

Supplementary Information 2

Name or Code	PAHIV	A _{HIV-IP}	Series	Prob.	Pred-A _{HIV-IP}
CHEMBL258205	CCR2	1	Training	55.75	1
CHEMBL1090893	CCR2	1	Prediction	82.81	1
CHEMBL497202	CCR2	1	Training	74.80	1
CHEMBL1092678	CCR2	1	Training	87.39	1
CHEMBL230281	CCR2	1	Training	99.17	1
CHEMBL256301	CCR2	1	Prediction	88.00	1
CHEMBL257191	CCR2	1	Training	92.98	1
CHEMBL389771	CCR2	1	Training	98.58	1
CHEMBL1092941	CCR2	1	Training	96.07	1
CHEMBL1091604	CCR2	1	Prediction	70.12	1
CHEMBL495924	CCR2	1	Training	50.34	1
CHEMBL1290636	CCR2	1	Training	92.24	1
CHEMBL403889	CCR2	1	Training	98.61	1
CHEMBL254772	CCR2	1	Prediction	99.73	1
CHEMBL404904	CCR2	1	Training	98.70	1
CHEMBL1091605	CCR2	1	Training	82.17	1
CHEMBL226066	CCR2	1	Training	51.89	1
CHEMBL397749	CCR2	1	Prediction	98.91	1
CHEMBL229316	CCR2	1	Training	81.42	1
CHEMBL502247	CCR2	1	Training	82.40	1
CHEMBL502793	CCR2	1	Training	77.57	1
CHEMBL397948	CCR2	1	Prediction	91.28	1
CHEMBL226065	CCR2	1	Training	57.31	1
CHEMBL526752	CCR2	1	Training	82.57	1
CHEMBL272369	CCR2	1	Training	51.84	1
CHEMBL388487	CCR2	1	Prediction	91.28	1
CHEMBL397996	CCR2	1	Training	94.77	1
CHEMBL230790	CCR2	1	Training	99.02	1
CHEMBL496343	CCR2	1	Training	57.73	1
CHEMBL402442	CCR2	1	Prediction	80.61	1
CHEMBL255302	CCR2	1	Training	99.23	1
CHEMBL502516	CCR2	1	Training	77.28	1
CHEMBL437552	CCR2	1	Training	99.40	1
CHEMBL1289203	CCR2	1	Prediction	90.02	1
CHEMBL1289083	CCR2	1	Training	85.71	1
CHEMBL505722	CCR2	1	Training	95.50	1
CHEMBL481010	CCR2	1	Training	61.90	1
CHEMBL387583	CCR2	1	Prediction	34.00	1
CHEMBL450231	CCR2	1	Training	97.17	1
CHEMBL1681819	CCR2	1	Training	98.77	1
CHEMBL1290637	CCR2	1	Training	92.86	1
CHEMBL230166	CCR2	1	Prediction	99.17	1

CHEMBL388486	CCR2	1	Training	98.95	1
CHEMBL438304	CCR2	1	Training	88.59	1
CHEMBL1683074	CCR2	1	Training	91.84	1
CHEMBL521275	CCR2	1	Prediction	60.81	1
CHEMBL1684712	CCR2	1	Training	98.54	1
CHEMBL1683059	CCR2	1	Training	32.66	1
CHEMBL256629	CCR2	1	Training	81.87	1
CHEMBL1683190	CCR2	1	Prediction	97.93	1
CHEMBL1684706	CCR2	1	Training	99.16	1
CHEMBL497788	CCR2	1	Training	55.31	1
CHEMBL230684	CCR2	1	Training	95.25	1
CHEMBL397997	CCR2	1	Prediction	34.00	1
CHEMBL1684694	CCR2	1	Training	98.77	1
CHEMBL1092748	CCR2	1	Training	94.00	1
CHEMBL496630	CCR2	1	Training	66.59	1
CHEMBL502513	CCR2	1	Prediction	93.55	1
CHEMBL516224	CCR2	1	Training	71.74	1
CHEMBL447937	CCR2	1	Training	99.56	1
CHEMBL230794	CCR2	1	Training	97.82	1
CHEMBL397747	CCR2	1	Prediction	92.40	1
CHEMBL441856	CCR2	1	Training	63.30	1
CHEMBL255478	CCR2	1	Training	98.44	1
CHEMBL257062	CCR2	1	Training	81.51	1
CHEMBL1684702	CCR2	1	Prediction	98.85	1
CHEMBL526859	CCR2	1	Training	64.01	1
CHEMBL1684713	CCR2	1	Training	97.67	1
CHEMBL1782377	CCR2	1	Training	93.31	1
CHEMBL1683063	CCR2	1	Prediction	34.21	1
CHEMBL402532	CCR2	1	Training	58.58	1
CHEMBL495368	CCR2	1	Training	34.18	1
CHEMBL481009	CCR2	1	Training	56.45	1
CHEMBL1684683	CCR2	1	Prediction	98.32	1
CHEMBL391459	CCR2	1	Training	98.89	1
CHEMBL1289316	CCR2	1	Training	74.76	1
CHEMBL273083	CCR2	1	Training	95.25	1
CHEMBL389888	CCR2	1	Prediction	94.77	1
CHEMBL270435	CCR2	1	Training	61.37	1
CHEMBL492569	CCR2	1	Training	63.76	1
CHEMBL522688	CCR2	1	Training	45.01	1
CHEMBL1683067	CCR2	1	Prediction	31.21	1
CHEMBL388868	CCR2	1	Training	98.58	1
CHEMBL499467	CCR2	1	Training	97.09	1
CHEMBL255499	CCR2	1	Training	97.56	1
CHEMBL257173	CCR2	1	Prediction	92.80	1
CHEMBL271725	CCR2	1	Training	78.57	1

CHEMBL496959	CCR2	1	Training	58.32	1
CHEMBL496344	CCR2	1	Training	64.80	1
CHEMBL497577	CCR2	1	Prediction	39.26	1
CHEMBL388867	CCR2	1	Training	91.28	1
CHEMBL452509	CCR2	1	Training	96.37	1
CHEMBL257628	CCR2	1	Training	44.45	1
CHEMBL495151	CCR2	1	Prediction	51.77	1
CHEMBL396517	CCR2	1	Training	85.32	1
CHEMBL1782376	CCR2	1	Training	95.96	1
CHEMBL395721	CCR2	1	Training	96.78	1
CHEMBL1290412	CCR2	1	Prediction	90.08	1
CHEMBL226017	CCR2	1	Training	64.80	1
CHEMBL480621	CCR2	1	Training	64.22	1
CHEMBL494540	CCR2	1	Training	46.99	1
CHEMBL526091	CCR2	1	Prediction	57.49	1
CHEMBL380258	CCR2	1	Training	42.15	1
CHEMBL502795	CCR2	1	Training	95.85	1
CHEMBL1782572	CCR2	1	Training	97.65	1
CHEMBL451340	CCR2	1	Prediction	84.04	1
CHEMBL1684700	CCR2	1	Training	94.04	1
CHEMBL449672	CCR2	1	Training	99.50	1
CHEMBL1782573	CCR2	1	Training	84.79	1
CHEMBL215020	CCR2	1	Prediction	69.33	1
CHEMBL257385	CCR2	1	Training	45.03	1
CHEMBL271828	CCR2	1	Training	90.72	1
CHEMBL438353	CCR2	1	Training	87.21	1
CHEMBL230727	CCR2	1	Prediction	98.24	1
CHEMBL1782578	CCR2	1	Training	92.80	1
CHEMBL481202	CCR2	1	Training	55.64	1
CHEMBL209411	CCR2	1	Training	1.45	1
CHEMBL403581	CCR2	1	Prediction	93.04	1
CHEMBL255500	CCR2	1	Training	97.03	1
CHEMBL403250	CCR2	1	Training	61.57	1
CHEMBL257768	CCR2	1	Training	98.44	1
Aceclofenac	CCR2	-1	Prediction	96.27	-1
Acetaminophen	CCR2	-1	Training	99.18	-1
Acetazolamide	CCR2	-1	Training	84.62	-1
Acetophenazine	CCR2	-1	Training	42.52	-1
Amantadine	CCR2	-1	Prediction	96.75	-1
Ambenonium	CCR2	-1	Training	37.65	-1
Amineptine	CCR2	-1	Training	93.86	-1
Amiodarone	CCR2	-1	Training	86.09	-1
Amitriptyline	CCR2	-1	Prediction	99.00	-1
Aprobarbital	CCR2	-1	Training	97.50	-1
Artane	CCR2	-1	Training	98.26	-1

Aspirin	CCR2	-1	Training	99.38	-1
Atenolol	CCR2	-1	Prediction	98.78	-1
Atropine	CCR2	-1	Training	76.97	-1
Baclofen	CCR2	-1	Training	98.37	-1
Beclomethasone	CCR2	-1	Training	99.66	-1
Benzonatate	CCR2	-1	Prediction	97.88	-1
Biperiden	CCR2	-1	Training	96.77	-1
Bromocriptine	CCR2	-1	Training	94.48	-1
Bucizine	CCR2	-1	Training	62.09	-1
Budesonide	CCR2	-1	Prediction	88.90	-1
Buprenorphine	CCR2	-1	Training	100.00	-1
Caffeine	CCR2	-1	Training	71.94	-1
Cantil	CCR2	-1	Training	97.87	-1
Carbachol	CCR2	-1	Prediction	93.39	-1
Carbamazepine	CCR2	-1	Training	87.58	-1
Carisoprodol	CCR2	-1	Training	78.02	-1
Carvedilol	CCR2	-1	Training	99.22	-1
Cefoperazone	CCR2	-1	Prediction	0.54	-1
Chloral hydrate	CCR2	-1	Training	99.20	-1
Chlordiazepoxide	CCR2	-1	Training	92.53	-1
Chlorpropamide	CCR2	-1	Training	79.22	-1
Chlorthalidone	CCR2	-1	Prediction	98.28	-1
Clidinium	CCR2	-1	Training	96.79	-1
Clobazam	CCR2	-1	Training	95.29	-1
Clofazimine	CCR2	-1	Training	99.96	-1
Clomipramine	CCR2	-1	Prediction	93.23	-1
Clonidine	CCR2	-1	Training	86.59	-1
Codeine	CCR2	-1	Training	99.84	-1
Colchicine	CCR2	-1	Training	99.12	-1
Cyclizine	CCR2	-1	Prediction	96.05	-1
Cyclosporin	CCR2	-1	Training	0.02	-1
Dextropropoxyphene	CCR2	-1	Training	99.03	-1
Diazepam	CCR2	-1	Training	94.85	-1
Diflucortolone	CCR2	-1	Prediction	82.23	-1
Dimercaprol	CCR2	-1	Training	99.68	-1
Diphenhydramine	CCR2	-1	Training	97.59	-1
Diphenidol	CCR2	-1	Training	98.72	-1
Dobutamine	CCR2	-1	Prediction	95.82	-1
Dofetilide	CCR2	-1	Training	70.70	-1
Domperidone	CCR2	-1	Training	9.13	-1
Dopamine	CCR2	-1	Training	99.41	-1
Doxazosin	CCR2	-1	Prediction	74.58	-1
Doxepin	CCR2	-1	Training	99.57	-1
Dronabinol	CCR2	-1	Training	99.12	-1
Droxicam	CCR2	-1	Training	97.83	-1

Entacapone	CCR2	-1	Prediction	98.59	-1
Epinephrine	CCR2	-1	Training	99.24	-1
Eprosartan	CCR2	-1	Training	59.75	-1
Ergotamine	CCR2	-1	Training	99.77	-1
Ethosuximide	CCR2	-1	Prediction	99.16	-1
Fentanyl	CCR2	-1	Training	93.22	-1
Fexofenadine	CCR2	-1	Training	94.61	-1
Flecainide	CCR2	-1	Training	86.32	-1
Flunarizine	CCR2	-1	Prediction	22.01	-1
Flunisolide	CCR2	-1	Training	85.88	-1
Fluoxetine	CCR2	-1	Training	96.86	-1
Fluvoxamine	CCR2	-1	Training	98.64	-1
Gabapentin	CCR2	-1	Prediction	99.13	-1
Gestodene	CCR2	-1	Training	97.79	-1
Glutethimide	CCR2	-1	Training	99.27	-1
Glycopyrrolate	CCR2	-1	Training	86.00	-1
Guanadrel	CCR2	-1	Prediction	91.23	-1
Halofantrine	CCR2	-1	Training	69.34	-1
Haloperidol	CCR2	-1	Training	30.44	-1
Halothane	CCR2	-1	Training	98.66	-1
Hydromorphone	CCR2	-1	Prediction	89.93	-1
Hydroxyzine	CCR2	-1	Training	92.91	-1
Indapamide	CCR2	-1	Training	88.42	-1
Indomethacin	CCR2	-1	Training	97.22	-1
Isoetharine	CCR2	-1	Prediction	98.02	-1
Isoproterenol	CCR2	-1	Training	98.67	-1
Isosorbide	CCR2	-1	Training	98.75	-1
Ketamine	CCR2	-1	Training	86.92	-1
Labetalol	CCR2	-1	Prediction	94.62	-1
Lacidipine	CCR2	-1	Training	99.79	-1
Lamotrigine	CCR2	-1	Training	38.38	-1
Leuprorelin	CCR2	-1	Training	7.77	-1
Levodopa	CCR2	-1	Prediction	98.72	-1
Lidocaine	CCR2	-1	Training	97.88	-1
Loratadine	CCR2	-1	Training	56.56	-1
Maprotiline	CCR2	-1	Training	99.25	-1
Meclizine	CCR2	-1	Prediction	78.37	-1
Medroxyprogesterone	CCR2	-1	Training	73.27	-1
Melfalan	CCR2	-1	Training	97.27	-1
Meprobamate	CCR2	-1	Training	87.05	-1
Methamphetamine	CCR2	-1	Prediction	99.20	-1
Methantheline	CCR2	-1	Training	95.14	-1
Methocarbamol	CCR2	-1	Training	99.03	-1
Methoxyflurane	CCR2	-1	Training	99.04	-1
Methscopolamine	CCR2	-1	Prediction	75.54	-1

Methylphenidate	CCR2	-1	Training	98.92	-1
Methysergide	CCR2	-1	Training	97.74	-1
Metoclopramide	CCR2	-1	Training	98.58	-1
Midodrine	CCR2	-1	Prediction	99.69	-1
Mirtazapine	CCR2	-1	Training	38.50	-1
Modafinil	CCR2	-1	Training	96.14	-1
Montelukast	CCR2	-1	Training	9.82	1*
Moricizine	CCR2	-1	Prediction	99.48	-1
Morphine	CCR2	-1	Training	99.71	-1
Nalmefene	CCR2	-1	Training	99.99	-1
Neostigmine	CCR2	-1	Training	99.85	-1
Nifedipine	CCR2	-1	Prediction	99.89	-1
Oxycodone	CCR2	-1	Training	99.81	-1
Paroxetine	CCR2	-1	Training	95.40	-1
Pecazine	CCR2	-1	Training	90.14	-1
Pergolide	CCR2	-1	Prediction	99.93	-1
Phenylbutazone	CCR2	-1	Training	98.67	-1
Phenytoin	CCR2	-1	Training	98.24	-1
Pilocarpine	CCR2	-1	Training	75.12	-1
Pimozide	CCR2	-1	Prediction	2.02	1*
Pramipexole	CCR2	-1	Training	96.19	-1
Probenecid	CCR2	-1	Training	97.08	-1
Procyclidine	CCR2	-1	Training	90.59	-1
Propranolol	CCR2	-1	Prediction	95.87	-1
Pseudoephedrine	CCR2	-1	Training	99.17	-1
Pyrantel	CCR2	-1	Training	98.94	-1
Quinidine	CCR2	-1	Training	39.65	-1
Ranitidine	CCR2	-1	Prediction	98.66	-1
Rifampin	CCR2	-1	Training	61.30	-1
Risperidone	CCR2	-1	Training	71.09	-1
Ropinirole	CCR2	-1	Training	97.00	-1
Salmeterol	CCR2	-1	Prediction	95.57	-1
Selegiline	CCR2	-1	Training	98.69	-1
Sulfinpyrazone	CCR2	-1	Training	93.98	-1
Tegafur	CCR2	-1	Training	62.47	-1
Terpin	CCR2	-1	Prediction	97.93	-1
Tolcapone	CCR2	-1	Training	71.39	-1
Tranlycypromine	CCR2	-1	Training	98.96	-1
Trazodone	CCR2	-1	Training	53.06	-1
Triamcinolone	CCR2	-1	Prediction	99.70	-1
Valproic acid	CCR2	-1	Training	99.34	-1
Vancomycin	CCR2	-1	Training	0.01	-1
Venlafaxine	CCR2	-1	Training	98.95	-1
Verapamil	CCR2	-1	Prediction	99.66	-1
Wytensin	CCR2	-1	Training	92.54	-1

Zafirlukast	CCR2	-1	Training	96.89	1*
Zileuton	CCR2	-1	Training	94.38	-1
Zonisamide	CCR2	-1	Prediction	95.96	-1
CHEMBL429323	CCR3	1	Training	99.10	1
CHEMBL399495	CCR3	1	Training	99.52	1
CHEMBL403838	CCR3	1	Prediction	99.70	1
CHEMBL217987	CCR3	1	Training	99.22	1
CHEMBL257029	CCR3	1	Training	99.65	1
CHEMBL402331	CCR3	1	Training	99.92	1
CHEMBL404585	CCR3	1	Prediction	99.80	1
CHEMBL361369	CCR3	1	Training	98.17	1
CHEMBL269933	CCR3	1	Training	99.58	1
CHEMBL404586	CCR3	1	Training	99.71	1
CHEMBL43423	CCR3	1	Prediction	99.15	1
CHEMBL362179	CCR3	1	Training	99.64	1
CHEMBL386073	CCR3	1	Training	99.53	1
CHEMBL404618	CCR3	1	Training	99.74	1
CHEMBL270806	CCR3	1	Prediction	99.97	1
CHEMBL256068	CCR3	1	Training	99.54	1
CHEMBL376737	CCR3	1	Training	99.99	1
CHEMBL218568	CCR3	1	Training	99.41	1
CHEMBL218262	CCR3	1	Prediction	99.50	1
CHEMBL401545	CCR3	1	Training	99.46	1
CHEMBL270583	CCR3	1	Training	99.55	1
CHEMBL257293	CCR3	1	Training	99.78	1
CHEMBL363840	CCR3	1	Prediction	99.76	1
CHEMBL272068	CCR3	1	Training	99.61	1
CHEMBL429846	CCR3	1	Training	96.33	1
CHEMBL180746	CCR3	1	Training	99.39	1
CHEMBL46404	CCR3	1	Prediction	99.22	1
CHEMBL257737	CCR3	1	Training	99.61	1
CHEMBL258322	CCR3	1	Training	99.50	1
CHEMBL257073	CCR3	1	Training	99.74	1
CHEMBL384199	CCR3	1	Prediction	99.46	1
CHEMBL182086	CCR3	1	Training	99.61	1
CHEMBL428775	CCR3	1	Training	99.44	1
CHEMBL219048	CCR3	1	Training	91.35	1
CHEMBL272067	CCR3	1	Prediction	100.00	1
CHEMBL257074	CCR3	1	Training	99.77	1
CHEMBL444568	CCR3	1	Training	99.42	1
CHEMBL270582	CCR3	1	Training	99.95	1
CHEMBL178503	CCR3	1	Prediction	99.74	1
CHEMBL178230	CCR3	1	Training	99.42	1
CHEMBL403839	CCR3	1	Training	99.94	1
CHEMBL218174	CCR3	1	Training	93.79	1

CHEMBL403331	CCR3	1	Prediction	99.68	1
CHEMBL270147	CCR3	1	Training	99.96	1
CHEMBL178506	CCR3	1	Training	99.88	1
CHEMBL258156	CCR3	1	Training	99.61	1
CHEMBL402983	CCR3	1	Prediction	99.72	1
CHEMBL437031	CCR3	1	Training	99.69	1
CHEMBL220765	CCR3	1	Training	99.50	1
CHEMBL180042	CCR3	1	Training	99.47	1
CHEMBL221067	CCR3	1	Prediction	94.59	1
CHEMBL427728	CCR3	1	Training	99.65	1
CHEMBL441334	CCR3	1	Training	100.00	1
CHEMBL250689	CCR3	1	Training	97.44	1
CHEMBL178671	CCR3	1	Prediction	99.62	1
CHEMBL360039	CCR3	1	Training	99.47	1
CHEMBL20921	CCR3	1	Training	28.30	1
CHEMBL220713	CCR3	1	Training	99.52	1
CHEMBL270146	CCR3	1	Prediction	99.75	1
CHEMBL220819	CCR3	1	Training	97.90	1
CHEMBL46905	CCR3	1	Training	91.40	1
CHEMBL429604	CCR3	1	Training	99.63	1
CHEMBL404122	CCR3	1	Prediction	99.75	1
CHEMBL295415	CCR3	1	Training	99.93	1
CHEMBL401879	CCR3	1	Training	99.97	1
CHEMBL258309	CCR3	1	Training	99.54	1
CHEMBL255399	CCR3	1	Prediction	99.85	1
CHEMBL255398	CCR3	1	Training	99.49	1
CHEMBL361130	CCR3	1	Training	99.80	1
CHEMBL180728	CCR3	1	Training	99.83	1
CHEMBL180351	CCR3	1	Prediction	99.89	1
CHEMBL366710	CCR3	1	Training	99.42	1
CHEMBL178287	CCR3	1	Training	98.21	1
CHEMBL385607	CCR3	1	Training	99.62	1
CHEMBL359609	CCR3	1	Prediction	96.87	1
CHEMBL383879	CCR3	1	Training	99.57	1
CHEMBL258323	CCR3	1	Training	99.44	1
CHEMBL221903	CCR3	1	Training	94.25	1
CHEMBL428071	CCR3	1	Prediction	99.56	1
CHEMBL220766	CCR3	1	Training	99.92	1
CHEMBL362490	CCR3	1	Training	99.08	1
CHEMBL180229	CCR3	1	Training	98.83	1
CHEMBL369331	CCR3	1	Prediction	99.37	1
CHEMBL384649	CCR3	1	Training	99.61	1
CHEMBL404202	CCR3	1	Training	99.49	1
CHEMBL181575	CCR3	1	Training	99.08	1
CHEMBL218581	CCR3	1	Prediction	65.51	1

CHEMBL220801	CCR3	1	Training	93.38	1
CHEMBL181528	CCR3	1	Training	99.44	1
CHEMBL360529	CCR3	1	Training	97.90	1
CHEMBL360062	CCR3	1	Prediction	99.41	1
CHEMBL386493	CCR3	1	Training	99.70	1
CHEMBL180694	CCR3	1	Training	99.08	1
CHEMBL178278	CCR3	1	Training	99.33	1
CHEMBL362613	CCR3	1	Prediction	99.16	1
CHEMBL21143	CCR3	1	Training	19.65	1
CHEMBL218997	CCR3	1	Training	94.26	1
CHEMBL426422	CCR3	1	Training	99.23	1
CHEMBL20532	CCR3	1	Prediction	24.32	1
CHEMBL182087	CCR3	1	Training	99.16	1
CHEMBL266181	CCR3	1	Training	28.33	1
CHEMBL180534	CCR3	1	Training	99.00	1
CHEMBL282285	CCR3	1	Prediction	16.95	1
CHEMBL181302	CCR3	1	Training	99.12	1
CHEMBL180860	CCR3	1	Training	95.48	1
CHEMBL220800	CCR3	1	Training	94.72	1
CHEMBL221901	CCR3	1	Prediction	93.75	1
CHEMBL181311	CCR3	1	Training	99.18	1
CHEMBL20612	CCR3	1	Training	16.68	1
CHEMBL360653	CCR3	1	Training	99.10	1
CHEMBL180082	CCR3	1	Prediction	98.38	1
CHEMBL220866	CCR3	1	Training	94.26	1
Aceclofenac	CCR3	-1	Training	99.09	-1
Acetaminophen	CCR3	-1	Training	99.81	-1
Acetazolamide	CCR3	-1	Prediction	95.88	-1
Acetophenazine	CCR3	-1	Training	75.80	-1
Amantadine	CCR3	-1	Training	99.21	-1
Ambenonium	CCR3	-1	Training	71.89	-1
Amineptine	CCR3	-1	Prediction	98.48	-1
Amiodarone	CCR3	-1	Training	96.32	-1
Amitriptyline	CCR3	-1	Training	99.76	-1
Aprobarbital	CCR3	-1	Training	99.40	-1
Artane	CCR3	-1	Prediction	99.58	-1
Aspirin	CCR3	-1	Training	99.85	-1
Atenolol	CCR3	-1	Training	99.71	-1
Atropine	CCR3	-1	Training	93.40	-1
Baclofen	CCR3	-1	Prediction	99.61	-1
Beclomethasone	CCR3	-1	Training	99.92	-1
Benzonatate	CCR3	-1	Training	99.49	-1
Biperiden	CCR3	-1	Training	99.22	-1
Bromocriptine	CCR3	-1	Prediction	98.64	-1
Bucizine	CCR3	-1	Training	87.40	-1

Budesonide	CCR3	-1	Training	97.14	-1
Buprenorphine	CCR3	-1	Training	100.00	-1
Caffeine	CCR3	-1	Prediction	91.56	-1
Cantil	CCR3	-1	Training	99.49	-1
Carbachol	CCR3	-1	Training	98.36	-1
Carbamazepine	CCR3	-1	Training	96.76	-1
Carisoprodol	CCR3	-1	Prediction	93.76	-1
Carvedilol	CCR3	-1	Training	99.81	-1
Cefoperazone	CCR3	-1	Training	2.24	-1
Chloral hydrate	CCR3	-1	Training	99.81	-1
Chlordiazepoxide	CCR3	-1	Prediction	98.13	-1
Chlorpropamide	CCR3	-1	Training	94.16	-1
Chlorthalidone	CCR3	-1	Training	99.59	-1
Clidinium	CCR3	-1	Training	99.22	-1
Clobazam	CCR3	-1	Prediction	98.85	-1
Clofazimine	CCR3	-1	Training	99.99	-1
Clomipramine	CCR3	-1	Training	98.31	-1
Clonidine	CCR3	-1	Training	96.47	-1
Codeine	CCR3	-1	Prediction	99.96	-1
Colchicine	CCR3	-1	Training	99.79	-1
Cyclizine	CCR3	-1	Training	99.04	-1
Cyclosporin	CCR3	-1	Training	0.08	-1
Dextropropoxyphene	CCR3	-1	Prediction	99.77	-1
Diazepam	CCR3	-1	Training	98.73	-1
Diflucortolone	CCR3	-1	Training	95.15	-1
Dimercaprol	CCR3	-1	Training	99.92	-1
Diphenhydramine	CCR3	-1	Prediction	99.42	-1
Diphenidol	CCR3	-1	Training	99.69	-1
Dobutamine	CCR3	-1	Training	98.98	-1
Dofetilide	CCR3	-1	Training	91.08	-1
Domperidone	CCR3	-1	Prediction	29.85	-1
Dopamine	CCR3	-1	Training	99.86	-1
Doxazosin	CCR3	-1	Training	92.55	-1
Doxepin	CCR3	-1	Training	99.90	-1
Dronabinol	CCR3	-1	Prediction	99.79	-1
Droxicam	CCR3	-1	Training	99.48	-1
Entacapone	CCR3	-1	Training	99.66	-1
Epinephrine	CCR3	-1	Training	99.82	-1
Eprosartan	CCR3	-1	Prediction	86.28	-1
Ergotamine	CCR3	-1	Training	99.95	-1
Ethosuximide	CCR3	-1	Training	99.80	-1
Fentanyl	CCR3	-1	Training	98.31	-1
Fexofenadine	CCR3	-1	Prediction	98.67	-1
Flecainide	CCR3	-1	Training	96.39	-1
Flunarizine	CCR3	-1	Training	54.44	1*

Flunisolide	CCR3	-1	Training	96.26	-1
Fluoxetine	CCR3	-1	Prediction	99.24	-1
Fluvoxamine	CCR3	-1	Training	99.68	-1
Gabapentin	CCR3	-1	Training	99.79	-1
Gestodene	CCR3	-1	Training	99.47	-1
Glutethimide	CCR3	-1	Prediction	99.83	-1
Glycopyrrolate	CCR3	-1	Training	96.30	-1
Guanadrel	CCR3	-1	Training	97.78	-1
Halofantrine	CCR3	-1	Training	90.54	-1
Haloperidol	CCR3	-1	Prediction	64.95	-1
Halothane	CCR3	-1	Training	99.68	-1
Hydromorphone	CCR3	-1	Training	97.42	-1
Hydroxyzine	CCR3	-1	Training	98.23	-1
Indapamide	CCR3	-1	Prediction	97.00	-1
Indomethacin	CCR3	-1	Training	99.33	-1
Isoetharine	CCR3	-1	Training	99.53	-1
Isoproterenol	CCR3	-1	Training	99.68	-1
Isosorbide	CCR3	-1	Prediction	99.70	-1
Ketamine	CCR3	-1	Training	96.57	-1
Labetalol	CCR3	-1	Training	98.67	-1
Lacidipine	CCR3	-1	Training	99.95	-1
Lamotrigine	CCR3	-1	Prediction	72.50	-1
Leuprorelin	CCR3	-1	Training	26.30	-1
Levodopa	CCR3	-1	Training	99.69	-1
Lidocaine	CCR3	-1	Training	99.49	-1
Loratadine	CCR3	-1	Prediction	84.65	-1
Maprotiline	CCR3	-1	Training	99.82	-1
Meclizine	CCR3	-1	Training	93.88	-1
Medroxyprogesterone	CCR3	-1	Training	92.07	-1
Melfalan	CCR3	-1	Prediction	99.34	-1
Meprobamate	CCR3	-1	Training	96.61	-1
Methamphetamine	CCR3	-1	Training	99.81	-1
Methantheline	CCR3	-1	Training	98.81	-1
Methocarbamol	CCR3	-1	Prediction	99.77	-1
Methoxyflurane	CCR3	-1	Training	99.77	-1
Methscopolamine	CCR3	-1	Training	92.89	-1
Methylphenidate	CCR3	-1	Training	99.74	-1
Methysergide	CCR3	-1	Prediction	99.46	-1
Metoclopramide	CCR3	-1	Training	99.66	-1
Midodrine	CCR3	-1	Training	99.93	-1
Mirtazapine	CCR3	-1	Training	72.61	-1
Modafinil	CCR3	-1	Prediction	99.06	-1
Montelukast	CCR3	-1	Training	31.55	-1
Moricizine	CCR3	-1	Training	99.88	-1
Morphine	CCR3	-1	Training	99.93	-1

Nalmefene	CCR3	-1	Prediction	100.00	-1
Neostigmine	CCR3	-1	Training	99.96	-1
Nifedipine	CCR3	-1	Training	99.97	-1
Oxycodone	CCR3	-1	Training	99.96	-1
Paroxetine	CCR3	-1	Prediction	98.87	-1
Pecazine	CCR3	-1	Training	97.48	-1
Pergolide	CCR3	-1	Training	99.98	-1
Phenylbutazone	CCR3	-1	Training	99.68	-1
Phenytoin	CCR3	-1	Prediction	99.58	-1
Pilocarpine	CCR3	-1	Training	92.75	-1
Pimozide	CCR3	-1	Training	8.03	-1
Pramipexole	CCR3	-1	Training	99.07	-1
Probenecid	CCR3	-1	Prediction	99.29	-1
Procyclidine	CCR3	-1	Training	97.61	-1
Propantheline	CCR3	-1	Training	98.99	-1
Pseudoephedrine	CCR3	-1	Training	99.80	-1
Pyrantel	CCR3	-1	Prediction	99.75	-1
Quinidine	CCR3	-1	Training	73.56	-1
Ranitidine	CCR3	-1	Training	99.68	-1
Rifampin	CCR3	-1	Training	87.02	-1
Risperidone	CCR3	-1	Prediction	91.24	-1
Ropinirole	CCR3	-1	Training	99.27	-1
Salmeterol	CCR3	-1	Training	98.92	-1
Selegiline	CCR3	-1	Training	99.69	-1
Sulfinpyrazone	CCR3	-1	Prediction	98.51	-1
Tegafur	CCR3	-1	Training	87.57	-1
Terpin	CCR3	-1	Training	99.50	-1
Tolcapone	CCR3	-1	Training	91.35	-1
Tranlycypromine	CCR3	-1	Prediction	99.75	-1
Trazodone	CCR3	-1	Training	82.72	-1
Triamcinolone	CCR3	-1	Training	99.93	-1
Valproic acid	CCR3	-1	Training	99.84	-1
Vancomycin	CCR3	-1	Prediction	0.05	-1
Venlafaxine	CCR3	-1	Training	99.75	-1
Verapamil	CCR3	-1	Training	99.92	-1
Wytensin	CCR3	-1	Training	98.13	-1
Zafirlukast	CCR3	-1	Prediction	99.25	-1
Zileuton	CCR3	-1	Training	98.61	-1
Zonisamide	CCR3	-1	Training	99.02	-1
CHEMBL515193	CCR5	1	Prediction	92.78	1
CHEMBL460845	CCR5	1	Training	64.89	1
CHEMBL21106	CCR5	1	Training	99.76	1
CHEMBL457043	CCR5	1	Training	69.96	1
CHEMBL20896	CCR5	1	Prediction	88.97	1
CHEMBL320386	CCR5	1	Training	85.92	1

CHEMBL316475	CCR5	1	Training	89.19	1
CHEMBL20345	CCR5	1	Training	99.67	1
CHEMBL473558	CCR5	1	Prediction	88.42	1
CHEMBL461687	CCR5	1	Training	82.22	1
CHEMBL319593	CCR5	1	Training	99.83	1
CHEMBL322422	CCR5	1	Training	99.84	1
CHEMBL99909	CCR5	1	Prediction	86.47	1
CHEMBL1201187	CCR5	1	Training	99.62	1
CHEMBL21147	CCR5	1	Training	99.38	1
CHEMBL20622	CCR5	1	Training	98.69	1
CHEMBL212731	CCR5	1	Prediction	94.48	1
CHEMBL520091	CCR5	1	Training	99.61	1
CHEMBL511493	CCR5	1	Training	99.60	1
CHEMBL480503	CCR5	1	Training	99.55	1
CHEMBL317710	CCR5	1	Prediction	82.01	-1*
CHEMBL194497	CCR5	1	Training	99.98	1
CHEMBL21117	CCR5	1	Training	99.76	1
CHEMBL455073	CCR5	1	Training	98.85	1
CHEMBL212689	CCR5	1	Prediction	98.92	1
CHEMBL459384	CCR5	1	Training	53.99	1
CHEMBL480693	CCR5	1	Training	99.18	1
CHEMBL193984	CCR5	1	Training	99.94	1
CHEMBL489513	CCR5	1	Prediction	93.89	1
CHEMBL103790	CCR5	1	Training	99.72	1
CHEMBL20453	CCR5	1	Training	99.66	1
CHEMBL464132	CCR5	1	Training	99.85	1
CHEMBL371584	CCR5	1	Prediction	99.47	1
CHEMBL456226	CCR5	1	Training	70.67	1
CHEMBL491319	CCR5	1	Training	93.89	1
CHEMBL371177	CCR5	1	Training	99.96	1
CHEMBL471920	CCR5	1	Prediction	99.62	1
CHEMBL472464	CCR5	1	Training	45.59	1
CHEMBL278085	CCR5	1	Training	97.78	1
CHEMBL513564	CCR5	1	Training	99.24	1
CHEMBL473759	CCR5	1	Prediction	89.39	1
CHEMBL500631	CCR5	1	Training	98.82	1
CHEMBL195753	CCR5	1	Training	99.97	1
CHEMBL472412	CCR5	1	Training	98.91	1
CHEMBL520755	CCR5	1	Prediction	99.71	1
CHEMBL377914	CCR5	1	Training	66.73	1
CHEMBL318406	CCR5	1	Training	80.76	1
CHEMBL211866	CCR5	1	Training	75.84	1
CHEMBL471251	CCR5	1	Prediction	98.18	1
CHEMBL193822	CCR5	1	Training	99.97	1
CHEMBL328297	CCR5	1	Training	99.00	1

CHEMBL471909	CCR5	1	Training	99.48	1
CHEMBL172854	CCR5	1	Prediction	99.52	1
CHEMBL281607	CCR5	1	Training	99.59	1
CHEMBL101961	CCR5	1	Training	83.14	1
CHEMBL511634	CCR5	1	Training	95.50	1
CHEMBL435886	CCR5	1	Prediction	99.97	1
CHEMBL193440	CCR5	1	Training	97.59	1
CHEMBL193988	CCR5	1	Training	99.94	1
CHEMBL449758	CCR5	1	Training	96.34	1
CHEMBL435727	CCR5	1	Prediction	99.51	1
CHEMBL470510	CCR5	1	Training	99.59	1
CHEMBL461690	CCR5	1	Training	78.70	1
CHEMBL379082	CCR5	1	Training	84.44	1
CHEMBL420465	CCR5	1	Prediction	99.86	1
CHEMBL93139	CCR5	1	Training	87.04	1
CHEMBL196497	CCR5	1	Training	100.00	1
CHEMBL471623	CCR5	1	Training	86.23	1
CHEMBL481068	CCR5	1	Prediction	98.74	1
CHEMBL480890	CCR5	1	Training	97.07	1
CHEMBL99788	CCR5	1	Training	78.62	1
CHEMBL198758	CCR5	1	Training	99.01	1
CHEMBL382435	CCR5	1	Prediction	96.66	1
CHEMBL207182	CCR5	1	Training	85.67	1
CHEMBL471542	CCR5	1	Training	95.51	1
CHEMBL175327	CCR5	1	Training	99.71	1
CHEMBL173095	CCR5	1	Prediction	99.70	1
CHEMBL353331	CCR5	1	Training	98.17	1
CHEMBL481080	CCR5	1	Training	97.79	1
CHEMBL1222769	CCR5	1	Training	99.55	1
CHEMBL455570	CCR5	1	Prediction	99.63	1
CHEMBL174304	CCR5	1	Training	99.41	1
CHEMBL481274	CCR5	1	Training	99.06	1
CHEMBL283788	CCR5	1	Training	99.61	1
CHEMBL457044	CCR5	1	Prediction	53.52	1
CHEMBL20598	CCR5	1	Training	99.63	1
CHEMBL480504	CCR5	1	Training	99.20	1
CHEMBL352514	CCR5	1	Training	97.89	1
CHEMBL380447	CCR5	1	Prediction	76.52	1
CHEMBL198150	CCR5	1	Training	75.84	1
CHEMBL207630	CCR5	1	Training	99.64	1
CHEMBL437494	CCR5	1	Training	88.44	1
CHEMBL204743	CCR5	1	Prediction	99.38	1
CHEMBL428104	CCR5	1	Training	100.00	1
CHEMBL204821	CCR5	1	Training	82.19	1
CHEMBL179141	CCR5	1	Training	96.68	1

CHEMBL179209	CCR5	1	Prediction	98.53	1
CHEMBL85086	CCR5	1	Training	74.25	1
CHEMBL214818	CCR5	1	Training	94.53	-1*
CHEMBL320149	CCR5	1	Training	91.79	1
CHEMBL469724	CCR5	1	Prediction	87.96	1
CHEMBL318210	CCR5	1	Training	80.27	1
CHEMBL511494	CCR5	1	Training	99.55	1
CHEMBL499483	CCR5	1	Training	97.52	1
CHEMBL202814	CCR5	1	Prediction	66.59	1
CHEMBL207487	CCR5	1	Training	89.58	1
CHEMBL172659	CCR5	1	Training	98.04	1
CHEMBL197641	CCR5	1	Training	76.47	1
CHEMBL366626	CCR5	1	Prediction	98.43	1
CHEMBL457960	CCR5	1	Training	64.32	1
CHEMBL203536	CCR5	1	Training	75.78	1
CHEMBL364070	CCR5	1	Training	96.07	1
CHEMBL193972	CCR5	1	Prediction	97.36	1
CHEMBL382252	CCR5	1	Training	82.10	1
CHEMBL436290	CCR5	1	Training	99.84	1
CHEMBL205539	CCR5	1	Training	82.32	1
CHEMBL1172035	CCR5	1	Prediction	94.96	1
CHEMBL1222771	CCR5	1	Training	97.13	1
CHEMBL318909	CCR5	1	Training	89.86	1
CHEMBL193678	CCR5	1	Training	99.97	1
CHEMBL366536	CCR5	1	Prediction	98.45	-1*
CHEMBL102675	CCR5	1	Training	73.56	1
CHEMBL472260	CCR5	1	Training	53.12	1
CHEMBL475606	CCR5	1	Training	99.99	1
CHEMBL368265	CCR5	1	Prediction	99.63	1
CHEMBL318681	CCR5	1	Training	85.74	1
CHEMBL82301	CCR5	1	Training	94.43	1
Aceclofenac	CCR5	-1	Training	97.33	-1
Acetaminophen	CCR5	-1	Prediction	99.42	-1
Acetazolamide	CCR5	-1	Training	88.59	-1
Acetophenazine	CCR5	-1	Training	51.08	-1
Amantadine	CCR5	-1	Training	97.68	-1
Ambenonium	CCR5	-1	Prediction	46.02	-1
Amineptine	CCR5	-1	Training	95.57	-1
Amiodarone	CCR5	-1	Training	89.73	-1
Amitriptyline	CCR5	-1	Training	99.29	-1
Aprobarbital	CCR5	-1	Prediction	98.22	-1
Artane	CCR5	-1	Training	98.76	-1
Aspirin	CCR5	-1	Training	99.56	-1
Atenolol	CCR5	-1	Training	99.14	-1
Atropine	CCR5	-1	Prediction	82.51	-1

Baclofen	CCR5	-1	Training	98.84	-1
Beclomethasone	CCR5	-1	Training	99.76	-1
Benzonatate	CCR5	-1	Training	98.49	-1
Biperiden	CCR5	-1	Prediction	97.69	-1
Bromocriptine	CCR5	-1	Training	96.03	-1
Bucizine	CCR5	-1	Training	69.81	-1
Budesonide	CCR5	-1	Training	91.87	-1
Buprenorphine	CCR5	-1	Prediction	100.00	-1
Caffeine	CCR5	-1	Training	78.35	-1
Cantil	CCR5	-1	Training	98.48	-1
Carbachol	CCR5	-1	Training	95.23	-1
Carbamazepine	CCR5	-1	Prediction	90.87	-1
Carisoprodol	CCR5	-1	Training	83.36	-1
Carvedilol	CCR5	-1	Training	99.44	-1
Cefoperazone	CCR5	-1	Training	0.76	-1
Chloral hydrate	CCR5	-1	Prediction	99.43	-1
Chlordiazepoxide	CCR5	-1	Training	94.59	-1
Chlorpropamide	CCR5	-1	Training	84.33	-1
Chlorthalidone	CCR5	-1	Training	98.78	-1
Clidinium	CCR5	-1	Prediction	97.71	-1
Clobazam	CCR5	-1	Training	96.62	-1
Clofazimine	CCR5	-1	Training	99.97	-1
Clomipramine	CCR5	-1	Training	95.11	-1
Clonidine	CCR5	-1	Prediction	90.12	-1
Codeine	CCR5	-1	Training	99.89	-1
Colchicine	CCR5	-1	Training	99.37	-1
Cyclizine	CCR5	-1	Training	97.17	-1
Cyclosporin	CCR5	-1	Prediction	0.03	-1
Dextropropoxyphene	CCR5	-1	Training	99.31	-1
Diazepam	CCR5	-1	Training	96.30	-1
Diflucortolone	CCR5	-1	Training	86.73	-1
Dimercaprol	CCR5	-1	Prediction	99.77	-1
Diphenhydramine	CCR5	-1	Training	98.28	-1
Diphenidol	CCR5	-1	Training	99.09	-1
Dobutamine	CCR5	-1	Training	97.00	-1
Dofetilide	CCR5	-1	Prediction	77.30	-1
Domperidone	CCR5	-1	Training	12.42	-1
Dopamine	CCR5	-1	Training	99.58	-1
Doxazosin	CCR5	-1	Training	80.55	-1
Doxepin	CCR5	-1	Prediction	99.70	-1
Dronabinol	CCR5	-1	Training	99.38	-1
Droxycam	CCR5	-1	Training	98.45	-1
Entacapone	CCR5	-1	Training	98.99	-1
Epinephrine	CCR5	-1	Prediction	99.46	-1
Eprosartan	CCR5	-1	Training	67.70	-1

Ergotamine	CCR5	-1	Training	99.84	-1
Ethosuximide	CCR5	-1	Training	99.40	-1
Fentanyl	CCR5	-1	Prediction	95.10	-1
Fexofenadine	CCR5	-1	Training	96.12	-1
Flecainide	CCR5	-1	Training	89.91	-1
Flunarizine	CCR5	-1	Training	28.49	-1
Flunisolide	CCR5	-1	Prediction	89.57	-1
Fluoxetine	CCR5	-1	Training	97.75	-1
Fluvoxamine	CCR5	-1	Training	99.03	-1
Gabapentin	CCR5	-1	Training	99.38	-1
Gestodene	CCR5	-1	Prediction	98.42	-1
Glutethimide	CCR5	-1	Training	99.48	-1
Glycopyrrolate	CCR5	-1	Training	89.66	-1
Guanadrel	CCR5	-1	Training	93.62	-1
Halofantrine	CCR5	-1	Prediction	76.15	-1
Haloperidol	CCR5	-1	Training	38.19	-1
Halothane	CCR5	-1	Training	99.05	-1
Hydromorphone	CCR5	-1	Training	92.65	-1
Hydroxyzine	CCR5	-1	Prediction	94.87	-1
Indapamide	CCR5	-1	Training	91.51	-1
Indomethacin	CCR5	-1	Training	98.02	-1
Isoetharine	CCR5	-1	Training	98.59	-1
Isoproterenol	CCR5	-1	Prediction	99.06	-1
Isosorbide	CCR5	-1	Training	99.11	-1
Ketamine	CCR5	-1	Training	90.37	-1
Labetalol	CCR5	-1	Training	96.13	-1
Lacidipine	CCR5	-1	Prediction	99.85	-1
Lamotrigine	CCR5	-1	Training	46.78	-1
Leuprorelin	CCR5	-1	Training	10.63	-1
Levodopa	CCR5	-1	Training	99.09	-1
Lidocaine	CCR5	-1	Prediction	98.49	-1
Loratadine	CCR5	-1	Training	64.76	-1
Maprotiline	CCR5	-1	Training	99.46	-1
Meclizine	CCR5	-1	Training	83.64	-1
Medroxyprogesterone	CCR5	-1	Prediction	79.46	-1
Melfalan	CCR5	-1	Training	98.05	-1
Meprobamate	CCR5	-1	Training	90.47	-1
Methamphetamine	CCR5	-1	Training	99.43	-1
Methantheline	CCR5	-1	Prediction	96.51	-1
Methocarbamol	CCR5	-1	Training	99.31	-1
Methoxyflurane	CCR5	-1	Training	99.32	-1
Methscopolamine	CCR5	-1	Training	81.34	-1
Methylphenidate	CCR5	-1	Prediction	99.23	-1
Methysergide	CCR5	-1	Training	98.39	-1
Metoclopramide	CCR5	-1	Training	98.99	-1

Midodrine	CCR5	-1	Training	99.78	-1
Mirtazapine	CCR5	-1	Prediction	46.91	-1
Modafinil	CCR5	-1	Training	97.24	-1
Montelukast	CCR5	-1	Training	13.32	-1
Moricizine	CCR5	-1	Training	99.63	-1
Morphine	CCR5	-1	Prediction	99.79	-1
Nalmefene	CCR5	-1	Training	99.99	-1
Neostigmine	CCR5	-1	Training	99.89	-1
Nifedipine	CCR5	-1	Training	99.92	-1
Oxycodone	CCR5	-1	Prediction	99.87	-1
Paroxetine	CCR5	-1	Training	96.69	-1
Pecazine	CCR5	-1	Training	92.81	-1
Pergolide	CCR5	-1	Training	99.95	-1
Phenylbutazone	CCR5	-1	Prediction	99.06	-1
Phenytoin	CCR5	-1	Training	98.75	-1
Pilocarpine	CCR5	-1	Training	81.00	-1
Pimozide	CCR5	-1	Training	2.83	-1
Pramipexole	CCR5	-1	Prediction	97.27	-1
Probenecid	CCR5	-1	Training	97.91	-1
Procyclidine	CCR5	-1	Training	93.15	-1
Propantheline	CCR5	-1	Training	97.03	-1
Pseudoephedrine	CCR5	-1	Prediction	99.41	-1
Pyrantel	CCR5	-1	Training	99.25	-1
Quinidine	CCR5	-1	Training	48.12	-1
Ranitidine	CCR5	-1	Training	99.04	-1
Rifampin	CCR5	-1	Prediction	69.10	-1
Risperidone	CCR5	-1	Training	77.64	-1
Ropinirole	CCR5	-1	Training	97.85	-1
Salmeterol	CCR5	-1	Training	96.82	-1
Selegiline	CCR5	-1	Prediction	99.07	-1
Sulfinpyrazone	CCR5	-1	Training	95.66	-1
Tegafur	CCR5	-1	Training	70.14	-1
Terpin	CCR5	-1	Training	98.52	-1
Tolcapone	CCR5	-1	Prediction	77.89	-1
Tranlycypromine	CCR5	-1	Training	99.26	-1
Trazodone	CCR5	-1	Training	61.47	-1
Triamcinolone	CCR5	-1	Training	99.79	-1
Valproic acid	CCR5	-1	Prediction	99.53	-1
Vancomycin	CCR5	-1	Training	0.02	-1
Venlafaxine	CCR5	-1	Training	99.26	-1
Verapamil	CCR5	-1	Training	99.76	-1
Wytensin	CCR5	-1	Prediction	94.60	-1
Zafirlukast	CCR5	-1	Training	97.78	1*
Zileuton	CCR5	-1	Training	95.95	-1
Zonisamide	CCR5	-1	Training	97.11	-1

CHEMBL1242210	CXCR4	1	Training	92.23	1
CHEMBL218806	CXCR4	1	Training	99.37	1
CHEMBL508054	CXCR4	1	Training	90.46	1
CHEMBL1096504	CXCR4	1	Prediction	98.63	-1*
CHEMBL219474	CXCR4	1	Training	99.18	1
CHEMBL1092637	CXCR4	1	Training	96.75	1
CHEMBL454896	CXCR4	1	Training	91.97	1
CHEMBL219339	CXCR4	1	Prediction	99.18	1
CHEMBL460298	CXCR4	1	Training	90.49	1
CHEMBL518501	CXCR4	1	Training	95.07	1
CHEMBL1682996	CXCR4	1	Training	94.98	1
CHEMBL373636	CXCR4	1	Prediction	99.42	1
CHEMBL375990	CXCR4	1	Training	99.42	1
CHEMBL518924	CXCR4	1	Training	83.57	1
CHEMBL1094864	CXCR4	1	Training	99.01	1
CHEMBL1682997	CXCR4	1	Prediction	74.21	1
CHEMBL1644080	CXCR4	1	Training	99.69	1
CHEMBL376219	CXCR4	1	Training	99.37	1
CHEMBL1088913	CXCR4	1	Training	83.57	1
CHEMBL374421	CXCR4	1	Prediction	99.37	1
CHEMBL541728	CXCR4	1	Training	89.65	1
CHEMBL436283	CXCR4	1	Training	99.18	1
CHEMBL1682998	CXCR4	1	Training	93.14	-1*
CHEMBL1644082	CXCR4	1	Prediction	73.79	1
CHEMBL375991	CXCR4	1	Training	99.25	1
CHEMBL577268	CXCR4	1	Training	81.13	1
CHEMBL452864	CXCR4	1	Training	88.77	1
CHEMBL516630	CXCR4	1	Prediction	89.97	1
CHEMBL1682995	CXCR4	1	Training	97.23	1
CHEMBL374108	CXCR4	1	Training	92.60	1
CHEMBL461358	CXCR4	1	Training	79.64	-1*
CHEMBL1091591	CXCR4	1	Prediction	93.11	1
CHEMBL461359	CXCR4	1	Training	98.44	1
CHEMBL1644081	CXCR4	1	Training	86.38	1
CHEMBL376811	CXCR4	1	Training	99.42	1
CHEMBL1682994	CXCR4	1	Prediction	81.15	1
CHEMBL436536	CXCR4	1	Training	99.37	1
CHEMBL506505	CXCR4	1	Training	98.94	1
CHEMBL1093137	CXCR4	1	Training	99.91	1
CHEMBL219096	CXCR4	1	Prediction	99.37	1
CHEMBL373440	CXCR4	1	Training	97.46	1
CHEMBL375993	CXCR4	1	Training	99.37	1
CHEMBL219075	CXCR4	1	Training	96.45	1
CHEMBL387120	CXCR4	1	Prediction	99.42	1
CHEMBL460299	CXCR4	1	Training	87.76	1

CHEMBL1093149	CXCR4	1	Training	83.57	1
CHEMBL384429	CXCR4	1	Training	92.60	1
CHEMBL375850	CXCR4	1	Prediction	99.40	1
CHEMBL1089434	CXCR4	1	Training	99.91	1
CHEMBL374862	CXCR4	1	Training	99.46	1
CHEMBL219135	CXCR4	1	Training	99.25	1
CHEMBL462588	CXCR4	1	Prediction	96.78	1
CHEMBL426169	CXCR4	1	Training	99.40	1
CHEMBL373637	CXCR4	1	Training	99.66	1
CHEMBL450815	CXCR4	1	Training	91.40	1
CHEMBL508684	CXCR4	1	Prediction	93.38	1
CHEMBL518041	CXCR4	1	Training	97.54	-1*
CHEMBL450041	CXCR4	1	Training	91.40	1
CHEMBL480502	CXCR4	1	Training	66.13	1
CHEMBL472323	CXCR4	1	Prediction	79.86	1
CHEMBL443092	CXCR4	1	Training	93.13	1
CHEMBL452868	CXCR4	1	Training	90.81	1
CHEMBL446868	CXCR4	1	Training	93.38	1
CHEMBL454689	CXCR4	1	Prediction	86.67	1
CHEMBL518004	CXCR4	1	Training	60.00	1
CHEMBL516989	CXCR4	1	Training	85.39	1
CHEMBL460484	CXCR4	1	Training	86.17	1
CHEMBL516480	CXCR4	1	Prediction	88.35	1
Aceclofenac	CXCR4	-1	Training	97.77	-1
Acetaminophen	CXCR4	-1	Training	99.52	-1
Acetazolamide	CXCR4	-1	Training	90.32	-1
Acetophenazine	CXCR4	-1	Prediction	55.65	1*
Amantadine	CXCR4	-1	Training	98.06	-1
Ambenonium	CXCR4	-1	Training	50.60	-1
Amineptine	CXCR4	-1	Training	96.29	-1
Amiodarone	CXCR4	-1	Prediction	91.30	-1
Amitriptyline	CXCR4	-1	Training	99.41	-1
Aprobarbital	CXCR4	-1	Training	98.51	-1
Artane	CXCR4	-1	Training	98.97	-1
Aspirin	CXCR4	-1	Prediction	99.63	-1
Atenolol	CXCR4	-1	Training	99.28	-1
Atropine	CXCR4	-1	Training	85.00	-1
Baclofen	CXCR4	-1	Training	99.03	-1
Beclomethasone	CXCR4	-1	Prediction	99.80	-1
Benzonatate	CXCR4	-1	Training	98.74	-1
Biperiden	CXCR4	-1	Training	98.07	-1
Bromocriptine	CXCR4	-1	Training	96.67	-1
Buclizine	CXCR4	-1	Prediction	73.53	-1
Budesonide	CXCR4	-1	Training	93.14	-1
Buprenorphine	CXCR4	-1	Training	100.00	-1

Caffeine	CXCR4	-1	Training	81.30	-1
Cantil	CXCR4	-1	Prediction	98.73	-1
Carbachol	CXCR4	-1	Training	96.00	-1
Carbamazepine	CXCR4	-1	Training	92.28	-1
Carisoprodol	CXCR4	-1	Training	85.75	-1
Carvedilol	CXCR4	-1	Prediction	99.54	1*
Cefoperazone	CXCR4	-1	Training	0.91	-1
Chloral hydrate	CXCR4	-1	Training	99.52	-1
Chlordiazepoxide	CXCR4	-1	Training	95.46	-1
Chlorpropamide	CXCR4	-1	Prediction	86.60	-1
Chlorthalidone	CXCR4	-1	Training	98.98	-1
Clidinium	CXCR4	-1	Training	98.08	-1
Clobazam	CXCR4	-1	Training	97.17	-1
Clofazimine	CXCR4	-1	Prediction	99.98	-1
Clomipramine	CXCR4	-1	Training	95.89	-1
Clonidine	CXCR4	-1	Training	91.64	-1
Codeine	CXCR4	-1	Training	99.91	-1
Colchicine	CXCR4	-1	Prediction	99.48	-1
Cyclizine	CXCR4	-1	Training	97.63	-1
Cyclosporin	CXCR4	-1	Training	0.03	-1
Dextropropoxyphene	CXCR4	-1	Training	99.42	-1
Diazepam	CXCR4	-1	Prediction	96.90	-1
Diflucortolone	CXCR4	-1	Training	88.70	-1
Dimercaprol	CXCR4	-1	Training	99.81	-1
Diphenhydramine	CXCR4	-1	Training	98.56	-1
Diphenidol	CXCR4	-1	Prediction	99.24	1*
Dobutamine	CXCR4	-1	Training	97.49	-1
Dofetilide	CXCR4	-1	Training	80.36	-1
Domperidone	CXCR4	-1	Training	14.56	-1
Dopamine	CXCR4	-1	Prediction	99.65	-1
Doxazosin	CXCR4	-1	Training	83.26	-1
Doxepin	CXCR4	-1	Training	99.75	-1
Dronabinol	CXCR4	-1	Training	99.48	-1
Droxicam	CXCR4	-1	Prediction	98.71	-1
Entacapone	CXCR4	-1	Training	99.16	-1
Epinephrine	CXCR4	-1	Training	99.55	-1
Eprosartan	CXCR4	-1	Training	71.58	-1
Ergotamine	CXCR4	-1	Prediction	99.86	-1
Ethosuximide	CXCR4	-1	Training	99.50	-1
Fentanyl	CXCR4	-1	Training	95.89	-1
Fexofenadine	CXCR4	-1	Training	96.75	-1
Flecainide	CXCR4	-1	Prediction	91.46	-1
Flunarizine	CXCR4	-1	Training	32.37	-1
Flunisolide	CXCR4	-1	Training	91.16	-1
Fluoxetine	CXCR4	-1	Training	98.12	-1

Fluvoxamine	CXCR4	-1	Prediction	99.19	-1
Gabapentin	CXCR4	-1	Training	99.49	-1
Gestodene	CXCR4	-1	Training	98.68	-1
Glutethimide	CXCR4	-1	Training	99.57	-1
Glycopyrrolate	CXCR4	-1	Prediction	91.24	-1
Guanadrel	CXCR4	-1	Training	94.63	-1
Halofantrine	CXCR4	-1	Training	79.32	-1
Haloperidol	CXCR4	-1	Training	42.60	-1
Halothane	CXCR4	-1	Prediction	99.21	-1
Hydromorphone	CXCR4	-1	Training	93.81	-1
Hydroxyzine	CXCR4	-1	Training	95.69	1*
Indapamide	CXCR4	-1	Training	92.83	-1
Indomethacin	CXCR4	-1	Prediction	98.34	-1
Isoetharine	CXCR4	-1	Training	98.82	-1
Isoproterenol	CXCR4	-1	Training	99.21	-1
Isosorbide	CXCR4	-1	Training	99.26	-1
Ketamine	CXCR4	-1	Prediction	91.85	-1
Labetalol	CXCR4	-1	Training	96.76	-1
Lacidipine	CXCR4	-1	Training	99.87	-1
Lamotrigine	CXCR4	-1	Training	51.37	-1
Leuprorelin	CXCR4	-1	Prediction	12.51	-1
Levodopa	CXCR4	-1	Training	99.24	-1
Lidocaine	CXCR4	-1	Training	98.74	-1
Loratadine	CXCR4	-1	Training	68.83	-1
Maprotiline	CXCR4	-1	Prediction	99.55	-1
Meclizine	CXCR4	-1	Training	86.00	-1
Medroxyprogesterone	CXCR4	-1	Training	82.30	-1
Melfalan	CXCR4	-1	Training	98.37	-1
Meprobamate	CXCR4	-1	Prediction	91.94	-1
Methamphetamine	CXCR4	-1	Training	99.53	-1
Methantheline	CXCR4	-1	Training	97.08	-1
Methocarbamol	CXCR4	-1	Training	99.43	-1
Methoxyflurane	CXCR4	-1	Prediction	99.43	-1
Methscopolamine	CXCR4	-1	Training	83.97	-1
Methylphenidate	CXCR4	-1	Training	99.36	-1
Methysergide	CXCR4	-1	Training	98.66	-1
Metoclopramide	CXCR4	-1	Prediction	99.16	-1
Midodrine	CXCR4	-1	Training	99.82	-1
Mirtazapine	CXCR4	-1	Training	51.50	-1
Modafinil	CXCR4	-1	Training	97.69	-1
Montelukast	CXCR4	-1	Prediction	15.58	-1
Moricizine	CXCR4	-1	Training	99.69	-1
Morphine	CXCR4	-1	Training	99.83	-1
Nalmefene	CXCR4	-1	Training	100.00	-1
Neostigmine	CXCR4	-1	Prediction	99.91	-1

Nifedipine	CXCR4	-1	Training	99.93	-1
Oxycodone	CXCR4	-1	Training	99.89	-1
Paroxetine	CXCR4	-1	Training	97.23	-1
Pecazine	CXCR4	-1	Prediction	93.94	-1
Pergolide	CXCR4	-1	Training	99.96	-1
Phenylbutazone	CXCR4	-1	Training	99.21	-1
Phenytoin	CXCR4	-1	Training	98.95	-1
Pilocarpine	CXCR4	-1	Prediction	83.67	-1
Pimozide	CXCR4	-1	Training	3.38	-1
Pramipexole	CXCR4	-1	Training	97.72	-1
Probenecid	CXCR4	-1	Training	98.26	-1
Procyclidine	CXCR4	-1	Prediction	94.23	-1
Propantheline	CXCR4	-1	Training	97.52	-1
Pseudoephedrine	CXCR4	-1	Training	99.51	-1
Pyrantel	CXCR4	-1	Training	99.37	-1
Quinidine	CXCR4	-1	Prediction	52.70	-1
Ranitidine	CXCR4	-1	Training	99.20	-1
Rifampin	CXCR4	-1	Training	72.87	-1
Risperidone	CXCR4	-1	Training	80.66	-1
Ropinirole	CXCR4	-1	Prediction	98.21	-1
Salmeterol	CXCR4	-1	Training	97.34	1*
Selegiline	CXCR4	-1	Training	99.22	-1
Sulfinpyrazone	CXCR4	-1	Training	96.36	-1
Tegafur	CXCR4	-1	Prediction	73.84	-1
Terpin	CXCR4	-1	Training	98.77	-1
Tolcapone	CXCR4	-1	Training	80.89	-1
Tranlycypromine	CXCR4	-1	Training	99.38	-1
Trazodone	CXCR4	-1	Prediction	65.72	-1
Triamcinolone	CXCR4	-1	Training	99.82	-1
Valproic acid	CXCR4	-1	Training	99.61	-1
Vancomycin	CXCR4	-1	Training	0.02	-1
Venlafaxine	CXCR4	-1	Prediction	99.38	-1
Verapamil	CXCR4	-1	Training	99.80	-1
Wyntensin	CXCR4	-1	Training	95.46	-1
Zafirlukast	CXCR4	-1	Training	98.14	-1
Zileuton	CXCR4	-1	Prediction	96.61	-1
Zonisamide	CXCR4	-1	Training	97.58	-1
CHEMBL433165	HIV-1 PR	1	Training	100.00	1
CHEMBL76289	HIV-1 PR	1	Training	98.92	1
CHEMBL53254	HIV-1 PR	1	Training	81.50	1
CHEMBL52669	HIV-1 PR	1	Prediction	58.03	1
CHEMBL421568	HIV-1 PR	1	Training	99.88	1
CHEMBL52702	HIV-1 PR	1	Training	54.27	1
CHEMBL319092	HIV-1 PR	1	Training	81.50	1
CHEMBL96352	HIV-1 PR	1	Prediction	100.00	1

CHEMBL430469	HIV-1 PR	1	Training	82.93	1
CHEMBL319408	HIV-1 PR	1	Training	81.50	1
CHEMBL319792	HIV-1 PR	1	Training	82.93	1
CHEMBL295414	HIV-1 PR	1	Prediction	87.11	1
CHEMBL300140	HIV-1 PR	1	Training	94.71	1
CHEMBL298189	HIV-1 PR	1	Training	69.55	1
CHEMBL433270	HIV-1 PR	1	Training	62.70	1
CHEMBL96697	HIV-1 PR	1	Prediction	99.80	1
CHEMBL100310	HIV-1 PR	1	Training	84.34	1
CHEMBL300754	HIV-1 PR	1	Training	74.83	1
CHEMBL96100	HIV-1 PR	1	Training	99.81	1
CHEMBL94824	HIV-1 PR	1	Prediction	98.79	1
CHEMBL52645	HIV-1 PR	1	Training	47.95	1
CHEMBL314510	HIV-1 PR	1	Training	99.00	1
CHEMBL297720	HIV-1 PR	1	Training	58.27	1
CHEMBL79236	HIV-1 PR	1	Prediction	99.52	1
CHEMBL49768	HIV-1 PR	1	Training	93.45	1
CHEMBL295442	HIV-1 PR	1	Training	92.69	1
CHEMBL416082	HIV-1 PR	1	Training	97.71	1
CHEMBL312238	HIV-1 PR	1	Prediction	99.29	1
CHEMBL297294	HIV-1 PR	1	Training	94.90	1
CHEMBL316454	HIV-1 PR	1	Training	99.80	1
CHEMBL295549	HIV-1 PR	1	Training	80.48	1
CHEMBL419923	HIV-1 PR	1	Prediction	84.28	1
CHEMBL44489	HIV-1 PR	1	Training	90.70	1
CHEMBL293992	HIV-1 PR	1	Training	95.45	1
CHEMBL285759	HIV-1 PR	1	Training	82.35	1
CHEMBL318777	HIV-1 PR	1	Prediction	99.88	1
CHEMBL294392	HIV-1 PR	1	Training	93.09	1
CHEMBL96645	HIV-1 PR	1	Training	99.81	1
CHEMBL297066	HIV-1 PR	1	Training	92.88	1
CHEMBL301571	HIV-1 PR	1	Prediction	95.79	1
CHEMBL318525	HIV-1 PR	1	Training	99.99	1
CHEMBL311953	HIV-1 PR	1	Training	99.17	1
CHEMBL295470	HIV-1 PR	1	Training	90.77	1
CHEMBL431999	HIV-1 PR	1	Prediction	85.38	1
CHEMBL299884	HIV-1 PR	1	Training	96.70	1
CHEMBL298316	HIV-1 PR	1	Training	88.76	1
CHEMBL291196	HIV-1 PR	1	Training	89.92	1
CHEMBL290987	HIV-1 PR	1	Prediction	88.76	1
CHEMBL295530	HIV-1 PR	1	Training	89.81	1
CHEMBL47610	HIV-1 PR	1	Training	99.94	1
CHEMBL46114	HIV-1 PR	1	Training	89.18	1
CHEMBL295471	HIV-1 PR	1	Prediction	95.69	1
CHEMBL111143	HIV-1 PR	1	Training	76.72	1

CHEMBL45451	HIV-1 PR	1	Training	92.05	1
CHEMBL292193	HIV-1 PR	1	Training	95.42	1
CHEMBL322984	HIV-1 PR	1	Prediction	86.80	1
CHEMBL77786	HIV-1 PR	1	Training	75.02	1
CHEMBL48565	HIV-1 PR	1	Training	99.01	1
CHEMBL297673	HIV-1 PR	1	Training	94.16	1
CHEMBL46274	HIV-1 PR	1	Prediction	92.61	1
CHEMBL276447	HIV-1 PR	1	Training	98.69	1
CHEMBL44578	HIV-1 PR	1	Training	94.88	1
CHEMBL99267	HIV-1 PR	1	Training	98.16	1
CHEMBL100040	HIV-1 PR	1	Prediction	99.22	1
CHEMBL98589	HIV-1 PR	1	Training	98.21	1
CHEMBL297189	HIV-1 PR	1	Training	88.57	1
CHEMBL95228	HIV-1 PR	1	Training	99.89	1
CHEMBL98954	HIV-1 PR	1	Prediction	99.24	1
CHEMBL9544	HIV-1 PR	1	Training	99.01	1
CHEMBL9705	HIV-1 PR	1	Training	99.01	1
CHEMBL295357	HIV-1 PR	1	Training	92.51	1
CHEMBL265514	HIV-1 PR	1	Prediction	87.62	1
CHEMBL413515	HIV-1 PR	1	Training	99.81	-1*
CHEMBL296115	HIV-1 PR	1	Training	86.38	1
CHEMBL47480	HIV-1 PR	1	Training	96.75	1
CHEMBL77497	HIV-1 PR	1	Prediction	98.35	1
CHEMBL52670	HIV-1 PR	1	Training	94.54	1
CHEMBL329750	HIV-1 PR	1	Training	91.43	1
CHEMBL410311	HIV-1 PR	1	Training	94.50	1
CHEMBL108918	HIV-1 PR	1	Prediction	89.72	1
CHEMBL164045	HIV-1 PR	1	Training	97.65	1
CHEMBL351834	HIV-1 PR	1	Training	99.45	1
CHEMBL296484	HIV-1 PR	1	Training	95.83	1
CHEMBL297620	HIV-1 PR	1	Prediction	95.23	1
CHEMBL295904	HIV-1 PR	1	Training	95.31	1
CHEMBL298393	HIV-1 PR	1	Training	54.27	1
CHEMBL305814	HIV-1 PR	1	Training	91.98	1
CHEMBL295924	HIV-1 PR	1	Prediction	96.78	1
CHEMBL265516	HIV-1 PR	1	Training	90.45	1
CHEMBL308780	HIV-1 PR	1	Training	86.38	1
CHEMBL296493	HIV-1 PR	1	Training	88.46	1
CHEMBL301269	HIV-1 PR	1	Prediction	92.73	1
CHEMBL101560	HIV-1 PR	1	Training	83.32	1
CHEMBL78261	HIV-1 PR	1	Training	56.04	1
CHEMBL277908	HIV-1 PR	1	Training	86.38	1
CHEMBL77431	HIV-1 PR	1	Prediction	70.79	1
CHEMBL297045	HIV-1 PR	1	Training	88.76	1
CHEMBL291195	HIV-1 PR	1	Training	97.03	1

CHEMBL82245	HIV-1 PR	1	Training	99.21	1
CHEMBL429722	HIV-1 PR	1	Prediction	99.01	1
CHEMBL310417	HIV-1 PR	1	Training	98.81	1
CHEMBL49002	HIV-1 PR	1	Training	98.56	1
CHEMBL73880	HIV-1 PR	1	Training	98.25	1
CHEMBL115	HIV-1 PR	1	Prediction	99.86	1
CHEMBL265975	HIV-1 PR	1	Training	79.26	1
CHEMBL289195	HIV-1 PR	1	Training	96.38	1
CHEMBL99357	HIV-1 PR	1	Training	99.71	1
CHEMBL75363	HIV-1 PR	1	Prediction	82.35	1
CHEMBL49544	HIV-1 PR	1	Training	96.73	1
CHEMBL298788	HIV-1 PR	1	Training	98.80	1
CHEMBL95413	HIV-1 PR	1	Training	79.23	1
CHEMBL296137	HIV-1 PR	1	Prediction	97.24	1
CHEMBL202345	HIV-1 PR	1	Training	5.13	1
CHEMBL306963	HIV-1 PR	1	Training	93.45	1
CHEMBL97253	HIV-1 PR	1	Training	79.33	1
CHEMBL98129	HIV-1 PR	1	Prediction	80.52	1
CHEMBL47712	HIV-1 PR	1	Training	94.22	1
CHEMBL60697	HIV-1 PR	1	Training	97.31	1
CHEMBL319053	HIV-1 PR	1	Training	99.99	1
CHEMBL100089	HIV-1 PR	1	Prediction	98.12	1
CHEMBL432550	HIV-1 PR	1	Training	99.31	1
CHEMBL316694	HIV-1 PR	1	Training	95.22	1
Aceclofenac	HIV-1 PR	-1	Training	97.10	-1
Acetaminophen	HIV-1 PR	-1	Prediction	99.37	-1
Acetazolamide	HIV-1 PR	-1	Training	87.70	-1
Acetophenazine	HIV-1 PR	-1	Training	48.95	-1
Amantadine	HIV-1 PR	-1	Training	97.48	-1
Ambenonium	HIV-1 PR	-1	Prediction	43.91	-1
Amineptine	HIV-1 PR	-1	Training	95.20	-1
Amiodarone	HIV-1 PR	-1	Training	88.92	-1
Amitriptyline	HIV-1 PR	-1	Training	99.23	-1
Aprobarbital	HIV-1 PR	-1	Prediction	98.06	-1
Artane	HIV-1 PR	-1	Training	98.65	-1
Aspirin	HIV-1 PR	-1	Training	99.52	-1
Atenolol	HIV-1 PR	-1	Training	99.06	-1
Atropine	HIV-1 PR	-1	Prediction	81.24	-1
Baclofen	HIV-1 PR	-1	Training	98.74	-1
Beclomethasone	HIV-1 PR	-1	Training	99.73	-1
Benzonatate	HIV-1 PR	-1	Training	98.36	-1
Biperiden	HIV-1 PR	-1	Prediction	97.49	-1
Bromocriptine	HIV-1 PR	-1	Training	95.69	-1
Bucizine	HIV-1 PR	-1	Training	67.98	-1
Budesonide	HIV-1 PR	-1	Training	91.22	-1

Buprenorphine	HIV-1 PR	-1	Prediction	100.00	-1
Caffeine	HIV-1 PR	-1	Training	76.87	-1
Cantil	HIV-1 PR	-1	Training	98.35	-1
Carbachol	HIV-1 PR	-1	Training	94.83	-1
Carbamazepine	HIV-1 PR	-1	Prediction	90.14	-1
Carisoprodol	HIV-1 PR	-1	Training	82.14	-1
Carvedilol	HIV-1 PR	-1	Training	99.40	-1
Cefoperazone	HIV-1 PR	-1	Training	0.70	-1
Chloral hydrate	HIV-1 PR	-1	Prediction	99.38	-1
Chlordiazepoxide	HIV-1 PR	-1	Training	94.14	-1
Chlorpropamide	HIV-1 PR	-1	Training	83.17	-1
Chlorthalidone	HIV-1 PR	-1	Training	98.67	-1
Clidinium	HIV-1 PR	-1	Prediction	97.51	-1
Clobazam	HIV-1 PR	-1	Training	96.33	-1
Clofazimine	HIV-1 PR	-1	Training	99.97	-1
Clomipramine	HIV-1 PR	-1	Training	94.69	-1
Clonidine	HIV-1 PR	-1	Prediction	89.33	-1
Codeine	HIV-1 PR	-1	Training	99.88	-1
Colchicine	HIV-1 PR	-1	Training	99.32	-1
Cyclizine	HIV-1 PR	-1	Training	96.93	-1
Cyclosporin	HIV-1 PR	-1	Prediction	0.02	-1
Dextropropoxyphene	HIV-1 PR	-1	Training	99.25	-1
Diazepam	HIV-1 PR	-1	Training	95.98	-1
Diflucortolone	HIV-1 PR	-1	Training	85.72	-1
Dimercaprol	HIV-1 PR	-1	Prediction	99.75	-1
Diphenhydramine	HIV-1 PR	-1	Training	98.13	-1
Diphenidol	HIV-1 PR	-1	Training	99.01	-1
Dobutamine	HIV-1 PR	-1	Training	96.75	-1
Dofetilide	HIV-1 PR	-1	Prediction	75.77	-1
Domperidone	HIV-1 PR	-1	Training	11.53	-1
Dopamine	HIV-1 PR	-1	Training	99.54	-1
Doxazosin	HIV-1 PR	-1	Training	79.18	-1
Doxepin	HIV-1 PR	-1	Prediction	99.67	-1
Dronabinol	HIV-1 PR	-1	Training	99.32	-1
Droxycam	HIV-1 PR	-1	Training	98.32	-1
Entacapone	HIV-1 PR	-1	Training	98.91	-1
Epinephrine	HIV-1 PR	-1	Prediction	99.41	-1
Eprosartan	HIV-1 PR	-1	Training	65.81	-1
Ergotamine	HIV-1 PR	-1	Training	99.82	-1
Ethosuximide	HIV-1 PR	-1	Training	99.35	-1
Fentanyl	HIV-1 PR	-1	Prediction	94.69	-1
Fexofenadine	HIV-1 PR	-1	Training	95.79	-1
Flecainide	HIV-1 PR	-1	Training	89.11	-1
Flunarizine	HIV-1 PR	-1	Training	26.78	-1
Flunisolide	HIV-1 PR	-1	Prediction	88.74	-1

Fluoxetine	HIV-1 PR	-1	Training	97.56	-1
Fluvoxamine	HIV-1 PR	-1	Training	98.95	-1
Gabapentin	HIV-1 PR	-1	Training	99.33	-1
Gestodene	HIV-1 PR	-1	Prediction	98.29	-1
Glutethimide	HIV-1 PR	-1	Training	99.43	-1
Glycopyrrolate	HIV-1 PR	-1	Training	88.84	-1
Guanadrel	HIV-1 PR	-1	Training	93.09	-1
Halofantrine	HIV-1 PR	-1	Prediction	74.57	-1
Haloperidol	HIV-1 PR	-1	Training	36.20	-1
Halothane	HIV-1 PR	-1	Training	98.97	-1
Hydromorphone	HIV-1 PR	-1	Training	92.05	-1
Hydroxyzine	HIV-1 PR	-1	Prediction	94.44	-1
Indapamide	HIV-1 PR	-1	Training	90.82	-1
Indomethacin	HIV-1 PR	-1	Training	97.84	-1
Isoetharine	HIV-1 PR	-1	Training	98.47	-1
Isoproterenol	HIV-1 PR	-1	Prediction	98.97	-1
Isosorbide	HIV-1 PR	-1	Training	99.04	-1
Ketamine	HIV-1 PR	-1	Training	89.60	-1
Labetalol	HIV-1 PR	-1	Training	95.80	-1
Lacidipine	HIV-1 PR	-1	Prediction	99.83	-1
Lamotrigine	HIV-1 PR	-1	Training	44.67	-1
Leuprorelin	HIV-1 PR	-1	Training	9.85	-1
Levodopa	HIV-1 PR	-1	Training	99.01	-1
Lidocaine	HIV-1 PR	-1	Prediction	98.35	-1
Loratadine	HIV-1 PR	-1	Training	62.80	-1
Maprotiline	HIV-1 PR	-1	Training	99.42	-1
Meclizine	HIV-1 PR	-1	Training	82.44	-1
Medroxyprogesterone	HIV-1 PR	-1	Prediction	78.04	-1
Melfalan	HIV-1 PR	-1	Training	97.88	-1
Meprobamate	HIV-1 PR	-1	Training	89.71	-1
Methamphetamine	HIV-1 PR	-1	Training	99.38	-1
Methantheline	HIV-1 PR	-1	Prediction	96.21	-1
Methocarbamol	HIV-1 PR	-1	Training	99.25	-1
Methoxyflurane	HIV-1 PR	-1	Training	99.26	-1
Methscopolamine	HIV-1 PR	-1	Training	80.01	-1
Methylphenidate	HIV-1 PR	-1	Prediction	99.17	-1
Methysergide	HIV-1 PR	-1	Training	98.25	-1
Metoclopramide	HIV-1 PR	-1	Training	98.90	-1
Midodrine	HIV-1 PR	-1	Training	99.76	-1
Mirtazapine	HIV-1 PR	-1	Prediction	44.80	-1
Modafinil	HIV-1 PR	-1	Training	97.00	-1
Montelukast	HIV-1 PR	-1	Training	12.37	-1
Moricizine	HIV-1 PR	-1	Training	99.60	-1
Morphine	HIV-1 PR	-1	Prediction	99.77	-1
Nalmefene	HIV-1 PR	-1	Training	99.99	-1

Neostigmine	HIV-1 PR	-1	Training	99.89	-1
Nifedipine	HIV-1 PR	-1	Training	99.91	-1
Oxycodone	HIV-1 PR	-1	Prediction	99.85	-1
Paroxetine	HIV-1 PR	-1	Training	96.41	-1
Pecazine	HIV-1 PR	-1	Training	92.22	-1
Pergolide	HIV-1 PR	-1	Training	99.95	-1
Phenylbutazone	HIV-1 PR	-1	Prediction	98.97	-1
Phenytoin	HIV-1 PR	-1	Training	98.64	-1
Pilocarpine	HIV-1 PR	-1	Training	79.65	-1
Pimozide	HIV-1 PR	-1	Training	2.60	-1
Pramipexole	HIV-1 PR	-1	Prediction	97.04	-1
Probenecid	HIV-1 PR	-1	Training	97.73	-1
Procyclidine	HIV-1 PR	-1	Training	92.58	-1
Proprantheline	HIV-1 PR	-1	Training	96.78	-1
Pseudoephedrine	HIV-1 PR	-1	Prediction	99.36	-1
Pyrantel	HIV-1 PR	-1	Training	99.18	-1
Quinidine	HIV-1 PR	-1	Training	45.99	-1
Ranitidine	HIV-1 PR	-1	Training	98.96	-1
Rifampin	HIV-1 PR	-1	Prediction	67.25	-1
Risperidone	HIV-1 PR	-1	Training	76.12	-1
Ropinirole	HIV-1 PR	-1	Training	97.67	-1
Salmeterol	HIV-1 PR	-1	Training	96.54	-1
Selegiline	HIV-1 PR	-1	Prediction	98.99	-1
Sulfinpyrazone	HIV-1 PR	-1	Training	95.29	-1
Tegafur	HIV-1 PR	-1	Training	68.33	-1
Terpin	HIV-1 PR	-1	Training	98.39	-1
Tolcapone	HIV-1 PR	-1	Prediction	76.39	-1
Tranlycypromine	HIV-1 PR	-1	Training	99.19	-1
Trazodone	HIV-1 PR	-1	Training	59.44	-1
Triamcinolone	HIV-1 PR	-1	Training	99.77	-1
Valproic acid	HIV-1 PR	-1	Prediction	99.49	-1
Vancomycin	HIV-1 PR	-1	Training	0.02	-1
Venlafaxine	HIV-1 PR	-1	Training	99.19	-1
Verapamil	HIV-1 PR	-1	Training	99.74	-1
Wytensin	HIV-1 PR	-1	Prediction	94.15	-1
Zafirlukast	HIV-1 PR	-1	Training	97.59	-1
Zileuton	HIV-1 PR	-1	Training	95.61	-1
Zonisamide	HIV-1 PR	-1	Training	96.86	-1
CHEMBL338099	HIV-1 RT	1	Training	99.06	-1*
CHEMBL88677	HIV-1 RT	1	Training	98.85	1
CHEMBL132756	HIV-1 RT	1	Prediction	99.89	1
CHEMBL253186	HIV-1 RT	1	Training	83.86	1
CHEMBL135380	HIV-1	1	Training	88.75	1

	RT				
CHEMBL57	HIV-1 RT	1	Training	94.94	-1*
CHEMBL37024	HIV-1 RT	1	Prediction	98.79	1
CHEMBL37835	HIV-1 RT	1	Training	96.20	1
CHEMBL541204	HIV-1 RT	1	Training	98.79	1
CHEMBL436376	HIV-1 RT	1	Training	99.90	1
CHEMBL436177	HIV-1 RT	1	Prediction	94.48	1
CHEMBL103706	HIV-1 RT	1	Training	99.77	1
CHEMBL341201	HIV-1 RT	1	Training	94.01	1
CHEMBL37762	HIV-1 RT	1	Training	99.22	1
CHEMBL38341	HIV-1 RT	1	Prediction	89.68	1
CHEMBL408273	HIV-1 RT	1	Training	99.98	-1*
CHEMBL134278	HIV-1 RT	1	Training	99.68	1
CHEMBL133658	HIV-1 RT	1	Training	99.94	1
CHEMBL382553	HIV-1 RT	1	Prediction	84.73	1
CHEMBL435600	HIV-1 RT	1	Training	100.00	1
CHEMBL398766	HIV-1 RT	1	Training	98.54	1
CHEMBL207512	HIV-1 RT	1	Training	87.37	1
CHEMBL334983	HIV-1 RT	1	Prediction	98.04	1
CHEMBL207839	HIV-1 RT	1	Training	86.23	1
CHEMBL133195	HIV-1 RT	1	Training	98.33	1
CHEMBL206522	HIV-1 RT	1	Training	93.73	-1*
CHEMBL381134	HIV-1 RT	1	Prediction	86.37	1
CHEMBL56135	HIV-1 RT	1	Training	50.09	1
CHEMBL287317	HIV-1 RT	1	Training	82.53	1
CHEMBL133559	HIV-1 RT	1	Training	99.67	1
CHEMBL134026	HIV-1 RT	1	Prediction	99.69	1
CHEMBL36424	HIV-1 RT	1	Training	93.38	1
CHEMBL253169	HIV-1 RT	1	Training	99.07	1
CHEMBL205152	HIV-1 RT	1	Training	91.48	1

CHEMBL379722	HIV-1 RT	1	Prediction	93.12	1
CHEMBL252964	HIV-1 RT	1	Training	98.07	1
CHEMBL207929	HIV-1 RT	1	Training	87.37	1
CHEMBL38318	HIV-1 RT	1	Training	99.94	1
CHEMBL206962	HIV-1 RT	1	Prediction	85.01	1
CHEMBL134630	HIV-1 RT	1	Training	82.73	1
CHEMBL340047	HIV-1 RT	1	Training	99.94	1
CHEMBL399976	HIV-1 RT	1	Training	89.26	1
CHEMBL377010	HIV-1 RT	1	Prediction	78.83	1
CHEMBL135254	HIV-1 RT	1	Training	99.89	1
CHEMBL236161	HIV-1 RT	1	Training	72.05	1
CHEMBL253822	HIV-1 RT	1	Training	55.12	-1*
CHEMBL399503	HIV-1 RT	1	Prediction	85.07	1
CHEMBL207920	HIV-1 RT	1	Training	93.32	1
CHEMBL306904	HIV-1 RT	1	Training	5.64	1
CHEMBL402265	HIV-1 RT	1	Training	98.06	1
CHEMBL429488	HIV-1 RT	1	Prediction	99.89	1
CHEMBL135259	HIV-1 RT	1	Training	99.30	1
CHEMBL400547	HIV-1 RT	1	Training	88.03	1
CHEMBL207900	HIV-1 RT	1	Training	82.96	1
CHEMBL291983	HIV-1 RT	1	Prediction	49.06	1
CHEMBL131972	HIV-1 RT	1	Training	98.92	1
CHEMBL135105	HIV-1 RT	1	Training	99.99	1
CHEMBL254007	HIV-1 RT	1	Training	99.79	1
CHEMBL398890	HIV-1 RT	1	Prediction	97.88	1
CHEMBL253369	HIV-1 RT	1	Training	91.07	1
CHEMBL253170	HIV-1 RT	1	Training	93.69	1
CHEMBL252137	HIV-1 RT	1	Training	89.46	1
CHEMBL129	HIV-1 RT	1	Prediction	3.63	1
CHEMBL132425	HIV-1	1	Training	99.99	1

	RT				
CHEMBL137111	HIV-1 RT	1	Training	84.97	1
CHEMBL299001	HIV-1 RT	1	Training	45.10	1
CHEMBL443063	HIV-1 RT	1	Prediction	99.21	1
CHEMBL37834	HIV-1 RT	1	Training	90.87	1
CHEMBL381513	HIV-1 RT	1	Training	79.33	1
CHEMBL83412	HIV-1 RT	1	Training	6.17	1
CHEMBL252963	HIV-1 RT	1	Prediction	99.18	1
CHEMBL35729	HIV-1 RT	1	Training	83.82	1
CHEMBL253171	HIV-1 RT	1	Training	94.20	1
CHEMBL593	HIV-1 RT	1	Training	90.99	1
CHEMBL135808	HIV-1 RT	1	Prediction	99.96	1
CHEMBL37025	HIV-1 RT	1	Training	96.14	1
CHEMBL46745	HIV-1 RT	1	Training	32.43	1
CHEMBL84621	HIV-1 RT	1	Training	21.33	1
CHEMBL383088	HIV-1 RT	1	Prediction	93.02	-1*
CHEMBL319224	HIV-1 RT	1	Training	99.99	1
CHEMBL78882	HIV-1 RT	1	Training	2.39	1
CHEMBL252136	HIV-1 RT	1	Training	96.46	1
CHEMBL381888	HIV-1 RT	1	Prediction	18.58	1
CHEMBL55187	HIV-1 RT	1	Training	26.71	1
CHEMBL142837	HIV-1 RT	1	Training	73.24	1
CHEMBL144744	HIV-1 RT	1	Training	73.61	-1*
CHEMBL438146	HIV-1 RT	1	Prediction	77.81	1
CHEMBL250438	HIV-1 RT	1	Training	76.18	1
CHEMBL103386	HIV-1 RT	1	Training	92.05	1
CHEMBL205764	HIV-1 RT	1	Training	95.62	1
CHEMBL366017	HIV-1 RT	1	Prediction	91.94	1
CHEMBL81227	HIV-1 RT	1	Training	89.23	1
CHEMBL79526	HIV-1 RT	1	Training	57.28	1

CHEMBL171919	HIV-1 RT	1	Training	27.74	-1*
CHEMBL309896	HIV-1 RT	1	Training	67.80	1
CHEMBL207105	HIV-1 RT	1	Training	86.04	1
CHEMBL398891	HIV-1 RT	1	Prediction	93.95	1
CHEMBL131643	HIV-1 RT	1	Training	96.20	1
CHEMBL368116	HIV-1 RT	1	Prediction	46.00	1
CHEMBL377820	HIV-1 RT	1	Training	82.05	1
CHEMBL177271	HIV-1 RT	1	Training	76.19	1
CHEMBL99235	HIV-1 RT	1	Training	23.59	-1*
CHEMBL192231	HIV-1 RT	1	Prediction	98.57	1
CHEMBL288971	HIV-1 RT	1	Training	29.21	1
CHEMBL191163	HIV-1 RT	1	Training	81.51	1
CHEMBL39999	HIV-1 RT	1	Training	98.80	-1*
CHEMBL189942	HIV-1 RT	1	Prediction	91.18	1
CHEMBL176362	HIV-1 RT	1	Training	40.95	1
CHEMBL336237	HIV-1 RT	1	Training	11.84	1
CHEMBL175162	HIV-1 RT	1	Training	79.72	1
CHEMBL317356	HIV-1 RT	1	Prediction	76.88	-1*
Aceclofenac	HIV-1 RT	-1	Training	98.03	1*
Acetaminophen	HIV-1 RT	-1	Training	99.57	-1
Acetazolamide	HIV-1 RT	-1	Training	91.38	-1
Acetophenazine	HIV-1 RT	-1	Prediction	58.78	-1
Amantadine	HIV-1 RT	-1	Training	98.29	-1
Ambenonium	HIV-1 RT	-1	Training	53.79	-1
Amineptine	HIV-1 RT	-1	Training	96.72	-1
Amiodarone	HIV-1 RT	-1	Prediction	92.26	-1
Amitriptyline	HIV-1 RT	-1	Training	99.48	-1
Aprobarbital	HIV-1 RT	-1	Training	98.69	-1
Artane	HIV-1 RT	-1	Training	99.09	-1
Aspirin	HIV-1	-1	Prediction	99.68	-1

	RT				
Atenolol	HIV-1 RT	-1	Training	99.37	-1
Atropine	HIV-1 RT	-1	Training	86.56	1*
Baclofen	HIV-1 RT	-1	Training	99.15	-1
Beclomethasone	HIV-1 RT	-1	Prediction	99.82	-1
Benzonatate	HIV-1 RT	-1	Training	98.89	-1
Biperiden	HIV-1 RT	-1	Training	98.30	-1
Bromocriptine	HIV-1 RT	-1	Training	97.06	-1
Bucizine	HIV-1 RT	-1	Prediction	75.94	1*
Budesonide	HIV-1 RT	-1	Training	93.92	-1
Buprenorphine	HIV-1 RT	-1	Training	100.00	-1
Caffeine	HIV-1 RT	-1	Training	83.17	-1
Cantil	HIV-1 RT	-1	Prediction	98.88	-1
Carbachol	HIV-1 RT	-1	Training	96.46	-1
Carbamazepine	HIV-1 RT	-1	Training	93.14	-1
Carisoprodol	HIV-1 RT	-1	Training	87.24	-1
Carvedilol	HIV-1 RT	-1	Prediction	99.59	-1
Cefoperazone	HIV-1 RT	-1	Training	1.03	-1
Chloral hydrate	HIV-1 RT	-1	Training	99.58	-1
Chlordiazepoxide	HIV-1 RT	-1	Training	95.98	-1
Chlorpropamide	HIV-1 RT	-1	Prediction	88.02	-1
Chlorthalidone	HIV-1 RT	-1	Training	99.10	-1
Clidinium	HIV-1 RT	-1	Training	98.31	-1
Clobazam	HIV-1 RT	-1	Training	97.50	-1
Clofazimine	HIV-1 RT	-1	Prediction	99.98	1*
Clomipramine	HIV-1 RT	-1	Training	96.37	-1
Clonidine	HIV-1 RT	-1	Training	92.56	-1
Codeine	HIV-1 RT	-1	Training	99.92	-1
Colchicine	HIV-1 RT	-1	Prediction	99.54	-1
Cyclizine	HIV-1 RT	-1	Training	97.91	-1

Cyclosporin	HIV-1 RT	-1	Training	0.04	-1
Dextropropoxyphene	HIV-1 RT	-1	Training	99.49	-1
Diazepam	HIV-1 RT	-1	Prediction	97.26	-1
Diflucortolone	HIV-1 RT	-1	Training	89.92	-1
Dimercaprol	HIV-1 RT	-1	Training	99.83	-1
Diphenhydramine	HIV-1 RT	-1	Training	98.73	-1
Diphenidol	HIV-1 RT	-1	Prediction	99.33	-1
Dobutamine	HIV-1 RT	-1	Training	97.79	-1
Dofetilide	HIV-1 RT	-1	Training	82.30	-1
Domperidone	HIV-1 RT	-1	Training	16.23	1*
Dopamine	HIV-1 RT	-1	Prediction	99.69	-1
Doxazosin	HIV-1 RT	-1	Training	84.97	-1
Doxepin	HIV-1 RT	-1	Training	99.78	-1
Dronabinol	HIV-1 RT	-1	Training	99.54	-1
Droxicam	HIV-1 RT	-1	Prediction	98.86	-1
Entacapone	HIV-1 RT	-1	Training	99.26	-1
Epinephrine	HIV-1 RT	-1	Training	99.60	-1
Eprosartan	HIV-1 RT	-1	Training	74.10	1*
Ergotamine	HIV-1 RT	-1	Prediction	99.88	-1
Ethosuximide	HIV-1 RT	-1	Training	99.56	-1
Fentanyl	HIV-1 RT	-1	Training	96.36	-1
Fexofenadine	HIV-1 RT	-1	Training	97.13	-1
Flecainide	HIV-1 RT	-1	Prediction	92.40	-1
Flunarizine	HIV-1 RT	-1	Training	35.23	1*
Flunisolide	HIV-1 RT	-1	Training	92.14	-1
Fluoxetine	HIV-1 RT	-1	Training	98.35	1*
Fluvoxamine	HIV-1 RT	-1	Prediction	99.29	-1
Gabapentin	HIV-1 RT	-1	Training	99.55	-1
Gestodene	HIV-1 RT	-1	Training	98.84	-1
Glutethimide	HIV-1	-1	Training	99.62	-1

	RT				
Glycopyrrolate	HIV-1 RT	-1	Prediction	92.21	-1
Guanadrel	HIV-1 RT	-1	Training	95.25	-1
Halofantrine	HIV-1 RT	-1	Training	81.34	-1
Haloperidol	HIV-1 RT	-1	Training	45.75	-1
Halothane	HIV-1 RT	-1	Prediction	99.30	-1
Hydromorphone	HIV-1 RT	-1	Training	94.51	-1
Hydroxyzine	HIV-1 RT	-1	Training	96.19	-1
Indapamide	HIV-1 RT	-1	Training	93.64	-1
Indomethacin	HIV-1 RT	-1	Prediction	98.54	1*
Isoetharine	HIV-1 RT	-1	Training	98.96	-1
Isoproterenol	HIV-1 RT	-1	Training	99.31	-1
Isosorbide	HIV-1 RT	-1	Training	99.35	-1
Ketamine	HIV-1 RT	-1	Prediction	92.76	-1
Labetalol	HIV-1 RT	-1	Training	97.13	1*
Lacidipine	HIV-1 RT	-1	Training	99.89	-1
Lamotrigine	HIV-1 RT	-1	Training	54.55	-1
Leuprorelin	HIV-1 RT	-1	Prediction	13.98	-1
Levodopa	HIV-1 RT	-1	Training	99.33	-1
Lidocaine	HIV-1 RT	-1	Training	98.89	-1
Loratadine	HIV-1 RT	-1	Training	71.50	1*
Maprotiline	HIV-1 RT	-1	Prediction	99.61	-1
Meclizine	HIV-1 RT	-1	Training	87.47	-1
Medroxyprogesterone	HIV-1 RT	-1	Training	84.08	-1
Melfalan	HIV-1 RT	-1	Training	98.57	-1
Meprobamate	HIV-1 RT	-1	Prediction	92.84	-1
Methamphetamine	HIV-1 RT	-1	Training	99.58	-1
Methantheline	HIV-1 RT	-1	Training	97.42	-1
Methocarbamol	HIV-1 RT	-1	Training	99.50	-1
Methoxyflurane	HIV-1 RT	-1	Prediction	99.50	-1

Methscopolamine	HIV-1 RT	-1	Training	85.61	-1
Methylphenidate	HIV-1 RT	-1	Training	99.44	-1
Methysergide	HIV-1 RT	-1	Training	98.82	-1
Metoclopramide	HIV-1 RT	-1	Prediction	99.26	-1
Midodrine	HIV-1 RT	-1	Training	99.84	-1
Mirtazapine	HIV-1 RT	-1	Training	54.68	-1
Modafinil	HIV-1 RT	-1	Training	97.96	-1
Montelukast	HIV-1 RT	-1	Prediction	17.34	-1
Moricizine	HIV-1 RT	-1	Training	99.73	-1
Morphine	HIV-1 RT	-1	Training	99.85	-1
Nalmefene	HIV-1 RT	-1	Training	100.00	-1
Neostigmine	HIV-1 RT	-1	Prediction	99.92	-1
Nifedipine	HIV-1 RT	-1	Training	99.94	1*
Oxycodone	HIV-1 RT	-1	Training	99.90	-1
Paroxetine	HIV-1 RT	-1	Training	97.56	-1
Pecazine	HIV-1 RT	-1	Prediction	94.63	-1
Pergolide	HIV-1 RT	-1	Training	99.97	-1
Phenylbutazone	HIV-1 RT	-1	Training	99.31	-1
Phenytoin	HIV-1 RT	-1	Training	99.08	-1
Pilocarpine	HIV-1 RT	-1	Prediction	85.34	1*
Pimozide	HIV-1 RT	-1	Training	3.82	1*
Pramipexole	HIV-1 RT	-1	Training	97.99	-1
Probenecid	HIV-1 RT	-1	Training	98.46	-1
Procyclidine	HIV-1 RT	-1	Prediction	94.89	-1
Propantheline	HIV-1 RT	-1	Training	97.81	-1
Pseudoephedrine	HIV-1 RT	-1	Training	99.57	-1
Pyrantel	HIV-1 RT	-1	Training	99.45	-1
Quinidine	HIV-1 RT	-1	Prediction	55.87	-1
Ranitidine	HIV-1 RT	-1	Training	99.30	-1
Rifampin	HIV-1	-1	Training	75.32	-1

	RT				
Risperidone	HIV-1 RT	-1	Training	82.58	1*
Ropinirole	HIV-1 RT	-1	Prediction	98.42	-1
Salmeterol	HIV-1 RT	-1	Training	97.65	-1
Selegiline	HIV-1 RT	-1	Training	99.32	-1
Sulfinpyrazone	HIV-1 RT	-1	Training	96.78	-1
Tegafur	HIV-1 RT	-1	Prediction	76.23	-1
Terpin	HIV-1 RT	-1	Training	98.91	-1
Tolcapone	HIV-1 RT	-1	Training	82.78	1*
Tranlycypromine	HIV-1 RT	-1	Training	99.46	-1
Trazodone	HIV-1 RT	-1	Prediction	68.54	-1
Triamcinolone	HIV-1 RT	-1	Training	99.84	-1
Valproic acid	HIV-1 RT	-1	Training	99.65	-1
Vancomycin	HIV-1 RT	-1	Training	0.02	1*
Venlafaxine	HIV-1 RT	-1	Prediction	99.45	-1
Verapamil	HIV-1 RT	-1	Training	99.82	-1
Wytensin	HIV-1 RT	-1	Training	95.99	-1
Zafirlukast	HIV-1 RT	-1	Training	98.36	-1
Zileuton	HIV-1 RT	-1	Prediction	97.00	-1
Zonisamide	HIV-1 RT	-1	Training	97.86	-1
CHEMBL414850	HIV-IN	1	Training	98.48	1
CHEMBL196391	HIV-IN	1	Prediction	78.64	1
CHEMBL212412	HIV-IN	1	Training	16.77	-1*
CHEMBL210234	HIV-IN	1	Training	98.77	1
CHEMBL212213	HIV-IN	1	Training	92.06	1
CHEMBL204656	HIV-IN	1	Prediction	34.88	1
CHEMBL206604	HIV-IN	1	Training	48.41	1
CHEMBL203443	HIV-IN	1	Training	20.66	1
CHEMBL371007	HIV-IN	1	Training	99.77	1
CHEMBL379658	HIV-IN	1	Prediction	98.32	1
CHEMBL193759	HIV-IN	1	Training	50.59	1
CHEMBL32865	HIV-IN	1	Training	99.95	1
CHEMBL425924	HIV-IN	1	Training	99.81	1
CHEMBL382965	HIV-IN	1	Prediction	99.82	1
CHEMBL378029	HIV-IN	1	Training	97.19	1

CHEMBL377501	HIV-IN	1	Training	99.94	1
CHEMBL210233	HIV-IN	1	Training	96.87	1
CHEMBL368084	HIV-IN	1	Prediction	83.39	1
CHEMBL379664	HIV-IN	1	Training	31.32	1
CHEMBL377759	HIV-IN	1	Training	96.19	1
CHEMBL209872	HIV-IN	1	Training	98.45	1
CHEMBL212982	HIV-IN	1	Prediction	99.51	1
CHEMBL199145	HIV-IN	1	Training	98.83	1
CHEMBL198160	HIV-IN	1	Training	99.84	1
CHEMBL212000	HIV-IN	1	Training	61.26	1
CHEMBL36070	HIV-IN	1	Prediction	99.61	1
CHEMBL380588	HIV-IN	1	Training	96.77	1
CHEMBL209307	HIV-IN	1	Training	99.79	1
CHEMBL441683	HIV-IN	1	Training	97.82	1
CHEMBL426686	HIV-IN	1	Prediction	97.93	1
CHEMBL270717	HIV-IN	1	Training	29.07	1
CHEMBL209440	HIV-IN	1	Training	68.21	1
CHEMBL421353	HIV-IN	1	Training	78.93	1
CHEMBL142072	HIV-IN	1	Training	99.61	1
CHEMBL208776	HIV-IN	1	Training	97.82	1
CHEMBL320261	HIV-IN	1	Prediction	45.81	1
CHEMBL384912	HIV-IN	1	Training	65.61	1
CHEMBL409132	HIV-IN	1	Training	15.72	1
CHEMBL365604	HIV-IN	1	Training	85.11	1
CHEMBL29660	HIV-IN	1	Prediction	5.18	1
CHEMBL209958	HIV-IN	1	Training	80.29	1
CHEMBL377267	HIV-IN	1	Training	67.18	1
CHEMBL216058	HIV-IN	1	Training	6.40	1
CHEMBL386055	HIV-IN	1	Prediction	59.19	1
CHEMBL403498	HIV-IN	1	Training	62.92	1
CHEMBL143614	HIV-IN	1	Training	82.15	1
CHEMBL194833	HIV-IN	1	Training	36.47	1
CHEMBL343646	HIV-IN	1	Prediction	88.03	1
CHEMBL147147	HIV-IN	1	Training	97.68	1
CHEMBL357909	HIV-IN	1	Training	92.26	1
CHEMBL19464	HIV-IN	1	Training	88.33	1
CHEMBL145705	HIV-IN	1	Prediction	80.96	1
CHEMBL148241	HIV-IN	1	Training	82.34	1
CHEMBL145280	HIV-IN	1	Training	97.45	1
CHEMBL145335	HIV-IN	1	Training	92.92	1
CHEMBL63592	HIV-IN	1	Prediction	5.18	1
CHEMBL147317	HIV-IN	1	Training	83.08	1
CHEMBL371471	HIV-IN	1	Training	39.90	1
CHEMBL197584	HIV-IN	1	Training	37.65	1
CHEMBL213852	HIV-IN	1	Prediction	64.57	1

CHEMBL20342	HIV-IN	1	Training	85.82	1
CHEMBL146777	HIV-IN	1	Training	81.70	1
CHEMBL379132	HIV-IN	1	Training	98.02	1
CHEMBL50605	HIV-IN	1	Prediction	96.52	1
CHEMBL198000	HIV-IN	1	Prediction	84.84	1
CHEMBL144727	HIV-IN	1	Training	97.64	1
CHEMBL214371	HIV-IN	1	Training	89.10	1
CHEMBL1159993	HIV-IN	1	Training	45.00	1
CHEMBL144613	HIV-IN	1	Prediction	2.13	-1*
CHEMBL213467	HIV-IN	1	Training	80.19	1
CHEMBL37869	HIV-IN	1	Training	17.08	1
CHEMBL209641	HIV-IN	1	Training	69.54	1
CHEMBL278545	HIV-IN	1	Prediction	93.66	-1*
CHEMBL1159989	HIV-IN	1	Training	66.65	-1*
CHEMBL32711	HIV-IN	1	Training	64.92	-1*
CHEMBL108253	HIV-IN	1	Training	32.73	1
CHEMBL18927	HIV-IN	1	Prediction	78.25	1
CHEMBL379974	HIV-IN	1	Training	43.42	-1*
CHEMBL1159988	HIV-IN	1	Training	61.33	1
CHEMBL20592	HIV-IN	1	Training	92.14	1
CHEMBL35842	HIV-IN	1	Prediction	91.22	1
CHEMBL145946	HIV-IN	1	Prediction	85.91	1
CHEMBL144118	HIV-IN	1	Training	93.04	1
CHEMBL358506	HIV-IN	1	Training	79.24	1
Aceclofenac	HIV-IN	-1	Training	97.23	1*
Acetaminophen	HIV-IN	-1	Prediction	99.40	-1
Acetazolamide	HIV-IN	-1	Training	88.22	-1
Acetophenazine	HIV-IN	-1	Training	50.16	-1
Amantadine	HIV-IN	-1	Training	97.59	-1
Ambenonium	HIV-IN	-1	Prediction	45.11	-1
Amineptine	HIV-IN	-1	Training	95.41	-1
Amiodarone	HIV-IN	-1	Training	89.39	-1
Amitriptyline	HIV-IN	-1	Training	99.26	-1
Aprobarbital	HIV-IN	-1	Prediction	98.15	-1
Artane	HIV-IN	-1	Training	98.71	-1
Aspirin	HIV-IN	-1	Training	99.54	-1
Atenolol	HIV-IN	-1	Training	99.10	-1
Atropine	HIV-IN	-1	Prediction	81.97	-1
Baclofen	HIV-IN	-1	Training	98.80	-1
Beclomethasone	HIV-IN	-1	Training	99.75	-1
Benzonatate	HIV-IN	-1	Training	98.43	-1
Biperiden	HIV-IN	-1	Prediction	97.61	-1
Bromocriptine	HIV-IN	-1	Training	95.89	-1
Bucizine	HIV-IN	-1	Training	69.02	-1
Budesonide	HIV-IN	-1	Training	91.60	-1

Buprenorphine	HIV-IN	-1	Prediction	100.00	-1
Caffeine	HIV-IN	-1	Training	77.72	-1
Cantil	HIV-IN	-1	Training	98.43	-1
Carbachol	HIV-IN	-1	Training	95.06	-1
Carbamazepine	HIV-IN	-1	Prediction	90.56	-1
Carisoprodol	HIV-IN	-1	Training	82.84	-1
Carvedilol	HIV-IN	-1	Training	99.42	-1
Cefoperazone	HIV-IN	-1	Training	0.73	-1
Chloral hydrate	HIV-IN	-1	Prediction	99.41	-1
Chlordiazepoxide	HIV-IN	-1	Training	94.40	-1
Chlorpropamide	HIV-IN	-1	Training	83.83	-1
Chlorthalidone	HIV-IN	-1	Training	98.73	-1
Clidinium	HIV-IN	-1	Prediction	97.62	-1
Clobazam	HIV-IN	-1	Training	96.50	-1
Clofazimine	HIV-IN	-1	Training	99.97	1*
Clomipramine	HIV-IN	-1	Training	94.93	-1
Clonidine	HIV-IN	-1	Prediction	89.78	-1
Codeine	HIV-IN	-1	Training	99.88	-1
Colchicine	HIV-IN	-1	Training	99.35	-1
Cyclizine	HIV-IN	-1	Training	97.07	-1
Cyclosporin	HIV-IN	-1	Prediction	0.03	-1
Dextropropoxyphene	HIV-IN	-1	Training	99.28	-1
Diazepam	HIV-IN	-1	Training	96.16	-1
Diflucortolone	HIV-IN	-1	Training	86.30	-1
Dimercaprol	HIV-IN	-1	Prediction	99.76	-1
Diphenhydramine	HIV-IN	-1	Training	98.22	-1
Diphenidol	HIV-IN	-1	Training	99.05	-1
Dobutamine	HIV-IN	-1	Training	96.90	1*
Dofetilide	HIV-IN	-1	Prediction	76.65	-1
Domperidone	HIV-IN	-1	Training	12.03	-1
Dopamine	HIV-IN	-1	Training	99.56	-1
Doxazosin	HIV-IN	-1	Training	79.96	-1
Doxepin	HIV-IN	-1	Prediction	99.69	-1
Dronabinol	HIV-IN	-1	Training	99.35	-1
Droxycam	HIV-IN	-1	Training	98.39	-1
Entacapone	HIV-IN	-1	Training	98.96	-1
Epinephrine	HIV-IN	-1	Prediction	99.44	-1
Eprosartan	HIV-IN	-1	Training	66.89	1*
Ergotamine	HIV-IN	-1	Training	99.83	-1
Ethosuximide	HIV-IN	-1	Training	99.38	-1
Fentanyl	HIV-IN	-1	Prediction	94.93	-1
Fexofenadine	HIV-IN	-1	Training	95.98	-1
Flecainide	HIV-IN	-1	Training	89.57	-1
Flunarizine	HIV-IN	-1	Training	27.74	-1
Flunisolide	HIV-IN	-1	Prediction	89.22	-1

Fluoxetine	HIV-IN	-1	Training	97.67	-1
Fluvoxamine	HIV-IN	-1	Training	99.00	-1
Gabapentin	HIV-IN	-1	Training	99.36	-1
Gestodene	HIV-IN	-1	Prediction	98.37	-1
Glutethimide	HIV-IN	-1	Training	99.46	-1
Glycopyrrolate	HIV-IN	-1	Training	89.31	-1
Guanadrel	HIV-IN	-1	Training	93.40	-1
Halofantrine	HIV-IN	-1	Prediction	75.47	-1
Haloperidol	HIV-IN	-1	Training	37.32	-1
Halothane	HIV-IN	-1	Training	99.02	-1
Hydromorphone	HIV-IN	-1	Training	92.40	-1
Hydroxyzine	HIV-IN	-1	Prediction	94.69	-1
Indapamide	HIV-IN	-1	Training	91.22	-1
Indomethacin	HIV-IN	-1	Training	97.94	1*
Isoetharine	HIV-IN	-1	Training	98.54	-1
Isoproterenol	HIV-IN	-1	Prediction	99.02	-1
Isosorbide	HIV-IN	-1	Training	99.08	-1
Ketamine	HIV-IN	-1	Training	90.04	-1
Labetalol	HIV-IN	-1	Training	95.99	1*
Lacidipine	HIV-IN	-1	Prediction	99.84	-1
Lamotrigine	HIV-IN	-1	Training	45.87	-1
Leuprorelin	HIV-IN	-1	Training	10.29	-1
Levodopa	HIV-IN	-1	Training	99.05	-1
Lidocaine	HIV-IN	-1	Prediction	98.43	-1
Loratadine	HIV-IN	-1	Training	63.92	-1
Maprotiline	HIV-IN	-1	Training	99.44	-1
Meclizine	HIV-IN	-1	Training	83.13	-1
Medroxyprogesterone	HIV-IN	-1	Prediction	78.85	-1
Melfalan	HIV-IN	-1	Training	97.98	-1
Meprobamate	HIV-IN	-1	Training	90.15	-1
Methamphetamine	HIV-IN	-1	Training	99.41	-1
Methantheline	HIV-IN	-1	Prediction	96.38	-1
Methocarbamol	HIV-IN	-1	Training	99.29	-1
Methoxyflurane	HIV-IN	-1	Training	99.29	-1
Methscopolamine	HIV-IN	-1	Training	80.77	-1
Methylphenidate	HIV-IN	-1	Prediction	99.21	-1
Methysergide	HIV-IN	-1	Training	98.33	-1
Metoclopramide	HIV-IN	-1	Training	98.96	-1
Midodrine	HIV-IN	-1	Training	99.78	-1
Mirtazapine	HIV-IN	-1	Prediction	46.00	-1
Modafinil	HIV-IN	-1	Training	97.13	-1
Montelukast	HIV-IN	-1	Training	12.90	-1
Moricizine	HIV-IN	-1	Training	99.62	-1
Morphine	HIV-IN	-1	Prediction	99.78	-1
Nalmefene	HIV-IN	-1	Training	99.99	-1

Neostigmine	HIV-IN	-1	Training	99.89	-1
Nifedipine	HIV-IN	-1	Training	99.92	-1
Oxycodone	HIV-IN	-1	Prediction	99.86	-1
Paroxetine	HIV-IN	-1	Training	96.57	-1
Pecazine	HIV-IN	-1	Training	92.56	-1
Pergolide	HIV-IN	-1	Training	99.95	-1
Phenylbutazone	HIV-IN	-1	Prediction	99.02	-1
Phenytoin	HIV-IN	-1	Training	98.70	-1
Pilocarpine	HIV-IN	-1	Training	80.43	-1
Pimozide	HIV-IN	-1	Training	2.73	-1
Pramipexole	HIV-IN	-1	Prediction	97.17	-1
Probenecid	HIV-IN	-1	Training	97.84	-1
Procyclidine	HIV-IN	-1	Training	92.91	-1
Proprantheline	HIV-IN	-1	Training	96.93	-1
Pseudoephedrine	HIV-IN	-1	Prediction	99.39	-1
Pyrantel	HIV-IN	-1	Training	99.22	-1
Quinidine	HIV-IN	-1	Training	47.20	-1
Ranitidine	HIV-IN	-1	Training	99.01	-1
Rifampin	HIV-IN	-1	Prediction	68.31	-1
Risperidone	HIV-IN	-1	Training	76.99	1*
Ropinirole	HIV-IN	-1	Training	97.77	-1
Salmeterol	HIV-IN	-1	Training	96.70	-1
Selegiline	HIV-IN	-1	Prediction	99.03	-1
Sulfinpyrazone	HIV-IN	-1	Training	95.50	-1
Tegafur	HIV-IN	-1	Training	69.37	-1
Terpin	HIV-IN	-1	Training	98.47	-1
Tolcapone	HIV-IN	-1	Prediction	77.25	1*
Tranlycypromine	HIV-IN	-1	Training	99.23	-1
Trazodone	HIV-IN	-1	Training	60.60	-1
Triamcinolone	HIV-IN	-1	Training	99.78	-1
Valproic acid	HIV-IN	-1	Prediction	99.51	-1
Vancomycin	HIV-IN	-1	Training	0.02	1*
Venlafaxine	HIV-IN	-1	Training	99.23	-1
Verapamil	HIV-IN	-1	Training	99.75	-1
Wytensin	HIV-IN	-1	Prediction	94.41	-1
Zafirlukast	HIV-IN	-1	Training	97.70	-1
Zileuton	HIV-IN	-1	Training	95.81	-1
Zonisamide	HIV-IN	-1	Training	97.00	-1

Compounds appear exactly in the same order as in **Supplementary Information 1** file.

A_{HIV-IP}: is referred to the observed anti-HIV activity through the inhibition of a specific protein.

Name or Code: in the specific case of codes, these are represented by numbers belonging to ChEMBL Database.

PAHIV: the code used for the different proteins associated to HIV.

Prob.: is the predicted probability (by the mt-QSAR-LDA model) to belong to the observed anti-HIV activity (active or inactive according to the variable $A_{\text{HIV-IP}}$).

Compounds with **Prob.**<50% are incorrectly classified by the mt-QSAR-LDA model.

Pred- $A_{\text{HIV-IP}}$: is the predicted activity (by the mt-QSAR-ANN model) to belong to the observed anti-HIV activity (active or inactive according to the variable $A_{\text{HIV-IP}}$).

* Compounds incorrectly classified by the mt-QSAR-ANN model.