S1 Table

Compound ID	MolNAME	plate	position	Content	cas#	Formula	MolWt	Bioactivity	Source	Status	Reference	Screen Score (z-score) rep1	rep2	rep3	rep4	Average
	empty	100122-01	A01	sample								NA	NA	NA	NA	NA
01500372	MAFENIDE HYDROCHLORIDE	100122-01	A02	sample	138-39-6	C7H11ClN2O2S	222.69492	antibacterial	synthetic	USAN, INN, BAN		0.28	-1.37	-0.82	-2.36	-1.07
01500373	MAPROTILINE HYDROCHLORIDE	100122-01	A03	sample	10347-81-6, 10262-69-8	C20H24ClN	313.87398	antidepressant	synthetic	USAN, INN, BAN		1.47	-1.74	-0.91	-0.61	-0.45
01500374	MECAMYLAMINE HYDROCHLORIDE	100122-01	A04	sample	826-39-1, 60-40-2	C11H22ClN	203.75769	antihypertensive	synthetic	USP, INN, BAN		0.88	4.29	-0.06	-0.38	1.18
01500375	MECHLORETHAMINE	100122-01	A05	sample	55-86-7, 51-75-2	C5H11Cl2N	156.05612	antineoplastic, alkylating agent	synthetic	USP, INN, BAN, JAN		-0.95	-1.74	-2.12	-1.98	-1.70
01500376	MECLIZINE HYDROCHLORIDE	100122-01	A06	sample	31884-77-2, 1104-22-9	C25H29Cl3N2	463.88228	antiemetic	synthetic	USP, INN, BAN, JAN		-0.32	-2.98	1.68	-1.87	-0.87
01500377	MECLOFENAMATE SODIUM	100122-01	A07	sample	6385-02-0	C14H10Cl2NNaO2	318.1371	antiinflammatory, antipyretic	synthetic	USP		0.38	-1.38	-1.05	-0.96	-0.75
01500380	MEDRYSONE	100122-01	A08	sample	2668-66-8	C22H32O3	344.49854	glucocorticoid	semisynthetic	USAN, INN		0.78	-1.19	-1.10	-0.47	-0.50
01500381	MEGESTROL ACETATE	100122-01	A09	sample	595-33-5, 3562-63-8	C24H32O4	384.52024	progestogen, antineoplastic	semisynthetic	USP, INN, BAN		-1.75	-2.51	-1.01	0.85	-1.11
01500382	MELPHALAN	100122-01	A10	sample	148-82-3	C13H18Cl2N2O2	305.20661	antineoplastic, alkylating agent	synthetic	USP, INN, BAN, JAN		-0.09	-0.74	0.03	-1.24	-0.51
01500388	MESTRANOL	100122-01	A11	sample	72-33-3	C21H26O2	310.44017	estrogen, with progesterone as oral contraceptive	semisynthetic	USP, INN, BAN, JAN		1.56	-2.14	-1.84	-1.27	-0.93
	0.04% JAK2inhib	100122-01	A12	0.04% jak2inhib								0.98	-3.38	1.79	-1.91	-0.63
	0.04% DMSO	100122-01	B01	0.04% dmso								-0.65	-1.33	-1.07	-1.61	-1.17
01500390	METAPROTERENOL	100122-01	B02	sample	586-06-1, 5874-97-5	C11H17NO3	211.26304	bronchodilator	synthetic	USP, JAN		-0.60	-0.91	0.30	2.05	0.21
01500391	METHACHOLINE CHLORIDE	100122-01	B03	sample	62-51-1, 55-92-5	C8H18ClNO2	195.69116	cholinergic, diagnostic aid	synthetic	USP, INN, BAN		0.43	0.36	1.17	-0.60	0.34
01500396	METHIMAZOLE	100122-01	B04	sample	60-56-0	C4H6N2S	114.16982	antihyperthyroid	synthetic	USP, INN, BAN, JAN		0.48	1.30	0.84	6.65	2.32
01500397	METHOCARBAMOL	100122-01	B05	sample	532-03-6	C11H15NO5	241.2459	muscle relaxant (skeletal)	synthetic	USP, INN, BAN, JAN		0.12	2.37	-0.22	-0.95	0.33
01500398	METHOTREXATE(+/-)	100122-01	B06	sample	60388-53-6	C20H22N8O5	454.44894	antineoplastic, antirheumatic, folic acid antagonist	synthetic; AMETHOPTERIN	USP, INN, BAN, JAN		-8.26	-9.36	-8.49	-8.77	-8.72
01500399	METHOXAMINE HYDROCHLORIDE	100122-01	B07	sample	61-16-5, 390-28-3	C11H18ClNO3	247.72401	alpha1 adrenoreceptor agonist, vasoconstrictor	synthetic	USP-XXII, INN, BAN, JAN		-1.43	-1.83	-0.45	-0.97	-1.17
01500403	METHYLDOPA	100122-01	B08	sample	41372-08-1, 555-30-6	C10H13NO4	211.21941	antihypertensive	synthetic	USP, INN, BAN, JAN		-0.35	0.13	-0.26	2.17	0.42
01500406	METHYLPREDNISOLONE	100122-01	B09	sample	83-43-2	C22H30O5	374.4814	glucocorticoid	semisynthetic	USP, INN, BAN, JAN		0.73	-0.59	-0.02	2.31	0.61
01500410	METOCLOPRAMIDE HYDROCHLORIDE	100122-01	B10	sample	54143-57-6, 7232-21-5	C14H23Cl2N3O2	336.26431	antiemetic	synthetic	USP, INN, BAN, JAN		0.04	-0.36	-0.30	0.01	-0.15
01500411	METOPROLOL TARTRATE	100122-01	B11	sample	56392-17-7, 37350-58-6	C19H31NO9	417.46022	antihypertensive, antianginal	synthetic	USP, JAN		-0.51	0.90	2.77	-0.01	0.79
	0.04% JAK2inhib	100122-01	B12	0.04% jak2inhib								-1.80	-2.00	-1.44	-1.48	-1.68
	0.04% DMSO	100122-01	C01	0.04% dmso								-1.93	-1.31	-2.32	4.04	-0.38
01500412	METRONIDAZOLE	100122-01	C02	sample	443-48-1, 69198-10-3	C6H9N3O3	171.15693	antiprotozoal	synthetic	USP, INN, BAN, JAN		-0.67	-0.09	-0.70	-1.46	-0.73
01500414	MINOCYCLINE HYDROCHLORIDE	100122-01	C03	sample	13614-98-7, 10118-90-8	C23H28ClN3O7	493.94851	antibacterial	semisynthetic	USAN, INN, BAN		-0.49	0.27	-0.30	-0.49	-0.25
01500415	MINOXIDIL	100122-01	C04	sample	38304-91-5	C9H15N5O	209.2528	antihypertensive, antialopecia agent	synthetic	USP, INN, BAN		0.35	0.54	-0.80	0.91	0.25
01500418	MOXALACTAM DISODIUM	100122-01	C05	sample	8031-09-2	C20H18N6Na2O9S	564.44486	antibacterial	semisynthetic	USAN, INN, BAN		-0.50	-0.01	-1.55	0.43	-0.41
01500419	NADIDE	100122-01	C06	sample	53-84-9	C21H27N7O14P2	663.43544	alcohol and narcotic antagonist	synthetic	USAN, INN, BAN, JAN		-0.15	3.17	-0.25	-0.45	0.58
01500420	NAFCILLIN SODIUM	100122-01	C07	sample	7177-50-6, 985-16-0	C21H21N2NaO5S	436.46572	antibacterial	semisynthetic	USP, INN, BAN		-0.26	4.97	-0.17	0.02	1.14
01500422	NALOXONE HYDROCHLORIDE	100122-01	C08	sample	357-08-4, 51481-60-8	C19H22ClNO4	363.84449	narcotic antagonist	synthetic	USP, INN, BAN, JAN	Brain Res 839:209 (1999); Brit J Pharmacol 127:605 (1999)	-0.06	0.01	0.33	0.37	0.16
01500424	NAPHAZOLINE HYDROCHLORIDE	100122-01	C09	sample	550-99-2, 835-31-4	C14H15ClN2	246.74205	adrenergic agonist, nasal decongestant	synthetic	USP, INN, BAN, JAN		-0.54	-0.16	2.17	0.11	0.40
01500425	NAPROXEN(+)	100122-01	C10	sample	22204-53-1	C14H14O3	230.26588	antiinflammatory, analgesic, antipyretic	synthetic	USP, INN, BAN, JAN		-0.72	0.44	-0.01	-0.06	-0.09
01500428	NEOSTIGMINE BROMIDE	100122-01	C11	sample	114-80-7, 59-99-4	C12H19BrN2O2	303.20143	cholinergic	synthetic	USP, INN, BAN, JAN		-0.29	-0.17	1.55	0.16	0.31
	0.11% JAK2inhib	100122-01	C12	0.11% jak2inhib								-4.94	-4.14	-3.27	-2.11	-3.61
	0.11% DMSO	100122-01	D01	0.11% dmso								-0.50	5.57	1.57	5.72	3.09
01500430	NIACIN	100122-01	D02	sample	59-67-6	C6H5NO2	123.11225	antihyperlipidemic, vitamin (enzyme cofactor)	widespread in the plant and fungal kingdom	USP, INN, JAN		1.29	0.18	1.83	3.66	1.74
01500431	NIFEDIPINE	100122-01	D03	sample	21829-25-4	C17H18N2O6	346.34281	antianginal, antihypertensive	synthetic	USP, INN, BAN, JAN		0.24	-0.08	-0.94	-0.99	-0.44
01500433	NITROFURANTOIN	100122-01	D04	sample	67-20-9, 54-87-5 [nitrofurantoin	C8H6N4O5	238.16082	antibacterial	synthetic	USP, INN, BAN, JAN		1.59	-1.95	-1.18	-1.67	-0.80
01505399	OXYBUTYNIN CHLORIDE	100122-01	D05	sample	1508-65-2	C22H32ClNO3	393.95824	anticholinergic	synthetic; MJ-4309-1, 5058	USP, JAN		1.65	-0.89	-2.25	-0.40	-0.47
01500436	NOREPINEPHRINE	100122-01	D06	sample	69815-49-2, 51-40-1	C8H11NO3	169.18177	adrenergic agonist, antihypotensive	synthetic	USP, INN, BAN		-0.31	0.94	0.26	5.84	1.68
01500437	NORETHINDRONE	100122-01	D07	sample	68-22-4	C20H26O2	298.42902	progestogen	synthetic	USP, INN, BAN, JAN		-0.41	-0.81	2.93	-0.06	0.42
01500439	NORETHYNODREL	100122-01	D08	sample	68-23-5	C20H26O2	298.42902	progestogen, in combination with estrogen as oral contraceptive	synthetic	USP		0.63	0.34	0.77	1.24	0.75
01500440	NORFLOXACIN	100122-01	D09	sample	70458-96-7	C16H18FN3O3	319.33856	antibacterial	synthetic	USP, INN, BAN, JAN		2.72	0.42	-0.26	-0.31	0.64
01500441	NORGESTREL	100122-01	D10	sample	6533-00-2	C21H28O2	312.45611	progestogen	synthetic	USP, INN, BAN		0.23	-0.77	0.64	2.91	0.75
01500442	NORTRIPTYLINE	100122-01	D11	sample	894-71-3, 72-69-5	C19H21N	263.38592	antidepressant	synthetic	USP, INN, BAN, JAN		-0.80	-1.22	0.17	-0.07	-0.48
	0.11% JAK2inhib	100122-01	D12	0.11% jak2inhib								-1.68	-4.14	-3.04	-2.86	-2.93
	0.11% JAK2inhib	100122-01	E01	0.11% jak2inhib								-3.42	-3.75	-3.75	-2.32	-3.31
01500443	NOSCAPINE HYDROCHLORIDE	100122-01	E02	sample	912-60-7, 128-62-1 [noscapine]	C22H24ClNO7	449.89208	antitussive	Corydalis cava and Papaver spp	USP, INN, BAN, JAN	Tetrahedron Letters 1965: 669	-0.20	1.23	-0.93	-0.10	0.00
01500444	NOVOBIOCIN SODIUM	100122-01	E03	sample	1476-53-5, 303-81-1	C31H35N2NaO11	634.6212	antibacterial	Streptomyces niveus and S griseus	USP		-0.59	-1.17	-0.93	-1.48	-1.04
01500445	NYLIDRIN HYDROCHLORIDE	100122-01	E04	sample	849-55-8	C19H26ClNO2	335.87757	vasodilator (peripheral)	synthetic	USP-XII, INN, BAN		1.32	1.43	-0.22	0.42	0.74
01500446	NYSTATIN	100122-01	E05	sample	114-90-9	C47H75NO17	926.1183	antifungal, binds to membrane sterols	Streptomyces noursei	USP, INN, BAN, JAN		-4.46	0.15	0.36	0.68	-0.82
01500447	ORPHENADRINE CITRATE	100122-01	E06	sample	4682-36-4, 83-98-7	C24H31NO8	461.51657	muscle relaxant (skeletal), antihistaminic	synthetic	USP, INN, BAN		1.74	0.44	1.18	-0.05	0.83
01500448	OXACILLIN SODIUM	100122-01	E07	sample	7240-38-2, 1173-88-2	C19H18N3NaO5S	423.42621	antibacterial	semisynthetic	USP, INN, BAN, JAN		-0.52	2.03	0.45	5.71	1.92
01500451	OXYBENZONE	100122-01	E08	sample	131-57-7	C14H12O3	228.24994	ultraviolet screen	synthetic	USP, INN		0.58	0.40	0.17	-0.34	0.20
01500453	OXYMETAZOLINE HYDROCHLORIDE	100122-01	E09	sample	2315-02-8, 1491-59-4	C16H25ClN2O	296.84345	adrenergic agonist, nasal decongestant	synthetic	USP, INN, BAN, JAN		0.83	-0.38	0.01	-0.29	0.04
01500455	OXYPHENBUTAZONE	100122-01	E10	sample	7081-38-1, 129-20-4	C19H20N2O3	324.38285	antiinflammatory	synthetic	USP-XXIII, INN, BAN		0.54	0.96	1.13	0.57	0.80
01500457	OXYTETRACYCLINE	100122-01	E11	sample	6153-64-6, 79-57-2	C22H25ClN2O9	496.90555	antibacterial	Streptomyces rimosus	USP, INN, BAN, JAN		3.08	-1.03	0.44	-0.33	0.54
	0.11% DMSO	100122-01	E12	0.11% dmso								-1.77	-1.56	-0.73	6.46	0.60
	0.11% JAK2inhib	100122-01	F01	0.11% jak2inhib								-2.79	-2.92	-2.46	-3.42	-2.90
01500459	PAPAVERINE HYDROCHLORIDE	100122-01	F02	sample	61-25-6, 58-74-2 [papaverine]	C20H22ClNO4	375.85564	muscle relaxant (smooth), cerebral vasodilator	Papaver somniferum, Rauwolfia serpentina	USP, BAN, JAN		-0.98	0.04	-1.75	-0.77	-0.87
01500460	PARACHLOROPHENOL	100122-01	F03	sample	106-48-9	C6H5ClO	128.55915	topical antibacterial (topical)	synthetic	USP		0.46	1.68	4.32	0.73	1.80
01500462	PARGYLINE HYDROCHLORIDE	100122-01	F04	sample	306-07-0, 555-57-7 [pargyline]	C11H14ClN	195.69393	antihypertensive	synthetic	USAN, INN, BAN		2.02	1.44	0.76	4.50	2.18
01500464	PENICILLAMINE	100122-01	F05	sample	52-67-5	C5H11NO2S	149.21292	chelating agent (Cu), antirheumatic	semisynthetic	USP, INN, BAN, JAN		0.77	0.18	-0.14	0.39	0.30
01500472	PHENACEMIDE	100122-01	F06	sample	63-98-9	C9H10N2O2	178.19225	anticonvulsant	synthetic	USP-XIII, INN, BAN		0.19	-0.27	0.02	0.27	0.05
01500473	PHENAZOPYRIDINE HYDROCHLORIDE	100122-01	F07	sample	136-40-3, 94-78-0	C11H12ClN5	249.70479	analgesic	synthetic	USP, INN, BAN		2.51	1.28	0.87	0.96	1.41
01500476	PHENELZINE SULFATE	100122-01	F08	sample	156-51-4, 51-71-8 [phenelzine]	C8H14N2O4S	234.27578	antidepressant	synthetic	USP, INN, BAN		0.36	0.94	1.00	1.11	0.85
01500477	PHENINDIONE	100122-01	F09	sample	83-12-5	C15H10O2	222.24575	anticoagulant	synthetic	USP-XXII, INN, BAN		-0.37	-1.00	0.24	0.29	-0.21
01500478	PHENIRAMINE MALEATE	100122-01	F10	sample	132-20-7, 86-21-5	C20H24N2O4	356.42528	antihistaminic	synthetic	USP, INN, BAN		0.01	0.20	0.68	0.17	0.27
01500482	PHENYLBUTAZONE	100122-01	F11	sample	50-33-9	C19H20N2O2	308.38345	antiinflammatory	synthetic	USP, INN, BAN, JAN		-0.27	-0.28	0.75	-0.54	-0.09
	0.04% DMSO	100122-01	F12	0.04% dmso								-1.10	-0.61	-0.05	1.20	-0.14
	0.04% JAK2inhib	100122-01	G01	0.04% jak2inhib								-0.88	-2.77	0.20	-2.83	-1.57
01500485	PHENYTOIN SODIUM	100122-01	G02	sample	630-93-3, 57-41-0 [phenytoin]	C15H11N2NaO2	274.25692	anticonvulsant, antieleptic	synthetic	USP, JAN		-1.30	-0.75	-0.39	-1.57	-1.00
01501010	FENOFIBRATE	100122-01	G03	sample	49562-28-9	C20H21ClO4	360.84097	antihyperlipidemic	synthetic	USAN, INN, BAN		0.32	-1.29	-0.86	-0.29	-0.53
01501011	FENOPROFEN	100122-01	G04	sample	31879-05-7	C15H14O3	242.27703	antiinflammatory	synthetic	USAN, INN, BAN		0.47	0.06	0.28	-0.24	0.14
01501015	FLUFENAMIC ACID	100122-01	G05	sample	530-78-9	C14H10F3NO2	281.2365	antiinflammatory, analgesic	synthetic	USAN, INN, BAN, JAN		-0.01	-0.23	0.13	5.94	1.46
01501016	FENBENDAZOLE	100122-01	G06	sample	43210-67-9	C15H13N3O2S	299.35376	anthelmintic	synthetic	USAN, INN, BAN		1.28	0.51	0.67	0.32	0.70
01501021	FENSPIRIDE HYDROCHLORIDE	100122-01	G07	sample	5053-08-7, 5053-06-5	C15H21ClN2O2	296.79982	antiinflammatory, bronchodilator	synthetic	USAN, INN		-0.96	0.08	-0.31	0.21	-0.25
01501103	MEFENAMIC ACID	100122-01	G08	sample	61-68-7	C15H15NO2	241.2923	antiinflammatory, analgesic	synthetic	USP, INN, BAN, JAN		-0.10	-0.77	-0.54	0.41	-0.25
01501104	METHACYCLINE HYDROCHLORIDE	100122-01	G09	sample	3963-95-9, 914-00-1	C22H23ClN2O8	478.89021	antibacterial	semisynthetic	USAN, INN, BAN		0.13	4.44	0.32	0.32	1.30
01501108	MEFEXAMIDE	100122-01	G10	sample	1227-61-8	C15H25ClN2O3	316.8311	stimulant (central)	synthetic	USAN, INN		-0.80	0.29	-0.30	0.62	-0.05
01501109	PROBUCOL	100122-01	G11	sample	23288-49-5	C31H48O2S2	516.85501	antihyperlipidemic	synthetic	USP, INN, BAN, JAN		-0.40	2.65	-0.43	-0.23	0.40
	0.04% DMSO	100122-01	G12	0.04% dmso								-0.23	-0.27	0.15	1.07	0.18
	0.04% JAK2inhib	100122-01	H01	0.04% jak2inhib								0.18	-2.88	-1.54	-3.26	-1.88
01501105	PUROMYCIN HYDROCHLORIDE	100122-01	H02	sample	58-58-2, 53-79-2 [puromycin]	C22H31Cl2N7O5	544.44227	antineoplastic, antiprotozoal	Streptomyces alboniger	USAN, INN, BAN		-7.85	-4.85	-7.96	-8.97	-7.41
01501110	MEBENDAZOLE	100122-01	H03	sample	31431-39-7	C16H13N3O3	295.30031	anthelmintic	synthetic	USP, INN, BAN, JAN		2.54	4.10	3.04	-0.74	2.24
01501115	NALBUPHINE HYDROCHLORIDE	100122-01	H04	sample	23277-43-2, 20594-83-6	C21H28ClNO4	393.91461	analgesic, narcotic antagonist	synthetic	USAN, INN, BAN		0.39	0.71	-0.68	-0.21	0.06
01501119	PROGLUMIDE	100122-01	H05	sample	6620-60-6	C18H26N2O4	334.41892	anticholinergic	synthetic	USAN, INN, BAN, JAN		-0.06	-0.16	0.23	-0.11	-0.02
01501120	MINAPRINE HYDROCHLORIDE	100122-01	H06	sample	25953-17-7, 25905-77-5	C17H24Cl2N4O	371.31303	psychotropic	synthetic	USAN		0.35	-0.75	-0.55	2.57	0.41
01501121	MEMANTINE HYDROCHLORIDE	100122-01	H07	sample	19982-08-2	C12H22ClN	215.76884	muscle relaxant (skeletal)	synthetic	USAN		-4.80	-0.16	0.10	0.05	-1.20
01501127	ATENOLOL	100122-01	H08	sample	29122-68-7	C14H22N2O3	266.34304	beta adrenergic blocker	synthetic	USP, INN, BAN, JAN		-0.18	0.27	0.33	0.56	0.25
01501129	CARBETAPENTANE CITRATE	100122-01	H09	sample	23142-01-0, 77-23-6	C26H39NO10	525.60143	antitussive	synthetic	NF-XIII, INN, BAN		-0.79	1.82	-0.07	0.44	0.35
01501134	PIMOZIDE	100122-01	H10	sample	2062-78-4	C28H29F2N3O	461.55963	antipsychotic	synthetic	USP, INN, BAN, JAN		0.62	-0.16	0.07	0.87	0.35
01501135	NICARDIPINE HYDROCHLORIDE	100122-01	H11	sample	54527-84-3, 55985-32-5	C26H30ClN3O6	515.9985	vasodilator	synthetic	USAN, INN, BAN, JAN		-0.39	-0.48	0.15	0.12	-0.15
	empty	100122-01	H12	sample								NA	NA	NA	NA	NA
	empty	100122-02	A01	sample								NA	NA	NA	NA	NA
01501137	NEFOPAM	100122-02	A02	sample	23327-57-3, 13669-70-0	C17H19NO	253.34708	analgesic	synthetic	USAN, INN, BAN		-0.28	-0.02	3.33	-0.48	0.64
01501138	PIRENZEPINE HYDROCHLORIDE	100122-02	A03	sample	29868-97-1, 28797-61-7	C19H23Cl2N5O2	424.33346	antiulcer	synthetic	USAN, INN, BAN, JAN		0.13	0.48	0.00	-2.43	-0.46
01501139	PRAMOXINE HYDROCHLORIDE	100122-02	A04	sample	637-58-1, 140-65-8	C17H28ClNO3	329.87061	anesthetic (topical)	synthetic	USAN, INN, BAN		-0.97	-0.74	-1.03	-1.58	-1.08
01501140	MEPHENESIN	100122-02	A05	sample	59-47-2	C10H14O3	182.22128	muscle relaxant (skeletal)	synthetic	NF-XII, INN, BAN		-1.17	-1.69	-0.17	-0.77	-0.95
01501142	SULFACHLORPYRIDAZINE	100122-02	A06	sample	80-32-0	C10H9ClN4O2S	284.72583	antibacterial	synthetic	USP, INN, BAN		0.77	-1.31	0.13	-0.86	-0.32
01501144	SULFADIMETHOXINE	100122-02	A07	sample	122-11-2	C12H14N4O4S	310.33378	antibacterial	synthetic	USP, INN, BAN, JAN		0.70	-0.56	0.00	-0.17	-0.01
01501146	SULFAGUANIDINE	100122-02	A08	sample	57-67-0	C7H10N4O2S	214.24735	antibacterial	synthetic	NF-XI, INN, BAN		-1.20	-0.59	-0.77	3.70	0.28
01501147	SULFAMONOMETHOXINE	100122-02	A09	sample	1220-83-3	C11H12N4O3S	280.30729	antibacterial	synthetic	USAN, INN, BAN, JAN		-1.54	-1.10	-0.79	-0.73	-1.04
01501148	SULCONAZOLE NITRATE	100122-02	A10	sample	61318-91-0, 61318-90-9	C18H15Cl3N3O3S	460.76952	antifungal	synthetic	USP, INN, BAN, JAN		-3.98	-2.48	-2.26	-1.35	-2.52
01501149	RITODRINE HYDROCHLORIDE	100122-02	A11	sample	23239-51-2, 26652-09-5	C17H22ClNO3	323.82279	muscle relaxant (smooth)	synthetic	USAN, INN, BAN		0.44	-0.49	0.03	0.15	0.03
	0.04% JAK2inhib	100122-02	A12	0.04% jak2inhib								-3.93	-3.30	-2.30	-1.59	-2.78
	0.04% DMSO	100122-02	B01	0.04% dmso								-0.38	-0.27	-1.05	-2.79	-1.12
01501150	SULPIRIDE	100122-02	B02	sample	15676-16-1	C15H23N3O4S	341.43226	dopamine receptor antagonist, antipsychotic	synthetic	USAN, INN, BAN, JAN		0.53	0.19	-0.07	-0.80	-0.04
01501151	RANITIDINE	100122-02	B03	sample	66357-35-5	C13H22N4O3S	314.40929	H2 antihistamine	synthetic	USAN, INN, BAN		-0.02	0.53	0.02	-1.78	-0.31
01501153	SULOCTIDIL	100122-02	B04	sample	54063-56-8	C20H35NOS	337.57205	peripheral vasodilator	synthetic	USAN, INN, BAN	hepatotoxic at clinical dose (600mg)	0.60	0.02	-0.03	-1.28	-0.17
01501154	RONIDAZOLE	100122-02	B05	sample	7681-76-7	C6H8N4O4	200.15506	antiprotozoal	synthetic	USAN, INN, BAN		-0.04	1.75	1.55	-0.76	0.63
01501155	SULFAMETER	100122-02	B06	sample	651-06-9	C11H12N4O3S	280.30729	antibacterial	synthetic	USAN, INN, BAN		-1.58	0.33	-0.31	0.05	-0.38
01501156	SULFAMETHOXYPYRIDAZINE	100122-02	B07	sample	80-35-3	C11H12N4O3S	280.30729	antibacterial	synthetic	USP-XVII, INN, BAN		-0.22	-0.89	-0.21	0.10	-0.31
01501161	SUPROFEN	100122-02	B08	sample	40828-46-4	C14H12O3S	260.31394	antiinflammatory	synthetic	USP, INN, BAN, JAN		-1.66	-0.61	-1.13	2.38	-0.26
01501171	SACCHARIN	100122-02	B09	sample	81-07-2	C7H5NO3S	183.1868	sweetener	synthetic	USAN, NF		-1.05	-0.44	-0.99	-0.94	-0.85
01501173	ACETANILIDE	100122-02	B10	sample	103-84-4	C8H9NO	135.16703	analgesic, antipyretic	synthetic	NF		-0.49	-0.45	1.61	2.03	0.67
01501175	FLURANDRENOLIDE	100122-02	B11	sample	1524-88-5	C24H33FO6	436.52541	antiinflammatory	semisynthetic	USP, INN, BAN, JAN		-1.51	-1.02	0.05	-1.00	-0.87
	0.04% JAK2inhib	100122-02	B12	0.04% jak2inhib								-4.04	-1.83	-1.12	-2.10	-2.27
	0.04% DMSO	100122-02	C01	0.04% dmso								-1.06	-1.31	-1.44	2.80	-0.25
01501184	ESTRADIOL ACETATE	100122-02	C02	sample	4245-41-4	C20H26O3	314.42842	estrogen	semisynthetic	USAN		-0.03	2.44	0.36	3.23	1.50
01501185	ECONAZOLE NITRATE	100122-02	C03	sample	68797-31-9, 27220-47-9	C18H16Cl3N3O4	444.70492	antifungal	SQ-13050; synthetic	USP, INN, BAN, JAN		-0.08	0.14	0.44	-2.00	-0.37
01501187	FLUNISOLIDE	100122-02	C04	sample	77326-96-6, 3385-03-3	C24H31FO6	434.50947	antiinflammatory	semisynthetic	USP, INN, BAN, JAN		-0.23	0.44	-0.02	-0.14	0.01
01501196	FLUMETHASONE	100122-02	C05	sample	2135-17-3	C22H28F2O5	410.46226	antiinflammatory	semisynthetic	USAN, INN, BAN		-0.83	-0.41	-0.74	-0.76	-0.68

Compound ID	MolNAME	plate	position	Content	cas#	Formula	MolWt	Bioactivity	Source	Status	Reference	Screen Score (z-score) rep1	rep2	rep3	rep4	Average
01501200	XYLAZINE	100122-02	C06	sample	23076-35-9, 7361-61-7	C12H16N2S	220.33872	analgesic	synthetic	USP, INN, BAN		0.26	-0.35	-0.53	0.12	-0.12
01501201	TOLAZAMIDE	100122-02	C07	sample	1156-19-0	C14H21N3O3S	311.40577	antidiabetic	synthetic	USP, INN, BAN, JAN		0.35	0.48	-0.46	2.09	0.62
01501202	GALANTHAMINE HYDROBROMIDE	100122-02	C08	sample	357-70-0, 1953-04-4	C17H22BrNO3	368.27379	anticholinesterase, analgesic, antiAlzheimer	Galanthus, Narcissus and other Lillaceae	USAN		-3.43	-0.69	0.35	5.13	0.34
01505602	FENRETINIDE	100122-02	C09	sample	65646-68-6	C26H33NO2	391.55841	antineoplastic	synthetic; MCN-R-1967	USAN, INN		1.12	-0.26	-0.49	0.07	0.11
01501214	ENALAPRIL MALEATE	100122-02	C10	sample	76095-16-4, 75847-73-3	C24H32N2O9	492.53064	ACE inhibitor, antihypertensive	synthetic	USP, INN, BAN, JAN		-0.77	-0.52	0.58	-0.10	-0.20
01501215	KETOPROFEN	100122-02	C11	sample	22071-15-4	C16H14O3	254.28818	antiinflammatory	synthetic	USP, INN, BAN, JAN		0.64	-0.58	-0.33	0.40	0.03
	0.11% JAK2inhib	100122-02	C12	0.11% jak2inhib								-4.66	-5.87	-2.92	-4.83	-4.57
	0.11% DMSO	100122-02	D01	0.11% dmso								-1.34	-1.67	-1.85	-2.92	-1.95
01501217	LISINOPRIL	100122-02	D02	sample	83915-83-7, 76547-98-3	C21H31N3O5	405.49832	ACE inhibitor	synthetic	USP, INN, BAN, JAN		0.88	0.75	2.50	-1.77	0.59
01502004	BUMETANIDE	100122-02	D03	sample	28395-03-1	C17H20N2O5S	364.42335	diuretic	synthetic	USP, INN, BAN, JAN		-0.67	5.11	0.12	2.91	1.87
01502005	CARBENOXOLONE SODIUM	100122-02	D04	sample	7421-40-1, 5697-56-3	C34H48Na2O7	614.73706	antiinflammatory, antisecretory, antiulcer	semisynthetic	USAN, INN, BAN, JAN		-0.28	-0.40	-0.40	-1.71	-0.70
01502020	FOLIC ACID	100122-02	D05	sample	59-30-3	C19H19N7O6	441.40658	hematopoietic vitamin	liver, kidney, green plants and fungi	USP, INN, BAN, JAN		-0.12	1.61	0.17	-1.17	0.12
01502021	PHTHALYLSULFATHIAZOLE	100122-02	D06	sample	85-73-4	C17H13N3O5S2	403.43826	antibacterial	synthetic	USP-XX, INN, BAN		1.01	0.79	1.32	0.03	0.79
01502025	SUCCINYLSULFATHIAZOLE	100122-02	D07	sample	116-43-8	C13H13N3O5S2	355.39366	antibacterial	synthetic	USP-XVIII, INN, BAN		-0.08	0.20	0.33	3.25	0.93
01502026	TRANEXAMIC ACID	100122-02	D08	sample	1197-18-8	C8H15NO2	157.21425	hemostatic	synthetic	USAN, INN, BAN, JAN		0.77	2.48	0.29	0.02	0.89
01502028	CEPHALEXIN	100122-02	D09	sample	23325-78-2, 15686-71-2	C16H17N3O4S	347.39559	antibacterial	semisynthetic	USP, INN, BAN, JAN		-0.66	-0.40	-0.46	-0.14	-0.41
01502030	OXOLINIC ACID	100122-02	D10	sample	14698-29-4	C13H11NO5	261.23632	antibacterial	synthetic	USAN, INN, BAN		-0.07	-0.90	0.07	1.30	0.10
01502031	CEFOXITIN SODIUM	100122-02	D11	sample	66309-69-1, 61622-34-2	C16H16N3NaO7S2	449.43962	antibacterial	semisynthetic	USP, INN, BAN, JAN		-0.83	-0.72	-0.58	0.69	-0.36
	0.11% JAK2inhib	100122-02	D12	0.11% jak2inhib								-3.40	-3.91	-2.35	-2.73	-3.10
	0.11% JAK2inhib	100122-02	E01	0.11% jak2inhib								-1.72	-3.33	-0.12	-3.52	-2.17
01502032	SURAMIN	100122-02	E02	sample	129-46-4, 145-63-1 [suramin]	C51H34N6Na6O23S6	1429.18883	antiprotozoal, trypanocidal, antiviral	synthetic; Bayer-205, 309F	USP		0.01	0.67	0.81	-0.79	0.18
01502033	CEFUROXIME SODIUM	100122-02	E03	sample	56238-63-2	C16H15N4NaO8S	446.37375	antibacterial	semisynthetic	USAN, INN, BAN		-0.21	-0.11	1.33	-1.41	-0.10
01502036	VIGABATRIN	100122-02	E04	sample	60643-86-9	C6H11NO2	129.16007	anticonvulsant	synthetic; MDL-71754	USAN, INN, BAN		0.26	0.86	0.24	-0.02	0.33
01502037	LOMEFLOXACIN HYDROCHLORIDE	100122-02	E05	sample	98079-52-8, 98079-51-7	C17H20ClF2N3O3	387.81705	antibacterial	synthetic	USAN, JAN		-0.26	0.41	0.73	0.14	0.26
01502038	CEFAMANDOLE SODIUM	100122-02	E06	sample	34444-01-4	C18H17N6NaO5S2	484.49119	antibacterial	semisynthetic	USAN, INN, BAN		2.01	1.57	1.80	1.01	1.60
01502040	CEFMETAZOLE SODIUM	100122-02	E07	sample	56796-39-5	C15H16N7NaO5S3	493.52047	antibacterial	semisynthetic	USP, INN		0.09	-0.33	-0.53	-0.49	-0.32
01502042	CEFOPERAZONE SODIUM	100122-02	E08	sample	62893-20-3, 62893-19-0	C25H26N9NaO8S2	667.65927	antibacterial	semisynthetic	USP, INN, BAN, JAN		-0.19	0.30	-0.21	0.21	0.03
01502044	OFLOXACIN	100122-02	E09	sample	82419-36-1	C18H20FN3O4	361.3762	antibacterial	synthetic	USP, INN, BAN, JAN		1.28	-0.51	-0.53	0.61	0.21
01502046	BEZAFIBRATE	100122-02	E10	sample	41859-67-0	C19H20ClNO4	361.82855	antihyperlipidemic	synthetic	USAN, INN, BAN, JAN		0.15	-0.47	-0.58	4.41	0.88
01505371	CETIRIZINE HYDROCHLORIDE	100122-02	E11	sample	83881-52-1	C21H27Cl3N2O3	461.81994	H1 antihistamine	synthetic	USAN, INN, BAN		-3.93	-0.97	0.42	-0.03	-1.13
	0.11% DMSO	100122-02	E12	0.11% dmso								-1.12	-2.34	-1.30	-1.82	-1.64
	0.11% JAK2inhib	100122-02	F01	0.11% jak2inhib								-1.89	-3.92	-2.73	-4.64	-3.30
01505398	PHENYLETHYL ALCOHOL	100122-02	F02	sample	60-12-8	C8H10O	122.1683	antimicrobial	synthetic	USP, BAN		0.50	0.37	0.29	-0.96	0.05
01501118	MECLOCYCLINE SULFOSALICYLATE	100122-02	F03	sample	73816-42-9, 2013-58-3	C29H27ClN2O14S	695.06054	antibacterial	semisynthetic; GS-2989, NSC-78502	USAN, INN, BAN		2.23	0.03	-0.25	4.73	1.68
01505347	RIBOFLAVIN	100122-02	F04	sample	83-88-5	C17H20N4O6	376.37215	Vitamin B2; Vitamin cofactor; LD50(rat) 560 mg/kg ip	retina, whey and urine	USP, INN, BAN, JAN	Helv Chim Acta 35:457 (1952); Tet. Lett.,1969:3489; JACS	0.64	0.14	0.05	0.21	0.26
01506665	ACEBUTOLOL HYDROCHLORIDE	100122-02	F05	sample	34381-68-5, 37517-30-9	C18H29ClN2O4	372.89583	antihypertensive, antianginal, antiarrhythmic	synthetic	USAN, INN, BAN		-0.14	0.53	-0.15	3.30	0.88
01505306	ASPARTAME	100122-02	F06	sample	22839-47-0	C14H18N2O5	294.30996	sweetener	synthetic	USAN, NF, INN, BAN		0.81	-0.18	2.62	0.88	1.03
01505374	VARDENAFIL HYDROCHLORIDE	100122-02	F07	sample	224789-15-5	C23H33ClN6O4S	525.07426	erectile dysfunction, PD5 inhibitor	synthetic	USAN, INN, BAN		-0.56	0.85	0.55	1.26	0.53
01505396	FLUORESCEIN	100122-02	F08	sample	2321-07-5	C20H12O5	332.31564	corneal trama indicator	synthetic	USP, BAN, JAN		0.98	0.34	0.01	0.82	0.54
01505397	NIACINAMIDE	100122-02	F09	sample	98-92-0	C6H6N2O	122.12752	Vitamin B3; enzyme cofactor; anti-pellagra	widespread in plants, yeasts, fungi	USP, INN, JAN		0.20	-0.22	-0.72	0.51	-0.06
01505270	PROPRANOLOL HYDROCHLORIDE (+/-)	100122-02	F10	sample	318-98-9, 525-66-6	C16H22ClNO2	295.81224	antihypertensive, antianginal, antiarrhythmic	synthetic	USP, INN, BAN, JAN		-1.21	-1.94	-0.07	0.44	-0.69
01500401	METHSCOPOLAMINE BROMIDE	100122-02	F11	sample	155-41-9	C18H24BrNO4	398.30028	anticholinergic	semisynthetic	USP-XXII, BAN, JAN		-1.37	0.13	-0.02	0.35	-0.23
	0.04% DMSO	100122-02	F12	0.04% dmso								-1.24	-0.53	0.77	-0.63	-0.41
	0.04% JAK2inhib	100122-02	G01	0.04% jak2inhib								-1.56	-2.11	-2.34	-4.22	-2.56
02300219	EDROPHONIUM CHLORIDE	100122-02	G02	sample	116-38-1, 312-48-1	C10H16ClNO	201.69812	acetylcholinesterase inhibitor	synthetic	USP, INN, BAN, JAN		2.69	-0.04	0.39	-1.01	0.50
01900005	THIOPENTAL SODIUM	100122-02	G03	sample	71-73-8, 76-75-5 [thiopental]	C11H17N2NaO2S	264.32414	anesthetic	synthetic	USP, INN, BAN, JAN		1.12	0.56	0.95	-0.60	0.51
02300061	CLOMIPRAMINE HYDROCHLORIDE	100122-02	G04	sample	17321-77-6, 303-49-1	C19H24Cl2N2	351.32253	antidepressant	synthetic	USP, INN, BAN, JAN		0.68	-0.14	-0.12	-0.81	-0.10
01505983	PHENFORMIN HYDROCHLORIDE	100122-02	G05	sample	834-28-6	C10H16ClN5	241.72552	antidiabetic	synthetic	USP-XIX, INN, BAN	JACS 81:2220 (1959); Ann Pharmacother27:1183 (1993)	0.20	0.25	0.52	0.87	0.46
01505691	PENFLURIDOL	100122-02	G06	sample	26864-56-2	C28H27ClF5NO	523.97849	antipsychotic	synthetic; McN-JR-16341, R-16341	USAN, INN, BAN		0.67	4.88	0.43	0.04	1.51
02300009	TILORONE	100122-02	G07	sample	27591-69-1, 27591-97-5	C25H34N2O3	410.56133	antiviral	synthetic	USAN, INN		-0.92	0.36	2.22	0.11	0.44
01505672	VINCRISTINE SULFATE	100122-02	G08	sample	2068-78-2	C46H58N4O14S	923.05756	antineoplastic	Vinca rosea; 37231, NSC-67574	USP, INN, BAN, JAN	Int Pharmacodyn Ther 157:299 (1965)	0.37	0.82	-0.24	1.59	0.63
01505693	OMEPRAZOLE	100122-02	G09	sample	73590-58-6	C17H19N3O3S	345.42328	gastric acid depressant	synthetic; H-168/68	USP, INN, BAN, JAN		-0.01	0.40	0.41	1.50	0.58
01505281	ZOLMITRIPTAN	100122-02	G10	sample	139264-17-8	C16H21N3O2	287.36467	antimigraine, 5HT[1B/1D] agonist	synthetic	USAN, INN, BAN		1.57	-0.81	-0.41	-0.20	0.04
01506066	DEBRISOQUIN SULFATE	100122-02	G11	sample	581-88-4	C10H15N3O4S	273.31275	anti-hypertensive	synthetic; RO-5-3307/1	USAN, INN, BAN		0.32	0.08	-0.02	0.97	0.34
	0.04% DMSO	100122-02	G12	0.04% dmso								0.12	-0.42	0.69	0.34	0.18
	0.04% JAK2inhib	100122-02	H01	0.04% jak2inhib								-0.51	-1.94	-0.86	-3.65	-1.74
01506086	SULFADOXINE	100122-02	H02	sample	2447-57-6	C12H14N4O4S	310.33378	antibacterial	synthetic; RO-4-4393	USP, INN, BAN, JAN		0.51	0.28	-0.69	3.03	0.78
01506069	FINASTERIDE	100122-02	H03	sample	98319-26-7	C23H36N2O2	372.55557	anti-androgen, alpha-reductase inhibitor	synthetic; MK=909	USP, INN, BAN		0.83	1.64	0.08	-0.88	0.42
01506082	PENTETIC ACID	100122-02	H04	sample	67-43-6	C14H23N3O10	393.35351	chelating agent, diagnostic aid	synthetic; DTPA	USP, INN, BAN		0.52	-0.65	0.81	-0.70	-0.01
01506084	PROSCILLARIDIN	100122-02	H05	sample	466-06-8	C29H40O9	532.63675	cardiotonic	Scilla spp; A-32686, 2936	USAN, INN, BAN, JAN		0.89	1.08	-0.36	-0.26	0.34
01505438	HYDROCORTISONE VALERATE	100122-02	H06	sample	57524-89-7	C26H38O6	446.58916	antiinflammatory, glucocorticoid	semisynthetic	USP		0.17	0.03	2.97	-1.28	0.47
01506035	REPAGLINIDE	100122-02	H07	sample	135062-02-1	C27H36N2O4	452.59897	antidiabetic	synthetic; AG-EE-623-ZW	USP, INN, BAN		0.49	0.74	0.08	-1.33	0.00
01505271	CROTAMITON	100122-02	H08	sample	483-63-6	C13H17NO	203.28654	antipruritic, scabicide	synthetic	USP, INN, BAN, JAN		-0.57	-0.40	-0.18	-0.68	-0.46
01505364	CEFPROZIL	100122-02	H09	sample	121123-17-9	C18H19N3O5S	389.43323	antibacterial	semisynthetic; BMY-28100-03-800	USP, INN, BAN		0.31	-0.11	-1.23	0.88	-0.04
01505384	METHYLDOPATE HYDROCHLORIDE	100122-02	H10	sample	2508-79-4	C10H15ClNO4	275.73456	antihypertensive	synthetic	USP, BAN		-0.13	-0.26	-0.50	-0.71	-0.40
01501145	SULFAQUINOXALINE SODIUM	100122-02	H11	sample	59-40-5	C14H11N4NaO2S	322.32317	antibacterial	synthetic	USP, INN, BAN		-1.55	-1.34	-0.03	-0.70	-0.90
	empty	100122-02	H12	sample								NA	NA	NA	NA	NA
	empty	100122-03	A01	sample								NA	NA	NA	NA	NA
01500113	POTASSIUM p-AMINOBENZOATE	100122-03	A02	sample	150-13-0 (acid)	C7H6KNO2	175.23337	ultraviolet screen	synthetic	USP		-0.41	0.02	-0.89	-0.90	-0.55
01500145	BETAMETHASONE VALERATE	100122-03	A03	sample	2152-44-5	C27H37FO6	476.59074	glucocorticoid	semisynthetic	USP, INN, BAN, JAN		-0.56	0.35	-1.07	0.93	-0.09
01500280	ERYTHROMYCIN	100122-03	A04	sample	114-07-8	C37H67NO13	733.94544	antibacterial	Streptomyces erythreus	USP, INN, BAN, JAN		-2.50	-0.98	-1.17	-0.68	-1.33
01500510	PROMETHAZINE HYDROCHLORIDE	100122-03	A05	sample	58-33-3, 60-87-7	C17H21ClN2S	320.88732	antihistaminic	synthetic	USP, INN, BAN, JAN		0.84	0.55	2.20	5.08	2.17
01500534	SCOPOLAMINE HYDROBROMIDE	100122-03	A06	sample	6533-68-2, 114-49-8	C17H22BrNO4	384.27319	anticholinergic, treatment of motion sickness	Scopolia, Datura, Atropa spp	USP, BAN, JAN		-0.93	-1.28	0.10	0.01	-0.52
01500568	THEOPHYLLINE	100122-03	A07	sample	5967-84-0, 58-55-9	C7H8N4O2	180.16741	bronchodilator	Camelia, thea, Paullinia cupana	USP, BAN, JAN		0.29	0.57	-0.42	-1.18	-0.19
01500583	TOLNAFTATE	100122-03	A08	sample	2398-96-1	C19H17NO3S	307.41744	antifungal	synthetic; SCH-10144	USP, INN, BAN, JAN		0.60	-0.48	0.57	-1.24	-0.14
01500594	TRIMETHOBENZAMIDE HYDROCHLORIDE	100122-03	A09	sample	554-92-7, 138-56-7	C21H29ClN2O5	424.92868	antiemetic	synthetic	USP, INN		-1.56	-1.18	0.52	-0.83	-0.77
01500611	VINBLASTINE SULFATE	100122-03	A10	sample	143-67-9, 865-21-4	C46H60N4O13S	909.0741	antineoplastic, spindle poison	Vinca rosea	USP, INN, BAN, JAN		-9.67	-8.05	-4.10	-8.26	-7.52
01504283	ARMODAFINIL	100122-03	A11	sample	112111-43-0	C15H15NO2S	273.3563	analeptic	synthetic; R-enatiomer of modafinil (01505361)	USAN		-6.12	-0.56	0.00	2.02	-1.16
	0.04% JAK2inhib	100122-03	A12	0.04% jak2inhib								-2.32	-3.68	-0.80	-4.07	-2.72
	0.04% DMSO	100122-03	B01	0.04% dmso								0.27	3.48	-1.05	-0.79	0.48
01502195	PIRACETAM	100122-03	B02	sample	7491-74-9	C6H10N2O2	142.1588	antinauseant	synthetic	USAN, INN, BAN		-0.46	0.07	-1.63	0.51	-0.37
01503092	GLUCONOLACTONE	100122-03	B03	sample	90-80-2	C6H10O6	178.143	chelating agent	synthetic	USP		-0.63	0.38	-0.31	-0.40	-0.24
01503101	AZLOCILLIN SODIUM	100122-03	B04	sample	37091-66-0	C20H22N5NaO6S	483.48204	antibacterial	semisynthetic	USAN, INN, BAN		-0.03	-0.10	-0.41	2.18	0.41
01503428	CHOLINE CHLORIDE	100122-03	B05	sample	67-48-1, 62-49-7 [choline]	C5H14ClNO	139.62643	choleretic, lipotropic, hepatoprotectant	widespread in the plant and animal kingdoms	USP, INN		0.88	-0.95	0.33	0.73	0.25
01503722	ATORVASTATIN CALCIUM	100122-03	B06	sample	134523-03-8, 134523-00-5	C33H33CaFNO5	582.71306	antihyperlipidemic, HMGCoA reductase inhibitor	synthetic	USAN, INN, BAN		3.11	2.24	-0.37	0.82	0.95
01503932	OXYPHENCYCLIMINE HYDROCHLORIDE	100122-03	B07	sample	125-52-0, 125-53-1	C20H29ClN2O3	380.91873	anticholinergic	synthetic	USP-XXII, INN, BAN, JAN		1.18	-0.29	0.64	0.43	0.49
01503935	PROPAFENONE HYDROCHLORIDE	100122-03	B08	sample	34183-22-7, 54063-53-5	C21H28ClNO3	377.91521	antiarrhythmic	synthetic	USP, INN, BAN, JAN		-0.55	-1.11	-0.11	3.12	0.34
01503975	FLUCONAZOLE	100122-03	B09	sample	86386-73-4	C13H12F2N6O	306.27699	antifungal	synthetic	USAN, INN, BAN, JAN		2.56	-0.12	-0.35	-0.19	0.48
01503977	LOVASTATIN	100122-03	B10	sample	75330-75-5	C24H36O5	404.55152	antihyperlipidemic, HMGCoA reductase inhibitor	Aspergillus spp; mevinolin	USP, INN, BAN	PNAS 77:3957 (1980); Int J Oncol 12:717 (1998)	0.83	-0.36	2.18	0.89	0.88
01505407	ATROPINE OXIDE	100122-03	B11	sample	4438-22-6	C17H25NO4	307.3931	anticholinergic	semisynthetic	USAN, INN		-0.36	-1.21	0.32	-0.67	-0.48
	0.04% JAK2inhib	100122-03	B12	0.04% jak2inhib								-1.10	-0.61	-0.97	-1.95	-1.16
	0.04% DMSO	100122-03	C01	0.04% dmso								0.11	0.23	-1.74	0.07	-0.33
01504078	SENNOSIDE A	100122-03	C02	sample	81-27-6	C42H38O20	862.75916	cathartic	Cassia & Rheum spp	USP, JAN	Helv Chim Acta 33: 313 (1950)	0.56	-0.25	-0.94	0.01	-0.16
01504094	TENIPOSIDE	100122-03	C03	sample	29767-20-2	C32H32O13S	656.66804	antineoplastic	semisynthetic	USAN, INN, BAN		-9.31	-11.19	-13.15	-12.42	-11.51
01504105	TANNIC ACID	100122-03	C04	sample	1401-55-4	C76H52O46	1701.23424	nonspecific enzyme/receptor blocker	principal constituent of tree galls, esp Quercus spp;	USP, JAN	mixed galloyl esters of penta-o-galloylglucose (m-digalloyl	2.78	4.32	2.71	3.41	3.30
01502006	CARPROFEN	100122-03	C05	sample	53716-49-7	C15H12ClNO2	273.72139	antiinflammatory, analgesic	synthetic	USAN, INN, BAN		0.28	0.24	0.07	0.42	0.25
01503978	HYDROXYCHLOROQUINE SULFATE	100122-03	C06	sample	747-36-4, 118-42-3	C18H28ClN3O5S	433.95796	antimalarial, lupus suppressant	synthetic	USP-XXII, INN		1.12	0.24	-0.45	-0.46	0.11
01504144	DIRITHROMYCIN	100122-03	C07	sample	62013-04-1	C42H78N2O14	835.09496	antibacterial	semisynthetic	USP, INN, BAN	Drugs 61: 443 (2001)	-0.29	-1.05	0.13	-0.82	-0.51
01504148	MEPIVACAINE HYDROCHLORIDE	100122-03	C08	sample	1722-62-9, 96-88-8	C15H23ClN2O	282.81636	anesthetic (local)	synthetic	USP, INN, BAN, JAN	Mol Pharmacol 54: 162 (1998)	-0.63	-1.05	0.23	-0.33	-0.44
01504152	NILUTAMIDE	100122-03	C09	sample	63612-50-0	C12H10F3N3O4	317.2264	antiandrogen	synthetic	USAN, INN, BAN	Pharmacotherapy 31: 65 (1997)	0.91	-0.75	-0.51	-1.54	-0.47
01504184	AMINOLEVULINIC ACID HYDROCHLORIDE	100122-03	C10	sample	5451-09-2	C5H10ClNO3	167.59335	antineoplastic	synthetic	USAN		0.68	-0.27	0.96	-0.04	0.33
01505456	PARAMETHADIONE	100122-03	C11	sample	115-67-3	C7H11NO3	157.17062	anticonvulsant	synthetic	USP-XXII, INN, BAN		0.93	-0.71	0.29	3.07	0.89
	0.11% JAK2inhib	100122-03	C12	0.11% jak2inhib								-4.30	-3.73	-2.42	-4.07	-3.63
	0.11% DMSO	100122-03	D01	0.11% dmso								1.03	1.26	-1.05	5.48	1.68
01504229	METAXALONE	100122-03	D02	sample	1665-48-1	C12H15NO3	221.25825	muscle relaxant (skeletal)	synthetic	USAN, INN, BAN		-0.34	0.23	-0.76	-0.59	-0.37
01504211	CHLOROGUANIDE HYDROCHLORIDE	100122-03	D03	sample	637-32-1	C11H17Cl2N5	290.19764	antimalarial	synthetic	USP-XIV, INN, BAN		1.16	0.63	3.00	1.23	1.50
01504231	CLARITHROMYCIN	100122-03	D04	sample	81103-11-9	C38H69NO13	747.97253	antibacterial	Streptomyces erythreus	USP, INN, BAN, JAN		1.32	0.38	-0.58	-0.31	0.20
01504237	HYDROQUINONE	100122-03	D05	sample	123-31-9	C6H6O2	110.11352	antioxidant	synthetic	USP		0.17	0.41	0.06	4.67	1.33
01504258	NATEGLINIDE	100122-03	D06	sample	105816-04-4	C19H27NO3	317.43194	antidiabetic	synthetic	USAN, INN, BAN		1.57	1.08	0.55	-0.53	0.67
01504261	CANDESARTAN CILEXTIL	100122-03	D07	sample	139481-59-7	C33H34N6O6	610.67553	angiotensin 1 receptor antagonist	synthetic	USAN, INN		-3.53	-1.16	-0.38	-0.88	-1.49
01504263	ROSIGLITAZONE	100122-03	D08	sample	122320-73-4	C18H19N3O3S	357.4443	antidiabetic	synthetic	USAN, INN, BAN		1.32	1.15	1.48	0.84	1.00
01504268	LOSARTAN	100122-03	D09	sample	124750-99-8, 114798-26-4	C22H23ClN6O	422.92121	antihypertensive, AT1 anglotensin II antagonist	synthetic	USAN, INN, BAN		0.14	0.61	1.59	0.77	0.78
01505020	HOMOSALATE	100122-03	D10	sample	118-56-9	C16H22O3	262.35194	UV screen, analgesic	synthetic	USP, INN		0.80	0.95	1.24	-0.01	0.75
00300618	SALICYLANILIDE	100122-03	D11	sample	87-17-2	C13H11NO2	213.23812	antipyretic, fungicide	synthetic	NF-XIII		-0.16	0.15	1.19	3.82	1.25
	0.11% JAK2inhib	100122-03	D12	0.11% jak2inhib								-4.00	-4.76	-2.01	-2.87	-3.41
	0.11% JAK2inhib	100122-03	E01	0.11% jak2inhib								-3.26	-2.86	0.84	-0.98	-1.57
01505022	PROPOFOL	100122-03	E02	sample	2078-54-8	C12H18O	178.27666	anesthetic	synthetic; ICI-35868	USAN, INN, BAN		0.04	2.17	-1.63	-0.11	0.12
00200046	GRISEOFULVIN	100122-03	E03	sample	126-07-8	C17H17ClO6	352.77444	antifungal, inhibits mitosis in metaphase	Penicillium griseofulvum	USP, INN, BAN, JAN	J Chem Soc 1952: 3949	-0.62	-0.94	-1.20	-0.49	-0.81
01505200	BENAZEPRIL HYDROCHLORIDE	100122-03	E04	sample	86541-74-4	C24H29ClN2O5	460.96213	ACE inhibitor, antihypertensive	synthetic	USAN, INN, BAN, JAN		-1.26	-0.12	-1.24	0.68	-0.48
01505209	VALSARTAN	100122-03	E05	sample	137862-53-4	C24H29N5O3	435.53043	Angiotensin II inhibitor, antihypertensive	synthetic; CGP-48933	USAN, INN, BAN		1.73	0.31	0.55	0.79	0.85
00200331	SALSALATE	100122-03	E06	sample	552-94-3	C14H10O5	258.2328	analgesic	synthetic	USP, INN, BAN		0.03	-1.25	0.24	-0.11	-0.27
00300024	HYDROCORTISONE	100122-03	E07	sample	50-23-7	C21H30O5	362.47025	glucocorticoid, antiinflammatory	adrenal glands	USP, INN, BAN, JAN		0.97	-0.30	0.09	-0.28	0.12
01505321	RIFAXIMIN	100122-03	E08	sample	80621-81-4	C43H51N3O11	785.89942	antibacterial, RNA synthesis inhibitor	semisynthetic	USAN, INN	Drugs 49:467 (1995)	0.41	0.06	0.00	-0.10	0.09
01505248	CANRENONE	100122-03	E09	sample	976-71-6	C22H28O3	340.46666	aldosterone antagonist; antifibrogenic	synthetic	USAN, INN	Eur J Clin Pharmacol 9: 253 (1976); Gastroenterology 124:	-0.72	-1.00	-0.14	-0.81	-0.67
01505361	MODAFINIL	100122-03	E10	sample	68693-11-8	C15H15NO2S	273.3563	analeptic	synthetic; CRL-40476, CEP-1538	USAN, INN, BAN		0.50	0.21	0.10	0.11	0.23
01505114	CLIOQUINOL	100122-03	E11	sample	130-26-7	C9H5ClINO	305.5037	antiseptic, antiamebic	synthetic	USP, INN, BAN		-0.33	0.45	0.04	-0.83	-0.17
	0.11% DMSO	100122-03	E12	0.11% dmso								-1.44	-2.17	-0.94	-2.04	-1.65
	0.11% JAK2inhib	100122-03	F01	0.11% jak2inhib								-1.97	-1.25	-2.49	-3.40	-2.28

Compound ID	MolNAME	plate	position	Content	cas#	Formula	MolWt	Bioactivity	Source	Status	Reference	Screen Score (z-score) rep1	rep2	rep3	rep4	Average
01505366	RANOLAZINE	100122-03	F02	sample	95635-55-5	C24H33N3O4	427.54831	antianginal, antiischemic	synthetic; RS-43285-003; CVT-303	USAN, INN		0.48	2.49	2.73	0.54	1.56
00211468	DANTHRON	100122-03	F03	sample	117-10-2	C14H8O4	240.21746	cathartic	Rheum palmatum, Xyris semifuscata	USP-XXI, INN, BAN	JACS 53: 4112 (1931)	-0.23	-0.02	-0.94	0.91	-0.07
01505376	ACEDAPSONE	100122-03	F04	sample	77-46-3	C16H16N2O4S	332.38092	antimalarial, leprostatic	synthetic; CI-556, CN-1883, DADDS, PAM-MAR-1165	USAN, INN, BAN		-0.33	0.90	-0.29	-0.32	-0.01
01505385	ATOMOXETINE HYDROCHLORIDE	100122-03	F05	sample	82248-59-7	C17H22ClNO	277.7969	norepinephrine reuptake inhibitor	synthetic; LY-139603	USAN, INN, BAN		0.29	0.48	-0.09	3.67	1.09
00300029	DESOXYCORTICOSTERONE ACETATE	100122-03	F06	sample	56-47-3	C23H32O4	372.50909	mineralocorticoid	adrenocortex	USP, INN, BAN		0.96	-0.68	2.04	-0.13	0.55
01505389	TRAMADOL HYDROCHLORIDE	100122-03	F07	sample	36282-47-0	C16H26ClNO2	299.84412	analgesic	synthetic; U-26225A, CG-315E	USAN, INN, BAN, JAN		0.41	-0.32	0.46	0.30	0.21
01505392	TERBINAFINE HYDROCHLORIDE	100122-03	F08	sample	78628-80-5, 91161-71-6(base)	C21H26ClN	327.90107	antifungal	synthetic, SF-86-327	USAN, INN, BAN		0.88	-1.14	1.01	0.09	0.21
01505801	TOPIRAMATE	100122-03	F09	sample	97240-79-4	C12H21NO8S	339.36707	anticonvulsant, antimigraine, GABA-A agonist, AMP/kinate	synthetic; RWJ-17021	USAN, INN, BAN		-1.08	-0.21	1.16	0.86	0.18
01505802	GEMIFLOXACIN MESYLATE	100122-03	F10	sample	204519-65-3	C19H24FN5O7S	485.49483	antibacterial	synthetic	USAN		-6.80	0.30	1.20	0.09	-1.30
01505803	PRAVASTATIN SODIUM	100122-03	F11	sample	81131-70-6	C23H35NaO7	446.521	antihyperlipidemic, HMGCoA reductase inhibitor	CS-514; SQ-31000	USAN, INN, BAN, JAN		-1.60	-0.45	0.38	-1.35	-0.75
	0.04% DMSO	100122-03	F12	0.04% dmso								0.24	-0.77	2.53	0.20	0.55
	0.04% JAK2inhib	100122-03	G01	0.04% jak2inhib								-0.96	2.50	0.95	-1.25	0.31
01505811	LEVALBUTEROL HYDROCHLORIDE	100122-03	G02	sample	50293-90-8	C13H22ClNO3	275.77819	bronchodilator, tocolytic	synthetic	USAN		-0.32	0.29	-0.94	0.84	-0.03
01505814	METFORMIN HYDROCHLORIDE	100122-03	G03	sample	1115-70-4, 657-24-	C4H12ClN5	165.62674	antidiabetic	synthetic; LA-6023	USAN, JAN		1.03	1.32	-0.31	0.78	0.71
01505816	PREGABALIN	100122-03	G04	sample	148553-50-8	C8H17NO2	159.23019	anticonvulsant	synthetic; CI-1008	USAN, INN		0.12	0.64	-0.85	0.60	0.13
01505820	TOPOTECAN HYDROCHLORIDE	100122-03	G05	sample	119413-54-6	C23H24ClN3O5	457.91783	antineoplastic; topoisomerase I inhibitor	semisynthetic	USAN, INN, BAN		0.17	1.04	-0.39	0.15	0.24
02300176	PHENOXYBENZAMINE HYDROCHLORIDE	100122-03	G06	sample	63-92-3, 59-96-1	C18H23Cl2NO	340.29611	alpha adrenergic blocker	synthetic	USP		-0.41	0.55	-0.14	-0.13	-0.03
02300270	PINACIDIL	100122-03	G07	sample	85371-64-8, 60560-33-0	C13H19N5	245.32988	K channel agonist, antihypertensive	synthetic	USAN, INN		-0.31	-0.46	-0.18	-0.10	-0.26
02300307	VERAPAMIL HYDROCHLORIDE	100122-03	G08	sample	152-11-4, 52-53-9 [verapamil]	C27H39ClN2O4	491.07588	adrenegic blocker, Ca channel blocker, coronary vasodilator,	synthetic	USP, INN, BAN, JAN		0.12	-0.30	-0.14	-0.10	-0.10
01505818	PANTOPRAZOLE	100122-03	G09	sample	102625-70-7	C16H15F2N3O4S	383.37645	proton pump inhibitor, gastric acid release inhibitor, antiulcer	synthetic; SK&F-96022, BY-1023	USAN, INN, BAN		-0.07	-0.03	0.49	1.93	0.58
02300241	LOPERAMIDE HYDROCHLORIDE	100122-03	G10	sample	34552-83-5, 53179-11-6	C29H34Cl2N2O2	513.51253	Ca channel blocker	synthetic	USP, INN, BAN, JAN		-1.89	-0.56	-0.38	1.54	-0.32
02300332	PODOFILOX	100122-03	G11	sample	518-28-5	C22H22O8	414.41584	antineoplastic, inhibits microtubule assembly, and human DNA	Podophylum peltatum; podophylotoxin	USAN, BAN	JACS 73: 2909 (1951); 75: 1308 (1953); J Med Chem 32:	-10.56	-6.56	-5.80	-3.21	-6.53
	0.04% DMSO	100122-03	G12	0.04% dmso								-0.10	5.78	0.17	5.24	2.77
	0.04% JAK2inhib	100122-03	H01	0.04% jak2inhib								-1.89	-1.52	-3.45	-2.43	-2.32
02300205	LEVODOPA	100122-03	H02	sample	59-92-7	C9H11NO4	197.19232	antiparkinsonian	Vicia faba seedlings, Sarothamnus spp, & other palnts	USP, INN, BAN, JAN		-0.65	-0.17	-1.13	0.30	-0.41
00300607	RUTOSIDE (rutin)	100122-03	H03	sample	153-18-4	C27H30O16	610.53055	vascular protectant	Ruta graveolens, widespread in plants	NF-XI, INN, BAN, JAN		-0.43	0.43	0.56	-0.41	0.04
01500615	ZOMEPIRAC SODIUM	100122-03	H04	sample	64092-49-5, 64092-48-4	C15H14ClNO3	291.73673	analgesic, antiinflammatory	synthetic	USAN, INN, BAN		0.05	1.02	-0.36	0.56	0.32
00300548	SPARTEINE SULFATE	100122-03	H05	sample	6160-12-9, 299-39-8	C15H28N2O4S	332.46541	oxytocic	Lupinus spp and other Leguminosae	USAN, BAN, JAN	J Chem Soc 1949: 663	-0.16	0.02	-0.89	-1.08	-0.53
00300034	TESTOSTERONE PROPIONATE	100122-03	H06	sample	57-85-2	C22H32O3	344.49854	androgen, antineoplastic	semisynthetic	USP, JAN		0.11	0.76	-0.10	-0.76	0.00
01506009	METHIMAZOLE	100122-03	H07	sample	60-56-0	C4H6N2S	114.16982	thyroid inhibitor	synthetic	USP, INN, BAN, JAN		-0.22	1.72	-0.45	5.54	1.65
01506067	ENILCONAZOLE	100122-03	H08	sample	35554-44-0	C14H14Cl2N2O	297.18648	antifungal	synthetic; R-23979	USAN, INN, BAN		-0.78	-0.37	0.22	-0.11	-0.26
01504526	FIROCOXIB	100122-03	H09	sample	189954-96-9	C17H20O5S	336.40995	analgesic, antiinflammatory, antipyretic, COX-II inhibitor	synthetic; ML-1785713	USAN, INN		0.51	0.59	0.24	-0.72	0.15
00330071	LINDANE	100122-03	H10	sample	58-89-9	C6H6Cl6	290.83272	insecticide	synthetic; gamma-BHC	USP, INN, BAN	Use: insecticide	-0.38	0.74	3.01	0.78	1.04
01504218	ACRISORCIN	100122-03	H11	sample	7527-91-5	C25H28N2O2	388.51411	antifungal	synthetic	USP-XXII, INN		-0.05	-0.04	0.73	-0.59	0.01
	empty	100122-03	H12	sample								NA	NA	NA	NA	NA
	empty	100122-04	A01	sample								NA	NA	NA	NA	NA
00305025	PHENYL AMINOSALICYLATE	100122-04	A02	sample	133-11-9	C13H11NO3	229.23752	antibacterial (tuberculostatic)	synthetic; NSC-40144	USAN, INN, BAN		-1.33	-1.12	-1.72	-0.52	-1.17
00307023	TESTOSTERONE	100122-04	A03	sample	58-22-0	C19H28O2	288.43381	androgen, antineoplastic	mamallian male hormone	USP, INN, BAN		-1.29	-0.98	1.04	1.99	0.19
00310035	SANGUINARINE SULFATE	100122-04	A04	sample	5578-73-4	C20H15NO8S	429.40845	antineoplastic, antiplaque agent	Sanguinaria canadensis	USAN, INN	J Heterocyclic Chem 9: 1453 (1972)	-1.60	-1.52	-2.51	-1.83	-1.86
00310039	alpha-TOCHOPHEROL	100122-04	A05	sample	59-02-9	C29H50O2	430.72065	vitamin E	soya, wheat germ and other plant oils	USP		-0.21	-0.91	-0.81	-1.66	-0.90
00310040	alpha-TOCHOPHERYL ACETATE	100122-04	A06	sample	58-95-7	C31H52O3	472.75829	vitamin E	derivative	USP		-0.23	0.44	-0.68	-0.90	-0.34
00330001	DACTINOMYCIN	100122-04	A07	sample	50-76-0	C62H86N12O16	1255.44752	antineoplastic, intercalating agent	Actinomyces spp	USP, INN, BAN, JAN		-3.11	-0.51	-2.64	1.26	-1.25
00330002	MITOMYCIN C	100122-04	A08	sample	50-07-7	C15H18N4O5	334.33451	antineoplastic	Streptomyces verticillatus	USP, INN, BAN, JAN		-1.03	-1.98	-0.90	-2.85	-1.69
00330018	DICHLORVOS	100122-04	A09	sample	62-73-7	C4H7Cl2O4P	220.97779	insecticide, cholinesterase inhibitor	synthetic	USAN, INN, BAN		-0.77	-1.84	2.03	-0.48	-0.26
00330062	TEMEFOS	100122-04	A10	sample	3383-96-8	C16H20O6P2S3	466.4738	insecticide	synthetic	USAN, INN		-1.23	-1.77	0.59	-2.04	-1.11
00330082	MITOTANE	100122-04	A11	sample	53-19-0	C14H10Cl4	320.0478	insecticide, antineoplastic	synthetic	USP, BAN, JAN		-0.32	-2.23	0.04	-1.84	-1.09
	0.04% JAK2inhib	100122-04	A12	0.04% jak2inhib								-2.29	-2.04	-0.72	-2.99	-2.01
	0.04% DMSO	100122-04	B01	0.04% dmso								-0.98	-0.24	-0.88	4.77	0.67
01300027	IVERMECTIN	100122-04	B02	sample	70288-86-7	C48H74O14	875.11658	antiparasitic	semisynthetic	USP, INN, BAN	Science 221:823 (1983); J Vet Pharmacol Ther 7:1 (1984)	-9.09	-4.82	-3.73	-2.40	-5.01
01300037	SODIUM NITROPRUSSIDE	100122-04	B03	sample	13755-38-9	C5FeN6Na2O	261.92195	antihypertensive	synthetic	USP	J Clin Pharmacol 14:494 (1974)	-3.52	-3.51	-3.55	-2.58	-3.29
01300038	SODIUM OXYBATE	100122-04	B04	sample	502-85-2	C4H7NaO3	126.08839	anesthetic	synthetic; WY-3478, NSC-84223	USAN		0.16	2.78	-1.47	-1.12	0.09
01400151	ETHYL PARABEN	100122-04	B05	sample	120-47-8	C9H10O3	166.17825	antifungal	synthetic	USAN, NF, JAN		-1.02	-0.48	4.52	0.02	0.76
01400208	COUMARIN	100122-04	B06	sample	91-64-5	C9H6O2	146.14697	antineoplastic, antiinflammatory, antihyperglycaemic	Coumarouna odorata, tonka beans, lavender oil	NF-X, INN	Prog Chem Org Nat Prod 9: 225 (1952)	0.09	-0.41	-0.65	-0.93	-0.47
01500101	ACETAMINOPHEN	100122-04	B07	sample	103-90-2	C8H9NO2	151.16643	analgesic, antipyretic	synthetic	USP, INN, BAN		-0.13	-0.01	0.71	0.18	0.19
01500102	ACETAZOLAMIDE	100122-04	B08	sample	59-66-5	C4H6N4O3S2	222.24542	carbonic anhydrase inhibitor, diuretic, antiglaucoma	synthetic	USP, INN, BAN, JAN		-0.58	-0.51	0.59	-0.63	-0.28
01500103	ACETOHYDROXAMIC ACID	100122-04	B09	sample	546-88-3	C2H5NO2	75.06765	urease inhibitor, antiurolithic, antbacterial	synthetic	USP, INN		0.20	0.35	0.55	0.01	0.28
01500104	ACETYLCHOLINE	100122-04	B10	sample	60-31-1, 51-84-3	C7H16ClNO2	181.66407	antiarrhythmic, miotic, vasodilator (peripheral)	synthetic	USP		0.36	0.74	0.40	-0.07	0.36
01500105	ACETYLCYSTEINE	100122-04	B11	sample	616-91-1	C5H9NO3S	163.19638	mucolytic	synthetic	USP, INN, BAN, JAN		0.82	-1.12	1.52	-0.60	0.16
	0.04% JAK2inhib	100122-04	B12	0.04% jak2inhib								-1.44	-1.55	4.40	-0.08	0.33
	0.04% DMSO	100122-04	C01	0.04% dmso								-0.33	-0.29	-1.76	1.45	-0.23
01500107	ADENOSINE	100122-04	C02	sample	58-61-7	C10H13N5O4	267.24621	antiarrhythmic, cardiac depressant	widespread in living tissue	USP, BAN		-1.02	-0.44	-0.78	-1.00	-0.81
01500108	ALLOPURINOL	100122-04	C03	sample	315-30-0	C5H4N4O	136.11383	antihyperuricemia, antigout, antiurolithic	synthetic	USP, INN, BAN, JAN		-0.77	-0.37	-0.97	-0.20	-0.58
01500109	ALVERINE CITRATE	100122-04	C04	sample	5560-59-8, 150-59-4 [alverine]	C26H35NO7	473.57135	anticholinergic	synthetic	USAN, INN, BAN		-0.94	-0.02	-0.96	0.16	-0.44
01500110	AMANTADINE HYDROCHLORIDE	100122-04	C05	sample	665-66-7, 768-94-5	C10H18ClN	187.71466	antiviral, antiparkinsonian; treatment of drug-induced	synthetic	USP, INN, BAN		-0.18	-0.73	-0.97	1.81	-0.02
01500111	AMIKACIN SULFATE	100122-04	C06	sample	39831-55-5, 37517-28-5	C22H47N5O21S2	781.76879	antibacterial	semisynthetic	USP, JAN		0.59	-0.22	0.12	2.51	0.75
01500112	AMILORIDE HYDROCHLORIDE	100122-04	C07	sample	17440-83-4, 2016-88-8	C6H9Cl2N7O	266.09093	Na+ channel inhibitor, diuretic	synthetic	USP, INN, BAN	Biochim Biophys Acta 944: 383 (1988)	0.69	0.00	0.51	-0.36	0.21
01500114	AMINOCAPROIC ACID	100122-04	C08	sample	60-32-2	C6H13NO2	131.17601	hemostatic	synthetic	USP, INN, BAN		-0.54	-0.15	-0.04	-0.34	-0.27
01500115	AMINOGLUTETHIMIDE	100122-04	C09	sample	125-84-8	C13H16N2O2	232.28467	aromatase inhibitor, antineoplastic, testosterone suppressant	synthetic	USP, INN, BAN		1.09	-0.03	0.54	-0.51	0.27
01500116	AMINOSALICYLATE SODIUM	100122-04	C10	sample	6018-19-5	C7H6NNaO3	175.12057	antibacterial, tuberculostatic	synthetic	USP		0.00	-0.57	1.37	1.11	0.48
01500117	AMITRIPTYLINE HYDROCHLORIDE	100122-04	C11	sample	549-18-8	C20H24ClN	313.87398	antidepressant	synthetic	USP, INN, BAN, JAN		0.22	-0.76	0.42	-0.02	-0.04
	0.11% JAK2inhib	100122-04	C12	0.11% jak2inhib								-3.07	-4.27	-1.80	-1.92	-2.76
	0.11% DMSO	100122-04	D01	0.11% dmso								-1.87	-2.11	-3.27	-2.04	-2.32
01500119	AMODIAQUINE DIHYDROCHLORIDE	100122-04	D02	sample	6398-98-7, 69-44-3	C20H24Cl3N3O	428.79278	antimalarial	synthetic	USP, INN, BAN		-0.08	2.24	-1.33	-0.53	0.07
01500120	AMOXICILLIN	100122-04	D03	sample	61336-70-7, 26787-78-0	C16H19N3O5S	365.41093	antibacterial	semisynthetic	USP, INN, BAN, JAN		-0.23	0.15	-1.61	-0.50	-0.55
01500122	AMPHOTERICIN B	100122-04	D04	sample	1397-89-3	C47H73NO17	924.10236	antifungal	Streptomycetes nodosus	USP, INN, BAN, JAN	New Engl J Med 296: 784 (1977)	0.32	-0.26	0.80	-0.87	0.00
01500123	AMPICILLIN SODIUM	100122-04	D05	sample	69-52-3, 69-53-4 [ampicillin]	C16H18N3NaO4S	371.39336	antibacterial	semisynthetic	USP, INN, BAN, JAN		0.33	0.85	-0.32	0.75	0.40
01500124	AMPROLIUM	100122-04	D06	sample	121-25-5	C14H20Cl2N4	315.2483	coccidiostat	synthetic	USP, INN, BAN		0.39	0.87	0.00	0.66	0.48
01500126	ANTAZOLINE PHOSPHATE	100122-04	D07	sample	154-68-7, 91-75-8 [antazoline]	C17H22N3O4P	363.35639	antihistaminic	synthetic	USP		0.46	0.01	0.70	3.82	1.25
01500127	ANTHRALIN	100122-04	D08	sample	480-22-8, 1143-38-0	C14H10O3	226.234	antipsoriatic	synthetic	USP		0.29	0.00	0.55	0.71	0.39
01500128	ANTIPYRINE	100122-04	D09	sample	60-80-0	C11H12N2O	188.23109	analgesic	synthetic	USP, INN, BAN, JAN		0.39	0.01	0.86	-0.29	0.24
01500129	APOMORPHINE HYDROCHLORIDE	100122-04	D10	sample	41372-20-7, 314-19-2	C17H18ClNO2	303.79151	emetic	synthetic	USP, BAN		0.41	-0.52	1.48	-0.58	0.20
01500130	ASPIRIN	100122-04	D11	sample	50-78-2	C9H8O4	180.16171	analgesic, antipyretic, antiinflammatory	synthetic	USP, BAN, JAN		1.71	1.16	2.34	1.07	1.57
	0.11% JAK2inhib	100122-04	D12	0.11% jak2inhib								-3.39	-3.26	-1.91	-3.28	-2.96
	0.11% JAK2inhib	100122-04	E01	0.11% jak2inhib								-3.73	-2.64	-3.46	-2.44	-3.07
01500131	ATROPINE SULFATE	100122-04	E02	sample	51-55-8, 5908-99-6 [atropine	C17H25NO7S	387.4553	anticholinergic, mydriatic	Atropa and Datura spp	USP, BAN		-0.28	-0.34	-1.30	-0.45	-0.59
01500132	AUROTHIOGLUCOSE	100122-04	E03	sample	12192-57-3	C6H11AuO5S	392.18257	antirheumatic	synthetic	USP		-0.32	0.22	-0.26	0.28	-0.02
01500133	AZATHIOPRINE	100122-04	E04	sample	446-86-6	C9H7N7O2S	277.26584	immunosuppressant, antineoplastic, antirheumatic	synthetic	USP, INN, BAN, JAN		-1.16	0.47	-0.79	-0.58	-0.52
01500134	BACITRACIN	100122-04	E05	sample	1405-87-4	C66H103N17O16S	1422.72511	antibacterial	Bacillus licheniformis and B subtilis	USP, INN, BAN, JAN		1.02	0.50	-0.27	-0.31	0.23
01500135	BACLOFEN	100122-04	E06	sample	1134-47-0	C10H12ClNO2	213.66564	muscle relaxant (skeletal)	synthetic	USP, INN, BAN, JAN		0.28	-0.19	-0.75	0.15	-0.13
01500136	BECLOMETHASONE DIPROPIONATE	100122-04	E07	sample	5534-09-8, 4419-39-0	C28H37ClO7	521.05589	antiasthmatic, topical antiinflammatory	synthetic	USP, INN, BAN, JAN		0.03	1.23	0.46	0.63	0.59
01500137	BENSERAZIDE HYDROCHLORIDE	100122-04	E08	sample	322-35-0	C10H16ClN3O5	293.70912	decarboxylase inhibitor	component of Madopa (Hoffmann-LaRoche)	USAN, INN, BAN, JAN		0.15	0.08	0.25	5.38	1.47
01500138	BENZETHONIUM CHLORIDE	100122-04	E09	sample	121-54-0	C27H42ClNO2	448.09429	antiinfective (topical)	synthetic	USP, INN, BAN, JAN		1.31	-0.53	0.75	-0.01	0.38
01500139	BENZOCAINE	100122-04	E10	sample	94-09-7	C9H11NO2	165.19352	anesthetic (topical)	synthetic	USP, INN, BAN		1.66	0.23	0.74	0.54	0.79
01500141	BENZTHIAZIDE	100122-04	E11	sample	91-33-8	C15H14ClN3O4S3	431.94153	diuretic, antihypertensive	synthetic	USP-XIII, INN, BAN, JAN		0.32	-0.14	1.17	-0.50	0.21
	0.11% DMSO	100122-04	E12	0.11% dmso								-0.61	1.27	0.68	-1.86	-0.13
	0.11% JAK2inhib	100122-04	F01	0.11% jak2inhib								-3.66	-3.68	-3.39	-3.40	-3.53
01500143	beta-CAROTENE	100122-04	F02	sample	7235-40-7	C40H56	536.89232	provitamin A	provitamin A; widespread in plants and animals	USP, INN		-7.36	-1.96	-1.78	-0.40	-2.87
01500144	BETAMETHASONE	100122-04	F03	sample	378-44-9	C22H29FO5	392.47183	glucocorticoid, antiinflammatory	semisynthetic	USP, INN, BAN, JAN		-0.87	0.63	-0.88	0.44	-0.17
01500146	BETHANECHOL CHLORIDE	100122-04	F04	sample	590-63-6, 674-38-4	C7H17ClN2O2	196.67874	cholinergic	synthetic	USP, BAN, JAN		0.00	1.37	-0.84	0.69	0.31
01500147	BISACODYL	100122-04	F05	sample	603-50-9	C22H19NO4	361.40103	cathartic	synthetic	USP, INN, BAN, JAN		0.15	0.06	-0.87	0.18	-0.12
01500148	BITHIONATE SODIUM	100122-04	F06	sample	97-18-7	C12H4Cl4Na2O2S	400.02008	anthelmintic, antiseptic	synthetic	USAN, INN, BAN, JAN		0.68	0.40	-0.44	-0.92	-0.07
01500151	BROMOCRIPTINE MESYLATE	100122-04	F07	sample	22260-51-1, 25614-03-3	C33H44BrN5O8S	750.71533	prolactin inhibitor, antiparkinsonian	semisynthetic	USP, BAN, JAN		-0.20	-1.18	-1.62	6.53	0.88
01500152	BUSULFAN	100122-04	F08	sample	55-98-1	C6H14O6S2	246.30288	antineoplastic, alkylating agent	synthetic	USP, INN, BAN, JAN		1.32	-0.59	0.85	0.77	0.59
01500155	CAFFEINE	100122-04	F09	sample	58-08-2, 5743-12-4	C8H10N4O2	194.1945	CNS stimulant	Cofea, Theobroma, Camelia and Cola spp	USP, INN, BAN, JAN		2.14	0.17	0.07	0.65	0.75
01500156	CAMPHOR (1R)	100122-04	F10	sample	464-49-3, 76-22-2	C10H16O	152.23842	analgesic, antiinfective, antipruritic	Cinnamomum camphora	USP, JAN		1.12	0.63	-0.14	0.47	0.52
01500157	CAPREOMYCIN SULFATE	100122-04	F11	sample	1405-37-4, 11003-38-6	C25H46N14O12S	766.79597	antibacterial, tuberculostatic	Streptomyces capreolis	USP, INN, BAN, JAN		0.74	-0.81	0.58	-0.12	0.10
	0.04% DMSO	100122-04	F12	0.04% dmso								0.81	-0.62	0.63	-0.89	-0.02
	0.04% JAK2inhib	100122-04	G01	0.04% jak2inhib								-2.50	-0.57	-2.72	-0.70	-1.62
01500158	CARBACHOL	100122-04	G02	sample	51-83-2	C6H15ClN2O2	182.65165	cholinergic, miotic	synthetic	USP, INN, BAN, JAN		-0.10	0.68	-1.33	-0.77	-0.38
01500159	CARBAMAZEPINE	100122-04	G03	sample	298-46-4	C15H12N2O	236.27569	analgesic, anticonvulsant	synthetic	USP, INN, BAN, JAN		-1.04	0.58	-1.34	0.02	-0.45
01500160	CARBENICILLIN DISODIUM	100122-04	G04	sample	4800-94-6, 4697-36-3	C17H16N2Na2O6S	422.37047	antibacterial	semisynthetic	USP, INN, BAN, JAN		-0.54	-0.16	-0.32	0.02	-0.25
01500161	CARBINOXAMINE MALEATE	100122-04	G05	sample	3505-38-2, 486-16-8	C20H23ClN2O5	406.86971	antihistaminic	synthetic	USP, INN, BAN, JAN		-0.07	3.24	-0.38	-0.08	0.68
01500162	CARISOPRODOL	100122-04	G06	sample	78-44-4	C12H24N2O4	260.33608	muscle relaxant (skeletal)	synthetic	USP, INN, BAN		-0.17	0.34	0.00	0.36	0.13
01500163	CEFADROXIL	100122-04	G07	sample	66592-87-8, 50370-12-2	C16H17N3O5S	363.39499	antibacterial	semisynthetic	USP, INN, BAN, JAN		0.12	-0.68	0.36	1.09	0.22
01500165	CEFOTAXIME SODIUM	100122-04	G08	sample	64485-93-4, 63527-52-6	C16H16N5Na07S2	477.45302	antibacterial	semisynthetic	USP, INN, BAN, JAN		-0.11	0.09	0.10	4.59	1.17
01500166	CEPHALOTHIN SODIUM	100122-04	G09	sample	58-71-9, 153-61-7 [cephalothin]	C16H15N2NaO6S2	418.42555	antibacterial	semisynthetic	USP, INN, BAN, JAN		1.09	0.14	0.13	-0.54	0.20
01500167	CEPHAPIRIN SODIUM	100122-04	G10	sample	24356-60-3, 21593-23-7	C17H16N3NaO6S2	445.45137	antibacterial	semisynthetic	USP, INN, BAN, JAN		0.91	0.34	0.79	0.87	0.73
01500168	CEPHRADINE	100122-04	G11	sample	38821-53-3 [anhydrous], 58456-	C16H19N3O4S	349.41153	antibacterial	semisynthetic	USP, INN, BAN, JAN		1.08	0.51	0.95	0.04	0.64
	0.04% DMSO	100122-04	G12	0.04% dmso								0.80	-1.06	0.73	-0.25	0.06
	0.04% JAK2inhib	100122-04	H01	0.04% jak2inhib								-2.28	-1.68	2.14	-2.64	-1.12
01500169	CETYLPYRIDINIUM CHLORIDE	100122-04	H02	sample	6004-24-6, 123-03-5	C21H38ClN	339.99671	antiinfective (topical)	synthetic	USP, INN, BAN, JAN		-0.40	2.54	0.36	1.92	1.10
01500171	CHLORAMBUCIL	100122-04	H03	sample	305-03-3	C14H19Cl2NO2	304.21903	antineoplastic, alkylating agent	synthetic	USP, INN, BAN		-0.48	0.12	-1.47	-0.36	-0.55
01500172	CHLORAMPHENICOL PALMITATE	100122-04	H04	sample	530-43-8	C27H42Cl2N2O6	561.55159	antibacterial, antirickettsial	semisynthetic	USP, BAN, JAN		-6.53	-0.54	-0.47	0.34	-1.80
01500173	CHLORAMPHENICOL HEMISUCCINATE	100122-04	H05	sample	982-57-0, 56-75-7	C15H16Cl2N2O8	423.20937	antibacterial, antirickettsial, inhibits protein synthesis	semisynthetic	USP, BAN, JAN		-0.24	0.17	-0.61	0.30	-0.10
01500174	CHLORAMPHENICOL	100122-04	H06	sample	56-75-7	C11H12Cl2N2O5	323.13469	antibacterial, antirickettsial, inhibits protein synthesis	Streptomyces venezuelae	USP, INN, BAN, JAN		0.93	0.60	-0.88	0.07	0.18
01500175	CHLORCYCLIZINE HYDROCHLORIDE	100122-04	H07	sample	1620-21-9, 82-93-9 [base]	C18H22Cl2N2	337.29544	H1-antihistamine	synthetic	USP XXI, INN, BAN		-0.49	0.30	-0.63	-1.20	-0.50
01500177	CHLORHEXIDINE	100122-04	H08	sample	3697-42-5, 55-56-1	C22H32Cl4N10	578.37934	antibacterial (topical), disinfectant	synthetic	USP, INN, BAN, JAN		0.92	0.17	0.53	0.28	0.48
01500178	CHLORACRESOL	100122-04	H09	sample	59-50-7	C7H7ClO	142.58624	antiinfectant	synthetic	USAN, NF, INN		0.14	1.20	0.14	1.08	0.64

Compound ID	MolNAME	plate	position	Content	cas#	Formula	MolWt	Bioactivity	Source	Status	Reference	Screen Score (z-score) rep1	rep2	rep3	rep4	Average
01500179	CHLOROQUINE DIPHOSPHATE	100122-04	H10	sample	54-05-7	C18H32ClN3O8P2	515.87164	antimalarial, antiamebic, antirheumatic, intercalating agent	synthetic	USP, BAN		0.80	-0.23	2.12	-0.10	0.65
01500180	CHLOROTHIAZIDE	100122-04	H11	sample	58-94-6	C7H6ClN3O4S2	295.72457	diuretic, antihypertensive	synthetic	USP, INN, BAN		2.17	0.30	0.53	0.29	0.82
	empty	100122-04	H12	sample								NA	NA	NA	NA	NA
	empty	100122-05	A01	sample								NA	NA	NA	NA	NA
01500181	CHLOROTRIANISENE	100122-05	A02	sample	569-57-3	C23H21ClO3	380.87502	estrogen	synthetic	USP-XIII, INN, BAN		-0.41	-0.50	-1.51	0.16	-0.56
01500182	CHLOROXYLENOL	100122-05	A03	sample	88-04-0	C8H9ClO	156.61333	antibacterial, topical and urinary antiseptic	synthetic	USP, INN, BAN		0.02	-0.53	-1.26	0.39	-0.35
01500183	CHLORPHENIRAMINE (S) MALEATE	100122-05	A04	sample	113-92-8, 132-22-9	C20H23ClN2O4	390.87031	antihistaminic	synthetic	USP, INN, BAN		-0.82	-0.44	0.35	-0.67	-0.39
01500184	CHLORPROMAZINE	100122-05	A05	sample	50-53-3	C17H19ClN2S	318.87138	antiemetic, antipsychotic	synthetic	USP, INN, BAN, JAN		-0.05	2.54	-0.76	-0.11	0.41
01500185	CHLORPROPAMIDE	100122-05	A06	sample	94-20-2	C10H13ClN2O3S	276.74371	antidiabetic	synthetic	USP, INN, BAN, JAN		0.05	-0.97	0.28	0.21	-0.11
01500186	CHLORTETRACYCLINE HYDROCHLORIDE	100122-05	A07	sample	64-72-2	C22H24Cl2N2O8	515.35118	antibacterial, antiamebic, Ca chelator, hepatotoxic; inhibits protein	Streptomyces aureofaciens	USP, BAN	Ann NY Acad Sci 51: 177 (1948); JACS 74: 4976 (1952);	0.05	-0.82	-0.43	-0.03	-0.31
01500187	CHLORTHALIDONE	100122-05	A08	sample	77-36-1	C14H11ClN2O4S	338.77177	diuretic, antihypertensive	synthetic	USP, INN, BAN, JAN		-0.49	-0.34	-0.52	-0.10	-0.36
01500188	CHLORZOXAZONE	100122-05	A09	sample	95-25-0	C7H4ClNO2	169.56843	muscle relaxant (skeletal)	synthetic	USP, INN, BAN, JAN		-0.40	-0.14	0.77	0.69	0.23
01500189	CICLOPIROX OLAMINE	100122-05	A10	sample	41621-49-2	C14H24N2O3	268.35898	antifungal	synthetic	USP, INN, BAN		-0.99	-1.94	-0.32	-0.57	-0.95
01500190	CINOXACIN	100122-05	A11	sample	28657-80-9	C12H10N2O5	262.2239	antibacterial	synthetic	USP, INN, BAN, JAN		0.00	-0.88	0.04	-0.50	-0.34
	0.04% JAK2inhib	100122-05	A12	0.04% jak2inhib								-1.16	-1.31	-0.18	-1.85	-1.12
	0.04% DMSO	100122-05	B01	0.04% dmso								0.35	0.24	-1.29	-0.20	-0.23
01500191	CLEMASTINE	100122-05	B02	sample	15686-51-8	C25H30ClNO5	459.97455	antihistaminic	synthetic	USAN, BAN		-0.44	-0.27	-0.67	-0.25	-0.41
01500192	CLIDINIUM BROMIDE	100122-05	B03	sample	3485-62-9	C22H26BrNO3	432.36142	anticholinergic	synthetic	USP, INN, BAN		0.29	0.14	-0.10	0.06	0.10
01500193	CLINDAMYCIN HYDROCHLORIDE	100122-05	B04	sample	21462-39-5, 58207-19-5	C18H34Cl2N2O5S	461.45208	antibacterial, inhibits protein synthesis	semisynthetic; U-21251	USAN, INN, BAN		-0.24	0.37	3.90	-0.38	0.91
01500196	CLOMIPHENE CITRATE	100122-05	B05	sample	50-41-9, 911-45-5 [clomiphene]	C32H36ClNO8	598.09862	gonad stimulating principle	synthetic	USP, INN, BAN		-0.70	-0.72	-0.01	0.50	-0.23
01500198	CLONIDINE HYDROCHLORIDE	100122-05	B06	sample	4205-91-8, 4205-90-7	C9H10Cl3N3	266.55915	antihypertensive	synthetic	USP, INN, BAN		0.37	-0.17	0.59	1.54	0.58
01500200	CLOTRIMAZOLE	100122-05	B07	sample	23593-75-1	C22H17ClN2	344.84719	antifungal	synthetic	USP, INN, BAN, JAN		-1.49	-1.42	-0.98	-2.76	-1.66
01500201	CLOXACILLIN SODIUM	100122-05	B08	sample	7081-44-9, 642-78-4	C19H17ClN3NaO5S	457.87124	antibacterial	semisynthetic	USP, INN, BAN, JAN		-0.58	0.55	0.32	1.29	0.40
01500202	CLOXYQUIN	100122-05	B09	sample	130-16-5	C9H6ClNO	179.60727	antibacterial, antifungal	synthetic	USAN, INN		0.69	0.54	0.39	0.26	0.47
01500205	COLCHICINE	100122-05	B10	sample	64-86-8	C22H25NO6	399.44765	antimitotic, antigout agent	Colchicum autumnale	USP, JAN	J Am Chem Soc 74: 487 (1952)	-8.48	-7.47	-7.62	-7.13	-7.67
01500206	COLISTIMETHATE SODIUM	100122-05	B11	sample	8068-28-8, 21362-08-3	C57H103N16Na5O28S	1735.81586	antibacterial	Bacillus colistinus	USP, INN, BAN, JAN	Brit.J.Pharmacol.Chemother. 23: 552 (1964)	-0.37	1.30	0.56	3.01	1.13
	0.04% JAK2inhib	100122-05	B12	0.04% jak2inhib								-0.82	-2.31	0.33	-1.12	-0.98
	0.04% DMSO	100122-05	C01	0.04% dmso								-0.90	-1.37	-2.33	-0.66	-1.31
01500207	CORTISONE ACETATE	100122-05	C02	sample	50-04-4, 53-06-5 [cortisone]	C23H30O6	402.49195	glucocorticoid	semisynthetic	USP, INN, BAN, JAN		0.50	0.46	-0.66	4.40	1.17
01500208	COTININE	100122-05	C03	sample	486-56-6, 5695-98-7[fumarate]	C10H12N2O	176.21994	antidepressant	Nicotiana tabacum	USAN, INN	JACS 79: 149 (1957)	0.66	0.53	-0.76	0.77	0.30
01500209	CRESOL	100122-05	C04	sample	1319-77-3	C7H8O	108.14121	antiinfectant	coal tar	USAN, NF, JAN		-0.12	0.51	-0.55	0.44	0.07
01500210	CROMOLYN SODIUM	100122-05	C05	sample	15826-37-6, 16110-51-3	C23H14Na2O11	512.34103	antiasthmatic, antiallergy	synthetic	USP, INN, BAN, JAN		0.17	0.75	0.01	0.49	0.36
01500211	CYCLIZINE	100122-05	C06	sample	82-92-8	C18H22N2	266.38944	H1 antihistamine	synthetic	USP, BAN		0.55	1.48	0.08	2.89	1.25
01500212	CYCLOPENTOLATE HYDROCHLORIDE	100122-05	C07	sample	5870-29-1, 512-15-2	C17H26ClNO3	327.85467	mydriatic	synthetic	USP, INN, BAN, JAN		0.06	-0.02	-0.02	0.82	0.21
01500213	CYCLOPHOSPHAMIDE HYDRATE	100122-05	C08	sample	6055-19-2, 50-18-0	C7H17Cl2N2O3P	279.10494	antineoplastic, alkylating agent	synthetic	USP, INN, BAN, JAN		0.86	-0.20	-0.32	0.18	0.13
01500215	CYCLOSERINE	100122-05	C09	sample	68-41-7	C3H6N2O2	102.09347	antibacterial (tuberculostatic)	Streptomyces spp	USP, INN, BAN, JAN		1.76	-0.42	0.07	1.40	0.70
01500216	CYPROTERONE ACETATE	100122-05	C10	sample	427-51-0	C24H29ClO4	416.94933	antiandrogen	synthetic	USP		0.16	0.60	0.79	-0.34	0.30
01500217	CYTARABINE	100122-05	C11	sample	147-94-4	C9H13N3O5	243.22106	antineoplastic, antiviral, antimetabolite	synthetic	USP, INN, BAN, JAN		-0.57	-1.88	-1.41	-1.86	-1.43
	0.11% JAK2inhib	100122-05	C12	0.11% jak2inhib								-1.78	-2.41	-1.01	-1.61	-1.70
	0.11% DMSO	100122-05	D01	0.11% dmso								-0.38	0.29	-0.78	-1.49	-0.59
01500218	DACARBAZINE	100122-05	D02	sample	4342-03-4	C6H10N6O	182.1862	antineoplastic	synthetic	USP, INN, BAN, JAN		0.13	-0.11	-0.39	0.43	0.01
01500220	DANAZOL	100122-05	D03	sample	17230-88-5	C22H27NO2	337.46599	anterior pituitary suppressant	synthetic	USP, INN, BAN, JAN		-0.71	0.71	1.61	-0.41	0.30
01500222	DAPSONE	100122-05	D04	sample	80-08-0	C12H12N2O2S	248.30564	antibacterial, leprostatic, dermatitis herpetiformis suppressant	synthetic	USP, INN, BAN		1.20	0.29	-0.08	0.23	0.41
01500223	DAUNORUBICIN	100122-05	D05	sample	20830-81-3	C27H29NO10	527.53288	antineoplastic	Streptomyces peucetius; FI-6339, NDC-0082-4155, RP-13057	USAN, INN, BAN, JAN		-8.14	-7.08	-5.60	-2.35	-5.79
01500225	SODIUM DEHYDROCHOLATE	100122-05	D06	sample	145-41-5	C24H33NaO5	424.51741	choleretic	synthetic	USP, INN, BAN, JAN		0.36	1.11	0.26	0.50	0.56
01500226	DEMECLOCYCLINE HYDROCHLORIDE	100122-05	D07	sample	127-33-3	C21H22Cl2N2O8	501.32409	antibacterial	Streptomyces aureofaiens	USP, BAN, JAN		2.37	0.49	0.75	0.65	1.07
01500227	DESIPRAMINE HYDROCHLORIDE	100122-05	D08	sample	58-28-6, 50-47-5 [desipramine]	C18H23ClN2	302.85041	antidepressant	synthetic	USP, INN, BAN, JAN		-0.47	0.02	-0.26	1.89	0.29
01500230	DEXAMETHASONE	100122-05	D09	sample	50-02-2	C22H29FO5	392.47183	glucocorticoid	semisynthetic	USP, INN, BAN, JAN		0.22	0.37	0.14	5.68	1.61
01500231	DEXAMETHASONE ACETATE	100122-05	D10	sample	55812-90-3, 1177-87-3	C24H31FO6	434.50947	glucocorticoid, antiinflammatory	semisynthetic	USP, INN, BAN, JAN		0.21	0.35	1.54	-0.60	0.37
01500224	DEFEROXAMINE MESYLATE	100122-05	D11	sample	138-14-7, 70-51-9	C26H52N6O11S	656.80194	chelating agent (Fe & Al)	Strptomyces pilosus	USAN, INN, BAN		1.23	0.75	0.33	-0.41	0.47
	0.11% JAK2inhib	100122-05	D12	0.11% jak2inhib								-3.78	-2.78	-3.01	1.96	-1.90
	0.11% JAK2inhib	100122-05	E01	0.11% jak2inhib								-2.05	-2.77	-4.04	-2.14	-2.75
01500232	DEXAMETHASONE SODIUM PHOSPHATE	100122-05	E02	sample	2392-39-4, 312-93-6	C22H28FNa2O8P	516.41546	glucocorticoid, antiinflammatory	semisynthetic	USP, BAN, JAN		-0.07	0.61	-0.06	-0.29	0.05
01500233	DEXTROMETHORPHAN HYDROBROMIDE	100122-05	E03	sample	6700-34-1, 125-69-9	C18H26BrNO	352.31802	antitussive	synthetic	USP, INN, BAN		-0.11	1.39	-0.79	1.32	0.45
01500235	DIBENZOTHIOPHENE	100122-05	E04	sample	132-65-0	C12H8S	184.26156	keratolytic	synthetic	USAN		-0.10	0.27	-0.46	-0.25	-0.14
01500236	DIBUCAINE HYDROCHLORIDE	100122-05	E05	sample	61-12-1, 85-79-0 [dibucaine]	C20H30ClN3O2	379.934	anesthetic (local)	synthetic	USP, INN, BAN		0.76	-0.12	-1.04	0.48	0.02
01500237	DICLOFENAC SODIUM	100122-05	E06	sample	15307-79-6	C14H10Cl2NNaO2	318.1371	antiinflammatory	synthetic	USP, JAN		0.41	-0.02	0.56	-0.11	0.21
01500238	DICLOXACILLIN SODIUM	100122-05	E07	sample	13412-64-1, 343-55-5	C19H16Cl2N3NaO5S	492.31627	antibacterial	semisynthetic	USAN, INN, BAN		0.17	0.16	-0.13	0.03	0.06
01500239	DICUMAROL	100122-05	E08	sample	66-76-2	C19H12O6	336.30389	anticoagulant	synthetic	USAN, INN	J Biol Chem 138:21, 513, 529 (1041); 142:941 (1942)	1.75	-0.29	2.15	2.08	1.42
01500240	DICYCLOMINE HYDROCHLORIDE	100122-05	E09	sample	67-92-5, 77-19-0 [dicyclomine]	C19H36ClNO2	345.95727	anticholinergic	synthetic	USP, INN, BAN, JAN		0.22	0.27	0.03	4.43	1.24
01500241	DIENESTROL	100122-05	E10	sample	84-17-3, 13029-44-2 [//E,E//]	C18H18O2	266.34296	estrogen	synthetic	USP, INN, BAN		0.83	0.17	0.54	-0.70	0.21
01500242	DIETHYLCARBAMAZINE CITRATE	100122-05	E11	sample	1642-54-2, 90-89-1	C16H29N3O8	391.42483	anthelmintic	synthetic	USP, INN, BAN, JAN		1.40	-0.08	1.15	4.60	1.77
	0.11% DMSO	100122-05	E12	0.11% dmso								-0.10	-1.03	0.69	-0.69	-0.28
	0.11% JAK2inhib	100122-05	F01	0.11% jak2inhib								-3.00	-2.94	-4.28	2.78	-1.86
01500244	DIETHYLSTILBESTROL	100122-05	F02	sample	56-53-1	C18H20O2	268.3589	estrogen	synthetic	USP, INN, BAN		-1.15	-1.36	-2.98	-0.48	-1.49
01500245	DIFLUNISAL	100122-05	F03	sample	22494-42-4	C13H8F2O3	250.20371	analgesic, antiinflammatory	synthetic	USP, INN, BAN, JAN		-0.67	0.31	-0.62	-0.07	-0.26
01500246	DIGITOXIN	100122-05	F04	sample	71-63-6	C41H64O13	764.95943	inotropic, cardiotonic	Digitalis spp	USP, INN, BAN, JAN	Chem Rev 17: 187 (1935); Anal Profiles Drug Subst 3:149	-5.20	-1.60	-3.04	-2.20	-3.01
01500247	DIGOXIN	100122-05	F05	sample	20830-75-5	C41H64O14	780.95883	cardiac stimulant	Digitalis lanata or D. orientalis Lam., Scrophulariaceae	USP, INN, BAN, JAN	J.Chem.Soc.1930: 508; 1954: 2012	-0.16	0.21	-0.51	3.36	0.73
01500248	DIHYDROERGOTAMINE MESYLATE	100122-05	F06	sample	6190-39-2	C34H41N5O8S	679.79857	vasoconstrictor, antimigraine	semisynthetic	USP, INN, BAN, JAN		0.12	0.35	0.05	-0.16	0.09
01500249	DIHYDROSTREPTOMYCIN SULFATE	100122-05	F07	sample	5490-27-7, 128-46-1	C21H43N7O16S	681.67816	antibacterial, tuberculostatic	Streptomyces humidus	USP, INN, BAN, JAN		0.24	1.01	0.37	2.42	1.01
01500251	DIMENHYDRINATE	100122-05	F08	sample	523-87-5	C24H28ClN5O3	469.97546	antiemetic	synthetic	USP, INN, BAN, JAN		0.00	0.14	-0.02	-0.49	-0.09
01500253	DIMETHADIONE	100122-05	F09	sample	695-53-4	C5H7NO3	129.11644	anticonvulsant	synthetic	USAN, INN		0.76	0.77	0.67	-0.64	0.39
01500255	DIOXYBENZONE	100122-05	F10	sample	131-53-3	C14H12O4	244.24934	ultraviolet screen	synthetic	USP, INN		0.78	-0.09	0.76	-1.33	0.03
01500256	DIPHENHYDRAMINE HYDROCHLORIDE	100122-05	F11	sample	147-24-0	C17H22ClNO	291.82399	antihistaminic	synthetic	USP, INN, BAN, JAN		0.77	0.15	0.31	-1.01	0.06
	0.04% DMSO	100122-05	F12	0.04% dmso								1.06	0.53	0.29	-1.38	0.12
	0.04% JAK2inhib	100122-05	G01	0.04% jak2inhib								-1.78	-1.48	-2.41	-1.37	-1.76
01500258	DIPHENYLPYRALINE HYDROCHLORIDE	100122-05	G02	sample	132-18-3 147-20-6	C19H24ClNO	317.86223	antihistaminic	synthetic	USP-XXI, INN, BAN, JAN		-0.48	-0.09	-0.70	-0.11	-0.35
01500259	DIPYRIDAMOLE	100122-05	G03	sample	58-32-2	C24H40N8O4	504.6376	coronary vasodilator	synthetic	USP, INN, BAN, JAN		0.10	-0.13	-1.83	-0.66	-0.63
01500260	PYRITHIONE ZINC	100122-05	G04	sample	13463-41-7	C10H10N2O2S2Zn	319.7014	antibacterial, antifungal, antiseborrheic	synthetic	USAN, INN, BAN		-2.57	-3.27	-4.17	-2.76	-3.19
01500261	DISOPYRAMIDE PHOSPHATE	100122-05	G05	sample	3737-09-5	C21H32N3O5P	437.48009	antiarrhythmic	synthetic	USP, INN, BAN, JAN		0.40	0.29	-0.61	0.79	0.22
01500262	DISULFIRAM	100122-05	G06	sample	97-77-8	C10H20N2S4	296.5403	alcohol antagonist	synthetic	USP, INN, BAN, JAN		-1.96	-3.75	-0.92	0.16	-1.62
01500263	DOPAMINE HYDROCHLORIDE	100122-05	G07	sample	62-31-7, 51-61-6 [dopamine]	C8H12ClNO2	189.64334	cardiotonic, antihypotensive	synthetic	USP, INN, BAN, JAN		-0.49	-0.07	0.71	-0.75	-0.15
01500264	DOXEPIN HYDROCHLORIDE	100122-05	G08	sample	1229-29-4, 1668-19-5	C19H22ClNO	315.84629	antidepressant	synthetic	USP, INN, BAN		-0.36	0.13	0.45	-1.13	-0.23
01500266	DOXYCYCLINE HYDROCHLORIDE	100122-05	G09	sample	17086-28-1, 564-25-0	C22H25ClN2O8	480.90615	antibacterial	semisynthetic; GS-3065	USP, INN, BAN		0.35	0.45	0.17	3.93	1.23
01500267	DOXYLAMINE SUCCINATE	100122-05	G10	sample	562-10-7, 469-21-6	C21H28N2O5	388.46771	antihistaminic, hypnotic	synthetic	USP, INN, BAN, JAN		0.49	-0.32	0.10	-0.59	-0.08
01500268	DYCLONINE HYDROCHLORIDE	100122-05	G11	sample	536-43-6, 586-60-7 [dyclonine]	C18H28ClNO2	325.88236	anesthetic (topical)	synthetic	USP, INN, BAN		-0.29	-0.19	0.50	0.04	0.01
	0.04% DMSO	100122-05	G12	0.04% dmso								0.71	-0.14	-0.16	0.05	0.12
	0.04% JAK2inhib	100122-05	H01	0.04% jak2inhib								-1.00	-2.40	-1.81	0.40	-1.20
01500269	DYPHYLLINE	100122-05	H02	sample	479-18-5	C10H14N4O4	254.24748	PDE inhibitor, bronchodilator, vasodilator	synthetic	USP, INN, BAN, JAN		-0.38	-0.52	-1.48	-0.62	-0.75
01500270	TRISODIUM ETHYLENEDIAMINE TETRACETATE	100122-05	H03	sample	150-38-9	C10H14N2Na3O8	361.21702	chelating agent, antioxidant	synthetic	USAN		-0.06	-0.03	-1.44	0.98	-0.14
01500272	EMETINE	100122-05	H04	sample	316-42-7, 483-18-1 [emetine]	C29H42Cl2N2O4	553.57509	inhibits RNA, DNA and protein synthesis	Uragoga ipecacuanha	USP, BAN	Nature 162: 524 (1948)	-4.57	-3.97	-5.54	-0.18	-3.57
01500274	ADRENALINE BITARTRATE	100122-05	H05	sample	51-42-3	C13H19NO9	333.29768	adrenergic agonist, bronchodilator, antiglaucoma agent	Portulaca grandiflora	USP, JAN		0.37	0.41	-0.17	0.05	0.17
01500275	EQUILIN	100122-05	H06	sample	474-86-2	C18H20O2	268.3589	estrogen	pregnant mare urine	USP		-0.31	0.27	0.71	3.53	1.05
01500276	ERGOCALCIFEROL	100122-05	H07	sample	50-14-6	C28H44O	396.66228	antirachitic vitamin; LD50 (rat) 56 mg/kg po	irradiation of ergosterol	USP, INN, BAN, JAN	Steroids 1959:90; Prog Chem Org Nat Prod 27:131 (1969)	-6.43	2.50	0.55	-0.40	-0.95
01500277	ERGONOVINE MALEATE	100122-05	H08	sample	129-51-1, 60-79-7 [ergonovine]	C23H27N3O6	441.48814	oxytocic, 5HT antagonist	ergot and Convolvulvaceae spp	USP, INN, BAN, JAN		-0.48	0.62	0.16	0.24	0.13
01500279	ERYTHROMYCIN ETHYLSUCCINATE	100122-05	H09	sample	1264-62-6, 114-07-8	C43H75NO16	862.0743	antibacterial	semisynthetic	USP, JAN		-2.89	-0.10	1.51	-0.40	-0.47
01500282	ESTRADIOL	100122-05	H10	sample	50-28-2	C18H24O2	272.39078	estrogen	pregnancy urine	USP, INN, BAN		0.60	-0.32	0.93	-0.09	0.28
01500283	ESTRADIOL CYPIONATE	100122-05	H11	sample	313-06-4	C26H36O3	396.57502	estrogen	semisynthetic	USP		-1.91	-0.22	0.07	-0.95	-0.76
	empty	100122-05	H12	sample								NA	NA	NA	NA	NA
	empty	100122-06	A01	sample								NA	NA	NA	NA	NA
01500284	ESTRADIOL VALERATE	100122-06	A02	sample	979-32-8	C23H32O3	356.50969	estrogen	semisynthetic	USP		0.22	0.69	1.01	-0.83	0.27
01500285	ESTRIOL	100122-06	A03	sample	50-27-1, 514-68-1 [as,	C18H24O3	288.39018	estrogen	mammalian hormone	USP, INN, BAN, JAN	JACS 76:2943 (1954); Biochem Prep 12:81 (1968); J	1.04	-0.84	-1.05	1.24	0.10
01500286	ESTRONE	100122-06	A04	sample	53-16-7	C18H22O2	270.37484	estrogen	pregnacy urine, dates and Punica granatum seeds	USP, INN, BAN		-0.39	-2.47	-1.79	-0.65	-1.32
01500287	ETHACRYNIC ACID	100122-06	A05	sample	58-54-8	C13H12Cl2O4	303.14419	diuretic	synthetic	USP, INN, BAN, JAN		0.23	-2.40	-0.51	-1.68	-1.09
01500288	ETHAMBUTOL HYDROCHLORIDE	100122-06	A06	sample	1070-11-7, 74-55-5	C10H24N2O2	277.23692	antibacterial (tuberculostatic)	synthetic	USP, INN, BAN, JAN		0.73	-0.56	0.11	-1.21	-0.23
01500291	ETHINYL ESTRADIOL	100122-06	A07	sample	57-63-6	C20H24O2	296.41308	estrogen, plus progestogen as oral contraceptive	semisynthetic	USP, INN, BAN, JAN		0.97	-2.10	-1.03	0.68	-0.71
01500292	ETHIONAMIDE	100122-06	A08	sample	536-33-4	C8H10N2S	166.2463	antibacterial, tuberculostatic	synthetic	USP, INN, BAN, JAN		-0.09	-1.20	-0.18	1.91	0.11
01500293	ETHOPROPAZINE HYDROCHLORIDE	100122-06	A09	sample	1094-08-2, 522-00-9	C19H25ClN2S	348.9415	antiparkinsonian, anticholinergic	synthetic	USP-XXIII, INN, BAN		0.90	-1.12	-0.18	1.42	0.25
01500295	EUCATROPINE HYDROCHLORIDE	100122-06	A10	sample	536-93-6, 100-91-4	C17H26ClNO3	327.85467	anticholinergic (opthalmic)	semisynthetic	USP, INN, BAN		1.55	-0.14	0.72	1.10	0.81
01500296	EUGENOL	100122-06	A11	sample	97-53-0	C10H12O2	164.20594	analgesic (topical), antiseptic, antifungal	common in plant essential oils	USP		1.51	0.13	0.45	0.25	0.58
	0.04% JAK2inhib	100122-06	A12	0.04% jak2inhib								0.63	-0.19	4.35	2.14	1.73
	0.04% DMSO	100122-06	B01	0.04% dmso								-3.15	-5.85	-3.30	5.34	-1.74
01500299	FLUDROCORTISONE ACETATE	100122-06	B02	sample	514-36-3, 127-31-1	C23H31FO6	422.49832	mineralocorticoid	semisynthetic	USP, INN, BAN, JAN		-2.15	-3.63	-1.82	-0.56	-2.04
01500300	FLUMETHAZONE PIVALATE	100122-06	B03	sample	2002-29-1, 2135-17-3	C27H36F2O6	494.58117	glucocorticoid, antiinflammatory	semisynthetic	USP, INN, BAN, JAN		-1.12	-2.38	-2.12	-0.31	-1.48
01500302	FLUOCINOLONE ACETONIDE	100122-06	B04	sample	67-73-2	C24H30F2O6	452.4999	glucocorticoid, antiinflammatory	semisynthetic	USP, INN, BAN, JAN		-0.56	-1.57	0.09	-1.32	-0.84
01500303	FLUOCINONIDE	100122-06	B05	sample	356-12-7	C28H32F2O7	494.53754	antiinflammatory, glucocorticoid	semisynthetic	USP, INN, BAN, JAN		-0.86	-0.89	0.09	-0.54	-0.55
01500304	FLUOROMETHOLONE	100122-06	B06	sample	426-13-1	C22H29FO4	376.47243	glucocorticoid, antiinflammatory	semisynthetic	USP, INN, BAN, JAN		0.28	-0.06	0.27	0.94	0.36
01500305	FLUOROURACIL	100122-06	B07	sample	51-21-8	C4H3FN2O2	130.07911	antineoplastic, pyrimidine antimetabolite	synthetic	USP, INN, BAN, JAN		-0.56	1.11	0.22	3.00	0.94
01500308	FLURBIPROFEN	100122-06	B08	sample	5104-49-4	C15H13FO2	244.26806	antiinflammatory, analgesic	synthetic	USP, INN, BAN, JAN		0.40	-0.29	-0.16	0.32	0.07
01500309	FURAZOLIDONE	100122-06	B09	sample	67-45-8	C8H7N3O5	225.16209	antibacterial	NF-180; synthetic	USP, INN, BAN		-1.84	-3.02	-3.21	-3.47	-2.88
01500310	FURESMIDE	100122-06	B10	sample	54-31-9	C12H11ClN2O5S	330.74887	diuretic, antihypertensive	synthetic	USP, INN, BAN, JAN		0.36	0.02	1.26	-0.28	0.34
01500311	FUSIDIC ACID	100122-06	B11	sample	6990-06-3	C31H48O6	516.72461	antibacterial	Fusidium spp	USAN, INN, BAN	Tetrahedron 21: 3505 (1965)	-0.97	0.61	-0.16	0.58	0.01
	0.04% JAK2inhib	100122-06	B12	0.04% jak2inhib								-0.74	-3.38	-0.72	-0.46	-1.33
	0.04% DMSO	100122-06	C01	0.04% dmso								-1.10	-3.87	-4.02	-1.81	-2.70
01500312	GALLAMINE TRIETHIODIDE	100122-06	C02	sample	65-29-2, 153-76-4 [gallamine]	C30H60I3N3O3	891.5442	muscle relaxant (skeletal)	synthetic	USP, INN		-0.58	-3.48	-3.54	-1.20	-2.20
01500313	GEMFIBROZIL	100122-06	C03	sample	25812-30-0	C15H22O3	250.34079	antihyperlipoproteinemic	synthetic	USP, INN, BAN		1.49	-2.41	-1.73	0.50	-0.54
01500314	GENTAMICIN SULFATE	100122-06	C04	sample	1405-41-0, 1403-66-3	C21H45N5O11S	575.6837	antibacterial	Micromonospora spp	USP, INN, BAN, JAN		-0.38	-0.35	2.60	0.58	0.61
01500315	GENTIAN VIOLET	100122-06	C05	sample	548-62-9	C25H30ClN3	407.99095	antibacterial, anthelmintic	synthetic	USP, INN, BAN, JAN		-3.58	-1.76	-1.73	-2.13	-2.30

Compound ID	MolNAME	plate	position	Content	cas#	Formula	MolWt	Bioactivity	Source	Status	Reference	Screen Score (z-score) rep1	rep2	rep3	rep4	Average
01500316	GLUCOSAMINE HYDROCHLORIDE	100122-06	C06	sample	3416-24-8	C6H14ClNO5	215.63518	antiarthritic	polysaccharides in bacteria, fungi, higher plants, invertebrates,	USAN, NF-XXI	Adv Carbohydr Chem 15:159 (1960); Methods Carbohydr	0.76	0.55	-0.38	0.58	0.38
01500319	GRAMICIDIN	100122-06	C07	sample	1405-97-6	C60H92N12O10	1141.47664	antibacterial	Bacillus brevis	USP		-2.65	-0.70	-1.74	-0.13	-1.30
01500321	GUAIFENESIN	100122-06	C08	sample	93-14-1	C10H14O4	198.22068	expectorant	synthetic	USP, INN, BAN, JAN		-0.81	0.37	0.28	0.31	0.04
01500322	GUANABENZ ACETATE	100122-06	C09	sample	23256-50-0	C10H12Cl2N4O2	291.13874	antihypertensive	synthetic	USP, JAN		2.04	1.89	1.46	0.74	1.53
01500323	GUANETHIDINE SULFATE	100122-06	C10	sample	60-02-6, 55-65-2	C10H24N4O4S	296.39118	antihypertensive, mitotic agent	synthetic	USP, INN, BAN		1.08	0.92	0.91	0.57	0.87
01500324	HALAZONE	100122-06	C11	sample	80-13-7	C7H5Cl2NO4S	270.0922	antiinfectant	synthetic	USP, INN		0.65	0.00	2.86	1.45	1.24
	0.11% JAK2inhib	100122-06	C12	0.11% jak2inhib								-1.45	-3.54	-2.08	-1.47	-2.14
	0.1% DMSO	100122-06	D01	0.1% dmso								-0.99	-0.12	3.81	0.93	0.91
01500325	HALOPERIDOL	100122-06	D02	sample	52-86-8	C21H23ClFNO2	375.87436	antidyskinetic, antipsychotic	synthetic	USP, INN, BAN, JAN		-1.75	-1.90	-0.97	-0.02	-1.16
01500327	HETACILLIN POTASSIUM	100122-06	D03	sample	5321-32-4, 3511-16-8	C19H22KN3O4S	427.57089	antibacterial	semisynthetic	USP-XIII, JAN		-0.47	-1.34	-0.58	4.54	0.54
01500328	HEXACHLOROPHENE	100122-06	D04	sample	70-30-4	C13H6Cl6O2	406.90957	antiinfective (topical)	synthetic	USP, INN, BAN		-0.31	1.10	1.92	0.45	0.79
01500330	HEXYLRESORCINOL	100122-06	D05	sample	136-77-6	C12H18O2	194.27606	anthelmintic, topical antiseptic	synthetic	USP, BAN		-0.12	1.34	-0.67	-0.23	0.08
01500331	HISTAMINE DIHYDROCHLORIDE	100122-06	D06	sample	51-45-6 [histamine]	C5H11Cl2N3	184.06952	H receptor agonist, induces edema in mammalian tissues; gastric	Claviceps purpurea, many plants and animals	USAN	JACS 40:1716 (1918); J Biol Chem 180:703 (1949);	0.13	0.66	2.16	-0.02	0.73
01500332	HOMATROPINE BROMIDE	100122-06	D07	sample	51-56-9, 87-00-3 [homatropine]	C16H22BrNO3	356.26264	anticholinergic (opthalmic)	semisynthetic	USP, JAN		0.24	1.02	0.58	1.17	0.75
01500333	HOMATROPINE METHYLBROMIDE	100122-06	D08	sample	80-49-9, 87-00-3 [homatropine]	C17H24BrNO3	370.28973	anticholinergic (opthalmic)	semisynthetic	USP, INN, BAN		0.02	0.80	0.80	0.70	0.58
01500334	HYDRALAZINE HYDROCHLORIDE	100122-06	D09	sample	304-20-1, 86-54-4 [hydralazine]	C8H9ClN4	196.64073	antihypertensive	semisynthetic	USP, INN, BAN		-1.47	-1.03	-0.18	-0.67	-0.84
01500335	HYDROCHLOROTHIAZIDE	100122-06	D10	sample	58-93-5	C7H8ClN3O4S2	297.74051	diuretic	semisynthetic	USP, INN, BAN, JAN		0.38	-0.47	1.40	0.93	0.56
01500338	HYDROCORTISONE ACETATE	100122-06	D11	sample	50-03-3	C23H32O6	404.50789	glucocorticoid, antiinflammatory	semisynthetic	USP, INN, BAN, JAN		1.59	-0.11	1.20	-0.45	0.56
	0.11% JAK2inhib	100122-06	D12	0.11% jak2inhib								-2.36	-3.85	-1.14	0.36	-1.75
	0.1% JAK2inhib	100122-06	E01	0.1% jak2inhib								2.17	0.94	-0.47	-2.11	0.13
01500339	HYDROCORTISONE HEMISUCCINATE	100122-06	E02	sample	83784-20-7, 2203-97-6	C25H34O8	462.54493	glucocorticoid	semisynthetic	USP, JAN		-1.89	0.45	-2.57	2.06	-0.49
01500340	HYDROCORTISONE PHOSPHATE TRIETHYLAMINE	100122-06	E03	sample	3863-59-0 [cortisol 21-	C33H61N2O8P	644.83652	glucocorticoid	semisynthetic	USP, INN, BAN, JAN		-0.60	2.37	-0.84	0.00	0.23
01500341	HYDROFLUMETHIAZIDE	100122-06	E04	sample	135-09-1	C8H8F3N3O4S2	331.29386	antihypertensive, diuretic	synthetic	USP, INN, BAN, JAN		0.12	0.20	-0.21	0.30	0.10
01500343	HYDROXYPROGESTERONE CAPROATE	100122-06	E05	sample	630-56-8, 68-96-2	C27H40O4	428.61745	progestogen	semisynthetic	USP, INN, JAN		0.01	0.38	-2.25	-1.38	-0.81
01500344	HYDROXYUREA	100122-06	E06	sample	127-07-1	CH4N2O2	76.05523	antineoplastic, inhibits ribonucleoside diphosphate reductase	synthetic	USP, INN, BAN		-4.05	-1.04	-2.79	1.43	-2.32
01500345	HYDROXYZINE PAMOATE	100122-06	E07	sample	10246-75-0, 68-88-2	C44H43ClN2O8	763.29491	anxiolytic, antihistaminic	synthetic	USP, JAN		-1.00	0.94	-0.93	-0.64	-0.41
01500346	HYOSCYAMINE	100122-06	E08	sample	101-31-5	C17H23NO3	289.37776	anticholinergic, analgesic	Atropa, Datura and Hyoscyamus spp	USP, BAN		-0.53	0.60	-1.02	0.25	-0.17
01500347	IBUPROFEN	100122-06	E09	sample	15687-27-1, 58560-75-1 [(+/-)	C13H18O2	206.28721	antiinflammatory	synthetic	USP, INN, BAN, JAN		1.04	0.77	0.23	0.16	0.55
01500348	IMIPRAMINE HYDROCHLORIDE	100122-06	E10	sample	113-52-0, 50-49-7 [imipramine]	C19H25ClN2	316.8775	antidepressant	synthetic	USP, INN, BAN, JAN		0.89	1.29	0.77	0.82	0.94
01500349	INDAPAMIDE	100122-06	E11	sample	26807-65-8	C16H16ClN3O3S	365.84122	diuretic, antihypertensive	synthetic	USP, INN, BAN, JAN		1.96	-0.32	2.31	0.77	1.18
	0.11% DMSO	100122-06	E12	0.11% dmso								0.18	1.70	0.01	0.61	0.63
	0.11% JAK2inhib	100122-06	F01	0.11% jak2inhib								-5.85	-2.47	-3.85	1.43	-2.68
01500350	INDOMETHACIN	100122-06	F02	sample	53-86-1	C19H16ClNO4	357.79667	antiinflammatory, antipyretic, analgesic	synthetic	USP, INN, BAN, JAN		-2.43	-1.95	-2.44	-0.85	-1.92
01500351	INDOPROFEN	100122-06	F03	sample	31842-01-0	C17H15NO3	281.314	analgesic, antiinflammatory	synthetic	USAN, INN, BAN		1.42	0.24	2.34	3.44	1.86
01500352	INOSITOL	100122-06	F04	sample	87-89-8	C6H12O6	180.15894	growth factor	synthetic	NF-XII		0.19	-0.44	0.39	0.00	0.03
01500353	IODOQUINOL	100122-06	F05	sample	83-73-8	C9H5I2NO	396.9551	antiamebic	synthetic	USP, INN, BAN		-0.69	1.17	4.21	0.15	1.21
01500354	IPRATROPIUM BROMIDE	100122-06	F06	sample	66985-17-9, 22254-24-6	C20H30BrNO3	412.371	bronchodilator, antiarrhythmic	synthetic	USAN, INN, BAN, JAN		-0.09	4.67	-0.61	0.21	1.04
01500355	ISONIAZID	100122-06	F07	sample	54-85-3	C6H7N3O	137.14219	antibacterial, tuberculostatic	synthetic	USP, INN, BAN, JAN		3.19	0.29	-0.36	-0.07	0.76
01500356	ISOPROPAMIDE IODIDE	100122-06	F08	sample	71-81-8, 7492-32-2	C23H33IN2O	480.43666	anticholinergic	synthetic	USP, INN, BAN, JAN		-0.22	1.85	2.15	-0.05	0.93
01500357	ISOPROTERENOL HYDROCHLORIDE	100122-06	F09	sample	51-30-9, 7683-59-2	C11H18ClNO3	247.72401	bronchodilator	synthetic	USP, INN, BAN, JAN		0.30	0.63	-0.09	-0.14	0.18
01500358	ISOSORBIDE DINITRATE	100122-06	F10	sample	87-33-2	C6H8N2O8	236.13926	antianginal	semisynthetic	USP, INN, BAN, JAN		1.59	1.33	2.85	1.75	1.88
01500359	ISOXSUPRINE HYDROCHLORIDE	100122-06	F11	sample	579-56-6, 395-28-8	C18H24ClNO3	337.84988	vasodilator	synthetic	USP, INN, BAN, JAN		2.33	1.25	2.47	2.12	2.04
	0.04% DMSO	100122-06	F12	0.04% dmso								1.07	-1.12	1.25	0.84	0.51
	0.04% JAK2inhib	100122-06	G01	0.04% jak2inhib								-4.74	-6.15	-3.45	-2.67	-4.25
01500360	KANAMYCIN A SULFATE	100122-06	G02	sample	25389-94-0, 133-92-6	C18H38N4O15S	582.58536	antibacterial	Streptomyces kanamyceticus	USP, INN, BAN, JAN		-0.01	-3.11	-2.16	-1.38	-1.66
01500362	KETOCONAZOLE	100122-06	G03	sample	65277-42-1	C26H28Cl2N4O4	531.44346	antifungal, PXR/SRC1 & CAR/SRC1 inhibitor	synthetic	USP, INN, BAN, JAN	Oncogene 26:258 (2007)	-2.23	-3.49	-3.16	-2.41	-2.82
01500363	LACTULOSE	100122-06	G04	sample	4618-18-2	C12H22O11	342.30254	laxative	synthetic	USP, INN, BAN, JAN		0.26	-0.48	-0.21	0.47	0.01
01500364	LEUCOVORIN CALCIUM	100122-06	G05	sample	1492-18-8	C20H21CaN7O7	511.51307	antianemic, antidote to folic acid antagonists	synthetic	USP, INN, BAN, JAN		-0.40	0.09	0.57	0.08	0.09
01500365	LEVONORDEFRIN	100122-06	G06	sample	829-74-3, 18829-78-2	C9H13NO3	183.20886	vasoconstrictor	synthetic	USP, INN		-0.18	0.89	0.55	0.10	0.34
01500368	LINCOMYCIN HYDROCHLORIDE	100122-06	G07	sample	7179-49-9, 859-18-7	C18H35ClN2O6S	443.00645	antibacterial	Streptomyces lincolnensis, S espinosus, S variabilis	USAN, INN, BAN		-0.13	0.70	0.38	0.39	0.34
01500379	MEDROXYPROGESTERONE ACETATE	100122-06	G08	sample	71-58-9, 520-85-4	C24H34O4	386.53618	contraceptive	semisynthetic	USP, INN, BAN, JAN		-1.23	0.00	-0.36	-0.74	-0.58
01500383	MEPENZOLATE BROMIDE	100122-06	G09	sample	76-90-4, 25990-43-6	C21H26BrNO3	420.35027	anticholinergic	synthetic	USP-XXIII, INN, BAN		1.05	0.32	0.26	-0.24	0.35
01500387	MERCAPTOPURINE	100122-06	G10	sample	6112-76-1, 50-44-2 [anhydrous]	C5H4N4S	152.17843	antineoplastic, purine antimetabolite	synthetic	USP, INN, BAN, JAN		1.57	0.92	0.22	-0.18	0.63
01500394	METHENAMINE	100122-06	G11	sample	100-97-0	C6H12N4	140.18934	antibacterial (urinary)	synthetic	USP, INN, JAN		1.71	2.36	0.87	1.18	1.53
	0.04% DMSO	100122-06	G12	0.04% dmso								1.57	-0.24	0.24	0.33	0.48
	0.04% JAK2inhib	100122-06	H01	0.04% jak2inhib								-4.33	-6.51	-3.76	-3.84	-4.61
01500395	METHICILLIN SODIUM	100122-06	H02	sample	7246-14-2, 132-92-3	C17H19N2NaO6S	402.40458	antibacterial	semisynthetic	USAN, INN, BAN, JAN		-1.89	-2.36	-1.34	-1.12	-1.68
01500400	METHOXSALEN	100122-06	H03	sample	298-81-7	C12H8O4	216.19516	antipsoriatic, pigmentation agent	amni visnaga	USP, BAN, JAN	Clin Pharmacol Therap 71:153 (2002)	-1.23	-0.70	1.79	-1.91	-0.51
01500404	METHYLERGONOVINE MALEATE	100122-06	H04	sample	57432-61-8, 7054-07-1	C24H29N3O6	455.51523	oxytocic	semisynthetic	USP, INN, BAN, JAN		-0.27	0.50	0.10	-1.05	-0.18
01500408	METHYLTHIOURACIL	100122-06	H05	sample	56-04-2	C5H6N2OS	142.18037	antithyroid agent	synthetic	USP-XXI, INN		-0.96	1.07	0.28	3.30	0.92
01500413	MICONAZOLE NITRATE	100122-06	H06	sample	22832-87-7, 22916-47-8	C18H15Cl4N3O4	479.14995	antifungal (topical)	synthetic	USP, JAN		1.01	-0.65	-1.00	1.97	0.33
01500427	NEOMYCIN SULFATE	100122-06	H07	sample	1405-10-3, 1404-04-2	C23H48N6O17S	712.73301	antibacterial	Streptomyces fradiae	USP, JAN		0.65	0.62	0.86	-0.10	0.51
01500434	NITROFURAZONE	100122-06	H08	sample	59-87-0	C6H6N4O4	198.13912	antiinfective (topical)	synthetic	USP, INN, BAN		-2.86	-0.79	-2.84	-3.01	-2.38
01500435	NITROMIDE	100122-06	H09	sample	121-81-3	C7H5N3O5	211.135	antibacterial, coccidiostat	synthetic	USAN		-0.54	-0.09	-2.39	-2.67	-1.42
01500438	NORETHINDRONE ACETATE	100122-06	H10	sample	51-98-9	C22H28O3	340.46666	oral contraceptive (in combination with estrogen)	synthetic	USP		0.35	-1.18	-1.32	-1.76	-0.98
01500450	OXIDOPAMINE HYDROCHLORIDE	100122-06	H11	sample	1199-18-4	C8H12ClNO3	205.64274	adrenergic agonist (opthalmic)	synthetic	USAN, INN		1.53	-0.86	0.71	-0.63	0.19
	empty	100122-06	H12	sample								NA	NA	NA	NA	NA
	empty	100122-07	A01	sample								NA	NA	NA	NA	NA
01500456	OXYQUINOLINE HEMISULFATE	100122-07	A02	sample	148-24-3	C9H9NO5S	243.23978	antiinfectant	synthetic	USAN		-0.70	-2.04	0.78	-1.21	-0.79
01500465	PENICILLIN G POTASSIUM	100122-07	A03	sample	69-57-8, 61-33-6 [penicillin, G]	C16H17KN2O4S	372.49089	antibacterial	Penicillium spp	USP, BAN, JAN		-0.18	-1.70	1.17	4.06	0.84
01500467	PENICILLIN V POTASSIUM	100122-07	A04	sample	132-98-9, 87-08-1 [penicillin, V]	C16H17KN2O5S	388.49029	antibacterial	semisynthetic	USP, JAN		-1.06	-1.77	-0.76	-1.99	-1.39
01500480	PHENOLPHTHALEIN	100122-07	A05	sample	77-09-8	C20H14O4	318.33218	cathartic	synthetic	USP-XXIII		0.61	-0.30	0.17	2.04	0.63
01500483	PHENYLEPHRINE HYDROCHLORIDE	100122-07	A06	sample	61-76-7, 59-42-7	C9H14ClNO2	203.67043	mydriatic, decongestant	synthetic	USP, INN, BAN, JAN		-0.17	-0.23	-0.53	-0.55	-0.37
01500484	PHENYLPROPANOLAMINE HYDROCHLORIDE	100122-07	A07	sample	154-41-6	C9H14ClNO	187.67103	vasoconstrictor, decongestant, anorexic	synthetic	USP, INN, BAN		0.06	0.42	-0.41	0.03	0.02
01500486	PHYSOSTIGMINE SALICYLATE	100122-07	A08	sample	57-64-7, 57-47-6	C22H27N3O5	413.47759	cholinergic, anticholinesterase, miotic	Physostigma venenosum	USP, JAN	J Chem Soc 1954: 3651	-0.06	0.87	0.93	-0.18	0.39
01500487	PILOCARPINE NITRATE	100122-07	A09	sample	148-72-1, 92-13-7 [pilocarpine]	C11H17N3O5	271.27524	antiglaucoma agent, miotic	Pilocarpus spp	USP		2.48	3.64	-0.67	2.39	1.96
01500488	PINDOLOL	100122-07	A10	sample	13523-86-9	C14H20N2O2	248.3277	antihypertensive, antianginal, antiarrhythmic, antiglaucoma agent	synthetic	USP, INN, BAN, JAN		1.15	-0.40	0.06	0.38	0.30
01500489	PIPERACILLIN SODIUM	100122-07	A11	sample	59703-84-3, 66258-76-2	C23H26N5NaO7S	539.54677	antibacterial	semisynthetic	USP, INN, BAN, JAN		2.46	1.93	0.65	-1.17	0.97
	0.04% JAK2inhib	100122-07	A12	0.04% jak2inhib								-0.69	-1.89	-1.64	-2.10	-1.58
	0.04% DMSO	100122-07	B01	0.04% dmso								-0.89	-2.06	0.81	-2.54	-1.17
01500490	PIPERAZINE	100122-07	B02	sample	110-85-0, 144-29-6	C4H10N2	86.1377	anthelmintic	synthetic	USP		-1.23	-1.41	-0.57	-0.59	-0.95
01500491	PIROXICAM	100122-07	B03	sample	36322-90-4	C15H13N3O4S	331.35256	antiinflammatory	synthetic	USP, INN, BAN, JAN		-0.44	-1.19	0.18	1.29	-0.04
01500492	POLYMYXIN B SULFATE	100122-07	B04	sample	1405-20-5, 1404-26-8	C56H100N16O17S	1301.5824	antibacterial	Bacillus polymyxa	USP, INN, BAN, JAN		0.41	-0.80	-0.29	-0.65	-0.33
01500494	PRAZIQUANTEL	100122-07	B05	sample	55268-74-1	C19H24N2O2	312.41533	anthelmintic	synthetic	USP, INN, BAN, JAN		-0.29	-0.87	0.09	-0.15	-0.30
01500495	PRAZOSIN HYDROCHLORIDE	100122-07	B06	sample	19237-84-4, 19216-56-9	C19H22ClN5O4	419.87129	antihypertensive	synthetic	USP, INN, BAN, JAN		-0.51	2.10	3.01	-0.90	0.92
01500496	PREDNISOLONE	100122-07	B07	sample	50-24-8 [anhydrous], 52438-85-	C21H28O5	360.45431	glucocorticoid	semisynthetic	USP, INN, BAN, JAN		0.30	0.45	1.29	1.53	0.89
01500497	PREDNISOLONE ACETATE	100122-07	B08	sample	52-21-1	C23H30O6	402.49195	glucocorticoid	semisynthetic	USP, JAN		0.27	0.35	-0.81	-0.07	-0.06
01500499	PREDNISONE	100122-07	B09	sample	53-03-2	C21H26O5	358.43837	glucocorticoid	semisynthetic	USP, INN, BAN		1.11	0.11	0.76	-0.30	0.42
01500500	PRIMAQUINE DIPHOSPHATE	100122-07	B10	sample	63-45-6, 90-34-6 [primaquine]	C15H27N3O9P2	455.34474	antimalarial	synthetic	USP, INN, BAN		1.13	2.77	-0.39	-0.18	0.83
01500501	PRIMIDONE	100122-07	B11	sample	125-33-7	C12H14N2O2	218.25758	anticonvulsant	synthetic	USP, INN, BAN, JAN		1.05	-0.01	0.72	0.57	0.58
	0.04% JAK2inhib	100122-07	B12	0.04% jak2inhib								-0.63	-1.03	-1.10	-1.01	-0.94
	0.04% DMSO	100122-07	C01	0.04% dmso								-1.81	1.97	3.34	-1.76	0.43
01500502	PROBENECID	100122-07	C02	sample	57-66-9	C13H19NO4S	285.36468	uricosuric	synthetic	USP, INN, BAN, JAN		-0.53	0.30	0.89	-0.50	0.04
01500503	PROCAINAMIDE HYDROCHLORIDE	100122-07	C03	sample	614-39-1, 51-06-9	C13H22ClN3O	271.79279	antiarrhythmic	synthetic	USP, INN, BAN, JAN		-0.77	0.06	-0.03	-0.72	-0.36
01500504	PROCAINE HYDROCHLORIDE	100122-07	C04	sample	51-05-8, 59-46-1 [procaine]	C13H21ClN2O2	272.77752	anesthetic (local)	synthetic	USP, JAN		-0.30	-0.91	1.35	0.21	0.09
01500505	PROCHLORPERAZINE EDISYLATE	100122-07	C05	sample	1257-78-9, 84-02-6	C22H30ClN3O6S3	564.1459	antiemetic, antipsychotic, treatment of vertigo	synthetic	USP, JAN		-0.28	-0.91	-0.62	-1.18	-0.75
01500507	PROCYCLIDINE HYDROCHLORIDE	100122-07	C06	sample	1508-76-5, 77-37-2	C19H30ClNO	323.91005	anticholinergic	synthetic	USP, INN, BAN		-1.46	-0.49	0.96	-0.82	-0.45
01500509	PROMAZINE HYDROCHLORIDE	100122-07	C07	sample	53-60-1, 58-40-2 [promazine]	C17H21ClN2S	320.88732	antipsychotic	synthetic	USP, INN, BAN		-0.24	0.55	-0.38	-0.29	-0.09
01500511	PROPANTHELINE BROMIDE	100122-07	C08	sample	50-34-0, 298-50-0	C23H30BrNO3	448.40445	anticholinergic	synthetic	USP, INN, BAN, JAN		-0.48	-0.04	2.76	0.52	0.69
01500514	DEXPROPRANOLOL HYDROCHLORIDE	100122-07	C09	sample	13071-11-9	C16H22ClNO2	295.81224	antihypertensive, antianginal, antiarrhythmic	synthetic	USAN, INN, BAN		-0.11	-0.85	-1.00	0.09	-0.47
01500515	PROPYLTHIOURACIL	100122-07	C10	sample	51-52-5	C7H10N2OS	170.23455	antihyperthyroid	synthetic	USP, INN, BAN, JAN		0.70	-0.20	-0.02	-0.06	0.10
01500516	PSEUDOEPHEDRINE HYDROCHLORIDE	100122-07	C11	sample	345-78-8, 90-82-4	C10H16ClNO	201.69812	decongestant	synthetic	USP, INN, BAN		3.13	0.47	3.59	0.08	1.81
	0.11% JAK2inhib	100122-07	C12	0.11% jak2inhib								-0.59	-4.34	0.83	-2.25	-1.59
	0.11% DMSO	100122-07	D01	0.11% dmso								-1.27	-1.42	-0.50	-2.56	-1.44
01500517	PYRANTEL PAMOATE	100122-07	D02	sample	22204-24-6, 15686-83-6	C34H30N2O6S	594.692	anthelmintic	synthetic	USP, INN, BAN, JAN		0.14	-0.11	0.55	-1.47	-0.22
01500518	PYRAZINAMIDE	100122-07	D03	sample	98-96-4	C5H5N3O	123.1151	antibacterial, tuberculostatic	synthetic	USP, INN, BAN, JAN		-1.24	-0.74	0.40	-0.58	-0.54
01500519	PYRILAMINE MALEATE	100122-07	D04	sample	59-33-6, 91-84-9 [pyrilamine]	C21H27N3O5	401.46644	antihistaminic	synthetic	USP, INN, BAN		0.61	-0.71	0.29	-0.50	-0.08
01500520	PYRIMETHAMINE	100122-07	D05	sample	58-14-0	C12H13ClN4	248.71721	antimalarial	synthetic	USP, INN, BAN, JAN		0.49	-0.41	-0.73	0.13	-0.13
01500521	PYRVINIUM PAMOATE	100122-07	D06	sample	3546-41-6	C49H43N3O6	769.90556	anthelmintic	synthetic	USP, BAN, JAN		-1.96	-1.34	0.15	0.68	-0.62
01500522	QUINACRINE HYDROCHLORIDE	100122-07	D07	sample	6151-30-0, 69-05-6	C23H32Cl3N3O	472.88999	antihelmintic, antimalarial, intercalating agent	synthetic	USP-XXII, INN, BAN		2.72	1.99	1.94	2.47	2.28
01500523	QUINIDINE GLUCONATE	100122-07	D08	sample	7054-25-3, 6591-63-5	C28H36N2O9	520.58482	antiarrhythmic, antimalarial	Cinchona spp	USP		2.70	-0.42	0.17	0.73	0.55
01500524	QUININE SULFATE	100122-07	D09	sample	6119-70-6, 804-63-7	C20H26N2O6S	422.50402	antimalarial, skeletal muscle relaxant	Cinchona spp	USP, JAN		0.94	0.01	-1.11	-0.03	-0.05
01500525	RACEPHEDRINE HYDROCHLORIDE	100122-07	D10	sample	134-71-4, 90-81-3	C10H16ClNO	201.69812	bronchodilator, decongestant	synthetic	USAN, INN, BAN		0.96	1.06	0.99	0.48	0.87
01500526	RESERPINE	100122-07	D11	sample	50-55-5	C33H40N2O9	608.69475	antihypertensive	Rauwolfia serpentina	USP, INN, BAN, JAN		0.48	-1.02	-1.07	0.15	-0.36
	0.11% JAK2inhib	100122-07	D12	0.11% jak2inhib								-0.34	-4.28	-0.33	-2.11	-1.77
	0.1% JAK2inhib	100122-07	E01	0.1% jak2inhib								-4.34	-4.99	-2.34	-2.64	-3.58
01500527	RESORCINOL	100122-07	E02	sample	108-46-3	C6H6O2	110.11352	keratolytic, antiseborheic	coal tar	USP, JAN		-0.98	-1.66	0.14	-1.13	-0.91
01500529	RIFAMPIN	100122-07	E03	sample	13292-46-1	C43H58N4O12	822.96131	antibacterial (tuberculostatic)	semisynthetic; L-5103, Ba-41166/E, NSC-113926	USP, INN, BAN, JAN		0.40	0.29	0.44	1.36	0.62
01500530	ROXARSONE	100122-07	E04	sample	121-19-7	C6H6AsNO6	263.03942	antibacterial	synthetic	USP, INN, BAN		-0.25	0.05	1.70	-0.23	0.32
01500531	SALICYL ALCOHOL	100122-07	E05	sample	90-01-7	C7H8O2	124.14061	anesthetic (local), antiinflammatory	Populus sieboldii	USAN	J Med Chem 13:957 (1970); Chem Pharm Bull 40:2191	-0.54	0.13	-0.13	-0.42	-0.24
01500532	SALICYLAMIDE	100122-07	E06	sample	65-45-2	C7H7NO2	137.13934	analgesic	synthetic	USP, INN, BAN, JAN		0.95	0.25	-0.28	1.71	0.66
01500533	SODIUM SALICYLATE	100122-07	E07	sample	54-21-7	C7H5NaO3	160.1059	keratolytic	synthetic	USP, JAN		-1.17	-0.42	-0.51	0.41	-0.42
01500536	SISOMICIN SULFATE	100122-07	E08	sample	53179-09-2, 32385-11-8	C19H39N5O11S	545.61358	antibacterial, binds to ribosomes	Micromonospora myoensis	USP, BAN, JAN		1.24	1.64	-0.28	1.36	0.99
01500538	SPECTINOMYCIN HYDROCHLORIDE	100122-07	E09	sample	22189-32-8, 21736-83-4	C14H26Cl2N2O7	405.27852	antibacterial	Streptomyces spectabilis	USP, INN, BAN, JAN		-0.10	0.37	-0.32	4.34	1.07
01500539	SPIRONOLACTONE	100122-07	E10	sample	52-01-7	C24H32O4S	416.58424	diuretic	synthetic	USP, INN, BAN, JAN		1.57	-0.73	-0.56	0.58	0.21
01500541	STREPTOMYCIN SULFATE	100122-07	E11	sample	3810-74-0, 57-92-1	C21H41N7O16S	679.66222	antibacterial (tuberculostatic)	Streptomyces griseus	USP, INN, BAN, JAN		0.75	0.35	-0.25	5.27	1.53
	0.11% DMSO	100122-07	E12	0.11% dmso								0.44	-1.38	-0.50	2.32	0.22
	0.11% JAK2inhib	100122-07	F01	0.11% jak2inhib								-3.73	-3.33	-2.21	-4.24	-3.37

Compound ID	MolNAME	plate	position	Content	cas#	Formula	MolWt	Bioactivity	Source	Status	Reference	Screen Score (z-score) rep1	rep2	rep3	rep4	Average
01500543	STREPTOZOSIN	100122-07	F02	sample	18883-66-4	C8H15N3O7	265.22465	antineoplastic, alkylating agent	synthetic	USAN, INN		-1.15	-1.25	-0.03	-1.23	-0.91
01500544	SULFABENZAMIDE	100122-07	F03	sample	127-71-9	C13H12N2O3S	276.31619	antibacterial	synthetic	USP, INN, BAN		0.69	-0.15	0.02	5.87	1.61
01500545	SULFACETAMIDE	100122-07	F04	sample	144-80-9, 127-56-0	C8H10N2O3S	214.2445	antibacterial	synthetic	USP, INN, BAN		-0.30	0.76	1.28	-0.41	0.33
01500546	SULFADIAZINE	100122-07	F05	sample	68-35-9	C10H10N4O2S	250.2808	antibacterial	synthetic	USP, INN, BAN, JAN		1.58	0.59	-0.51	-0.22	0.36
01500547	SULFAMERAZINE	100122-07	F06	sample	127-79-7	C11H12N4O2S	264.30789	antibacterial	synthetic	USP-XXIII, INN, BAN		0.89	0.59	-0.24	5.24	1.62
01500548	SULFAMETHAZINE	100122-07	F07	sample	57-68-1	C12H14N4O2S	278.33498	antibacterial	synthetic	USP, INN, BAN		-1.62	0.73	-0.89	-0.59	-0.59
01500549	SULFAMETHIZOLE	100122-07	F08	sample	144-82-1	C9H10N4O2S2	270.33365	antibacterial	synthetic	USP, INN, BAN, JAN		-0.82	0.48	0.72	1.86	0.56
01500550	SULFAMETHOXAZOLE	100122-07	F09	sample	723-46-6	C10H11N3O3S	253.28147	antibacterial, antipneumocystis	synthetic	USP, INN, BAN, JAN		0.66	-0.11	2.69	1.30	1.14
01500551	SULFAPYRIDINE	100122-07	F10	sample	144-83-2	C11H11N3O2S	249.29322	antibacterial	synthetic	USP, INN, BAN		1.41	0.29	1.69	0.31	0.92
01500552	SULFASALAZINE	100122-07	F11	sample	599-79-1	C18H14N4O5S	398.40008	anticolitis and Crohn's disease	synthetic	USP, INN, BAN		1.24	0.49	-0.87	-0.29	0.14
	0.04% DMSO	100122-07	F12	0.04% dmso								0.18	-0.25	-0.31	-0.01	-0.10
	0.04% JAK2inhib	100122-07	G01	0.04% jak2inhib								-3.03	-2.72	-0.83	-3.50	-2.52
01500553	SULFATHIAZOLE	100122-07	G02	sample	72-14-0	C9H9N3O2S2	255.31898	antibacterial	synthetic	USP, INN, BAN		-0.80	-1.64	-0.56	-0.69	-0.93
01500554	SULFINPYRAZONE	100122-07	G03	sample	57-96-5	C23H20N2O3S	404.49145	uricosuric	synthetic	USP, INN, BAN, JAN		-0.65	0.29	0.88	-0.51	0.00
01500555	SULFISOXAZOLE	100122-07	G04	sample	127-69-5	C11H13N3O3S	267.30856	antibacterial	synthetic	USP, INN, BAN, JAN		-1.36	-0.96	-0.35	-0.24	-0.73
01500556	SULINDAC	100122-07	G05	sample	38194-50-2	C20H17FO3S	356.41909	antiinflammatory	synthetic	USP, INN, BAN, JAN		-1.53	-0.21	-0.76	-0.41	-0.73
01500557	TAMOXIFEN CITRATE	100122-07	G06	sample	54965-24-1, 10540-29-1	C32H37NO8	563.65359	estrogen antagonist, antineoplastic	synthetic	USP, INN, BAN, JAN		0.53	0.54	0.16	1.21	0.61
01500558	TERBUTALINE HEMISULFATE	100122-07	G07	sample	23031-32-5, 23031-25-6	C12H21NO7S	323.36767	betaadrenergic agonist, bronchodilator	synthetic	USP, INN, BAN, JAN		-0.31	4.48	0.76	-0.06	1.22
01500564	TETRACAINE HYDROCHLORIDE	100122-07	G08	sample	136-47-0, 94-24-6 [tetracaine]	C15H25ClN2O2	300.8317	anesthetic (local)	synthetic	USP, BAN, JAN		-0.73	0.94	-0.60	1.23	0.21
01500566	TETRACYCLINE HYDROCHLORIDE	100122-07	G09	sample	64-75-5, 60-54-8 [tetracycline]	C22H25ClN2O8	480.90615	antibacterial, antiamebic, antirickettsial	Streptomyces spp	USP, INN, BAN, JAN		0.28	-0.38	-0.26	1.30	0.23
01500567	TETRAHYDROZOLINE HYDROCHLORIDE	100122-07	G10	sample	522-48-5, 84-22-0	C13H17ClN2	236.74684	adrenergic agonist, nasal decongestant	synthetic	USP, INN, BAN, JAN		0.35	-1.00	-0.88	0.67	-0.21
01500570	THIABENDAZOLE	100122-07	G11	sample	148-79-8	C10H7N3S	201.25139	anthelmintic	synthetic	USP, INN, BAN, JAN		1.89	3.90	2.31	1.85	2.49
	0.04% DMSO	100122-07	G12	0.04% dmso								0.39	2.25	-0.93	0.11	0.45
	0.04% JAK2inhib	100122-07	H01	0.04% jak2inhib								-0.71	-3.94	-2.27	-4.12	-2.76
01500572	THIMEROSAL	100122-07	H02	sample	54-64-8	C9H9HgNaO2S	404.81468	antiinfective, preservative	synthetic	USP, INN, BAN, JAN		-8.47	-6.08	-6.93	-7.86	-7.34
01500573	THIOGUANINE	100122-07	H03	sample	154-42-7, 5580-03-0	C5H5N5S	167.1931	antineoplastic, purine antimetabolite	synthetic	USP, INN, BAN		-0.44	-0.56	-0.66	-0.04	-0.42
01500575	THIORIDAZINE HYDROCHLORIDE	100122-07	H04	sample	130-61-0, 50-52-2 [thioridazine]	C21H27ClN2S2	407.04374	antipsychotic	synthetic	USP, INN, BAN		-1.98	-1.90	-0.89	3.75	-0.26
01500576	THIOTHIXENE	100122-07	H05	sample	5591-45-7, 3313-26-6 [//Z//]	C23H29N3O2S2	443.63448	antipsychotic	synthetic	USP, INN, BAN, JAN		-5.29	-4.29	-3.73	-4.77	-4.52
01500578	TIMOLOL MALEATE	100122-07	H06	sample	26921-17-5, 91524-16-2	C17H28N4O7S	432.49931	betaadrenergic blocker	synthetic	USP, JAN		-0.98	3.73	-0.23	0.12	0.66
01500579	TOBRAMYCIN	100122-07	H07	sample	32986-56-4	C18H37N5O9	467.52369	antibacterial, inhibits protein synthesis	Streptomyces spp	USP, INN, BAN, JAN		-0.30	0.34	0.75	0.70	0.37
01500580	TOLAZOLINE HYDROCHLORIDE	100122-07	H08	sample	59-97-2, 59-98-3 [tolazoline]	C10H13ClN2	196.68151	adrenergic blocker	synthetic	USP, INN, BAN, JAN		0.59	-0.36	-0.13	1.19	0.32
01500581	TOLBUTAMIDE	100122-07	H09	sample	64-77-7	C12H18N2O3S	270.35286	antidiabetic	synthetic	USP, INN, BAN, JAN		1.08	1.25	0.14	0.74	0.80
01500584	TRANYLCYPROMINE SULFATE	100122-07	H10	sample	13492-01-8, 7081-36-9	C9H13NO4S	231.27226	antidepressant, MAO inhibitor	synthetic	USP-XXI, INN, BAN	Arch Pharmacol Res 10: 50 (1987)	0.20	0.19	0.65	-0.03	0.25
01500585	TRIACETIN	100122-07	H11	sample	102-76-1	C9H14O6	218.20833	antifungal (topical)	synthetic	USP, INN, BAN		0.35	0.27	0.40	0.31	0.33
	empty	100122-07	H12	sample								NA	NA	NA	NA	NA
	empty	100122-08	A01	sample								NA	NA	NA	NA	NA
01500586	TRIAMCINOLONE	100122-08	A02	sample	124-94-7	C21H27FO6	394.44414	glucocorticoid	semisynthetic	USP, INN, BAN, JAN		-1.09	-1.50	-1.06	-2.44	-1.52
01500587	TRIAMCINOLONE ACETONIDE	100122-08	A03	sample	76-25-5	C24H31FO6	434.50947	antiinflammatory	semisynthetic	USP, INN, BAN, JAN		-0.18	-0.72	0.79	1.46	0.34
01500588	TRIAMCINOLONE DIACETATE	100122-08	A04	sample	67-78-7	C25H31FO8	478.51942	antiinflammatory	semisynthetic	USP, JAN		-0.67	-1.57	-0.70	-1.38	-1.08
01500589	TRIAMTERENE	100122-08	A05	sample	396-01-0	C12H11N7	253.26837	antihypertensive	semisynthetic	USP, INN, BAN, JAN		-1.34	-1.00	-0.24	-0.89	-0.87
01500590	TRICHLORMETHIAZIDE	100122-08	A06	sample	133-67-5	C8H8Cl3N3O4S2	380.65766	diuretic, antihypertensive	synthetic	USP, INN, JAN		-0.08	-1.80	-0.90	-0.66	-0.86
01500591	TRIFLUOPERAZINE HYDROCHLORIDE	100122-08	A07	sample	440-17-5, 117-89-5	C21H26Cl2F3N3S	480.42667	antipsychotic	synthetic	USP, INN, BAN, JAN		0.21	-1.11	0.34	0.02	-0.14
01500592	TRIHEXYPHENIDYL HYDROCHLORIDE	100122-08	A08	sample	52-49-3	C20H32ClNO	337.93714	anticholinergic, antiparkinsonian	synthetic	USP, INN, BAN, JAN		0.21	-1.29	-1.14	0.18	-0.51
01500593	TRIMEPRAZINE TARTRATE	100122-08	A09	sample	4330-99-8, 41375-66-0	C22H28N2O6S	448.54226	antipruritic	synthetic	USP, INN, BAN, JAN		0.36	-0.75	-1.45	-0.45	-0.58
01500595	TRIMETHOPRIM	100122-08	A10	sample	738-70-5	C14H18N4O3	290.32456	antibacterial	synthetic	USP, INN, BAN, JAN		0.29	3.54	-0.24	4.47	2.02
01500596	TRIOXSALEN	100122-08	A11	sample	3902-71-4	C14H12O3	228.24994	melanizing agent, antipsoriatic	synthetic	USP, INN, JAN		0.67	-1.92	-1.07	-1.14	-0.87
	0.04% JAK2inhib	100122-08	A12	0.04% jak2inhib								-1.02	-2.28	-1.65	-2.89	-1.96
	0.04% DMSO	100122-08	B01	0.04% dmso								-1.79	-0.98	-0.28	1.23	-0.45
01500597	TRIPELENNAMINE CITRATE	100122-08	B02	sample	6138-56-3, 91-81-6	C22H29N3O7	447.49233	antihistaminic	synthetic	USP, BAN		-1.15	-0.50	-0.27	-0.40	-0.58
01500598	TRIPROLIDINE HYDROCHLORIDE	100122-08	B03	sample	6138-79-0, 550-70-9	C19H23ClN2	314.86156	antihistaminic	synthetic	USP, INN, BAN, JAN		0.26	0.06	-0.30	0.93	0.24
01500599	TROPICAMIDE	100122-08	B04	sample	1508-75-4	C17H20N2O2	284.36115	anticholinergic (opthalmic)	synthetic	USP, INN, BAN, JAN		0.18	0.64	0.67	0.50	0.50
01500600	TRYPTOPHAN	100122-08	B05	sample	73-22-3 ['L']	C11H12N2O2	204.23049	antidepressant, nutrient; LD50(rat) 1634 mg/kg ip	many plants, animal protein	USP, INN, JAN	Biochem J 29:2256 (1935); JACS 67:36 (1945); Aust J	0.04	-0.66	-0.70	-0.04	-0.34
01500601	TUAMINOHEPTANE SULFATE	100122-08	B06	sample	6411-75-2, 123-82-0	C7H19NO4S	213.29778	adrenergic agonist	synthetic	USP-XX		-0.39	3.30	0.00	-0.49	0.61
01500603	TYROTHRICIN	100122-08	B07	sample	1404-88-2	C66H85N11O15	1272.47805	topical antibacterial (topical)	Bacillus aneurinolyticus; mixture of gramicidins & tyrocidines	USP, INN, BAN		-0.27	-1.02	-1.11	0.03	-0.59
01500604	UREA	100122-08	B08	sample	57-13-6	CH4N2O	60.05583	diuretic	synthetic	USP, JAN		0.09	-0.17	0.00	-0.02	-0.03
01500605	URSODIOL	100122-08	B09	sample	128-13-2	C24H40O4	392.584	anticholelithogenic; LD50(rat) 890 mg/kg ip	bear bile	USP, INN, BAN, JAN	Hoppe Seyler's Z Physiol Chem 244:181 (1936); Drugs	-11.01	-4.11	-1.54	-0.62	-4.32
01500606	VALPROATE SODIUM	100122-08	B10	sample	1069-66-5, 99-66-1 [valproic	C8H15NaO2	166.19735	anticonvulsant	synthetic	USAN, JAN		-2.27	-0.35	-0.73	-1.14	-1.12
01500607	VANCOMYCIN HYDROCHLORIDE	100122-08	B11	sample	1404-93-9, 1404-90-6	C67H77Cl3N8O24	1484.75894	antibacterial	Streptomyces orientalis	USP, INN, BAN, JAN		0.74	-0.01	0.40	1.86	0.75
	0.04% JAK2inhib	100122-08	B12	0.04% jak2inhib								0.07	-2.46	-1.57	-3.50	-1.87
	0.04% DMSO	100122-08	C01	0.04% dmso								1.92	-0.41	-1.19	-1.96	-0.41
01500609	VIDARABINE	100122-08	C02	sample	24356-66-9, 5536-17-4	C10H13N5O4	267.24621	antiviral	synthetic	USP, INN, BAN, JAN		-1.08	-0.29	-1.01	-1.11	-0.87
01500613	WARFARIN	100122-08	C03	sample	81-81-2, 2610-86-8 [warfarin	C19H16O4	308.33697	anticoagulant, rodenticide	synthetic	USP, INN, BAN, JAN	Pharmacol Res Commun 10:445 (1978); Chest 102:312S	0.47	-0.64	-0.59	-0.64	-0.35
01500614	XYLOMETAZOLINE HYDROCHLORIDE	100122-08	C04	sample	1218-35-5, 526-36-3	C16H25ClN2	280.84405	adrenergic agonist, nasal decongestant	synthetic	USP, INN, BAN		-1.12	0.09	0.07	-0.85	-0.45
01500616	ACETARSOL	100122-08	C05	sample	97-44-9	C8H10AsNO5	275.0942	antiprotozoal; diethylamine salt as antiphilitic	synthetic	NF, INN, BAN		-0.76	1.42	0.59	0.01	0.31
01500637	MERBROMIN	100122-08	C06	sample	129-16-8	C20H8Br2HgNa2O6	750.66076	antibacterial	synthetic	NF-XII, INN, BAN		0.33	0.81	0.24	-0.04	0.34
01500642	PHENACETIN	100122-08	C07	sample	62-44-2	C10H13NO2	179.22061	analgesic, antipyretic	synthetic	USP-XX, INN, BAN		0.93	0.01	0.01	-0.80	0.04
01500644	PHENYLMERCURIC ACETATE	100122-08	C08	sample	62-38-4	C8H8HgO2	336.74176	antifungal	synthetic	USAN, NF		2.99	-1.00	0.19	0.47	0.66
01500646	SULFANILAMIDE	100122-08	C09	sample	63-74-1	C6H8N2O2S	172.20686	antibacterial	synthetic	NF-XI, INN		0.70	-0.46	-0.41	-0.62	-0.20
01500648	AZELAIC ACID	100122-08	C10	sample	123-99-9	C9H16O4	188.22547	antiacne, antiproliferative agent	rancid fats and Lycopodium spp	USAN, INN		1.21	0.14	0.32	5.59	1.81
01500643	PHENETHICILLIN POTASSIUM	100122-08	C11	sample	132-93-4, 147-55-7	C17H19KN2O5S	402.51738	antibacterial	semisynthetic	USP-XX, INN, BAN, JAN		1.46	-1.83	-1.38	1.66	-0.02
	0.11% JAK2inhib	100122-08	C12	0.11% jak2inhib								-1.81	-2.40	-2.95	-2.20	-2.34
	0.11% DMSO	100122-08	D01	0.11% dmso								-1.37	-0.78	-0.80	-2.60	-1.39
01500649	THEOBROMINE	100122-08	D02	sample	83-67-0	C7H8N4O2	180.16741	diuretic, bronchodilator, cardiotonic	Camellia, Theobroma, Cola spp	NF-XII, BAN		2.03	0.16	1.42	-1.21	0.60
01500651	STRYCHNINE	100122-08	D03	sample	57-24-9	C21H22N2O2	334.42169	central stimulant	Strychnos nux-vomica and other Strychnos spp	NF-X		-1.35	-0.56	-1.39	-0.92	-1.05
01500655	ACONITINE	100122-08	D04	sample	302-27-2	C34H47NO11	645.75379	anesthetic (gastric), antipyretic, and cardiotoxin	Aconitum spp	USP-X, BP-1934	Neuropharmacol 34: 1139 (1995); Biochem Pharmacol 55:	0.65	0.31	3.11	0.39	1.12
01500663	YOHIMBINE HYDROCHLORIDE	100122-08	D05	sample	65-19-0	C21H27ClN2O3	390.91394	alpha adrenergic blocker, mydriatic, antidepressant	Corynanthe spp	USP	J Chem Soc 1950: 1534; Alkaloids 2: 406 (1952);	-0.13	0.35	1.14	1.04	0.60
01500667	ADENOSINE PHOSPHATE	100122-08	D06	sample	61-19-8	C10H14N5O7P	347.22618	vasodilator, neuromodulator	widespread in living tissue	USAN, INN, BAN		-0.44	0.04	0.31	-0.04	-0.03
01500668	KETOTIFEN FUMARATE	100122-08	D07	sample	34580-14-8, 34580-13-7	C23H23NO5S	425.50746	antiasthmatic	synthetic	USAN, INN, BAN, JAN		-0.26	-0.25	4.27	0.64	1.10
01500670	BETAHISTINE HYDROCHLORIDE	100122-08	D08	sample	5579-84-0, 5638-76-6	C8H14ClN2	209.12018	vasodilator	synthetic	USAN, INN, BAN, JAN		1.52	0.83	-0.08	4.13	1.60
01500673	MOLSIDOMINE	100122-08	D09	sample	25717-80-0	C9H14N4O4	242.23633	antianginal	synthetic	USAN, INN, BAN, JAN		0.13	-0.31	-0.67	0.20	-0.16
01500674	MYCOPHENOLIC ACID	100122-08	D10	sample	24280-93-1	C17H20O6	320.34535	immune suppressant, antineoplastic, antiviral	Penicillium brevicompactum and other Penicillium spp	USAN, INN, BAN	Biochem J 26:1411 (1932); J Antibiot 22:358 (1969);	0.90	-0.79	1.36	1.78	0.81
01500675	OLEANDOMYCIN PHOSPHATE	100122-08	D11	sample	3922-90-5 (base)	C35H64NO16P	785.87123	antibacterial	Streptomyces antibioticus	NF-XIII, INN, BAN, JAN		-1.58	-0.33	-4.42	-3.43	-2.44
	0.11% JAK2inhib	100122-08	D12	0.11% jak2inhib								-1.79	-3.26	-2.96	-3.04	-2.76
	0.11% JAK2inhib	100122-08	E01	0.11% jak2inhib								-3.61	-2.94	-2.30	-2.82	-2.92
01500676	OUABAIN	100122-08	E02	sample	11018-89-6, 630-60-4	C29H44O12	584.66683	antiarrhythmic, cardiotonic, hypertensive, Na/K ATPase inhibitor	Acokanthera and Strophanthus spp	USP-XX, JAN	Ann Rev Biochem 15: 155 (1946); Helv Chim Acta 42: 1418	-0.44	0.52	-0.41	0.24	-0.02
01500677	ALBUTEROL (+/-)	100122-08	E03	sample	18559-94-9	C13H21NO3	239.31722	bronchodilator, tocolytic	synthetic	USP, INN, BAN		-1.22	0.34	-1.22	0.35	-0.44
01500680	ARECOLINE HYDROBROMIDE	100122-08	E04	sample	300-08-3, 63-75-2 [arecoline]	C8H14BrNO2	236.11028	anthelmintic (Cestodes), hypotensive, cathartic	betel nuts (Arica catechu)	NF-XIII	Ber 21: 3404 (1888); Biochem J 122: 503 (1971)	-0.87	-1.00	2.47	0.17	0.19
01500682	CAPTOPRIL	100122-08	E05	sample	62571-86-2	C9H15NO3S	217.2888	antihypertensive	synthetic	USP, INN, BAN, JAN		-1.44	-0.27	0.09	0.63	-0.25
01500684	CIMETIDINE	100122-08	E06	sample	51481-61-9	C10H16N6S	252.34322	antiulcer	synthetic	USP, INN, BAN, JAN		0.21	0.19	0.11	0.39	0.23
01500685	CLOZAPINE	100122-08	E07	sample	5786-21-0	C18H19ClN4	326.83193	antipsychotic	synthetic	USP, INN, BAN		-0.84	-0.41	-0.11	3.34	0.50
01500687	HYDRASTINE (1R, 9S)	100122-08	E08	sample	118-08-1	C21H21NO6	383.40462	antihypertensive, sedative, antibacterial	Corydalis spp	USP-IX	J Nat Prod 45:105 (1982)	1.14	0.90	0.12	-0.28	0.47
01500689	LIDOCAINE HYDROCHLORIDE	100122-08	E09	sample	6108-05-0, 73-78-9	C14H23ClN2O	270.80521	anesthetic (local), antiarrhythmic	synthetic	USP, INN, JAN		-0.04	-0.38	2.24	0.06	0.47
01500691	PHENTOLAMINE HYDROCHLORIDE	100122-08	E10	sample	73-05-2, 50-60-2	C17H20ClN3O	317.82145	antihypertensive	synthetic	USP-XX, INN, BAN		0.91	-0.92	3.33	-1.14	0.54
01500767	BUTAMBEN	100122-08	E11	sample	94-25-7	C11H15NO2	193.2477	anesthetic (local)	synthetic	USP		1.44	-0.62	-0.22	-0.54	0.01
	0.11% DMSO	100122-08	E12	0.11% dmso								1.31	-2.44	-0.48	-1.92	-0.88
	0.11% JAK2inhib	100122-08	F01	0.11% jak2inhib								-2.44	-1.86	-0.33	-2.99	-1.90
01500771	CEFACLOR	100122-08	F02	sample	70356-03-5, 53994-73-3	C15H14ClN3O4S	367.81353	antibacterial	semisynthetic	USP, INN, BAN, JAN		-0.40	0.93	-1.30	1.72	0.24
01500772	IODIPAMIDE	100122-08	F03	sample	606-17-7, 2618-26-0	C12H11I3N2O4	627.94567	radiopaque agent	synthetic; L-isomer: spectrum	USAN, INN, BAN, JAN		-0.14	1.17	2.54	-0.01	0.89
01500778	LIOTHYRONINE	100122-08	F04	sample	6893-02-3	C15H12I3NO4	650.98039	thyroid hormone blocker	semisynthetic	USP, BAN, JAN		-0.10	0.21	0.66	0.44	0.30
01500801	ALLANTOIN	100122-08	F05	sample	97-59-6	C4H6N4O3	158.1142	wound healing agent	allantoic fluid; widely distributed in plants	USP, BAN, JAN		-29.23	-23.29	-25.52	-22.66	-25.17
01500804	ALTHIAZIDE	100122-08	F06	sample	5588-16-9	C11H14ClN3O4S3	383.89693	diuretic	synthetic	USAN, INN		0.19	1.01	1.86	-0.99	0.52
01500807	ADENINE	100122-08	F07	sample	73-24-5	C5H5N5	135.1291	Vitamin B4	widespread in nature	USP, JAN	Ber 18: 79, 1928 (1885)	0.76	0.90	1.97	4.25	1.97
01500810	AMINACRINE	100122-08	F08	sample	90-45-9, 134-50-9 [aminacrine	C13H10N2	194.23805	local antiseptic	synthetic	USAN, IN, BAN		-0.11	-0.64	-0.44	-0.49	-0.42
01500812	BEKANAMYCIN SULFATE	100122-08	F09	sample	4696-76-8 (base)	C18H39N5O14S	581.60063	antibacterial	semisynthetic; Streptomyces kanamyceticus; NK-1006	USP, INN, BAN, JAN	JACS 80:2911 (1958); 85:1547 (1963)	1.12	-0.55	-0.49	-0.28	-0.05
01500813	BUDESONIDE	100122-08	F10	sample	51333-22-3 [11(gr b), 16(gr a)]	C25H34O6	430.54613	antiinflammatory	semisynthetic	USAN, INN, BAN, JAN		0.42	0.66	-1.43	-0.53	-0.22
01500822	BRUCINE	100122-08	F11	sample	4845-99-2, 357-57-3 [brucine]	C23H26N2O4	394.47467	central stimulant	Strychnos nux-vomica	NF-IX	Progress in Organic Chemistry 1: 1 (1952)	1.47	-0.66	0.35	-1.08	0.02
	0.04% DMSO	100122-08	F12	0.04% dmso								4.26	2.22	3.15	-1.39	2.06
	0.04% JAK2inhib	100122-08	G01	0.04% jak2inhib								-2.12	-0.64	-1.55	-1.81	-1.53
01500828	CANRENOIC ACID, POTASSIUM SALT	100122-08	G02	sample	2181-04-6, 4138-96-9	C22H29KO4	396.57603	aldosterone antagonist, diuretic	semisynthetic	USAN, INN, BAN, JAN		-0.89	0.78	-0.86	-1.12	-0.52
01500837	CHENODIOL	100122-08	G03	sample	474-25-9	C24H40O4	392.584	anticholithogenic, antilipemic agent	human bile	USAN, INN, BAN, JAN	Helv Chim Acta 43: 1595 (1960)	-0.51	0.67	-0.42	0.07	-0.05
01500838	CHOLECALCIFEROL	100122-08	G04	sample	67-97-0	C27H44O	384.65113	vitamin D3	fish oils	USP, INN, BAN, JAN	J Biol Chem 247: 2328 (1972)	-0.36	2.10	1.41	0.85	1.00
01500839	CINCHONIDINE	100122-08	G05	sample	485-71-2	C19H22N2O	294.39999	antimalarial	Cinchona spp	NF-IX		-0.21	0.61	0.60	0.07	0.27
01500841	CINCHONINE	100122-08	G06	sample	118-10-5	C19H22N2O	294.39999	antimalarial	Cinchona spp	NF-IX		-0.44	-3.24	-1.55	0.09	-1.28
01500844	COENZYME B12	100122-08	G07	sample	13870-90-1	C72H104CoN18O17P	1583.64908	vitamin	Vitamin B12; cyanocobalamin	USP-XXI		0.35	0.23	0.66	1.08	0.58
01500847	CHOLESTEROL	100122-08	G08	sample	57-88-5	C27H46O	386.66707	emulsifying agent	common animal sterol	USAN, NF		-0.26	0.19	-0.18	-0.34	-0.15
01500873	PIPERINE	100122-08	G09	sample	94-62-2	C17H19NO3	285.34588	analeptic, antibacterial	black pepper (Piper nigrum L.)	USP-VIII	Tet Lett 1979: 1043	0.42	1.06	-0.07	0.57	0.50
01500903	ETOPOSIDE	100122-08	G10	sample	33419-42-0	C29H32O13	588.57059	antineoplastic	semisynthetic	USP, INN, BAN, JAN		1.23	-0.72	-0.33	-1.06	-0.22
01500907	DEHYDROCHOLIC ACID	100122-08	G11	sample	81-23-2	C24H34O5	402.53558	choleretic	derivative of cholic acid	USP, INN, BAN, JAN		1.83	0.60	2.40	-0.73	1.02
	0.04% DMSO	100122-08	G12	0.04% dmso								1.48	2.85	-0.92	-0.97	0.61
	0.04% JAK2inhib	100122-08	H01	0.04% jak2inhib								-3.12	-1.04	-1.89	-2.63	-2.17
01500992	FLUMEQUINE	100122-08	H02	sample	42835-25-6	C14H12FNO3	261.25504	antibacterial	synthetic	USAN, INN, BAN		-1.21	1.17	1.01	-0.58	0.10
01500993	FLUNARIZINE HYDROCHLORIDE	100122-08	H03	sample	30484-77-6, 52468-60-7	C26H28Cl2F2N2	477.42926	vasodilator	synthetic	USAN, INN, BAN, JAN		0.14	1.14	0.40	0.09	0.44
01500994	FLUPHENAZINE HYDROCHLORIDE	100122-08	H04	sample	146-56-5	C22H28Cl2F3N3OS	510.45316	H1 antihistamine	synthetic	USP, BAN, JAN		-0.48	1.15	-0.21	-2.40	-0.48
01500995	FLUTAMIDE	100122-08	H05	sample	13311-84-7	C11H11F3N2O3	276.21712	antiandrogen, antineoplastic, Nuclear Hormone receptor	synthetic	USP, INN, BAN		-0.41	1.35	0.22	3.91	1.27
01501002	DROPERIDOL	100122-08	H06	sample	548-73-2	C22H22FN3O2	379.43794	neuroleptic	synthetic	USP, INN, BAN, JAN		-1.07	-0.77	1.57	-0.27	-0.13
01501003	FAMOTIDINE	100122-08	H07	sample	76824-35-6	C8H15N7O2S3	337.44645	H2 antihistamine	synthetic	USP, INN, BAN, JAN		-0.64	1.41	0.71	1.08	0.64
01501005	ETODOLAC	100122-08	H08	sample	41340-25-4	C17H21NO3	287.36182	antiinflammatory	synthetic	USP, INN, BAN		0.66	0.95	0.14	0.18	0.48
01501007	FENOTEROL HYDROBROMIDE	100122-08	H09	sample	13392-18-2	C17H22BrNO4	384.27319	betaadrenergic agonist	synthetic	USAN, INN, BAN, JAN		1.46	0.54	0.50	0.35	0.71

Compound ID	MolNAME	plate	position	Content	cas#	Formula	MolWt	Bioactivity	Source	Status	Reference	Screen Score (z-score) rep1	rep2	rep3	rep4	Average
01501008	FENBUFEN	100122-08	H10	sample	36330-85-5	C16H14O3	254.28818	antiinflammatory	synthetic	USAN, INN, BAN, JAN		0.16	0.80	4.36	0.40	1.43
01501117	MEBEVERINE HYDROCHLORIDE	100122-08	H11	sample	2753-45-9, 3625-06-7	C25H36ClNO5	466.02237	muscle relaxant (smooth)	synthetic	USAN, INN, BAN		0.59	-0.35	-0.08	-0.65	-0.12
	empty	100122-08	H12	sample								NA	NA	NA	NA	NA
	empty	100122-09	A01	sample								NA	NA	NA	NA	NA
01501124	ACECLIDINE	100122-09	A02	sample	827-61-2	C9H15NO2	169.2254	cholinergic	synthetic	USAN, INN	Mol Pharm 21:594 (1982); Eur J Pharmacol 238:343 (1993);	-1.06	-1.39	-1.71	-1.15	-1.33
01501128	CAPSAICIN	100122-09	A03	sample	404-86-4	C18H27NO3	305.42079	analgesic (topical), depletes Substance P, neurotoxic	Capsicum spp	USP	J Chem Soc 1955: 1025; Life Sci 25: 1273 (1979); Trends	-0.51	0.87	-0.40	0.47	0.11
01501130	FAMPRIDINE	100122-09	A04	sample	504-24-5	C5H6N2	94.11697	K channel blocker; multiple sclerosis therapy	synthetic	USAN, INN	J Pharmacol Exp Ther 275: 864 (1995)	-0.08	-1.38	0.47	-0.34	-0.33
01501133	NICERGOLINE	100122-09	A05	sample	27848-84-6	C24H26BrN3O3	484.39712	vasodilator	synthetic	USAN, INN, BAN, JAN		-0.89	-0.66	-0.72	0.22	-0.51
01501152	SPIPERONE	100122-09	A06	sample	749-02-0	C23H26FN3O2	395.48097	antipsychotic	synthetic; R-5147	USAN, INN, BAN, JAN		-0.07	-1.85	0.26	0.58	-0.27
01501176	ERYTHROMYCIN ESTOLATE	100122-09	A07	sample	134-36-1, 114-07-8	C52H97NO18S	1056.41279	antibacterial	Streptomyces erythreus	USP, INN, BAN, JAN		-2.45	-2.85	-2.26	-1.05	-2.15
01501179	ESTRADIOL PROPIONATE	100122-09	A08	sample	113-38-2	C21H28O3	328.45551	estrogen	semisynthetic	NF-XIV, JAN		-0.65	-0.34	-0.69	2.13	0.11
01501182	ESTRADIOL BENZOATE	100122-09	A09	sample	50-50-0	C25H28O3	376.50011	estrogen	semisynthetic	USP-XX, INN, BAN, JAN		0.25	-1.25	-0.41	-0.60	-0.50
01501203	RETINOL	100122-09	A10	sample	68-26-8	C20H30O	286.4615	vitamin A	fish & liver oils, eggs, milk	USP, INN, BAN		2.09	-0.92	4.16	-0.14	1.30
01502013	ISOTRETINON	100122-09	A11	sample	4759-48-2	C20H28O2	300.44496	antiacne, antineoplastic	semisynthetic	USP, INN, BAN	Science 195: 487 (9177); N Eng J Med 300: 329 (1979)	0.77	2.23	0.75	-0.46	0.82
	0.04% JAK2inhib	100122-09	A12	0.04% jak2inhib								-2.73	-3.20	-1.00	-2.27	-2.30
	0.04% DMSO	100122-09	B01	0.04% dmso								-0.36	-1.10	-0.99	-0.36	-0.70
01502014	MESNA	100122-09	B02	sample	19767-45-4, 3375-50-6 [2-	C2H5NaO3S2	164.17815	mucolytic	synthetic	USAN, INN, BAN		-0.33	0.06	-0.45	0.29	-0.11
01502016	TRETINON	100122-09	B03	sample	302-79-4	C20H28O2	300.44496	keratolytic	semisynthetic	USP, INN, BAN	Science 195: 487 (9177); N Eng J Med 300: 329 (1979)	0.32	-0.30	-0.03	0.84	0.21
01502018	BRETYLIUM TOSYLATE	100122-09	B04	sample	61-75-6, 59-41-6 [bretylium]	C18H24BrNO3S	414.36488	inhibitor of norepinephrine release	synthetic	USP, INN, BAN		0.27	0.28	0.15	0.96	0.41
01502019	FOSCARNET SODIUM	100122-09	B05	sample	63585-09-1	CNa3O5P	191.95135	antiviral	synthetic	USAN, INN, BAN		-0.31	-0.75	-0.18	0.68	-0.14
01502029	CEFSULODIN SODIUM	100122-09	B06	sample	52152-93-9, 62587-73-9	C22H19N4NaO8S2	554.53653	antibacterial	semisynthetic	USAN, INN, BAN, JAN		-0.11	-0.58	-0.35	-0.70	-0.44
01502039	FOSFOMYCIN CALCIUM	100122-09	B07	sample	26472-47-9, 23112-90-5(acid)	C3H5CaO4P	176.1247	antibacterial	Streptomyces spp	USAN, INN, BAN		0.59	-0.47	0.83	0.86	0.46
01502041	CEFAMANDOLE NAFATE	100122-09	B08	sample	42540-40-9, 34444-01-4	C19H17N6NaO6S2	512.50174	antibacterial	semisynthetic	USP, BAN		-0.10	-1.13	0.52	0.15	-0.14
01502047	LIOTHYRONINE (L- isomer) SODIUM	100122-09	B09	sample	55-06-1, 6893-02-3	C15H11I3NNaO4	672.96222	thyroid hormone	synthetic; L-isomer	USP, BAN, JAN		0.58	-0.88	2.52	0.34	0.64
01502053	ALRESTATIN	100122-09	B10	sample	51411-04-2, 51876-97-2	C14H9NO4	255.23213	aldose reductase inhibitor	synthetic; FK-222284A	USAN, INN		0.82	-1.11	0.72	-0.12	0.08
01502084	PROADIFEN HYDROCHLORIDE	100122-09	B11	sample	78997-40-7	C23H32ClNO2	389.96999	cytochrome P450 inhibitor, Ca antagonist	synthetic; SKF-525A	USAN, INN		0.19	0.20	1.61	-0.58	0.36
	0.04% JAK2inhib	100122-09	B12	0.04% jak2inhib								-0.28	-3.89	-1.40	-1.82	-1.85
	0.04% DMSO	100122-09	C01	0.04% dmso								-0.08	-1.30	-1.29	-0.82	-0.87
01502106	CARBOPLATIN	100122-09	C02	sample	41575-94-4	C6H12N2O4Pt	371.26354	antineoplastic, convulsant	synthetic	USP, INN, BAN, JAN		-0.01	-1.01	-0.64	-0.17	-0.46
01502107	CISPLATIN	100122-09	C03	sample	15663-27-1	H6Cl2N2Pt	300.05722	antineoplastic, convulsant	synthetic	USP, INN, BAN, JAN		-0.81	-0.63	-0.45	-0.46	-0.58
01502109	ZIDOVUDINE [AZT]	100122-09	C04	sample	30516-87-1	C10H13N5O4	267.24621	RT transferase inhibitor, antiviral	synthetic	USP, INN, BAN, JAN		-0.17	3.57	-0.58	0.02	0.71
01502111	AZACITIDINE	100122-09	C05	sample	320-67-2	C8H12N4O5	244.20864	antineoplastic, pyrimidine antimetabolite	synthetic; U-18496; NSC-102816	USAN, INN		0.62	-0.15	0.16	0.57	0.30
01502112	CYCLOHEXIMIDE	100122-09	C06	sample	66-81-9	C15H23NO4	281.35486	protein synthesis inhibitor	synthetic	USAN, INN		0.59	0.40	4.27	-0.24	1.26
01502127	TINIDAZOLE	100122-09	C07	sample	19387-91-8	C8H13N3O4S	247.27451	antiprotozoal	synthetic	USP, INN, BAN, JAN		-0.07	-0.82	0.04	-0.22	-0.27
01502150	CARBIDOPA	100122-09	C08	sample	38821-49-7, 28860-95-9	C10H14N2O4	226.23408	decarboxylase inhibitor, antiparkinsonism	synthetic	USP, INN, BAN, JAN		1.47	-0.08	0.58	-0.41	0.39
01502196	ETHOSUXIMIDE	100122-09	C09	sample	77-67-8	C7H11NO2	141.17122	anticonvulsant	synthetic	USP, INN, BAN, JAN		2.35	-0.83	0.42	-0.20	0.44
01502197	PIPERIDOLATE HYDROCHLORIDE	100122-09	C10	sample	129-77-1, 82-98-4	C21H26ClNO2	359.89987	antispasmodic	synthetic	USP-XX, INN, BAN, JAN		-0.88	-1.95	4.18	-1.61	-0.06
01502198	ANISINDIONE	100122-09	C11	sample	117-37-3	C16H12O3	252.27224	anticoagulant	synthetic	NF-XIII, INN, BAN		-0.26	-1.32	-0.24	-0.37	-0.55
	0.11% JAK2inhib	100122-09	C12	0.11% jak2inhib								-2.77	-4.45	-1.65	-1.45	-2.58
	0.11% DMSO	100122-09	D01	0.11% dmso								-1.53	-0.06	-2.80	-1.75	-1.54
01502202	CYCLOSPORINE	100122-09	D02	sample	59865-13-3	C62H111N11O12	1202.64247	immunosuppressant	Tolypocladium inflatum	USP, INN, BAN, JAN	Helv Chim Acta 60: 1568 (1977)	1.75	0.41	0.60	-0.84	0.48
01502230	ASCORBIC ACID	100122-09	D03	sample	50-81-7	C6H8O6	176.12706	antiscorbutic, antiviral	Vitamin C	USP, INN, BAN, JAN		0.93	1.10	-0.41	1.52	0.78
01502254	MENADIONE	100122-09	D04	sample	58-27-5	C11H8O2	172.18521	prothrombogenic agent	Asplenium and Juglans spp.	USP, BAN	J Nat Prod 47: 901 (1984)	0.36	-0.31	-0.38	-0.18	-0.13
01502255	SALICIN	100122-09	D05	sample	138-52-3	C13H18O7	286.28421	analgesic, antipyretic	Salix spp	USP-IX		2.68	0.17	3.27	-0.09	1.51
01502258	MONENSIN SODIUM (monensin A is shown)	100122-09	D06	sample	22373-78-0, 17090-79-8	C37H63NaO11	690.89846	antibacterial	Streptomyces cinnamonensis	USP, INN, BAN	J Am Chem Soc 89: 5737 (1967)	0.77	0.38	-0.61	-0.20	0.09
01502260	ABAMECTIN	100122-09	D07	sample	65195-55-3	C48H72O14	873.10064	antiparisitic (avermectin A1a shown)	Streptomyces avermitilis	USP, INN, BAN		1.55	0.20	0.27	0.93	0.74
01503001	BENZOIC ACID	100122-09	D08	sample	65-85-0	C7H6O2	122.12467	antifungal	synthetic	USP, JAN		-0.13	1.28	-0.37	1.57	0.59
01503002	BENZYL BENZOATE	100122-09	D09	sample	120-51-4	C14H12O2	212.25054	scabicide	synthetic	USP, JAN		2.47	0.40	0.76	-0.77	0.72
01503004	BENZOYL PEROXIDE	100122-09	D10	sample	94-36-0	C14H10O4	242.2334	keratolytic	synthetic; NSC-675	USP		1.30	3.39	0.37	-0.25	1.20
01503007	BETAINE HYDROCHLORIDE	100122-09	D11	sample	590-46-5, 141-58-2 [replaced],	C5H12ClNO2	153.60989	antiarteriosclerotic, hypolipaemic, hepatoprotectant	widespread in fungi and plants	USP		1.57	0.28	0.99	-0.27	0.64
	0.11% JAK2inhib	100122-09	D12	0.11% jak2inhib								-3.07	-3.55	-2.89	-2.74	-3.06
	0.11% JAK2inhib	100122-09	E01	0.11% jak2inhib								-3.64	-2.93	-4.01	-1.90	-3.12
01503009	BIOTIN	100122-09	E02	sample	58-85-5	C10H16N2O3S	244.31462	vitamin B complex	Vitamin B complex	USP, INN, JAN		-0.62	-0.80	-1.67	2.40	-0.17
01503014	AKLOMIDE	100122-09	E03	sample	3011-89-0	C7H5ClN2O3	200.5825	antiprotozoal, coccidiostat	synthetic	USAN, INN, BAN	JACS 75: 4675 (1953)	0.04	0.60	-0.19	0.00	0.11
01503038	NICOTINYL ALCOHOL TARTRATE	100122-09	E04	sample	100-55-0	C10H13NO7	259.21761	vasodilator	synthetic	USAN, JAN		0.48	1.08	-0.21	1.94	0.82
01503059	FLOXURIDINE	100122-09	E05	sample	50-91-9	C9H11FN2O5	246.19682	antineoplastic, antimetabolite	synthetic	USP		0.35	0.29	-0.16	-0.50	0.00
01503065	ALTRETAMINE	100122-09	E06	sample	645-05-6	C9H18N6	210.28401	antineoplastic	synthetic	USP, INN, BAN		0.57	-0.36	-1.11	1.16	0.07
01503069	AMINOHIPPURIC ACID	100122-09	E07	sample	61-78-9, 94-16-6	C9H10N2O3	194.19165	renal function diagnosis	synthetic	USP		-0.58	-0.81	0.36	0.38	-0.16
01503070	MEFLOQUINE	100122-09	E08	sample	53230-10-7	C17H17ClF6N2O	414.78124	antimalarial	synthetic	USAN, INN, BAN		-0.06	1.76	0.32	5.41	1.86
01503073	ADIPHENINE HYDROCHLORIDE	100122-09	E09	sample	50-42-0, 64-95-9 [adiphenine]	C20H26ClNO2	347.88672	muscle relaxant (smooth)	synthetic	USAN, INN		-0.47	0.74	-0.07	-0.48	-0.07
01503076	QUINAPRIL HYDROCHLORIDE	100122-09	E10	sample	82586-55-8, 85441-61-8	C25H31ClN2O5	474.98922	antihypertensive, ACE inhibitor	synthetic	USP, INN, BAN		-8.06	-1.88	-0.42	-0.39	-2.69
01503081	AMIFOSTINE	100122-09	E11	sample	20537-88-6	C5H15N2O3PS	214.2247	radioprotectant	synthetic	USP, INN, BAN		0.39	0.14	0.69	-0.19	0.26
	0.11% DMSO	100122-09	E12	0.11% dmso								-0.60	-1.08	-0.22	-2.19	-1.02
	0.11% JAK2inhib	100122-09	F01	0.11% jak2inhib								-3.11	-0.30	-2.56	-3.19	-2.29
01503083	AMIPRILOSE	100122-09	F02	sample	56824-20-5, 60414-06-4	C14H28ClNO6	341.83536	immunomodulator, antiinflammatory	semisynthetic	USAN, INN		-0.17	2.84	-1.28	-0.07	0.33
01503086	TIAPRIDE HYDROCHLORIDE	100122-09	F03	sample	51012-32-9	C15H25ClN2O4S	364.8945	neuroleptic	synthetic	USAN, INN, BAN		-0.38	0.25	-0.88	0.12	-0.22
01503102	BACAMPICILLIN HYDROCHLORIDE	100122-09	F04	sample	37661-08-8, 50972-17-3	C21H28ClN3O7S	501.99021	antibacterial	semisynthetic	USP, INN, BAN, JAN		-0.02	0.93	-0.52	1.26	0.41
01503104	BENDROFLUMETHIAZIDE	100122-09	F05	sample	73-48-3	C15H14F3N3O4S2	421.41973	diuretic, antihypertensive	synthetic	USP, INN, BAN, JAN		0.51	0.99	-0.80	-0.45	0.06
01503106	BEPRIDIL HYDROCHLORIDE	100122-09	F06	sample	74764-40-2	C24H35ClN2O	403.01235	antiarrhythmic	synthetic; CERM-1978	USAN, INN, BAN, JAN		-0.26	0.56	-0.76	0.00	-0.12
01503107	BROMHEXINE HYDROCHLORIDE	100122-09	F07	sample	611-75-6, 3572-43-8	C14H21Br2ClN2	412.59787	expectorant	synthetic	USAN, INN, BAN, JAN		0.71	5.10	0.50	0.84	1.79
01503110	CARMUSTINE	100122-09	F08	sample	154-93-8	C5H9Cl2N3O2	214.05238	antineoplastic, alkylating agent	synthetic	USAN, INN, BAN	Toxicol Appl Pharmacol 21: 405 (1972)	2.39	0.42	0.71	3.75	1.82
01503111	CEFTRIAXONE SODIUM TRIHYDRATE	100122-09	F09	sample	104376-79-6, 73384-59-5	C18H22N8Na2O10S3	652.59524	antibacterial	semisynthetic; RO-13-9904	USP, INN, BAN, JAN		0.27	0.54	0.53	-0.39	0.24
01503117	TRIMIPRAMINE MALEATE	100122-09	F10	sample	521-78-8, 739-71-9	C24H30N2O4	410.5177	antidepressant	synthetic	USAN, JAN		0.67	-0.56	0.22	3.61	0.98
01503118	TRIFLUPROMAZINE HYDROCHLORIDE	100122-09	F11	sample	1098-60-8, 146-54-3	C18H20ClF3N2S	388.8857	antipsychotic	synthetic	USP, INN, BAN		0.59	-0.91	-0.67	2.76	0.44
	0.04% DMSO	100122-09	F12	0.04% dmso								0.33	-0.40	0.50	-0.27	0.04
	0.04% JAK2inhib	100122-09	G01	0.04% jak2inhib								-2.54	-3.09	-2.67	-1.95	-2.56
01503121	TRAZODONE HYDROCHLORIDE	100122-09	G02	sample	25332-39-2, 19794-93-5	C19H23Cl2N5O	408.33406	antidepressant	synthetic	USP, INN, BAN, JAN		-0.48	-0.35	-1.25	-0.79	-0.72
01503134	MENTHOL(-)	100122-09	G03	sample	1490-04-6	C10H20O	156.2703	analgesic (topical), antipruritic agent	Mentha piperita and other Mentha spp	USP, JAN		0.71	0.47	1.39	0.35	0.73
01503135	THONZYLAMINE HYDROCHLORIDE	100122-09	G04	sample	63-56-9, 91-85-0	C16H23ClN4O	322.84091	antihistamine	synthetic	USAN, INN, BAN		-0.31	-0.06	0.03	0.09	-0.06
01503136	THIAMPHENICOL	100122-09	G05	sample	15318-45-3	C12H15Cl2NO5S	356.22705	antibacterial	synthetic	USAN, INN, BAN, JAN		0.71	2.17	-0.24	0.41	0.76
01503142	TENOXICAM	100122-09	G06	sample	59804-37-4	C13H11N3O4S2	337.37832	antiinflammatory	synthetic	USAN, INN, BAN, JAN		-0.52	-0.14	-1.08	-0.12	-0.46
01503202	CHLOROXINE	100122-09	G07	sample	773-76-2	C9H5ClN2NO	214.0523	chelating agent	synthetic	USAN		0.17	1.27	0.18	3.16	1.20
01503203	CHLORPROTHIXENE HYDROCHLORIDE	100122-09	G08	sample	113-59-7	C18H19Cl2NS	352.32883	antipsychotic	synthetic	USP-XIII, INN, BAN, JAN	J Med Chem 36: 2219 (1993)	0.72	0.28	1.17	0.45	0.66
01503204	CINNARAZINE	100122-09	G09	sample	298-57-7	C26H28N2	368.52646	H1 antihistamine	synthetic	USAN, INN, BAN, JAN		-0.11	0.71	0.09	0.14	0.21
01503209	DANTROLENE SODIUM	100122-09	G10	sample	24868-20-0, 14663-23-1	C14H9N4NaO5	336.2143	muscle relaxant (skeletal)	synthetic	USAN, INN, BAN, JAN		-0.37	-0.75	-0.31	-1.74	-0.79
01503210	BETAMETHASONE 17,21-DIPROPIONATE	100122-09	G11	sample	5593-20-4	C28H37FO7	504.60129	glucocorticoid, antiinflammatory	semisynthetic	USP, INN, BAN, JAN		0.49	0.15	1.50	0.79	0.73
	0.04% DMSO	100122-09	G12	0.04% dmso								-0.24	-0.34	1.72	-1.48	-0.09
	0.04% JAK2inhib	100122-09	H01	0.04% jak2inhib								-2.49	-2.97	-1.98	-2.40	-2.46
01503212	DOBUTAMINE HYDROCHLORIDE	100122-09	H02	sample	49745-95-1, 34368-04-2	C18H24ClNO3	337.84988	cardiotonic	synthetic	USP, INN, BAN		-0.53	0.96	-0.32	0.11	0.05
01503214	EDOXUDINE	100122-09	H03	sample	15176-29-1	C11H16N2O5	256.26057	antiviral	synthetic; EDU; EUDR; ORF-15817; RWJ-15817	USAN, INN		0.91	-0.33	-0.29	1.21	0.38
01503215	ENOXACIN	100122-09	H04	sample	74011-58-8	C15H17FN4O3	320.32614	antibacterial	synthetic	USAN, INN, BAN, JAN		-0.33	-0.69	0.77	-0.35	-0.15
01503221	ETHISTERONE	100122-09	H05	sample	434-03-7	C21H28O2	312.45611	progestogen	synthetic; NSC-9565	NF-XIII, INN, BAN		-0.52	-0.13	-0.85	-0.20	-0.43
01503223	PARAROSANILINE PAMOATE	100122-09	H06	sample	7232-51-1, 569-61-9	C42H33N3O6	675.74781	anthelmintic, antischistosomal	synthetic	USAN, INN		-2.47	-1.64	-4.32	-4.54	-3.24
01503227	PERHEXILINE MALEATE	100122-09	H07	sample	6724-53-4, 6621-47-2	C23H39NO4	393.57158	coronary vasodilator	synthetic	USAN, INN, BAN	hepatotoxic at clinical dose (300mg)	0.01	0.63	-0.37	0.81	0.27
01503228	PAROMOMYCIN SULFATE	100122-09	H08	sample	1263-89-4, 7542-37-2	C23H47N5O18S	713.71774	antiamoebic, antiamebic	Streptomyces rimosis paramomycinus	USP, INN, BAN		-0.04	0.06	0.17	0.20	0.10
01503229	METHAPYRILENE HYDROCHLORIDE	100122-09	H09	sample	135-23-9, 91-80-5	C14H20ClN3S	297.8526	H1 antihistamine	synthetic	USP-XX, INN, BAN		-0.45	1.20	0.09	-0.40	0.11
01503234	BETA-PROPIOLACTONE	100122-09	H10	sample	57-57-8	C3H4O2	72.06413	antiinfective	synthetic; NSC-21626	USAN, INN		-0.18	-0.15	0.66	0.31	0.16
01503237	HALCINONIDE	100122-09	H11	sample	3093-35-4	C24H32ClFO5	454.97104	glucocorticoid, antiinflammatory	synthetic	USP, INN, BAN, JAN		-1.29	-1.46	0.03	-1.35	-1.02
	empty	100122-09	H12	sample								NA	NA	NA	NA	NA
	empty	100122-10	A01	sample								NA	NA	NA	NA	NA
01503239	HYCANTHONE	100122-10	A02	sample	3105-97-3	C20H24N2O2S	356.49048	anthelmintic, hepatotoxic	synthetic	USAN, INN		-0.86	-1.09	-0.91	-0.20	-0.77
01503240	PYRIDOSTIGMINE BROMIDE	100122-10	A03	sample	101-26-8, 155-97-5	C9H13BrN2O2	261.12016	cholinergic	synthetic	USP, INN, BAN, JAN		-0.46	1.49	-0.78	0.43	0.17
01503242	ISOXICAM	100122-10	A04	sample	34552-84-6	C14H13N3O5S	335.34081	antiinflammatory	synthetic	USAN, INN, BAN		-1.07	-1.73	-0.54	-0.53	-0.96
01503243	LABETALOL HYDROCHLORIDE	100122-10	A05	sample	32780-64-6, 36894-69-6	C19H25ClN2O3	364.8757	adrenergic blocker	synthetic	USP, INN, BAN, JAN		-0.81	-1.06	0.54	0.60	-0.18
01503245	LEVAMISOLE HYDROCHLORIDE	100122-10	A06	sample	16595-80-5, 14769-73-4	C11H13ClN2S	240.75666	immunomodulator	synthetic	USP, INN, BAN		-0.26	-0.66	0.86	0.52	0.12
01503250	MEPHENTERMINE SULFATE	100122-10	A07	sample	1212-72-2, 6190-60-9	C11H19NO4S	261.34238	vasoconstrictor	synthetic	USP-XXIII, INN, BAN		-0.81	-0.97	-0.53	-0.94	-0.81
01503251	METARAMINOL BITARTRATE	100122-10	A08	sample	33402-03-8	C13H19NO8	317.29828	antihypotensive	synthetic	USP, INN, BAN, JAN		0.60	-0.43	0.94	0.70	0.45
01503252	METHAZOLAMIDE	100122-10	A09	sample	554-57-4	C5H8N4O3S2	236.27251	carbonic anhydrase inhibitor	synthetic	USP, INN, BAN, JAN		-0.17	-0.69	-0.06	-0.56	-0.37
01503253	METHYLBENZETHONIUM CHLORIDE	100122-10	A10	sample	1320-44-1, 25155-18-4	C28H44ClNO2	462.12138	antiinfective	synthetic	USP, INN, BAN		0.85	-0.37	-0.19	4.04	1.08
01503255	METHYLPREDNISOLONE SODIUM SUCCINATE	100122-10	A11	sample	2375-03-3	C26H33NaO8	496.53791	glucocorticoid, antiinflammatory	semisynthetic	USP, JAN		-0.08	-1.14	3.60	-1.12	0.32
	0.04% JAK2inhib	100122-10	A12	0.04% jak2inhib								-2.24	-3.03	-2.20	-3.54	-2.75
	0.04% DMSO	100122-10	B01	0.04% dmso								-1.21	-2.17	-1.65	-1.63	-1.67
01503256	AMSACRINE	100122-10	B02	sample	51264-14-3	C22H20N2O3S	392.4803	antineoplastic, immune suppressive	synthetic	USAN, INN, BAN	Pharmacother 5: 78 (1985)	-4.36	-4.39	-3.64	-3.95	-4.09
01503257	MIDODRINE HYDROCHLORIDE	100122-10	B03	sample	3092-17-9, 42794-76-3	C12H19ClN2O4	290.74923	antihypertensive, vasoconstrictor	synthetic	USAN, INN, BAN, JAN		-0.25	-0.96	0.29	1.56	0.16
01503260	NADOLOL	100122-10	B04	sample	42200-33-9	C17H27NO4	309.40904	betaadrenergic blocker	synthetic	USP, INN, BAN, JAN		0.01	0.12	1.50	0.84	0.62
01503262	NALTREXONE HYDROCHLORIDE	100122-10	B05	sample	16676-29-2, 16590-41-3	C20H23NO4	341.41061	mucosal antagonist	synthetic	USP		-0.61	0.22	0.26	0.84	0.18
01503263	CYCLOTHIAZIDE	100122-10	B06	sample	2259-96-3	C14H16ClN3O4S2	389.88232	diuretic	synthetic	USP XXII, INN, BAN		0.31	1.38	0.29	0.67	0.67
01503265	NICLOSAMIDE	100122-10	B07	sample	50-65-7	C13H8Cl2N2O4	327.12571	anthelmintic, teniacide	synthetic; BAY-2353	USAN, INN, BAN		0.40	0.36	3.31	0.92	1.25
01503267	NOMIFENSINE MALEATE	100122-10	B08	sample	32795-47-4, 24526-64-5	C20H22N2O4	354.40934	antidepressant, dopamine uptake inhibitor	synthetic	USAN, INN, BAN	J Clin Psychiatry 45: 12 (1984); Int Pharmacopsychiatry 17:	0.33	-0.21	0.25	-0.71	-0.08
01503269	PERGOLIDE MESYLATE	100122-10	B09	sample	66104-23-2, 66104-22-1	C20H30N2O3S2	410.6017	dopamine receptor agonist	semisynthetic	USP, INN, BAN		1.29	-0.96	-1.11	-0.40	-0.29
01503270	PRILOCAINE HYDROCHLORIDE	100122-10	B10	sample	1786-81-8, 721-50-6	C13H21ClN2O	256.77812	anesthine (local)	synthetic	USAN, INN, BAN		0.70	4.97	0.73	-0.09	1.58
01503273	HYDROCORTISONE BUTYRATE	100122-10	B11	sample	13609-67-1	C25H36O6	432.56207	glucocorticoid, antiinflammatory	semisynthetic	USP, INN, BAN, JAN		-0.05	-1.05	0.86	-0.35	-0.15
	0.04% JAK2inhib	100122-10	B12	0.04% jak2inhib								-0.77	-3.38	-1.77	-1.57	-1.87
	0.04% DMSO	100122-10	C01	0.04% dmso								-1.27	-1.33	-1.58	-1.20	-1.34
01503276	ROXITHROMYCIN	100122-10	C02	sample	80214-83-1	C41H76N2O15	837.06727	antibacterial	semisynthetic; RU-28965, RU-965	USAN, INN, JAN		1.58	0.62	-0.55	1.20	0.71
01503278	MITOXANTHRONE HYDROCHLORIDE	100122-10	C03	sample	70476-82-3, 65271-80-9	C22H30Cl2N4O6	517.4136	antineoplastic	semisynthetic	USP, INN, BAN, JAN		-0.57	-0.53	-0.32	2.65	0.31
01503279	OXETHAZAINE	100122-10	C04	sample	126-27-2	C28H41N3O3	467.65727	anesthetic (local)	synthetic	USAN, INN, BAN, JAN		-0.56	-0.56	1.56	0.54	0.24
01503298	DIPYRONE	100122-10	C05	sample	5907-38-0, 68-89-3	C13H16N3NaO4S	333.34397	analgesic, antipyretic	synthetic	USAN, INN, BAN, JAN		-0.54	0.38	0.52	0.38	0.19

											Screen Score (z-score)				
Compound ID	MolNAME	plate	position	Content	cas#	Formula	MolWt	Bioactivity	Source	Status	Reference	rep1	rep2	rep3	rep4	Average
01503301	SULFANILATE ZINC	100122-10	C06	sample	31884-76-1	C12H12N2O6S2Zn	409.73724	antibacterial	synthetic	USAN		-0.31	0.22	0.32	1.37	0.40
01503304	URETHANE	100122-10	C07	sample	51-79-6	C3H7NO2	89.09474	antineoplastic, cytotoxic	synthetic; NSC-746	NF-XIII, INN		-0.47	0.27	0.34	0.04	0.05
01503322	THIRAM	100122-10	C08	sample	137-26-8	C6H12N2S4	240.43194	antifungal	synthetic	USAN, INN		-3.80	-5.76	-2.37	-5.84	-4.44
01503324	THIOTEPA	100122-10	C09	sample	52-24-4	C6H12N3PS	189.22044	antineoplastic, alkylating agent	synthetic	USP, INN, BAN, JAN		1.09	0.31	3.78	-0.21	1.24
01503330	TETROQUINONE	100122-10	C10	sample	319-89-1	C6H4O6	172.09518	keratolytic	synthetic	USAN, INN		1.78	-0.17	0.26	-0.61	0.31
01503339	SULFANITRAN	100122-10	C11	sample	122-16-7	C14H13N3O5S	335.34081	antibacterial	synthetic; NSC-77120	USAN, INN, BAN		-0.56	-1.07	-0.74	-0.57	-0.73
	0.11% JAK2inhib	100122-10	C12	0.11% jak2inhib								-0.64	-3.62	-2.49	-0.64	-1.85
	0.11% DMSO	100122-10	D01	0.11% dmso								-1.89	-1.49	-3.03	-0.89	-1.83
01503373	OXIBENDAZOLE	100122-10	D02	sample	20559-55-1	C12H15N3O3	249.27165	anthelmintic	synthetic	USAN, INN, BAN	Am J Vet Res 38:809 (1977); J Parasitol 66:929 (1980)	1.31	0.03	1.04	1.25	0.91
01503393	PIPOBROMAN	100122-10	D03	sample	54-91-1	C10H16Br2N2O2	356.05922	antineoplastic, alkylating agent	synthetic	USP-XXII, INN		1.20	0.27	-0.12	5.49	1.71
01503412	ETANIDAZOLE	100122-10	D04	sample	22668-01-5	C7H10N4O4	214.18215	antineoplastic, hypoxic cell radiosensitizer	synthetic	USAN, INN		0.69	2.64	-0.37	0.53	0.87
01503419	NAFRONYL OXALATE	100122-10	D05	sample	3200-06-4, 31329-57-4	C26H35NO7	473.57135	vasodilator	synthetic	USAN, INN, BAN		0.02	-0.25	0.35	2.92	0.76
01503420	QUIPAZINE MALEATE	100122-10	D06	sample	5786-68-5, 4774-24-7	C17H19N3O4	329.35868	antidepressant, oxytocic	synthetic	USAN, INN		0.76	-0.03	-0.37	5.43	1.45
01503421	RITANSERIN	100122-10	D07	sample	87051-43-2	C27H25F2N3O3S	477.5806	antiserotonin	synthetic	USAN, INN, BAN		0.39	1.26	3.31	0.81	1.44
01503422	SEMUSTINE	100122-10	D08	sample	13909-09-6	C10H18ClN3O2	247.72686	antineoplastic	synthetic	USAN, INN		0.47	4.90	1.18	0.26	1.70
01503423	SPIRAMYCIN	100122-10	D09	sample	8025-81-8	C43H74N2O14	843.07423	antibacterial	Streptomyces ambofaciens	USAN, INN, BAN	J Am Chem Soc 91: 3401 (1969)	1.36	0.31	0.96	-0.05	0.65
01503429	CLOFIBRATE	100122-10	D10	sample	637-07-0	C12H15ClO3	242.70455	antihyperlipidemic	synthetic	USP, INN, BAN, JAN		1.07	0.05	-0.75	-0.51	-0.04
01503500	RESORCINOL MONOACETATE	100122-10	D11	sample	102-29-4	C8H8O3	152.15116	antiseborrheic, antipruritic	synthetic	USP		0.93	0.21	1.41	-0.48	0.52
	0.11% JAK2inhib	100122-10	D12	0.11% jak2inhib								-2.00	-4.27	0.63	-4.22	-2.47
	0.11% JAK2inhib	100122-10	E01	0.11% jak2inhib								-3.67	-3.01	-3.71	-1.88	-3.07
01503600	NIMODIPINE	100122-10	E02	sample	66085-59-4	C21H26N2O7	418.45057	vasodilator	synthetic	USP, INN, BAN		-0.68	-1.50	-3.05	-1.18	-1.60
01503603	ACYCLOVIR	100122-10	E03	sample	59277-89-3	C8H11N5O3	225.20857	antiviral	synthetic	USP, INN, BAN, JAN		-0.27	0.41	-0.71	1.48	0.23
01503604	RETINYL PALMITATE	100122-10	E04	sample	79-81-2	C36H60O2	524.8784	provitamin, antixerophthalamic	semisynthetic; Vitamin A palmitate	USP, JAN		-9.56	-0.62	-0.83	-0.54	-2.88
01503607	THALIDOMIDE	100122-10	E05	sample	50-35-1	C13H10N2O4	258.23565	hypnotic	synthetic	USP, INN, BAN		-0.50	0.35	0.29	1.01	0.29
01503609	NITRENDIPINE	100122-10	E06	sample	84845-75-0	C18H20N2O6	360.3699	antihypertensive	synthetic	USAN, INN, BAN, JAN		-0.55	-0.49	0.44	-0.36	-0.24
01503610	BENZALKONIUM CHLORIDE	100122-10	E07	sample	8001-54-5	C22H40ClN	354.0238	antiinfective (topical)	synthetic	USAN, NF, INN, BAN, JAN		0.69	-0.28	1.67	2.80	1.22
01503614	CIPROFLOXACIN	100122-10	E08	sample	85721-33-1	C17H18FN3O3	331.34971	antibacterial, fungicide	synthetic	USP, INN, BAN		2.61	1.73	0.11	0.22	1.17
01503678	CELECOXIB	100122-10	E09	sample	169590-42-5	C17H14F3N3O2S	381.37923	antiarthritic, cyclooxygenase2 inhibitor	synthetic; SC-58635	USAN, INN, BAN		0.17	-0.12	0.62	-0.57	0.03
01503679	AZITHROMYCIN	100122-10	E10	sample	83905-01-5, 117772-70-0	C38H72N2O12	749.00374	antibacterial	semisynthetic	USP, INN, BAN		-6.05	0.15	0.39	0.66	-1.21
01503705	ANETHOLE	100122-10	E11	sample	4180-23-8	C10H12O	148.20654	expectorant, gastric stimulant, insecticide	anise, fennel and other plant oils	USAN, NF		-5.60	-1.20	-0.80	-0.13	-1.93
	0.11% DMSO	100122-10	E12	0.11% dmso								-0.60	-1.67	-0.18	-1.23	-0.92
	0.11% JAK2inhib	100122-10	F01	0.11% jak2inhib								-3.30	-3.72	-3.29	-3.59	-3.48
01503708	TERFENADINE	100122-10	F02	sample	50679-08-8	C32H41NO2	471.68907	H1 antihistamine, nonsedating	synthetic	USP XXIII, INN, BAN, JAN		-5.66	-2.37	-2.45	3.21	-1.82
01503710	CLOPIDOGREL SULFATE	100122-10	F03	sample	113665-84-2	C16H18ClNO6S2	419.90596	platelet aggregation inhibitor	synthetic	USP, INN, BAN		-3.36	0.38	-1.23	-0.66	-1.22
01503712	LORATADINE	100122-10	F04	sample	79794-75-5	C22H23ClN2O2	382.89381	H1 antihistamine	synthetic	USP, INN, BAN		-0.17	0.39	-0.25	0.60	0.14
01503720	SELAMECTIN	100122-10	F05	sample	165108-07-6	C43H63NO11	769.98166	antiparasitic, antimite	semisynthetic	USAN, INN		-0.25	1.15	-0.73	0.42	0.14
01503801	NAPROXOL	100122-10	F06	sample	26159-36-4	C14H16O2	216.28242	antiinflammatory, analgesic, antipyretic	synthetic	USAN, INN		-0.12	0.71	1.07	0.22	0.47
01503804	COLFORSIN	100122-10	F07	sample	66575-29-9	C22H34O7	410.51208	adenylate cyclase activator, antiglaucoma, hypotensive,	Coleus forskohlii; HL-362; L-75-1362B	USAN, INN	J Biol Chem 258:2960 (1983); J Med Chem 26:436, 486	-1.15	-1.11	-1.34	-0.75	-1.09
01503807	ISOSORBIDE MONONITRATE	100122-10	F08	sample	16051-77-7	C6H9NO6	191.14173	antianginal	semisynthetic; BM-22145, IS-5-MN, AHR-4698	USAN, INN, BAN, JAN		0.30	-0.08	-0.36	0.03	-0.03
01503816	AMCINONIDE	100122-10	F09	sample	51022-69-6	C28H35FO7	502.58535	glucocorticoid, antiinflammatory	synthetic	USP, INN, BAN, JAN		0.20	0.66	-0.16	-0.17	0.13
01503818	BUPIVACAINE HYDROCHLORIDE	100122-10	F10	sample	14252-80-3, 2180-92-9	C18H29ClN2O	324.89763	anesthetic (local)	synthetic	USP, INN, BAN, JAN		1.04	-1.45	-0.06	-1.09	-0.39
01503903	ALBENDAZOLE	100122-10	F11	sample	54965-21-8	C12H15N3O2S	265.33625	anthelmintic	synthetic	USP		1.28	0.49	0.18	-0.59	0.34
	0.04% DMSO	100122-10	F12	0.04% dmso								-0.02	-1.37	2.92	-1.35	0.04
	0.04% JAK2inhib	100122-10	G01	0.04% jak2inhib								-2.91	-2.24	-3.23	-3.24	-2.90
01503908	PACLITAXEL	100122-10	G02	sample	33069-62-4	C47H51NO14	853.92882	antineoplastic	Taxus breviofolia	USP, INN, BAN	J Am Chem Soc 93: 2325 (1971)	-3.93	-3.92	-4.85	-4.08	-4.19
01503914	BUTACAINE	100122-10	G03	sample	149-15-5, 149-16-6 [butacaine]	C18H30N2O2	306.452	anesthetic (local)	synthetic	USP-XX, INN, BAN		-0.33	-1.25	-2.10	-1.12	-1.20
01503918	CLOBETASOL PROPIONATE	100122-10	G04	sample	25122-46-7, 25122-41-2	C25H32ClFO5	466.98219	glucocorticoid, antiinflammatory	synthetic	USP, INN, BAN, JAN		0.03	0.62	0.02	1.47	0.54
01503923	IOPANIC ACID	100122-10	G05	sample	96-83-3	C11H12I3NO2	570.93699	radioopaque agent	synthetic	USP, INN, BAN, JAN		0.41	0.20	-1.27	1.73	0.27
01503925	KETOROLAC TROMETHAMINE	100122-10	G06	sample	74103-07-4, 74103-06-3	C19H24N2O6	376.41293	antiinflammatory	synthetic	USP, INN, BAN		0.44	0.13	-0.83	-0.79	-0.26
01503926	LANSOPRAZOLE	100122-10	G07	sample	103577-45-3	C16H14F3N3O2S	369.36808	antisecretory, proton pump inhibitor	synthetic	USP, INN, BAN		0.27	-0.28	0.28	0.70	0.24
01503929	MEXILETINE HYDROCHLORIDE	100122-10	G08	sample	5370-01-4, 31828-71-4	C11H18ClNO	215.72521	antiarrhythmic	synthetic; KO-1173	USP, INN, BAN, JAN		0.85	0.10	0.12	0.00	0.27
01503931	MORANTEL CITRATE	100122-10	G09	sample	26155-31-7, 20574-50-9	C18H24N2O7S	412.46518	anthelmintic	synthetic	USAN, INN, BAN		0.52	0.31	-0.41	-0.83	-0.10
01503934	PERPHENAZINE	100122-10	G10	sample	58-39-9	C21H26ClN3OS	403.97787	antipsychotic	synthetic	USP, INN, BAN, JAN		1.42	0.04	0.80	-0.59	0.42
01503938	RIBAVIRIN	100122-10	G11	sample	36791-04-5	C8H12N4O5	244.20864	antiviral	synthetic	USP, INN, BAN		1.10	-0.34	1.33	-0.74	0.34
	0.04% DMSO	100122-10	G12	0.04% dmso								0.45	-0.38	-0.37	-1.21	-0.38
	0.04% JAK2inhib	100122-10	H01	0.04% jak2inhib								1.20	-1.88	-2.57	1.26	-0.50
01503968	TACROLIMUS	100122-10	H02	sample	109581-93-3, 104987-11-3	C44H69NO12	804.04003	immune suppressant, antifungal	Streptomyces tsukubaensis	USAN, INN, BAN, JAN		-9.14	-3.31	-3.47	-2.82	-4.68
01503985	BROMPHENIRAMINE MALEATE	100122-10	H03	sample	980-71-2, 86-22-6	C20H23BrN2O4	435.32131	H1 antihistamine	synthetic	USP, INN, BAN		-1.58	-0.42	-0.82	-0.62	-0.86
01504008	SIROLIMUS	100122-10	H04	sample	53123-88-9	C51H79NO13	914.19718	immunosuppressant, antineoplastic; rapamycin	Streptomyces hygroscopicus	USAN, INN, BAN		0.35	-0.38	-0.17	1.31	0.28
01504085	PAROXETINE HYDROCHLORIDE	100122-10	H05	sample	61869-08-7	C19H21ClFNO3	365.83552	antidepressant	synthetic	USP, INN, BAN		-6.61	-1.28	-0.79	-1.44	-2.53
01504088	ETHYLNOREPINEPHRINE HYDROCHLORIDE	100122-10	H06	sample	3198-07-0, 536-24-3	C10H16ClNO3	233.69692	bronchodilator	synthetic	USP-XXII, INN		-0.01	0.87	-0.29	0.37	0.24
01504136	ALAPROCLATE	100122-10	H07	sample	60719-82-6	C13H18ClNO2	255.74691	antidepressant	synthetic	USAN, INN		0.30	1.53	-0.48	3.63	1.24
01504142	ACETRIAZOIC ACID	100122-10	H08	sample	85-36-9, 129-63-5 [acetrizoate	C9H6I3NO3	556.86627	X-ray contrast medium	synthetic	USP	JACS 74: 4365 (1952); J Pharmacol Exp Therap 116: 394	-0.13	0.16	-0.02	0.00	0.00
01504171	VENLAFAXINE	100122-10	H09	sample	99300-78-4, 93413-69-5	C17H27NO2	277.41024	antidepressant	synthetic	USAN, INN, BAN		-0.93	0.62	1.23	-0.78	0.04
01504172	CITALOPRAM	100122-10	H10	sample	59729-33-8	C20H21FN2O	324.40157	antidepressant, 5HT reuptake inhibitor	synthetic	USAN		1.51	0.80	1.20	-0.17	0.83
01504173	FLUOXETINE	100122-10	H11	sample	54910-89-3	C17H19ClF3NO	345.79528	antidepressant	synthetic	USAN, INN, BAN		0.98	-0.98	0.14	-1.13	-0.25
	empty	100122-10	H12	sample								NA	NA	NA	NA	NA
	empty	100122-11	A01	sample								NA	NA	NA	NA	NA
01504174	BUPROPION	100122-11	A02	sample	31677-93-7, 34911-55-2	C13H19Cl2NO	276.20848	antidepressant	synthetic	USP, INN, BAN		-2.30	-1.08	-2.17	-1.20	-1.69
01504175	CEFUROXIME AXETIL	100122-11	A03	sample	64544-07-6, 55268-75-2	C20H22N4O10S	510.48314	antibacterial	synthetic	USP, BAN, JAN		0.90	-1.35	2.65	-0.36	0.46
01504179	FEXOFENADINE HYDROCHLORIDE	100122-11	A04	sample	138452-21-8	C32H40ClNO4	538.1329	nonsedating H1-antihistamine	synthetic	USAN, INN, BAN		-0.88	-2.02	-1.57	3.00	-0.37
01504183	TRIFLURIDINE	100122-11	A05	sample	70-00-8	C10H11F3N2O5	296.20477	antiviral (opthalmic)	synthetic	USP, INN		-5.02	-5.92	-5.88	-6.78	-5.90
01504188	PIRENPERONE	100122-11	A06	sample	75444-65-4	C23H24FN3O2	393.46503	5HT2 receptor antagonist	synthetic	USAN, INN, BAN	Psychopharmacol 119: 222 (1995)	-0.92	1.19	-0.79	-0.64	-0.29
01504190	AVOBENZONE	100122-11	A07	sample	70356-09-1	C20H22O3	310.39654	sunscreen	synthetic	USP, INN		0.06	0.82	-0.77	-0.65	-0.14
01504210	ATOVAQUONE	100122-11	A08	sample	95233-18-4	C22H19ClO3	366.84793	antipneumocystic, antimalarial	synthetic	USP, INN, BAN		3.49	1.57	2.34	0.78	2.04
01504214	TRIMETOZINE	100122-11	A09	sample	635-41-6	C14H19NO5	281.31123	sedative, neurosedative	synthetic	USAN, INN	J Med Pharm Chem 5: 800 (1962)	0.55	1.09	-0.32	-1.02	0.08
01504216	ZOXAZOLAMINE	100122-11	A10	sample	61-80-3	C7H5ClN2O	168.5837	muscle relaxant, antirrheumatic	synthetic	NF-XI, INN, BAN		1.97	0.69	0.43	1.04	1.03
01504226	CYSTEAMINE HYDROCHLORIDE	100122-11	A11	sample	60-23-1	C2H8ClNS	113.60976	antiurolithic, depigmentation, radiation protectant	cysteamine; CL-9148	USAN, INN, BAN		0.71	-0.40	-0.79	-0.08	-0.14
	0.04% JAK2inhib	100122-11	A12	0.04% jak2inhib								-0.84	-0.26	-1.67	-2.55	-1.33
	0.04% DMSO	100122-11	B01	0.04% dmso								-2.86	-3.54	-2.36	-2.38	-2.78
01504235	ROFECOXIB	100122-11	B02	sample	162011-90-7	C17H14O4S	314.36273	COX2 inhibitor, antiinflammatory, antiarthritic	synthetic	USAN, INN, BAN		-2.92	-3.19	-2.28	-1.52	-2.48
01504236	SIMVASTATIN	100122-11	B03	sample	79902-63-9	C25H38O5	418.57861	antihyperlipidemic, HMGCoA reductase inhibitor	synthetic	USP, INN, BAN		7.09	3.08	1.56	1.54	3.32
01504243	OXCARBAZEPINE	100122-11	B04	sample	28721-07-5	C15H12N2O2	252.27509	antipsychotic	synthetic	USAN, INN, BAN		2.74	-1.94	-0.16	-0.46	0.05
01504150	MELOXICAM SODIUM	100122-11	B05	sample	71125-38-7	C14H12N3NaO4S2	373.38724	antiinflammatory	synthetic	USAN, INN, BAN	Neuropharmacol 39: 1653 (2000)	-1.09	-0.28	0.20	-0.36	-0.38
01504257	CARVEDILOL	100122-11	B06	sample	72956-09-3	C24H26N2O4	406.48582	beta-adrenergic blocker	synthetic	USAN, INN, BAN, JAN		0.44	-0.71	-1.05	-1.69	-0.75
01504259	IRBESARTAN	100122-11	B07	sample	138402-11-6	C25H28N6O	428.54151	angiotensin 2 receptor antagonist	synthetic	USP, INN, BAN		1.70	-1.85	-0.34	-1.91	-0.60
01504260	LEVOFLOXACIN	100122-11	B08	sample	138199-71-0	C18H20FN3O4	361.3762	antibacterial	synthetic	USAN, INN, BAN, JAN		0.92	0.48	-0.29	0.78	0.47
01504269	LITHIUM CITRATE	100122-11	B09	sample	6080-58-6, 919-16-4	C6H5Li3O7	209.91955	antidepressant	synthetic	USP		0.59	-0.07	-0.61	0.14	0.01
01504272	GATIFLOXACIN	100122-11	B10	sample	160738-57-8	C19H22FN3O4	375.40329	antibacterial	synthetic; BMS-206584-01, AM-1155	USAN, INN		1.25	0.65	1.48	2.62	1.50
01504273	MIGLITOL	100122-11	B11	sample	72432-03-2	C8H17NO5	207.22839	alpha-glucosidase inhibitor, antidiabetic	synthetic; BAYm-1099	USAN, INN, BAN		-1.74	0.51	1.30	1.79	0.46
	0.04% JAK2inhib	100122-11	B12	0.04% jak2inhib								0.25	-0.11	0.11	-2.15	-0.47
	0.04% DMSO	100122-11	C01	0.04% dmso								-0.98	-2.19	-3.39	-2.34	-2.23
01504300	ORLISTAT	100122-11	C02	sample	96829-58-2	C29H53NO5	495.74946	reversible lipase inhibitor, antiobesity	synthetic	USAN, INN, BAN		-4.16	-3.71	-2.26	-1.68	-2.95
01504303	MOXIFLOXACIN HYDROCHLORIDE	100122-11	C03	sample	186826-86-8	C23H29ClFN3O4	465.95668	antibacterial	synthetic	USAN		0.39	-1.13	-0.11	-0.60	-0.36
01504401	PIOGLITAZONE HYDROCHLORIDE	100122-11	C04	sample	111025-46-8 (pioglitazone)	C19H21ClN2O3S	392.90782	antidiabetic	synthetic	USAN, INN, BAN		-0.06	0.17	0.79	-0.14	0.19
01504403	DONEPEZIL HYDROCHLORIDE	100122-11	C05	sample	142057-77-0	C24H30ClNO3	415.9646	acetylcholinesterase inhibitor (reversible), cognitive enhancer	synthetic; E-2020, BNAG	USAN, INN, BAN		-11.77	-3.00	-0.80	-1.32	-4.22
01504911	FLUVASTATIN	100122-11	C06	sample	93957-54-1	C24H26FNO4	411.47752	antihyperlipidemic, HMGCoA reductase inhibitor	synthetic; XU-62-320	USAN, INN, BAN		4.74	6.36	6.76	6.02	5.97
01505003	PIZOTYLINE MALATE	100122-11	C07	sample	5189-11-7	C23H27NO5S	429.53934	5HT antagonist, antimigraine	synthetic; PIZOTIFEN; BC-105	USAN, INN, BAN	J Cardiovas Pharmacol 8:805 (1986); Eur Neurol 38:31	-1.82	0.14	0.50	0.25	-0.23
01505012	EXEMESTANE	100122-11	C08	sample	107868-30-4	C20H24O2	296.41308	antineoplastic, aromatase inhibitor	synthetic; PNU-155971, FCE-24304	USAN, INN, BAN	J Steroid Biochem 30:391 (1988)	-0.11	0.26	0.30	-0.44	0.00
01505112	TILMICOSIN	100122-11	C09	sample	108050-54-0	C46H80N2O13	869.1561	antibacterial	semisynthetic	USP, INN, BAN		-1.76	0.84	0.23	0.45	-0.06
01505113	FLUNIXIN MEGLUMINE	100122-11	C10	sample	42461-84-7	C21H28F3N3O7	491.46841	analgesic, antiinflammatory	synthetic; SCH-14714	USP		1.85	3.19	1.05	1.57	1.92
01505115	CLORSULON	100122-11	C11	sample	60200-06-8	C8H6Cl3N3O4S2	380.65766	antiparasitic, fasciolicide	synthetic; MK-401	USP, INN, BAN		1.36	0.04	-0.23	1.28	0.61
	0.11% JAK2inhib	100122-11	C12	0.11% jak2inhib								-2.13	-0.23	-1.69	-2.16	-1.55
	0.11% DMSO	100122-11	D01	0.11% dmso								-0.09	-2.90	-2.90	-2.71	-2.15
01505116	ESTROPIPATE	100122-11	D02	sample	7280-37-7	C22H32N2O5S	436.57474	estrogen	semisynthetic	USP, BAN		-0.54	-0.05	-1.75	0.38	-0.49
01505124	CLAVULANATE LITHIUM	100122-11	D03	sample	58001-44-8(acid)	C8H10LiNO5	207.1116	beta-lactamase inhibitor	synthetic	USP		0.71	0.93	0.01	0.82	0.62
01505125	ALCLOMETAZONE DIPROPIONATE	100122-11	D04	sample	66734-13-2	C28H37ClO7	521.05589	antiinflammatory, glucocorticoid	semisynthetic; SCH-22219	USP, INN, JAN		-1.29	-0.98	-0.69	-0.94	-0.98
01505166	ALENDRONATE SODIUM	100122-11	D05	sample	121268-17-5	C4H19NNaO10P2	326.13413	bone resorption inhibitor, farnesyldiphosphate synthetase inhibitor,	synthesis	USAN	Nature 223:211 (1969); Cancer Res 62:2708 (2002); Mol	-1.22	-1.52	-0.27	-1.26	-1.07
01505172	ACARBOSE	100122-11	D06	sample	56180-94-0	C25H43NO18	645.61736	alpha-glucosidase & saccharase inhibitor, antidiabetes,	Actinoplanes spp	USAN, INN, BAN	Naturwissenschaften 64:535 (1977); Carbohydr Res	-1.58	-0.92	0.65	0.02	-0.46
01505178	ROPINIROLE	100122-11	D07	sample	91374-21-9	C16H24N2O	260.38248	dopamine receptor agonist, antiParkinsonian	synthetic; SK&F-101468	USAN, INN, BAN	J Med Chem 28:1533 (1985)	-1.87	0.11	0.43	1.42	0.02
01505187	QUETIAPINE	100122-11	D08	sample	111974-69-7	C21H25N3O2S	383.5163	antipsychotic; 5HT antagonist, dopamine antagonist, H1-	synthetic; ICI-204636, ZD-5077, ZM-204639	USAN, INN, BAN		-1.01	0.60	1.38	3.34	1.08
01505189	RIZATRIPTAN BENZOATE	100122-11	D09	sample	144034-80-0	C22H25N5O2	391.47685	5HT-1B/1D agonist, antimigraine	synthetic; MK-0462 (benzoate)	USAN, INN, BAN		0.54	0.82	0.37	-0.41	0.33
01505201	FAMCICLOVIR	100122-11	D10	sample	104227-87-4	C14H19N5O4	321.33863	antiviral	synthetic	USAN, INN, BAN		-1.51	1.68	1.08	0.45	0.42
01505202	AMLODIPINE BESYLATE	100122-11	D11	sample	111470-99-6	C26H31ClN2O8S	567.06257	Ca channel blocker	synthetic	USAN, INN, BAN, JAN		-6.82	-0.34	-1.41	0.27	-2.07
	0.11% JAK2inhib	100122-11	D12	0.11% jak2inhib								1.40	2.55	-3.01	-2.27	-0.33
	0.11% JAK2inhib	100122-11	E01	0.11% jak2inhib								-4.25	-4.72	-3.69	-0.06	-3.18
01505203	EZETIMIBE	100122-11	E02	sample	163222-33-1	C24H21F2NO3	409.43667	sterol absorption inhibitor	synthetic	USAN, INN, BAN		-1.18	-1.16	-1.81	-0.71	-1.22
01505205	OLMESARTAN MEDOXOMIL	100122-11	E03	sample	144689-63-4	C29H30N6O6	558.59905	Angiotensin II inhibitor prodrug, antihypertensive	synthetic	USAN, INN, BAN		-3.57	-2.28	-1.79	-1.25	-2.22
01505207	CEFTIBUTEN	100122-11	E04	sample	97519-39-6	C15H14N4O6S2	410.43003	antibacterial	semisynthetic	USAN, INN, BAN		-0.19	-0.75	2.75	-0.15	0.42
01505208	CEFDINIR	100122-11	E05	sample	91832-40-5	C14H13N5O5S2	395.41821	antibacterial	semisynthetic; CL-983, FK-482	USAN, INN, BAN		-0.53	0.18	0.14	0.22	0.00
01505210	SIBUTRAMINE HYDROCHLORIDE	100122-11	E06	sample	84485-00-7; 106650-56-0	C17H27Cl2N	316.31744	anorexic, antidepressant, uptake inhibitor (5HT, norepinephrine,	synthetic	USAN, INN, BAN		-0.87	-1.26	0.04	-0.52	-0.65
01505212	PERINDOPRIL ERBUMINE	100122-11	E07	sample	107133-36-8; 82834-16-0	C23H43N3O5	441.61626	antihypertensive, ACE inhibitor	synthetic; S9490-3, McN-A2833-109	USAN		0.06	1.05	1.98	0.70	0.95
01505213	ROSUVASTATIN CALCIUM	100122-11	E08	sample	287714-14-4, 147098-20-2(Ca	C22H27CaFN3O6S	520.61939	antihyperlipidemic	synthetic	USAN, INN, BAN		10.66	7.99	5.77	7.05	7.87
01505214	RAMIPRIL	100122-11	E09	sample	87333-19-5	C23H32N2O5	416.52189	antihypertensive, ACE inhibitor	synthetic; HOE-498	USP, INN, BAN		0.56	0.70	0.44	-0.49	0.30
01505216	ESCITALOPRAM OXALATE	100122-11	E10	sample	219861-08-2	C22H23FN2O5	414.43741	antidepressant, 5HT reuptake inhibitor	synthetic; LU26-054-0	USAN		-6.72	-0.51	1.15	-0.67	-1.69
01505222	DERACOXIB	100122-11	E11	sample	169590-41-4	C17H14F3N3O3S	397.37863	antiinflammatory, antiarthritic, COX-2 inhibitor	synthetic	USAN, INN		1.32	-0.61	-0.72	-2.04	-0.51
	0.11% DMSO	100122-11	E12	0.11% dmso								0.62	1.44	-0.33	-1.21	0.13
	0.11% JAK2inhib	100122-11	F01	0.11% jak2inhib								-4.06	-5.17	-5.12	-4.27	-4.66

Compound ID	MolNAME	plate	position	Content	cas#	Formula	MolWt	Bioactivity	Source	Status	Reference	Screen Score (z-score)				
												rep1	rep2	rep3	rep4	Average
01505230	CILOSTAZOL	100122-11	F02	sample	73963-72-1	C20H27N5O2	369.47049	phosphodiesterase inhibitor	synthetic	USAN, INN, BAN, JAN		-1.21	-2.36	-0.97	-0.46	-1.25
01505244	CITICOLINE	100122-11	F03	sample	987-78-0	C14H26N4O11P2	488.33112	cognition enhancer, phosphocholine cytidyltransferase activator	cytidine-5'-diphosphocholine	USAN, INN, JAN	J Neurochem 65: 889 (1995); Neurosci Lett 273: 163 (1999)	-0.13	-0.69	-1.08	-0.59	-0.62
01505249	APRAMYCIN	100122-11	F04	sample	37321-09-8	C21H41N5O11	539.58782	antibacterial; LD50(iv) 280mg/kg(mouse)	Streptomyces tenebrarius, Saccharomyces porispora hiltus	USAN, INN, BAN	J Org Chem 41: 2087 (1976); 43: 1430 (1978); Eur J	-0.13	1.49	-0.46	1.25	0.54
01505262	SERTRALINE HYDROCHLORIDE	100122-11	F05	sample	79559-97-0; 79617-96-2(base)	C17H18Cl3N	342.69871	antidepressant, 5HT uptake inhibitor	synthetic	USAN, INN, BAN		1.13	1.10	0.53	0.80	0.89
01505263	ALFLUZOSIN	100122-11	F06	sample	81403-80-7	C19H27N5O4	389.45814	alpha(1)-adrenergic blocker	synthetic; SL-77499	USAN, INN, BAN		-6.54	0.37	-0.27	1.58	-1.22
01505265	TELITHROMYCIN	100122-11	F07	sample	191114-48-4	C43H65N5O10	812.025	antibacterial	semisynthetic; HMR-3647	USAN, INN, BAN		-3.05	0.29	-0.21	-0.68	-0.91
01505267	OXAPROZIN	100122-11	F08	sample	21256-18-8	C18H15NO3	293.32515	antiinflammatory	synthetic; WY-21743	USP, INN, BAN, JAN		0.38	2.48	0.82	-0.05	0.91
01505296	OXFENDAZOLE	100122-11	F09	sample	53716-50-0	C15H13N3O3S	315.35316	anthelmintic	synthetic	USP, INN, BAN	Am J Vet Res 38:465 (1977)	0.29	-0.28	-0.27	-0.92	-0.30
01505299	AMITRAZ	100122-11	F10	sample	33089-61-1	C19H23N3	293.41526	scabicide	synthetic; U-36059	USP, INN, BAN	Toxicol Appl Pharmacol 73:411 (1984); Toxicol Lett 28:99	1.26	1.26	1.20	0.83	1.14
01505305	PEFLOXACINE MESYLATE	100122-11	F11	sample	149676-40-4	C18H24FN3O6S	429.47088	antibacterial, antiproliferative	synthetic	USAN, INN, BAN	J Med Chem 31:221 (1988); J Pharmacol Exp Ther 248:415	1.45	3.69	2.00	5.61	3.19
	0.04% DMSO	100122-11	F12	0.04% dmso								0.39	1.76	0.90	1.24	1.07
	0.04% JAK2inhib	100122-11	G01	0.04% jak2inhib								-4.63	-5.02	-4.09	-1.52	-3.82
01505308	CHLOROPHYLLIDE Cu COMPLEX Na SALT	100122-11	G02	sample	15611-43-5	C34H28CuN4Na2O5	682.15166	antineoplastic	water soluble derivative of chlorophyll	USP, JAN	Mutat Res 308:191 (1994)	-2.69	-1.77	-1.85	-0.88	-1.80
01505309	BIFONAZOLE	100122-11	G03	sample	60628-96-8	C22H18N2	310.40216	antifungal, calmodulin antagonist	synthetic	USAN, INN, BAN, JAN	Eur J Pharmacol 313:265 (1996)	-0.88	-1.47	-1.44	-1.26	-1.26
01505312	TYLOSIN TARTRATE	100122-11	G04	sample	1405-54-5, 1401-69-0(base)	C46H77NO17	916.12309	antibacterial	Streptomyces fradiae	USP, INN, BAN	Chem Ber 108:2481 (1975); Infection 5:183 (1977);	0.09	-0.94	-0.17	-0.82	-0.46
01505314	SARAFLOXACIN HYDROCHLORIDE	100122-11	G05	sample	91296-87-6	C20H18ClF2N3O3	421.83456	antibacterial	synthetic	USAN, INN, BAN	J Med Chem 28:1558 (1985); J Antimicrob Chemother	1.05	-0.02	-0.01	-0.15	0.22
01505319	CLOPIDOL	100122-11	G06	sample	2971-90-6	C7H7Cl2NO	192.04594	coccidiostat, antiplatelet	synthetic	USAN, INN, BAN	Clin Appl Thromb Hemost 8:169 (2002)	0.79	0.86	0.59	0.30	0.64
01505327	CHLORMADINONE ACETATE	100122-11	G07	sample	302-22-7	C23H29ClO4	404.93818	progestin, antiandrogen	semisynthetic	USAN, INN, BAN, JAN	Cancer Metastasis Rev 6:615 (1987); Endocrin J 42:505	-1.64	-3.05	-3.09	0.64	-1.78
01505330	OXICONAZOLE NITRATE	100122-11	G08	sample	64211-46-7	C18H14Cl4N4O4	492.14868	antifungal	synthetic	USAN, INN, BAN, JAN	Arzneimittelforschung 32:17 (1992)	0.06	0.20	0.36	0.70	0.33
01505332	AZAPERONE	100122-11	G09	sample	1649-18-9	C19H22FN3O	327.40509	tranquilizer, neuroleptic, alpha adrenergic blocker	synthetic; R-1929	USP, INN, BAN	J Vet Pharmacol Ther 9:164 (1986); Psychopharmacol	1.33	0.38	0.07	0.35	0.53
01505333	TRANILAST	100122-11	G10	sample	53902-12-8	C18H17NO5	327.33989	antiallergic, mast cell degranulation inhibitor, angiogenesis blocker	synthetic; MK-341	USAN, INN, JAN	Br J Pharmacol 118:915 (1996); 122:1061 (1997); Eur J	2.34	0.31	0.60	0.29	0.89
01505340	AZELASTINE HYDROCHLORIDE	100122-11	G11	sample	58581-89-8	C22H25Cl2N3O	418.37005	H1 antihistamine (nonsedating); leucotriene synthesis blocker	synthetic	USAN, INN, BAN, JAN	Int Arch Allergy Appl Immun 83:284 (1987)	1.16	-0.01	-0.38	-2.06	-0.32
	0.04% DMSO	100122-11	G12	0.04% dmso								3.58	1.54	1.11	-0.93	1.33
	0.04% JAK2inhib	100122-11	H01	0.04% jak2inhib								-4.05	-3.93	-3.88	-3.93	-3.95
01505346	KETANSERIN TARTRATE	100122-11	H02	sample	83846-83-7, 74050-98-9(base)	C22H22FN3O3	395.43734	5HT2/5HT1C seritonin antagonist	synthetic; R41468	USAN, INN, BAN	J Pharmacol Exp Therap 218:217 (1981); Drug Dev Res	0.29	-0.82	-1.14	0.55	-0.28
01505354	FIPRONIL	100122-11	H03	sample	120068-37-3	C12H4Cl2F6N4OS	437.15228	GABA Cl channel agonist, antiparasitic	synthetic; RM-1601, MB-46030	USAN, BAN		-3.48	-1.60	-0.75	-0.59	-1.61
01505356	DECOQUINATE	100122-11	H04	sample	18507-89-6	C24H35NO5	417.55025	coccidiostat	synthetic; M&B-15497, HC-1528	USP, INN, BAN		-7.38	-2.46	-0.28	-0.02	-2.53
01505360	CEFDITORIN PIVOXIL	100122-11	H05	sample	117467-28-4	C25H28N6O7S3	620.72991	antibacterial	semisynthetic	USAN, INN, JAN		-1.62	-1.28	-0.81	1.42	-0.57
01505368	VALACYCLOVIR HYDROCHLORIDE	100122-11	H06	sample	124832-27-5	C13H21ClN6O4	360.80312	antiviral	synthetic; BW-256-U-87	USAN, INN, BAN		-6.65	-0.62	0.63	0.26	-1.59
01505387	DULOXETINE HYDROCHLORIDE	100122-11	H07	sample	136434-34-9	C18H20ClNOS	333.8832	antidepressant	synthetic; LY-248686	USAN, INN, BAN		0.53	-0.49	0.32	0.04	0.10
01505390	NISOLDIPINE	100122-11	H08	sample	63675-72-9	C20H24N2O6	388.42408	vasodilator (coronary)	synthetic; bayk-5552	USAN, INN, BAN, JAN		0.93	0.63	0.59	4.89	1.76
01505391	MONTELUKAST SODIUM	100122-11	H09	sample	151767-02-1	C34H33ClNNaO3S	594.15381	leucotriene antagonist, antiasthmatic	synthetic; MK-476	USAN, INN, BAN		-6.49	0.01	1.07	0.27	-1.29
01505410	BENURESTAT	100122-11	H10	sample	38274-54-3	C9H9ClN2O3	228.63668	urease inhibitor	synthetic; EU-2826	USAN, INN		1.36	2.94	0.53	0.06	1.22
01505411	BENZOXIQUINE	100122-11	H11	sample	86-75-9	C16H11NO2	249.27157	antiinfective	synthetic; NSC-3951	USAN, INN		2.09	1.88	0.74	-0.78	0.98
	empty	100122-11	H12	sample								NA	NA	NA	NA	NA
	empty	100122-12	A01	sample								NA	NA	NA	NA	NA
01505412	BISMUTH SUBSALICYLATE	100122-12	A02	sample	14882-18-9	C7H5BiO4	362.0955	antidiarrheal, antacid, antiulcer	synthetic	USP, JAN		-0.43	-0.77	-0.50	-0.47	-0.54
01505413	BENZOYLPAS	100122-12	A03	sample	13898-58-3	C14H11NO4	257.24807	antibacterial, tuberculostatic	synthetic	USP-XX		-0.71	-0.56	-1.81	0.15	-0.73
01505414	BROMINDIONE	100122-12	A04	sample	1146-98-1	C15H9BrO2	301.14178	anticoagulant	synthetic	USAN, INN, BAN	Farmaco Ed Sci 10:710 (1955)	-0.95	-0.83	-2.14	1.86	-0.51
01505417	CAPOBENIC ACID	100122-12	A05	sample	21434-91-3	C16H23NO6	325.36481	antiarrhythmic	synthetic; C-3	USAN, INN		-0.25	0.84	-0.81	-0.48	-0.18
01505425	ACETOHEXAMIDE	100122-12	A06	sample	968-81-0	C15H20N2O4S	324.40165	antidiabetic	synthetic; 33006	USP, INN, BAN, JAN		0.02	-1.53	-1.12	-1.75	-1.10
01505426	ETHOXZOLAMIDE	100122-12	A07	sample	452-35-7	C9H10N2O3S2	258.31965	carbonic anhydrase inhibitor, antiulcer, antiglaucoma	synthetic	USP-XX		0.58	0.91	-0.34	-1.15	0.00
01505429	FLUCYTOSINE	100122-12	A08	sample	2022-85-7	C4H4FN3O	129.09438	antifungal	synthetic; RO-2-9915	USP, INN, BAN, JAN		-0.77	0.48	-0.77	2.35	0.32
01505432	FOMEPIZOLE HYDROCHLORIDE	100122-12	A09	sample	56010-888	C4H7ClN2	118.56679	alcohol dehydrogenase inhibitor	synthetic; 4-MP	USAN, INN, BAN		0.61	0.06	-0.61	-0.25	-0.05
01505433	GLIPIZIDE	100122-12	A10	sample	29094-61-9	C21H27N5O4S	445.54444	antidiabetic	synthetic; CP-28720, K-4024	USP, INN, BAN		0.66	0.90	-0.54	-0.89	0.03
01505435	GUANFACINE	100122-12	A11	sample	29110-47-2	C9H9Cl2N3O	246.09758	antihypertensive	synthetic; BS-100-141	USP, INN, BAN, JAN		2.48	0.50	-0.16	-0.65	0.54
	0.04% JAK2inhib	100122-12	A12	0.04% jak2inhib								-2.58	-1.23	-1.11	-1.11	-1.51
	0.04% DMSO	100122-12	B01	0.04% dmso								0.49	-0.86	-0.99	1.54	0.05
01505436	D-LACTITOL MONOHYDRATE	100122-12	B02	sample	81025-04-9, 585-86-4	C12H26O12	362.33382	sweetener, treatment of portoencephalopathy	semisynthetic	USAN, NF, INN, BAN	Zhonghua Yi Xue Za Zhi 55:31 (1995)	-0.38	-0.54	-1.79	0.78	-0.48
01505437	LEVOCARNITINE	100122-12	B03	sample	541-15-1	C7H15NO3	161.2025	cofactor for fatty acid metabolism, replenisher in arterial disease	semisynthetic	USP, INN, BAN, JAN		-0.11	-0.23	2.01	-0.05	0.41
01505440	LOBENDAZOLE	100122-12	B04	sample	6306-71-4	C10H11N3O2	205.21807	anthelmintic	synthetic; SK&F-24529; NSC-42044	USAN, INN		-1.13	-1.83	-2.14	-1.40	-1.63
01505444	METHYLENE BLUE	100122-12	B05	sample	7220-79-3	C16H20ClN3OS	337.8743	antimethemoglobinemic, cyanide antidote	synthetic	USP, INN, BAN		-3.22	-3.83	-4.25	-2.67	-3.49
01505445	METHYLATROPINE NITRATE	100122-12	B06	sample	52-88-0	C18H26N2O6	366.41772	anticholinergic	semisynthetic	USAN, INN, BAN, JAN		0.05	-0.18	0.05	-0.56	-0.16
01505448	NITHIAMIDE	100122-12	B07	sample	140-40-9	C5H5N3O3S	187.1779	antibacterial	synthetic; CI-5279	USAN, INN, BAN		-0.41	0.46	-0.37	-0.32	-0.16
01505449	PRALIDOXIME CHLORIDE	100122-12	B08	sample	51-15-0	C7H9ClN2O	172.61558	cholesterase agonist	synthetis; 2-PAM	USP, INN, BAN		-0.25	-0.51	-0.58	-1.02	-0.59
01505450	PREDNISOLONE HEMISUCCINATE	100122-12	B09	sample	2920-86-7	C25H32O8	460.52899	antiinflammatory, glucocorticoid	semisynthetic	USP, JAN		0.48	0.15	0.40	0.25	0.32
01505453	PYRIDOXINE	100122-12	B10	sample	65-23-6	C8H11NO3	169.18177	vitamin B6, enzyme cofactor	rice husks, wheat germ, yeast	USP, INN, BAN, JAN		1.75	1.00	0.03	-0.29	0.62
01505460	RIMANTADINE HYDROCHLORIDE	100122-12	B11	sample	1501-84-4	C12H22ClN	215.76884	antiviral	synthetic; EXP-126	USP, INN, BAN		0.87	1.38	0.45	4.80	1.87
	0.04% JAK2inhib	100122-12	B12	0.04% jak2inhib								0.15	1.01	-1.31	-0.12	-0.07
	0.04% DMSO	100122-12	C01	0.04% dmso								1.23	-1.72	-1.97	-0.43	-0.72
01505461	SULFISOXAZOLE ACETYL	100122-12	C02	sample	80-74-0	C13H15N3O4S	309.3462	antibacterial	synthetic	USP		0.22	1.06	0.50	1.47	0.81
01505463	TAURINE	100122-12	C03	sample	107-35-7	C2H7NO3S	125.14699	neuroprotectant, inhibitory neurotransmitter, GABA agonist	widespread in animal tissue	USP, INN, JAN	Am J Clin Nutrition 47:660 (1988); Amino Acids 23:381	-0.24	-0.77	0.32	-0.08	-0.19
01505464	THIAMINE	100122-12	C04	sample	67-03-8	C12H18Cl2N4OS	337.27346	vitamin B1, enzyme cofactor	rice husks, wheat germ, yeast	USP, INN, BAN, JAN		0.32	-0.88	0.38	3.78	0.90
01505465	TRICLOSAN	100122-12	C05	sample	3380-34-5	C12H7Cl3O2	289.54739	antiinfective	synthetic; CH-3565	USP, INN, BAN		-0.42	2.99	-0.32	0.74	0.75
01505466	TRIMETHADIONE	100122-12	C06	sample	127-48-0	C6H9NO3	143.14353	anticonvulsant	synthetic	USP-XXIII, INN, BAN, JAN		0.53	0.44	0.13	0.62	0.43
01505467	ZINC UNDECYLENATE	100122-12	C07	sample	557-08-4	C22H38O4Zn	431.91576	antifungal	synthetic	USP, JAN		0.62	-1.10	-0.04	3.96	0.86
01505468	UNDECYLENIC ACID	100122-12	C08	sample	112-38-9	C11H20O2	184.28085	antifungal	semisynthetic	USP, JAN		0.21	-0.61	0.09	0.49	0.04
01505470	CLINDAMYCIN PALMITATE HYDROCHLORIDE	100122-12	C09	sample	25507--04-4	C34H64Cl2N2O6S	699.86898	antibacterial, inhibits protein synthesis	semisynthetic; U-25179E	USP, JAN		-0.44	1.30	0.58	0.35	0.45
01505474	CEFONICID SODIUM	100122-12	C10	sample	71420-79-6	C18H17N6NaO8S3	564.55339	antibacterial	semisynthetic; SK&F-D-75073-Z	USAN, INN, BAN		1.22	1.03	-0.02	-0.44	0.45
01505480	IFOSFAMIDE	100122-12	C11	sample	3778-73-2	C7H15Cl2N2O2P	261.0896	antineoplastic	synthetic; MJF-9325, Z-4942, NSC-109724	USP, INN, BAN, JAN		0.84	1.06	4.99	0.45	1.84
	0.11% JAK2inhib	100122-12	C12	0.11% jak2inhib								-2.80	-3.38	-1.85	-1.97	-2.50
	0.11% DMSO	100122-12	D01	0.11% dmso								-1.37	0.03	-1.11	1.37	-0.27
01505482	NETILMICIN SULFATE	100122-12	D02	sample	56391-56-1	C21H45N5O15S2	671.7453	antibacterial	semisynthetic; SCH-20569	USP, INN, BAN, JAN		3.19	0.58	-0.60	0.59	0.94
01505483	DOXORUBICIN	100122-12	D03	sample	23214-92-8	C27H29NO11	543.53228	antineoplastic	semisynthetic	USAN, INN, BAN		-7.58	-9.64	-6.87	-3.89	-6.99
01505492	METHYSERGIDE MALEATE	100122-12	D04	sample	129-49-7	C25H31N3O6	469.54232	vasoconstrictor, antimigraine	semisynthetic	USP		-0.57	0.24	0.28	0.06	0.00
01505497	SOLIFENACIN SUCCINATE	100122-12	D05	sample	242478-37-1	C27H32N2O6	480.56589	muscarinic M3 antagonist	synthetic; YM-905, YM-67905	USAN, INN		-10.04	-0.18	3.00	-0.33	-1.89
01505498	ACEPROMAZINE MALEATE	100122-12	D06	sample	3598-37-6	C23H26N2O5S	442.53807	sedative	synthetic	USP,INN, BAN		0.14	-0.27	0.20	2.85	0.73
01505514	BIPERIDEN	100122-12	D07	sample	514-65-8	C21H29NO	311.47138	anticholinergic, antiparkinsonian	synthetic	USP, INN, BAN, JAN		-1.04	-0.19	0.94	-0.08	-0.09
01505530	DEXCHLORPHENIRAMINE MALEATE	100122-12	D08	sample	2438-32-6	C20H23ClN2O4	390.87031	antihistamine	synthetic	USP, INN, BAN, JAN		0.36	0.09	0.50	0.68	0.41
01505532	DILOXANIDE FUROATE	100122-12	D09	sample	3736-81-0	C14H11Cl2NO4	328.15407	amoebicide	synthetic	USP		-0.17	0.87	0.09	-0.31	0.12
01505537	ETIDRONATE DISODIUM	100122-12	D10	sample	7414-83-7	C2H6Na2O7P2	249.99312	bone resorption inhibitor	synthetic	USP, BAN, JAN		0.53	0.30	0.61	1.30	0.68
01505560	NATAMYCIN	100122-12	D11	sample	7681-93-8	C33H47NO13	665.74144	antibacterial	Steptomyces natalensis; CL-12625, A-5283	USP, INN, BAN, JAN		-6.17	2.01	1.15	1.45	-0.39
	0.11% JAK2inhib	100122-12	D12	0.11% jak2inhib								-2.32	-2.45	2.06	-0.97	-0.92
	0.11% JAK2inhib	100122-12	E01	0.11% jak2inhib								-3.68	-3.04	-4.02	-3.00	-3.43
01505562	NORGESTIMATE	100122-12	E02	sample	35189-28-7	C23H31NO3	369.50842	progestin	semisynthetic	USP, INN, BAN		-0.25	-0.90	-1.58	0.79	-0.48
01505576	TERAZOSIN HYDROCHLORIDE	100122-12	E03	sample	70024-40-7	C19H26ClN5O4	423.90317	antihypertensive	synthetic; Abbott-45975	USP, INN, BAN, JAN		-0.70	-1.17	-0.21	-0.03	-0.53
01505581	TIOCONAZOLE	100122-12	E04	sample	65899-73-2	C16H13Cl3N2OS	387.71781	antifungal	synthetic; UK-20349	USP, INN, BAN, JAN		-1.00	-0.83	-0.77	-0.11	-0.68
01505584	ERGOTAMINE TARTRATE	100122-12	E05	sample	379-79-3	C38H43N5O10	729.79391	analgesic, antimigraine	Claviceps purpurea	USP, INN, BAN, JAN		-2.83	-1.15	-0.84	-2.06	-1.72
01505590	ANAGRELIDE HYDROCHLORIDE	100122-12	E06	sample	58579-51-4	C10H8Cl3N3O	292.55376	antithrombotic	synthetic; BL-4162a	USAN, INN, BAN		0.58	0.73	0.36	0.36	0.51
01505599	ETOMIDATE	100122-12	E07	sample	33125-97-2	C14H16N2O2	244.29582	sedative	synthetic	USAN, INN, BAN		-0.97	-1.40	0.17	-0.99	-0.80
01505610	LAMOTRIGINE	100122-12	E08	sample	84057-84-1	C9H7Cl2N5	256.09564	anticonvulsant	synthetic; BW-430C	USAN, INN, BAN		-0.57	0.42	1.91	0.59	0.59
01505622	RALOXIFENE HYDROCHLORIDE	100122-12	E09	sample	82640-04-8	C28H28ClNO4S	510.05666	antiestrogen	synthetic-LY-156758	USAN, INN, BAN		-0.12	-0.08	-0.67	1.19	0.08
01505637	CEFPODOXIME PROXETIL	100122-12	E10	sample	87239-81-4	C21H27N5O9S2	557.60544	antibacterial	semisynthetic; U-76252, CS-807	USP, INN, BAN, JAN		-5.69	-0.31	0.10	0.94	-1.24
01505639	TADALAFIL	100122-12	E11	sample	171596-29-5	C22H19N3O4	389.41443	erectile dysfunction therapy	synthetic; IC-351	USAN, INN		-8.01	-0.39	-0.15	0.27	-2.07
	0.11% DMSO	100122-12	E12	0.11% dmso								0.17	-0.32	-0.65	-0.71	-0.38
	0.11% JAK2inhib	100122-12	F01	0.11% jak2inhib								-3.06	-3.22	-3.78	-2.16	-3.05
01505650	AMINOPENTAMIDE	100122-12	F02	sample	119793-66-7	C19H26N2O5S	394.49347	antispasmodic, antiemetic	synthetic; NND-1962	USP		-0.90	-1.22	-1.45	-0.25	-0.96
01505652	ARSANILIC ACID	100122-12	F03	sample	98-50-0	C6H8AsNO3	217.05716	antibacterial	synthetic; AS-101	USP, INN, BAN		1.12	-0.24	-0.38	0.40	0.22
01505656	PANTHENOL	100122-12	F04	sample	16485-10-2	C9H19NO4	205.25608	vitamin B5 precursor, radioprotectant	various plants	USP, INN, BAN, JAN		-0.33	1.10	0.60	0.72	0.52
01505660	PHENTERMINE	100122-12	F05	sample	122-09-8	C10H15N	149.23775	anorexic	synthetic	USAN, INN, BAN		-0.58	-1.50	-0.41	-0.24	-0.68
01505675	TRIENTINE HYDROCHLORIDE	100122-12	F06	sample	38260-01-4	C6H20Cl2N4	219.1591	chelating agent	synthetic; MK-0681	USP, INN, BAN		1.08	-0.21	3.37	-0.47	0.94
01505677	TICLOPIDINE HYDROCHLORIDE	100122-12	F07	sample	53885-35-1	C14H15Cl2NS	300.25235	PAF inhibitor	synthetic; 53-32C, 4-C-32	USAN, INN, BAN, JAN		0.11	0.07	-0.03	-0.58	-0.11
01505678	TICARCILLIN DISODIUM	100122-12	F08	sample	4697-14-7	C15H14N2Na2O6S2	428.39623	antibacterial	synthetic	USP, INN, BAN		0.56	0.62	0.74	0.01	0.48
01505679	TETRAMIZOLE HYDROCHLORIDE	100122-12	F09	sample	5086-74-8	C11H13ClN2S	240.75666	anthelmintic	synthetic; R-8299, McN-JR-8299-11	USAN, INN, BAN		-0.25	0.24	0.76	0.91	0.41
01505681	TOLTRAZURIL	100122-12	F10	sample	69004-03-1	C18H14F3N3O4S	425.38918	coccidiostat	synthetic; BAY-Vi-9142	USAN, INN, BAN		0.06	0.34	-0.91	-0.01	-0.13
01505682	TOREMIPHENE CITRATE	100122-12	F11	sample	89778-27-8	C32H36ClNO8	598.09862	antineoplastic, anti-estrogen	synthetic; FC-1157a	USAN, INN, BAN		1.06	0.62	0.26	0.47	0.60
	0.04% DMSO	100122-12	F12	0.04% dmso								0.70	0.60	0.51	0.36	0.54
	0.04% JAK2inhib	100122-12	G01	0.04% jak2inhib								-2.11	-2.50	0.54	-1.58	-1.41
01505683	ROLIPRAM	100122-12	G02	sample	61413-54-5	C16H21NO3	275.35067	tranquilizer	synthetic; ZK-62711	USAN, INN		0.23	-0.88	-1.06	-0.13	-0.46
01505684	ROLITETRACYCLINE	100122-12	G03	sample	751-97-3	C27H33N3O8	527.57936	antibacterial	semisynthetic; SQ-15659	USP-XXII, INN, BAN, JAN		1.26	0.01	1.03	0.67	0.74
01505690	PIPAMPERONE	100122-12	G04	sample	1893-33-0	C21H30FN3O2	375.49055	antipsychotic	synthetic; R-3345	USAN, INN, BAN		0.54	-0.68	-0.94	-1.37	-0.61
01505692	PANCURONIUM BROMIDE	100122-12	G05	sample	15500-66-0	C35H60Br2N2O4	732.68745	neuromuscular blocker	synthetic; ORG-NA-97	USAN, INN, BAN, JAN		-0.39	-0.30	0.02	-0.01	-0.17
01505701	FUMAZENIL	100122-12	G06	sample	78755-81-4	C15H14FN3O3	303.29553	benzodiazepine antagonist	synthetic; Ro-15-1788/000	USP, INN, BAN		0.39	-0.01	0.02	-0.19	0.05
01505703	ALTRENOGEST	100122-12	G07	sample	850-52-2	C21H26O2	310.44017	progestinantineoplastic	synthetic; RU-2267, A-35957	USAN, INN, BAN		-0.06	-0.19	-0.47	-0.14	-0.22
01505704	BISOPROLOL FUMARATE	100122-12	G08	sample	104344-23-2	C22H35NO8	441.52615	beta-blocker, antihypertensive	synthetic; CL-297939	USP, JAN		0.41	2.81	-0.32	0.13	0.76
01505705	FLUDARABINE PHOSPHATE	100122-12	G09	sample	75607-67-9	C10H13FN5O7P	365.21661	antineoplastic	synthetic;	USP, INN, BAN		0.71	3.78	0.27	0.13	1.22
01505706	MUPIROCIN	100122-12	G10	sample	12650-69-0	C26H44O9	500.63518	antibacterial, antimycoplasmal, isoleucyl-tRNA synthetase inhibitor	Pseudomonas fluorescens; BRL-4910A	USP, INN, BAN	J Antibiotics 31:330 (1978); Biochem J 176:305 (1978);	0.66	1.22	0.87	0.01	0.69
01505707	TEICOPLANIN [A(2-1) shown]	100122-12	G11	sample	61036-62-2	C88H95Cl2N9O33	1877.68485	antibacterial	Actinoplanes teichomyceticus; MDL-507	USAN, INN, BAN		1.15	1.55	0.80	-0.04	0.87
	0.04% DMSO	100122-12	G12	0.04% dmso								0.91	2.70	-0.19	0.22	0.91
	0.04% JAK2inhib	100122-12	H01	0.04% jak2inhib								-2.94	-2.46	-3.48	-4.68	-3.39
01505708	EPIRUBICIN HYDROCHLORIDE	100122-12	H02	sample	56390-09-1	C27H30ClNO11	579.99325	antineoplastic	synthetic; IMI-28	USAN, INN, BAN, JAN		-11.12	-16.09	-12.37	-5.86	-11.36
01505709	VECURONIUM BROMIDE	100122-12	H03	sample	50700-72-6	C34H57BrN2O4	637.74839	neuromuscular blocker	synthetic; ORG-NC-45	USAN, INN, BAN, JAN		-0.02	-0.57	-0.57	-0.39	-0.39
01505710	ALISKIREN HEMIFUMARATE	100122-12	H04	sample	173334-57-1	C34H57N3O10	667.84749	renin inhibitor	synthetic	USAN, INN		-5.92	-1.53	3.00	1.89	-0.64
01505711	ACAMPROSATE CALCIUM	100122-12	H05	sample	77337-73-6	C10H20CaN2O8S2	400.4875	alcohol antagonist	synthetic	USAN, INN, BAN		0.46	0.82	-0.60	-0.38	0.07
01505712	PREDNISOLONE SODIUM PHOSPHATE	100122-12	H06	sample	125-02-0	C21H27Na2O8P	484.39794	antiinflammatory, glucocorticoid	semisynthetic	USP, JAN		0.24	0.74	-0.64	0.24	0.15
01505713	PREGNENOLONE SUCCINATE	100122-12	H07	sample	4598-67-8	C25H36O5	416.56267	glucocortcoid, antiinflammatory	semisynthetic	USAN, INN, BAN		-5.05	-0.28	0.79	-0.16	-1.18
01505714	DARIFENACIN HYDROBROMIDE	100122-12	H08	sample	133099-07-7	C28H31BrN2O2	507.47547	M3 muscarinic antagonist, bladder suppressant	synthetic; UK-88525-04	USAN, INN, BAN		-8.25	-1.46	-0.50	-0.50	-2.68
01505722	DESOXYMETASONE	100122-12	H09	sample	382-67-2	C22H29FO4	376.47243	antiinflammatory	semisynthetic; HOE-304, R-2113, A-41-304	USP		1.73	1.63	0.70	1.79	1.46

Compound ID	MolNAME	plate	position	Content	cas#	Formula	MolWt	Bioactivity	Source	Status	Reference	Screen Score (z-score) rep1	rep2	rep3	rep4	Average
01505723	BETAMETHASONE ACETATE	100122-12	H10	sample	987-24-6	C24H31FO6	434.50947	antiinflammatory	semisynthetic	USP, BAN, JAN		1.34	1.22	1.12	1.09	1.19
01505751	ERYTHROSINE SODIUM	100122-12	H11	sample	16423-68-0	C20H6I4Na2O5	879.86502	color additive	synthetic	USP-XXII	JACS 49:1594 (1927); Food Cosmet Toxicol 14:525 (1976)	2.54	0.22	1.95	0.48	1.29
	empty	100122-12	H12	sample								NA	NA	NA	NA	NA
	empty	100122-13	A01	sample								NA	NA	NA	NA	NA
01505724	ISOFLUPREDNONE ACETATE	100122-13	A02	sample	338-98-7	C23H29FO6	420.48238	antiinflammatory	semisynthetic; U-6013	USP		0.60	0.80	-0.82	-0.22	0.09
01505725	BETAMETHAZONE SODIUM PHOSPHATE	100122-13	A03	sample	151-73-5	C22H28FNa2O8P	516.41546	antiinflammatory, glucocorticoid	semisynthetic	USP, BAN, JAN		1.84	-1.34	-1.03	0.31	-0.05
01505727	MELENGESTROL ACETATE	100122-13	A04	sample	2919-66-6	C25H32O4	396.53139	antineoplastic, progestin	semisynthetic; BDH-1921, 5373, NSC-70968	USAN, INN, BAN		-0.38	0.46	-0.42	-0.83	-0.29
01505728	PHTHALYLSULFACETAMIDE	100122-13	A05	sample	131-69-1	C16H14N2O6S	362.36378	antibacterial	synthetic	NF-XIII, BAN	J Indian Chem Soc 26:130 (1949)	-0.47	-0.27	-0.62	-1.59	-0.74
01505765	TRICHLORFON	100122-13	A06	sample	52-68-6	C4H8Cl3O4P	257.43876	antihelmintic	synthetic; Bayer-L-1359, DETF	USAN	Biochem Pharmacol 24:717 (1975); Arch Toxicol 41:31	-0.79	-0.72	0.04	-1.14	-0.66
01505778	BEPHENIUM HYDROXYNAPTHOATE	100122-13	A07	sample	3818-50-6	C28H29NO4	443.54763	anthelmintic	synthetic	USP-XXI, INN, BAN	Experientia 30:1265 (1974)	-1.21	0.01	0.41	-0.82	-0.40
01505780	DIPERODON HYDROCHLORIDE	100122-13	A08	sample	537-12-2	C22H28ClN3O4	433.93916	analgesic, anesthetic	synthetic	USP-XXII, INN, BAN		-0.10	-1.26	-0.49	-0.14	-0.50
01505777	DIATRIZOIC ACID	100122-13	A09	sample	117-96-4	C11H9I3N2O4	613.91858	radiopaque agent	synthetic	USP, BAN, JAN	Anal Profiles Drug Subst 4:137 (1975)	-0.45	-1.20	0.72	-0.53	-0.37
01505715	PANTOTHENIC ACID(d) Na salt	100122-13	A10	sample	63409-48-3	C9H16NNaO5	241.22137	vitamin B5	rice bran, queen bee jelly	USP, INN, JAN	Biophys Res Commun 38:181 (1970)	-0.29	-0.03	3.48	0.57	0.93
01505726	DESONIDE	100122-13	A11	sample	638-94-8	C24H32O6	416.51904	antiinflammatory, glucocorticoid	semisynthetic; D-2083	USAN, INN, BAN		-0.74	-3.03	-2.82	-3.05	-2.41
	0.04% JAK2inhib	100122-13	A12	0.04% jak2inhib								-1.68	-2.18	-2.38	-1.07	-1.83
	0.04% DMSO	100122-13	B01	0.04% dmso								-0.59	-0.74	-2.58	-1.22	-1.29
01505753	GLYCOPYRROLATE	100122-13	B02	sample	596-51-0	C19H28BrNO3	398.34391	anticholinergic	synthetic; AHR-504	USAN, INN, BAN, JAN	J Pharm Pharmacol 26:352 (1974); Toxicol Appl Pharmacol	0.03	-0.32	-1.55	3.24	0.35
01505756	ITRACONAZOLE	100122-13	B03	sample	84625-61-6	C35H38Cl2N8O4	705.65031	antifungal	synthetic; R51211	USAN, INN, BAN, JAN		-0.85	-0.57	2.24	0.34	0.29
01505760	OCTISALATE	100122-13	B04	sample	118-60-5	C15H22O3	250.34079	sunscreen	synthetic	USP, INN		0.40	0.80	0.01	0.69	0.48
01505763	RIBOFLAVIN 5-PHOSPHATE SODIUM	100122-13	B05	sample	130-40-5	C17H20N4NaO9P	478.33395	vitamin, enzyme cofactor	widespread in plants and animals	USP, JAN	Helv Chim Acta 35:457 (1952)	1.84	-0.21	-1.01	-0.42	0.05
01505781	SELEGILINE HYDROCHLORIDE	100122-13	B06	sample	14611-52-0	C13H18ClN	223.74811	antidepressant, MAO inhibitor, antiparkinsonian	synthetic	USP, INN, BAN	J Org Chem 42:2637 (1977); Am J Psychiatry 150:321	0.01	-0.45	1.93	0.00	0.37
01505782	CEFTAZIDIME	100122-13	B07	sample	72558-82-8	C22H22N6O7S2	546.58464	antibacterial	semisynthetic	USP, INN, BAN, JAN	J Antimicrobial Chemother 12(suppl A):1 (1983); Drugs	-0.77	-0.67	0.74	0.20	-0.13
01505805	GABAPENTIN	100122-13	B08	sample	60142-96-3	C9H17NO2	171.24134	anticonvulsant	synthetic; CI-945; GOE-3450	USAN, INN, BAN		-0.72	0.12	0.84	-0.03	0.05
01505819	ELETRIPTAN HYDROBROMIDE	100122-13	B09	sample	177834-92-3, 143322-58-	C22H27BrN2O2S	463.44069	5-HT agonist, anti-migrane	synthetic; UK-116044-04	USAN, INN, BAN		-4.08	-1.71	0.52	2.39	-0.72
01505851	ARIPIPRAZOLE	100122-13	B10	sample	129722-12-9	C23H27Cl2N3O2	448.39654	antipsychotic, 5HT2A antagonist	synthetic; OPC-14597, OPC-31	USAN, INN, BAN	J Med Chem 41:658 (1998); J Clin Psychiatry 63:763	-7.58	-2.90	-0.98	-0.78	-3.06
01505906	ZILEUTON	100122-13	B11	sample	111406-87-2	C11H12N2O2S	236.29449	5-lipoxygenase inhibitor	synthetic; Abbott-64077	USP, INN, BAN		1.24	-0.76	0.53	0.71	0.43
	0.04% JAK2inhib	100122-13	B12	0.04% jak2inhib								0.81	-3.14	0.95	-1.03	-0.60
	0.04% DMSO	100122-13	C01	0.04% dmso								-0.34	-0.59	-2.73	0.60	-0.76
01505907	METHYLPHENIDATE HYDROCHLORIDE	100122-13	C02	sample	298-59-9, 113-45-1(base)	C14H20ClNO2	269.774	CNS stimulant	synthetic	USP, INN, BAN, JAN	Helv Chim Acta 27:1748 (1944); J Pharmacol Exp Therap	-0.78	1.90	1.14	1.20	0.86
01505943	RABEPRAZOLE SODIUM	100122-13	C03	sample	117976-90-6	C18H20N3NaO3S	381.4322	gastric acid secretion inhibitor	synthetic; LY-307640, E-3810	USAN, INN, BAN		0.40	0.76	-0.66	-0.70	-0.05
01505944	RISEDRONATE SODIUM HYDRATE	100122-13	C04	sample	115436-72-1	C7H16NNaO10P2	359.14367	calcium regulator	synthetic; NE-58095	USAN		-3.53	-0.33	-0.46	2.59	-0.43
01505953	SUCRALOSE	100122-13	C05	sample	56038-13-2	C12H19Cl3O8	397.63943	sweetener	semisynthetic	NF, BAN	Arch Oral Biol 27:693 (1982); Trends Biochem Sci 3:61	1.43	-0.41	0.02	0.02	0.26
01505955	COLISTIN SULFATE	100122-13	C06	sample	1264-72-8	C52H102N16O21S2	1351.61534	antibacterial	Bacillus polymyxa colistinus; polymyxin E	USP, INN, BAN, JAN	J Biochem (Tokyo) 54:25, 173, 412 (1963); J Chem Soc	-4.17	-0.61	-1.46	-0.20	-1.61
01505957	ARSENIC TRIOXIDE	100122-13	C07	sample	1327-53-3	As4O6	395.6828	antineoplastic, antileukemia	mineral	USAN, JAN	Pharmacol Ther 76:141 (1997); Blood 93:268 (1999); N	0.59	-0.44	0.48	0.22	0.21
01505958	CLONAZEPAM	100122-13	C08	sample	1622-61-3	C15H10ClN3O3	315.71825	anticonvulsant, sedative	synthetic	USP-XII	Pediatr Neurol 9:465 (1993); J Forensic Sci 40:382 (1995);	-7.28	-1.78	-0.72	-1.03	-2.70
01505971	BENZBROMARONE	100122-13	C09	sample	117976-90-6	C17H12Br2O3	424.09139	uricosuric	synthetic; MJ-10061, L-2214	USAN, INN, BAN		-0.62	0.00	0.08	-0.64	-0.29
01505972	BROMPERIDOL	100122-13	C10	sample	10457-90-6	C21H23BrFNO2	420.32536	antipsychotic	synthetic; R-11333	USAN, INN, BAN, JAN		1.19	0.80	1.37	0.30	0.92
01505973	CYPROHEPTADINE HYDROCHLORIDE	100122-13	C11	sample	41354-29-4	C21H22ClN	323.86919	H1-antihistamine, antipruritic	synthetic	USP, INN, BAN, JAN		-2.16	-2.01	0.54	1.77	-0.46
	0.11% JAK2inhib	100122-13	C12	0.11% jak2inhib								-0.04	-4.47	0.73	-3.66	-1.86
	0.11% DMSO	100122-13	D01	0.11% dmso								-1.62	-1.66	-2.50	-2.23	-2.00
01505974	CLOFAZIMINE	100122-13	D02	sample	2030-63-9	C27H22Cl2N4	473.40919	antibacterial, antilepretic, antituberculosis	synthetiNSC-141046c; G-30320	USP, INN, BAN		0.78	1.62	-0.77	5.31	1.73
01505975	BENZYDAMINE HYDROCHLORIDE	100122-13	D03	sample	132-69-4	C19H24ClN3O	345.87563	analgesic, antipyretic, antiinflammatory	synthetic; AF-864	USAN, INN, BAN, JAN		-1.43	2.78	-1.33	3.98	1.00
01505976	DOXAZOSIN MESYLATE	100122-13	D04	sample	77883-43-3	C24H29N5O8S	547.59143	antihypertensive	synthetic; UK-33274-27	USAN, INN, BAN, JAN		2.46	0.09	-1.52	2.32	0.84
01505977	ISOETHARINE MESYLATE	100122-13	D05	sample	7279-75-6	C14H25NO6S	335.42245	bronchodilator	synthetic	USP		-0.18	-0.31	0.50	-0.03	-0.01
01505978	FLORFENICOL	100122-13	D06	sample	76639-94-6	C12H14Cl2FNO4S	358.21808	antibacterial	synthetic; SCH-25298	USAN, INN, BAN		-0.02	0.66	1.77	0.40	0.70
01505979	ETHYNODIOL DIACETATE	100122-13	D07	sample	297-76-7	C24H32O4	384.52024	progestin	semisynthetic; SC-11800	USP, INN, BAN, JAN		0.33	-0.29	-0.42	-0.73	-0.28
01505981	ORNIDAZOLE	100122-13	D08	sample	16773-42-5	C7H10ClN3O3	219.62905	antiinfective	synthetic; 16773-42-5	USAN, INN		0.82	0.42	0.42	-0.49	0.29
01505982	OXANTEL PAMOATE	100122-13	D09	sample	68813-55-8	C36H32N2O7	604.66564	anthelmintic	synthetic; CP-14445-16	USAN, INN, BAN		0.21	0.03	0.79	1.48	0.63
01505984	PROTRYPTYLINE HYDROCHLORIDE	100122-13	D10	sample	1225-55-4	C19H22ClN	299.84689	antidepressant	synthetic; MK-240	USP, INN, BAN	J Med Chem 11:325 (1968); N Engl J Med 307:1037 (1982)	-0.86	-0.55	0.13	-0.48	-0.44
01505485	PHYTONADIONE	100122-13	D11	sample	84-80-0	C31H46O2	450.71107	vitamin	semisynthetic	USP, INN, BAN		-4.03	-1.53	0.48	-0.82	-1.47
	0.11% JAK2inhib	100122-13	D12	0.11% jak2inhib								-1.96	-2.90	-2.01	-2.28	-2.29
	0.11% JAK2inhib	100122-13	E01	0.11% jak2inhib								-3.06	-3.64	-5.68	2.56	-2.45
01505987	DENATONIUM BENZOATE	100122-13	E02	sample	3734-33-6	C28H34N2O3	446.59478	denaturing agent, bitter principle	synthetic	USAN, NF, INN, BAN	Chem Ind 22:721 (1988)	-0.07	0.28	0.99	0.44	0.41
01505993	MESALAMINE	100122-13	E03	sample	89-57-6	C7H7NO3	153.13874	antiinflammatory	synthetic; 5-ASA	USP, INN, BAN	Gastroenterology 83:1062 (1982); Am J Gastroenterol	-0.19	-0.86	-1.16	-0.53	-0.69
01505994	ETHAMIVAN	100122-13	E04	sample	304-84-7	C12H17NO3	223.27419	CNS & respiratory stimulant	synthetic; NCS-406087	USAN, USP-XX, INN, BAN	Compt Rendu 243:609 (1956)	0.84	0.39	-0.52	0.97	0.42
01505996	AZTREONAM	100122-13	E05	sample	78110-38-0	C13H21N5O7S2	423.46962	antibacterial	synthetic; SQ-26776	USPXX11, USAN, INN, BAN		0.52	1.23	0.32	-0.46	0.40
01506053	TYLOXAPOL	100122-13	E06	sample	25301-02-4	C70H124O13	1173.76098	polymeric nonionic detergent	synthetic	USP, INN, BAN		0.94	0.51	-0.04	-0.13	0.32
01900002	THIAMYLAL SODIUM	100122-13	E07	sample	337-47-3, 77-27-0 [thiamylal]	C12H17N2NaO2S	276.33529	anesthetic	synthetic	USP-XXII, JAN		0.65	-0.70	-0.46	-0.67	-0.29
01900004	CHLORDIAZEPOXIDE	100122-13	E08	sample	438-41-5, 58-25-3	C16H14ClN3O	299.76248	minor tranquilizer, sedative	synthetic	USP, INN, BAN, JAN		-0.57	0.73	0.32	0.67	0.29
02300094	ASTEMIZOLE	100122-13	E09	sample	68844-77-9	C28H31FN4O	458.58387	H1 antihistamine (nonsedating)	synthetic	USP, INN, BAN, JAN		-0.56	-0.55	0.84	0.16	-0.03
02300154	ACECAINIDE HYDROCHLORIDE	100122-13	E10	sample	34118-92-8, 32795-44-1	C15H24ClN3O2	313.83043	antiarrhythmic	synthetic	USAN, INN		-0.21	0.20	0.70	0.52	0.30
01505430	FLUROTHYL	100122-13	E11	sample	333-36-8	C4H4F6O	182.06628	central stimulant, convulsant	synthetic; SK&F-6539	USP-XXI, INN, BAN	Anesth Analag 95:1611 (2002); 96:1010 (2003)	0.97	-0.06	0.80	0.62	0.58
	0.11% DMSO	100122-13	E12	0.11% dmso								-0.42	-0.57	-0.52	-0.80	-0.58
	0.11% JAK2inhib	100122-13	F01	0.11% jak2inhib								-1.61	-2.85	-3.79	-2.53	-2.69
02300166	ALPRENOLOL	100122-13	F02	sample	13655-52-2, 13707-88-5	C15H24ClNO2	285.81703	betaadrenergic blocker	synthetic	USAN, INN, BAN, JAN		0.18	0.00	-0.87	0.07	-0.16
02300165	AMIODARONE HYDROCHLORIDE	100122-13	F03	sample	1951-25-3	C25H30ClI2NO3	681.78455	adrenergic agonist, coronary vasodilator, Ca channel blocker	synthetic	USAN, INN, BAN, JAN	Adv Drug Res 16: 309 (1987)	0.86	0.84	-0.91	0.40	0.30
02300173	BUSPIRONE HYDROCHLORIDE	100122-13	F04	sample	33386-08-2, 36505-84-7	C21H32ClN5O2	421.97449	5HT1a receptor agonist, anxiolytic	synthetic	USP, INN, BAN		0.29	0.79	-0.16	0.54	0.36
02300242	LOXAPINE SUCCINATE	100122-13	F05	sample	27833-64-3, 1977-10-2	C22H24ClN3O5	445.90668	antipsychotic	synthetic	USP		-0.14	0.61	-0.05	-0.11	0.08
02300206	DIAZOXIDE	100122-13	F06	sample	364-98-7	C8H7ClN2O2S	230.67419	antihypertensive, diuretic, activates K channels and AMPA	synthetic; SCH-6783; NSC-64198	USP, INN, BAN		0.19	-0.59	-1.19	2.96	0.34
02300214	DILTIAZEM HYDROCHLORIDE	100122-13	F07	sample	33286-22-5, 42399-41-7	C22H27ClN2O4S	450.98849	Ca channel blocker, coronary vasodilator	synthetic	USP, INN, BAN, JAN		-0.01	0.58	0.54	-0.42	0.17
02300229	GLYBURIDE	100122-13	F08	sample	10238-21-8	C23H28ClN3O5S	494.01371	antihyperglycemic	synthetic	USP, INN, BAN, JAN		-0.24	1.01	0.15	-0.24	0.17
02300292	MIANSERIN HYDROCHLORIDE	100122-13	F09	sample	21535-47-7, 24219-97-4	C18H21ClN2	300.83447	5HT antagonist	synthetic	USAN, INN, BAN, JAN		0.45	-0.11	1.79	3.41	1.38
02300309	VESAMICOL HYDROCHLORIDE	100122-13	F10	sample	120447-62-3	C17H26ClNO	295.85587	acetylcholine transport blocker (vesicular)	synthetic	USAN		0.01	0.10	0.57	-1.03	-0.09
01505985	NIZATIDINE	100122-13	F11	sample	76963-41-2	C12H21N5O2S2	331.46147	antiulcer, H2 antagonist	synthetic; LY-139037	USP, INN, BAN, JAN	Clin Pharmacol Ther 37:162 (1985); Arzneim Forsch 39:240	0.82	0.25	1.20	0.05	0.58
	0.04% DMSO	100122-13	F12	0.04% dmso								0.48	-0.78	0.38	-0.23	-0.04
	0.04% JAK2inhib	100122-13	G01	0.04% jak2inhib								-1.11	-1.75	-3.41	-0.95	-1.81
02300347	PENTYLENETETRAZOL	100122-13	G02	sample	54-95-5	C6H10N4	138.1734	analeptic, circulation stimulant	synthetic	NF-XIII, INN, BAN		-0.13	0.38	-0.65	-0.79	-0.30
02300259	NICOTINE DITARTRATE	100122-13	G03	sample	65-31-6	C18H26N2O12	462.41412	nicotinyl acetylcholine receptor agonist, ectoparasiticide	Nicotiana tabacum	USAN		0.06	1.21	-0.91	0.04	0.10
02300104	TACRINE HYDROCHLORIDE	100122-13	G04	sample	1684-40-8	C13H15ClN2	234.7309	anticholinesterase, cognitive adjuvant, K channel blocker	synthetic; CL-970	USP		0.67	0.72	-0.41	0.77	0.44
01500252	DIMERCAPROL	100122-13	G05	sample	59-52-9	C3H8OS2	124.22461	chelating agent (As, Au, Hg antidote)	synthetic	USP, INN, BAN, JAN		0.57	0.03	0.03	0.46	0.27
02300325	METOLAZONE	100122-13	G06	sample	17560-51-9	C16H16ClN3O3S	365.84122	diuretic, antihypertensive	synthetic	USP, INN, BAN, JAN		1.12	0.29	0.24	-0.12	0.38
02300161	AMOXAPINE	100122-13	G07	sample	14028-44-5	C17H16ClN3O	313.78957	antidepressant, inhibits norepinephrine uptake	synthetic	USP, INN, BAN, JAN		-2.73	-2.77	-2.58	-2.06	-2.54
01505995	BUTYL PARABEN	100122-13	G08	sample	94-26-8	C11H14O3	194.23243	antifungal, preservative	synthetic	USAN, NF, BAN		-0.80	0.19	-0.18	3.27	0.62
01505991	DECAMETHONIUM BROMIDE	100122-13	G09	sample	541-22-0	C16H38Br2N2	418.30266	neuromuscular blocker	synthetic	USP-XX, INN, BAN		0.68	-0.46	-0.02	-0.47	-0.07
01505294	CARBADOX	100122-13	G10	sample	6804-07-5	C11H10N4O4	262.22675	antibacterial	synthetic	USAN, INN, BAN	J Vet Med Sci 65:1275 (2003)	0.23	-0.29	0.55	-1.13	-0.16
01503721	ENROFLOXACIN	100122-13	G11	sample	93106-60-6	C19H22FN3O3	359.40389	antibacterial	synthetic	USAN, INN, BAN		0.74	3.39	0.40	-0.08	1.11
	0.04% DMSO	100122-13	G12	0.04% dmso								0.90	-0.01	1.05	0.16	0.52
	0.04% JAK2inhib	100122-13	H01	0.04% jak2inhib								-1.26	-1.42	-3.17	-2.76	-2.15
01505420	DEXPANTHENOL	100122-13	H02	sample	81-13-0	C9H19NO4	205.25608	cholinergic	semisynthetic	USP, INN, BAN		-0.01	-0.05	-1.28	-0.31	-0.41
01505292	NONOXYNOL-9	100122-13	H03	sample	26027-38-3	C33H60O10	616.84015	spermatocide, contraceptive	synthetic	USP, INN	J Steroid Biochem Mol Biol 65:143 (1998)	-1.57	-1.94	-2.31	-2.11	-1.98
01505729	DOCOSANOL	100122-13	H04	sample	661-19-8	C22H46O	326.61132	antiviral	Pygeum africanum	USAN	Antiviral Res 40:85 (1998)	-0.45	-0.16	-0.87	-0.16	-0.41
01505447	OCTODRINE	100122-13	H05	sample	543-82-8	C8H19N	129.24733	vasoconstrictor, anesthetic (local)	synthetic; SK&F-51	USAN, INN		-0.16	-0.56	-0.90	-0.93	-0.64
01503078	ANIRACETAM	100122-13	H06	sample	72432-10-1	C12H13NO3	219.24231	cognitive enhancer	synthetic	USAN, INN, JAN		1.90	0.03	-0.76	-0.37	0.20
01503611	PENTOXIFYLLINE	100122-13	H07	sample	6493-05-6	C13H18N4O3	278.31341	PDE inhibitor, bronchodilator, vasodilator	synthetic	USP, INN, BAN, JAN		0.02	1.09	-0.35	3.19	0.99
01505122	AZTREONAM	100122-13	H08	sample	78110-38-0	C13H17N5O8S2	435.43714	antibiotic	semisynthetic; SQ-26776	USP, INN, BAN, JAN		0.41	1.05	1.29	0.00	0.69
01500164	CEFAZOLIN SODIUM	100122-13	H09	sample	27164-46-1, 25953-19-9	C14H13N8NaO4S3	476.49271	antibacterial	semisynthetic	USP, INN, BAN		0.39	0.92	-0.13	1.07	0.56
01500602	TUBOCURARINE CHLORIDE	100122-13	H10	sample	6989-98-6, 57-94-3	C37H41ClN2O6	645.20212	muscle relaxant (skeletal)	Chondodendron spp	USP, INN, BAN, JAN	Nature 158: 515 (1946); Chem Commun 1970: 1020	1.54	0.76	0.69	1.33	1.08
01500582	TOLMETIN SODIUM	100122-13	H11	sample	64490-92-2, 26171-23-3	C15H14NNaO3	279.27353	antiinflammatory	synthetic	USP, JAN		-1.06	-1.88	-0.01	5.97	0.76
	empty	100122-13	H12	sample								NA	NA	NA	NA	NA
	empty	100122-14	A01	sample								NA	NA	NA	NA	NA
01505990	CLEMIZOLE HYDROCHLORIDE	100122-14	A02	sample	1163-36-6, 442-52-4(base)	C19H21Cl2N3	362.30532	H1-antihistamine	synthetic; AL-20	INN, BAN, JAN	Ann 575:162 (1952)	-1.67	-1.50	-0.97	-1.15	-1.32
01500632	HEXESTROL	100122-14	A03	sample	5635-50-7	C18H22O2	270.37484	estrogen, antineoplastic (hormonal)	synthetic; NSC-9894	NF-XI, INN		-0.78	-0.50	-1.56	-0.72	-0.89
01504523	FTAXILIDE	100122-14	A04	sample	19368-18-4	C16H15NO3	269.30285	antiulcer	synthetic; MP-12	INN		-1.34	-1.35	-1.17	-1.30	-1.29
01503045	ACEXAMIC ACID	100122-14	A05	sample	57-08-9	C8H15NO3	173.21365	wound healing agent	synthetic	INN, BAN		0.43	-0.75	-0.70	-0.34	-0.34
01503032	DIPYROCETYL	100122-14	A06	sample	486-79-3	C11H10O6	238.19875	antirheumatic, analgesic	synthetic	INN	Bul Chem Soc Japan 16: 284 (1941); J Pharm Pharmacol	-0.37	-0.72	-1.16	-1.06	-0.83
01505117	ESTRAGOLE	100122-14	A07	sample	140-67-0	C10H12O	148.20654	insect attractant, skin irritant, carcinogen	numerous plant essential oils	experimental	JACS 55:1556 (1933); Food Chem Toxicol 28:537 (1990)	-0.84	-0.26	-0.45	1.91	0.09
01503017	AMINOTHIAZOLE	100122-14	A08	sample	96-50-4	C3H4N2S	100.14273	antithyroid agent	synthetic; RP-2921	INN		0.79	-0.15	0.62	-1.14	0.03
01503105	BENFOTIAMINE	100122-14	A09	sample	22457-89-2	C19H23N4O6PS	466.45616	vitamin B1	Vitamin B1; 8088-CB	INN, JAN		0.08	0.29	-1.40	-0.88	-0.48
01500679	AMINOPTERIN	100122-14	A10	sample	54-62-6, 58602-66-7	C19H20N8O5	440.42185	antineoplastic, antirheumatic, folic acid antagonist	synthetic; NSC-739	INN, BAN		-6.65	-7.74	-7.80	-10.61	-8.20
00201606	RUTILANTINONE	100122-14	A11	sample	21288-61-9	C22H20O9	428.3993	coccidiostat	Streptomyces species	experimental	Chem Ber 92: 1880 (1959); 100: 2561 (1967)	0.10	0.57	-0.60	-1.16	-0.27
	0.04% JAK2inhib	100122-14	A12	0.04% jak2inhib								0.84	-1.06	-1.25	-2.86	-1.08
	0.04% DMSO	100122-14	B01	0.04% dmso								-1.73	-2.03	-0.23	-1.03	-1.26
01500195	CLOFIBRIC ACID	100122-14	B02	sample	882-09-7	C10H11ClO3	214.65037	antihyperlipoproteinemic	synthetic	INN		-0.92	-0.91	-0.85	2.48	-0.05
01505807	AVOCADENOFURAN	100122-14	B03	sample	25346-24-1	C17H28O	248.41211		Persea spp	undetermined activity	Tetrahedron 25:4617(1969); An Acad Brasil Cienc 42	-0.52	-0.34	-0.07	-0.02	-0.24
00330086	DIBUTYL PHTHALATE	100122-14	B04	sample	84-74-2	C16H22O4	278.35134	plasticiser, suspect endocrine disruptor	synthetic	NF		-0.03	-1.16	-1.37	-0.94	-0.87
01503320	TIMONACIC	100122-14	B05	sample	444-27-9	C4H7NO2S	133.16989	hepatoprotectant	synthetic	INN		-0.94	0.13	-1.69	-0.95	-0.86
00210925	METHYL ORSELLINATE	100122-14	B06	sample	3187-58-4	C9H10O4	182.17765		lichens and lichen acids	undetermined activity	Ber 56: 2556 (1923); JACS 88: 2053 (1966); Tetrahedron	-0.14	-0.55	-0.03	-1.02	-0.43
01503114	DIBEKACIN	100122-14	B07	sample	34493-98-6	C18H39N5O12S	549.60183	antibacterial	semisynthetic	INN, BAN		0.50	0.29	0.75	0.61	0.54
01503920	CLOPERASTINE HYDROCHLORIDE	100122-14	B08	sample	3703-76-2	C20H25Cl2NO	366.33435	antitussive	synthetic; HT-11	INN, JAN		-1.41	-0.05	-1.67	-1.87	-1.25
01504104	DIHYDROJASMONIC ACID	100122-14	B09	sample	98674-52-3	C12H20O3	212.2914	plant growth regulator	Jasminium spp and Vicia faba	experimental	Helv Chim Acta 57: 1301 (1974); Tet Lett 3413 (1974);	0.76	0.27	0.01	-0.24	0.20
01500641	PENTAMIDINE ISETHIONATE	100122-14	B10	sample	100-33-4	C23H36N4O10S2	592.69217	antiprotozoal, inhibits nucleic acid & protein synthesis	synthetic; MB-800, RP-2512	INN, BAN, JAN		-0.98	-1.53	-0.67	-1.54	-1.18
00310006	HYDRASTININE HYDROCHLORIDE	100122-14	B11	sample	4884-68-8, 6592-85-4	C11H14ClNO3	243.69213	cardiotonic, uterine hemostatic	derivative of hydrastine (01501009)	INN, NF-VIII		0.91	0.15	-1.45	-2.07	-0.62
	0.04% JAK2inhib	100122-14	B12	0.04% jak2inhib								0.11	-0.57	-1.57	-1.66	-0.92
	0.04% DMSO	100122-14	C01	0.04% dmso								-2.04	-1.52	-0.85	-0.30	-1.18
01500281	ERYTHROMYCIN STEARATE	100122-14	C02	sample	643-22-1; 114-07-8(base)	C55H103NO15	1018.43186	antibacterial	Streptomyces erythreus	INN, BAN, JAN		-7.55	-2.98	-1.38	0.62	-2.82
01300042	SODIUM TETRADECYL SULFATE	100122-14	C03	sample	139-88-8	C14H29NaO4S	316.43863	sclerosing agent	synthetic	INN	J Ind Hyg Toxicol 30:63 (1948)	2.55	-0.07	-0.59	-0.57	0.33
01505256	SILIBININ	100122-14	C04	sample	22888-70-6	C25H22O10	482.44809	hepatoprotective agent, antioxidant	Silybum marianum	INN	Arzneim-Forsch 20: 1248 (1970); Chem Ber 108: 790, 1482	-2.12	-1.02	-1.89	-2.06	-1.77
01500633	HEXETIDINE	100122-14	C05	sample	141-94-6	C21H45N3	339.6129	antifungal	synthetic	BAN		-0.12	1.16	0.93	1.08	0.76

Compound ID	MolNAME	plate	position	Content	cas#	Formula	MolWt	Bioactivity	Source	Status	Reference	Screen Score (z-score) rep1	rep2	rep3	rep4	Average
01503222	FIPEXIDE HYDROCHLORIDE	100122-14	C06	sample	34161-24-5	C20H22Cl2N2O4	425.31534	psychostimulant	synthetic	INN	hepatotoxic at clinical dose (600mg)	1.89	-0.44	-0.98	-0.44	0.01
01500898	EMODIN	100122-14	C07	sample	518-82-1	C15H10O5	270.24395	antibacterial, antineoplastic, cathartic, tyrosine kinase inhibitor	Cascara, Rheum and Rhamnnus species	experimental	Oncogene 17: 913 (1998); Planta Med 65: 9 (1999); Clin	1.63	-0.10	-0.20	-0.26	0.27
01505168	ETHACRIDINE LACTATE	100122-14	C08	sample	1837-57-6; 6402-23-9 (hydrate)	C18H21N3O4	343.38577	antiseptic, abortifaceant	synthetic	INN, BAN, JAN	Clin Obster Gynacol 11:573 (1984)	-0.99	-0.53	-0.82	0.00	-0.58
01506049	meta-CRESYL ACETATE	100122-14	C09	sample	122-46-3	C9H10O2	150.17885	antiseptic (topical)	synthetic	INN		0.02	0.38	0.33	0.38	0.28
01505300	PURPURIN	100122-14	C10	sample	81-54-9	C14H8O5	256.21686	xanthin oxidase inhibitor, irritant	Rubia and Galllium spp	experimental	J Chem Soc 1928:229; 1929:1399; 1931:3206; Anticancer	-0.13	1.65	1.08	3.05	1.41
01502012	FOSFOSAL	100122-14	C11	sample	6064-83-1	C7H7O6P	218.10404	analgesic, antiinflammatory	synthetic	INN		1.24	2.23	3.78	0.00	1.81
	0.11% JAK2inhib	100122-14	C12	0.11% jak2inhib								-1.91	-1.34	-1.15	3.03	-0.34
	0.11% DMSO	100122-14	D01	0.11% dmso								-2.09	-0.60	-2.10	-0.74	-1.38
01503080	AMBROXOL HYDROCHLORIDE	100122-14	D02	sample	23828-92-4, 18683-91-5	C13H19Br2ClN2O	414.57018	expectorant	synthetic	INN, BAN, JAN		-1.35	-1.32	-1.11	0.76	-0.75
01505276	CAPSANTHIN	100122-14	D03	sample	465-42-9	C40H56O3	584.89052	antineoplastic	Capsicum annum	experimental		-0.35	0.79	1.80	1.46	0.93
01505155	3-HYDROXYTYRAMINE	100122-14	D04	sample	62-31-7	C8H11NO2	153.18237	dopaminergic	synthetic	experimental	Am J Physiol 267:R628 (1994); FEBS Lett 325:215 (1993)	-1.01	-0.94	-0.33	-1.19	-0.87
00201664	CELASTROL	100122-14	D05	sample	34157-83-0	C29H38O4	450.62381	antineoplastic, antiinflamatory, NO synthesis inhibitor, chaperone	Celastrus scandens & Tripterygium wilfordii	experimental	J Chem Soc 1963: 2884; 1972: 330; J Org Chem 30: 1729	0.03	1.85	0.98	0.27	0.78
01505293	DIALLYL SULFIDE	100122-14	D06	sample	592-88-1	C6H10S	114.2106	antibacterial, antifungal, antineoplastic, antihypercholesterolaemic,	Allium spp, Wasabia japonica	experimental	Arch Biochem Biophys 107:137 (1964); JACS 104:312	-0.04	-0.21	-1.50	-0.01	-0.44
00100528	PEUCENIN	100122-14	D07	sample	578-72-3	C11H16O4	260.29237		Peucedanum ostruthium, Ptaeroxylon obliquum	undetermined activity	Ber 74:1851 (1941); J Chem Soc (C) 1967:145	-0.06	0.19	-0.01	-1.32	-0.30
00107108	5alpha-ANDROSTAN-3,17-DIONE	100122-14	D08	sample		C19H28O2	288.43381	androgen	human urine & adrenal cortex	experimental		1.22	0.84	0.09	2.39	1.13
00212151	CHLORQUINALDOL	100122-14	D09	sample	72-80-0	C10H7Cl2NO	228.07939	antiinfectant, antifungal	synthetic	INN, BAN		1.56	1.17	0.43	-0.49	0.67
01503711	ORBIFLOXACIN	100122-14	D10	sample	113617-63-3	C19H20F3N3O3	395.38475	antibacterial	synthetic	INN		0.89	0.98	-0.16	-0.89	0.21
01501199	ZAPRINAST	100122-14	D11	sample	37762-06-4	C13H13N5O2	271.28086	cGMP phosphodiesterase inhibitor	synthetic; M&B-22948	INN, BAN		0.38	0.57	0.28	0.18	0.35
	0.11% JAK2inhib	100122-14	D12	0.11% jak2inhib								-2.14	-0.83	-1.51	-3.94	-2.10
	0.11% JAK2inhib	100122-14	E01	0.11% jak2inhib								-3.69	-2.92	-4.31	-2.30	-3.30
00102058	OLEANOLIC ACID ACETATE	100122-14	E02	sample	4339-72-4	C32H50O4	498.7529		birch bark	undetermined activity	J Chem Soc 1939: 1047	-2.60	-3.35	1.67	-2.43	-1.68
00210658	DEHYDROVARIABILIN	100122-14	E03	sample		C17H14O4	282.29873		Dalbergia variabilis	undetermined activity	Phytochemistry 17: 1417 (1978)	0.22	0.28	-0.05	0.75	0.30
00211475	4'-METHOXYCHALCONE	100122-14	E04	sample	22966-19-4	C16H14O2	238.28878		Citrus limon	undetermined activity	Acta Cryst C 48:741 (1992)	-0.95	0.32	-0.86	0.64	-0.21
00200141	2-ETHOXYCARBONYL-2-	100122-14	E05	sample		C24H24O9	456.45348		mp 111-114 C	undetermined activity		-0.46	0.81	0.70	1.40	0.61
01506073	IDAZOXAN HYDROCHLORIDE	100122-14	E06	sample	79944-58-4	C11H13ClN2O2	240.69146	alpha2-adrenergic blocker	synthetic	INN, BAN	Ann NY Acad Sci 881:272 (1999); CNS Drug Reviews	-0.02	-0.44	0.46	0.36	0.09
01505827	BECLAMIDE	100122-14	E07	sample	501-68-8	C10H12ClNO	197.66624	anticonvulsant, antiepileptic	synthetic; mp 94 deg C	INN, BAN	J Org Chem 16:1283 (1951)	-0.34	0.98	-0.14	-0.60	-0.02
00231043	1,3,5-TRIMETHOXYBENZENE	100122-14	E08	sample	621-23-8	C9H12O3	168.19419	spasmolytic	synthetic	experimental		-0.22	0.38	0.73	0.20	0.27
00270043	3beta-HYDROXY-23,24-BISNORCHOL-5-ENIC ACID	100122-14	E09	sample		C22H34O3	346.51448		semisynthetic	undetermined activity		1.17	2.88	1.40	0.91	1.59
01504070	PHYSCION	100122-14	E10	sample	521-61-9	C16H12O5	284.27104	antibacterial, cathartic	Xanthoria lichens, Rumex spp and various Aspergillus spp.	experimental	Helv Chim Acta 8: 140 (1925); Pharmacology 14: 1 (1976)	0.12	1.19	1.16	-0.16	0.58
01503939	RIBOSTAMYCIN SULFATE	100122-14	E11	sample	25546-65-0	C17H36N4O14S	552.55887	antibacterial	Streptomyces ribosidificus	INN, BAN, JAN		1.71	0.16	-0.88	-0.13	0.21
	0.11% DMSO	100122-14	E12	0.11% dmso								0.81	1.69	0.10	-1.97	0.16
	0.11% JAK2inhib	100122-14	F01	0.11% jak2inhib								-4.15	-3.28	-3.35	-3.41	-3.55
02300345	NIPECOTIC ACID	100122-14	F02	sample	498-95-3	C6H11NO2	129.16007	GABA uptake inhibitor	synthetic	experimental	J Neurochem 25: 797 (1975); Life Sci 19: 701 (1976)	-1.55	-1.53	-0.31	0.49	-0.73
02300348	1-(2-METHOXYPHENYL)PIERAZINE HYDROCHLORIDE	100122-14	F03	sample		C11H17ClN2O	228.72394	5HT1 receptor agonist	synthetic	experimental	Biochem Pharmacol 29: 833 (1980); J Med Chem 30: 1	0.21	0.00	-1.68	-1.15	-0.66
01505870	4-HYDROXYANTIPYRINE	100122-14	F04	sample	1672-63-5	C11H12N2O2	204.23049	analgesic	synthetic	experimental		1.38	1.41	0.04	-0.03	0.70
01400010	IPRIFLAVONE	100122-14	F05	sample	35212-22-7	C18H16O3	280.32642	anabolic	synthetic	INN, JAN		-0.45	0.97	1.64	0.29	0.61
01502085	CYCLOCREATINE	100122-14	F06	sample	35404-50-3	C5H9N3O2	143.14638	regulator of creatine biosynthesis	heart & muscle tissue	experimental		0.16	0.58	1.04	0.70	0.62
01502096	alpha-CYANO-4-HYDROXYCINNAMIC ACID	100122-14	F07	sample		C10H7NO3	189.17219	inhibitor of mitochondrial pyruvate transport	synthetic	experimental		0.72	0.24	0.57	0.27	0.45
01506052	TROLOX	100122-14	F08	sample	53188-07-1	C14H18O4	250.29716	antioxidant	synthetic	experimental	Food Chem Toxicol 42:45 (2004); Bioorg Med Chem Letts	1.05	0.33	0.70	0.07	0.53
00330009	SODIUM FLUOROACETATE	100122-14	F09	sample	62-74-8	C2H2FNaO2	100.02524	inhibitor of citric acid cycle	synthetic	experimental		0.35	1.43	2.07	0.59	1.11
01505899	HYDROQUININE HYDROBROMIDE HYDRATE	100122-14	F10	sample	207386-86-5	C20H29BrN2O3	425.36973	depigmentor	semisynthetic; derivatice of quinine	experimental		0.61	2.00	1.34	0.26	1.05
01505761	OXYTHIAMINE CHLORIDE HYDROCHLORIDE	100122-14	F11	sample	614-05-1	C12H17Cl2N3O2S	338.25819	thiamine antagonist	synthesis	experimental	Science 110:162 (1949); Proc Soc Exp Med 72:165 (1949)	0.95	1.37	0.88	0.06	0.81
	0.04% DMSO	100122-14	F12	0.04% dmso								1.43	5.50	-0.06	-0.64	1.56
	0.04% JAK2inhib	100122-14	G01	0.04% jak2inhib								-1.67	-1.99	-0.30	-1.21	-1.29
00307123	ESTRONE BENZOATE	100122-14	G02	sample		C25H26O3	374.48417		semisynthetic	undetermined activity		0.16	-1.05	-1.05	-0.40	-0.58
01501126	5-AMINOPENTANOIC ACID HYDROCHLORIDE	100122-14	G03	sample		C5H12ClNO2	153.60989	GABAb antagonist	synthetic	experimental	Biochem Pharmacol 30: 1105 (1981)	0.83	2.15	0.96	0.90	1.21
01500699	ACETYLTRYPTOPHANAMIDE	100122-14	G04	sample		C13H15N3O2	245.2834	antidepressant, nutrient	synthetic	experimental		-0.79	-0.64	0.79	0.30	-0.09
01500702	ACETYLTRYPTOPHAN	100122-14	G05	sample	1218-34-4	C13H14N2O3	246.26813	antidepressant	synthetic	experimental		0.83	0.01	-0.41	0.59	0.26
01500762	ROSOLIC ACID	100122-14	G06	sample		C19H14O3	290.32163	diagnostic aid	synthetic	experimental		0.26	-0.01	0.41	0.98	0.41
01505862	2-AMINOBENZENESULFONAMIDE	100122-14	G07	sample		C6H8N2O2S	172.20686	antibacterial	synthetic	experimental		0.28	-0.36	-0.09	-0.17	-0.09
01504617	ISAXONINE	100122-14	G08	sample	4214-72-6	C7H11N3	137.18582	nerve growth stimulant	synthetic	INN	hepatotoxic at clinical dose (1500mg)	-0.29	1.22	1.05	2.59	1.14
00210515	PYROGALLIN	100122-14	G09	sample		C11H8O4	204.18401	antiinfectant	synthetic	experimental	aq KIO4 + catechol + pyrogallol	-0.37	-0.45	0.27	-0.33	-0.22
00201505	METHYL 7-DESHYDROXYPYROGALLIN-4-	100122-14	G10	sample	77-41-8	C13H10O6	262.22105		synthetic	undetermined activity		2.15	-0.57	0.54	0.63	0.69
01503207	CYCLOBENZAPRINE HYDROCHLORIDE	100122-14	G11	sample	6202-23-9, 303-53-7	C20H22ClN	311.85804	muscle relaxant (skeletal)	synthetic	USP, INN		-0.80	-0.87	-0.03	-1.00	-0.67
	0.04% DMSO	100122-14	G12	0.04% dmso								1.30	0.94	0.66	0.21	0.78
	0.04% JAK2inhib	100122-14	H01	0.04% jak2inhib								-2.55	-2.34	-2.77	1.77	-1.47
00300563	TRICHLORMETHINE	100122-14	H02	sample	555-77-1	C6H13Cl4N	240.98921	antineoplastic, cytotoxic	synthetic	INN, BAN		-0.12	-1.08	-1.13	1.75	-0.15
01500736	3,6-DIMETHOXYFLAVONE	100122-14	H03	sample		C17H14O4	282.29873		semisynthetic	undetermined activity		-0.56	-1.28	-0.22	0.22	-0.46
01500734	3,4'-DIMETHOXYFLAVONE	100122-14	H04	sample		C17H14O4	282.29873		derivative Milettia flowers	undetermined activity		-0.52	-0.05	0.04	0.11	-0.11
01505770	FURALTADONE	100122-14	H05	sample	139-91-3	C13H16N4O6	324.29567	antibacterial	synthetic; NF-260	INN, BAN		-1.41	-1.54	1.21	-0.89	-0.66
01300010	ARGININE HYDROCHLORIDE	100122-14	H06	sample	1119-34-2	C6H15ClN4O2	210.66505	ammonia detoxicant, diagnostic aid	widespread in nature	USP		0.73	1.87	0.40	1.03	1.01
01505241	SPARTEINE HYDROIODIDE	100122-14	H07	sample		C15H27IN2	362.30024	oxytocic	Lupinus spp and other Leguminosae	experimental	J Chem Soc 1949: 663	0.74	-0.68	0.01	1.14	0.30
00100114	3alpha-HYDROXY-3-DEOXYANGOLENSIC ACID	100122-14	H08	sample		C27H36O7	472.58377		Meliaceae spp	undetermined activity		-0.27	-0.17	1.02	-0.24	0.09
01300019	OXIGLUTATIONE DISODIUM SALT	100122-14	H09	sample	103239-24-3; 27025-41-8(acid)	C20H30N6Na2O12S2	656.6027	antioxidant	synthetic	JAN		0.41	0.52	0.04	0.17	0.28
00201580	POMIFERIN	100122-14	H10	sample	572-03-2	C25H24O6	420.46643	antioxidant	Maclura pomifera	experimental	JACS 61:2832 (1939); 62:651 (1940); 63:1253 (1941);	0.19	0.00	2.21	-0.66	0.44
01505895	GLYCOCHOLIC ACID	100122-14	H11	sample	475-31-0	C26H43NO6	465.63571		mammalian bile	undetermined activity		0.46	0.67	1.19	0.16	0.62
	empty	100122-14	H12	sample								NA	NA	NA	NA	NA
	empty	100122-15	A01	sample								NA	NA	NA	NA	NA
01500623	BROXYQUINOLINE	100122-15	A02	sample	521-74-4	C9H5Br2NO	302.9543	antiinfectant, disinfectant	synthetic	INN		-1.00	-1.66	-2.18	-0.89	-1.43
1503424	ALFAXALONE	100122-15	A03	sample	23930-19-0	C21H32O3	332.48739	anesthetic	semisynthetic	INN, BAN, JAN		-1.26	-0.86	-1.42	-0.11	-0.91
01500999	DROFENINE HYDROCHLORIDE	100122-15	A04	sample	1679-76-1	C20H32ClNO2	353.93654	antispasmodic	synthetic	INN		-1.82	-3.70	-2.21	-3.23	-2.74
01501000	ETHAVERINE HYDROCHLORIDE	100122-15	A05	sample	985-13-7, 486-47-5	C24H30ClNO4	431.964	antispasmodic	synthetic	INN		-0.84	0.18	-0.88	-0.80	-0.58
01501026	FENDILINE HYDROCHLORIDE	100122-15	A06	sample	113042-18-7	C23H26ClN	351.92337	coronary vasodilator	synthetic	INN		-0.43	-0.78	0.68	-0.94	-0.37
01501114	PIMETHIXENE MALEATE	100122-15	A07	sample	314-03-4	C23H23NO4S	409.50806	H1 antihistamine	synthetic; BP-400	INN		-1.48	-2.31	-3.02	-3.19	-2.50
01501159	SULMAZOLE	100122-15	A08	sample	73384-60-8	C14H13N3O2S	287.34261	cardiotonic	synthetic	INN		-0.10	0.01	0.48	-1.40	-0.25
01501170	ACETAMINOSALOL	100122-15	A09	sample	118-57-0	C15H13NO4	271.27516	analgesic, antipyretic	synthetic	INN		-0.01	1.02	1.59	-1.06	0.39
01501188	EBSELEN	100122-15	A10	sample	60940-34-3	C13H9NOSe	274.18278	antioxidant, lipoxygenase inhibitor, inhibits oxidation of LDL	synthetic	INN		-0.39	-0.64	0.29	-1.18	-0.48
01502001	ACETYL-L-LEUCINE	100122-15	A11	sample	99-15-0	C8H15NO3	173.21365	antivertigo	synthetic	INN		0.96	0.79	0.22	2.47	1.11
	0.04% JAK2inhib	100122-15	A12	0.04% jak2inhib								0.01	-1.44	-2.93	-3.84	-2.05
	0.04% DMSO	100122-15	B01	0.04% dmso								-0.08	2.03	-1.31	-0.45	0.05
01800031	URSOLIC ACID	100122-15	B02	sample	77-52-1	C30H48O3	456.71526	diuretic, antineoplastic, antiulcer	Rhododendron spp, Epigaea asiatica, surface wax of fruits	experimental	Phytochemistry 10:3279 (1971)	-0.91	-0.61	-1.53	-0.79	-0.96
00300062	METAMECONINE	100122-15	B03	sample		C10H10O4	194.1888		Accacia crombei	undetermined activity		-0.55	-1.22	-0.47	-0.09	-0.58
01503085	PYRITHYLDIONE	100122-15	B04	sample	77-04-3	C9H13NO2	167.20946	hypnotic, sedative	synthetic	INN		0.15	-0.63	-0.46	-0.02	-0.24
00201182	IRIGENOL	100122-15	B05	sample	4935-93-7	C15H10O8	318.24215		Iris spp	undetermined activity		0.62	-0.97	3.93	2.35	1.48
1503381	PASINIAZID	100122-15	B06	sample	2066-89-9	C13H14N4O4	290.28093	antibacterial (tuberculostatic)	synthetic; RD-325	INN		0.80	-0.57	0.50	-0.52	0.05
01505864	3-ACETYLCOUMARIN	100122-15	B07	sample		C11H8O3	188.18461		synthetic	experimental		0.78	-0.06	0.52	-0.77	0.12
01505863	3-ACETAMIDOCOUMARIN	100122-15	B08	sample		C11H9NO3	203.19928		synthetic	experimental		0.52	1.06	1.87	0.37	0.96
01503648	GABOXADOL HYDROCHLORIDE	100122-15	B09	sample	64603-91-4	C6H9ClN2O2	176.60383	GABAa agonist, GABAc antagonist	synthetic; THIP hydrochloride	INN	J Med Chem 24: 1377 (1981); 26: 895 (1983); Drugs of the	0.06	0.87	0.39	1.09	0.60
01503822	RAMIFENAZONE	100122-15	B10	sample	3615-24-5	C14H20ClN3O	281.788	analgesic, antipyretic, antiinflammatory	synthetic	INN		0.75	1.76	0.06	-0.27	0.57
01504100	METHOPRENE (S)	100122-15	B11	sample	40596-69-8	C19H34O3	310.48103	ectoparasiticide	synthetic	INN		-5.34	-3.30	-5.12	-4.46	-4.55
	0.04% JAK2inhib	100122-15	B12	0.04% jak2inhib								0.50	0.70	-1.76	-1.64	-0.55
	0.04% DMSO	100122-15	C01	0.04% dmso								-2.02	0.01	-2.13	-1.65	-1.45
01504187	TELENZEPINE HYDROCHLORIDE	100122-15	C02	sample	80880-90-6	C19H23ClN4O2S	406.93776	antiulcer, M1 muscarinic antagonist	synthetic	INN	Gen Pharmacol 21: 17 (1990)	-0.78	-1.17	-0.43	0.11	-0.56
01505865	6-HYDROXYTROPINONE	100122-15	C03	sample		C8H13NO2	155.19831		synthetic	experimental		-0.45	-0.55	0.36	6.26	1.41
01505779	DICHLORISONE ACETATE	100122-15	C04	sample	79-61-8	C23H28Cl2O5	455.38261	antipruretic	semisynthetic; R-25788	INN	JACS 81:2191 (1959)	2.04	-1.15	-0.46	0.14	0.14
01505788	NIFUROXAZIDE	100122-15	C05	sample	965-52-6	C12H9N3O5	275.22263	antiseptic	synthetic	INN	Ann Pharm Fr 21:287 (1963)	-1.19	-1.81	-0.24	-1.25	-1.12
00300104	2-METHYLENE-5-(2,5-DIOXOTETRAHYDROFURAN-3-	100122-15	C06	sample		C18H24O4	304.38958		derivative	undetermined activity		-1.00	-0.15	0.01	0.59	-0.14
00300105	beta-CARYOPHYLLENE ALCOHOL	100122-15	C07	sample		C15H26O	222.37387		palmarosa oil, Cymbopogon martini	undetermined activity	Aust J Chem 41: 1755 (1988)	0.08	-0.33	0.14	-0.43	-0.13
01505892	FUSARIC ACID	100122-15	C08	sample	536-69-6	C9H11NO2	165.19352	antiproliferative, dopamine beta-hydroxylase inhibitor	Fusarium spp	experimental		-0.04	-0.48	0.95	3.29	0.93
00300106	3-AMINO-beta-PINENE	100122-15	C09	sample		C10H18ClN	187.71466		synthetic	undetermined activity	Helv Chim Acta 46: 1480 (1963)	2.16	-0.01	0.34	5.70	2.05
00210505	PURPUROGALLIN	100122-15	C10	sample	569-77-7	C11H8O5	220.18341	xanthine oxidase inhibitor, antioxidant	gall of Dryophanta divisa	experimental	J Chem Soc 1949: 3271; Biotechnol Biochem 61: 890	0.51	-0.01	2.25	-0.79	0.49
00300565	METERGOLINE	100122-15	C11	sample	17692-51-2	C25H29N3O2	403.52878	analgesic, antipyretic	synthetic; FI-6337, MCE	INN, BAN		0.01	-0.29	3.02	-0.56	0.54
	0.11% JAK2inhib	100122-15	C12	0.11% jak2inhib								0.39	-1.67	-2.48	5.76	0.50
	0.11% DMSO	100122-15	D01	0.11% dmso								-1.91	-2.14	-1.71	-2.29	-2.01
01300030	OMEGA-3-ACID ESTERS (EPA shown)	100122-15	D02	sample	86227-47-6	C22H34O2	330.51508	hypolipidemic	semisynthetic; K-85	USAN		-5.26	-1.61	-1.50	-1.19	-2.39
01500626	DICHLOROPHENE	100122-15	D03	sample	97-23-4	C13H10Cl2O2	269.12945	anthelmintic	synthetic	INN, BAN		-1.14	-0.91	-0.01	0.25	-0.45
01505876	CHICAGO SKY BLUE	100122-15	D04	sample	2610-05-1	C34H24N6Na4O16S4	992.81618	inhibitor of aminoacid uptake	synthetic	experimental	J.Neurochem. 63 Suppl 1:S49A (1994); 65:96 (1995)	-0.50	-0.01	-0.54	1.45	0.10
01500636	MECYSTEINE HYDROCHLORIDE	100122-15	D05	sample	2485-62-3, 18598-63-5	C4H10ClNO2S	171.6468	mucolytic	synthetic	INN, BAN		0.48	0.54	0.46	1.34	0.71
01505992	BUFLOMEDIL HYDROCHLORIDE	100122-15	D06	sample	35543-24-9, 55837-25-7(base)	C17H26ClNO4	343.85407	vasodilator (peripheral)	synthetic	INN, BAN	Therapie 30:207, 259 (1975); Drugs 33:430 (1987)	0.33	0.81	0.00	-0.96	0.04
01503628	PRONETALOL HYDROCHLORIDE	100122-15	D07	sample	54-80-8	C15H20ClNO	265.78575	beta adrenergic agonist, antiarrhythmic	synthetic; ICI-38174, AY-6204	INN, BAN		0.21	0.37	0.17	0.79	0.39
01505898	HEMICHOLINIUM BROMIDE	100122-15	D08	sample	312-45-8	C24H34Br2N2O4	574.35758	acetylcholine antagonist	synthetic	experimental		0.96	0.06	0.16	-0.60	0.24
01503806	HOMIDIUM BROMIDE	100122-15	D09	sample	1239-45-8	C21H20BrN3	394.31765	antiprotozoal, intercalcate with DNA	synthetic	INN, BAN	J Mol Biol 13: 269 (1965); 27: 87 (1967)	-0.24	0.58	1.57	0.31	0.56
01500645	PREGNENOLONE	100122-15	D10	sample	145-13-1, 4598-67-8	C21H32O2	316.48799	glucocortcoid, antiinflammatory	semisynthetic	INN, BAN		-0.33	0.46	0.97	-0.17	0.23
01504098	PHENOTHRIN	100122-15	D11	sample	26002-80-2	C23H26O3	350.46187	ectoparasiticide	synthetic; S-2539-F	INN, BAN		-0.64	0.51	2.58	0.44	0.72
	0.11% JAK2inhib	100122-15	D12	0.11% jak2inhib								-1.62	1.52	-2.89	-4.26	-1.81
	0.11% JAK2inhib	100122-15	E01	0.11% jak2inhib								-3.98	-3.55	-3.47	-3.58	-3.64
01500669	BENFLUOREX HYDROCHLORIDE	100122-15	E02	sample	23602-78-0	C19H21ClF3NO2	387.83292	antihyperlipoproteinemic	synthetic	INN, BAN		-0.99	0.30	0.26	-1.91	-0.58
01505180	6,2'-DIMETHOXYFLAVONE	100122-15	E03	sample		C17H14O4	282.29873		derivative	undetermined activity		2.77	0.20	-0.67	-0.02	0.57
01504116	FORMESTANE	100122-15	E04	sample	566-48-3	C20H28O2	300.44496	antineoplastic, aromatase inhibitor	synthetic; CGP-32349	INN, BAN	Steroids 65: 171 (2000)	-0.11	-0.04	-0.32	0.59	0.03
01505173	BAMBUTEROL HYDROCHLORIDE	100122-15	E05	sample	81732-46-9	C18H30ClN3O5	403.9099	beta adrenergic agonist, bronchodilator, cholinesterase inhibitor	synthetic	INN, BAN	Acta Anaeth Scand 34:595 (1990); Chest c103:771 (1993)	1.02	0.17	2.89	1.58	1.42
01501004	DROPROPIZINE	100122-15	E06	sample	17692-31-8	C13H20N2O2	236.31655	antitussive	synthetic; UCB-1967	INN, BAN		1.31	1.51	2.34	2.45	1.90
01503036	DINITOLMIDE	100122-15	E07	sample	148-01-6	C8H7N3O5	225.16209	antiprotozoal	synthetic	INN, BAN		0.47	-1.22	1.90	-1.00	0.04
01505245	TROXERUTIN	100122-15	E08	sample	7085-55-4	C33H42O19	742.69129	vasoprotectant	derivative; rutin 7,3',4'-trihydroxyethyl ether; Z-6000, THR	INN, BAN		0.39	0.21	1.52	1.07	0.80
01503053	PIPENZOLATE BROMIDE	100122-15	E09	sample	125-51-9, 13473-38-6	C22H28BrNO3	434.37736	spasmolytic	synthetic	INN, BAN		0.20	0.64	-0.97	1.22	0.28
01505323	CARBIMAZOLE	100122-15	E10	sample	22232-54-8	C7H10N2O2S	186.23395	antithyroid	synthetic	INN, BAN	Clin Endocrinol 10:655 (1979)	1.52	3.36	-0.23	-0.33	1.08
01503230	NIFENAZONE	100122-15	E11	sample	2139-47-1	C17H16N4O2	308.34267	analgesic, antiinflammatory	synthetic	INN, BAN		1.73	0.47	1.21	0.50	0.98
	0.11% DMSO	100122-15	E12	0.11% dmso								-0.39	-0.28	-0.15	0.23	-0.15
	0.11% JAK2inhib	100122-15	F01	0.11% jak2inhib								-3.82	-4.34	-4.39	-4.75	-4.32

Compound ID	MolNAME	plate	position	Content	cas#	Formula	MolWt	Bioactivity	Source	Status	Reference	Screen Score (z-score) rep1	rep2	rep3	rep4	Average
01505355	LUFENURON	100122-15	F02	sample	103055-07-8	C17H8Cl2F8N2O3	511.15811	molt inhibitor, chitin synthesis inhibitor; insecticide	synthetic; CGA-184699	INN, BAN	Pakistan J Biol Sci 6:1125 (2003)	-5.29	-1.64	-2.27	-1.88	-2.77
01503231	NIMESULIDE	100122-15	F03	sample	51803-78-2	C13H12N2O5S	308.31499	antiinflammatory	synthetic; R-805	INN, BAN		-0.89	-0.31	-1.17	-1.45	-0.95
01505755	IDEBENONE	100122-15	F04	sample	58186-27-9	C19H30O5	338.44795	cognition enhancer, nootropic	synthetic	INN, BAN	Chem Pharm Bull 30:2797 (1982); Biochemistry 21:4096	0.11	1.04	-0.16	0.28	0.32
01505783	OXYPHENONIUM BROMIDE	100122-15	F05	sample	50-10-2	C21H34BrNO3	428.41403	anticholinergic, anticonvulsant	synthetic; BA-5473, C-5473	INN, BAN		-0.05	-0.09	2.67	-0.28	0.56
01503383	PEMPIDINE TARTRATE	100122-15	F06	sample	79-55-0	C14H27NO6	305.37439	ganglionic blocker, antihypertensive	synthetic	INN, BAN		0.67	0.71	-0.50	-0.35	0.13
01500634	IPRONIAZID SULFATE	100122-15	F07	sample	54-92-2, 305-33-9 [as	C9H15N3O5S	277.301	monoamine oxidase inhibitor, antidepressant	synthetic	INN, BAN		0.24	0.05	2.32	0.08	0.67
01503974	DIMETHYL 4,4-o-PHENYLENE-BIS (3-THIOPHANATE)	100122-15	F08	sample		C12H14N4O4S2	342.39778	antifungal (systemic plant)	synthetic	agricultural use		0.75	1.00	0.20	0.39	0.59
01504021	LUPININE	100122-15	F09	sample	486-70-4	C10H19NO	169.26903	antifeedant, antiinflammatory, oxytoxic	Anabasis aphylla, Lupinus spp	experimental	Helv Chim Acta 11:1062 (1928); JACS 56:2434 (1934)	-0.07	-0.53	0.09	0.02	-0.12
01504101	TETRACHLOROISOPHTHALONITRILE	100122-15	F10	sample		C8Cl4N2	265.9146	antifungal	synthetic	experimental		-1.93	-1.48	-1.58	-0.83	-1.45
00100568	SARMENTOSIDE B	100122-15	F11	sample		C34H48O13	664.75386		Strophanthus sarmentosis; mp 193-195	undetermined activity	Helv Chim Acta 31: 1719 (1948); 40: 980 (1957); 41: 736	0.74	1.74	-0.14	0.47	0.70
	0.04% DMSO	100122-15	F12	0.04% dmso								0.95	1.18	-0.13	-1.72	0.07
	0.04% JAK2inhib	100122-15	G01	0.04% jak2inhib								-2.28	-2.60	-2.89	-2.51	-2.57
01503206	CLOFOCTOL	100122-15	G02	sample	37693-01-9	C21H26Cl2O	365.34677	antibacterial	synthetic	INN		-0.57	0.42	-0.30	0.55	0.03
1300048	XYLOSE	100122-15	G03	sample	58-86-6	C5H10O5	150.13245	diagnostic aid	many woods, straw, corncobs, cottonseed hulls and pecan shells.	undetermined activity		0.40	-0.35	-1.86	-1.22	-0.76
01505786	TRICLABENDAZOLE	100122-15	G04	sample	68786-66-3	C14H9Cl3N2OS	359.66363	anthelmintic	synthetic	INN, BAN	Vet Parasitol 13:145 (1983); Vet Rec 113:315 (1983)	-0.06	1.75	-1.13	0.46	0.25
01502034	METAMPICILLIN SODIUM	100122-15	G05	sample	6489-97-0	C17H18N3NaO4S	383.40451	antibacterial	semisynthetic	INN		-0.33	0.55	-0.66	0.73	0.07
01506039	ETICLOPRIDE HYDROCHLORIDE	100122-15	G06	sample	97612-24-3, 84226-12-0 (base)	C17H26Cl2N2O3	377.31437	dopamine D2 blocker	synthetic	INN	Eur J Pharmacol 111:191 (1985); Physiol Behav 61:563	-0.11	0.32	-1.19	-1.39	-0.59
01600654	CHAULMOSULFONE	100122-15	G07	sample	473-32-5	C48H76N2O4S	777.21592	antilepretic	synthetic	INN		0.13	1.43	1.19	0.77	0.88
01504512	DEFERIPRONE	100122-15	G08	sample	30652-11-0	C7H9NO2	139.15528	iron chelating agent	synthetic	INN, BAN		-1.03	0.14	0.49	1.04	0.16
01506047	TIRATRICOL	100122-15	G09	sample	51-24-1	C14H9I3O4	621.93863	thyroid agent	synthetic	INN		2.32	-0.26	-0.16	0.14	0.51
01504504	CARSALAM	100122-15	G10	sample	2037-95-8	C8H5NO3	163.13395	analgesic	synthetic	INN, BAN		0.66	-0.58	-1.11	0.20	-0.21
01504501	beta-NAPHTHOL	100122-15	G11	sample	135-19-3	C10H8O	144.17466	anthelmintic, antiseptic	synthetic	INN, NF-XI	Austral J Chem 27:2385 (1974); Tetrahedron Letts 31:6977	0.63	0.72	0.30	-0.36	0.32
	0.04% DMSO	100122-15	G12	0.04% dmso								1.21	2.51	-0.09	0.02	0.91
	0.04% JAK2inhib	100122-15	H01	0.04% jak2inhib								-2.53	-2.52	-3.07	1.82	-1.57
01504511	CHLORALOSE	100122-15	H02	sample	158-79-93-3	C8H11Cl3O6	309.53227	anesthetic	synthetic	INN, DCF		-0.75	-0.09	-1.51	0.27	-0.52
01300099	CYSTINE	100122-15	H03	sample	56-89-3	C6H12N2O4S2	240.30154	nutrient	widespread in plants and animals	INN		1.04	-0.56	-1.81	-0.94	-0.57
01504073	UVAOL	100122-15	H04	sample	545-46-0	C30H50O2	442.7318	antineoplastic	Arctostaphylos spp, Leucothoe keiskei, Crataegus cuneata,	experimental	Bull Chem Soc Jpn 39:2313 (1966); J Pharm Sci 55:1378	-0.41	0.42	-1.81	1.51	-0.07
01506065	CLORGILINE HYDROCHLORIDE	100122-15	H05	sample	17780-72-2 (base)	C13H16Cl3NO	308.63757	MAO-A inhibitor, antidepressant, antiparkinsonian	synthetic	INN, BAN	J Neural Transm Suppl. 52:39 (1998)	-0.45	0.32	1.56	1.69	0.78
01504520	EPIESTRIOL	100122-15	H06	sample	547-81-9	C18H24O3	288.39018	estrogen	semisynthetic	INN, BAN		0.37	0.16	-0.38	0.40	0.14
1300018	GLUTAMINE (L)	100122-15	H07	sample	56-85-9	C5H10N2O3	146.14705	dietary suppliment	beetroot; widely distributed in plants	USP, INN		-0.96	1.05	0.00	-0.22	-0.03
01506027	OXALAMINE CITRATE	100122-15	H08	sample	959-14-8 (base)	C20H27N3O8	437.45349	antitussive	synthetic; SKF-9976, AF-438	INN		-0.01	-0.18	-0.37	-0.67	-0.31
01503100	URAPIDIL HYDROCHLORIDE	100122-15	H09	sample	34661-75-1	C20H30ClN5O3	423.9468	antihypertensive	synthetic	INN, BAN, JAN		0.48	3.05	0.26	1.08	1.21
01504506	TOSYLCHLORAMIDE SODIUM	100122-15	H10	sample	127-65-1	C7H7ClNNaO2S	227.64614	antiseptic, disinfestant, antiproliferative	synthetic	INN, BAN		0.50	-0.25	-0.06	-0.08	0.03
01504508	CINCHOPHEN	100122-15	H11	sample	132-60-5	C16H11NO2	249.27157	analgesic, antipyretic, antiinflammatory	synthetic	INN		1.23	0.18	-0.05	2.30	0.92
	empty	100122-15	H12	sample								NA	NA	NA	NA	NA
	empty	100122-16	A01	sample								NA	NA	NA	NA	NA
01504510	CHINIOFON	100122-16	A02	sample	8002-90-2	C9H5IiNNaO4S	373.1027	antiprotozoal, amebicide	synthetic	INN, DCF, NF-XI		-0.82	-0.82	-0.24	1.85	-0.01
01506031	PIRIBEDIL HYDROCHLORIDE	100122-16	A03	sample	3605-01-4	C16H18N4O2	298.34746	dopamine agonist	synthetic; EU-4200, ET-495	INN		-1.06	-0.70	-0.54	0.26	-0.51
01502015	NIFLUMIC ACID	100122-16	A04	sample	4394-00-7	C13H9F3N2O2	282.22408	analgesic, antiinflammatory	synthetic; UP-83	INN		1.27	-0.86	-0.77	-0.22	-0.15
1506077	METICRANE	100122-16	A05	sample	1084-65-7	C10H13NO4S2	275.34741	diuretic, antihypertensive	synthetic; SD-17102	INN, JAN		-1.78	-2.11	-1.85	-2.23	-1.99
01500938	PROTOVERATRINE B	100122-16	A06	sample	124-97-0	C41H63NO15	809.95696	antihypertensive, emetic; LD50(mouse) 0.21 mg/kg sc	Veratrum album, V viride	INN	J Biol Chem 149:271 (1943); JACS 82:2242, 2252 (1960);	0.12	-0.80	-0.13	5.76	1.24
01500618	ACRIFLAVINIUM HYDROCHLORIDE	100122-16	A07	sample	8018-07-3	C14H14ClN3	259.74078	antiinfective, intercalating agent	synthetic	NF, INN		1.20	0.53	1.27	-2.38	0.16
01505037	3-BROMO-4-METHYL-3,4-HEXAMETHYLENE-3,4-	100122-16	A08	sample		C7H11BrN2O2	235.08192	guanyl cyclase activator, NO donor, vasodilator	synthetic; DD2	experimental		0.30	0.77	0.84	-0.53	0.35
01503094	TIOXOLONE	100122-16	A09	sample	4991-65-5	C7H4O3S	168.17213	antiseborrhoic	synthetic	INN, BAN		0.26	2.39	-0.47	-0.14	0.51
00100566	DEOXYCHOLIC ACID	100122-16	A10	sample	88-44-3	C24H40O4	392.584	bile constituent	undetermined activity	J Biol Chem 238: 3846 (1963)		0.52	-0.15	-0.44	-0.87	-0.23
01504507	CHLORINDIONE	100122-16	A11	sample	1146-99-2	C15H9ClO2	256.69078	antcoagulant, Vitamine K antagonist	synthetic; G25766	INN, BAN		0.39	0.00	-1.15	2.88	0.53
	0.04% JAK2inhib	100122-16	A12	0.04% jak2inhib								-1.83	-0.70	-3.39	-2.44	-2.09
	0.04% DMSO	100122-16	B01	0.04% dmso								-1.43	-1.02	-1.39	2.76	-0.27
01503917	CLENBUTEROL HYDROCHLORIDE	100122-16	B02	sample	37148-27-9	C12H19Cl3N2O	313.65703	bronchodilator, beta2 adrenergic agonist	synthetic; NAB-365	INN, BAN, JAN		-1.01	-0.05	-1.44	-0.86	-0.84
01503606	CYPERMETHRIN	100122-16	B03	sample	52315-07-8	C22H19Cl2NO3	416.30763	insecticide	synthetic	BAN		0.45	-1.27	-1.35	-1.41	-0.90
01506079	MOXISYLYTE HYDROCHORIDE	100122-16	B04	sample	54-32-0	C16H25NO3	279.38255	alpha-adrenergic blocker	synthetic	INN, BAN, JAN	J Auton Nerv Syst 79: 191 (2000); hepatotoxic at clinical	-0.38	-1.67	-1.73	-1.26	-1.26
01900040	BARBITAL	100122-16	B05	sample	57-44-3	C8H12N2O3	184.19644	sedative	synthetic	INN	Therapeutische Monatsh 17:208 (1903)	-0.28	-0.88	-0.49	-0.62	-0.57
01506085	OXEDRINE	100122-16	B06	sample	94-07-5	C9H13NO2	167.20946	anti-obesity	citrus aurantium; SYNEPHRINE	BAN		-0.01	0.70	0.03	1.30	0.50
01506024	NAFTOPIDIL DIHYDROCHLORIDE	100122-16	B07	sample	57149-07-2	C24H30Cl2N2O3	465.4243	antihypertensive	synthetic	INN		0.57	0.41	0.31	0.21	0.38
01506056	ZARDAVERINE	100122-16	B08	sample	101975-10-4	C12H10F2N2O3	268.2219	PDE III & IV inhibitor, antiallergic	synthetic	INN	Eur Repir J 5:982 (1992); J. Pharmacol Exp Ther 270:250	0.54	0.10	-0.26	-1.24	-0.22
01505082	CYCLANDELATE	100122-16	B09	sample	456-59-7	C17H24O3	276.37903	vasodilator	synthetic; BS-572	INN, BAN, JAN	Arzneim Forsch 2:165 (1952); 3:503 (1953)	0.07	-0.33	1.80	-0.67	0.22
01505434	HALOTHANE	100122-16	B10	sample	151-67-7	C2HBrClF3	197.38247	anesthetic	synthesis	USP, INN, BAN, JAN		0.86	0.71	0.34	-0.21	0.43
01500647	VINCAMINE	100122-16	B11	sample	1617-90-9	C21H26N2O3	354.45297	vasodilator	Vinca minor	INN, BAN		0.22	1.23	0.48	-1.65	0.07
	0.04% JAK2inhib	100122-16	B12	0.04% jak2inhib								-1.22	-1.66	-2.55	-1.46	-1.72
	0.04% DMSO	100122-16	C01	0.04% dmso								-0.43	-1.37	-0.61	-0.18	-0.65
00270029	PRASTERONE ACETATE	100122-16	C02	sample	53-43-0 (praesterone)	C21H30O3	330.47145	adrenocortical hormone, antidepressant	semisynthetic	INN		-1.51	-0.78	-1.83	-1.17	-1.32
00212064	HYDROXYTOLUIC ACID	100122-16	C03	sample	83-40-9	C8H8O3	152.15116	analgesic, antiseptic	synthetic; 3-MS	INN, BAN		-0.62	0.01	-0.53	0.44	-0.18
00100424	XYLOCARPUS A	100122-16	C04	sample		C31H38O11	586.64191		Meliaceae spp	undetermined activity	Adv Med Phytochemistry 1986: 179	-3.33	-2.65	-4.47	-2.24	-3.17
01504517	DOXIFLURIDINE	100122-16	C05	sample	3094-09-5	C9H11FN2O5	246.19682	antineoplastic	synthetic	INN, JAN		0.01	3.40	2.00	-0.20	1.31
1504518	EFLOXATE	100122-16	C06	sample	119-41-5	C19H16O5	324.33637	coronary vasodilator	synthetic	INN, JAN		1.98	3.68	-0.04	3.02	2.16
01504502	BITOSCANATE	100122-16	C07	sample	4044-65-9	C8H4N2S2	192.26248	anthelmintic	synthetic; 16842	INN, MI		4.45	0.07	-0.03	2.29	1.70
01504515	DIACETAMATE	100122-16	C08	sample	2623-33-8	C10H11NO3	193.20407	analgesic, antiinflammatory	synthetic	INN, BAN		0.49	0.62	1.40	-1.19	0.33
00211175	METACETAMOL	100122-16	C09	sample	621-42-1	C8H9NO2	151.16643	analgesic	synthetic; BS-749	INN, BAN		1.03	0.93	1.51	5.18	2.16
00100447	DEACETOXY(7)-7-OXOKHIVORINIC ACID	100122-16	C10	sample		C27H36O10	520.58197		derivative	undetermined activity		-0.05	-0.36	-0.73	-1.19	-0.58
01503416	MIZORIBINE	100122-16	C11	sample	50924-49-7	C9H13N3O6	259.22046	immunosuppressant	synthetic	INN, JAN		0.62	0.72	4.16	-0.51	1.25
	0.11% JAK2inhib	100122-16	C12	0.11% jak2inhib								-0.67	-0.94	-3.76	-3.61	-2.24
	0.11% DMSO	100122-16	D01	0.11% dmso								1.94	-1.43	-1.38	-0.77	-0.41
00310050	QUININE ETHYL CARBONATE	100122-16	D02	sample	83-75-0	C23H28N2O4	396.49061	antimalarial	semisynthetic	JAN, NF-VIII		-1.80	-0.69	-1.62	-0.53	-1.16
01503200	CETRIMONIUM BROMIDE	100122-16	D03	sample	57-09-0, 6899-10-1	C19H42BrN	364.45729	antiinfectant	synthetic	NF, INN, BAN		1.16	1.48	1.16	-0.98	0.71
00100583	EUPHOL ACETATE	100122-16	D04	sample		C32H52O2	468.77004		Euphorbia spp	undetermined activity	Helv Chim Acta 37: 2306 (1954)	-4.29	-1.16	-0.54	-0.28	-1.57
00330008	2,4-DINITROPHENOL	100122-16	D05	sample	51-28-5	C6H4N2O5	184.10918	uncouples oxidative phosphorylation	synthetic	Martindale 28		-0.08	0.00	0.44	1.33	0.42
01300044	TARTARIC ACID	100122-16	D06	sample	87-69-4	C4H6O6	150.08882	pharmaceutical aid	common plant constituent	NF, JAN		0.14	2.00	-0.02	0.62	0.68
01505772	BUCETIN	100122-16	D07	sample	1083-57-4	C12H17NO3	223.27419	analgesic	synthetic	INN, BAN, JAN	Arnzneim Forsch 15:727 (1965); Chem Pharm Bull 16:1726,	0.06	0.69	2.09	0.38	0.80
01505310	REBAMIPIDE	100122-16	D08	sample	90098-04-7	C19H15ClN2O4	370.7954	antiulcer, antioxidant	synthetic	INN, JAN	Chem Pharm Bull39:2906 (1991); Dig Dis Sci 43:35S	0.15	1.27	0.68	-0.31	0.45
1300046	TYROSINE	100122-16	D09	sample	60-18-4	C9H11NO3	181.19292		widespread in nature	USP		1.03	-0.36	-0.27	-0.30	0.03
01504181	PRISTIMERIN	100122-16	D10	sample	1258-84-0	C30H40O4	464.6509	antineoplastic, antiinflammatory	Celastrus and Maytenus spp	experimental		-18.99	-4.61	-4.08	-0.96	-7.16
01505740	LIPOAMIDE	100122-16	D11	sample	3206-73-3	C8H15NOS2	205.34285	hepatoprotectant	semisynthetic; thioctic acid amide	JAN		0.07	-0.23	0.19	-0.93	-0.23
	0.11% JAK2inhib	100122-16	D12	0.11% jak2inhib								-2.40	-3.60	-3.64	-5.34	-3.74
	0.11% JAK2inhib	100122-16	E01	0.11% jak2inhib								-3.80	-3.58	-4.63	-3.06	-3.77
01502045	PIROMIDIC ACID	100122-16	E02	sample	19562-30-2	C14H16N4O3	288.30862	antibacterial	synthetic; PD-93	INN, JAN		-0.45	-0.69	3.13	-0.27	0.43
01503084	AMRINONE	100122-16	E03	sample	60719-84-8	C10H9N3O	187.20273	cardiac stimulant	synthetic	experimental		-0.16	-0.43	-0.24	0.28	-0.14
01505005	L-DEOXYALLIIN	100122-16	E04	sample	21593-77-1	C6H11NO2S	161.22407	antineoplastic	Allium spp	experimental	J Cancer Res 50:5084 (1990)	-1.42	0.00	0.62	0.59	-0.05
01506043	SOTALOL HYDROCHLORIDE	100122-16	E05	sample	959-24-0	C12H21ClN2O3S	308.82977	beta-adrenergic agonist	synthetic; MJ-1999	USP		-0.64	-0.64	0.54	0.91	0.04
01505688	PROPARACAINE HYDROCHLORIDE	100122-16	E06	sample	575-06-98	C16H27ClN2O3	330.85819	local anesthetic	synthetic	USP, INN, BAN		-0.85	0.17	0.51	3.78	0.90
1506064	CHLOROPYRAMINE HYDROCHLORIDE	100122-16	E07	sample	6170-42-9, 59-32-5 (base)	C16H21ClN3	326.27187	antihistamine	synthetic	INN, BAN		1.05	-0.71	0.09	1.23	0.41
01505315	6-AMINONICOTINAMIDE	100122-16	E08	sample	329-89-5	C6H7N3O	137.14219	antineoplastic, apoptosis inducer	synthetic	experimental	Biochem Pharmacol 50:1943 (1995); Cancer Chemother	1.06	1.67	2.38	0.38	1.37
01502102	QUINOLINIC ACID	100122-16	E09	sample		C7H5NO4	167.1222	differentiates between cerebral and forebrain NMDA receptors	synthetic	experimental		0.97	0.18	-0.63	1.04	0.39
01503205	CITIOLONE	100122-16	E10	sample	1195-16-0	C6H9NO2S	159.20813	hepatoprotectant	synthetic	INN		0.91	0.85	0.58	0.47	0.70
00100749	STROPHANTHIDINIC ACID LACTONE ACETATE	100122-16	E11	sample		C25H32O7	444.52959		semisynthetic	undetermined activity	J Biol Chem 64: 123; 65: 491 (1925)	-2.15	-2.65	-3.42	-3.33	-2.89
	0.11% DMSO	100122-16	E12	0.11% dmso								0.08	-0.25	-0.48	-1.18	-0.46
	0.11% JAK2inhib	100122-16	F01	0.11% jak2inhib								0.75	-3.61	-3.24	-1.33	-1.86
00270078	5alpha-CHOLESTANOL	100122-16	F02	sample	80-97-7	C27H48O	388.68301		eggs, faces, gall stones, adrenal tissue	undetermined activity		-3.56	-1.47	-0.93	-0.04	-1.50
01504912	OLSELTAMIVIR PHOSPHATE	100122-16	F03	sample	196618-13-0	C15H29N2O8P	396.38078	antiviral	synthetic	USAN	N Engl J Med 353:2667 (2005); Lancet 369:1056 (2007)	-6.06	-0.91	-1.15	2.72	-1.35
01300028	MANNITOL	100122-16	F04	sample	69-65-8	C6H14O6	182.17488	diuretic, sweetener, diagnostic aid	manna and seaweeds; exudates of olive and plane trees	USP		1.13	-0.54	1.10	0.78	0.62
00210242	THEAFLAVIN MONOGALLATES	100122-16	F05	sample		C36H28O16	716.61496		mixed isomers black tea (3' shown)	undetermined activity	Tet Lets 1970: 5237	0.08	-0.09	-0.15	1.72	0.39
01505762	PYRITINOL	100122-16	F06	sample	1098-97-1	C16H20N2O4S2	368.4768	cognition enhancer, nootropic	synthetic; pyrithioxin	INN, BAN, JAN	Chem Pharm Bull 25:1335 (1977; Arzniem) Forsch 19:5	0.32	-0.81	0.00	0.16	-0.08
01501111	PROTOPORPHYRIN IX	100122-16	F07	sample	553-12-8	C34H34N4O4	562.67448	hepatoprotectant	mamalian feces, avian pigment	JAN		-0.32	3.85	4.36	-0.56	1.84
01503973	2-THIOURACIL	100122-16	F08	sample	141-90-2	C4H4N2OS	128.15328	thyroid depressant	synthetic	BP-1948		-0.60	1.49	0.52	0.97	0.59
00100595	COTARNINE CHLORIDE	100122-16	F09	sample	10018-19-6, 82-54-2	C12H14ClNO3	255.70328	vasoconstrictor	Papaver pseudo-orientale	experimental	J Indian Chem Soc 12: 421 (1935); J Nat Prod 53:1302	-0.01	1.18	0.68	0.15	0.50
00100655	DIHYDROGEDUNIC ACID, METHYL ESTER	100122-16	F10	sample		C26H36O8	476.57202		derivative	undetermined activity		2.40	-1.00	0.28	-1.25	0.11
01505372	SUMATRIPTAN	100122-16	F11	sample	103628-46-2	C14H21N3O2S	295.40637	5HT agonist	synthetic; GR-43175	USAN, INN, BAN		0.91	0.40	1.83	1.63	1.19
	0.04% DMSO	100122-16	F12	0.04% dmso								1.62	1.09	-0.81	-0.38	0.38
	0.04% JAK2inhib	100122-16	G01	0.04% jak2inhib								-1.27	-0.28	-1.62	0.75	-0.61
01300043	SORBITOL	100122-16	G02	sample	50-70-4	C6H14O6	182.17488	sweetening agent and humectant	fruits of Sorbus and Crataegus spp	NF, JAN		-1.08	-0.23	1.59	-0.12	0.04
01503108	BROMOPRIDE	100122-16	G03	sample	4093-35-0	C14H22BrN3O2	344.25434	antiemetic	synthetic	INN		-1.09	-0.64	-1.77	0.09	-0.85
01505108	L-BUTHIONINE SULFOXIMINE	100122-16	G04	sample	83730-53-4	C8H18N2O3S	222.30826	inhibitor of gamma-glutamylcysteine synthetase	synthetic	experimental	J Biol Chem 254:7558 (1979); 257:13704 (1982); Bone	-0.45	1.25	1.69	3.11	1.40
01503074	ALEXIDINE HYDROCHLORIDE	100122-16	G05	sample	22573-93-9, 22782-69-0	C26H58Cl2N10	581.72516	antibacterial	synthetic	INN		-2.88	-5.07	-2.51	-1.49	-2.99
00240929	AVOCADYNE ACETATE	100122-16	G06	sample	24607-06-5	C19H34O4	326.48043	antifungal	Persea spp	experimental	Ann Acad Brasil Cienc 42 (suplemento): 45 (1970);	-0.05	0.35	2.36	-0.24	0.61
01500833	CANAVANINE	100122-16	G07	sample	543-38-4	C5H12N4O3	176.17639	NO synthase inhibitor	Canavalia ensiformis	experimental	Phytochemistry 6: 863 (1967); Eur J Pharmacol 269: 269;	0.12	-0.10	0.71	0.66	0.35
01502010	DIACERIN	100122-16	G08	sample	13739-02-1	C19H12O8	368.30269	antiinflammatory	synthetic	INN		-0.14	1.63	1.46	0.04	0.75
1401414	CRESOPIRINE	100122-16	G09	sample	4386-39-4	C10H10O4	194.1888	antiinflammatory, antpyretic	synthetic	INN		1.58	1.08	0.54	0.93	1.03
00380004	DIHYDROCELASTRYL DIACETATE	100122-16	G10	sample		C33H44O6	536.71503	chaperone stimulant	celastrol derivative	undetermined activity	J Org Chem 30: 1729 (1965)	-23.45	-1.52	-0.59	-1.41	-6.74
01504616	MEPIROXOL	100122-16	G11	sample	6968-72-5	C6H7NO2	125.12819	antihyperlipemic	synthetic	INN		0.11	2.04	0.91	0.73	0.95
	0.04% DMSO	100122-16	G12	0.04% dmso								0.97	0.80	-0.63	0.10	0.31
	0.04% JAK2inhib	100122-16	H01	0.04% jak2inhib								-3.34	-3.24	-2.28	0.92	-1.98
01300029	MEGLUMINE	100122-16	H02	sample	6284-40-8	C7H17NO5	195.21724	diagnostic aid	semisynthetic	USP, INN, BAN, JAN		-1.03	-0.98	-1.17	-0.30	-0.87
02300218	EFAROXAN HYDROCHLORIDE	100122-16	H03	sample	89197-32-0	C13H17ClN2O	252.74624	insulin secretagogue, alpha2 adrenorecetor antagonist	synthetic	INN, BAN	Naunyn Schmiedebergs Arch Pharmacol 359: 262 (1999)	-0.64	-0.46	-0.13	0.77	-0.11
01503044	CHROMOCARB	100122-16	H04	sample	4940-39-0	C10H6O4	190.15692	vascular protectant	synthetic	INN		-0.17	0.08	3.33	0.28	0.88
01502024	PIPEMIDIC ACID	100122-16	H05	sample	51940-44-4	C14H17N5O3	303.32329	antibacterial	synthetic	INN, BAN, JAN		-0.12	1.26	0.00	-0.06	0.27
01504505	CARZENIDE	100122-16	H06	sample	138-41-0	C7H7NO4S	201.20214	diuretic, carbonic anhydrase inhibitor	synthetic	INN		-0.01	1.50	-0.33	1.79	0.74
01504082	DIHYDROCELASTROL	100122-16	H07	sample		C29H40O4	452.63975		celastrol derivative	undetermined activity	J Org Chem 30: 1729 (1965)	-0.77	1.16	0.13	1.02	0.39
00100612	TOTAROL-19-CARBOXYLIC ACID, METHYL ESTER	100122-16	H08	sample		C21H30O3	330.47145		Podocarpus spp	undetermined activity	J Chem Soc 1963: 1553	1.55	0.50	-0.79	-1.03	0.06
00310016	CHAULMOOGRIC ACID	100122-16	H09	sample	502-30-7	C18H32O2	280.45454	antibacterial (mycobacteria)	Hydnocarpus and Oncola spp	experimental	J Chromatography 39: 182 (1969); Am Rev Respir Dis	-5.97	2.06	-0.42	0.20	-1.03

Compound ID	MolNAME	plate	position	Content	cas#	Formula	MolWt	Bioactivity	Source	Status	Reference	Screen Score (z-score) rep1	rep2	rep3	rep4	Average
00201716	NORSTICTIC ACID	100122-16	H10	sample	571-67-5	C18H12O9	372.29094	antibacterial	Lobaria pulmonaria, Usnea japonica, Lecanora radiosa, Parmelia	experimental	Z Naturforsch 59c: 384 (2004)	1.02	1.07	1.36	0.53	0.99
00200413	2,6-DIMETHOXYQUINONE	100122-16	H11	sample	35069-70-6	C8H8O4	168.15056	antibacterial, induces dermatitis, mutagen	Picrasmus & Ailanthus spp	experimental		3.25	0.00	-0.21	-1.97	0.27
	empty	100122-16	H12	sample								NA	NA	NA	NA	NA
	empty	100122-17	A01	sample								NA	NA	NA	NA	NA
00201538	DECAHYDROGAMBOGIC ACID	100122-17	A02	sample		C38H54O8	638.84928		derivative	undetermined activity	Tetrahedron 21: 1453 (1965)	-5.44	-1.23	-3.08	-2.90	-3.16
00201595	OSAJIN	100122-17	A03	sample	482-53-1	C25H24O5	404.46703		Maclura pomifera	undetermined activity	J Am Chem Soc 63: 1253 (1941); 68: 406 (1946)	0.04	0.93	-0.87	-1.49	-0.35
00201605	BISANHYDRORUTILANTINONE	100122-17	A04	sample	749-18-8	C22H16O7	392.36862	antibacterial	Streptomyces spp; also rutilantinone	experimental	Naturwissenschaften 52: 539 (1965); Chem Ber 100: 256	-0.99	-0.82	-0.30	-1.03	-0.79
00205071	HAEMATOMMIC ACID, ETHYL ESTER	100122-17	A05	sample	39503-14-5	C11H12O5	224.21529		various lichens, e.g. Evernia spp, Parmelia spp	undetermined activity	J Org Chem 42: 2526 (1977); Helv Chim Acta 72: 1061	1.39	-0.67	-0.54	0.12	0.07
00201696	LANOSTEROL ACETATE	100122-17	A06	sample		C32H52O2	468.77004		derivative of lanosterol	undetermined activity	J Chem Soc 1953: 571	-7.93	-1.99	-0.78	-2.18	-3.22
01505746	7-AMINOCEPHALOSPORANIC ACID	100122-17	A07	sample	957-68-6	C10H12N2O5S	272.28154		derivative of Cephalosporin C	undetermined activity	Biochem J 79:48 (1961); JACS 84:3400 (1962)	0.74	-0.46	0.02	0.25	0.14
00201539	GARCINOLIC ACID	100122-17	A08	sample		C38H46O9	646.78492		Garcinia spp.; also hydrolysis product of gambogic acid	undetermined activity	Ann Chim 56: 232 (1966)	0.28	0.23	6.15	-0.53	1.53
00210369	GALLIC ACID	100122-17	A09	sample	149-91-7	C7H6O5	170.12287	antineoplastic, astringent, antibacterial	insect galls	INN, NF-VII	J Chem Soc 1961:1854; Agric Biol Chem 30:617 (1966);	0.66	-0.44	0.66	-0.65	0.06
00100006	BUSSEIN	100122-17	A10	sample	41060-14-4	C43H54O18	858.89903		Entandrophragma species	undetermined activity	Chem Commun 1965:302	-0.84	-0.11	-0.24	-2.29	-0.87
01502248	GLUTATHIONE	100122-17	A11	sample	70-18-8	C10H17N3O6S	307.32749	antioxidant	plant and animal tissue	JAN	Pharm Biol 11: 539 (1968)	1.14	-0.38	1.30	-0.20	0.47
	0.04% JAK2inhib	100122-17	A12	0.04% jak2inhib								-1.05	-1.69	-1.14	-2.24	-1.53
	0.04% DMSO	100122-17	B01	0.04% dmso								-1.08	-0.62	-1.38	-1.26	-1.08
00100049	KHAYANTHONE	100122-17	B02	sample	25279-68-9	C32H42O9	570.68614		Khaya species	undetermined activity	Chem Commun 1967:379	-8.16	-0.51	-2.26	1.51	-2.36
00200463	BRAZILEIN	100122-17	B03	sample	600-76-0	C16H12O5	284.27104		Caesalpinia spp	undetermined activity	Phytochemistry 46: 177 (1997)	0.12	0.40	-1.69	0.13	-0.26
00100008	CARAPIN	100122-17	B04	sample	3463-88-5	C27H32O7	468.55189		Carapa and Cedrela species; mp 180-185	undetermined activity	Chem Commun 1965: 302	-4.95	-4.19	-4.00	-1.81	-3.74
01502256	SHIKIMIC ACID	100122-17	B05	sample	138-59-0	C7H10O5	174.15475		common constituent in plants	undetermined activity	Helv Chim Acta 20: 705 (1937)	0.05	-0.13	1.50	-0.86	0.11
01504412	PODOPHYLLIN ACETATE	100122-17	B06	sample	1180-34-3	C24H24O9	456.45348		derivative	undetermined activity		-8.29	-7.27	-9.07	-8.36	-8.25
00300423	DIFUCOL HEXAMETHYL ETHER	100122-17	B07	sample	14262-07-8	C18H22O6	334.37244		derivative	undetermined activity	J Chem Soc 1969: 2403; Phytochemistry 31: 279	0.48	0.77	0.52	-0.09	0.42
00100005	ANTHOTHECOL	100122-17	B08	sample	10410-83-0	C28H32O7	480.56304		also as 11-ACETOXYCEDRELONE	undetermined activity	J Chem Soc 1963:983; 1970: 205; Nature 207:1101(1965)	-16.35	-24.62	-23.30	-13.70	-19.49
00100009	CEDRELONE	100122-17	B09	sample	1254-85-9	C26H30O5	422.526		Cedrela species	undetermined activity	J Chem Soc 1963: 2506, 2515	-21.11	-9.87	-6.22	-3.16	-10.09
00100303	ALLOPREGNANOLONE	100122-17	B10	sample		C21H34O2	318.50393		semisynthetic	undetermined activity	J Am Chem Soc 59: 616 (1937)	1.93	0.08	2.88	-0.22	1.17
00100012	DEACETYLGEDUNIN	100122-17	B11	sample		C26H32O6	440.54134		Khaya, Azadirachta and other West African timbers; mp 264-266	undetermined activity	J Chem Soc 1961: 3705; Phytochemistry 10: 1845 (1971)	-0.99	-0.77	0.04	1.21	-0.13
	0.04% JAK2inhib	100122-17	B12	0.04% jak2inhib								0.53	1.20	-0.25	-0.87	0.15
	0.04% DMSO	100122-17	C01	0.04% dmso								-1.23	0.82	-1.60	2.99	0.24
00100013	3-DEACETYLKHIVORIN	100122-17	C02	sample		C30H40O9	544.6479		Meliaceae spp	undetermined activity		-1.39	-0.69	-2.20	-0.04	-1.08
00100014	7-DEACETYLKHIVORIN	100122-17	C03	sample		C30H40O9	544.6479		Khaya species and other West African timbers	undetermined activity	J Chem Soc 1970: 1710	-0.38	1.37	-0.95	0.32	0.09
00100358	1,7-DIDEACETOXY-1,7-DIOXO-3-DEACETYLKHIVORIN	100122-17	C04	sample		C26H32O7	456.54074		Meliaceae spp	undetermined activity		0.31	0.81	0.74	-0.65	0.30
00100346	PICROTIN	100122-17	C05	sample	21416-53-5	C15H18O7	310.30651	GABAa receptor antagonist	nontoxin component of PICROTOXIN	experimental	J Chem Soc 1952: 1042; 1958: 2987	-0.09	0.54	0.41	-1.30	-0.11
00100222	3-DEOXO-3beta-HYDROXYMEXICANOLIDE 16-ENOL	100122-17	C06	sample		C28H36O7	484.59492		derivative	undetermined activity		-1.81	-1.73	-2.58	-1.36	-1.87
00100173	EPOXYGEDUNIN	100122-17	C07	sample		C28H34O8	498.57838		Meliaceae spp	undetermined activity		-2.67	-3.34	-2.35	3.33	-1.26
00100101	PRENYLETIN	100122-17	C08	sample	15870-91-4	C14H14O4	246.25528		Ptaeroxylon obliquum	undetermined activity	J Chem Soc (C) 1967:145; Tet Lett 1967:2147	0.99	-1.31	0.53	0.27	0.12
00100060	MEXICANOLIDE	100122-17	C09	sample	1915-67-9	C27H32O7	468.55189		Meliaceae spp	undetermined activity	Tetrahedron 24: 1489 (1968)	0.47	1.25	1.40	0.37	0.87
00100315	TIGOGENIN	100122-17	C10	sample	77-60-1	C27H44O3	416.64993		Agavaceae, Dioscoreaceae, Solanaceae, Scrophulariaceae,	undetermined activity	Chem Ind 1954:1320	2.26	-0.70	0.80	-0.55	0.45
00100513	PTAEROXYLIN	100122-17	C11	sample	14729-11-4	C15H14O4	258.27643		Ptaeroxylon obliquum, Cedrelopsis grevei	undetermined activity	J Chem Soc (C) 1966:114; 1967:145; Tet Lett 1967:3459	0.37	-0.13	2.94	1.06	1.06
	0.11% JAK2inhib	100122-17	C12	0.11% jak2inhib								-2.28	-3.35	-1.16	-1.35	-2.03
	0.11% DMSO	100122-17	D01	0.11% dmso								-1.77	-1.10	-1.21	-1.38	-1.37
00100223	1,2alpha-EPOXYDEACETOXYDIHYDROGEDUNIN	100122-17	D02	sample		C26H32O7	456.54074		Meliaceae spp	undetermined activity		-6.80	-1.65	-0.16	-1.73	-2.59
00100105	8beta-HYDROXYCARAPIN, 3,8-HEMIACETAL	100122-17	D03	sample		C27H32O8	484.55129		derivative	undetermined activity		-0.20	0.33	0.97	0.35	0.36
00100359	3,16-DIDEOXYMEXICANOLIDE-3beta-DIOL	100122-17	D04	sample		C27H36O7	472.58377		derivative	undetermined activity	Taylor (unpublished)	0.04	1.95	-0.91	1.19	0.57
00100267	TOTAROL ACETATE	100122-17	D05	sample		C22H32O2	328.49914		Podocarpus totara	undetermined activity	J Chem Soc 1951: 2979	0.14	0.15	2.80	0.11	0.80
00100117	HYDROLYSIS PRODUCT OF BUSSEIN	100122-17	D06	sample		C32H40O14	648.6672		structure tentative	undetermined activity		1.92	1.01	0.05	-0.79	0.55
00100550	OLEANOIC ACID	100122-17	D07	sample	508-02-1	C30H48O3	456.71526		leaves of Olea europea and Viscum album L.	undetermined activity	J Chem Soc (C) 1939: 1047	0.69	0.25	0.07	1.94	0.74
00100520	LUNARINE	100122-17	D08	sample	24185-51-1	C25H31N3O4	437.54352		Lunaria spp	undetermined activity	Bull Soc Chim France 1956:1840; Naturwissenschaften	-0.61	2.06	0.42	-0.01	0.47
00100551	FRIEDELIN	100122-17	D09	sample	559-74-0	C30H50O	426.7324		Ceratopetalum apetalum D. Don, Cunoniaceae	undetermined activity	J Chem Soc 1954: 473	0.51	1.26	0.57	0.33	0.67
00100096	3-DEOXY-3beta-HYDROXYANGOLENSIC ACID METHYL	100122-17	D10	sample		C27H36O7	472.58377		Meliaceae spp	undetermined activity		3.19	-0.94	-0.42	0.02	0.46
00100081	UTILIN	100122-17	D11	sample	31218-22-1	C41H52O17	816.86139		Entandrophragma utile	undetermined activity	J Chem Soc 1960:3827; Chem Commun 1970:1388	-0.04	-1.52	-1.40	-0.59	-0.89
	0.11% JAK2inhib	100122-17	D12	0.11% jak2inhib								0.15	-2.77	-2.08	-2.59	-1.82
	0.11% JAK2inhib	100122-17	E01	0.11% jak2inhib								-3.55	-2.58	-0.17	-1.87	-2.04
00100201	3-DEOXO-3beta-ACETOXYDEOXYDIHYDROGEDUNIN	100122-17	E02	sample		C30H40O7	512.6491		Meliaceae spp	undetermined activity		0.54	-0.24	-0.12	2.95	0.79
00100455	MEROGEDUNIN	100122-17	E03	sample		C21H28O4	344.45491		derivative	undetermined activity	J Chem Soc 1966: 506	-0.74	1.69	-0.23	-0.64	0.02
00100517	ENTANDROPHRAGMIN	100122-17	E04	sample	11013-05-1	C43H56O17	844.91557		Entangrophragma spp.	undetermined activity	J. Chem. Res. Synop. 1977: 154	1.62	0.38	1.87	-0.51	0.84
00100355	1,3-DIDEACETYL-7-DEACETOXY-7-OXOKHIVORIN	100122-17	E05	sample		C26H34O7	458.55668		Meliaceae spp	undetermined activity		-2.53	-2.20	-2.98	-1.07	-2.19
00100497	3beta-ACETOXYDEOXODIHYDROGEDUNIN	100122-17	E06	sample		C30H40O8	528.6485		Meliaceae spp	undetermined activity		-8.19	-2.99	-1.93	-1.18	-3.57
00100305	3beta-HYDROXYISOALLOSPIROST-9(11)-ENE	100122-17	E07	sample		C27H42O3	414.63399		semisynthetic	undetermined activity		-0.44	-0.14	-0.80	1.57	0.05
01505959	DIPTERYXIN	100122-17	E08	sample	53948-01-9	C17H14O6	314.29753		Dipteryx odorata	undetermined activity	Phytochemistry 13:1943 (1974)	0.79	0.58	-0.47	0.78	0.42
01100296	PODOTOTARIN	100122-17	E09	sample		C40H58O2	570.90706		Podocarpus spp	undetermined activity	Tetrahedron 19: 209 (1963); Phytochemistry 6: 883 (1967)	-3.50	0.56	0.48	1.46	-0.25
00100360	beta-AMYRIN	100122-17	E10	sample	559-70-6	C30H50O	426.7324		widespread in plants	undetermined activity	Phytochemistry 9: 1669 (1970)	-3.52	-0.32	0.64	1.16	-0.51
00100129	8-HYDROXYCARAPINIC ACID	100122-17	E11	sample		C26H30O8	470.5242		Meliaceae spp	undetermined activity		1.01	-0.59	2.23	3.98	1.66
	0.11% DMSO	100122-17	E12	0.11% dmso								-0.35	0.58	0.49	0.39	0.28
	0.11% JAK2inhib	100122-17	F01	0.11% jak2inhib								-2.67	-3.09	-3.10	-3.24	-3.02
00100024	DIHYDROGEDUNIN	100122-17	F02	sample		C28H36O7	484.59492		Meliaceae spp.	undetermined activity		-2.11	-3.36	-1.89	-3.29	-2.66
00100287	TOTAROL	100122-17	F03	sample	511-15-9	C20H30O	286.4615		Podocarpus spp, Dacrydium cupressinum, Tetraclinis articulata	undetermined activity	Aust J Chem 48: 883 (1995)	-1.88	-0.42	-1.99	-1.53	-1.45
00100031	FISSINOLIDE	100122-17	F04	sample	1915-69-1	C29H36O8	512.60547		Cedrela fissilis, Khaya grandifoliola	undetermined activity	Tetrahedron 26: 219 (1970); Tet Letters 1970: 2797; J Chem	0.47	0.67	-0.13	1.86	0.72
00100432	DEOXYGEDUNIN	100122-17	F05	sample		C28H34O6	466.57958		Meliaceae spp	undetermined activity		-0.61	0.76	1.09	-0.22	0.26
00100139	DEOXYKHIVORIN	100122-17	F06	sample		C32H42O9	570.68614		Meliaceae spp	undetermined activity		-1.65	-3.20	-3.28	0.59	-1.89
01100298	SMILAGENIN ACETATE	100122-17	F07	sample		C29H46O4	458.68757		Smilax ornata, Agave & Yucca spp	undetermined activity		-6.57	-0.48	-1.16	-0.94	-2.29
00100047	DEACETOXY-7-OXOGEDUNIN	100122-17	F08	sample		C26H30O6	438.5254		Meliaceae spp	undetermined activity		2.86	2.84	1.13	-0.10	1.68
00100162	KHIVORIN	100122-17	F09	sample	2524-38-1	C32H42O10	586.68554		Khaya and other West African timbers	undetermined activity	J Chem Soc 1962: 768	0.06	-1.46	-1.85	-1.56	-1.20
01504524	ORNITHINE	100122-17	F10	sample	70-26-8	C5H12N2O2	132.16359	hepatoprotectant, anticholesteremic	widespread in nature	INN		1.11	0.87	0.40	0.37	0.69
01505484	LUPEOL	100122-17	F11	sample	545-47-1	C30H50O	426.7324	antineoplastic	widespread in plants	experimental	Bull Soc Chim Belg 70:585 (1961)	-5.92	4.21	0.73	1.16	0.04
	0.04% DMSO	100122-17	F12	0.04% dmso								2.12	-0.87	0.59	-0.18	0.41
	0.04% JAK2inhib	100122-17	G01	0.04% jak2inhib								-1.00	-1.23	-2.44	-2.10	-1.69
01500733	ALPINETIN METHYL ETHER	100122-17	G02	sample	36052-66-1	C17H16O4	284.31467		Eucalyptus spp	undetermined activity		-0.52	-0.30	-0.35	1.01	-0.04
01505488	SALIDROSIDE	100122-17	G03	sample	10338-51-9	C15H22O7	314.33839		Salix triandra, Rhodiola spp	undetermined activity	Naturwissenschaften 51:360 (1964)	3.13	1.44	0.89	-0.22	1.31
01400242	N-METHYLBENZYLAMINE HYDROCHLORIDE	100122-17	G04	sample	13426-94-3, 103-67-3(base)	C8H12ClN	157.64454		Ephedra sp.	undetermined activity		-0.72	-0.09	1.06	0.62	0.22
01504036	3-DESHYDROXYSAPPANOL TRIMETHYL ETHER	100122-17	G05	sample		C19H22O5	330.38419		derivative	undetermined activity		-0.52	0.94	-0.31	0.02	0.03
01504030	beta-ESCIN	100122-17	G06	sample	6805-41-0	C55H86O24	1131.28427	membrane permeabilizer	principal saponin Aesculus hippocastanum	INN	Arzneimittel-Forsch 13: 385 (1963)	-1.25	2.97	0.12	2.73	1.14
01500741	6,4'-DIMETHOXYFLAVONE	100122-17	G07	sample	54401-47-7	C17H14O4	282.29873		derivative Cassia spectabilis	undetermined activity		0.05	0.07	0.72	0.70	0.38
01504120	CARNOSIC ACID	100122-17	G08	sample	3650-09-7	C20H28O4	332.44376		Salvia spp, Rosmarinus officinalis	undetermined activity		0.39	0.38	-0.23	0.81	0.34
01504206	BOVINOCIDIN (3-nitropropionic acid)	100122-17	G09	sample	504-88-1	C3H5NO4	119.0776	antineoplastic	Aspergillus, Streptomyces spp & other microorganisms	experimental	Nature 164: 575 (1949)	0.87	1.37	1.02	1.65	1.23
01500709	CHRYSIN	100122-17	G10	sample	480-40-0	C15H10O4	254.2455	diuretic	Ulnus sieboldiana, Flourensia resinosa, Oroxylum indicum, Pinus	experimental	J Chem Soc 1938:1320; Biochem J 59:58 (1955)	1.02	1.27	2.70	0.47	1.37
01503006	BENZYL ISOTHIOCYANATE	100122-17	G11	sample	622-78-6	C8H7NS	149.21569	antineoplastic, antibacterial, antifungal	Tropaeolum majus, Lepidium sativum and other Cruciferae	INN	J Agr Food Chem 12: 127 ((1964)	0.14	0.50	0.06	2.34	0.76
	0.04% DMSO	100122-17	G12	0.04% dmso								0.33	2.52	0.86	-0.39	0.83
	0.04% JAK2inhib	100122-17	H01	0.04% jak2inhib								-4.02	-2.08	-2.64	-3.00	-2.94
01503042	ARTEMISININ	100122-17	H02	sample	63968-64-9	C15H22O5	282.33959	antimalarial	Artemisia annua	INN	Science 228:1049 (1985); Drugs 52:818 (1996); Trends	-2.06	0.06	-0.40	0.01	-0.60
01500721	7,4'-DIHYDROXYFLAVONE	100122-17	H03	sample	2196-14-7	C15H10O4	254.2455	antioxidant	Pterocarpus marsupium	experimental	Phytochemistry 4: 523 (1965); J Nat Prod 47:179 (1984)	-0.36	2.50	-0.31	-0.10	0.43
01500158	LOBELINE HYDROCHLORIDE	100122-17	H04	sample	90-69-7	C22H28ClNO2	373.92696	antiasthmatic, respiratory stimulant	Lobelia spp	INN, BAN, JAN		-0.55	-0.54	-0.02	-0.18	-0.32
01505349	4-O-METHYLPHLORACETOPHENONE	100122-17	H05	sample	7507-89-3	C9H10O4	182.17765	antifungal	Prunus domesticus	experimental		-0.75	-0.06	-0.78	-0.06	-0.41
01500706	ARCAINE SULFATE	100122-17	H06	sample	36587-93-6	C6H18N6O4S	270.31216		Arca noae	undetermined activity	Chem Abstracts 41: 4455 (1947)	-0.33	0.48	-0.80	0.81	0.04
01505274	3,4-DIHYDROXYCARANE	100122-17	H07	sample		C10H18O2	170.25376		monoterpene	undetermined activity		0.16	1.37	0.53	0.05	0.53
01700330	MUNDULONE ACETATE	100122-17	H08	sample		C28H28O7	476.53116		derivative	undetermined activity		5.82	7.49	8.19	8.93	7.61
01500656	AJMALINE	100122-17	H09	sample	4360-17-7	C20H26N2O2	326.44242	antiarrhythmic (Class Ia): inhibits glucose uptake by mitochondria,	Rauwolfia spp., Melodinus balansae, Tonduzia longifolia	JAN	J Chem Soc 1954: 1242; Angew Chem., 68: 13 (1956)	0.09	2.54	0.08	0.69	0.85
01503219	DIOSMIN	100122-17	H10	sample	520-27-4	C28H32O15	608.55824	vascular protectant	Zanthoxylum avicennae	INN, BAN		0.95	0.71	0.10	-0.25	0.38
01500760	HECOGENIN	100122-17	H11	sample	467-55-0	C27H42O4	430.63339	antiinflammatory	Agave and Yucca spp	experimental	Planta Med 63:199 (1997)	0.89	-0.23	1.02	-0.33	0.34
	empty	100122-17	H12	sample								NA	NA	NA	NA	NA
	empty	100122-18	A01	sample								NA	NA	NA	NA	NA
01500872	PALMATINE CHLORIDE	100122-18	A02	sample	10605-02-4	C21H22ClNO4	387.86679	antibacterial, antimalarial, uterine contractant	Jateorhiza palmata (Calumba root)	experimental	J Nat Prod 28: 73 (1965); Can J Chem 58: 2770 (1980)	1.04	1.08	-1.65	1.09	0.39
01505812	CRYPTOTANSHINONE	100122-18	A03	sample	35825-57-1	C19H20O3	296.36945	inhibits angiogenesis	Salvia miltiorrhiza, Rosmarinus officinalis	experimental	Chem Pharm Bull 10:112 (1962); Planta Med 24:190	-0.66	-1.55	-2.91	-1.75	-1.72
01500754	XANTHURENIC ACID	100122-18	A04	sample	59-00-7	C10H7NO4	205.17159	caspase activator, guanylyl cyclase stimulant	pathological metabolite of tryptophan and kynurenine	experimental	Mol Microbiol 42:553 (2001); BMC Physiology 1:7 (2001)	0.05	-1.58	-1.77	-2.05	-1.34
01505177	RUBESCENSIN A	100122-18	A05	sample	28957-04-2	C20H28O6	364.44256	antibacterial, antineoplastic, insect growth inhibitor	Isodon trichocarpus, I japonicus, Rabdosia spp	experimental	Chem Pharm Bull 18:871 (1970); 20:1752 (1972); 24:2118	-1.77	-1.24	-1.35	4.38	0.00
01501017	FERULIC ACID	100122-18	A06	sample	1135-24-6	C10H10O4	194.1888	antineoplastic, choleretic, food preservative	widely distributed in plants	experimental	J Org Chem 16: 216 (1951)	-1.62	-1.32	-0.68	-2.48	-1.52
01504019	GOSSYPOL	100122-18	A07	sample	303-45-7	C30H30O8	518.5688	antispermatogenic, antineoplastic, antiHIV	Lobelia spp	experimental	J Am Chem Soc 80: 2193 (1938)	2.41	0.99	0.52	0.28	1.05
01500811	BERBERINE CHLORIDE	100122-18	A08	sample	633-65-8, 2086-83-1	C20H18ClNO4	371.82376	antiarrhythmic, alpha2 agonist, cholinesterase, anticonvulsant,	Berberis and Mahonia spp	JAN	Coll Czech Chem Comm 35:124 (1970); J Nat Prod 40:384	-1.31	-2.72	-2.76	-4.18	-2.74
01503982	AGMATINE SULFATE	100122-18	A09	sample	2482-00-0	C5H16N4O4S	228.27167	NMDA blocker, alpha-2 adrenergic agonist; NO synthase inhibitor	Ambrosia entemisifolia	experimental	JACS 41:681 (1919); Science 263:966 (1994); Biochem J	-0.31	0.75	0.16	1.07	0.42
01503602	SALINOMYCIN, SODIUM	100122-18	A10	sample	53003-10-4	C42H69NaO11	773.00143	antibacterial	Streptomyces albus	INN, BAN	J Antibiotics 27: 814 (1954)	-3.33	-2.60	0.14	-3.28	-2.27
01505038	KASUGAMYCIN HYDROCHLORIDE	100122-18	A11	sample	19408-46-9, 6980-18-3 (base)	C14H26ClN3O9	415.83102	antifungal	Streptomyces kasugaensis	agricultural use	J Antibiot Ser A 18:101 (1965); Tet Lett 1966:1239	-0.01	0.66	-1.31	-3.09	-0.93
	0.04% JAK2inhib	100122-18	A12	0.04% jak2inhib								-1.66	-0.79	-0.69	-2.13	-1.32
	0.04% DMSO	100122-18	B01	0.04% dmso								0.86	-1.11	-1.33	2.51	0.23
01505920	PANTETHINE	100122-18	B02	sample	16816-67-4	C22H42N4O8S2	554.73004	antilipemic	semisynthetic	JAN	J Chem Soc 1954:1171; Atherosclerosis 50:73 (1984)	-0.18	-0.82	0.02	-1.80	-0.70
01500944	CARNOSINE	100122-18	B03	sample	305-84-0	C9H14N4O3	226.23693		mammalian skeletal muscle	undetermined activity	Science 184: 909 (1974); Proc Soc Exp Biol Med 158: 402	2.75	-0.33	1.82	0.26	1.13
01500987	GLUTAMINE (D)	100122-18	B04	sample	6899-04-3	C5H10N2O3	146.14705		widely distributed in plants	undetermined activity		1.12	-0.20	-0.07	-0.66	0.05
01502227	CADAVERINE TARTRATE	100122-18	B05	sample	462-94-2(base)	C7H16N2O6	224.21537		putrifaction of lysine; sectrition of the fox Vulpes vulpes	undetermined activity		-0.73	-0.49	-0.58	-2.25	-1.01
01502245	ELLAGIC ACID	100122-18	B06	sample	476-66-4	C14H6O8	302.19912	hemostatic, antineoplastic, antimutagenic	widely distributed in higher plants	INN		1.47	2.03	1.83	-0.12	1.31
01502232	CAMPTOTHECIN	100122-18	B07	sample	7689-03-4	C20H16N2O4	348.36152	antineoplastic	Camptotheca acuminata	experimental	J Am Chem Soc 88: 3888 (1966)	0.10	2.14	1.69	1.47	1.35
01504002	BAICALEIN	100122-18	B08	sample	491-67-8	C15H10O5	270.24395	antiviral (HIV)	Scutellaria baicalensis	experimental	Gazz Chim acta 49 (II): 47 (1919); Acta Phytochim 1: 109	-1.53	4.84	-0.65	-0.99	0.42
01500819	BERGENIN	100122-18	B09	sample	477-90-7	C14H18O10	346.29356	hepatoprotectant	Bergenia spp.	JAN	J Chem Soc 1958: 2231; Org Biomol Chem. 6:2713 (2008)	0.17	0.92	1.05	-0.03	0.53
01500906	LITHOCHOLIC ACID	100122-18	B10	sample	434-13-9	C24H40O3	376.5846	LD50(mouse) 3900 mg/kg po	mammalian bile and gallstones, faecal matter	experimental	JACS 71:4126 (1949)	-4.92	0.16	2.45	-0.82	-0.78
01500901	AESCULIN	100122-18	B11	sample	531-75-9	C15H16O9	340.28937	antiinflammatory	Aesculus hippocastanum, Fraxinus spp	experimental	Naturwiss 29: 650 (1941); Phytochemistry 11: 657 (1972)	-0.35	-0.03	-1.60	-1.13	-0.78
	0.04% JAK2inhib	100122-18	B12	0.04% jak2inhib								0.93	0.93	2.45	-1.18	0.78
	0.04% DMSO	100122-18	C01	0.04% dmso								0.60	-1.46	1.58	-0.54	0.04
01501204	LAPACHOL	100122-18	C02	sample	84-79-7	C15H14O3	242.27703	antineoplastic, antifungal	heartwood of Bignoniaceae	experimental	Phytochemistry 14: 1829 (1975)	0.43	-0.78	-0.62	0.06	-0.23
01503904	PATULIN	100122-18	C03	sample	149-29-1	C7H6O4	154.12347	antibacterial	Aspergillus clavatus, Penicillium patulum	experimental	J Chem Soc 1944: 415	-13.10	-12.18	-8.02	-5.32	-9.65
01500990	ENOXOLONE	100122-18	C04	sample	471-53-4	C30H46O4	470.69872	antitussive, antiinflammatory, antibacterial	derivative	INN, BAN, JAN		-2.20	-1.17	-0.44	-0.09	-0.98
01505824	TANSHINONE IIA	100122-18	C05	sample	568-72-9	C19H18O3	294.35351	antineoplastic, bone resorption inhibitor, antiproliferative, apoptosis	Salvia miltiorrhiza	experimental	Chem Pharm Bull 10:112 (1962); Phytochemistry 24:815	-0.75	-1.46	-2.50	-2.00	-1.67

Compound ID	MolNAME	plate	position	Content	cas#	Formula	MolWt	Bioactivity	Source	Status	Reference	Screen Score (z-score) rep1	rep2	rep3	rep4	Average
01505810	PEONIFLORIN	100122-18	C06	sample	23180-57-6	C23H30O11	482.48895	antiinflammatory, antispasmodic, antihypertensive, antidiuretic	Peonia spp	experimental	Tetrahedron 25:1825 (1969)	-1.24	-0.67	1.09	0.05	-0.19
00100146	7-DESACETOXY-6,7-DEHYDROGEDUNIN	100122-18	C07	sample		C26H30O5	422.526		derivative of gedunin	undetermined activity		-0.60	-0.04	-0.91	-0.49	-0.51
01500867	HARMINE	100122-18	C08	sample	442-51-3	C13H12N2O	212.25339	antiparkinsonian, CNS stimulant	Peganum harmala	experimental	Phytochemistry 7: 503 (1968)	4.31	3.06	3.47	2.80	3.41
00100102	CARAPIN-8(9)-ENE	100122-18	C09	sample		C22H30O7	466.53595		Carapa and Cedrela species	undetermined activity	Chem Commun 1965: 302	5.05	6.11	5.60	1.38	4.54
01504525	OROTIC ACID	100122-18	C10	sample	65-86-1	C5H4N2O4	156.09863	hepatoprotectant, uricosuric agent	widespread in animals	INN	J Biol Chem 202:91 (1953)	0.16	4.13	3.05	-0.65	1.67
00300047	ANISODAMINE HYDROBROMIDE	100122-18	C11	sample	17659-49-3	C17H23NO4	305.37716	anticholinergic, antispasmodic	Scopolia tanguticus	CHINA	Naturwissenschaften 49: 281 (1962)	0.05	2.85	0.34	0.88	1.03
	0.11% JAK2inhib	100122-18	C12	0.11% jak2inhib								-3.22	-2.23	-1.75	-2.48	-2.42
	0.11% DMSO	100122-18	D01	0.11% dmso								-0.49	-2.96	-0.95	-2.49	-1.72
01503630	SPAGLUMIC ACID	100122-18	D02	sample	4910-46-7	C11H16N2O8	304.25877	neurotransmitter; mGluR3 receptors	brain tissue	INN	PNAS 80:1116 (1983); Eur J Pharmacol 98:193 (1984); J	1.61	-0.57	-0.99	-1.35	-0.32
00201508	7-DESHYDROXYPYROGALLIN-4-CARBOXYLIC ACID	100122-18	D03	sample		C12H8O6	248.19396		synthetic	undetermined activity		1.15	-1.35	-0.36	-1.48	-0.51
01506011	6-METHOXYHARMALAN	100122-18	D04	sample	3589-73-9	C13H14N2O	214.26933	convulsant, halucinogen	Peganum spp	experimental	Int J Biochem 14:581 (1982); Neurosci Let 189:121 (1995);	0.79	0.85	0.48	1.01	0.78
00107113	ANDROSTERONE ACETATE	100122-18	D05	sample	1164-95-0	C21H32O3	332.48739	androgen	semisynthetic	experimental		0.26	0.20	-0.29	1.52	0.42
00270049	alpha-HYDROXYDEOXYCHOLIC ACID	100122-18	D06	sample	83-49-8	C24H40O4	392.584		pig bile	undetermined activity	J Chem Soc 1990: 1	0.01	0.30	-0.02	1.22	0.38
10100003	BIOCHANIN A	100122-18	D07	sample	491-80-5	C16H12O5	284.27104	phytoestrogen	widely distributed in Leguminosae	experimental	J Chem soc 1953: 1852	0.94	-0.25	0.45	0.02	0.29
00270051	METHYL DEOXYCHOLATE	100122-18	D08	sample	3245-38-3	C25H42O4	406.61109		rabbit bile & feces	undetermined activity	Helv Chim Acta 25:797 (1942); J Biol Chem 238: 3846	-2.29	-2.50	-1.20	-0.49	-1.62
00300038	JUGLONE	100122-18	D09	sample	481-39-0	C10H6O3	174.15752	antineoplastic, antifungal	leaves and nuts of Juglans spp., Carya spp and Pterocarya spp.	experimental		-3.48	0.37	1.12	1.74	-0.06
01504051	STIGMASTEROL	100122-18	D10	sample		C29H48O	412.70531		soya and calabar beans; widely distributed in plant oils	undetermined activity		-4.79	-0.36	1.08	-0.06	-1.03
01506004	LACTOBIONIC ACID	100122-18	D11	sample	96-82-2	C12H22O12	358.30194	food additive	semisynthetic	undetermined activity		-0.29	4.84	-0.06	0.08	1.14
	0.11% JAK2inhib	100122-18	D12	0.11% jak2inhib								-3.57	-1.47	1.54	-2.33	-1.46
	0.11% JAK2inhib	100122-18	E01	0.11% jak2inhib								-2.71	-4.03	-4.01	-1.51	-3.07
01600025	2,6-DIHYDROXY-4-METHOXYTOLUENE	100122-18	E02	sample		C8H10O3	154.1671		synthetic	undetermined activity		0.54	1.94	-0.15	0.33	0.66
01600075	QUERCETIN PENTAMETHYL ETHER	100122-18	E03	sample		C20H20O7	372.3782		derivative	undetermined activity		-0.54	-1.07	-0.34	-0.44	-0.60
01600919	3-METHOXYCATECHOL	100122-18	E04	sample	934-00-9	C7H8O3	140.14001		Machaerium kuhlmanni	undetermined activity	Phytochemistry 17: 1383, 1401 (1990)	0.18	-0.49	-1.48	0.60	-0.30
01506091	MENAQUINONE-4	100122-18	E05	sample		C21H24O2	308.42423	antioxidant, alkaline phosphatase enhancer	synthetic; VITAMIN K2	experimental	Biochem J 162:297 (1977); J Vasc Res 40:531 (2003)	-4.62	-0.71	-0.30	0.36	-1.32
01505896	GRAMINE	100122-18	E06	sample	87-52-5	C11H14N2	174.24763		Arundo, Hordeum, Phalaris spp	experimental	J Org Chem 24:1285 (1959); Phytochemistry 33:741 (1993)	0.25	0.37	0.62	-0.49	0.19
01505884	ESEROLINE FUMARATE	100122-18	E07	sample	469-22-7	C17H22N2O5	334.37529	μ-opioid receptor agonist, analgesic	Coynanthe yohimbe	experimental	Can J Physiol Pharmacol 59:307 (1981); Eur J Pharmacol	-0.47	-0.92	0.65	-1.15	-0.47
00100032	GEDUNIN	100122-18	E08	sample	2753-30-2	C28H34O7	482.57898	antifeedant; heat shock inducer	numerous Meliaceae species	experimental	J Chem Soc 1960:3827; 1962:5095; 1967:1026; 1969:864;	-4.10	-0.80	-2.68	-2.65	-2.56
00100618	3alpha-HYDROXY-4,4-BISNOR-8,11,13-	100122-18	E09	sample		C15H20O	216.32605		semisynthetic	undetermined activity		0.31	0.06	0.03	-0.93	-0.13
00100291	STROPHANTHIDIN	100122-18	E10	sample	66-28-4	C23H32O6	404.50789	cardiotonic	Strophanthus kombe	experimental	J Soc Chem Ind 53: 956 (1934)	-2.61	-1.36	-1.98	-2.85	-2.20
00100318	DIOSGENIN	100122-18	E11	sample	512-04-9	C27H42O3	414.63399	antiinflammatory, estrogen; LD50(rat) 4872 mg/kg ip. LD50	Clintonia, Dioscorea and Solanum spp, Trillium erectum, Balanites	experimental	Konstitution und Vorkommen der Organischen	-1.56	1.33	0.84	0.11	0.18
	0.11% DMSO	100122-18	E12	0.11% dmso								0.39	1.26	0.59	0.08	0.58
	0.11% JAK2inhib	100122-18	F01	0.11% jak2inhib								-2.50	-3.77	-3.85	-3.13	-3.31
00100375	alpha-DIHYDROGEDUNOL	100122-18	F02	sample		C28H38O7	486.61086		derivative	undetermined activity	J Chem Soc 1961: 3705	-0.22	-3.79	-2.55	-1.01	-1.89
00100434	DIHYDRODEOXYGEDUNIN	100122-18	F03	sample		C28H36O6	468.59552		Meliaceae spp	undetermined activity		2.10	2.27	1.50	2.44	2.08
00270088	CHOLESTAN-3-ONE	100122-18	F04	sample	566-88-1	C27H46O	386.66707		minor mammalian sterol	undetermined activity		-1.29	0.46	0.55	1.55	0.32
01505764	SPERMINE	100122-18	F05	sample	71-44-3	C10H26N4	202.34552	immune modulator	all animal tissue, fungi	experimental	Differentiation 19:1 (1981); Cancer Res 42:3248 (1982)	-0.29	-1.28	-0.18	0.90	-0.21
00100529	HETEROPEUCENIN, METHYL ETHER	100122-18	F06	sample	26213-95-6	C16H18O4	274.31946		Ptaeroxylon obliquum, Harrisonia perforate ,Neochamaelea	undetermined activity	Tetrahedron Letters 1967:2737	0.34	-0.98	0.22	-1.76	-0.54
00200115	PECTOLINARIN	100122-18	F07	sample	28978-02-1	C29H34O15	622.58533		Cirsium and Linaria spp, Kickxia elatine, Duranta plumieri	undetermined activity	Phytochemistry 12:421 (1973); Chem Pharm Bull 26:2036	0.10	0.33	-0.12	0.89	0.30
00200139	ISOTECTORIGENIN, 7-METHYL ETHER	100122-18	F08	sample		C18H16O6	328.32462		Dalbergia spp	undetermined activity		0.11	-0.49	0.65	5.16	1.36
00200258	2,4'-DIHYDROXYCHALCONE 4'-GLUCOSIDE	100122-18	F09	sample		C21H22O8	402.40469	anthelmintic & antiulcerocenic	aglycone Flamingia chappar, Acacia neovernicosa	experimental	Phytochemistry 21: 1063 (1982); Planta Medica 58: 389	-0.06	2.04	5.09	1.39	2.12
00200004	12a-HYDROXY-9-DEMETHYLMUNDUSERONE-8-	100122-18	F10	sample		C19H16O9	388.33397		derivative	undetermined activity		-0.06	0.91	2.62	0.25	0.93
00200208	ASARYLALDEHYDE	100122-18	F11	sample	4460-86-0	C10H12O4	196.20474	fly attractant	Daucus carota, Acorus calamus, Asarum europaeum	experimental	J Nat Prod 39: 412 (1976)	0.10	1.04	-0.77	-1.26	-0.22
	0.04% DMSO	100122-18	F12	0.04% dmso								-0.46	1.66	1.12	-0.02	0.57
	0.04% JAK2inhib	100122-18	G01	0.04% jak2inhib								0.44	-2.00	1.17	-1.61	-0.50
00200215	2-METHYL-5,7,8-TRIMETHOXYISOFLAVONE	100122-18	G02	sample		C19H18O5	326.35231		derivative	undetermined activity		1.22	-0.24	0.57	1.58	0.78
00200243	GRISEOFULVIC ACID	100122-18	G03	sample	469-54-5	C16H15ClO6	338.74735		semisynthetic	undetermined activity		0.42	0.50	-0.62	-0.45	-0.04
00200412	2,3,4'-TRIHYDROXY-4-METHOXYBENZOPHENONE	100122-18	G04	sample		C14H12O5	260.24874		derivative	undetermined activity		1.10	1.37	-0.14	0.50	0.71
00200422	KOPARIN	100122-18	G05	sample	65048-75-1	C16H12O6	300.27044		Castanospermum australe	undetermined activity	Aust J Chem 30:1827 (1977)	-0.16	-0.19	0.98	0.78	0.35
00200425	2,3-DIHYDROXY-4-METHOXY-4'-	100122-18	G06	sample		C16H16O5	288.30292		derivative	undetermined activity		-0.07	-0.97	-0.68	2.60	0.22
00200090	OBTUSAQUINONE	100122-18	G07	sample	21105-15-7	C16H14O3	254.28618		Dalbergia retusa	undetermined activity	Phytochemistry 17: 1395 (1978)	-0.67	0.37	-0.95	0.40	-0.21
00200427	PISCIDIC ACID	100122-18	G08	sample	35388-57-9	C11H12O7	256.21409		Piscidia piscipula	undetermined activity	J Chem Soc 1954: 3981; Acta Chem Scand 18: 1979	0.04	0.09	0.24	0.21	0.14
00200110	ANTIAROL	100122-18	G09	sample	642-71-7	C9H12O4	184.19359		Antiaris toxicaria	undetermined activity	Helv Chim Acta 45: 1183, 1206, 2285 (1992)	1.56	1.40	0.18	-1.21	0.48
00200111	THEAFLAVIN	100122-18	G10	sample	4670-05-7	C29H24O12	564.50743	antioxidant	pigment in black tea	experimental	Tet Lett 1966:1193, 4024; Tetrahedron 29:125 (1973)	0.25	1.15	2.43	-0.02	0.96
00200010	HAEMATOXYLIN	100122-18	G11	sample	517-26-2	C16H14O6	302.28638		Haematoxylon campechianum	undetermined activity	Bul Soc Chim Fr 1972: 3292	-0.73	0.89	1.31	0.41	0.47
	0.04% DMSO	100122-18	G12	0.04% dmso								0.22	4.10	1.52	0.13	1.49
	0.04% JAK2inhib	100122-18	H01	0.04% jak2inhib								-1.51	-3.15	-1.61	-2.02	-2.07
00200011	MUNDULONE	100122-18	H02	sample	481-94-7	C26H26O6	434.49352		Mundulea sericea	undetermined activity	Tet Letters 1963, 281	6.03	7.66	5.40	8.33	6.86
00200012	BRAZILIN	100122-18	H03	sample	474-07-7	C16H14O5	286.28698		Haematoxylin campechianum	undetermined activity	J Chem Soc 1928, 1504	-0.15	-1.56	-1.59	1.79	-0.38
00200054	FUMARPROTOCETRARIC ACID	100122-18	H04	sample	489-50-9	C22H16O12	472.36562		Cetraria islandica	undetermined activity	Chem Ber 67: 411, 766 (1934)	0.76	-0.43	0.60	0.25	0.30
00200035	GANGALEOIDIN	100122-18	H05	sample	55365-63-4	C18H14Cl2O7	413.21408		Lecanora gangaleoides	undetermined activity	J Chem Soc 1986: 1491	0.98	0.55	0.27	1.25	0.76
00200070	LECANORIC ACID	100122-18	H06	sample	480-56-8	C16H14O7	318.28578		Common constituent of lichens	undetermined activity	Monatsh Chem 61:147 (1932)	0.28	-0.08	0.54	-0.10	0.16
00100584	GITOXIGENIN DIACETATE	100122-18	H07	sample	5996-03-2	C27H38O7	474.59971		aglycon of GITOXIN	undetermined activity	Helv Chim Acta 33: 76 (1950)	-4.38	-3.20	-6.13	-5.36	-4.76
00100599	2-METHYL GRAMINE	100122-18	H08	sample		C12H16N2	188.27472		derivative	undetermined activity		0.17	-0.60	-1.42	-1.09	-0.74
00100609	XANTHYLETIN	100122-18	H09	sample	553-19-5	C14H12O3	228.24994		Brosimum rubescens, Ruta, Boenninghausenia, Flindersia,	undetermined activity	J Chem Soc (C) 1969:33; Phytochemistry 11:3479 (1972)	0.24	1.37	1.20	2.24	1.26
00100615	CHUKRASIN METHYL ETHER	100122-18	H10	sample		C43H58O16	830.93211		Meliaceae	undetermined activity	Helv Chim Acta 61: 1814 (1978)	-2.47	0.03	-0.74	-0.37	-0.89
00100616	ANGOLENSIN (R)	100122-18	H11	sample	4842-48-2	C16H16O4	272.30352		Pericopsis and Pterocarpus spp	undetermined activity	J Chem Soc 1959: 2679; 1963: 5573	-0.28	1.78	0.62	-0.19	0.48
	empty	100122-18	H12	sample								NA	NA	NA	NA	NA
	empty	100122-19	A01	sample								NA	NA	NA	NA	NA
00200428	ROCCELLIC ACID	100122-19	A02	sample	22139-54-4	C17H32O4	300.44219		Lecanora and Roccella spp	undetermined activity	J Chem Soc 1971: 1318	-1.78	-2.12	-1.48	-1.78	-1.79
00200446	METHYLXANTHOXYLIN	100122-19	A03	sample	23121-32-6	C11H14O4	210.23183		Acradenia franklinii, Eugenia jambolana	undetermined activity	J Chem Soc 1955:105	-0.76	-0.97	-0.20	-0.03	-0.49
00200457	ANHYDROBRAZILIC ACID	100122-19	A04	sample		C12H10O5	234.2105		derivative	undetermined activity		-0.80	-0.03	-0.77	-0.40	-0.50
00200484	DEOXYSAPPANONE B 7,4'-DIMETHYL ETHER	100122-19	A05	sample		C18H18O5	314.34116		Caesalpinia sappan	undetermined activity	Chem Pharm Bull 34: 2506 (1986); 35: 3597 (1987)	-1.44	0.06	-0.42	-0.47	-0.57
00200523	XANTHONE	100122-19	A06	sample	90-47-1	C13H8O2	196.20751		gentian and other flowers	undetermined activity	Phytochemistry 4: 411 (1968)	0.67	0.26	1.16	-0.90	0.30
00200640	3-METHYLORSELLINIC ACID	100122-19	A07	sample	4707-46-4	C9H10O4	182.17765		Aspergillus terreus	undetermined activity	Helv Chim Acta 11: 864 (1928)	-0.68	0.11	-0.84	-0.85	-0.57
00200690	2-BENZOYL-5-METHOXYBENZOQUINONE	100122-19	A08	sample		C14H10O4	242.2334		synthetic dalbergione analog	undetermined activity		0.16	0.59	-0.46	-0.42	-0.03
00200743	ERGOSTEROL	100122-19	A09	sample	57-87-4	C28H44O	396.66228		yeast	undetermined activity	J Biol Chem 80: 15 (1928)	-2.98	-1.34	-0.03	-1.46	-1.45
00200744	ERGOSTEROL ACETATE	100122-19	A10	sample	2418-45-3	C32H50O2	466.7541		derivative; mp 179-181 C	undetermined activity		-6.19	-1.55	-0.24	-1.25	-2.31
00200488	NORSTICTIC ACID PENTAACETATE	100122-19	A11	sample		C28H24O15	600.49448		derivative of norsticitic acid (00240916)	undetermined activity		1.22	-0.69	0.68	-0.93	0.07
	0.04% JAK2inhib	100122-19	A12	0.04% jak2inhib								-0.76	-0.55	1.06	-2.43	-0.67
	0.04% DMSO	100122-19	B01	0.04% dmso								-2.51	-1.41	1.06	-1.44	-1.07
00200759	IRETOL	100122-19	B02	sample		C7H8O4	156.13941		semisynthetic	undetermined activity	J Chem Soc 1927: 3028	-1.37	-0.85	-0.82	-0.30	-0.83
00200763	IRIGENIN, 7-BENZYL ETHER	100122-19	B03	sample		C25H22O8	450.44929		derivative of irigenin from Iris spp.	undetermined activity		-0.80	-0.45	-0.80	-0.12	-0.54
00200793	IRIDIN	100122-19	B04	sample	491-74-7	C24H26O13	522.46702		Iris spp.	undetermined activity	J Chem Soc 1928:1022; Phytochemistry 22:2061 (1983);	-1.63	-0.75	-0.31	-1.77	-1.12
00200798	DALBERGIONE, 4-METHOXY-4'-HYDROXY-	100122-19	B05	sample		C16H14O4	270.28758		Dalbergia spp	undetermined activity	Chem Commun 1968: 1392; mp 174-176 C (blackens)	-0.57	-0.66	0.52	-0.33	-0.26
00200833	ACACETIN DIACETATE	100122-19	B06	sample	5892-39-7	C20H16O7	368.34632		derivative of acacetin	undetermined activity	J Chem Soc 128: 2344 (1926)	0.86	0.30	0.10	-0.85	0.10
00200846	APIGENIN	100122-19	B07	sample	520-36-5	C15H10O5	270.24395	antispasmodic, antineoplastic, topoisomerase I inhibitor	parsley seed	experimental	J Chem Soc 1963: 1477; Eur J Cancer 32A: 146 (1996); J	-1.37	0.86	0.09	1.41	0.25
00200848	DEOXYSAPPANONE B 7,3'-DIMETHYL ETHER	100122-19	B08	sample		C18H18O5	314.34116		Caesalpinia sappan	undetermined activity	Chem Pharm Bull 34: 2506 (1986); 35: 3597 (1987)	-0.18	0.43	0.52	-0.08	0.17
00200873	IRIGENIN TRIMETHYL ETHER	100122-19	B09	sample		C21H22O8	402.40469		derivative	undetermined activity	Prog Chem Org Nat Prod 43: 1 (1983)	-0.26	-1.35	0.42	0.29	-0.23
00201136	SAPPANONE A DIMETHYL ETHER	100122-19	B10	sample		C18H16O5	312.32522		Caesalpinia sappan	undetermined activity	Chem Pharm Bull 34: 2506 (1986); 35: 3597 (1987)	1.90	0.71	0.38	-0.20	0.70
00201078	VIOLASTYRENE	100122-19	B11	sample	19034-96-9	C17H18O3	270.33121		Dalbergia miscolobium	undetermined activity	Chem Commun 1968:1390; Phytochemistry 17:1375,1395	1.29	0.64	0.70	-0.10	0.63
	0.04% JAK2inhib	100122-19	B12	0.04% jak2inhib								-0.58	-1.41	-0.46	-2.08	-1.13
	0.04% DMSO	100122-19	C01	0.04% dmso								-0.21	-1.67	-0.47	-0.75	-0.77
00201154	DEHYDROROTENONE	100122-19	C02	sample	30990-44-4	C23H20O6	392.41225		Derris spp; rotenone derivative	undetermined activity	Chem Rev 12: 181 (1933)	0.36	-0.04	2.33	1.28	0.98
00201177	DUARTIN (-)	100122-19	C03	sample	52305-04-1	C18H20O6	332.3565		Dalbergia variabilis	undetermined activity	Phytochemistry 17: 1401 (1978)	0.45	-0.14	-0.50	0.86	0.17
00201181	IRIGENIN, DIBENZYL ETHER	100122-19	C04	sample		C32H28O8	540.57516		derivative of Irigenin	undetermined activity		0.51	-1.66	0.72	0.28	-0.04
00201227	NONIC ACID	100122-19	C05	sample		C9H16O4	188.22547		hydroysis product of actinonin	undetermined activity		0.33	-0.89	-1.27	-0.62	-0.61
00201281	DALBERGIONE	100122-19	C06	sample		C15H12O2	224.26169		Dalbergia spp	undetermined activity		1.54	0.09	0.82	-1.16	0.32
00201310	2'-METHOXYFORMONETIN	100122-19	C07	sample		C17H14O5	298.29813		Eschscholtzia californica	undetermined activity	Phytochemistry 41: 661 (1996)	0.90	-0.15	-0.21	1.40	0.49
00201331	DEOXYSAPPANONE B TRIMETHYL ETHER	100122-19	C08	sample		C19H20O5	328.36825		Caesalpinia sappan	undetermined activity	Chem Pharm Bull 34: 2506 (1986); 35: 3597 (1987)	1.34	2.16	0.85	0.49	1.21
00201342	DEOXYSAPPANONE B 7,3'-DIMETHYL ETHER	100122-19	C09	sample		C20H20O6	356.3788		derivative Caesalpinia sappan	undetermined activity	Chem Pharm Bull 34: 2506 (1986); 35: 3597 (1987)	0.23	0.03	-0.03	-1.87	-0.41
00201364	DUARTIN, DIMETHYL ETHER	100122-19	C10	sample		C20H24O6	360.41068		derivative of DUARTIN (00201177)	undetermined activity		0.47	2.02	2.40	2.70	1.90
00201448	4,4'-DIMETHOXYDALBERGIONE	100122-19	C11	sample		C17H16O4	284.31467		Dalbergia nigra	undetermined activity	Tetrahedron 21: 2683 (1965)	0.17	-0.95	0.07	4.54	0.95
	0.11% JAK2inhib	100122-19	C12	0.11% jak2inhib								-3.39	-3.58	3.03	-3.78	-1.93
	0.11% DMSO	100122-19	D01	0.11% dmso								-1.52	-2.51	1.49	-0.66	-0.80
00201477	MUNDOSERONE	100122-19	D02	sample	3564-85-0	C19H18O6	342.35171		Mundulea suberosa; mp 156-161 C	undetermined activity	Proc Chem Soc 1960:176; 1969:177	4.06	3.79	3.83	4.02	3.93
00201602	PACHYRRHIZIN	100122-19	D03	sample	10091-01-7	C19H12O6	336.30389	insecticide	Pachyrrhizus erosus; mp 206-207 C	experimental	J Am Chem Soc 67: 1609 (1945)	-0.78	-2.03	-1.28	-2.28	-1.59
00202130	PERSEITOL	100122-19	D04	sample	527-06-0	C7H16O7	212.20137		Persia spp.	undetermined activity	J Am Chem Soc 61: 339 (1939); Carbohydr Res 150: 35	-0.46	-0.55	0.62	0.16	-0.06
00202178	EPIAFZELECHIN (2R,3R)(-)	100122-19	D05	sample	24808-04-6	C15H14O5	274.27583		Larix sibirica, Actinidia chinensis, Juniperus communis, Cassia	undetermined activity	J Chem Soc 1955: 2948; Aust. J. Chem 13: 390 (1960);	-0.42	0.36	-0.70	-0.74	-0.37
00201727	EVERNINIC ACID	100122-19	D06	sample	570-10-5	C8H8O5	184.14996		oak moss lichen	undetermined activity	Ber 56: 2556 (1923); JACS 88: 2053 (1966); Tetrahedron	0.75	0.93	1.27	0.72	0.92
00210211	EPIAFZELECHIN TRIMETHYL ETHER	100122-19	D07	sample		C18H20O5	316.3571		derivative	undetermined activity		0.26	0.23	0.70	0.33	0.38
00210296	GENISTEIN	100122-19	D08	sample	446-72-0	C15H10O5	270.24395		widely distributed in Leguminoseae	undetermined activity	Phytochemistry 7: 791 (1968)	0.36	1.00	0.20	0.58	0.54
01504166	ISOOSAJIN	100122-19	D09	sample	5745-54-0	C25H24O5	404.46703		Maclura pomifera	undetermined activity	J Am Chem Soc 61: 2832 (1939)	1.09	0.03	1.10	0.31	0.63
00211949	APOTOXICAROL	100122-19	D10	sample		C18H14O7	342.30808		derivative	undetermined activity		-0.88	-0.36	-0.21	0.08	-0.34
00107023	SITOSTERYL ACETATE	100122-19	D11	sample		C31H52O2	456.75889		widespread in plants	undetermined activity	J Am Chem Soc 48: 2987 (1926)	-2.47	-1.77	0.26	-2.30	-1.57
	0.11% JAK2inhib	100122-19	D12	0.11% jak2inhib								-2.26	-2.49	-1.28	-4.34	-2.59
	0.11% JAK2inhib	100122-19	E01	0.11% jak2inhib								-3.37	-4.33	-3.29	-2.23	-3.30
00300001	ORSELLINIC ACID	100122-19	E02	sample	480-64-8	C8H8O4	168.15056		common lichen constituent	undetermined activity		-0.09	1.68	-0.74	1.45	0.58
00300003	SOLIDAGENONE	100122-19	E03	sample	23534-56-7	C20H28O3	316.44436		Solidago canadensis L.; mp 133-134 C	undetermined activity	Tetrahedron 25, 2233 (1969)	-0.31	-0.59	-0.70	-0.03	-0.41
00300005	SPHONDIN	100122-19	E04	sample	483-66-9	C12H8O4	216.19516		Heracleum maximum root; mp 191-192 C	undetermined activity	Ber 74:595 (1941); Monatsh Chem 84:217 (1953)	1.55	0.63	0.46	1.82	1.11
00300007	EUPARIN	100122-19	E05	sample	532-48-9	C13H12O3	216.23879		Eupatorium macculatum	undetermined activity	J Chem Soc 1939:925	0.28	1.16	0.87	0.03	0.58
00300006	STICTIC ACID	100122-19	E06	sample	549-06-4	C19H14O9	386.31803		numerous lichens, e.g. Parmelia sp.	undetermined activity	Ber 66, 943 (1933); Tetrahedron 24, 2707 (1966)	-0.43	0.55	-0.32	0.12	-0.02
00300010	AGELASINE (stereochemistry of diterpene unknown)	100122-19	E07	sample		C26H40ClN5	458.0952	cytotoxic, antineoplastic	Agelas dispar	experimental	Can J Chem 53:1690 (1975)	-0.52	1.46	-0.32	0.63	0.31
00300012	ISOPIMPINELLIN	100122-19	E08	sample	482-27-9	C13H10O5	246.22165		Hercaleum maximum; mp 150-153 C dimorphic (142-145 C)	undetermined activity	J Chem Soc 1945: 540	-1.90	-0.17	-1.99	-0.27	-1.08
00300032	ISOBERGAPTENE	100122-19	E09	sample	482-48-4	C12H8O4	216.19516		Heracleum and other Umbelliferaceae; mp 223-224 C	undetermined activity	Ber 70: 1253 (1937)	-0.94	-0.62	0.84	-1.42	-0.54
00300021	GIBBERELLIC ACID	100122-19	E10	sample	77-06-5	C19H22O6	346.38359		Gibberella fujikuroi	undetermined activity	J Chem Soc 1954: 1066	1.72	0.03	0.71	1.76	1.05
00300013	PIMPINELLIN	100122-19	E11	sample	131-12-4	C13H10O5	246.22165	GABA receptor antagonist, phototoxin	Heracleum maximum root; mp 118-119 C	experimental	Monatsh 59: 161 (1932); J Org Chem 35: 2294 (1970)	0.44	-1.33	-0.84	-2.28	-1.00
	0.11% DMSO	100122-19	E12	0.11% dmso								-0.22	0.92	-0.13	-1.15	-0.14
	0.11% JAK2inhib	100122-19	F01	0.11% jak2inhib								-4.01	-3.83	-3.35	-3.20	-3.60

Compound ID	MolNAME	plate	position	Content	cas#	Formula	MolWt	Bioactivity	Source	Status	Reference	Screen Score (z-score) rep1	rep2	rep3	rep4	Average
00300020	1-MONOPALMITIN	100122-19	F02	sample	542-44-9	C19H38O4	330.51231		Asparagus, Momodica spp; widespread in plants	undetermined activity		-1.13	-0.61	1.79	0.05	0.03
00300058	EPI(13)TORULOSOL	100122-19	F03	sample	3650-30-4	C20H34O2	306.49278		Cryptomeria japonica and Larix sibirica	undetermined activity	J Org Chem 29: 1554 (1964); Phytochemistry 13:471 (1974)	-1.05	-0.62	0.03	1.77	0.03
00300055	CADIN-4-EN-10-OL	100122-19	F04	sample		C15H26O	222.37387		Chamaecyparis spp and Juniperus spp.	undetermined activity	Tet Lett 1968: 1913	-0.17	2.27	0.69	1.16	0.99
00300056	LARIXOL	100122-19	F05	sample		C20H34O2	306.49278		Larix sibiricia	undetermined activity	Tet Letters 1965: 3523; 1967: 219	0.28	0.67	-0.25	2.41	0.78
00300057	LARIXOL ACETATE	100122-19	F06	sample		C22H36O3	348.53042		Larix europaea	undetermined activity	Tet Letters 1965: 3523; 1967: 220	0.22	0.82	-0.73	-0.16	0.04
00300146	VULPINIC ACID	100122-19	F07	sample	521-52-8	C19H14O5	322.32043	antiinflammatory, antibacterial, plant growth inhibitor	numerous lichens, e.g. Letharia vulpina	experimental	J Am Chem Soc 72:1824 (1950)	-0.12	0.74	-0.44	0.31	0.12
00300110	3-NOR-3-OXOPANASINSAN-6-OL	100122-19	F08	sample		C14H22O2	222.33024		derivative Panax ginseng	undetermined activity	Chem Pharm Bull 35: 1975 (1987)	1.40	-0.19	1.13	0.08	0.60
00300111	2-METHOXY-5 (6)EPOXY-	100122-19	F09	sample		C16H28O2	252.40036		derivative	undetermined activity		-0.08	-0.29	0.23	-1.04	-0.30
00300117	ISOKORBUSONE	100122-19	F10	sample	24173-72-6	C14H22O2	222.33024		Cyperus rotundus, Sindora sumatrana	undetermined activity	Chem Pharm Bull 17:1390 (1969); 42:138 (1994)	0.55	0.61	3.57	1.27	1.50
00300118	3,7-EPOXYCARYOPHYLLAN-6-OL	100122-19	F11	sample		C15H26O2	238.37327		derivative Lippia spp	undetermined activity		-2.74	0.20	3.88	-0.85	0.12
	0.04% DMSO	100122-19	F12	0.04% dmso								1.43	0.20	1.55	-0.31	0.72
	0.04% JAK2inhib	100122-19	G01	0.04% jak2inhib								-2.05	-2.61	-2.78	-1.47	-2.23
00300119	2-HYDROXY-5 (6)EPOXY-	100122-19	G02	sample		C15H26O2	238.37327		derivative	undetermined activity		-0.87	-0.34	-0.15	0.28	-0.27
00300132	3,7-EPOXYCARYOPHYLLAN-6-ONE	100122-19	G03	sample		C15H24O2	236.35733		derivative Lippia spp	undetermined activity		0.34	1.36	-0.08	0.77	0.60
00300133	CLOVANEDIOL DIACETATE	100122-19	G04	sample		C19H30O4	322.44855		derivative Dipterocarpus pilosus, Salvia canariensis, Viguiera	undetermined activity	Chem Pharm Bull 42: 138 (1994)	-1.44	-1.33	-0.65	-1.24	-1.16
00307047	3-OXOURSAN (28-13)OLIDE	100122-19	G05	sample		C30H44O3	452.68338		semisynthetic	undetermined activity		0.03	2.51	-0.50	1.49	0.88
00307050	DEHYDROABIETAMIDE	100122-19	G06	sample		C20H29NO	299.46023		derivative	undetermined activity		-4.53	-3.47	-3.72	-2.96	-3.67
00307056	MUUROLLADIE-3-ONE	100122-19	G07	sample		C15H22O	218.34199		derivative of muurolene	undetermined activity	Coll Czech Chem Comm 31: 3373 (1966)	-0.31	-0.04	0.24	-0.06	-0.04
00300160	3-PINANONE OXIME	100122-19	G08	sample		C10H17NO	167.25309		derivative	undetermined activity		0.77	0.95	0.72	3.41	1.46
00300531	MELEZITOSE	100122-19	G09	sample		C18H32O16	504.44614		honey & plant exudates	undetermined activity	J Org Chem 11: 610 (1946)	2.09	1.17	0.72	0.83	1.20
00300539	ARBUTIN	100122-19	G10	sample	497-76-7	C12H16O7	272.25712		Berginia crassifolia; also in Pyrus and Vaccinium spp.	undetermined activity	Pharmazie 15: 650 (1960)	0.76	0.41	0.94	3.43	1.39
00300533	ISOSAFROLE	100122-19	G11	sample	120-58-1	C10H10O2	162.19		Illicium religiosum	undetermined activity	J Chem Soc 1927:2489; J Biol Chem 255:7941 (1980); J	1.40	0.23	0.47	3.70	1.45
	0.04% DMSO	100122-19	G12	0.04% dmso								0.29	0.32	0.40	0.18	0.30
	0.04% JAK2inhib	100122-19	H01	0.04% jak2inhib								-2.68	-2.12	-0.13	1.06	-0.97
00300540	HYMECROMONE METHYL ETHER	100122-19	H02	sample	2555-28-4	C11H10O3	190.20055		Dalbergia volubilis, Eupatorium pauciflorum	undetermined activity	Indian J Chem 15:94, 492 (1977)	-0.62	-0.93	-2.12	0.15	-0.88
00300537	XANTHOPTERIN	100122-19	H03	sample	119-44-8	C6H5N5O2	179.13905	cell proliferation inhibitor	human urine, butterfly wing pigment	experimental	J Het Chem 29:583 (1992); Int J Biochem 25:1873 (1993)	2.46	-0.04	-0.76	0.52	0.55
00300542	SANTONIN	100122-19	H04	sample	481-06-1	C15H18O3	246.30891		Artemisia spp.	undetermined activity	J Chem Soc 1930: 1110	-1.26	-0.67	-1.26	-0.17	-0.84
00300547	PHLORIDZIN	100122-19	H05	sample	60-81-1	C21H24O10	436.41943	induces experimental glucosuria, antifeedant	Rosaceae spp	experimental	J Chem Soc 1933: 1170; Physiol Rev 25: 255 (1945)	-1.48	0.35	-1.13	-0.31	-0.64
00300558	GEDUNOL	100122-19	H06	sample		C28H36O7	484.59492		Meliaceae spp	undetermined activity		1.07	-1.14	-0.51	-0.26	-0.21
00300566	CHRYSANTHEMYL ALCOHOL	100122-19	H07	sample	5617-92-5	C10H18O	154.25436		reduction product of pyrrethrin constituent	undetermined activity		-1.14	-0.35	-0.52	-1.23	-0.81
00300564	MENTHONE	100122-19	H08	sample	14073-97-3	C10H18O	154.25436		pennyroyal and peppermint oils	undetermined activity	J Org Chem 25: 1434 (1960)	0.66	2.21	1.06	0.25	1.05
00300556	CHRYSAROBIN	100122-19	H09	sample	491-58-7	C15H12O3	240.26109		Andira araroba (glacial AcOH)	undetermined activity	J Am Chem Soc 53: 4114 (1931)	0.67	1.41	2.98	1.72	1.69
00300553	PELLETIERINE HYDROCHLORIDE	100122-19	H10	sample		C8H16ClNO	177.67582		Punica granatum	undetermined activity	Bull Soc Chim Fr 1961: 1993	0.94	-0.26	-0.30	-1.77	-0.35
00300554	PHLORETIN	100122-19	H11	sample	60-82-2	C15H14O5	274.27583		Prunus spp	undetermined activity	Ann Rev Biochem 20: 4955 (1951)	-0.03	-1.08	-0.52	-2.24	-0.97
	empty	100122-19	H12	sample								NA	NA	NA	NA	NA
	empty	100122-20	A01	sample								NA	NA	NA	NA	NA
00210220	CATECHIN TETRAMETHYLETHER	100122-20	A02	sample		C19H22O6	346.38359		derivative	undetermined activity		-2.32	-2.28	-0.88	-1.30	-1.70
00200499	ACACETIN	100122-20	A03	sample	480-44-4	C16H12O5	284.27104	antiinflammatory, spasmolytic agent, antioxidant	Robinia pseudoacacia	experimental	J Pharm Soc Japan 73: 481 (1953); Experientia 47: 195	1.30	-0.98	-1.12	-1.99	-0.70
01504256	EPICATECHIN PENTAACETATE	100122-20	A04	sample		C25H24O11	500.46343		derivative	undetermined activity		-2.10	-1.79	-0.18	0.00	-1.02
00205113	EPIGALLOCATECHIN	100122-20	A05	sample	970-74-1	C15H14O7	306.27463		green tea	undetermined activity		2.32	-1.48	0.05	-1.14	-0.06
01600537	CATECHIN PENTAACETATE	100122-20	A06	sample		C25H24O11	500.46343		derivative	undetermined activity		-1.88	-1.25	-0.85	-0.72	-1.17
00201513	EPIGALLOCATECHIN 3,5-DIGALLATE	100122-20	A07	sample		C29H22O15	610.48969		tea pigment	undetermined activity		-0.45	-1.61	-0.38	3.52	0.27
00210206	EPICATECHIN	100122-20	A08	sample	490-46-0	C15H14O6	290.27523	antioxidant	tea and cocoa constituent	experimental	J Chem Soc 1969: 1824; Acta Cryst C 40: 2068 (1984)	-1.51	0.65	-1.44	-1.85	-1.04
00210239	EPIGALLOCATECHIN-3-MONOGALLATE	100122-20	A09	sample	989-51-5	C22H18O11	458.38216		tea pigment	undetermined activity		3.06	-0.26	0.86	0.43	1.02
00201507	2,2-BISEPIGALLOCATECHIN DIGALLATE	100122-20	A10	sample		C44H34O22	914.74838		tea pigment	undetermined activity		-0.01	0.24	4.90	0.00	1.28
00210238	EPICATECHIN MONOGALLATE	100122-20	A11	sample	1257-08-5	C22H18O10	442.38276		tea pigment	undetermined activity		0.18	0.38	0.82	2.89	1.07
	0.04% JAK2inhib	100122-20	A12	0.04% jak2inhib								-1.18	-0.12	-0.31	-2.59	-1.05
	0.04% DMSO	100122-20	B01	0.04% dmso								-2.60	-4.61	3.44	-3.90	-1.92
00310041	VISNAGIN	100122-20	B02	sample	82-57-5	C13H10O4	230.22225		Ammi visnaga	undetermined activity	Tetrahedron 3: 230 (1958)	-2.22	-2.74	3.95	-1.20	-0.55
00310298	GLUCOSAMINIC ACID	100122-20	B03	sample		C6H13NO6	195.17361		oxidation product of glucosamine (01500316)	undetermined activity		1.09	-1.83	-0.10	-0.11	-0.24
00310030	RHODINYL ACETATE	100122-20	B04	sample		C12H22O2	198.30794		common constituent of plant essential oils	undetermined activity		3.94	-0.67	-0.59	2.72	1.35
00310010	HELENINE	100122-20	B05	sample	546-43-0	C15H20O2	232.32545	anthelmintic, antibacterial, antineoplastic	Inula spp	experimental	J Am Chem Soc 79: 5721 (1957); 88: 3408 (1966); J Org	-0.32	-1.02	-0.59	-0.60	-0.63
00310012	HESPERETIN	100122-20	B06	sample	520-33-2	C16H14O6	302.28638		aglycone of hesperidin (00310011)	undetermined activity	J Chem Soc 1956: 632	-1.42	0.14	-0.92	-0.58	-0.70
00310009	EPIANDROSTERONE	100122-20	B07	sample		C19H30O2	290.44975		in normal human urine	undetermined activity	J Am Chem Soc 75: 2275 (9153)	-0.52	0.27	0.09	-0.55	-0.18
00310008	DJENKOLIC ACID	100122-20	B08	sample	498-59-9	C7H14N2O4S2	254.32863		djenkol bean (Pithecolobium lobatum)	undetermined activity	J Biol Chem 168: 373 (1947)	-0.48	0.73	0.65	4.80	1.42
00310015	CEDRYL ACETATE	100122-20	B09	sample	77-54-3	C17H28O2	264.41151		semisynthetic	undetermined activity		-0.41	0.98	1.65	-0.40	0.46
00310023	HYPOXANTHINE	100122-20	B10	sample	68-94-0	C5H4N4O	136.11383		widely distributed in the plant and animal kingdom	undetermined activity		2.03	0.59	1.31	-0.08	0.96
00310021	PHYTOL	100122-20	B11	sample		C19H38O	282.51411		nettles	undetermined activity	J Chem Soc 1966: 2144	-6.25	-1.35	-0.65	-1.83	-2.52
	0.04% JAK2inhib	100122-20	B12	0.04% jak2inhib								-1.62	-0.43	-0.25	-2.91	-1.30
	0.04% DMSO	100122-20	C01	0.04% dmso								-4.08	-0.94	-1.77	-3.50	-2.57
00310019	CHRYSANTHEMIC ACID, ETHYL ESTER	100122-20	C02	sample		C12H20O2	196.292	insecticide	pyrethrum flowers	experimental	J Chem Soc 1945: 283	-1.14	-2.08	-0.97	2.19	-0.50
00310004	ANABASINE HYDROCHLORIDE	100122-20	C03	sample	13078-04-1 (anabasine)	C10H15ClN2	198.69745	insecticide	Anabasis aphylla & Nicotiana spp	agricultural use	J Am Chem Soc 57: 959 (9154)	0.10	-1.42	-0.61	0.37	-0.39
00310001	ACONITIC ACID	100122-20	C04	sample	585-84-2	C6H6O6	174.11112		Aconitum and Achillea spp	undetermined activity	Ind Eng Chem 33: 637 (1941)	3.20	-0.37	0.02	3.59	1.61
00310011	HESPERIDIN	100122-20	C05	sample	520-26-3	C28H34O15	610.57418	capillary protectant	Citrus spp.	experimental		0.02	2.12	0.91	1.33	1.09
00310025	LARIXINIC ACID	100122-20	C06	sample	118-71-8	C6H6O3	126.11292		Larix decidua	undetermined activity	Ber 27: 3115 (1984); 34: 1804 (1901); 43: 2398 (1910)	-0.76	0.63	0.60	0.25	0.18
00310018	QUINIC ACID	100122-20	C07	sample	77-95-2	C7H12O6	192.17009		Cinchona spp	undetermined activity	Ber 65: 1009 (1932)	3.20	1.70	-0.21	2.49	1.79
00310028	QUASSIN	100122-20	C08	sample	76-78-8	C22H28O6	388.46486	insecticide, antiamoebic	Quassia amara, Picrasma excelsa and Ailanthus glandulosa	experimental	JACS 60:1146 (1938); 72:375 (1950); Tetrahedron 15:100	1.51	0.16	0.50	-0.93	0.31
00350025	APIIN	100122-20	C09	sample	26544-34-3	C26H28O14	564.50466		parsley seed; flowers of Anthemis nobilis. 80% + other glycosides	undetermined activity	Chem Ind 1953: 85; Can J Chem 43: 2085 (1965)	1.13	0.72	-0.32	-0.60	0.23
10101011	BIXIN	100122-20	C10	sample	39937-23-0	C25H30O4	394.51545		Bixa orellana seeds	undetermined activity	Helv Chim Acta 40: 1242 (1957); J Chem Soc 1961: 1625;	-3.94	-0.20	0.55	-0.68	-1.07
00203008	JUAREZIC ACID	100122-20	C11	sample	1552-94-9	C11H10O2	174.20115		propolis and Populus spp	undetermined activity	JACS 108: 3016 (1986); Phytochemistry 29: 2551 (1990)	0.72	0.64	0.99	1.71	1.02
	0.11% JAK2inhib	100122-20	C12	0.11% jak2inhib								-2.13	2.31	-1.62	-3.91	-1.34
	0.11% DMSO	100122-20	D01	0.11% dmso								0.32	-0.38	-2.96	-3.53	-1.64
01600759	4-HYDROXY-6-METHYLPYRAN-2-ONE	100122-20	D02	sample	675-10-5	C6H6O3	126.11292		Pennicillium stipitatum	undetermined activity	J Am Chem Soc 89: 676, 681 (1967)	1.10	-1.80	0.66	-0.56	-0.15
01400164	2-HYDROXY-3,4-DIMETHOXYBENZOIC ACID	100122-20	D03	sample		C9H10O5	198.17705	prostaglandin synthetase inhibitor	Dalbergia odorifera	experimental		1.14	-1.07	-0.56	-0.22	-0.18
01400131	HAEMATOMMIC ACID	100122-20	D04	sample	479-25-4	C9H8O5	196.16111		Alectoria spp, Haematomma spp and Lethariella spp	undetermined activity	J Org Chem 42: 2526 (1977); Helv Chim Acta 72: 1061	-0.35	-1.57	-0.05	-0.47	-0.61
01400156	ISOPEONOL	100122-20	D05	sample	493-33-4	C9H10O3	166.17825		Paeonia spp	undetermined activity		-0.85	-0.05	0.17	0.46	-0.07
01400136	N-METHYLISOLEUCINE	100122-20	D06	sample	5125-98-8	C7H15NO2	145.2031		Phasealus vulgaris	undetermined activity	Phytochemistry 42: 443 (1996)	0.15	0.12	0.09	-0.13	0.06
01600300	CREATININE	100122-20	D07	sample	60-27-5	C4H7N3O	113.11989	metabolic enhancer	metabolite in muscle and urine; renal metabolite	undetermined activity	J Biol Chem 81:73 (1929); JACS 93:5552 (1971)	-0.18	-0.38	0.51	0.58	0.13
01601000	MEVASTATIN	100122-20	D08	sample	73573-88-3	C23H34O5	390.52443	antihyperlipidemic, HMGCoA reductase inhibitor	Penicillium brevicompactum; Compactin	INN		0.68	0.00	0.78	1.60	0.76
01600964	N-METHYLANTHRANILIC ACID	100122-20	D09	sample	119-68-6	C8H9NO2	151.16643		grapefruit peel oil	undetermined activity	Ber 42: 3194 (1909)	0.69	4.87	0.89	0.01	1.61
01600480	TETRAHYDROSAPPANONE A TRIMETHYL ETHER	100122-20	D10	sample		C19H22O5	330.38419		derivative Caesalpinia sappan	undetermined activity	Chem Pharm Bull 34: 2506 (1986); 35: 3597 (1987)	0.99	0.24	-0.07	0.38	0.38
00300610	ACETOSYRINGONE	100122-20	D11	sample	2478-38-8	C10H12O4	196.20474	insect attractant, plant hormone	several commercial woods	experimental	Can J Chem 34: 1562 (1956)	2.71	1.06	1.08	3.35	2.05
	0.11% JAK2inhib	100122-20	D12	0.11% jak2inhib								-2.88	-1.21	-1.80	-3.45	-2.33
	0.11% JAK2inhib	100122-20	E01	0.11% jak2inhib								-5.31	-1.33	-4.36	-2.93	-3.48
01601021	PAEONOL	100122-20	E02	sample	552-41-0	C9H10O3	166.17825	antibacterial	Paeonia montan, Xanthorrhoea spp	experimental		-0.56	-1.98	-1.78	-0.70	-1.25
01503218	HEPTAMINOL HYDROCHLORIDE	100122-20	E03	sample	543-15-7, 372-66-7	C8H20ClNO	181.7077	vasodilator	synthetic	INN, BAN		1.19	-0.55	-0.90	0.35	0.02
00270083	5alpha-CHOLESTAN-3beta-OL-6-ONE	100122-20	E04	sample		C27H46O2	402.66647		Mandevilla pentlandiana	undetermined activity		-0.11	0.10	0.95	-0.31	0.16
00240437	PERSEITOL HEPTAACETATE	100122-20	E05	sample	19147-10-5	C21H30O14	506.46485		derivative of perseitol	undetermined activity		1.17	-0.18	0.53	2.44	0.99
00240429	3,4-DIDESMETHYL-5-DESHYDROXY-3'-	100122-20	E06	sample		C15H14O5	274.27583		synthetic	undetermined activity	Tetrahedron 21: 2697 (1965)	-0.62	0.02	-0.33	0.13	-0.20
00500580	PIPERONYLIC ACID	100122-20	E07	sample	94-53-1	C8H6O4	166.13462		Piper longum, Cinnamumum spp	undetermined activity	J Chem Soc 1950: 2376	-0.20	-0.78	0.38	0.95	0.08
00501332	PHENACYLAMINE HYDROCHLORIDE	100122-20	E08	sample	5468-37-1, 613-89-8(base)	C8H10ClNO	171.628		Castanopsis cuspidata, Vitis spp	undetermined activity	Planta Med 22: 434 (1972)	3.24	2.75	1.42	0.14	1.89
00500123	CYCLOVERATRYLENE	100122-20	E09	sample		C27H30O6	450.53655		Halopythus spp	undetermined activity	Tet Lett 1978: 1699; 33: 5846 (1992)	0.10	0.36	0.50	-0.25	0.18
00501000	d,l-threo-3-HYDROXYASPARTIC ACID	100122-20	E10	sample		C4H7NO5	149.10409	L-aspartate beta-carboxylase inhibitor	Streptomyces spp, Arthrinium phaeospermum,	experimental		1.74	0.63	1.28	-0.84	0.70
00390001	APIOLE	100122-20	E11	sample	523-80-8	C12H14O4	222.24298	antipyretic, diuretic, insecticide	Petroselimum spp, Anethum graveolens	experimental	Phytochemistry 15: 1773 (1976); Pharmazie 34: 426 (1979)	-2.30	-0.03	-0.56	3.01	0.03
	0.11% DMSO	100122-20	E12	0.11% dmso								0.07	0.39	0.12	-1.44	-0.22
	0.11% JAK2inhib	100122-20	F01	0.11% jak2inhib								-5.81	-2.11	-4.33	-5.27	-4.38
01401406	DERRUSNIN	100122-20	F02	sample	14736-62-0	C19H16O7	356.33517		Derris robusta	undetermined activity	J Chem Soc 1969:365	-0.49	-2.02	3.35	4.21	1.26
01401419	DERRUSTONE	100122-20	F03	sample	2204-59-3	C18H14O6	326.30868		Derris robusta	undetermined activity	J Chem Soc 1959: 2679; Phytochemistry 7: 701 (1968); 11:	-1.66	-1.59	-0.11	1.40	-0.49
01401401	METHYL ROBUSTONE	100122-20	F04	sample		C22H18O6	378.38516		Derris spp	undetermined activity	J Indian Chem Soc 18: 471 (9179)	-3.24	-3.33	-3.41	-4.56	-3.64
00100048	7-DEACETOXY-7-OXOKHIVORIN	100122-20	F05	sample	15004-51-0	C30H38O9	542.63196		Khaya senegalensis and other Meliaceae; mp 225	undetermined activity	J Chem Soc 1963: 980	0.25	-0.58	-0.39	0.13	-0.15
00100650	DESACETYL (7)KHIVORINIC ACID, METHYL ESTER	100122-20	F06	sample		C28H40O10	536.625		semisynthetic	undetermined activity		-0.70	-0.82	-0.41	-0.32	-0.56
00100572	FRAXIDIN METHYL ETHER	100122-20	F07	sample		C12H12O5	236.22644		derivative	undetermined activity		0.51	0.39	0.05	0.11	0.27
00100652	DIHYDROXY (3alpha,12alpha)PREGNAN-20-ONE	100122-20	F08	sample		C21H34O3	334.50333		semisynthetic	undetermined activity		-0.05	0.20	5.29	-0.78	1.17
00200033	LEOIDIN	100122-20	F09	sample	105350-54-7	C18H14Cl2O7	413.21408		lichen metabolite	undetermined activity	J Chem Soc 1986: 1491	1.11	1.04	1.09	-0.07	0.79
00300147	USNIC ACID	100122-20	F10	sample	125-46-2	C18H16O7	344.32402	antibacterial	Usnea, Cladonia and other lichen spp	experimental	J Chem Soc, 1953, 603; Antibiotics I (Verlag), 1967, p 611	0.60	0.19	-0.05	0.06	0.20
00307059	CEDROL	100122-20	F11	sample	77-53-2	C15H26O	222.37387	acaricide	Common constitutent in the Family Cupressaceae	experimental	J Org Chem 43: 1964 (1978)	1.15	2.51	0.59	-0.08	1.04
	0.04% DMSO	100122-20	F12	0.04% dmso								1.03	0.56	1.23	-0.47	0.59
	0.04% JAK2inhib	100122-20	G01	0.04% jak2inhib								-4.78	-5.54	-3.89	-0.54	-3.69
00300384	5,7,4'-TRIMETHOXYFLAVONE	100122-20	G02	sample	5631-70-9	C18H16O5	312.32522		Cassia siamia, Citrus reticulata	undetermined activity	Phytochemistry 22: 625 (1983)	-2.90	-2.84	0.54	-0.04	-1.31
00300604	PHLORACETOPHENONE	100122-20	G03	sample	480-66-0	C8H8O4	168.1506		Prunus domesticus	undetermined activity	JACS 54:2452 (1932); J Chem Soc 1953:1241;	-0.47	0.52	0.64	-0.16	0.13
01500624	CARNITINE (dl) HYDROCHLORIDE	100122-20	G04	sample	461-06-3	C7H16ClNO3	197.66347	antihyperlipoproteinemic, gastric/ pancreatic secretion stimulant	striated muscle, liver; also in Pisum sativum	INN, JAN		0.63	0.42	-0.27	0.21	0.25
01500672	QUERCETIN	100122-20	G05	sample	117-39-5	C15H10O7	302.24275	capillary protectant, antioxidant. antineoplastic, anti-HIV;	Solanaceae, Rhamnaceae, Passifloraceae, Umbelliferae genera	experimental	Chem Ber 103:3674 (1970); Experientia 28:380 (1972);	-2.17	-2.59	-1.10	1.40	-1.11
01500678	gamma-AMINOBUTYRIC ACID	100122-20	G06	sample	56-12-2	C4H9NO2	103.12183	antihypertensive	widely distributed in higher plants	JAN		0.00	-0.20	-0.35	1.15	0.15
01500690	MELATONIN	100122-20	G07	sample	73-31-4	C13H16N2O2	232.28467	sleep induction, modifies circadian rhythm	pineal gland	experimental		0.00	1.06	-0.32	-0.19	0.14
01500707	CITROPTEN	100122-20	G08	sample	487-06-9	C11H10O4	206.19995	photosensitizing agent	Bergamot oil	experimental	Indian J Chem 13: 835 (1975)	-0.22	-0.15	-0.81	-1.72	-0.72
01500717	6,4'-DIHYDROXYFLAVONE	100122-20	G09	sample	63046-09-3	C15H10O4	254.24455	antihaemorrhagic	Cassia spp as glycoside	experimental		1.96	1.38	3.84	3.95	2.78
01500719	7,2'-DIHYDROXYFLAVONE	100122-20	G10	sample	77298-66-9	C15H10O4	254.24455	antihaemorrhagic	Primula spp	experimental		1.45	1.15	0.14	-0.19	0.64
01500729	4-METHYLESCULETIN	100122-20	G11	sample		C10H8O4	192.17286		analog of esculetin	undetermined activity		0.70	2.17	3.15	0.04	1.51
	0.04% DMSO	100122-20	G12	0.04% dmso								0.87	1.10	0.27	-0.34	0.48
	0.04% JAK2inhib	100122-20	H01	0.04% jak2inhib								-5.13	-5.01	-3.99	-5.75	-4.97
01500737	3,7-DIMETHOXYFLAVONE	100122-20	H02	sample	20950-52-1	C17H14O4	282.29873		Pongamia pinnata	undetermined activity		-1.18	-3.33	-1.33	-2.72	-2.14
01500730	4-METHYLDAPHNETIN	100122-20	H03	sample		C10H8O4	192.17286		analog of daphnetin	undetermined activity		-0.36	0.23	-0.03	2.10	0.48
01500739	CHRYSIN DIMETHYL ETHER	100122-20	H04	sample	21392-57-4	C17H14O4	282.29873		Boesenburgia pandurata, Leptosermum scoparium	undetermined activity		-0.19	-0.65	-1.10	-0.06	-0.50
01500746	NARINGENIN	100122-20	H05	sample	480-41-1	C15H12O5	272.25989	antiulcer, gibberellin antagonist	widely distributed in plants	experimental		-0.55	0.03	-0.44	1.24	0.07
01500752	QUERCITRIN	100122-20	H06	sample	522-12-3	C21H20O11	448.38695	antihemmorrhagic	widespread in plants	experimental		-5.42	-2.53	-0.02	-0.44	-2.10
01500764	KINETIN	100122-20	H07	sample	525-79-1	C10H9N5O	215.21613	auxin, plant growth regulator, plant cell division promotor	yeast	experimental	JACS 77: 1392, 2662 (1955); 78: 1375, 3693 (1956); 82:	0.30	0.11	-0.45	-1.79	-0.46
01500765	NARINGIN	100122-20	H08	sample	10236-47-2	C27H32O14	580.54769	antihaemorrhagic, antiinflammatory	Citrus spp	experimental	JACS 61: 175 (1939); Tetrahedron 19: 773 (1963)	0.04	0.00	-0.30	0.54	0.07
01500814	CANTHARIDIN	100122-20	H09	sample	56-25-7	C10H12O4	196.20474	irritant	active principle of cantharides and other insects	experimental	J Am Chem Soc 63: 3167 (1941)	-1.03	-0.97	1.91	-2.14	-0.56

Compound ID	MolNAME	plate	position	Content	cas#	Formula	MolWt	Bioactivity	Source	Status	Reference	Screen Score (z-score) rep1	rep2	rep3	rep4	Average
01500815	BETULIN	100122-20	H10	sample	473-98-3	C30H50O2	442.7318		Betula spp	undetermined activity	J Am Chem Soc 78: 2312 (1956)	0.50	0.73	-0.55	0.00	0.17
01500817	CARMINIC ACID	100122-20	H11	sample	1260-17-9	C22H20O14	508.3963		Dactylopius coccus (cochineal)	undetermined activity		1.38	0.47	5.74	0.99	2.15
	empty	100122-20	H12	sample								NA	NA	NA	NA	NA
	empty	100122-21	A01	sample								NA	NA	NA	NA	NA
01500821	BICUCULLINE (+)	100122-21	A02	sample	485-49-4	C20H17NO6	367.36159	GABAa antagonist	Dicentra cucullaria, Corydalis spp	experimental	Coll Czech Chem Commun, 29, 2328 (1964); Nature	-1.75	-1.34	1.25	-2.26	-1.03
01500832	CARYLOPHYLLENE OXIDE	100122-21	A03	sample	1139-30-6	C14H22O	206.33084		clove, cinnamon and many other oils	undetermined activity		-1.20	-2.17	-2.82	-2.24	-2.11
01500835	URSOCHOLANIC ACID	100122-21	A04	sample	546-18-9	C24H40O2	360.5852		Abrus pecatorius	undetermined activity	Steroids 23:357 (1974)	-12.11	-4.31	-2.60	-3.50	-5.63
01500836	CEPHALOSPORIN C SODIUM	100122-21	A05	sample	61-24-5	C16H20N3NaO8S	437.4069	antibacterial	Cephalosporium acremonium	BAN		-0.60	-1.63	-0.95	-1.38	-1.14
01500842	CARYOPHYLLENE [(-)]	100122-21	A06	sample	87-44-5	C14H22	190.33144		clove, cinnamon and many other oils	undetermined activity		-6.70	-1.40	-1.04	2.95	-1.55
01500849	CHOLEST-5-EN-3-ONE	100122-21	A07	sample	601-54-7	C27H44O	384.65113		animal fats; mp 79-80 C	undetermined activity	J Am Chem Soc 75: 3500 (1953)	-4.24	-1.61	-1.29	-3.20	-2.59
01500851	CHOLEST-4,6-DIEN-3-ONE	100122-21	A08	sample	566-93-8	C27H42O	382.63519		Pinus spp	undetermined activity	Hoppe Seyler's Z Physiol Chem 245:80 (1936); J Chem Soc	-8.09	0.06	-1.17	0.14	-2.27
01500854	7-OXOCHOLESTEROL	100122-21	A09	sample	566-28-9	C27H44O2	400.65053		Cliona copiosa	undetermined activity	Annalen 543, 240 (1940); JACS 71:2226 (1949); J Chem	-6.99	-0.54	-0.63	1.29	-1.72
01500855	CITRULLINE	100122-21	A10	sample	627-77-0	C6H13N3O3	175.18881		Citrullis vulgaris and the alga Grateloupia filicina	undetermined activity	Tetrahedron 40: 235 (1984)	2.29	-0.14	0.50	-0.36	0.57
01500856	CHOL-11-ENIC ACID	100122-21	A11	sample		C24H36O3	372.55272		semisynthetic	undetermined activity		1.10	-0.93	3.61	-2.32	0.36
	0.04% JAK2inhib	100122-21	A12	0.04% jak2inhib								-0.39	-2.55	-1.85	-2.90	-1.92
	0.04% DMSO	100122-21	B01	0.04% dmso								-2.41	-1.29	-1.34	1.19	-0.96
01500857	BILIRUBIN	100122-21	B02	sample	635-65-4	C33H36N4O6	584.67807		pigment mamalian gallstones, blood and urine	undetermined activity		-1.01	-0.75	0.90	-0.52	-0.34
01500860	S-ISOCORYDINE (+)	100122-21	B03	sample	475-67-2	C20H23NO4	341.41061	sedative, cholinergic	Dicentra canadensis, Artabotyris suaveoleus and Cordyalis	experimental	J Org Chem 19:1774 (1954); Aust J Chem 20: 1277 (1967)	-1.31	-1.45	-2.45	-2.63	-1.96
01500861	CORALYNE CHLORIDE	100122-21	B04	sample	38989-38-7	C22H22ClNO4	399.87794	cytostatic, intercalating agent	semisynthetic	experimental	Int J Immunopharmacol 6: 587 (1984); Nucleic Acids Res	-0.67	-2.06	-1.70	-1.91	-1.59
01500862	BOLDINE	100122-21	B05	sample	476-70-0	C19H21NO4	327.38352		Peumus boldus	undetermined activity	J Chem Soc Perkin I 1977: 706	-0.31	1.22	-0.29	2.58	-0.49
01500864	HARMALINE	100122-21	B06	sample	304-21-2	C13H14N2O	214.26933	CNS stimulant, antiparkinsonian agent	Peganium harmala	experimental	Ber 63: 120 (1930)	-0.02	0.02	-0.49	-2.60	-0.78
01500866	HARMANE	100122-21	B07	sample	486-84-0	C12H10N2	182.2269	intercalating agent, sedative	Arariba rubra.	experimental	J Am Chem Soc 76: 2792 (1954)	0.93	0.08	0.65	-2.13	-0.12
01500869	MIMOSINE	100122-21	B08	sample		C8H10N2O4	198.1799	depilatory agent	Mimosa and Leucena spp	experimental	Z Physiol Chem 244: 153 (1936)	0.75	3.22	2.07	-2.03	1.00
01500871	NORHARMAN	100122-21	B09	sample	244-63-3	C11H8N2	168.19981	plant growth inhibitor; mutagen	Chrysophyllum and Nocardia spp	experimental	J Chem Soc 119: 1602 (1921); 1929: 2926; Phytochemistry	1.30	0.74	-0.65	-3.58	-0.55
01500876	CORYNANTHINE	100122-21	B10	sample	123333-62-0	C21H26N2O3	354.45297		bark of Pseudocinchona africana Chev.	undetermined activity	Helv Chim Acta 9: 1207 (1951)	2.33	-0.86	-0.71	-2.66	-0.48
01500877	KYNURAMINE	100122-21	B11	sample		C9H12N2O	164.20879		urine of various animals	undetermined activity	Z Naturforsch 8b: 454 (1953)	1.97	-0.03	0.10	-0.98	0.27
	0.04% JAK2inhib	100122-21	B12	0.04% jak2inhib								-0.02	-2.47	-1.74	-1.12	-1.34
	0.04% DMSO	100122-21	C01	0.04% dmso								-2.25	-1.22	-1.33	-2.01	-1.70
01500879	KYNURENINE	100122-21	C02	sample		C10H12N2O3	208.21874		mamalian urine	undetermined activity	J Am Chem Soc 71: 4158 (1955)	-1.15	-0.91	1.34	-1.13	-0.46
01500899	ESCULETIN	100122-21	C03	sample	305-01-1	C9H6O4	178.14577	antifungal	Aesculus and Solanaceae spp	experimental		-2.31	-0.30	-0.88	-0.58	-1.02
01500904	CHOLIC ACID, METHYL ESTER	100122-21	C04	sample	1448-36-8	C25H42O5	422.61049		acid as primary bile constituent	undetermined activity		2.27	0.41	0.85	0.03	0.89
01500984	GINKGOLIDE A	100122-21	C05	sample	15291-75-5	C20H24O11	440.40768	antibacterial	Ginkgo biloba	experimental	J Am Chem Soc 93: 3546 (1971)	2.78	0.50	-0.04	-0.47	0.69
01500986	GITOXIN	100122-21	C06	sample	4562-36-1	C41H64O14	780.95883	cardiotonic	Digitalis spp.	experimental	Chem Pharm Bull 18: 1080 (1970); Mol Pharmacol 11:653	-5.35	-2.90	-3.56	-3.25	-3.77
01500989	18alpha-GLYCYRRHETINIC ACID	100122-21	C07	sample		C30H46O4	470.69872	antiinflammatory	epimer of aglycone Glycyrrhiza glabra	experimental		-2.35	-0.97	-0.40	0.42	-0.82
01501012	3-HYDROXYFLAVONE	100122-21	C08	sample	577-85-5	C15H10O3	238.24515		cabbage	undetermined activity		0.95	0.04	-0.10	0.61	0.37
01501019	BERBAMINE HYDROCHLORIDE	100122-21	C09	sample	478-61-5 (berbamine)	C37H42Cl2N2O6	681.66309	antihypertensive, skeletal muscle relaxant	Berberis spp	experimental	J Indian Chem Soc 28: 225 (1951); 30: 705 (1953); Aust J	0.87	1.61	-0.43	-1.08	0.25
01501107	PICROTOXININ	100122-21	C10	sample	17617-45-7	C15H16O6	292.29117	convulsant, GABA receptor antagonist, ichthyotoxin	Anamirta cocculus, Menispermum cocculus	experimental	JACS 57: 1111 (1935); 79: 5550 (1957); Chem Rev 67: 441	1.91	2.22	0.80	-1.76	0.79
01504027	CYTISINE	100122-21	C11	sample	485-35-8	C11H14N2O	190.24703	antiinflammatory, respiratory stimulant	Thermopsis lanceolata	INN	J Chem Soc 1932: 2778; Martindale 28th Ed, 1700 (1982)	2.29	0.50	0.43	-1.23	0.50
	0.11% JAK2inhib	100122-21	C12	0.11% jak2inhib								-1.33	-3.43	-0.09	-2.21	-1.76
	0.11% DMSO	100122-21	D01	0.11% dmso								-3.26	3.56	1.03	-0.38	0.24
01501197	PRIMULETIN	100122-21	D02	sample	491-78-1	C15H10O3	238.24515		Primula spp	undetermined activity	Helv Chim Acta 24:297 (1941)	2.26	-0.04	0.18	-0.32	0.52
01501207	KINETIN RIBOSIDE	100122-21	D03	sample		C15H17N5O5	347.33324		semisynthetic	undetermined activity		-0.58	1.87	0.47	-0.14	0.41
01501208	KARANJIN	100122-21	D04	sample	521-88-0	C17H10O4	278.26685		Derris and Tephrosia spp.	undetermined activity	Indian Acad Sci 17: 16 (1943)	2.28	1.20	1.24	-0.18	1.13
01501212	LINALOOL (+)	100122-21	D05	sample		C10H18O	154.25436		Mentha arvensis and related essential oils	undetermined activity		0.77	-0.75	0.16	1.12	0.33
01502113	AZASERINE	100122-21	D06	sample	115-02-6	C5H7N3O4	173.12924	antineoplastic, amino acid antagonist	Streptomyces fragilis	USAN, INN		0.92	2.21	0.65	-0.21	0.89
00330058	CHLORPYRIFOS	100122-21	D07	sample	2921-88-2	C9H11Cl3NO3PS	350.58972	insecticide	synthetic; DURSBAN	BAN		0.14	-0.19	0.07	0.52	0.14
01502223	RESVERATROL	100122-21	D08	sample	501-36-0	C14H12O3	228.24994	antifungal, antibacterial	Veratrum grandiflorum, Pinus sibirica, Vitis vinifera, Arachis	experimental	Aust J Chem 24:2427 (1971); Tet Lett 1972:2965;	1.12	1.62	1.19	0.55	1.12
01502231	CELLOBIOSE (D[+])	100122-21	D09	sample	528-50-7	C12H22O11	342.30254		enzymatic hydrolysis of cellulose	undetermined activity	J Am Chem Soc 75: 1916 (1953)	-0.45	0.22	2.80	-1.91	0.16
01502235	ASTAXANTHIN	100122-21	D10	sample	71772-51-5	C40H52O4	596.85804		Carotenoid pigment plant and animal sources	undetermined activity	Nature 184: 1714 (1959)	-0.08	-0.53	0.55	2.26	0.55
01502237	HARMOL HYDROCHLORIDE	100122-21	D11	sample	40580-83-4	C12H11ClN2O	234.68727	MAO inhibitor	common plant alkaloid	experimental	Phytochemistry 19:1573 (1980)	1.09	-0.07	0.04	-1.71	-0.16
	0.11% JAK2inhib	100122-21	D12	0.11% jak2inhib								-1.39	-4.26	-4.14	-4.10	-3.47
	0.11% JAK2inhib	100122-21	E01	0.11% jak2inhib								-4.72	-3.21	-4.22	1.95	-2.55
01502238	DEOXYADENOSINE	100122-21	E02	sample	16373-93-6	C10H13N5O3	251.24681		synthetic	undetermined activity		0.46	0.60	-0.36	0.28	0.25
01502242	SCOPOLETIN	100122-21	E03	sample	92-61-5	C10H8O4	192.17286	NO synthesis (inducible) inhibitor, anticoagulant	Scopolia spp.	experimental	J Org Chem 26: 1215 (1961)	0.58	0.37	-0.13	0.48	0.33
01502244	AMYGDALIN	100122-21	E04	sample	29883-15-6	C20H27NO11	457.43829	antiinflammatory, experimental antineoplastic	Rosaceae spp	experimental		0.80	0.18	-1.08	2.98	0.72
01502253	HEMATEIN	100122-21	E05	sample	475-25-2	C16H12O6	300.27044		logwood, Haematoxylon spp.	undetermined activity	J Chem Soc 93: 115 (1908)	0.91	1.37	-0.77	1.16	0.67
01502247	FISETIN	100122-21	E06	sample	528-48-3	C15H10O6	286.24335	antioxidant	Rhus and Acacia spp.	experimental	Biochem J 77: 315 (1960)	-1.11	-0.07	1.07	-0.29	-0.10
01502252	MONOCROTALINE	100122-21	E07	sample	315-22-0	C16H23NO6	325.36481	antineoplastic, insect sterilant	Crotalaria spp	experimental	J Am Chem Soc 72: 158 (1950)	-0.44	-0.08	-0.50	0.34	-0.17
01502261	QUEBRACHITOL	100122-21	E08	sample	642-38-6	C7H14O6	194.18603		common in dicotyledons	undetermined activity		0.98	0.12	1.55	1.12	0.94
01503346	URIDINE TRIPHOSPHATE TRISODIUM	100122-21	E09	sample	19817-92-6	C9H12N2Na3O15P3	550.09119	psychostimulant	yeast	experimental	JACS 75:5449 (1953); 105:115 (1983)	0.72	2.25	0.22	-1.57	0.40
01503427	ALOIN	100122-21	E10	sample	5133-19-7	C21H22O10	434.40349	cathartic, laxative	aloe	BAN	J Chem Soc 1932: 2573	1.85	0.29	1.04	2.19	1.34
01503620	SAFROLE	100122-21	E11	sample	94-59-7	C10H10O2	162.19	anesthetic (topical) and antiseptic, pediculicide	sassafras officinale	experimental	J Org Chem 13: 448 (1948)	1.94	-0.64	1.70	0.00	0.75
	0.11% DMSO	100122-21	E12	0.11% dmso								0.69	-1.25	0.37	-1.40	-0.40
	0.11% JAK2inhib	100122-21	F01	0.11% jak2inhib								-4.48	-1.68	-3.41	1.77	-1.95
01503639	RAUWOLSCINE HYDROCHLORIDE	100122-21	F02	sample	6211-32-1	C21H27ClN2O3	390.91394	alpha2 adrenergic antagonist	Rauwolfia, Aspidosperma and Vinca spp	experimental		-0.63	-0.39	-0.83	-0.66	-0.63
01503640	PARTHENOLIDE	100122-21	F03	sample	20554-84-1	C15H20O3	248.32485	5HT antagonist, antineoplastic, smooth muscle relaxant	Chrysanthemum parthenium, Michelia champaca	experimental	Tetrahedron 21:1509 (1965); Phytochemistry 17:957 (1978);	-0.14	1.94	-0.23	1.27	0.71
01503802	AZADIRACHTIN	100122-21	F04	sample	11141-17-6	C35H44O16	720.73133	antifeedant, insecticide	Melia azadirach and Azadirachta indica	experimental	Phytochemistry 12: 391 (1973)	1.34	1.71	0.31	1.72	1.27
01503805	DESACETYLCOLFORSIN	100122-21	F05	sample	64657-20-1	C20H32O6	368.47444		Coleus forskohlii; 8,13-epoxy-1,6,7,9-tetrahydroxy-14-labden-11-	undetermined activity		-0.04	-1.40	0.70	-0.23	-0.24
01503815	CEVADINE	100122-21	F06	sample	62-59-9	C32H49NO9	591.74863	antihypertensive	Veratrum alba; contains 20% veratridine	experimental		-1.64	0.10	-0.65	-0.05	-0.56
01503922	TRYPTAMINE	100122-21	F07	sample	61-54-1	C10H12N2	160.22054	psychotropic	Acacia spp, Lens esculenta, Prosopsis juliflora and fungi	experimental	J Chem Soc 99:270 (1911); J Sci Technol Sect B 25:157	-0.84	0.38	0.71	0.29	0.13
01503983	BATYL ALCOHOL	100122-21	F08	sample	544-62-7	C21H44O3	344.58303		fish oils	undetermined activity		-1.70	0.04	-0.12	0.69	-0.27
01503986	CAFESTOL ACETATE	100122-21	F09	sample	81760-48-7	C22H30O4	358.482		coffee bean oil	undetermined activity	Chem Ber 96: 2489 (1963); Tetrahedron 20: 1339 (1964)	0.47	-0.78	-0.42	-1.86	-0.65
01503987	CAFFEIC ACID	100122-21	F10	sample	331-39-5	C9H8O4	180.16171		widespread in plants	undetermined activity		0.43	0.56	-0.24	1.09	0.46
01503989	GLUCITOL-4-GUCOPYANOSIDE	100122-21	F11	sample		C12H24O11	344.31848		derivative cotton	undetermined activity		1.75	-0.38	-0.90	0.33	0.20
	0.04% DMSO	100122-21	F12	0.04% dmso								2.02	0.56	0.49	0.20	0.82
	0.04% JAK2inhib	100122-21	G01	0.04% jak2inhib								-3.94	-3.70	-2.62	-1.99	-3.06
01503990	CONESSINE	100122-21	G02	sample	5913-82-6, 546-06-5	C24H40N2	356.5998		Holarrhena spp	undetermined activity		-2.43	-0.67	-2.14	1.66	-0.89
01503994	CONVALLATOXIN	100122-21	G03	sample	508-75-8	C29H42O10	550.65209	cardiotonic	Convallaria majalis	experimental	Phytochemistry 13: 1805 (1974)	-3.04	-3.32	-2.24	-1.47	-2.52
01504001	CAFESTOL	100122-21	G04	sample	469-83-0	C20H28O3	316.44436		coffee bean oil	undetermined activity	Chem Ber 96: 2489 (1963); Tetrahedron 20: 1339 (1964)	-0.43	-0.35	-0.97	0.01	-0.43
01504005	TRIPTOPHENOLIDE	100122-21	G05	sample	74285-86-2	C20H24O3	312.41248		Tripterygium wilfordii	undetermined activity	Chin Chem Lett 5:217 (1994)	-0.19	-0.10	1.82	3.31	1.21
01504013	UBIDECARENEONE	100122-21	G06	sample	303-98-0	C59H90O4	863.37275	cardiovascular agent	widespread in aerobic organisms (solubility limits concentration to	experimental		-2.06	0.58	-0.33	0.88	-0.23
01504015	alpha-MANGOSTIN	100122-21	G07	sample	6147-11-1	C24H26O6	410.47122		Garcinia mangostana, Hydnocarpus octandra, H venenata	undetermined activity	JACS 80:1691 (1958); Aust J Chem 23:2539 (1970);	0.00	0.71	-0.64	0.00	0.01
01504016	HEDERAGENIN	100122-21	G08	sample	465-99-6	C30H48O4	472.71466		Clematis, Hedera spp	undetermined activity		-2.62	-0.68	0.41	-0.35	-0.81
01504018	HEDERACOSIDE C	100122-21	G09	sample		C59H96O26	1221.40737		Hedera helix	undetermined activity	(structure tentative)	1.17	0.90	0.48	-1.82	0.18
01504020	EVOXINE	100122-21	G10	sample	522-11-2	C18H21NO6	347.37117		Evodia xanthoxyloides	undetermined activity	Aust J Sci Res, Ser A 5:401 (1952); Planta Med 42:400 (1981)	2.21	0.75	2.62	1.58	1.79
01504022	SALSOLIDINE	100122-21	G11	sample	493-48-1	C12H17NO2	207.27479	antihypertensive	Salsola Richteri	experimental	Bull Soc Chim France 4L1265 (1937); Phytochemistry 12:193 (1973); 13:1628 (1974); J Nat Prod 39:175,197 (1976); 45:277 (1982)	1.54	-0.15	-0.15	0.68	0.48
	0.04% DMSO	100122-21	G12	0.04% dmso								1.27	0.88	-0.15	2.36	1.09
	0.04% JAK2inhib	100122-21	H01	0.04% jak2inhib								-3.83	-3.96	-3.45	-2.38	-3.40
01504044	RESVERATROL 4'-METHYL ETHER	100122-21	H02	sample	33626-08-3	C15H14O3	242.27703		derivative	undetermined activity	Chem Pharm Bull 25:2300 (1977); Phytochemistry 32:1083 (1993)	-1.09	-1.71	-1.12	2.52	-0.35
01504024	LAGOCHILIN	100122-21	H03	sample	23554-81-6	C20H36O5	356.50692		Lagochilus inebrians	undetermined activity	Chem Commun 1974:249	1.91	3.97	-1.00	0.54	1.36
01504025	SALSOLINE	100122-21	H04	sample	89-31-6	C11H15NO2	193.2477	antihypertensive, antihistamine	Salsola richteri	experimental	Phytochemistry 12:193 (1973); J Med Chem 33:147 (1990)	0.00	-0.06	-0.85	2.32	0.36
01504075	RHOIFOLIN	100122-21	H05	sample	17306-46-6	C27H30O14	578.53175		Chorisia, Citrus and Rhus spp	undetermined activity	Experientia 20: 562 (1964); Chem Ber 102: 2083 (1969)	0.57	0.85	2.34	1.73	1.37
01504023	THERMOPSINE PERCHLORATE	100122-21	H06	sample	486-90-8(base)	C15H21ClN2O5	344.79802		Anabasis aphylla, Thermopsis spp	undetermined activity	Ber 66:625 (1933); Can J Chem 29:13 29, 22 (1951)	-0.14	-0.02	1.16	0.34	0.34
01504053	FUCOSTANOL	100122-21	H07	sample	83-45-4	C29H52O	416.73719		Calendula officinalis	undetermined activity	J Am Chem Soc 60: 2431 (1938)	-3.55	0.10	1.82	0.34	-0.32
01504079	TOMATINE	100122-21	H08	sample	86273-92-9	C47H79NO21	994.14778	antifungal, antibacterial, antiinflammatory agent	Solanum spp.	experimental	Chem Ber 90: 203 (1957)	-3.48	2.22	2.93	0.45	0.53
01504068	DIOSMETIN	100122-21	H09	sample	520-34-3	C16H12O6	300.27044		Valeriana, Digitalis spp	undetermined activity	J Indian Chem Soc 31: 565 (1954)	-0.61	-0.07	0.10	0.10	-0.12
01504041	TRIACETYLRESVERATROL	100122-21	H10	sample	42206-94-0	C20H18O6	354.36286		Kirkpatrickia variolosa (sponge)	undetermined activity	Aust J Chem 24:2427 (1971); Phytochemistry 32:1083 (1993); J Nat Prod 58:1958 (1995)	2.07	1.13	1.88	1.83	1.73
01504065	MYRICETIN	100122-21	H11	sample	529-44-2	C15H10O8	318.24215	antiHIV, topoisomerase II inhibitor	Myrica spp	experimental	J Chem Soc 81: 203 (1902); PNAS 97: 4790 (2000)	2.05	0.44	0.57	0.64	0.92
	empty	100122-21	H12	sample								NA	NA	NA	NA	NA
	empty	100122-22	A01	sample								NA	NA	NA	NA	NA
01504081	BETULINIC ACID	100122-22	A02	sample	472-15-1	C29H46O3	442.68817	antineoplastic	Betula spp.	experimental	Acta Chem Scand 19: 1661 (1965); Nature Medicine 1: 1046 (1995)	-5.50	-2.58	1.75	-1.05	-1.84
01504115	HIERACIN	100122-22	A03	sample	1621-84-7	C15H10O7	302.24275		Ginkgo biloba, Hieracium pilosella and Isoetes spp	undetermined activity	Chem Pharm Bull 32:4935 (1984)	-0.79	-1.41	-1.54	-1.53	-1.32
01504118	DIFFRACTAIC ACID	100122-22	A04	sample	436-32-8	C20H22O7	374.39414		Usnea spp	undetermined activity	Chem Ber 65: 175, 1668 (1932)	-2.25	2.73	-0.72	-0.63	-0.22
01504123	10-HYDROXYCAMPTOTHECIN	100122-22	A05	sample	19685-09-7	C20H16N2O5	364.36092	antineoplastic	Camptotheca acuminata	experimental	J Med Chem 29:1553 (1986); J Nat Prod 53:186 (1990)	0.45	1.96	1.62	1.93	1.49
01504124	LINAMARIN	100122-22	A06	sample	554-35-8	C10H17NO6	247.25009		Linum usitatissimum, Manihot utilissimus	undetermined activity	Phytochemistry 4: 127 (1965)	0.94	-0.44	1.05	0.52	0.52
01504130	3,7-DIHYDROXYFLAVONE	100122-22	A07	sample	492-00-2	C15H10O4	254.24455		Platymiscium praecox	undetermined activity	Phytochemistry 11: 3515 (1972)	0.36	-0.92	-0.30	-0.48	-0.34
01504132	6,3'-DIMETHOXYFLAVONE	100122-22	A08	sample	79786-40-6	C17H14O4	282.29873		Pimelia decora	undetermined activity	Aust J Chem 34:1779 (1981)	0.82	-0.41	0.35	0.42	0.29
01504149	LEUCODIN	100122-22	A09	sample	17946-87-1	C15H18O3	246.30891	antiinflammatory, hypolipidemic	Artemesia & Achillea spp	experimental	Pharmacol Toxicol USSR 54: 35 (1991); J Gen Chem 33: 2663 (1963)	0.11	-1.40	-0.22	-0.65	-0.54
01504155	APHYLLIC ACID	100122-22	A10	sample	642-67-1	C15H26N2O2	266.38667		Anabasis aphylla	undetermined activity		1.53	0.25	3.88	0.02	1.42
01504156	ANABASAMINE HYDROCHLORIDE	100122-22	A11	sample	20410-87-1(base)	C16H20ClN3	289.8109		Anabasis aphylla	undetermined activity		0.85	-1.05	0.65	-1.93	-0.37
	0.04% JAK2inhib	100122-22	A12	0.04% jak2inhib								-1.09	-2.60	-1.34	-2.07	-1.78
	0.04% DMSO	100122-22	B01	0.04% dmso								-0.81	-0.69	-1.45	-0.02	-0.74
01504167	URSINOIC ACID	100122-22	B02	sample	30265-59-9	C15H16O5	276.29177		Angelica ursina	undetermined activity	Khim Prir Soedin 6:421 (1970); Chem Nat Compd (Eng Trans) 6:429 (1970)	-0.48	-0.76	0.87	0.50	0.03
01504176	RHETSININE	100122-22	B03	sample	526-43-2	C19H17N3O2	319.36624		Zanthoxylum rhetsa, Evodia rutaecarpa	undetermined activity	Tetrahedron 7: 257 (1959)	-0.78	-1.72	-2.49	-0.36	-1.34
01504180	ASARININ (-)	100122-22	B04	sample	13079-95-3	C20H18O6	354.36286	antibacterial (tuberculostatic)	Asarum & Xanthoxylum spp	experimental	Aust J Chem 1: 384 (1954); 26: 687 (1973)	1.96	0.04	-1.01	-0.14	0.21
01504185	TETRANDRINE	100122-22	B05	sample	518-34-3	C38H42N2O6	622.76824	analgesic, antineoplastic, antihypertensive, lymphotoxin	Triclisia and Cyclea spp	experimental	Phytochemistry 14: 2524 (1975); Life Sci 68: 841 (2001)	0.09	0.84	-0.05	0.84	0.43
01504200	ISOLIQUIRITIGENIN	100122-22	B06	sample	961-29-5	C15H12O4	256.26049	aldose reductase inhibitor, antineoplastic, antiinflammatory	widespread in Fabaceae	experimental	J Chem Soc 1953: 2183; Eur J Biochem 212: 87 (1992)	0.02	0.18	0.05	-2.18	-0.48
01504204	CANTHAXANTHIN (euglenanone)	100122-22	B07	sample	514-78-3	C40H52O2	564.85924		Cantharellus cinnabarinus	undetermined activity	Arch Biochem Biophys 91: 271 (1960); Biochem J 101: 735 (1966)	0.75	-0.27	0.15	0.88	0.38
01504234	18-AMINOABIETA-8,11,13-TRIENE SULFATE	100122-22	B08	sample		C20H33NO4S	383.55431		derivative of abietic acid	undetermined activity		-0.11	-0.36	0.46	-0.17	-0.05

Compound ID	MolNAME	plate	position	Content	cas#	Formula	MolWt	Bioactivity	Source	Status	Reference	Screen Score (z-score) rep1	rep2	rep3	rep4	Average
01504410	PICROPODOPHYLLIN	100122-22	B09	sample	477-47-4	C22H22O8	414.41584	Insulin growth factor 1 receptor inhibitor, antineoplastic	Podophylum peltatum; epimer of podophyllotoxin; 10% cytotoxicity of podophyllotoxin	experimental	JACS 73: 2909 (1951); 75: 1308 (1953); J Med Chem 32: 604 (1989); Pharmacol Ther 59: 163 (1993); Cancer Res 64:236 (2004); Int. J. Cancer 121:1857 (2007)	0.11	-0.74	0.67	-0.01	0.01
01504519	7-HYDROXYFLAVONE	100122-22	B10	sample	6665-86-7	C15H10O3	238.24515	antifungal, analgesic	Virola spp	experimental	Mycol Res 101:920 (1997); Indian J Exp Biol 38:1172 (2000); Chem Pharm Bull 52:1255 (2004)	0.52	-0.41	0.49	-2.43	-0.46
01504614	GYROMITRIN	100122-22	B11	sample	16568-02-8	C4H8N2O	100.12116	hepatotoxin, carcinogen	Gyromitra mushroom species; metabolized to to the hepatotoxin formylmethylhydrazine	experimental	Arch Pharmazie 302:294 (1968); Z Lebensm Unters Forsch 160:325 (1976); Cancer Res 37:3458 (1977); J Appl Toxicol 11:235 (1991)	0.47	-0.66	0.83	0.15	0.20
	0.04% JAK2inhib	100122-22	B12	0.04% jak2inhib								0.38	-1.75	2.13	-3.03	-0.57
	0.04% DMSO	100122-22	C01	0.04% dmso								-1.28	-0.05	-1.16	0.05	-0.61
01504800	CHRYSANTHEMIC ACID	100122-22	C02	sample	10453-89-1	C10H16O2	168.23782	esters as insecticide	esters as constituent of pyrethrum flowers	experimental	J Chem Soc 1945: 283	1.90	-0.88	-1.52	-0.10	-0.15
01505002	LAPPACONITINE	100122-22	C03	sample	32854-75-4	C32H44N2O8	584.71608	analgesic, antiarrhythmic	Aconitum spp and Delphinium cashmirianum	experimental	Tet Lett 1964:2711; Can J Chem 45:969 (1967); J Nat Prod 42:615 (1979); Planta Medica 64:22 (1998); Mol Pharm 59:183 (2001)	-0.02	-0.59	-1.02	0.09	-0.39
01505006	DIHYDROMYRISTICIN	100122-22	C04	sample	607-91-0	C11H14O3	194.23243	GSH transferase inducer	derivative; myristicin	experimental	J Agr Food Chem 40:107 (1992)	-0.39	-1.81	-0.81	-1.60	-1.15
01505010	EUPHORBIASTEROID	100122-22	C05	sample	28649-59-4	C32H40O8	552.6708		Euphorbia lathyris, Macaranga tanarius	undetermined activity	Tet Lett 1970:2241, 3071; Experientia 27:1393 (1971)	-0.35	-0.43	-0.57	-1.07	-0.60
01505018	ASTRAGALOSIDE IV	100122-22	C06	sample	84687-43-4	C41H68O14	784.99071		Astragalus species	undetermined activity	Chem Pharm Bull 31:689, 698, 709, 716 (1983)	-6.58	0.71	-0.10	0.06	-1.48
01505030	DEMETHYLNOBILETIN	100122-22	C07	sample	2174-59-6	C20H20O8	388.3776		Citrus, Sideritis, Heteropappus and Thymus spp; Mentha piperita, Amaracus pampanini	undetermined activity	Tetrahedron 8:64 (1960); Phytochemistry 11:2283 (1972); 24:1027 (1985)	-0.68	-1.11	-0.92	-1.97	-1.17
01505034	BACCATIN III	100122-22	C08	sample	27548-93-2	C31H38O11	586.64191		Taxus baccata	undetermined activity	J Org Chem 51:3239 (1986)	0.06	-0.12	0.15	0.05	0.04
01505080	SALVINORIN A	100122-22	C09	sample	83729-01-5	C23H28O8	432.47481	k-opiod receptor agonist, psychotropic	Salvia divinorum	experimental	J Chem Soc 1982:2505; J Org Chem 49:4716 (1984); Chem Lett 1990:2015	-0.04	-1.09	1.25	-1.24	-0.28
01505121	11a-ACETOXYPROGESTERONE	100122-22	C10	sample	2268-98-6	C23H32O4	372.50909	metabolite of progesterone	semisynthetic	undetermined activity	Endocrinology 53:221 (1953); Biochem Biophys Res Commun 319:677 (2004)	-0.22	-1.30	-1.40	-2.04	-1.24
01505123	21-ACETOXYPREGNENOLONE	100122-22	C11	sample	566-78-9	C23H34O4	374.52503	precursor in corticoid biosynthesis, derivative	semisynthetic	undetermined activity	PNAS 94:4895 (1997)	2.30	-0.87	0.29	-0.57	0.29
	0.11% JAK2inhib	100122-22	C12	0.11% jak2inhib								-2.72	-2.13	2.20	-2.61	-1.31
	0.11% DMSO	100122-22	D01	0.11% dmso								-1.47	-0.92	-0.99	2.32	-0.26
01505127	GOSSYPIN	100122-22	D02	sample	652-78-8	C21H20O13	480.38575		Gossypium spp, Hibiscus spp	undetermined activity	Proc Indian Acad Sci Sect A, 24:352, 375 (1946); 25:397 (1947)	-2.15	-0.89	-1.65	-0.36	-1.26
01505129	PLUMBAGIN	100122-22	D03	sample	481-42-5	C11H8O3	188.18461	antibacterial, antifungal, tuberculostatic; antifeedant (African army worms)	Aristea, Diospyros & Plumbago spp; Dyerophyton, Drosera, Dioncophyllum, Nepenthe, Sisyrinchium and Sparaxis tricolor	experimental	JACS 58:572 (1936); Indian J Chem 6:681 (1968); Fitoterapia 1990:387	-0.16	0.08	-1.42	-1.07	-0.64
01505130	3,4-DIMETHOXYCINNAMIC ACID	100122-22	D04	sample	14737-89-4	C11H12O4	208.21589		Piper methysticum, Veronica virginica	undetermined activity		-0.27	-1.07	-0.24	-1.79	-0.84
01505132	2',4'-DIHYDROXYCHALCONE	100122-22	D05	sample	1776-30-3	C15H12O3	240.26109	anthelmintic, antiulcer	Flemingia chappar, Ceratiola ericoides, Acacia neovernicosa, Flourensia spp	experimental	J Chem Soc 1937:1737; Tetrahedron 27:2111 (1971); Planta Med 58:389 (1992)	1.07	1.75	3.19	3.27	2.32
01505134	MANGIFERIN	100122-22	D06	sample	4773-96-0	C19H18O11	422.34871	MAO inhibitor, immunostimulant	Mangifera indica, Iris & Salacia spp, Aphloia, Athyrium, Anemarrhena, Belamcanda chinensis, Hedysarum ussuriense	experimental	J Chem Soc (C) 1966:1685; Phytochemistry 6:741, 1597 (1967); Tetrahedron 23:1363 (1967); Pharm Res 3:307 (1986); Naturwissenschaften 59:651 (1972)	-0.12	-0.19	-0.96	-0.49	-0.44
01505135	PIPLARTINE	100122-22	D07	sample	20069-09-4	C17H19NO5	317.34468	anti-asthma, antibronchitis	Piper spp	experimental	Tetrahedron 23:1769 (1967); Phytochemistry 13:2327 (1974)	0.21	0.95	3.58	1.33	1.52
01505140	2',4-DIHYDROXY-3,4',6'-TRIMETHOXYCHALCONE	100122-22	D08	sample	112572-59-5	C18H18O6	330.34056		Viscum album (glucoside)	undetermined activity	Annalen 550:146 (1942); Planta 95:133 (1970); Phytochemistry 13:1561 (1974)	-0.52	0.36	0.06	2.48	0.59
01505141	2',4-DIHYDROXYCHALCONE	100122-22	D09	sample	13323-66-5	C15H12O3	240.26109		Adhatoda vasica (as glucoside)	undetermined activity	JACS 68:697 (1946)	0.80	1.53	0.76	0.04	0.78
01505142	2',5'-DIHYDROXY-4-METHOXYCHALCONE	100122-22	D10	sample	6342-92-3	C16H14O4	270.28758		Cassia javanica	undetermined activity	Chem Abs 92:55042v (1980)	1.19	0.42	0.97	2.06	1.16
01505143	GOSSYPETIN	100122-22	D11	sample	489-35-0	C15H10O8	318.24215		widespread in plants	undetermined activity	J Chem Soc 1929:24	-0.62	-0.10	0.99	0.45	0.18
	0.11% JAK2inhib	100122-22	D12	0.11% jak2inhib								-2.75	-3.99	-0.48	-2.36	-2.40
	0.11% JAK2inhib	100122-22	E01	0.11% jak2inhib								-3.60	-1.00	-3.35	-3.05	-2.75
01505151	HARPAGOSIDE	100122-22	E02	sample	19210-12-9	C23H28O11	480.47301		Melittis melissophyllum, Harpagophytum procumbens	undetermined activity	J Chem Soc Perkin 1 1979:2473; Phytochemistry 40:1569 (1995)	-1.02	0.59	1.83	0.24	0.41
01505152	2',4'-DIHYDROXY-4-METHOXYCHALCONE	100122-22	E03	sample	81674-91-1	C16H14O4	270.28758		Bauhinia manca	undetermined activity		-30.32	-30.46	-26.93	-24.85	-28.14
01505169	DESOXYPEGANINE HYDROCHLORIDE	100122-22	E04	sample	61939-05-7	C11H13ClN2	208.69266	acetylcholinesterase inhibitor, antiParkinsonism	derivative of peganine Peganum spp	experimental	Naunyn Schmeidebergs Arch Pharmacol 363:429 (2001)	2.50	0.34	-1.14	-0.79	0.23
01505153	2',3-DIHYDROXY-4,4',6'-TRIMETHOXYCHALCONE	100122-22	E05	sample	38186-71-9	C18H18O6	330.34056		Merrillia caloxylon	undetermined activity	Annalen 550:146 (1942); Planta 95:133 (1970); Phytochemistry 13:1561 (1974)	0.55	3.70	0.30	0.40	1.24
01505174	GARLICIN	100122-22	E06	sample	2179-57-9	C6H10S2	146.2746	antineoplastic, antibacterial, apoptosis inducer, insecticide	Allium spp, Descurainia sophia	experimental	Pharmazie 20:441 (1965); J Org Chem 40:1567 (1975); Food Chem Toxicol 26:297 (1988); Cancer Res 35:3493 (1993); Biochim Biophys Acta 1315:15 (1996)	-0.45	0.47	-0.42	0.59	0.05
01505175	ASIATIC ACID	100122-22	E07	sample	464-92-6	C30H48O5	488.71406	wound healing, experimental carcinogen	Dipterocarpus pilosus, Dryobalanops aromatica	experimental	Bull Soc Chim Fr 1959:880; 1961:1586; J Chem Soc 1961:646; Phytochemistry 8:917 (1969)	0.63	-1.11	2.90	0.35	0.69
01505176	AURAPTENE	100122-22	E08	sample	495-02-3	C19H22O3	298.38539	antineoplastic, apoptosis inducer	Citrus aurantium, Feronia elephantum, Aegle marmelos, Libanotis intermedia	experimental	Chem Pharm Bull 1:119 (1959); Cancer Res 12:2550 (1998); Mutat Res 480:201 (2001)	0.26	-0.16	-0.82	-0.62	-0.33
01505190	L(+/-)-ALLIIN	100122-22	E09	sample	556-27-4(-)	C6H11NO3S	177.22347	antibacterial, antioxidant	Allium species	experimental	Helv Chim Acta 34:481 (1951); Phytochemistry 15:521 (1976)	2.26	0.29	0.22	0.24	0.75
01505195	EPITESTOSTERONE	100122-22	E10	sample	481-30-1	C19H28O2	288.43381	androgen	cooccurs with testosterone in mammals	experimental		1.04	0.07	0.70	0.46	0.57
01505217	RHODOCLADONIC ACID	100122-22	E11	sample	26984-15-6	C15H10O8	318.24215		Cladonia spp	undetermined activity	Can J Chem 47: 2733 (1969); 61: 2055 (1983); Phytochemistry 12: 937 (1973)	-3.62	0.50	1.31	1.96	0.04
	0.11% DMSO	100122-22	E12	0.11% dmso								0.22	-0.76	0.67	-1.33	-0.30
	0.11% JAK2inhib	100122-22	F01	0.11% jak2inhib								-2.78	-3.13	-3.37	0.82	-2.12
01505234	AVOCADYNE	100122-22	F02	sample	34524-38-4	C17H32O3	284.44279	antibacterial, antifungal	Persea spp	experimental	An Acad Brasil Cienc 42 (suplemento): 45 (1970); Tetrahedron 25:4617 (1969)	-0.17	-0.69	-0.97	-0.22	-0.51
01505240	LUPANYL ACID HYDROCHLORIDE	100122-22	F03	sample		C14H25ClN2O2	288.82055		Anabasis aphylla	undetermined activity		-0.72	1.01	-1.02	0.12	-0.15
01505242	LUPANINE PERCHLORATE	100122-22	F04	sample	550-90-3 (base)	C15H25ClN2O5	348.8299		Lupinus and Cystisus spp	undetermined activity		-0.35	-0.04	-0.58	2.70	0.43
01505254	THEANINE	100122-22	F05	sample	3081-61-6	C7H14N2O3	174.20123		Thea sinensis	undetermined activity	JACS 64: 1021 (1942); J Sci Food Agric 5: 597 (1954); Biochim Biophys Acta 39: 462 (1960)	-0.47	1.18	-0.19	-0.17	0.09
01505255	HUPERZINE A	100122-22	F06	sample	102518-79-6	C15H18N2O	242.32351	anticholinesterase, cognition enhancer	Lycopodium spp	experimental	Tet Lett 1960 (10): 26; Can J Chem 64: 837 (1986); Adv Med 1: 175 (1992)	0.71	0.89	-0.49	-0.21	0.23
01505257	ICARIIN	100122-22	F07	sample	489-32-7	C33H40O15	676.67775	hepatoprotective	Epimedium spp	experimental	Planta Med 61: 523 (1995); J Chromatog A 963: 239 (2002)	0.08	1.12	2.69	0.28	1.04
01505268	NOBILETIN	100122-22	F08	sample	478-01-3	C21H22O8	402.40469	matrix metaloproteinase inhibitor; antineoplastic	Citrus spp	experimental	J Chem Soc 1938:1004; Phytochemistry 14:309 (1975); J Cancer Res 92:1322 (2001); Biochem Pharmacol 65:2065 (2003); Mol Cancer Ther 3:839 (2004)	-0.36	-0.88	-0.54	-1.43	-0.80
01505269	TANGERITIN	100122-22	F09	sample	481-53-8	C20H20O7	372.3782		Citrus spp, Fortunella japonica	undetermined activity	Chem Ind 1957: 47; Phytochemistry 14: 309 (1975)	0.35	-0.08	0.47	-0.97	-0.06
01505278	3-HYDROXY-3',4'-DIMETHOXYFLAVONE	100122-22	F10	sample	6889-80-1	C17H14O5	298.29813		synthetic	undetermined activity	Tetrahedron 32: 565 (1976); Lebensmittelchem Gerichtl.Chem 39: 9 (1985)	0.91	2.59	1.25	-0.77	1.00
01505297	PERILLYL ALCOHOL	100122-22	F11	sample	536-59-4, 18457-55-1	C10H16O	152.23842	antineoplastic, apoptosis inducer; skin irritant, LD50(rat) 2100 mg/kg po	Ocimum gratissimum	experimental	CR Hebd Seances Acad Sci 249:306 (1959); Cancer Res 57:420 (1997)	-0.14	0.09	0.66	0.41	0.25
	0.04% DMSO	100122-22	F12	0.04% dmso								0.05	-0.33	0.36	-0.12	-0.01
	0.04% JAK2inhib	100122-22	G01	0.04% jak2inhib								-1.91	-1.51	-2.94	-1.52	-1.97
01505326	SOLANESYL ACETATE	100122-22	G02	sample		C47H76O2	673.12857		Nicotiana tabacum; Murraya exotica; Pinus spp	undetermined activity	Phytochemistry 39:1383 (1995)	-5.56	2.01	-1.29	0.01	-1.21
01505320	INDOLE-3-CARBINOL	100122-22	G03	sample	700-06-1	C9H9NO	147.17818	antineoplastic	Brassica spp	experimental	Anticancer Res 15:709 (1995); Biochem Mol Biol Int 39:1125 (1996)	0.64	0.94	0.33	0.97	0.72
01505325	SOLANESOL	100122-22	G04	sample	13190-97-1	C45H74O	631.09093		Nicotiana tabacum; Betulaprenol 9: mp 42 C	undetermined activity	Biochem J 102:313, 325 (1966); 128: 11P (1972); Nature 1966: 212, 1364; Phytochemistry 39:1383 (1995); J Nat Prod 46:174 (1983); J Org Chem 54:3390 (1989)	0.21	0.78	2.05	1.53	1.14
01505302	GENETICIN	100122-22	G05	sample	108321-42-2, 49863-47-0(base)	C20H44N4O18S2	692.71768	antibacterial	Micromonospora spp; G-418	experimental	Antimicrob Agents Chemother 6:144 (1974); J Antibiotics 28:573 (1975); 30:945 (1977); 35:1 (1982)	0.02	1.58	-0.06	0.77	0.58
01505334	SECURININE	100122-22	G06	sample	5610-40-2	C13H15NO2	217.27	GABAA receptor blocker, CNS stimulant	Securinega spp and Phyllanthus discoides	INN	Chem Ind 1962:1652; 1964:838, 1691; Naturwissenschaften 50:155 (1963)	-1.67	0.47	-2.00	-2.37	-1.39
01505345	CURCUMIN	100122-22	G07	sample	458-37-7	C21H20O6	368.38995	antiedemic, antiinflammatory, bile stimulant; antibacterial, antifungal, lipo/cyclooxygenase inhibitor	Curcuma spp	experimental	Ber 51: 1347 (1918); J Pharm Pharmacol 5: 448 (1953); Cancer Res 51:813 (1991)	2.17	1.04	-0.35	0.33	0.80
01505380	3,4',5,6,7-PENTAMETHOXYFLAVONE	100122-22	G08	sample	4472-73-5	C20H20O7	372.3782		Citrus spp	undetermined activity		1.49	0.21	-0.16	-0.09	0.36
01505381	SINENSETIN	100122-22	G09	sample	2306-27-6	C20H20O7	372.3782		Citrus spp	undetermined activity		-0.42	-0.13	-0.58	-0.55	-0.42
01505382	5-HYDROXY-2',4',7,8-TETRAMETHOXYFLAVONE	100122-22	G10	sample	123316-61-0	C19H18O7	358.35111		Citrus spp, Limnophilia rugosa	undetermined activity	Chem Pharm Bull 33:3982 (1985): Phytochemistry 28:1778 (1989)	0.99	0.78	0.28	0.22	0.57
01505383	HEXAMETHYLQUERCETAGETIN	100122-22	G11	sample	1251-84-9	C21H22O8	402.40469		Citrus spp	undetermined activity	Phytochemistry 11:2283 (1972)	-0.37	-1.38	0.99	1.16	0.10
	0.04% DMSO	100122-22	G12	0.04% dmso								0.60	0.31	1.07	2.38	1.09
	0.04% JAK2inhib	100122-22	H01	0.04% jak2inhib								-3.55	-2.58	-3.73	-2.35	-3.05
01505476	HELICIN	100122-22	H02	sample	618-65-5	C13H16O7	284.26827		Spiraea spp	undetermined activity	J Chem Soc 1930:2729; Bull Chem Soc Japan 44:526 (1971)	-1.16	-0.56	-0.75	-0.99	-0.87
01505475	RHIZOCARPIC ACID	100122-22	H03	sample	18463-11-1	C28H23NO6	469.49861		Rhizocarpon spp, Calicium hyperelium; mp 178 C	undetermined activity	JACS 72:4454 (1950); Pharmazie 23:583 (1968)	-1.35	-0.43	-2.40	-1.32	-1.37
01505745	ANDROSTERONE	100122-22	H04	sample	53-41-8	C19H30O2	290.44975	androgen	male urine	experimental	Helv Chim Acta 25:988 (1942); JACS 57:1755 (1935)	0.39	-0.20	-1.79	0.31	-0.48
01505754	SEROTONIN HYDROCHLORIDE	100122-22	H05	sample	50-67-9	C10H13ClN2O	212.68091	neurotransmitter	CNS, GI tract, all animals, many mushrooms & plants	experimental	Agents Actions 15:627 (1984)	-1.11	0.43	-1.88	-1.49	-1.01
01505766	SYRINGIC ACID	100122-22	H06	sample	530-57-4	C9H10O5	198.17705		Glycine max; widespread in plants	undetermined activity		0.22	0.33	-0.93	0.73	0.09
01505775	AGARIC ACID	100122-22	H07	sample	666-99-9	C22H40O7	416.5599	antiperspirant	Fomes and Polyporus spp	experimental	J Bacteriol 98:23 (1969)	-4.64	1.40	0.47	0.69	-0.52
01505758	SKATOLE	100122-22	H08	sample	83-34-1	C9H9N	131.17878	insect attractant	feces, beetroot, nectandra wood	experimental		-0.70	0.31	0.57	0.85	0.26
01505757	MELIBIOSE	100122-22	H09	sample	585-99-9	C12H22O11	342.30254		yeast	undetermined activity	JACS 37:2734 (1915); J Chem Soc 113:188 (1918)	0.11	2.56	0.52	1.11	1.07
01505743	ALEURETIC ACID	100122-22	H10	sample	533-87-9	C16H32O5	304.43044		shellac constituent	undetermined activity	J Chem Soc 1944:306; J Sci Ind Res 11B:458 (1952)	-1.69	0.44	0.90	1.56	0.30
01505883	alpha-ERGOCRYPTINE	100122-22	H11	sample	511-09-1	C32H41N5O5	575.71407		ergot	experimental		-0.76	-1.54	-0.33	-0.58	-0.80
	empty	100122-22	H12	sample								NA	NA	NA	NA	NA
	empty	100122-23	A01	sample								NA	NA	NA	NA	NA
01505842	PIPERIC ACID	100122-23	A02	sample	5285-18-7	C12H10O4	218.2111		Piper nigrum, Minthostachys verticillata, Menta piperita	undetermined activity	Chem Ber 103:3752 (1970)	0.34	-0.68	-0.17	0.80	0.07
01505847	LACCAIC ACID A	100122-23	A03	sample	15979-35-8	C26H19NO12	537.44083		Coccus laccae exudate; lac resin	undetermined activity	J Chem Soc C 1967:842; Indian J Chem Soc 7:977 (1969)	0.53	1.11	1.81	0.64	1.02
01505840	STRYCHNINE METHIODIDE	100122-23	A04	sample		C22H25IN2O2	476.36115	neuromuscular blocker	derivative	experimental	J Physiol 82:432 (1934); Phytochemistry 11:2547 (1972)	-1.27	-1.47	-2.11	-2.93	-1.95
01505921	PANGAMIC ACID SODIUM	100122-23	A05	sample	20858-86-0	C10H18NNaO8	303.24666		vitamin B15	experimental	Int Rec Med 164:18 (1951); Chim Ther 7:103 (1972); Indian Drugs 20:185 (1983)	-0.51	-0.06	-2.09	-2.25	-1.23
01505909	1-HYDROXY-3,6,7-TRIMETHOXY-2,8-DIPRENYLXANTHONE	100122-23	A06	sample	15404-76-9	C26H30O6	438.5254		Garcinia mangostana	undetermined activity	JACS 80:1891 (1958); Aust J Chem 23:2539 (1970); Tetrahedron 27:3919 (1971); Phytochemistry 12:232 (1973)	-2.31	-1.42	0.42	-1.07	-1.10
01505908	MANGOSTIN TRIMETHYL ETHER	100122-23	A07	sample		C27H32O6	452.55249		derivative	undetermined activity		0.90	3.20	0.41	0.77	1.32
01506003	KAEMPFEROL	100122-23	A08	sample	520-18-3	C15H10O6	286.24335		Citrus, Delphinium, Acacia spp.	undetermined activity	J Agric Food Chem 54:2951 (2006); Am J Epidem 166: 924 (2007)	-0.81	0.90	-1.96	-0.78	-0.66
01506015	MEVALONIC ACID LACTONE	100122-23	A09	sample	503-48-0	C6H10O3	130.1448		common primary metabolite	undetermined activity	JACS 78:5273 (1956)	0.13	1.18	-1.87	-0.62	-0.29
01506020	N-ACETYLMURAMIC ACID	100122-23	A10	sample	10597-89-4	C11H19NO8	293.27598		bacterial cell wall component	undetermined activity		-0.69	0.72	-2.24	-1.13	-0.83
01506075	KAWAIN	100122-23	A11	sample	3155-48-4	C14H14O3	230.26588		Piper methysticum	experimental	Tet Letts 25:4059 (1984)	-0.17	1.18	0.10	3.26	1.09
	0.04% JAK2inhib	100122-23	A12	0.04% jak2inhib								-2.13	-0.80	-3.33	-2.39	-2.16
	0.04% DMSO	100122-23	B01	0.04% dmso								-0.24	-1.52	-1.80	-0.90	-1.12

Compound ID	MolNAME	plate	position	Content	cas#	Formula	MolWt	Bioactivity	Source	Status	Reference	Screen Score (z-score) rep1	rep2	rep3	rep4	Average
01701001	ANDROSTA-1,4-DIEN-3,17-DIONE	100122-23	B02	sample	897-06-3	C19H24O2	284.40193		mammary neoplasms; cholesterol metabolite	undetermined activity	J Am Chem Soc 80: 6148 (1958); 83: 4627 (1961)	0.85	-0.30	-0.50	0.22	0.07
01701060	HYDROXYPROGESTERONE	100122-23	B03	sample	3168-01-2	C21H30O3	330.47145	progestagen	urine and blood	INN, BAN		-0.07	-0.85	1.90	-0.61	0.09
01800018	LIMONIN	100122-23	B04	sample	1180-71-8	C26H30O8	470.5242		Citrus, Evodia, Dictamnus and Luvunga spp	undetermined activity	JACS 62:1307 (1940); J Chem Soc 1961:255; Citrus Sci Technol 1:355 (1977)	-0.38	-0.61	-1.52	-0.49	-0.75
01800009	GUAIOL(-)	100122-23	B05	sample	489-86-1	C15H26O	222.37387		Callitris intratropica, Eucalyptus maculata, Drimys lancelolata	undetermined activity	Tetrahedron 13: 308 (1961)	-0.36	-1.04	-0.60	-2.85	-1.21
01800005	MENTHYL BENZOATE	100122-23	B06	sample		C17H24O2	260.37963		derivative	undetermined activity		0.28	-0.71	-1.62	-2.28	-1.08
02300253	1R,2S-PHENYLPROPYLAMINE	100122-23	B07	sample	14838-15-4	C9H13NO	151.21006	decongestant	Ephedra vulgaris (MaHuang)	experimental	Phytochemistry 16: 9 (1977)	0.03	0.47	-0.58	-0.24	-0.08
02300228	KAINIC ACID	100122-23	B08	sample	487-79-6	C10H15NO4	213.23535	glutamate receptor agonist, anthelmintic	Digenia simplex	INN, JAN		-0.25	1.00	-1.98	0.66	-0.14
00300018	LOBARIC ACID	100122-23	B09	sample		C29H28O8	456.49711		lichens of the genus Stereocaulon and others	undetermined activity	Z Naturforsch 21b: 714 (1966)	1.09	1.12	-0.08	0.88	0.75
00100743	HOMOPTEROCARPIN	100122-23	B10	sample	606-91-7	C17H16O4	284.31467		mp 82-84 C; Pterocarpus santalinus	undetermined activity	J Chem Soc 1940:787	-0.99	0.21	-1.84	-0.27	-0.72
00201092	4-METHOXYDALBERGIONE	100122-23	B11	sample	4646-86-0	C16H14O3	254.28818		Dalbergia retusa and D. nigra	undetermined activity	Phytochemistry 17: 1395 (1978); Tetrahedron 21: 2683 (1965)	-0.70	1.16	-1.04	-0.44	-0.26
	0.04% JAK2inhib	100122-23	B12	0.04% jak2inhib								-2.36	-1.46	-0.08	-1.64	-1.38
	0.04% DMSO	100122-23	C01	0.04% dmso								-0.06	-0.62	-0.21	-0.76	-0.41
00231084	UMBELLIFERONE	100122-23	C02	sample	93-35-6	C9H6O3	162.14637	antifungal, phytoalexin	Angelica, Artemisia, Coronilla, Ferula and Ruta spp	experimental	Chem Pharm Bull 19:640 (1971); Phytochemistry 14:1083 (1975)	0.22	-1.14	-1.77	-1.41	-1.03
00200441	XANTHOXYLIN	100122-23	C03	sample	90-24-4	C10H12O4	196.20474		Xanthoxylium spp, Artemisia brevifolia	undetermined activity		1.36	-1.01	-0.38	0.37	0.09
00201138	DEGUELIN(-)	100122-23	C04	sample	522-17-8	C23H22O6	394.42819	antineoplastic, antiviral, insecticide	Tephrosia & Derris spp	experimental	J Am Chem Soc 56: 2415 (1934); J Org Chem 44: 2580 (1979); Applied Microbiol 18: 660 (1969); Proc Natl Acad Sci 95: 3380 (1998); J Natl Cancer Inst 95: 291 (2003)	5.10	4.22	4.74	6.25	5.08
00201315	7,8-DIHYDROXYFLAVONE	100122-23	C05	sample	38183-03-8	C15H10O4	254.24455	vascular protectant, antihaemorrhagic	Godmania aesculifolia	experimental	J Chem Soc 1939: 956, 958; 1956:4170	-0.78	-1.53	-2.26	-2.34	-1.73
00201466	MANDELIC ACID, METHYL ESTER	100122-23	C06	sample		C9H10O3	166.17825		free acid found in Poria spp.	undetermined activity		2.51	-0.14	-0.82	-1.63	-0.02
00210186	CITRININ	100122-23	C07	sample	518-75-2	C13H14O5	250.25353	antibacterial	Penicillium citrinum	experimental	J Chem Soc 1963: 3777	-1.17	-0.38	0.46	1.52	0.11
00210477	ACTINONIN	100122-23	C08	sample	13434-13-4	C19H35N3O5	385.5079	antibacterial	Streptomyces spp.	experimental	Nature 195: 701 (1962)	-2.84	-1.70	-1.09	-2.45	-2.02
00210567	DIMETHYLCAFFEIC ACID	100122-23	C09	sample	14737-89-4	C11H12O4	208.21589		Piper methysticum, Veronica virginica	undetermined activity		0.28	1.11	-0.12	-0.76	0.12
00201697	EUPHOL	100122-23	C10	sample	514-47-6	C30H50O	426.7324		Euphorbia spp.	undetermined activity	J Chem Soc 1944:249; 1958:179	-8.68	-2.36	0.85	-0.46	-2.66
00201515	THEAFLAVIN DIGALLATE	100122-23	C11	sample	30462-35-2	C43H32O20	868.72249		pigment in black tea	undetermined activity		1.20	3.65	0.96	-0.03	1.44
	0.11% JAK2inhib	100122-23	C12	0.11% jak2inhib								-4.20	-0.88	-4.20	-2.54	-2.96
	0.11% DMSO	100122-23	D01	0.11% dmso								-1.75	-1.56	-0.09	-1.43	-1.21
01505031	GARDENIN B	100122-23	D02	sample	2798-20-1	C19H18O7	358.35111		Gardenia lucida; Brickellia, Citrus and Mentha spp	undetermined activity	Tetrahedron 21:1441, 3741 (1965); Chem Pharm Bull 28:708, 717 (1980); Phytochemistry 23:2972 (1984)	-0.37	-0.91	3.10	1.47	0.82
00107022	beta-SITOSTEROL	100122-23	D03	sample	83-46-5	C29H50O	414.72125		widespread in plants	undetermined activity	J Am Chem Soc 48: 2987 (1926)	0.48	-2.23	-0.06	0.63	-0.29
00102007	FORMONONETIN	100122-23	D04	sample	485-72-3	C16H12O4	268.27164	phytoestrogen	soyabean and clover species	experimental	J Chem Soc 1933: 274	0.31	0.61	0.42	0.42	0.44
00300545	CHRYSOPHANOL	100122-23	D05	sample	481-74-3	C15H10O4	254.24455		Cassia and Rumex spp	undetermined activity	Phytochemistry 11: 2122 (1972)	0.37	-0.45	1.87	-1.32	0.12
00240565	5,7-DIHYDROXYISOFLAVONE	100122-23	D06	sample	4044-00-2	C15H10O4	254.24455		Arachis hypogaea & Derris spp	undetermined activity	J Chem Soc 1953:1852; CA 104:165440 (1986)	0.78	-0.02	-0.20	0.33	0.22
01500294	CINEOLE	100122-23	D07	sample	470-82-6	C10H18O	154.25436	anthelminthic, antiseptic, expectorant	eucalyptus and lavender oils	experimental		0.00	0.23	-0.11	-0.55	-0.11
01501210	HUMULENE (alpha)	100122-23	D08	sample	6753-98-6	C15H24	204.35853		hops and clove oils	undetermined activity	JACS 99: 3864 (1977); J Chem Soc 1980: 311	-4.42	-0.02	0.53	0.22	-0.92
01504076	YOHIMBIC ACID HYDRATE	100122-23	D09	sample	522-87-2	C20H26N2O4	358.44122		derivative; yohimbinic acid	undetermined activity	J Chem Soc 123: 3003 (1923)	-0.24	0.06	0.32	1.00	0.29
00202175	12a-HYDROXY-5-DEOXYDEHYDROMUNDUSERONE	100122-23	D10	sample		C19H18O6	342.35171		derivative	undetermined activity		0.41	0.51	-0.75	-0.77	-0.15
00212061	PYROCATECHUIC ACID	100122-23	D11	sample	303-38-8	C7H6O4	154.12347	antioxidant	Erythraea centaurium, Gentiana lutea	experimental		0.23	1.35	-0.09	0.20	0.42
	0.11% JAK2inhib	100122-23	D12	0.11% jak2inhib								-3.93	-2.83	-2.68	0.55	-2.22
	0.11% JAK2inhib	100122-23	E01	0.11% jak2inhib								-4.09	-4.72	-3.69	-2.77	-3.82
00212097	ONONETIN	100122-23	E02	sample	487-49-0	C15H14O4	258.27643		Trifolium subterraneum	undetermined activity	Monatsh Chem 63: 201 (1933); Aust J Chem 19: 1755 (1966)	0.92	-1.22	0.32	-1.02	-0.25
00211539	ARABITOL(D)	100122-23	E03	sample	488-82-4	C5H12O5	152.14839		Lecanora sordida & other lichen & fungi	undetermined activity		-0.01	-1.37	0.57	-0.27	-0.27
00211249	7,4'-DIMETHOXYISOFLAVONE	100122-23	E04	sample		C17H14O4	282.29873		Dalbergia violaceae, Pterodon apparicioi	undetermined activity		1.33	0.80	2.49	2.70	1.83
00211012	IRIGINOL HEXAACETATE	100122-23	E05	sample		C27H22O14	570.46799		semisynthetic	undetermined activity		0.03	0.69	1.81	-0.64	0.47
00211066	2-METHOXYRESORCINOL	100122-23	E06	sample	29267-67-2	C7H8O3	140.14001		Peltophorum africanum	undetermined activity	Phytochemistry 29:283 (1990)	-0.50	-0.29	2.37	-0.62	0.24
00300048	KOBUSONE	100122-23	E07	sample	24173-71-5	C14H22O2	222.33024		Cyperus rotundus, Sindora sumatrana	undetermined activity	J Chem Soc 1957: 2988; Chem Pharm Bull 17: 1390 (1969); 42: 138 (1994); Helv Chim Acta 66: 1843 (1983)	0.04	0.06	2.99	1.66	1.19
00240645	RETUSIN 7-METHYL ETHER	100122-23	E08	sample		C17H14O5	298.29813		derivative Dalbergia spp	undetermined activity		-0.27	-0.05	0.89	1.09	0.42
00240673	ROBUSTIC ACID	100122-23	E09	sample	5307-59-5	C22H20O6	380.4011		Derris robusta	undetermined activity	J Chem Soc 1969:365	-0.87	0.10	-0.46	0.42	-0.20
00240914	PSEUDO-ANISATIN	100122-23	E10	sample	31090-37-6	C15H22O6	298.33899	GABA antagonist	Illicium anisatum	experimental	J Am Chem Soc 74: 3211 (1952)	-0.24	2.99	2.05	-0.23	1.14
00240958	4'-METHOXYFLAVONE	100122-23	E11	sample	4143-74-2	C16H12O3	252.27224		Sapindus saponaria.	undetermined activity		0.36	1.79	-0.12	-0.19	0.46
	0.11% DMSO	100122-23	E12	0.11% dmso								-0.59	1.73	-0.56	3.93	1.13
	0.11% JAK2inhib	100122-23	F01	0.11% jak2inhib								-1.46	-2.94	-2.30	-3.98	-2.67
00240944	HAEMATOXYLIN PENTAACETATE	100122-23	F02	sample		C26H24O12	528.47398		derivative	undetermined activity	Bul Soc Chim Fr 1972: 3292	-0.72	-0.85	0.26	-0.95	-0.57
01505825	DIHYDROTANSHINONE I	100122-23	F03	sample		C18H14O3	278.31048		Salvia miltiorrhiza	undetermined activity	Acta Chim Sin36:199 (1978); J Org Chem 55:3537 (1990)	-4.07	-3.08	-3.20	-2.41	-3.19
00240862	KUHLMANNIN	100122-23	F04	sample		C17H14O5	298.29813		Manchaerium spp	undetermined activity	Phytochemistry 17: 1383 (1978)	0.00	-0.66	2.85	1.98	1.04
00203010	beta-TOXICAROL	100122-23	F05	sample	82-11-1	C23H22O7	410.42759		Derris species & isomeration of alpha-toxicarol	undetermined activity	J Chem Soc 1938: 513,734; 1939: 812	3.02	3.31	4.29	2.18	3.20
00100058	6-HYDROXYANGOLENSIC ACID METHYL ESTER	100122-23	F06	sample		C27H34O8	486.56723		Meliaceae spp	undetermined activity		-1.66	-1.07	-0.36	-0.96	-1.01
01504029	LIGUSTILIDE	100122-23	F07	sample	4431-01-0	C12H14O2	190.24418	antispasmodic, smooth muscle relaxant	Ligusticum and Angelica spp	experimental	Phytochemistry 23: 2033 (1984); J Nat Prod 58: 1047 (1995)	0.18	0.02	0.20	1.84	0.56
00300532	ANDROGRAPHOLIDE	100122-23	F08	sample	5508-58-7	C20H30O5	350.4591		Adrographis peniculata	undetermined activity	Indian J Chem 6: 252 (1968)	0.61	1.05	2.95	2.14	1.69
00100576	TRIDESACETOXYKHIVORIN	100122-23	F09	sample		C26H36O7	460.57262		Khaya spp	undetermined activity		-2.05	0.69	-0.01	-0.02	-0.35
00100465	DIHYDROFISSINOLIDE	100122-23	F10	sample		C29H38O8	514.62141		derivative of fissinolide (00100031)	undetermined activity		-0.08	-0.06	2.53	-0.72	0.42
00211224	alpha-TOXICAROL	100122-23	F11	sample	82-09-7	C23H22O7	410.42759		Derris spp	undetermined activity	J Chem Soc 1938: 513	3.40	4.07	3.60	3.92	3.75
	0.04% DMSO	100122-23	F12	0.04% dmso								0.55	1.34	-0.73	0.06	0.30
	0.04% JAK2inhib	100122-23	G01	0.04% jak2inhib								-0.42	-3.27	-2.21	-1.31	-1.80
00300549	ACETYL ISOGAMBOGIC ACID	100122-23	G02	sample		C40H46O9	670.80722		derivative	undetermined activity	J Chem Soc 1966:772; Magn Reson Chem 31: 340 (1993)	-5.38	-2.18	2.30	-0.25	-1.38
00240828	3,4-DIMETHOXYDALBERGIONE	100122-23	G03	sample	41043-20-3	C17H16O4	284.31467	induces dermatitis	Dalbergia spp, Machaerium spp	undetermined activity	Tetrahedron 21: 2697 (9165)	0.50	1.59	0.64	0.69	0.85
01500657	HYDROQUINIDINE	100122-23	G04	sample	1435-55-8	C20H26N2O2	326.44242	antiarrhythmic, antimalarial	Cinchona bark	INN		0.45	-1.00	0.89	1.16	0.37
01500639	OCTOPAMINE HYDROCHLORIDE	100122-23	G05	sample	104-14-3	C8H12ClNO2	189.64334	adrenergic agonist	salivary glands of Octopus vulgaris; also Capsicum frutescens & Cyperus spp; ND-50	INN		0.43	-0.38	0.07	0.17	0.07
00270067	STIGMASTA-4,22-DIEN-3-ONE	100122-23	G06	sample	20817-72-5	C29H46O	410.68937		plant constituent	undetermined activity	J Chem Soc 1942:391; Phytochemistry 22:2087 (1983)	-2.96	-0.41	1.56	0.75	-0.26
01500843	LATHOSTEROL	100122-23	G07	sample		C27H46O	386.66707		Austeria rubens	undetermined activity	J Biol Chem 248: 6697 (1973)	-5.87	-0.31	0.86	1.48	-0.96
01500880	TRIGONELLINE	100122-23	G08	sample	535-83-1	C7H7NO2	137.13934	antihyperglycemic	Trigonella foenumgraecum and in coffee beans	experimental	J Org Chem 26: 1318 (1961)	0.75	0.81	-0.73	4.21	1.26
01500659	ARTEMISIN	100122-23	G09	sample	481-05-0	C16H20O4	276.3354	anthelmintic	Artemesia spp	undetermined activity	J Chem Soc 1963: 5235	0.09	0.19	-0.08	-0.76	-0.14
01502108	ANTIMYCIN A (A1 shown)	100122-23	G10	sample	1397-94-0	C27H38N2O9	534.61191	antifungal, antiviral, interferes in cytochrome oxidation	Streptomyces spp	experimental		-1.88	0.13	-1.19	-0.83	-0.94
01500704	N-ACETYLPROLINE	100122-23	G11	sample		C7H11NO3	157.17062	antirheumatic	synthetic	experimental		0.17	2.06	0.72	0.03	0.75
	0.04% DMSO	100122-23	G12	0.04% dmso								-1.04	0.74	-1.16	0.28	-0.29
	0.04% JAK2inhib	100122-23	H01	0.04% jak2inhib								-2.49	-2.53	-1.81	-2.98	-2.45
01503431	CYTIDINE	100122-23	H02	sample	65-46-3	C9H13N3O5	243.22106		nucleoside	undetermined activity		0.09	-0.88	-0.40	2.10	0.23
00100325	DIGITONIN	100122-23	H03	sample	11024-24-1	C56H92O29	1229.34024		Digitalis purpurea	undetermined activity	Tetrahedron 19: 621 (1963)	-5.38	-1.85	-0.33	0.67	-1.72
01500848	LITHOCHOL-11-ENIC ACID	100122-23	H04	sample		C24H38O3	374.56866		Curvularia spp.	undetermined activity	J Chem Soc 1974: 1797	-3.05	-1.49	0.37	0.02	-1.04
00300053	BROMO-3-HYDROXY-4-(SUCCIN-2-YL)-CARYOLANE gamma-LACTONE	100122-23	H05	sample		C19H27BrO4	399.32864		derivative of caryophyllene	undetermined activity		-0.20	-0.33	-0.87	-0.29	-0.42
01501022	FARNESOL	100122-23	H06	sample	4602-84-0	C15H26O	222.37387		major component in oil of Hibiscus abelmoschus	undetermined activity	J Org Chem 28:1086 (1963)	0.31	0.20	0.27	-0.34	0.11
01501132	NEROL	100122-23	H07	sample	106-25-2	C10H18O	154.25436	weak estrogen receptor blocker	neroli and bergamot oils	experimental	J Pharm Pharmacol 54:1521 (2002)	1.91	0.83	0.36	0.57	0.92
01502094	ROSMARINIC ACID	100122-23	H08	sample	537-15-5	C18H16O8	360.32342	antiinflammatory, antithrombotic, antiplatelet, cytostatic, antiviral	Rosmarinus officinalis, Melissa officinalis, Momordica balsamina, Mentha piperita, Salvia officinalis, Teucrium scorodonia, Sanicula europaea, Coleus blumei, Thymus spp	experimental	J Org Chem 40: 1804 (1975); 41: 449 (1976); Drugs of the Future 10: 756 (1985)	-1.41	0.72	-0.09	-0.77	-0.39
01502003	BUFEXAMAC	100122-23	H09	sample	2438-72-4	C12H17NO3	223.27419	antiinflammatory, analgesic, antipyretic	synthetic; CP-1044-J3	INN, BAN, JAN		-0.22	2.17	-0.16	0.98	0.69
00100310	HECOGENIN ACETATE	100122-23	H10	sample	915-35-5	C29H44O5	472.67103		Hechtia texensis, Agave & Yucca spp	undetermined activity		-0.12	-0.49	-0.78	0.62	-0.19
01502101	PERILLIC ACID (-)	100122-23	H11	sample	7694-45-3	C10H14O2	166.22188	inhibits posttranslational cys isoprenylation, blocks G-protein	Salvia dorisiana	experimental	J Am Chem Soc 72: 2381 (1950); Experientia 26: 473 (1970); J Agric Food Chem 24: 377 (1976)	0.56	1.51	0.01	0.68	0.69
	empty	100122-23	H12	sample								NA	NA	NA	NA	NA
	empty	100122-24	A01	sample								NA	NA	NA	NA	NA
00100552	beta-AMYRIN ACETATE	100122-24	A02	sample	1616-93-9	C32H52O2	468.77004		latof various species of rubber tree	undetermined activity	J Chem Soc 1952:2916; Phytocehmistry 9: 1669 (1970)	-0.62	-1.72	-1.99	-2.04	-1.59
00200015	ISOROTENONE	100122-24	A03	sample		C23H22O6	394.42819		semisynthetic	undetermined activity	Chem Rev 12, 181 (1933); J Chem Soc 1966:749	4.37	2.48	3.23	3.51	3.40
00100537	SOLASODINE	100122-24	A04	sample	126-17-0	C27H43NO2	413.64926	antineoplastic, antiinflammatory	numerous Solanum spp	experimental	J Am Chem Soc 76: 4245 (1954); Alkaloids 19: 81 (1981)	-1.08	-0.94	-0.75	-1.68	-1.11
00100541	DICTAMNINE	100122-24	A05	sample	484-29-7	C12H9NO2	199.21103		Dictamnus albus and other Rutaceae	undetermined activity	Chem & Ind 1956: 1091	0.38	1.21	0.77	0.51	0.72
00200013	ROTENONE	100122-24	A06	sample	83-79-4	C23H22O6	394.42819	acaricide, ectoparasiticide, antineoplastic, mitochondrial poison	Derris spp	agricultural use	Chem Rev 12: 181 (1933); Prog Chem Ord Nat Prod 43: 1 (1983)	5.27	6.03	5.29	5.34	5.48
00200007	GAMBOGIC ACID	100122-24	A07	sample	2752-65-0	C38H44O8	628.76958	antiinflammatory, cytotoxic, inhibits HeLa cells in vitro; LD50(rat) 88 mg/kg ip	Garcinia morella, G hanburyii	experimental	Tetrahedron 21: 1453 (1965); J Chem Soc(C) 1966:772; Tet Lett 1967:4201; Phytochemistry 41,: 815 (1996)	-6.21	-6.26	-0.28	2.20	-2.64
00200002	ORSELLINIC ACID, ETHYL ESTER	100122-24	A08	sample	2524-37-0	C10H12O4	196.20474		Roccella and Lecanora lichens	undetermined activity	J Org Chem 30: 3566 (1965)	-5.14	-4.51	-3.64	-0.58	-3.47
00201604	PYRROMYCIN	100122-24	A09	sample	668-17-7	C30H35NO11	585.61355	antibacterial	Streptomyces spp	experimental	Tet Letters 1959: 17; Chem Ber 92: 1904 (1959)	-0.53	-0.53	-0.85	1.97	0.01
00100540	OBLIQUIN	100122-24	A10	sample		C14H12O4	244.24934		sneezewood or umtati, Ptaeroxylon Obliquum	undetermined activity	J Chem Soc 1966: 114	0.75	-0.09	-0.11	-0.93	-0.10
00700024	HAEMATOPORPHYRIN	100122-24	A11	sample	14459-29-1	C34H38N4O6	598.70516	antidepressant, antineoplastic	Chlorella vulgaris; derived blood	experimental	J Biol Chem 202:801 (1953); Photochem Photobiol 39:851 (1984); 55:145 (1992)	0.48	5.53	3.92	1.93	2.97
	0.04% JAK2inhib	100122-24	A12	0.04% jak2inhib								-2.51	-1.23	-2.91	-2.75	-2.35
	0.04% DMSO	100122-24	B01	0.04% dmso								-0.57	-2.21	-2.15	3.03	-0.48
00240740	4-ACETOXYPHENOL	100122-24	B02	sample	3233-32-7	C8H8O3	152.15116	antioxidant	Ferulago aucheri, Salvia yosgadensis	experimental		-1.32	-1.82	-2.56	-2.11	-1.95
00300015	CHOLESTANE	100122-24	B03	sample	481-21-0	C27H48	372.68361		semisynthetic	undetermined activity		-0.15	-1.36	-0.86	-0.80	-0.79
00100688	DIGOXIGENIN	100122-24	B04	sample	1672-46-4	C23H34O5	390.52443		aglycon of digitoxin, thevetin, cerberin, echujin, evomonoside; mp 217-218	undetermined activity	J Chem Soc 1954: 2012	-0.47	-1.27	-0.13	-0.69	-0.64
00200774	IRIGENIN	100122-24	B05	sample	548-76-5	C18H16O8	360.32342		Iris spp	experimental	J Chem Soc 1928:1022; 1970:1219	-0.36	-0.05	-0.84	0.40	-0.21
01505490	APIGENIN DIMETHYL ETHER	100122-24	B06	sample	5728-44-9	C17H14O5	298.29813		common plant metabolite	undetermined activity		0.17	0.68	-0.72	-0.72	-0.15
00100254	5beta-12-METHOXY-4,4-BISNOR-8,11,13-PODOCARPATRIEN-3-ONE	100122-24	B07	sample		C16H20O2	244.3366		semisynthetic	undetermined activity		0.00	-0.84	-0.17	0.17	-0.21
00200424	2,3,4-TRIHYDROXY-4'-ETHOXYBENZOPHENONE	100122-24	B08	sample		C15H14O5	274.27583		semisynthetic	undetermined activity		-1.67	-1.58	-1.25	-0.94	-1.36
00310299	THYMOQUINONE	100122-24	B09	sample		C10H12O2	164.20594		Callitris, Monarda spp, Juniperus cedrus, Nigella sativa	undetermined activity	Planta Med 11: 465 (1963)	2.86	-0.48	0.04	0.09	0.63
00107013	SMILAGENIN	100122-24	B10	sample	126-18-1	C27H44O3	416.64993		Smilax spp.	undetermined activity	J Chem Soc 1936: 1399	-4.71	-0.74	-1.22	-0.27	-1.73
00200407	4'-HYDROXYCHALCONE	100122-24	B11	sample	2657-25-2	C15H12O2	224.26169		Shorea robusta aglycone	undetermined activity	JACS 52:2538 (1930)	1.49	0.78	-0.36	0.38	0.57
	0.04% JAK2inhib	100122-24	B12	0.04% jak2inhib								-0.44	-1.67	-1.40	-1.03	-1.13
	0.04% DMSO	100122-24	C01	0.04% dmso								0.10	-1.22	-1.70	-0.59	-0.85
00200034	ATRANORIN	100122-24	C02	sample	479-20-9	C19H18O8	374.35051		Common lichen metabolite	undetermined activity	Helv Chim Acta 9:650 (1926); 17:1319 (1934); J Chem Soc 1933:130; Chem Pharm Bull 24:2340 (1976); Gaia D1000	-1.44	-1.65	-0.41	-1.83	-1.33

Compound ID	MolNAME	plate	position	Content	cas#	Formula	MolWt	Bioactivity	Source	Status	Reference	Screen Score (z-score) rep1	rep2	rep3	rep4	Average
00100205	3alpha-ACETOXYDIHYDRODEOXYGEDUNIN	100122-24	C03	sample		C30H40O7	512.6491		Meliaceae spp	undetermined activity		-0.79	-1.89	-0.39	-1.97	-1.26
00240927	CAPERATIC ACID	100122-24	C04	sample	29227-64-3	C21H38O7	402.53281	antibacterial (tuberculostatic)	lichens: Parmelia, Mycoblastus, Nephromopsis spp	undetermined activity	J Nat Prod 29:43 (1966); J Pharm Sci, 56:1611 (1967); 57:1804 (1968); Acta Chem Scand, 29:889 (1975)	-0.57	-1.60	-0.54	1.75	-0.24
00307033	3-HYDROXY-4-(SUCCIN-2-YL)-CARYOLANE delta-LACTONE	100122-24	C05	sample		C19H28O4	320.43261		derivative of caryophyllene	undetermined activity		-1.33	-1.10	-1.12	-0.70	-1.06
00100563	OXONITINE	100122-24	C06	sample		C33H43NO12	645.71016		derivative of aconitine	undetermined activity	J Am Chem Soc 76: 4048 (1954)	0.80	0.53	-0.25	-1.14	-0.02
00240942	ARTHONIOIC ACID	100122-24	C07	sample	25556-24-5	C29H36O9	528.60487		Arthonia impolita	undetermined activity	Z Naturforsch B 25: 49 (1970)	0.58	0.16	0.36	-0.76	0.09
00310002	ADONITOL	100122-24	C08	sample	488-81-3	C5H12O5	152.14839		Adonis spp	undetermined activity	Pharm Acta Helv 23: 153 (1948); JACS 104: 1109 (1982); J Chem Soc 1983: 1553	1.66	-0.39	-1.21	2.05	0.53
00240736	2-METHOXYXANTHONE	100122-24	C09	sample	1214-20-6	C14H10O3	226.234		Mammea and Keilmeyera spp.	undetermined activity	Phytochemistry 9: 447, 2537 (1970)	-0.33	0.31	-0.55	-0.51	-0.27
01500716	ALANYL-dl-LEUCINE	100122-24	C10	sample		C9H18N2O3	202.25541		synthetic	undetermined activity		-0.01	1.58	0.16	-0.30	0.36
01500865	HARMALOL HYDROCHLORIDE	100122-24	C11	sample	6028-07-5	C12H13ClN2O	236.70321	anthelmintic, narcotic agent	Peganium harmala	experimental	Biochem J 27: 727 (1933); Phytochemistry 19: 1573 (1980)	0.83	-0.18	-0.90	-0.28	-0.13
	0.11% JAK2inhib	100122-24	C12	0.11% jak2inhib								-2.67	-3.22	-3.25	-2.39	-2.88
	0.11% DMSO	100122-24	D01	0.11% dmso								-1.10	-2.00	-1.76	-0.90	-1.44
01500870	MYOSMINE	100122-24	D02	sample	532-12-7	C9H10N2	146.19345	mitogen	tobacco, nuts	undetermined activity	Tetrahedron Letters, 1967: 5185	0.00	-0.02	0.19	2.14	0.58
01500996	GLAFENINE	100122-24	D03	sample	3820-67-5	C19H17ClN2O4	372.81134	analgesic	synthetic; R-11707	INN, JAN		0.37	0.12	0.57	0.00	0.26
01501116	MEBHYDROLIN NAPHTHALENESULFONATE	100122-24	D04	sample	524-81-2	C29H28N2O6S2	564.68431	H1 antihistamine	synthetic	INN, BAN, JAN		-0.77	0.39	-0.08	-1.89	-0.59
01501113	PERUVOSIDE	100122-24	D05	sample	1182-67-2	C30H44O9	548.67978	cardiotonic	Thevetia peruviana	experimental	Helv Chim Acta 35:673, 730, 1073; 36:370 (1952); 45:907 (1962); 46:2886 (1963)	-2.69	-3.69	-2.83	2.57	-1.66
01500909	PROTOVERATRINE A	100122-24	D06	sample	143-57-7	C41H63NO14	793.95756	antihypertensive, emetic; LD50 (rat) 5 mg/kg po	Veratrum album, V viride, V nigrum	INN	J Biol Chem 149:271 (1943); JACS 82:2242, 2252 (1960); Planta Med 10:138 (1962)	1.13	0.63	1.04	-0.42	0.59
01501125	3-AMINOPROPANESULPHONIC ACID	100122-24	D07	sample	3687-18-1	C3H9NO3S	139.17408	antibacterial; GABA agonist	synthetic	experimental	Br J Pharmacol 59:373 (1977); Neuropharmacology 17:13 (1978)	-0.15	0.73	1.21	0.17	0.49
01501143	SULFAPHENAZOLE	100122-24	D08	sample	526-08-9	C15H14N4O2S	314.36843	antibacterial	synthetic	INN, BAN, JAN		0.81	0.11	0.62	-0.57	0.24
01501157	SUXIBUZONE	100122-24	D09	sample	27470-51-5	C24H26N2O6	438.48462	analgesic, antipyretic, antiinflammatory	synthetic	INN, BAN, JAN		0.91	0.11	0.82	0.71	0.64
01501172	AZOBENZENE	100122-24	D10	sample	103-33-3	C12H10N2	182.2269	acaricide	synthetic	experimental		3.99	-0.08	0.49	0.11	1.13
01501174	TODRALAZINE HYDROCHLORIDE	100122-24	D11	sample	14679-73-3	C11H13ClN4O2	268.70486	antihypertensive, peripheral vasodilator	synthetic; CEPH, BT-621	INN, BAN, JAN		0.56	0.17	0.12	2.79	0.91
	0.11% JAK2inhib	100122-24	D12	0.11% jak2inhib								-4.08	0.39	-3.16	-2.90	-2.44
	0.11% JAK2inhib	100122-24	E01	0.11% jak2inhib								-3.96	-2.55	-3.89	-3.47	-3.47
01501183	ESTRADIOL METHYL ETHER	100122-24	E02	sample	1035-77-4	C19H26O2	286.41787	estrogen	semisynthetic	experimental	JACS 100: 6218 (1978)	-2.09	-1.40	0.86	1.21	-0.36
01501198	TOLFENAMIC ACID	100122-24	E03	sample	13710-19-5	C14H12ClNO2	261.71024	antiinflammatory, analgesia	synthetic	INN, BAN, JAN		0.40	0.78	1.92	0.48	0.90
01501192	ESTRADIOL-3-SULFATE, SODIUM SALT	100122-24	E04	sample		C18H23NaO5S	374.43481	estrogen	semisynthetic	experimental		-0.41	-0.92	-0.59	4.46	0.63
01502070	6,7-DICHLORO-3-HYDROXY-2-QUINOXALINECARBOXYLIC ACID	100122-24	E05	sample		C9H4Cl2N2O3	259.04983	NMDA and kainate receptor antagonist	synthetic	experimental	Neurosci Lett 91: 194 (1988)	0.20	1.10	-0.25	4.15	1.30
01502074	4-NAPHTHALIMIDOBUTYRIC ACID	100122-24	E06	sample		C16H13NO4	283.28631	aldose reductase inhibitor	synthetic	experimental		0.60	0.83	1.26	1.22	0.98
01502073	IMIDAZOL-4-YLACETIC ACID SODIUM SALT	100122-24	E07	sample	56368-58-2	C5H5N2NaO2	148.0976	GABAc antagonist	synthetic	experimental	Brit J Pharmacol 109: 200 (1993); Gen Pharmacol 31:503 (1998)	2.77	0.02	0.82	0.17	0.95
01502083	N- (9-FLUORENYLMETHOXYCARBONYL)-L-LEUCINE	100122-24	E08	sample	35661-60-0	C21H23NO4	353.42176	antiinflammatory	synthetic; NPC-15199	experimental	PNAS 88:355 (1991); J Pharmacol Exp Ther 266:468 (1993)	0.58	0.26	-0.27	0.11	0.17
01502095	alpha-CYANO-3-HYDROXYCINNAMIC ACID	100122-24	E09	sample		C10H7NO3	189.17219	inhibit mitochondrial pyruvate transport	synthetic	experimental		-0.02	-0.09	0.32	0.52	0.18
01502092	5-FLUOROINDOLE-2-CARBOXYLIC ACID	100122-24	E10	sample	399-76-8	C9H6FNO2	179.15207	NMDA receptor antagonist (gly)	synthetic	experimental		-0.64	0.46	-0.60	-0.07	-0.21
01502114	p-FLUOROPHENYLALANINE	100122-24	E11	sample	51-65-0	C9H10FNO2	183.18395	amino acid antagonist, protein synthesis inhibitor	synthetic	experimental	J Biol Chem 269: 24637 ((1994); Biochemistry 35: 6969 (1996); Eur J Cell Biol 23: 312 (1981)	0.20	0.21	0.31	1.43	0.54
	0.11% DMSO	100122-24	E12	0.11% dmso								-0.43	0.51	-0.96	2.48	0.40
	0.11% JAK2inhib	100122-24	F01	0.11% jak2inhib								-3.64	-4.73	-2.88	-1.60	-3.21
01502103	ANTHRAQUINONE	100122-24	F02	sample	84-65-1	C14H8O2	208.21866	irritant	synthetic	experimental		-0.35	-0.82	-1.20	-0.52	-0.72
01502130	AMINOCYCLOPROPANECARBOXYLIC ACID	100122-24	F03	sample	68781-13-5	C4H7NO2	101.10589	NMDA partial agonist (gly)	synthetic; ACPC	experimental		0.76	-0.36	-0.18	-0.48	-0.07
01502128	CYCLOLEUCINE	100122-24	F04	sample	52-52-8	C6H11NO2	129.16007	NMDA receptor antagonist (gly)	synthetic	experimental		1.15	2.20	0.19	-0.46	0.77
01502129	ISOGUVACINE HYDROCHLORIDE	100122-24	F05	sample	64603-90-3	C6H10ClNO2	163.6051	GABA agonist	synthetic	experimental		-0.18	0.42	0.37	-2.09	-0.37
01502162	p-CHLOROPHENYLALANINE	100122-24	F06	sample	7424-00-2(dl); 14173-39-8(l)	C9H10ClNO2	199.63855	Irreversible inhibitor of tryptophan hydroxylase	synthetic	experimental		0.51	-0.52	0.78	-0.55	0.06
01502229	ABIETIC ACID	100122-24	F07	sample	514-10-3	C20H30O2	302.4609		common diterpene acid in conifers	undetermined activity		0.31	0.36	1.12	0.69	0.62
01502209	PHENETHYL CAFFEATE (CAPE)	100122-24	F08	sample	104594-70-9	C17H16O4	284.31467	antineoplastic, antiinflammatory, immunomodulator, NFkB blocker	synthetic	experimental	PNAS 93:9090 (1996)	0.42	-0.12	2.07	0.93	0.82
01502207	L-LEUCYL-L-ALANINE	100122-24	F09	sample	7298-84-2	C9H18N2O3	202.25541	ubiquitin blocker, neurite growth inhibitor	synthetic	experimental	Biochim Biophys Res Commun 189:280 (1992); Experientia 52:865 (1996)	-0.16	0.37	0.29	1.22	0.43
01503254	6alpha-METHYLPREDNISOLONE ACETATE	100122-24	F10	sample		C24H32O6	416.51904	glucocorticoid	semisynthetic	experimental		1.00	0.48	-0.23	1.68	0.73
01503127	DEQUALINIUM CHLORIDE	100122-24	F11	sample	522-51-0, 6707-58-0 [dequalinium]	C30H40Cl2N4	527.5861	antiinfectant	synthetic; BAQD-10	INN, BAN, JAN		0.76	0.42	2.46	-0.09	0.89
	0.04% DMSO	100122-24	F12	0.04% dmso								-0.39	0.42	-0.86	-0.41	-0.31
	0.04% JAK2inhib	100122-24	G01	0.04% jak2inhib								-2.30	-2.64	-1.36	-2.23	-2.13
01503077	PRIDINOL METHANESULFONATE	100122-24	G02	sample	511-45-5	C21H29NO4S	391.53358	anticholinergic	synthetic; C-238	INN, JAN		-1.21	-1.05	-2.05	-1.53	-1.46
01503043	BUCLADESINE	100122-24	G03	sample	362-74-3	C18H24N5O8P	469.39448	vasodilator	synthetic	INN, JAN		-1.27	0.44	-0.26	-0.55	-0.41
01502259	MORIN	100122-24	G04	sample	480-16-0	C15H10O7	302.24275	P450 and ATPase inhibitor	Chlorophora tinctoria	experimental	J Chem Soc 67: 649 (1895)	-0.59	0.09	0.52	0.00	0.00
01503391	D-PHENYLALANINE	100122-24	G05	sample	673-06-3	C9H11NO2	165.19352	antidepressant	synthetic	INN		0.38	0.26	-0.04	-0.42	0.05
01503403	EXALAMIDE	100122-24	G06	sample	53370-90-4	C13H19NO2	221.30188	antifungal	synthetic	INN, JAN	J Pharm Pharmacol 9: 855 (1957)	0.73	0.42	0.92	-0.25	0.45
01503297	HEXAMETHONIUM BROMIDE	100122-24	G07	sample	55-97-0, 60-26-4 [hexamethonium]	C12H30Br2N2	362.1943	antihypertensive, ganglionic blocker	synthetic	INN, BAN, JAN		-0.69	-0.46	0.76	0.23	-0.04
01503425	ZOPICLONE	100122-24	G08	sample	43200-80-2	C17H17ClN6O3	388.81644	hypnotic, sedative	synthetic	INN, BAN, JAN		0.00	-0.06	1.06	0.42	0.35
01503637	METITEPINE MALEATE	100122-24	G09	sample	20229-30-5	C24H28N2O4S2	472.62976	5HT1&2 receptor antagonist	synthetic	INN		-0.18	1.44	0.39	0.23	0.47
01503641	1-PHENYLBIGUANIDE HYDROCHLORIDE	100122-24	G10	sample	55-57-2	C8H12ClN5	213.67134	5HT3 receptor agonist	synthetic	experimental		2.04	-0.08	-0.27	4.73	1.60
01503672	SODIUM THIOGLYCOLATE	100122-24	G11	sample	367-51-1	C2H3NaO2S	114.09881	dipilatory, irritant	synthetic	experimental		-0.20	0.41	0.04	-0.37	-0.03
	0.04% DMSO	100122-24	G12	0.04% dmso								0.04	-0.05	-0.08	-0.56	-0.16
	0.04% JAK2inhib	100122-24	H01	0.04% jak2inhib								-2.22	-3.05	-0.08	-3.76	-2.28
01503636	N-METHYL-D-ASPARTIC ACID (NMDA)	100122-24	H02	sample	6384-92-5	C5H9NO4	147.13178	NMDA agonist	synthetic	experimental		-0.19	0.84	0.99	-1.28	0.09
01503051	RETINYL ACETATE	100122-24	H03	sample	127-47-9	C22H32O2	328.49914	vitamin precursor	semisynthetic	JAN		0.33	0.55	-0.22	3.04	0.92
01503936	PERICIAZINE	100122-24	H04	sample	2622-26-6	C21H23N3OS	365.50096	antipsychotic	synthetic	INN, BAN, JAN		-0.60	-0.65	-0.09	-0.79	-0.53
01503906	ANISOMYCIN	100122-24	H05	sample	22862-76-6	C14H19NO4	265.31183	antiprotozoal, antifungal, protein synthesis inhibitor	Streptomyces griseolus	experimental	JACS 76:4053 (1954); Chem Pharm Bull 17:1405 (1969); Prog Neurobiology 16:155 (1981); Mol Cell Biochem 14:7352 (1994)	0.79	2.19	2.55	1.29	1.71
01503947	CACODYLIC ACID	100122-24	H06	sample	75-60-5	C2H7AsO2	137.99849	antieczema, dermatologic, herbicide	synthetic	experimental		-1.26	-1.40	0.08	-0.62	-0.80
01503941	THIOCTIC ACID	100122-24	H07	sample	1077-24-7	C8H14O2S2	206.32758	hepatoprotectant	synthetic; alpha-lipoic acid	JAN	JACS 74:1868, 3455 (1992); Angewante Chemie Int Ed 4:846 (1965); Arzneim Forsch 20:1210 (1970)	-0.41	-0.13	2.91	0.73	0.78
01503928	5-METHYLFURMETHIDE	100122-24	H08	sample	1197-60-0	C9H16INO	281.13837	muscarinic agonist	synthetic	experimental	Eur J Pharmacol 186:257 (1990); 244:21 (1993)	-0.55	-0.75	3.75	-0.27	0.54
01504009	LEVULINIC ACID, 3-BENZYLIDENYL-	100122-24	H09	sample		C12H12O3	204.22764		derivative	undetermined activity		0.83	0.09	-0.12	0.05	0.21
01503970	METHOXYAMINE HYDROCHLORIDE	100122-24	H10	sample	593-56-6	CH6ClNO	83.51807	hydroxymethyltransferase inhibitor	synthetic	experimental		0.88	-0.71	0.59	-1.32	-0.14
01503954	TULOBUTEROL	100122-24	H11	sample	41570-61-0	C12H19Cl2NO	264.19733	bronchodilator, beta adrenergic agonist	synthetic	INN, BAN, JAN		0.94	-0.21	-1.25	-1.92	-0.61
	empty	100122-24	H12	sample								NA	NA	NA	NA	NA
	empty	100122-25	A01	sample								NA	NA	NA	NA	NA
01504135	TRIMEDLURE	100122-25	A02	sample	12002-53-8	C12H21ClO2	232.75297	arthropod pheromone	synthetic; 5-Cl isomer present	agricultural use	J Econ Entomol 59:1450 (1966)	NA	1.94	-1.63	-0.11	0.07
01504143	ARTENIMOL	100122-25	A03	sample	81496-81-3	C15H24O5	284.35553	antimalarial, antiinflammatory	semisynthetic; dihydroartemisinin	INN	Med Res Rev 7: 29 (1987); Am J Trop Med Hyg 61:187 (199); Trends Pharmacol Sci 20:199 (1999)	NA	-1.44	-2.41	-2.53	-2.13
01504145	GLICLAZIDE	100122-25	A04	sample	21187-98-4	C15H21N3O3S	323.41692	antidiabetic, adhesion inhibitor	synthetic; SE-1702	INN, BAN, JAN	Drugs 27:301 (1984); J Diabetes Complications 14:201 (2000); Metabolism 50: 688 (2001)	NA	-1.00	-0.75	-0.09	-0.61
01504137	ANCITABINE HYDROCHLORIDE	100122-25	A05	sample	10212-25-6	C9H12ClN3O4	261.66669	antineoplastic	synthetic	INN, JAN	Carcinogenesis 7:1167 (1992)	NA	-1.12	-0.10	-0.67	-0.63
01500840	CHOLIC ACID	100122-25	A06	sample	81-25-4	C24H40O5	408.5834		mammalian bile	undetermined activity	Biochem J 85: 236 (1962)	NA	1.33	-0.23	-0.17	0.31
01504182	3-METHYLXANTHINE	100122-25	A07	sample	1076-22-8	C6H6N4O2	166.14032	phosphodiesterase inhibitor	synthetic	experimental	Clin Exp Pharmacol Physiol 18: 163 (1991)	NA	-1.10	-0.44	-0.83	-0.79
01504151	NIMUSTINE	100122-25	A08	sample	42471-28-3	C9H13ClN6O2	272.69596	antineoplastic	synthetic	INN, JAN	Carcinogenesis 21: 1879 (2000)	NA	-0.11	1.00	-0.65	0.08
01504153	NORCANTHARIDIN	100122-25	A09	sample		C8H8O4	168.15056	antineoplastic, protein phosphatase inhibitor	synthetic	experimental	Biochem Biophys Res Comm 276: 278 (2000)	NA	2.01	-1.10	0.09	0.34
01504209	DIPLOSALSALATE	100122-25	A10	sample	530-75-6	C16H12O6	300.27044	analgesic, antipyretic	synthetic	experimental		NA	0.45	0.56	-0.88	0.04
01504221	PHENYLBUTYRATE SODIUM	100122-25	A11	sample	90-27-7 (phenylbutyric acid)	C10H11NaO2	186.18777	antihyperlipidemic	synthetic; R-757, Th-22	experimental		NA	0.43	1.18	-1.20	0.13
	0.04% JAK2inhib	100122-25	A12	0.04% jak2inhib								NA	-0.51	-1.49	-4.34	-2.11
	0.04% DMSO	100122-25	B01	0.04% dmso								NA	0.45	1.35	-1.21	0.19
01504225	2-MERCAPTOBENZOTHIAZOLE	100122-25	B02	sample	149-30-4	C7H5NS2	167.2526	antifungal	synthetic; AG-63	experimental		NA	-1.71	-0.90	0.48	-0.71
01504228	CRUSTECDYSONE	100122-25	B03	sample	5289-74-7	C27H44O7	480.64753	insect molting hormone	silkworm moth Bombyx mori & the plant Achyranthes fauriei	experimental	Yakugaku Zasshi 87: 325 (1967); Arch Insect Biochem Physiol 33: 231 (1996); J Neurosci 18: 8886 (1998)	NA	0.23	-1.28	0.03	-0.34
01504215	N,N-HEXAMETHYLENEAMILORIDE	100122-25	B04	sample		C12H18ClN7O	311.77656	Na/H+ antiporter inhibitor, diuretic	synthetic	experimental	Biochim Biophys Acta 944: 383 (1988)	NA	0.16	-1.47	1.66	0.11
01504223	FENBUTYRAMIDE	100122-25	B05	sample	90-26-6	C10H13NO	163.22121	antihyperlipidemic	synthetic	experimental		NA	-0.75	-1.03	-0.62	-0.80
01505007	2,3-DIMERCAPTOSUCCINIC ACID	100122-25	B06	sample	304-55-2	C4H6O4S2	182.21802	chelating agent, antihypertensive	synthetic; DMSA	experimental	Biochem Pharmacol 65:1741 (2003)	NA	-0.41	-1.16	-1.03	-0.87
01505001	PUERARIN	100122-25	B07	sample	3681-99-0	C21H20O9	416.38815	beta-adrenergic blocker	Pueraria spp	experimental	Chem Pharm Bull 8:688 (1960)	NA	-0.30	-1.10	-0.85	-0.75
01504244	BETAMIPRON	100122-25	B08	sample	3440-28-6	C10H11NO3	193.20407	sweetener	synthetic	INN, JAN		NA	0.19	0.13	0.15	0.16
01504232	2,3-DIHYDROXY-6,7-DICHLOROQUINOXALINE	100122-25	B09	sample		C8H4Cl2N2O2	231.03928	NMDA receptor antagonist (gly)	synthetic	experimental	J Neurochem 54: 699 (1990)	NA	-0.14	0.35	2.47	0.89
01505015	3H-1,2-DITHIOLE-3-THIONE	100122-25	B10	sample		C3H2S3	134.24139	antioxidant, antineoplastic	synthetic; D3T	experimental	Free Rad Biomed 28:944 (2000)	NA	-0.01	0.31	-1.84	-0.51
01505011	TRIMEBUTINE MALEATE	100122-25	B11	sample	34140-59-5(base)	C26H33NO9	503.55421	antispasmodic, opiod receptor agonist	synthetic	INN, BAN, JAN	Japan J Pharmacol 33:301 (1983); Hepato-Gastroenterology 49:193 (2002)	NA	0.15	2.85	-2.29	0.23
	0.04% JAK2inhib	100122-25	B12	0.04% jak2inhib								NA	0.25	3.44	-2.38	0.44
	0.04% DMSO	100122-25	C01	0.04% dmso								NA	-1.21	-1.76	-0.19	-1.05
01505036	TANSHINONE IIA SULFONATE SODIUM	100122-25	C02	sample		C19H17NaO6S	396.39754	free radical scavenger	semisynthetic	experimental	Biochem Pharmacol 46:2327 (1993); 65:51 (2003); Biochem Mol Biol Int 38:1171 (1996)	NA	-0.91	-1.18	0.25	-0.62
01505039	2,5-DI-t-BUTYL-4-HYDROXYANISOLE	100122-25	C03	sample	1991-52-2	C15H24O2	236.35733	antioxidant	synthetic	experimental		NA	-0.34	-1.20	1.95	0.14
01505107	VALINOMYCIN	100122-25	C04	sample	2001-95-8	C54H90N6O18	1111.3488	antibiotic; LD50 (rat, po) 4 mg/kg	Streptomyces spp	experimental	Chem Ber 88:57 (1955); Biochem Biophys Res Commun 15:1964 (1964); JACS 99:2032 (1977)	NA	-0.43	1.76	0.08	0.47
01505041	BISPHENOL A	100122-25	C05	sample	80-05-7	C15H16O2	228.29357	endocrine disruptor, plastic monomer	synthetic	experimental		NA	-0.70	-0.93	-0.89	-0.84
01505104	4-(3-BUTOXY-4-METHOXYBENZYL)IMIDAZOLIDIN-2-ONE	100122-25	C06	sample	29925-17-5	C15H22N2O3	278.35419	cAMP PDE inhibitor, inhibits cellular adhesion and superoxide & platelet aggregation	synthetic; RO-20-1724	experimental	Mol Pharmacol 13: 38 (1977); Biochem Biophs Acta 763: 276 (1983); Life Sci 63: 265 (1998)	NA	2.61	0.49	0.36	1.15
01505109	MANGANESE TETRAKIS(4-CARBOXYPHENYL)PORPHYRIN CHLORDE	100122-25	C07	sample		C48H28ClMnN4O8	879.17136	SOD mimetic	synthetic	experimental	J Biol Chem 269:23471 (1994); Br J Pharmacol 120:259 (1997); Toxicol Appl Pharmacol 26:25 (1998)	NA	0.12	-0.45	-0.08	-0.14
01505083	PRASTERONE	100122-25	C08	sample	53-43-0	C19H28O2	288.43381	androgen, estrogen, treatment of menopausal syndrome	adrenal glands, male urine	INN	Lancet 343:1479 (1994)	NA	0.43	1.01	0.36	0.60
01505158	2,3-DICHLORO-5,8-DIHYDROXYNAPTHOQUINONE	100122-25	C09	sample	14918-65-5	C10H4Cl2O4	259.04698	apoptosis inducer, antiproliferative	synthetic	experimental	Bioorg Med Chem Lett 8:2507 (1998); J Biol Chem 276:24638 (2001)	NA	0.22	0.95	0.13	0.43
01505157	2,2'-AZO-bis-2-AMINOPROPANE	100122-25	C10	sample	2997-92-4	C8H20Cl2N6	271.1948	free radical initiator, apoptosis inducer	synthetic	undetermined activity	Biochemistry 36:7706 (1997); 40:1719 (2001); Biochem Biophys Acta 1543:69 (2000)	NA	1.22	0.90	-1.17	0.31

Compound ID	MolNAME	plate	position	Content	cas#	Formula	MolWt	Bioactivity	Source	Status	Reference	Screen Score (z-score) rep1	rep2	rep3	rep4	Average
01505156	N-PHENYLANTHRANILIC ACID	100122-25	C11	sample	91-40-7	C13H11NO2	213.23812	ion channel (Cl) blocker	synthetic	experimental	Am J Physiol 253:C79 (1987); J Biol Chem 276:11575 (2001)	NA	1.00	0.74	-0.21	0.51
	0.11% JAK2inhib	100122-25	C12	0.11% jak2inhib								NA	-2.07	0.04	-3.71	-1.91
	0.11% DMSO	100122-25	D01	0.11% dmso								NA	-1.86	-1.71	-0.43	-1.34
01505154	3-AMINO-1,2,4-TRIAZOLE	100122-25	D02	sample	61-82-5	C2H4N4	84.08098	catalase inhibitor	synthetic	experimental	Biochem Pharmacol 42:699 (1991); Am J Physiol 270:H1165	NA	-0.92	-0.89	-0.21	-0.67
01505250	MADECASSIC ACID	100122-25	D03	sample	18449-41-7	C30H48O6	504.71346	wound healing	Centella asiatica	experimental	Bull Soc Chim Fr 1967: 1890; Phytochemistry 7: 1385 (1968); 28: 2852 (1989)	NA	-1.28	-1.39	2.24	-0.14
01505163	AURIN TRICARBOXYLIC ACID	100122-25	D04	sample	4431-00-9	C22H14O9	422.35148	apoptosis inhibitor, topoisomerase II inhibitor	synthetic	experimental	Eur J Biochem 248:30 (1997)	NA	-0.42	-0.88	-0.06	-0.45
01505167	ACADESINE	100122-25	D05	sample	2627-69-2	C9H14N4O5	258.23573	glucose uptake stimulant; AMPK activator	synthetic	INN	Eur J Biochem 229:558 (1995)Biochem J 338:783 (1999); J Mol Neurosci 17:45 (2001)	NA	-0.07	0.18	0.04	0.05
01505165	2-METHYL-4-(PIPERIDIN-1-YLCARBOXY)-5-ISOPROPYLPHENYLTRIMETHYLAMMONIUM CHLORIDE	100122-25	D06	sample		C19H31ClN2O2	354.92412	squalene-2,3-oxide cyclase inhibitor, anticholesterolemic	synthetic	experimental	Steroids 58:74 (1993); J Biol Chem 250:1571 (1975)	NA	-0.92	0.61	-0.20	-0.17
01505164	4,4'-DIISOTHIOCYANOSTILBENE-2,2'-SUFONIC ACID SODIUM SALT	100122-25	D07	sample	67483-13-0	C16H8N2Na2O6S4	498.48756	ATP transport inhibitor, anion transport inhibitor, antiulcer	synthetic; DIDS	undetermined activity	EMBO J 12:69 (1993); Biochem Biophys Res Commun 207:375 (1995)	NA	-0.29	-0.07	-0.12	-0.16
01505298	3-ISOBUTYL-1-METHYLXANTHINE (IBMX)	100122-25	D08	sample	28822-58-4	C10H14N4O2	222.24868	phosphodiesterase inhibitor	synthetic	experimental		NA	0.23	0.75	0.72	0.57
01505324	BISSALICYL FUMARATE	100122-25	D09	sample		C18H12O8	356.29154	crosslinking agent (hemoglobin)	synthetic	experimental	J Biol Chem 255:2816 (1980)	NA	0.72	4.72	-1.46	1.33
01505316	PROTIONAMIDE	100122-25	D10	sample	14222-60-7	C9H12N2S	180.27339	antibacterial	synthetic; TH-1321, RP-9778	INN, BAN, JAN	Chemotherapy 26:276 (1980)	NA	-0.27	3.87	-0.17	1.14
01505317	CARMOFUR	100122-25	D11	sample	61422-45-5	C11H16FN3O3	257.26687	antineoplastic	synthetic	INN, JAN	Am J Clin Oncology 13:477 (1990)	NA	0.13	1.97	0.43	0.84
	0.11% JAK2inhib	100122-25	D12	0.11% jak2inhib								NA	-2.77	-0.86	-2.49	-2.04
	0.11% JAK2inhib	100122-25	E01	0.11% jak2inhib								NA	-4.02	-2.61	0.84	-1.93
01505328	4'-DEMETHYLEPIPODOPHYLLOTOXIN	100122-25	E02	sample		C21H20O8	400.38875	antineoplastic	semisynthetic	experimental	Eur J Cancer Clin Oncol 24:1415 (1988)	NA	-6.87	-2.24	-1.62	-3.58
01505339	L-PHENYLALANINOL	100122-25	E03	sample	3182-95-4	C9H13NO	151.21006	antiulcer	synthetic	experimental	Chem Pharm Bull 40:3113 (1992)	NA	-1.39	-0.42	1.22	-0.20
01505336	VALERYL SALYCILATE	100122-25	E04	sample	64206-54-8	C12H14O4	222.24298	COX-1 inhibitor	synthetic	experimental	Arch Biochem Biophys 317:19 (1995); OphthalmolVis Sci 39:1888 (1998)	NA	0.11	-0.12	0.02	0.00
01505331	3,3'-DIINDOLYLMETHANE	100122-25	E05	sample	1968-05-4	C17H14N2	246.31453	apoptosis inducer	synthetic	experimental	Biochem Biophys Res Commun 228:153 (1996)	NA	1.20	-0.96	0.37	0.20
01505337	ELAIDYLPHOSPHOCHOLINE	100122-25	E06	sample		C23H48NO4P	433.61711	antineoplastic	synthetic	experimental		NA	0.76	0.85	0.42	0.68
01505342	7-NITROINDAZOLE	100122-25	E07	sample	2942-42-9	C7H5N3O2	163.1368	NO synthetase inhibitor	synthetic	experimental	Eur J Pharmacol 310:115 (1996); TIPS 18:204 (1997)	NA	0.82	0.09	0.45	0.45
01505253	SINOMENINE	100122-25	E08	sample	115-53-7	C19H23NO4	329.39946	weak abortifacient, immunosuppressant, analgesic, antiinflammatory; LD50 (po) 580 mg/kg; (ip) 285 mg/kg(mouse)	Sinomenium acutum and Stephania cepharantha	experimental	Annalen 485: 247 (1931); J Chem Soc 1955: 3252; J Immunopharmacol 7: 33 (1985); Arzneim-Forsch 44: 1223 (1994)	NA	0.29	0.61	-0.71	0.06
01505252	PALMATINE	100122-25	E09	sample	3486-67-7	C21H24NO5	370.42913	uterine contractant, antibacterial, antiarrhythmic, inotropic, adrenocorticotropic, anticholinesterase, analgesic	Jateorhesa palmata, Berberis spp	experimental	Ber 58: 2267 (1925); J Nat Prod 28: 73 (1965)	NA	2.60	0.50	0.41	1.17
01505395	BICUCULLINE(-) METHIODIDE	100122-25	E10	sample	55950-07-7	C21H20INO6	509.30105	GABAa antagonist	semisynthetic; water soluble derivative of bicuculline (01500821)	experimental	Brain Res 465:243 (1989); TiPS 20:268 (1999)	NA	0.56	-0.41	-0.30	-0.05
01505930	SR-2640	100122-25	E11	sample	105350-26-3	C23H18N2O3	370.41151	LTD4/ LTE4 antagonist	synthetic; 2[3-(quinolin-2-ylmethoxy)phenylamino]benzoic acid	experimental	Am Rev Respir Dis 137(suppl):427 (1988); Eur J Pharmacol 155:117 (1988); Biochem Pharmacol 38:2291 (1989); Agents Actions 29:299 (1990)	NA	0.52	1.07	-0.02	0.52
	0.11% DMSO	100122-25	E12	0.11% dmso								NA	-0.26	3.29	-0.73	0.77
	0.11% JAK2inhib	100122-25	F01	0.11% jak2inhib								NA	-4.29	-4.42	-1.94	-3.55
01505915	PROXYPHYLLINE	100122-25	F02	sample	6003-00-9	C10H14N4O3	238.24808	PDE inhibitor, bronchodilator, vasodilator	synthetic	INN, BAN, JAN		NA	-1.42	-1.22	0.29	-0.78
01505785	CAMYLOFINE DIHYDROCHLORIDE	100122-25	F03	sample	54-30-8	C19H34Cl2N2O2	393.40103	anticholinergic	synthetic	INN, JAN		NA	-2.00	-1.07	-0.17	-1.08
01505849	ETHIONINE	100122-25	F04	sample	67-21-0	C6H13NO2S	163.24001	antineoplastic; inhibitor DNA methylation	synthetic	experimental	J Org Chem 16:749 (1971); Adv Can Res 7:383 (1963)	NA	-0.60	0.22	1.75	0.46
01505846	11alpha-HYDROXYPROGESTERONE HEMISUCCINATE	100122-25	F05	sample	41238-98-6	C25H34O6	430.54613	glucocorticoid	semisynthetic	experimental		NA	0.15	1.71	-0.01	0.62
01505880	DIFLORASONE DIACETATE	100122-25	F06	sample	33564-31-7	C26H32F2O7	494.53754	antiinflammatory, glucocorticoid	semisynthetic; U-34865	USP, INN, BAN, JAN		NA	-0.87	-1.11	-0.79	-0.92
01505986	NIALAMIDE	100122-25	F07	sample	51-12-7	C16H18N4O2	298.34746	MAO inhibitor	synthetic	INN, BAN, NF-VIII	Toxicol Appl Pharmacol 1:524 (1959); hepatotoxic at clinical dose (100mg)	NA	0.89	1.78	-0.60	0.69
01505869	AMPYRONE	100122-25	F08	sample	83-07-8	C11H13N3O	203.24576	analgesic, antiinflammatory, antipyretic	synthetic	experimental		NA	1.04	0.05	-0.71	0.13
01505742	ASCORBYL PALMITATE	100122-25	F09	sample	137-66-6	C22H38O7	414.54396	antioxidant	semisynthetic	USAN, NF		NA	-1.41	-1.11	2.27	-0.09
01505773	FAMPROFAZONE	100122-25	F10	sample	22881-35-2	C24H31N3O	377.53417	analgesic, antipyretic, CNS stimulant	synthetic	INN, BAN	J Forensic Sci 52:479 (2007)	NA	-0.44	1.19	-0.41	0.11
01505774	OXELAIDIN CITRATE	100122-25	F11	sample	52432-72-1, 468-61-1 (base)	C26H41NO10	527.61737	antitussive	synthetic	INN, BAN	J Pharm Pharmacol 10:40 (1958)	NA	0.01	1.71	-0.38	0.45
	0.04% DMSO	100122-25	F12	0.04% dmso								NA	0.49	1.07	0.10	0.56
	0.04% JAK2inhib	100122-25	G01	0.04% jak2inhib								NA	-3.66	-3.14	-1.64	-2.81
01506010	METHIONINE SULFOXIMINE (L)	100122-25	G02	sample	15985-39-4	C5H12N2O3S	180.22699	glutamine synthetase inhibitor, ornithine decarboxylase enhancer	synthetic	experimental		NA	-1.79	-0.12	0.73	-0.39
01506041	SALSOLINOL HYDROBROMIDE	100122-25	G03	sample	38221-21-5	C10H14BrNO2	260.13258	prolactin-releasing factor	dopamine derivative	experimental	Neurosignals 12:315 (2003); Physiol Res 55:353 (2006)	NA	-0.44	-0.34	-0.26	-0.35
01506051	TRIMETHYLCOLCHICINIC ACID	100122-25	G04	sample	3482-37-9	C19H21NO5	343.38292	antineoplastic	derivative	experimental	JACS 75:5292 (1953)	NA	-0.12	-0.05	0.61	0.14
01506044	THIOGUANOSINE	100122-25	G05	sample	85-31-4	C10H13N5O4S	299.31021	antineoplastic	synthetic	experimental	Can Res 21:1015 (1961)	NA	-0.36	-0.12	4.27	1.26
01506078	MOROXYDINE HYDROCHLORIDE	100122-25	G06	sample	3731-59-7	C6H14ClN5O	207.66438	antiviral	synthetic; SKF-8898A, ABOB	INN, BAN	Acta Derm Venereol Suppl (Stockh) 183:1 [1994]	NA	-0.46	0.18	1.13	0.28
01506088	TRIMETAZIDINE DIHYDROCHLORIDE	100122-25	G07	sample	5011-34-7	C14H24Cl2N2O3	339.26498	anti-anginal	synthetic; 400045	INN, BAN, JAN	Circ Res 86:580 (2000); Am J Cardiovasc Drugs 3:361 (2003); Circulation 118:1250 (2008)	NA	1.19	-0.48	0.86	0.52
01601020	DIETHYLTOLUAMIDE	100122-25	G08	sample	134-62-3	C12H17NO	191.27539	insect repellant	synthetic; DEET	USP, INN, BAN		NA	1.41	-0.52	-0.06	0.28
01400666	METHOXYVONE	100122-25	G09	sample		C17H14O3	266.29933	anabolic	synthetic	experimental		NA	0.65	0.37	2.48	1.17
01500629	FLOPROPIONE	100122-25	G10	sample	2295-58-1	C9H10O4	182.17765	antispasmodic	synthetic	INN, JAN		NA	0.46	1.04	0.57	0.69
01500666	ACEMETACIN	100122-25	G11	sample	53164-05-9	C21H18ClNO6	415.83371	antiinflammatory	synthetic	INN, BAN, JAN		NA	0.19	1.21	-0.15	0.42
	0.04% DMSO	100122-25	G12	0.04% dmso								NA	0.24	2.75	-0.70	0.76
	0.04% JAK2inhib	100122-25	H01	0.04% jak2inhib								NA	-2.82	-1.74	-2.01	-2.19
01500671	DIHYDROFOLIC ACID	100122-25	H02	sample	4033-27-6	C19H21N7O6	443.42252	antidote to methotrexate toxicity	dihydrofolate reductase product	experimental	Nature 188:231 (1960); Compr Biochem 21:111 (1971); J Chem Soc(Perkin 1) 1985:1349; Tetrahedron 42:117 (1986)	NA	-1.00	-2.85	0.50	-1.12
01500703	ACETYLGLUTAMIC ACID	100122-25	H03	sample		C7H11NO5	189.16942	excitatory aminoacid	synthetic	experimental		NA	-1.36	-0.77	0.01	-0.70
01500998	ETHOXYQUIN	100122-25	H04	sample		C14H19NO	217.31363	antioxidant	synthetic	experimental		NA	-2.15	-0.98	0.50	-0.88
01500705	O-BENZYL-l-SERINE	100122-25	H05	sample		C10H13NO3	195.22001		synthetic	undetermined activity		NA	-0.95	0.80	1.04	0.29
01500715	ACETYLGLUCOSAMINE	100122-25	H06	sample		C8H15NO6	221.21185	antiarthritic	synthetic	experimental		NA	0.34	-0.50	0.70	0.18
01500710	ACETYLPHENYLALANINE	100122-25	H07	sample		C11H13NO3	207.23116		synthetic	undetermined activity		NA	0.72	0.06	-0.02	0.25
01500728	5,7-DIHYDROXY-4-METHYLCOUMARIN	100122-25	H08	sample		C10H8O4	192.17286		semisynthetic	undetermined activity		NA	0.81	0.94	2.64	1.46
01500802	ALLOXAN	100122-25	H09	sample	2244-11-3	C4H2N2O4	142.07154	specific cytotoxin (pacreatic islet betacell)	synthetic	experimental		NA	0.24	2.51	0.35	1.03
01500902	SODIUM DEOXYCHOLATE	100122-25	H10	sample	302-95-4	C24H39NaO4	414.56583	choleretic	bile constituent	experimental		NA	-0.61	0.40	-0.70	-0.31
01501194	TOLPERISONE HYDROCHLORIDE	100122-25	H11	sample	70312-00-4	C16H24ClNO	281.82878	muscle relaxant (skeletal)	synthetic; N-553	INN, BAN, JAN		NA	1.26	1.74	0.26	1.09
	empty	100122-25	H12	sample								NA	NA	NA	NA	NA