

Supplementary Table 1: Initial Hits

Compound	%Inhib	% Viability (Viab*inhib)	Grouping/Target	
		/100		
Chlorambucil	67	66	44	alkylating agent
Pararosaniline Pamoate	98	63	62	aniline dye
Anthothecol	102	48	49	anthothecol
Phenethyl Caffate (Cape)	80	100	80	anti-inflammatory
Gramicidin	103	35	37	antibiotic
Fexofenadine Hydrochloride	88	60	53	antihistamine /choline
Alexidine Hydrochloride	42	101	43	antiseptic
Tetrachloroisophthalonitrile	62	87	54	antiseptic
Dequalinium Chloride	83	75	62	antiseptic
Cetylpyridinium Chloride	63	64	41	antiseptic
Gentian Violet	102	62	64	antiseptic
Thiram	91	59	54	antiseptic
Thimerosal	97	50	48	antiseptic
Artemimol	62	68	42	artemisinin
Avocadynone Acetate	85	93	79	avocado
Oxfendazole	46	100	47	benzimidazole anti-helminth
Oxibendazole	86	67	57	benzimidazole anti-helminth
Methicillin Sodium	60	53	32	beta lactam antibiotic
Nisoldipine	56	62	35	calcium channel blocker
Monensin Sodium	71	46	33	cation ionophor
Lasalocid Sodium	93	43	40	cation ionophor
Celastrol	72	73	52	celestroid
Cantharidin	100	66	66	cell adhesion
Mundoserone	32	74	23	chemo hematopoeisis
4-Nonylphenol	34	97	33	detergent
Methotrexate	79	67	53	DHFR
Cedrelone	86	66	57	differentiation
Mitomycin C	97	62	60	DNA crosslinker
Amsacrine	100	58	58	DNA intercalator
Apomorphine Hydrochloride	35	89	31	dopamine antagonist
Chlorpromazine	88	48	42	dopamine antagonist
Antimycin A (A1 Shown)	59	58	34	electron transport
Deferoxamine Mesylate	44	84	37	Fe chelation
Tacrolimus	34	75	25	FKBP
Aminacrine	39	65	25	fluorescent dye/nucleotide
Evans Blue	47	116	54	fusion
Dihydrogambogic Acid	101	61	62	gambogic acid
Gambogic Acid Amide	102	55	55	gambogic acid
Acetyl Isogambogic Acid	91	53	48	gambogic acid
Acivicin	35	73	26	glutamine analog
Mycophenolic Acid	89	55	49	immuno T cell supp
Cloxyquin	93	62	58	ion channel
Valinomycin	86	54	46	K ionophore
Salinomycin, Sodium	89	46	40	K ionophore
Nigericin	84	46	38	K ionophore
Methyl Deoxycholate	35	102	36	lipid
Simvastatin	69	64	44	lipid
Picropodophyllotoxin	105	87	91	microtubule
4'-Demethylepipodophyllotoxin	92	85	77	microtubule
Albendazole	89	75	67	microtubule
Podophyllotoxin Acetate	100	74	74	microtubule
Podofilox	99	70	70	microtubule
Vinblastine Sulfate	94	69	65	microtubule
Paclitaxel	102	68	69	microtubule
Vincristine Sulfate	97	66	64	microtubule

Compound	%Inhib	% Viability (Viab*inhib)	Grouping/Target	
		/100		
Beta-Peltatin	97	65	63	microtubule
Colchicine	96	64	62	microtubule
Dihydroclastryl Diacetate	97	63	61	microtubule
Colchicine	99	63	62	microtubule
Apigenin	31	84	26	monoamine transporter activator
Sanguinarine Sulfate	99	50	49	Na/K ATPase inhib
Gitoxigenin Diacetate	97	40	39	Na/K ATPase inhib
Peruvoside	101	40	40	Na/K ATPase inhib
Gitoxin	101	39	39	Na/K ATPase inhib
Convallatoxin	107	39	41	Na/K ATPase inhib
Strophanthidin	100	37	37	Na/K ATPase inhib
Digoxigenin	100	37	37	Na/K ATPase inhib
Lanatoside C	87	36	31	Na/K ATPase inhib
Ouabain	92	33	30	Na/K ATPase inhib
6-Aminonicotinamide	40	84	34	NAD
Ciclopirox Olamine	67	57	38	NaK ATPase
Trichlormethine	83	70	58	nitrogen mustard
Oxyphenbutazone	33	76	25	NSAID
Celecoxib	99	62	61	NSAID
5-Fluoro-5'-Deoxyuridine	33	101	34	nucleoside
Thioguanine	58	84	49	nucleoside
5-Azacytidine	94	77	73	nucleoside
Edoxudine	51	70	36	nucleoside
Floxuridine	91	63	58	nucleoside
Ancitabine Hydrochloride	92	61	57	nucleoside
Cytarabine	87	61	53	nucleoside
Phenylmercuric Acetate	72	52	37	organomercuric
Orlistat	35	115	40	protease
Meclocyline Sulfosalicylate	57	80	46	protein synthesis
Puromycin Hydrochloride	54	77	42	protein synthesis
Cycloheximide	98	73	72	protein synthesis
Anisomycin	100	59	58	protein synthesis
Emetine	93	66	61	protozoa
Lefunamide	42	72	30	pyrimidine synthesis inhib
Rotenone	90	71	63	rotenoid
Deguelin(-)	52	71	36	rotenoid
Isorotenone	67	67	45	rotenoid
Dihydrorotenone	84	59	49	rotenoid
Sappanone A Dimethyl Ether	91	60	54	sappanone
Deoxysappanone B 7,3'-Dimethyl Ether	94	56	53	sappanone
Acetate				
Deoxysappanone B 7,4'-Dimethyl Ether	91	55	50	sappanone
3,4-Dimethoxydalbergione	100	52	52	sappanone
Sertaline Hydrochloride	54	96	52	serotonin
Clomipramine Hydrochloride	31	78	24	serotonin
Prednisolone Hemisuccinate	49	88	43	steroid
Prednisolone Hemisuccinate	96	68	65	steroid
Cetrimonium Bromide	76	93	70	surfactant
Benzalkonium Chloride	34	91	31	surfactant
Noxynol-9	52	80	41	surfactant
Minocycline Hydrochloride	48	80	38	tetracycline antibiotic
Camptothecin	108	74	80	topoisomerase
Mitoxanthrone Hydrochloride	109	73	80	topoisomerase
Teniposide	104	56	58	topoisomerase
Bleomycin	74	55	41	topoisomerase
Etoposide	97	50	49	topoisomerase
Patulin	101	52	52	toxin

Compound	%Inhib	% Viability (Viab*inhib)	Grouping/Target	
		/100		
Dactinomycin	101	58	58	transcription
Niclosamide	76	63	47	worms
Tomatine	39	91	36	
4,4'-Dimethoxydalbergione	37	87	32	
Methylbenzethonium Chloride	48	85	40	
Mundulone	58	82	47	
7-Oxocallitric Acid, Methyl Ester	63	75	48	
Rubescensin A	39	72	28	
P-Fluorophenylalanine	55	72	39	
2,6-Dimethoxyquinone	45	71	32	
Obtusaquinone	73	70	51	
1-	103	68	69	
Benzyloxycarbonylamino phenethyl Chloromethyl Ketone				
2,3-Dichloro-5,8-Dihydroxynapthoquinone	89	66	59	
7-Desacetoxy-6,7-Dehydrogedunin	67	58	39	
Aklavine Hydrochloride	72	53	38	
Piplartine	83	51	42	
Crinamine	64	48	31	

Supplementary Table 2: Follow up Titrations

Compound	CF IC50 (µM)	CC IC50 (µM)	Cell Free LC50 (µM)	Cell Cell LC50 (µM)	Cell Free TI (µM)	Cell Cell TI (µM)	CC/CF IC50	Celltiter TI	TZM TI	Mechanism of Action	Therapeutic Uses	Published anti-HIV activity
Colchicine	0.01	0.01	>100	>100	>10663	>8920	1.2	0.5		Inhibits microtubule polymerization	NA	Yes
Celecoxib	0.1	0.1	>100	>100	>836	>986	0.8	3.3	1.5	(NSAID) and selective COX-2 inhibitor	Arthritis, Pain Relief	Yes
Rotenone	0.1	0.1	>100	>100	>836	>986	0.8	0.0		Interferes with the electron transport chain in mitochondria	NA	
Celastrol	0.3	0.3	>100	>100	>398	>291	1.4	0.8		Antioxidant, anti-inflammatory, anticancer, and insecticidal activities	NA	Yes (Tat)
Obtusaquinone	1.7	1.9	>100	>100	>57	>53	1.1	NA		Fungicide	NA	
Phenethyl Caffate (Cape)	1.7	4.4	>100	>100	>57	>22	2.6	0.8		Antioxidant, immunomodulatory, anti-inflammatory	NA	Yes
5-Azacytidine	1.2	4.7	>100	>100	>84	>21	4.0	0.5		Inhibits DNA methylation and protein synthesis	NA	Yes (Ribonucleoside)
Artemimol	0.8	5.1	0.8	>100	1.0	>19	6.8	1.0		Believed to alter parasite Glucose metabolism in erythrocytes	Malaria	
Mundulone	4.8	11.1	>100	>100	21.0	9.0	2.3	1.5		Inhibitors of human tyrosyl-DNA phosphodiesterase 1	NA	
Cloxyquin	12.5	11.3	>100	>100	>8	>8.8	0.9	0.4		Activates Potassium Channel TRESK	NA	
Minocycline Hydrochloride	8.7	13.7	>100	>100	>11.4	>7.3	1.6	3.6		Binds to bacterial 30S ribosome	broad-spectrum tetracycline antibiotic	Yes
1Benzyloxycarbonylamino phenethyl Chloromethyl Ketone	0.6	0.5	0.6	1.9	1.0	3.8	0.9	0.9			NA	
Pararosaniline Pamoate	0.4	0.4	32.4	1.6	88.1	3.7	1.2	NA		Structurally related crystal violet	Anti-Schistosome	
3,4-Dimethoxydalbergione	2.9	1.4	2.9	2.3	1.0	1.7	0.5	0.8			NA	
Valinomycin	0.1	0.1	0.4	0.2	5.7	1.6	1.6	1.2		Potassium transporter	Antibiotic	
Sertaline Hydrochloride	15.9	8.0	28.2	12.2	1.8	1.5	0.5	NA		Inhibitor of the selective serotonin reuptake inhibitor (SSRI) class I	Anti-depressant (Zoloft)	
Sanguinarine Sulfate	2.3	1.5	7.3	2.2	3.2	1.4	0.7	NA		Toxin that affects Na ⁺ -K ⁺ -ATPase transmembrane protein	NA	Yes (Protease)
Nisoldipine	9.7	7.1	>100	8.5	>10.3	1.2	0.7	6.6	1.5	Nisoldipine (INN) is a calcium channel blocker of the dihydropyridine class	High Blood Pressure (Sular)	
Gambogic Acid Amide	0.8	0.6	1.3	0.7	1.6	1.2	0.7	1.4		Caspase activator and apoptosis inducer, causes G2/M arrest	NA	
2,3-Dichloro-5,8-Dihydroxynaphthoquinone	0.8	0.4	0.7	0.4	0.9	1.1	0.5	0.6			NA	
Patulin	1.1	0.8	1.0	0.8	1.0	1.1	0.7	0.7		Mycotoxin produced by a variety of molds, high affinity for sulfhydryl groups	NA	
Picropodophyllotoxin	0.2	0.2	0.7	0.2	3.4	1.0	1.0	0.1		IGF1R and microtubule inhibitor	NA	
7-Oxocallitric Acid	>100	>100	>100	>100	>1	>1	1.0	NA			NA	
Chlorpromazine	5.9	5.8	40.9	5.8	6.9	1.0	1.0	0.9		Dopamine antagonist, also anti-adrenergic, anti-serotonergic, anti-cholinergic, anti-histaminic	antipsychotic	Yes
Piplartine	3.3	2.8	2.0	2.6	0.6	0.9	0.9	0.2		Induces caspase-mediated apoptosis in PC-3 human prostate cancer cells	NA	
Oxibendazole	0.9	1.0	>100	0.7	107.1	0.7	1.0	0.6			anti parasitic in domesticated animals	
Niclosamide	2.8	2.9	1.4	2.0	0.5	0.7	1.0	0.7		Uncouples oxidative phosphorylation in the tapeworm	teniacide	
Gentian Violet	0.2	0.3	9.6	0.2	47.2	0.6	1.6	1.8	0.9	Crystal violet has antibacterial, antifungal, and anthelmintic	Topical antiseptic	
Monensin	0.1	0.2	0.1	0.1	1.3	0.6	2.2	8.3	<0.1	Ionophore for ions such as Li ⁺ , Na ⁺ , K ⁺ , Rb ⁺ , Ag ⁺ , and Tl ⁺	Anti-parasitic in livestock	Yes (glycosylation)
Fexofenadine Hydrochloride	1.7	1.5	1.3	0.7	0.8	0.4	0.9	1.0		H1-blocker of the GI tract, large blood vessels, and bronchial smooth muscle.	Allergies (Zyrtec)	
Lasalocid Sodium	2.2	2.2	0.9	0.9	0.4	0.4	1.0	5.1	3.1	Cation Transport through membrane.	Antibacterial animal food additive (Bovatec)	
Digoxigenin	1.5	1.8	>100	0.7	>66	0.4	1.2	0.5		Highly antigenic, used in immuno tagging	NA	
Dequalinium	0.5	3.2	0.3	0.7	0.6	0.2	5.9			Dequalinium is a quaternary ammonium cation	Topical bacteriostat	
Mitoxantrone Hydrochloride	0.1	0.2	>100	0.0	>1676	0.2	2.6	0.5	1.1	Type II topoisomerase inhibitor	NA	
Nigericin Sodium	0.1	0.2	0.1	0.0	0.7	0.1	1.7	9.6	72.2	H ⁺ , K ⁺ , Pb ²⁺ ionophore. It inhibits Golgi functions.	Antibiotic active against gram positive bacteria	Yes
Simvastatin	5.9	3.4	NA	NA	NA	NA	0.6	6.5	20.9	Statin that inhibits HMG-CoA Reductase	hypercholesterolemia	
Emetine	1.4	0.4	NA	NA	NA	NA	0.3	0.4		Inhibitor of protein synthesis.	Induce Vomiting, anti protozoal	Yes (RNA processing)