

Prediction of Anti-Hiv Activity of Flavanoid Constituents Through PASS

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ABSTRACT

Prediction of Activity Spectra for Substances (PASS), a new computer program, has been generated to evaluate the biological activity of four major flavanoids from a medicinal herb, *Boesenbergia pandurata* Holtt. (Zingiberaceae). Principal anti-HIV and other biological activities of pinostrobin, pinocembrin, cardamonin and alpinetin were predicted through PASS, their similarity and difference in the mechanisms of action with reference to accessory biological activities have been compared (Tables 1-4) and verified with the available data (<http://195.178.207.233/PASS/socket1.php>.) on pharmacological and toxicological activity of these compounds.

KEY WORDS: Anti-HIV Drugs, Flavanoids, *Boesenbergia pandurata*, Pinostrobin, Pinocembrin, Cardamonin, Alpinetin.

INTRODUCTION

Acquired immunodeficiency syndrome (AIDS) has evolved rapidly into an epidemic and world-wide health crisis. The number of people infected with HIV rose to just over 40 million in 2006, an increase of over 2 million since 2004 (WHO/UNAIDS (2006)). More than 60% of infected people live in sub-Saharan Africa, where at least 2 million deaths from HIV/AIDS occurred in 2006. Novel therapeutic strategies are urgently needed for deployment alongside conventional antiretroviral drugs, vaccines, and microbicides to prevent the spread of the disease.

Many attempts have been carried out to discover compounds as anti-HIV-1 agents and enzyme inhibitors of the HIV-1. However, the effective agents for treatment of this disease are still in demand since HIV-1 is resistant to some synthetic anti-HIV-1 PR inhibitors (Borman *et al.*, 1996). HIV-1 PR hydrolyzes viral polyproteins into functional enzymes and structural proteins that are essential for viral assembly (Kohl *et al.*, 1988). Therefore, HIV-1 PR is considered to be an important target for development of anti-HIV-1 drugs.

A number of plants have exhibited a potent anti-HIV-1 effect and their valid utilization for the formulation of such drugs have been reported during recent past and several active plant based secondary metabolites have been recognized. Most of them are able to act specifically on enzymatic targets. Different parts of twelve Thai medicinal plants - *Zingiber zerumbet* (rhizome), *Boesenbergia pandurata* (rhizome), *Piper chaba* (fruit), *Eclipta prostrata* (whole plant), *Barleria lupulina* (leaf, stem), *Acanthus ilicifolius* (leaf and stem), *Alpinia galangal* (rhizome), *Piper betel* (leaf), *Spilanthes acmella* (whole plant), and *Coccinia grandis* (leaf) have been reported to have a potent HIV-1 PR inhibitory activities (Tewtrakul *et al.*, 2003). Moreover, Tewtrakul *et al.*, (2003) reported that four major flavonoids (pinostrobin, pinocembrin, cardamonin and alpinetin) isolated from the ethanol extract of *Boesenbergia pandurata* (yellow rhizome) to show inhibitory activity against HIV-1 protease (HIV-PR).

Recently, Computer Aided Drug Design (CADD) is widely used in new drug R & D (Franke and Herrmann, 1994). Such a newly developed computerized system - PASS (Prediction of Activity Spectra for Substance) that estimates simultaneously the probability of more than 100 pharmacological activity, effects and mechanisms (Filimonov *et al.*, 1995, Filimonov and Poroikov (1996). Therefore, the present study was designed towards the Prediction of Activity Spectra for four flavonoid constituents viz; pinostrobin, pinocembrin, cardamonin and alpinetin. A specific server has been generated which predicts the possibility of a drug to be active against a target based on the physico-chemical methods using comparisons and several algorithms. It is observed that the approach, used in PASS, may be applied to other biological activities (Filimonov *et al.*, 1995; Filimonov *et al.*, 1996).

MATERIALS AND METHODS

PASS 4.20 prediction search includes 9314 biologically active substances. PASS 4.20 predicts the probabilities of presence/absence for 114 biological actions simultaneously (main and side pharmacological effects, mechanisms, specific toxicity). The biological activity spectrum of PASS was designed and prediction was made with the comparison from the source data available in <http://195.178.207.233/PASS/predict.php>. Biological activity spectrum of a compound presents exhibit its activity despite the difference in essential conditions of its experimental determination.

RESULTS AND DISCUSSION

Four flavonoids constituents like pinostrobin, pinocembrin, cardamonin and alpinetin were predicted. PASS predicted search results shows that the available information on the pharmacological and toxicological activity of these compounds and are corroborative with the previous reports (Tewtrakul *et al.*, 2003). The results showed that pinocembrin could possess several biological activities including anti-HIV(throughtheserver) <http://195.178.207.233/PASS/socket1.php>, (Table-1). More interestingly, this compound showed antineoplastic, antiseborrheic, and activity against membrane permeability inhibitor. Next active constituent of the plant extract i.e., alpinetine was predicted with such a similar multitude activity through the same server - <http://195.178.207.233/PASS/socket1.php> (Table.2). Pinostrobin was predicted with numerous biological activities principally with anti-HIV (Table.3) and other accessory activities like membrane integrity agonist, phosphatase inhibitor, free radical scavenger, apoptosis agonist, cell adhesion inhibitor, testosterone 17beta-dehydrogenase inhibitor and antineurotoxic activity (<http://195.178.207.233/PASS/socket1.php>). The extended PASS prediction strategy was revealed with an interesting data yield regarding the biological activities of cardamonin like antiseborrheic and arminative, etc., (Table.4) other than the anti-HIV effects (<http://195.178.207.233/PASS/socket1.php>). After having a biological activity prediction, a comparative analysis was made regarding the individual mechanism of action of these four active flavanoids of this plant extract. Controversially, four active flavanoids have shown much variability despite their similarity in their inhibitory activities (Tables 1-4). This difference may be due to the diversity among the target sites and the reciprocal activity of the specific drug towards such diversified targets and their differential physiological conditions too.

CONCLUSION

All the four flavanoids observed to have a multi potentials as hepatoprotectant, antipruritic, allergic, anti inflammatory, neuroprotector other than their principal anti-HIV activity.

While planning experiments and choosing the activities on which the compound has to be tested, it is necessary to keep in mind the balance between the novelty of pharmacological action and the risk to obtain negative result in experimental testing. Certainly, in this present study, such a vital approach has been made to take into account the particular interest in some kinds of activities other than the principal anti- HIV activity of the four flavanoids from this plant extract. The accuracy of biological activity prediction through PASS with reference to four flavanoid constituents is about 90%. Moreover, a thorough study regarding the legend, mode of action of the drugs with reference to the specific targets, their differential physiological conditions need to be mooted up to arrive with a final design of life saving drugs of this kind.

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Table-1: Biological Activity Spectrum Of Anti HIV constituent - Pinocebrin

28 Substructure descriptors; 0 new. 9

Possible	activities	at Pa > 70% Pa Pi for Activity:
0,901	0,005	Antineoplastic (brain cancer)
0,900	0,013	Antiseborrheic
0,764	0,007	Membrane permeability inhibitor
0,754	0,009	2,6-Dihydropyridine 3-monooxygenase inhibitor
0,802	0,061	Membrane integrity agonist
0,751	0,021	Pulmonary hypertension treatment
0,736	0,007	Nerve growth factor agonist
0,716	0,010	Neurotrophic factor enhancer
0,736	0,035	Cardiovascular analeptic

EFFECTS

0,802	0,007	Antiviral
0,802	0,007	Antiviral (HIV)
0,802	0,061	Membrane integrity agonist
0,764	0,007	Membrane permeability inhibitor
0,802	0,061	Membrane integrity agonist
0,764	0,007	Antitoxic
0,764	0,007	Hepatoprotectant
0,764	0,007	Membrane permeability inhibitor
0,802	0,007	Antipruritic
0,764	0,007	Antipruritic, allergic
0,764	0,007	Membrane permeability inhibitor
0,802	0,061	Membrane integrity agonist
0,802	0,007	Antiinflammatory
0,802	0,061	Membrane integrity agonist
0,764	0,007	Membrane permeability inhibitor
0,764	0,007	Neuroprotector
0,764	0,007	Membrane permeability inhibitor

0,736	0,007	Nerve growth factor agonist
0,736	0,007	Antiparkinsonian
0,736	0,007	Nerve growth factor agonist
0,736	0,035	Analeptic
0,736	0,035	Cardiovascular analeptic
0,736	0,007	Cognition disorders treatment
0,736	0,007	Alzheimer's disease treatment
0,736	0,007	Nerve growth factor agonist
0,716	0,010	Neurotrophic factor enhancer
0,736	0,007	Nerve growth factor agonist
0,716	0,010	Neurotrophic factor enhancer
0,900	0,013	Dermatologic
0,802	0,061	Antieczematic
0,802	0,061	Membrane integrity agonist
0,900	0,013	Antiseborrheic
0,802	0,061	Membrane integrity agonist
0,764	0,007	Hemostatic
0,764	0,007	Membrane permeability inhibitor
0,802	0,007	Psychotropic
0,736	0,007	Nootropic
0,736	0,007	Nerve growth factor agonist
0,802	0,061	Antiepileptic
0,802	0,061	Membrane integrity agonist
0,764	0,007	Vasoprotector
0,764	0,007	Membrane permeability inhibitor
0,736	0,007	Antiischemic, cerebral
0,736	0,007	Nerve growth factor agonist
0,736	0,007	Amyotrophic lateral sclerosis treatment
0,736	0,007	Nerve growth factor agonist

0,764	0,007	Septic shock treatment
0,764	0,007	Membrane permeability inhibitor
0,901	0,005	Antineoplastic (brain cancer)
0,751	0,021	Pulmonary hypertension treatment
MECHANISMS		
0,764	0,007	Membrane permeability inhibitor
0,754	0,009	2,6-Dihydropyridine 3-monooxygenase inhibitor
0,802	0,061	Membrane integrity agonist
0,900	0,013	Antiseborrheic
0,736	0,007	Nerve growth factor agonist
0,716	0,010	Neurotrophic factor enhancer
0,736	0,035	Cardiovascular analeptic

Table-2: Biological Activity Spectrum Of Anti HIV constituent - Alpinetine		
22 Substructure descriptors; 0 new. 19 Possible activities at Pa > 70% Pa Pifor Activity:		
0,935	0,007	Membrane integrity agonist
0,858	0,024	Mucomembranous protector
0,821	0,011	Antineurotoxic
0,811	0,004	NAD(P)H dehydrogenase (quinone) inhibitor
0,802	0,004	Capillary fragility treatment
0,799	0,013	Membrane integrity antagonist
0,761	0,005	Cytochrome P450 inhibitor
0,761	0,006	Free radical scavenger
0,762	0,011	Apoptosis agonist
0,747	0,003	Testosterone 17beta-dehydrogenase inhibitor
0,745	0,006	Cell adhesion inhibitor
0,736	0,001	Leucoanthocyanidin reductase inhibitor
0,742	0,007	CYP2A11 substrate
0,732	0,003	Naringenin-chalcone synthase inhibitor

0,745	0,016	Pectate lyase inhibitor
0,712	0,007	Scytalone dehydratase inhibitor
0,704	0,004	Iodide peroxidase inhibitor
0,761	0,061	Phosphatase inhibitor
0,702	0,015	Carbonyl reductase (NADPH) inhibitor

EFFECTS

0,935	0,007	Antiviral
0,935	0,007	Antiviral (HIV)
0,935	0,007	Membrane integrity agonist
0,935	0,007	Membrane integrity agonist
0,799	0,013	Membrane integrity antagonist
0,799	0,013	Antiprotozoal
0,799	0,013	Membrane integrity antagonist
0,821	0,006	Antitoxic
0,821	0,011	Antineurotoxic
0,761	0,006	Hepatoprotectant
0,761	0,006	Free radical scavenger
0,935	0,005	Antipruritic
0,761	0,006	Antieczematic atopic
0,761	0,006	Free radical scavenger
0,761	0,005	Antipruritic, allergic
0,761	0,006	Free radical scavenger
0,761	0,005	Cytochrome P450 inhibitor
0,935	0,007	Membrane integrity agonist
0,761	0,061	Antidiabetic
0,761	0,061	Phosphatase inhibitor
0,935	0,006	Antiinflammatory
0,935	0,007	Membrane integrity agonist
0,761	0,006	Free radical scavenger

0,799	0,013	Antineoplastic
0,799	0,013	Membrane integrity antagonist
0,761	0,061	Phosphatase inhibitor
0,761	0,006	Neuroprotector
0,761	0,006	Free radical scavenger
0,799	0,013	Anesthetic
0,799	0,013	Membrane integrity antagonist
0,799	0,013	Antifungal
0,799	0,013	Membrane integrity antagonist
0,935	0,006	Antiischemic
0,761	0,006	Antiischemic, cerebral
0,761	0,006	Free radical scavenger
0,935	0,007	Antiischemic renal
0,935	0,007	Membrane integrity agonist
0,761	0,006	Free radical scavenger
0,935	0,006	Dermatologic
0,761	0,006	Antipsoriatic
0,761	0,006	Free radical scavenger
0,935	0,006	Antieczematic
0,935	0,007	Membrane integrity agonist
0,761	0,006	Free radical scavenger
0,935	0,007	Antiseborrheic
0,935	0,007	Membrane integrity agonist
0,935	0,006	Psychotropic
0,761	0,006	Nootropic
0,761	0,006	Alzheimer's disease treatment
0,761	0,006	Free radical scavenger
0,761	0,006	Free radical scavenger

0,935	0,007	Antiepileptic
0,935	0,007	Membrane integrity agonist
0,799	0,013	Antibiotic
0,799	0,013	Membrane integrity antagonist
0,799	0,013	Antiarrhythmic
0,799	0,013	Membrane integrity antagonist
0,761	0,005	Prostate cancer treatment
0,761	0,005	Cytochrome P450 inhibitor
0,858	0,024	Antiulcerative
0,858	0,024	Mucomembranous protector
0,799	0,013	Contraceptive female
0,799	0,013	Membrane integrity antagonist
0,762	0,011	Apoptosis agonist
0,745	0,006	Cell adhesion inhibitor
0,802	0,004	Capillary fragility treatment
MECHANISMS		
0,935	0,007	Membrane integrity agonist
0,858	0,024	Mucomembranous protector
0,811	0,004	NAD(P)H dehydrogenase (quinone) inhibitor
0,799	0,013	Membrane integrity antagonist
0,761	0,005	Cytochrome P450 inhibitor
0,761	0,006	Free radical scavenger
0,747	0,003	Testosterone 17beta-dehydrogenase inhibitor
0,745	0,006	Cell adhesion inhibitor
0,736	0,001	Leucoanthocyanidin reductase inhibitor
0,742	0,007	CYP2A11 substrate
0,732	0,003	Naringenin-chalcone synthase inhibitor
0,745	0,016	Pectate lyase inhibitor
0,712	0,007	Scytalone dehydratase inhibitor

0,704	0,004	Iodide peroxidase inhibitor
0,761	0,061	Phosphatase inhibitor
0,702	0,015	Carbonyl reductase (NADPH) inhibitor

Table-3: Biological Activity Spectrum Of Anti HIV constituent - Pinostrobin

32 Substructure descriptors; 0 new. 237 Possible activities at Pa > 30% Pa Pi for Activity:

0,939	0,007	Membrane integrity agonist
0,857	0,020	Phosphatase inhibitor
0,793	0,005	Free radical scavenger
0,770	0,010	Apoptosis agonist
0,752	0,006	Cell adhesion inhibitor
0,745	0,003	Testosterone 17beta-dehydrogenase inhibitor
0,758	0,020	Antineurotoxic
0,771	0,048	Mucomembranous protector
0,727	0,006	Cytochrome P450 inhibitor
0,717	0,004	Naringenin-chalcone synthase inhibitor
0,732	0,019	Pectate lyase inhibitor
0,725	0,023	Membrane integrity antagonist
0,710	0,007	Naringenin 3-dioxygenase inhibitor
0,703	0,006	Antioxidant
0,698	0,016	L-ascorbate oxidase inhibitor
0,685	0,004	Iodide peroxidase inhibitor
0,685	0,005	Capillary fragility treatment
0,693	0,014	Membrane permeability inhibitor
0,683	0,006	NAD(P)H dehydrogenase (quinone) inhibitor

0,670	0,001	Leucoanthocyanidin reductase inhibitor
0,656	0,014	P-benzoquinone reductase (NADPH) inhibitor
0,640	0,005	Creatine kinase inhibitor
0,653	0,026	Carbonyl reductase (NADPH) inhibitor
0,694	0,083	Myocardial ischemia treatment
0,613	0,005	Chemopreventive
0,610	0,006	Phenylalanine ammonia-lyase inhibitor
0,614	0,012	CYP1A substrate
0,630	0,033	Neurotrophic factor enhancer
0,583	0,011	Caffeate O-methyltransferase inhibitor
0,589	0,029	Emetic
0,620	0,064	Nerve growth factor agonist
0,570	0,018	Aryl-alcohol dehydrogenase (NADP+) inhibitor
0,612	0,069	NAD(P)+-arginine ADP-ribosyltransferase inhibitor
0,546	0,004	Antihemorrhagic
0,575	0,040	1-Alkylglycerophosphocholine O-acetyltransferase inhibitor
0,591	0,072	Fibrinolytic
0,537	0,023	CYP2A11 substrate
0,663	0,153	Antiseborrheic
0,556	0,046	CYP2A3 substrate
0,562	0,060	Antidyskinetic
0,523	0,021	Beta-carotene 15,15'-monooxygenase inhibitor
0,522	0,022	Antiviral (Herpes)
0,535	0,036	Histamine release stimulant
0,532	0,034	CDK2/cyclin A inhibitor
0,536	0,041	Antiinflammatory
0,509	0,015	Lipid peroxidase inhibitor
0,533	0,042	NADPH-ferrihemoprotein reductase inhibitor
0,504	0,015	CYP1A1 substrate

0,529	0,046	Cytochrome P450 CYP2C9 inhibitor
0,497	0,023	5 Lipoxygenase inhibitor
0,508	0,035	Dihydroxy-acid dehydratase inhibitor
0,474	0,002	Cytochrome P450 CYP3A4 inhibitor
0,482	0,010	Glutathione-disulfide reductase inhibitor
0,558	0,096	Oxidoreductase inhibitor
0,503	0,040	Kinase inhibitor
0,485	0,025	Hepatoprotectant
0,495	0,038	Carminative
0,507	0,058	Antineoplastic
0,543	0,094	Hydroxylamine reductase (NADH) inhibitor
0,468	0,030	CYP1A2 substrate
0,466	0,031	Hemostatic
0,465	0,033	Scytalone dehydratase inhibitor
0,444	0,013	Osteoarthritis treatment
0,508	0,082	Trans-cinnamate 4-monooxygenase inhibitor
0,469	0,044	Nephrotoxic
0,448	0,023	Reductant
0,464	0,043	CYP2C11 substrate
0,488	0,068	Nitrite reductase [NAD(P)H] inhibitor
0,498	0,080	Steroid N-acetylglucosaminyltransferase inhibitor
0,592	0,178	Cardioprotectant
0,430	0,023	Sweetener
0,434	0,031	Hepatic disorders treatment
0,446	0,049	Polarisation stimulant
0,495	0,100	CYP3A2 substrate
0,399	0,007	Histidine decarboxylase inhibitor
0,425	0,034	Xenobiotic-transporting ATPase inhibitor

0,449	0,059	Histamine release inhibitor
0,394	0,005	CYP1B substrate
0,401	0,013	Epoxide hydrolase inhibitor
0,482	0,096	Trans-pentaprenyltranstransferase inhibitor
0,416	0,031	Plastoquinol-plastocyanin reductase inhibitor
0,517	0,138	CYP3A1 substrate
0,410	0,036	Protein-tyrosine kinase (PTK, not ETK, WZC) inhibitor
0,395	0,029	Antidiabetic symptomatic
0,370	0,005	CYP1B1 substrate
0,423	0,058	Vitamin-K-epoxide reductase (warfarin-insensitive) inhibitor
0,379	0,017	Dihydrobenzophenanthridine oxidase inhibitor
0,412	0,051	Analeptic
0,409	0,049	Trypanothione-disulfide reductase inhibitor
0,369	0,013	Quercetin 2,3-dioxygenase inhibitor
0,440	0,084	CYP2B5 substrate
0,437	0,082	Bilirubin oxidase inhibitor
0,361	0,010	Expectorant
0,379	0,029	Flavone apiosyltransferase inhibitor
0,446	0,095	Toxic
0,375	0,028	2-Enoate reductase inhibitor
0,476	0,129	Cardiovascular analeptic
0,378	0,031	Narcotic
0,373	0,028	Myc inhibitor
0,517	0,172	Ecdysone 20-monooxygenase inhibitor
0,438	0,097	Gonadotropin antagonist
0,356	0,016	(S)-canadine synthase inhibitor
0,389	0,051	Cytostatic
0,365	0,027	Imidazoline I1 receptor agonist
0,387	0,050	L-lysine 6-transaminase inhibitor

0,436	0,099	Membrane permeability enhancer
0,377	0,042	Antidote
0,382	0,050	CYP2C6 substrate
0,381	0,050	DNA ligase (ATP) inhibitor
0,380	0,053	Asparagine-tRNA ligase inhibitor
0,442	0,115	Indole-3-acetaldehyde oxidase inhibitor
0,401	0,074	Cholestanetriol 26-monooxygenase inhibitor
0,382	0,060	Antifungal
0,432	0,111	4-Methoxybenzoate monooxygenase (O-demethylating) inhibitor
0,376	0,060	Antiulcerative
0,419	0,107	Antipruritic
0,400	0,088	Psychosexual dysfunction treatment
0,426	0,114	CYP2A2 substrate
0,318	0,009	Mucolytic
0,333	0,025	Salutaridinol 7-O-acetyltransferase inhibitor
0,439	0,132	Leukotriene C antagonist
0,406	0,100	2,6-Dihydroxypyridine 3-monooxygenase inhibitor
0,371	0,067	Phenol 2-monooxygenase inhibitor
0,402	0,098	CYP2B11 substrate
0,412	0,109	Immunosuppressant
0,371	0,071	CYP2A5 substrate
0,331	0,030	Indoleamine-pyrrole 2,3-dioxygenase inhibitor
0,375	0,075	CYP2F1 substrate
0,374	0,074	Inositol 4-methyltransferase inhibitor
0,398	0,099	Nitrate reductase inhibitor
0,371	0,073	Thiamine-triphosphatase inhibitor
0,313	0,014	Tubulin antagonist
0,312	0,015	Glycerol dehydrogenase (NADP+) inhibitor

0,440	0,147	Adenylate cyclase stimulant
0,302	0,013	2-Dehydropantolactone reductase (A-specific) inhibitor
0,326	0,038	Deoxyribonuclease I inhibitor
0,314	0,026	CYP2A10 substrate
0,430	0,144	Proteasome endopeptidase complex inhibitor
0,322	0,035	3-Demethylubiquinone-9 3-O-methyltransferase inhibitor
0,352	0,066	Respiratory analeptic
0,389	0,104	Antipsoriatic
0,399	0,113	Hypothermic
0,368	0,089	Carcinogenic, male rats
0,327	0,049	RNA synthesis inhibitor
0,301	0,026	Lipoxygenase inhibitor
0,495	0,223	Hematotoxic
0,332	0,069	Interferon antagonist
0,321	0,060	Contraceptive
0,319	0,058	Bronchodilator
0,308	0,048	Imidazoline receptor agonist
0,315	0,056	Trans-1,2-dihydrobenzene-1,2-diol dehydrogenase inhibitor
0,315	0,058	Contraceptive female
0,331	0,074	Phloroglucinol reductase inhibitor
0,387	0,131	L-glucuronate reductase inhibitor
0,326	0,071	Fumarate reductase (NADH) inhibitor
0,380	0,127	Alcohol oxidase inhibitor
0,330	0,083	Antineoplastic (multiple myeloma)
0,394	0,147	Thromboxane B2 antagonist
0,352	0,106	CYP3A4 substrate
0,304	0,061	Tetrahydroxynaphthalene reductase inhibitor
0,390	0,147	Antialcoholic
0,388	0,149	Antitoxic

0,306	0,067	Biphenyl-2,3-diol 1,2-dioxygenase inhibitor
0,304	0,069	Antiosteoporotic
0,398	0,163	Neurotrophic factor
0,350	0,117	Miotic
0,426	0,194	Peroxidase inhibitor
0,390	0,158	Antipruritic, allergic
0,375	0,145	Teratogen
0,319	0,091	Anorexiant
0,382	0,155	Glucan 1,4-beta-glucosidase inhibitor
0,395	0,171	Cyclooxygenase 1 inhibitor
0,303	0,079	AMP deaminase inhibitor
0,359	0,137	Prostaglandin antagonist
0,361	0,140	Chemoprotective
0,312	0,094	Hypertensive
0,326	0,108	CYP3A substrate
0,340	0,122	Gentisate 1,2-dioxygenase inhibitor
0,410	0,195	Tumour necrosis factor alpha antagonist
0,394	0,179	Cathepsin G inhibitor
0,384	0,172	Lactaldehyde reductase inhibitor
0,392	0,181	Quinoprotein glucose dehydrogenase inhibitor
0,366	0,158	Interferon agonist
0,319	0,118	Anthranilate 3-monooxygenase (deaminating) inhibitor
0,349	0,150	Dermatologic
0,342	0,145	Pulmonary hypertension treatment
0,377	0,182	Magnesium-protoporphyrin IX monomethyl ester (oxidative) cyclase inhibitor
0,341	0,152	H ⁺ -transporting two-sector ATPase inhibitor
0,399	0,213	CYP2D16 substrate
0,355	0,171	Pyruvate decarboxylase inhibitor

0,361	0,179	Antihelmintic (Nematodes)
0,391	0,218	CYP2A1 substrate
0,310	0,142	Antileukemic
0,306	0,139	Monoamine uptake inhibitor
0,386	0,221	Lipid metabolism regulator
0,366	0,203	Penicillin amidase inhibitor
0,321	0,162	Octopamine antagonist
0,337	0,178	Antineoplastic (solid tumors)
0,316	0,161	Glutaminase inhibitor
0,329	0,177	Glycerol-3-phosphate dehydrogenase inhibitor
0,351	0,202	Antineoplastic (brain cancer)
0,313	0,166	CYP2C8 substrate
0,327	0,180	Atherosclerosis treatment
0,326	0,183	L-idoitol 2-dehydrogenase inhibitor
0,314	0,175	Microtubule formation stimulant
0,311	0,177	CYP2B6 substrate
0,308	0,212	Myosin ATPase inhibitor
0,333	0,243	ATPase inhibitor
0,311	0,222	Antiinflammatory, ophthalmic
0,360	0,277	Uroporphyrinogen-III synthase inhibitor
0,323	0,243	Dependence treatment
0,302	0,225	Ovulation inhibitor
0,319	0,245	Platelet adhesion inhibitor
0,337	0,264	Vasodilator, cerebral
0,340	0,268	Leukotriene C4 antagonist
0,311	0,240	CC chemokine 2 receptor antagonist
0,301	0,230	Laccase inhibitor
0,306	0,236	Vomilenine glucosyltransferase inhibitor

0,362	0,296	Antihypoxic
0,349	0,287	Cystic fibrosis treatment
0,321	0,263	Membrane dipeptidase inhibitor
0,316	0,259	Lysase inhibitor
0,329	0,289	2-Oxoglutarate decarboxylase inhibitor
0,335	0,301	Glyceryl-ether monooxygenase inhibitor
0,343	0,311	NADPH oxidase inhibitor
0,350	0,324	Cardiotoxic
0,324	0,301	3-Hydroxybenzoate 4-monooxygenase inhibitor
0,322	0,299	Monodehydroascorbate reductase (NADH) inhibitor
0,335	0,316	Insulysin inhibitor
0,321	0,304	Integrin antagonist
0,301	0,291	Gingipain K inhibitor
0,302	0,300	[acyl-carrier-protein] S-acetyltransferase inhibitor
0,327	0,328	General pump inhibitor
0,305	0,312	2,3-Dihydroxybenzoate 2,3-dioxygenase inhibitor
0,303	0,319	Convulsant
0,309	0,328	N-carbamoyl-L-amino-acid hydrolase inhibitor
0,313	0,332	Chitinase inhibitor

EFFECTS

0,939	0,007	Antiviral
0,522	0,022	Antiviral (Herpes)
0,367	0,158	Antiviral (Hepatitis)
0,367	0,158	Interferon agonist
0,939	0,007	Antiviral (HIV)
0,939	0,007	Membrane integrity agonist
0,701	0,014	Membrane permeability inhibitor
0,939	0,007	Membrane integrity agonist

0,727	0,023	Membrane integrity antagonist
0,438	0,099	Membrane permeability enhancer
0,367	0,158	Interferon agonist
0,332	0,049	RNA synthesis inhibitor
0,727	0,023	Antiprotozoal
0,727	0,023	Membrane integrity antagonist
0,438	0,099	Membrane permeability enhancer
0,564	0,010	Antitussive
0,564	0,010	Expectorant
0,727	0,023	Antibacterial
0,727	0,023	Antibiotic
0,727	0,023	Membrane integrity antagonist
0,438	0,099	Membrane permeability enhancer
0,438	0,099	Antimycobacterial
0,438	0,099	Membrane permeability enhancer
0,438	0,099	Membrane permeability enhancer
0,797	0,005	Antitoxic
0,758	0,020	Antineurotoxic
0,797	0,005	Hepatoprotectant
0,485	0,025	Liver fibrosis treatment
0,797	0,005	Hepatoprotectant
0,797	0,005	Free radical scavenger
0,701	0,014	Membrane permeability inhibitor
0,939	0,005	Antipruritic
0,684	0,026	Allergic conjunctivitis treatment
0,684	0,026	Lipoxygenase inhibitor
0,939	0,005	Antipruritic
0,646	0,107	Antiacne
0,939	0,005	Antipruritic

0,797	0,005	Antieczematic atopic
0,797	0,005	Free radical scavenger
0,939	0,005	Antipruritic
0,507	0,109	Immunosuppressant
0,797	0,005	Antipruritic, allergic
0,797	0,005	Free radical scavenger
0,728	0,006	Cytochrome P450 inhibitor
0,701	0,014	Membrane permeability inhibitor
0,523	0,023	5 Lipoxygenase inhibitor
0,507	0,109	Immunosuppressant
0,400	0,007	Histidine decarboxylase inhibitor
0,646	0,107	Antipruritic, non-allergic
0,939	0,005	Antipruritic
0,939	0,007	Membrane integrity agonist
0,386	0,221	Hypolipemic
0,386	0,221	Lipid metabolism regulator
0,857	0,020	Antidiabetic
0,395	0,029	Antidiabetic symptomatic
0,857	0,020	Phosphatase inhibitor
0,727	0,023	Cardiotonic
0,727	0,023	Antiarrhythmic
0,727	0,023	Membrane integrity antagonist
0,440	0,027	Heart failure treatment
0,440	0,147	Adenylate cyclase stimulant
0,365	0,027	Imidazoline I1 receptor agonist
0,440	0,147	Adenylate cyclase stimulant
0,939	0,005	Antiinflammatory
0,311	0,222	Antiinflammatory, ophthalmic

0,939	0,007	Membrane integrity agonist
0,797	0,005	Free radical scavenger
0,701	0,014	Membrane permeability inhibitor
0,684	0,026	Lipoxygenase inhibitor
0,523	0,023	5 Lipoxygenase inhibitor
0,507	0,109	Immunosuppressant
0,410	0,195	Tumour necrosis factor alpha antagonist
0,394	0,179	Cathepsin G inhibitor
0,363	0,137	Prostaglandin antagonist
0,321	0,304	Integrin antagonist
0,523	0,023	Autoimmune disorders treatment
0,523	0,023	Rheumatoid arthritis treatment
0,523	0,023	5 Lipoxygenase inhibitor
0,410	0,195	Tumour necrosis factor alpha antagonist
0,507	0,109	Systemic lupus erythematosus treatment
0,507	0,109	Immunosuppressant
0,507	0,109	Multiple sclerosis treatment
0,507	0,109	Immunosuppressant
0,367	0,158	Interferon agonist
0,327	0,328	Radioprotector
0,327	0,328	General pump inhibitor
0,857	0,014	Antineoplastic
0,315	0,014	Antileukemic
0,315	0,014	Tubulin antagonist
0,351	0,202	Antineoplastic (brain cancer)
0,315	0,014	Antineoplastic (breast cancer)
0,315	0,014	Tubulin antagonist
0,315	0,014	Antineoplastic (colorectal cancer)
0,315	0,014	Tubulin antagonist

0,315	0,014	Antineoplastic (lung cancer)
0,315	0,014	Tubulin antagonist
0,330	0,083	Antineoplastic (multiple myeloma)
0,337	0,178	Antineoplastic (solid tumors)
0,857	0,020	Phosphatase inhibitor
0,727	0,023	Membrane integrity antagonist
0,503	0,040	Kinase inhibitor
0,373	0,028	Myc inhibitor
0,367	0,158	Interferon agonist
0,332	0,049	RNA synthesis inhibitor
0,321	0,304	Integrin antagonist
0,315	0,014	Tubulin antagonist
0,314	0,175	Microtubule formation stimulant
0,797	0,005	Neuroprotector
0,797	0,005	Free radical scavenger
0,701	0,014	Membrane permmeability inhibitor
0,620	0,064	Nerve growth factor agonist
0,575	0,015	Lipid peroxidase inhibitor
0,438	0,099	Membrane permeability enhancer
0,440	0,099	Ophthalmic drug
0,440	0,099	Antiglaucomic
0,440	0,147	Adenylate cyclase stimulant
0,438	0,099	Membrane permeability enhancer
0,727	0,023	Anesthetic
0,727	0,023	Membrane integrity antagonist
0,620	0,040	Antiparkinsonian
0,620	0,064	Nerve growth factor agonist
0,503	0,040	Kinase inhibitor

0,438	0,099	Prostate disorders treatment
0,438	0,099	Membrane permeability enhancer
0,495	0,044	Toxic
0,350	0,324	Cardiotoxic
0,495	0,223	Hematotoxic
0,469	0,044	Nephrotoxic
0,449	0,059	Analgesic
0,449	0,059	Analgesic, non-opioid
0,449	0,059	Histamine release inhibitor
0,394	0,147	Thromboxane B2 antagonist
0,363	0,137	Prostaglandin antagonist
0,365	0,027	Antihypertensive
0,365	0,027	Imidazoline I1 receptor agonist
0,438	0,099	Antiparasitic
0,438	0,099	Membrane permeability enhancer
0,476	0,051	Analeptic
0,476	0,129	Cardiovascular analeptic
0,352	0,066	Respiratory analeptic
0,449	0,007	Antiallergic
0,449	0,059	Antiallergic rhinitis
0,449	0,059	Histamine release inhibitor
0,449	0,059	Histamine release inhibitor
0,439	0,132	Leukotriene C antagonist
0,400	0,007	Histidine decarboxylase inhibitor
0,727	0,023	Antifungal
0,727	0,023	Membrane integrity antagonist
0,503	0,040	Kinase inhibitor
0,438	0,099	Membrane permeability enhancer
0,367	0,158	Antiinfective

0,367	0,158	Interferon agonist
0,939	0,005	Antiischemic
0,797	0,005	Antiischemic, cerebral
0,797	0,005	Free radical scavenger
0,620	0,064	Nerve growth factor agonist
0,575	0,015	Lipid peroxidase inhibitor
0,438	0,099	Membrane permeability enhancer
0,337	0,264	Vasodilator, cerebral
0,939	0,007	Antiischemic renal
0,939	0,007	Membrane integrity agonist
0,694	0,083	Myocardial ischemia treatment
0,440	0,147	Adenylate cyclase stimulant
0,797	0,005	Free radical scavenger
0,311	0,240	Antineurogenic pain
0,311	0,240	CC chemokine 2 receptor antagonist
0,797	0,005	Antioxidant
0,703	0,006	Acute neurologic disorders treatment
0,797	0,005	Antioxidant
0,575	0,015	Lipid peroxidase inhibitor
0,797	0,005	Alzheimer's disease treatment
0,797	0,005	Free radical scavenger
0,797	0,005	Antioxidant
0,630	0,033	Neurotrophic factor enhancer
0,620	0,064	Nerve growth factor agonist
0,398	0,163	Neurotrophic factor
0,395	0,171	Cyclooxygenase 1 inhibitor
0,703	0,006	Amyotrophic lateral sclerosis treatment
0,797	0,005	Antioxidant

0,620	0,064	Nerve growth factor agonist
0,398	0,163	Neurotrophic factor
0,575	0,015	Lipid peroxidase inhibitor
0,368	0,089	Carcinogenic
0,368	0,089	Carcinogenic, male rats
0,630	0,033	Cognition disorders treatment
0,630	0,033	Neurotrophic factor enhancer
0,620	0,064	Nerve growth factor agonist
0,398	0,163	Neurotrophic factor
0,939	0,005	Dermatologic
0,797	0,005	Antipsoriatic
0,797	0,005	Free radical scavenger
0,523	0,023	5 Lipoxygenase inhibitor
0,939	0,005	Antieczematic
0,939	0,007	Membrane integrity agonist
0,797	0,005	Free radical scavenger
0,507	0,109	Immunosuppressant
0,939	0,007	Antiseborrheic
0,939	0,007	Membrane integrity agonist
0,701	0,014	Hemostatic
0,466	0,031	Antihemophilic
0,701	0,014	Hemostatic
0,701	0,014	Membrane permeability inhibitor
0,939	0,005	Psychotropic
0,797	0,005	Nootropic
0,797	0,005	Free radical scavenger
0,640	0,005	Creatine kinase inhibitor
0,620	0,064	Nerve growth factor agonist
0,438	0,099	Membrane permeability enhancer

0,939	0,007	Antiepileptic
0,939	0,007	Membrane integrity agonist
0,701	0,014	Vasoprotector
0,701	0,014	Membrane permeability inhibitor
0,684	0,023	Antiasthmatic
0,684	0,026	Lipoxygenase inhibitor
0,523	0,023	5 Lipoxygenase inhibitor
0,449	0,059	Histamine release inhibitor
0,439	0,132	Leukotriene C antagonist
0,410	0,195	Tumour necrosis factor alpha antagonist
0,340	0,268	Leukotriene C4 antagonist
0,321	0,304	Integrin antagonist
0,684	0,023	Antiarthritic
0,684	0,026	Lipoxygenase inhibitor
0,523	0,023	5 Lipoxygenase inhibitor
0,507	0,109	Immunosuppressant
0,311	0,240	CC chemokine 2 receptor antagonist
0,728	0,006	Prostate cancer treatment
0,728	0,006	Cytochrome P450 inhibitor
0,523	0,023	Inflammatory Bowel disease treatment
0,523	0,023	5 Lipoxygenase inhibitor
0,507	0,109	Immunosuppressant
0,367	0,158	Interferon agonist
0,321	0,304	Integrin antagonist
0,438	0,099	Antiemetic
0,438	0,099	Membrane permeability enhancer
0,333	0,069	Antiosteoporotic
0,333	0,243	ATPase inhibitor

0,321	0,304	Integrin antagonist
0,684	0,026	Antithrombotic
0,684	0,026	Lipoxygenase inhibitor
0,440	0,147	Adenylate cyclase stimulant
0,394	0,147	Thromboxane B2 antagonist
0,321	0,304	Integrin antagonist
0,319	0,245	Platelet adhesion inhibitor
0,771	0,048	Antiulcerative
0,771	0,048	Mucomembranous protector
0,333	0,243	ATPase inhibitor
0,727	0,023	Contraceptive female
0,727	0,023	Membrane integrity antagonist
0,438	0,099	Cystic fibrosis treatment
0,438	0,099	Membrane permeability enhancer
0,438	0,099	Prostatic (benign) hyperplasia treatment
0,438	0,099	Membrane permeability enhancer
0,373	0,028	Restenosis treatment
0,373	0,028	Myc inhibitor
0,701	0,014	Septic shock treatment
0,701	0,014	Membrane permeability inhibitor
0,363	0,137	Vasodilator, peripheral
0,363	0,137	Prostaglandin antagonist
0,770	0,010	Apoptosis agonist
0,752	0,006	Cell adhesion inhibitor
0,613	0,005	Chemopreventive
0,444	0,013	Osteoarthritis treatment
0,448	0,023	Reductant
0,592	0,178	Cardioprotectant
0,430	0,023	Sweetener

0,434	0,031	Hepatic disorders treatment
0,389	0,051	Cytostatic
0,377	0,042	Antidote
0,400	0,088	Psychosexual dysfunction treatment
0,399	0,113	Hypothermic
0,321	0,060	Contraceptive
0,375	0,145	Teratogen
0,319	0,091	Anorexiant
0,361	0,140	Chemoprotective
0,312	0,094	Hypertensive
0,327	0,180	Atherosclerosis treatment
0,362	0,296	Antihypoxic
0,685	0,005	Capillary fragility treatment
0,546	0,004	Antihemorrhagic
0,591	0,072	Fibrinolytic
0,562	0,060	Antidyskinetic
0,318	0,009	Mucolytic
0,319	0,058	Bronchodilator
0,390	0,147	Antialcoholic
0,350	0,117	Miotic
0,342	0,145	Pulmonary hypertension treatment
0,361	0,179	Anthelmintic (Nematodes)
0,323	0,243	Dependence treatment
0,302	0,225	Ovulation inhibitor
MECHANISMS		
0,939	0,007	Membrane integrity agonist
0,939	0,007	Antiseborrheic
0,939	0,005	Antiinflammatory
0,939	0,005	Antipruritic

0,857	0,020	Phosphatase inhibitor
0,857	0,014	Antineoplastic
0,797	0,005	Free radical scavenger
0,939	0,005	Antiinflammatory
0,797	0,005	Hepatoprotectant
0,797	0,005	Antipruritic, allergic
0,797	0,005	Antipsoriatic
0,752	0,006	Cell adhesion inhibitor
0,745	0,003	Testosterone 17beta-dehydrogenase inhibitor
0,771	0,048	Mucomembranous protector
0,728	0,006	Cytochrome P450 inhibitor
0,474	0,002	Cytochrome P450 CYP3A4 inhibitor
0,529	0,046	Cytochrome P450 CYP2C9 inhibitor
0,797	0,005	Antipruritic, allergic
0,717	0,004	Naringenin-chalcone synthase inhibitor
0,732	0,019	Pectate lyase inhibitor
0,727	0,023	Membrane integrity antagonist
0,857	0,014	Antineoplastic
0,727	0,023	Antifungal
0,727	0,023	Contraceptive female
0,710	0,007	Naringenin 3-dioxygenase inhibitor
0,797	0,005	Antioxidant
0,698	0,016	L-ascorbate oxidase inhibitor
0,685	0,004	Iodide peroxidase inhibitor
0,701	0,014	Membrane permeability inhibitor
0,939	0,005	Antiinflammatory
0,797	0,005	Hepatoprotectant
0,701	0,014	Hemostatic

0,797	0,005	Antipruritic, allergic
0,683	0,006	NAD(P)H dehydrogenase (quinone) inhibitor
0,670	0,001	Leucoanthocyanidin reductase inhibitor
0,656	0,014	P-benzoquinone reductase (NADPH) inhibitor
0,640	0,005	Creatine kinase inhibitor
0,653	0,026	Carbonyl reductase (NADPH) inhibitor
0,610	0,006	Phenylalanine ammonia-lyase inhibitor
0,614	0,012	CYP1A substrate
0,504	0,015	CYP1A1 substrate
0,468	0,030	CYP1A2 substrate
0,630	0,033	Neurotrophic factor enhancer
0,583	0,011	Caffeate O-methyltransferase inhibitor
0,620	0,064	Nerve growth factor agonist
0,570	0,018	Aryl-alcohol dehydrogenase (NADP+) inhibitor
0,612	0,069	NAD(P)+-arginine ADP-ribosyltransferase inhibitor
0,575	0,040	1-Alkylglycerophosphocholine O-acetyltransferase inhibitor
0,537	0,023	CYP2A11 substrate
0,556	0,046	CYP2A3 substrate
0,523	0,021	Beta-carotene 15,15'-monooxygenase inhibitor
0,535	0,036	Histamine release stimulant
0,532	0,034	CDK2/cyclin A inhibitor
0,575	0,015	Lipid peroxidase inhibitor
0,797	0,005	Antioxidant
0,533	0,042	NADPH-ferrihemoprotein reductase inhibitor
0,508	0,035	Dihydroxy-acid dehydratase inhibitor
0,482	0,010	Glutathione-disulfide reductase inhibitor
0,558	0,096	Oxidoreductase inhibitor
0,503	0,040	Kinase inhibitor
0,857	0,014	Antineoplastic

0,727	0,023	Antifungal
0,543	0,094	Hydroxylamine reductase (NADH) inhibitor
0,701	0,014	Hemostatic
0,465	0,033	Scytalone dehydratase inhibitor
0,508	0,082	Trans-cinnamate 4-monooxygenase inhibitor
0,464	0,043	CYP2C11 substrate
0,488	0,068	Nitrite reductase [NAD(P)H] inhibitor
0,498	0,080	Steroid N-acetylglucosaminyltransferase inhibitor
0,446	0,049	Polarisation stimulant
0,400	0,007	Histidine decarboxylase inhibitor
0,797	0,005	Antipruritic, allergic
0,425	0,034	Xenobiotic-transporting ATPase inhibitor
0,449	0,059	Histamine release inhibitor
0,394	0,005	CYP1B substrate
0,370	0,005	CYP1B1 substrate
0,482	0,096	Trans-pentaprenyltranstransferase inhibitor
0,416	0,031	Plastoquinol-plastocyanin reductase inhibitor
0,410	0,036	Protein-tyrosine kinase (PTK, not ETK, WZC) inhibitor
0,423	0,058	Vitamin-K-epoxide reductase (warfarin-insensitive) inhibitor
0,379	0,017	Dihydrobenzophenanthridine oxidase inhibitor
0,409	0,049	Trypanothione-disulfide reductase inhibitor
0,369	0,013	Quercetin 2,3-dioxygenase inhibitor
0,440	0,084	CYP2B5 substrate
0,564	0,010	Expectorant
0,318	0,009	Mucolytic
0,379	0,029	Flavone apiosyltransferase inhibitor
0,375	0,028	2-Enoate reductase inhibitor
0,476	0,129	Cardiovascular analeptic

0,373	0,028	Myc inhibitor
0,857	0,014	Antineoplastic
0,517	0,172	Ecdysone 20-monooxygenase inhibitor
0,438	0,097	Gonadotropin antagonist
0,356	0,016	(S)-canadine synthase inhibitor
0,387	0,050	L-lysine 6-transaminase inhibitor
0,438	0,099	Membrane permeability enhancer
0,727	0,023	Antifungal
0,438	0,099	Cystic fibrosis treatment
0,382	0,050	CYP2C6 substrate
0,381	0,050	DNA ligase (ATP) inhibitor
0,380	0,053	Asparagine-tRNA ligase inhibitor
0,442	0,115	Indole-3-acetaldehyde oxidase inhibitor
0,401	0,074	Cholestanetriol 26-monooxygenase inhibitor
0,432	0,111	4-Methoxybenzoate monooxygenase (O-demethylating) inhibitor
0,939	0,005	Antipruritic
0,797	0,005	Antipruritic, allergic
0,426	0,114	CYP2A2 substrate
0,333	0,025	Salutaridinol 7-O-acetyltransferase inhibitor
0,439	0,132	Leukotriene C antagonist
0,340	0,268	Leukotriene C4 antagonist
0,406	0,100	2,6-Dihydropyridine 3-monooxygenase inhibitor
0,371	0,067	Phenol 2-monooxygenase inhibitor
0,402	0,098	CYP2B11 substrate
0,507	0,109	Immunosuppressant
0,939	0,005	Antiinflammatory
0,797	0,005	Antipruritic, allergic
0,371	0,071	CYP2A5 substrate
0,331	0,030	Indoleamine-pyrrole 2,3-dioxygenase inhibitor

0,375	0,075	CYP2F1 substrate
0,374	0,074	Inositol 4-methyltransferase inhibitor
0,398	0,099	Nitrate reductase inhibitor
0,371	0,073	Thiamine-triphosphatase inhibitor
0,315	0,014	Tubulin antagonist
0,857	0,014	Antineoplastic
0,315	0,014	Antileukemic
0,312	0,015	Glycerol dehydrogenase (NADP+) inhibitor
0,440	0,147	Adenylate cyclase stimulant
0,694	0,083	Myocardial ischemia treatment
0,302	0,013	2-Dehydropantolactone reductase (A-specific) inhibitor
0,326	0,038	Deoxyribonuclease I inhibitor
0,314	0,026	CYP2A10 substrate
0,430	0,144	Proteasome endopeptidase complex inhibitor
0,322	0,035	3-Demethylubiquinone-9 3-O-methyltransferase inhibitor
0,332	0,049	RNA synthesis inhibitor
0,857	0,014	Antineoplastic
0,684	0,026	6 Lipoxygenase inhibitor
0,523	0,023	5 Lipoxygenase inhibitor
0,939	0,005	Antiinflammatory
0,797	0,005	Antipruritic, allergic
0,797	0,005	Antipsoriatic
0,939	0,005	Antiinflammatory
0,332	0,069	Interferon antagonist
0,561	0,048	Imidazoline receptor agonist
0,365	0,027	Imidazoline I1 receptor agonist
0,315	0,056	Trans-1,2-dihydrobenzene-1,2-diol dehydrogenase inhibitor
0,331	0,074	Phloroglucinol reductase inhibitor

0,387	0,131	L-glucuronate reductase inhibitor
0,326	0,071	Fumarate reductase (NADH) inhibitor
0,380	0,127	Alcohol oxidase inhibitor
0,394	0,147	Thromboxane B2 antagonist
0,304	0,061	Tetrahydroxynaphthalene reductase inhibitor
0,306	0,067	Biphenyl-2,3-diol 1,2-dioxygenase inhibitor
0,398	0,163	Neurotrophic factor
0,426	0,194	Peroxidase inhibitor
0,382	0,155	Glucan 1,4-beta-glucosidase inhibitor
0,395	0,171	Cyclooxygenase 1 inhibitor
0,303	0,079	AMP deaminase inhibitor
0,363	0,137	Prostaglandin antagonist
0,939	0,005	Antiinflammatory
0,361	0,140	Chemoprotective
0,326	0,108	CYP3A substrate
0,517	0,138	CYP3A1 substrate
0,495	0,100	CYP3A2 substrate
0,352	0,106	CYP3A4 substrate
0,340	0,122	Gentisate 1,2-dioxygenase inhibitor
0,410	0,195	Tumour necrosis factor alpha antagonist
0,939	0,005	Antiinflammatory
0,394	0,179	Cathepsin G inhibitor
0,384	0,172	Lactaldehyde reductase inhibitor
0,392	0,181	Quinoprotein glucose dehydrogenase inhibitor
0,367	0,158	Interferon agonist
0,857	0,014	Antineoplastic
0,319	0,118	Anthranilate 3-monooxygenase (deaminating) inhibitor
0,377	0,182	Magnesium-protoporphyrin IX monomethyl ester (oxidative) cyclase inhibitor

0,341	0,152	H ⁺ -transporting two-sector ATPase inhibitor
0,399	0,213	CYP2D16 substrate
0,355	0,171	Pyruvate decarboxylase inhibitor
0,391	0,218	CYP2A1 substrate
0,306	0,139	Monoamine uptake inhibitor
0,386	0,221	Lipid metabolism regulator
0,366	0,203	Penicillin amidase inhibitor
0,321	0,162	Octopamine antagonist
0,316	0,161	Glutaminase inhibitor
0,329	0,177	Glycerol-3-phosphate dehydrogenase inhibitor
0,313	0,166	CYP2C8 substrate
0,326	0,183	L-iditol 2-dehydrogenase inhibitor
0,314	0,175	Microtubule formation stimulant
0,311	0,177	CYP2B6 substrate
0,308	0,212	Myosin ATPase inhibitor
0,333	0,243	ATPase inhibitor
0,771	0,048	Antiulcerative
0,333	0,069	Antiosteoporotic
0,360	0,277	Uroporphyrinogen-III synthase inhibitor
0,319	0,245	Platelet adhesion inhibitor
0,337	0,264	Vasodilator, cerebral
0,311	0,240	CC chemokine 2 receptor antagonist
0,301	0,230	Laccase inhibitor
0,306	0,236	Vomilenine glucosyltransferase inhibitor
0,321	0,263	Membrane dipeptidase inhibitor
0,329	0,289	2-Oxoglutarate decarboxylase inhibitor
0,335	0,301	Glyceryl-ether monooxygenase inhibitor
0,343	0,311	NADPH oxidase inhibitor
0,324	0,301	3-Hydroxybenzoate 4-monooxygenase inhibitor

0,322	0,299	Monodehydroascorbate reductase (NADH) inhibitor
0,335	0,316	Insulysin inhibitor
0,321	0,304	Integrin antagonist
0,939	0,005	Antiinflammatory
0,857	0,014	Antineoplastic
0,333	0,069	Antiosteoporotic
0,301	0,291	Gingipain K inhibitor
0,302	0,300	[acyl-carrier-protein] S-acetyltransferase inhibitor
0,327	0,328	General pump inhibitor
0,305	0,312	2,3-Dihydroxybenzoate 2,3-dioxygenase inhibitor
0,309	0,328	N-carbamoyl-L-amino-acid hydrolase inhibitor
0,313	0,332	Chitinase inhibitor

Table-4:Biological Activity Spectrum Of Anti HIV constituent - Cardamonin		
28 Substructure descriptors; 0 new. 7 Possible activities at Pa > 70% Pa Pi for Activity:		
0,899	0,014	Mucomembranous protector
0,878	0,001	Sodium/bile acid cotransporter inhibitor
0,884	0,021	Membrane integrity agonist
0,769	0,008	2,6-Dihydropyridine 3-monooxygenase inhibitor
0,763	0,030	CC chemokine 2 receptor antagonist
0,789	0,083	Antiseborrheic
0,703	0,015	Carminative
EFFECTS		
0,884	0,021	Antiviral

0,884	0,021	Antiviral (HIV)
0,884	0,021	Membrane integrity agonist
0,884	0,021	Membrane integrity agonist
0,884	0,021	Antipruritic
0,884	0,021	Membrane integrity agonist
0,884	0,021	Antiinflammatory
0,884	0,021	Membrane integrity agonist
0,763	0,030	Antineurogenic pain
0,763	0,030	CC chemokine 2 receptor antagonist
0,878	0,001	Atherosclerosis treatment
0,878	0,001	Sodium/bile acid cotransporter inhibitor
0,884	0,021	Dermatologic
0,884	0,021	Antieczematic
0,884	0,021	Membrane integrity agonist
0,884	0,021	Antiseborrheic
0,884	0,021	Membrane integrity agonist
0,884	0,021	Psychotropic
0,884	0,021	Antiepileptic
0,884	0,021	Membrane integrity agonist
0,763	0,030	Antiarthritic
0,763	0,030	CC chemokine 2 receptor antagonist
0,878	0,001	Antihypercholesterolemic
0,878	0,001	Sodium/bile acid cotransporter inhibitor
0,000	0,000	Antiulcerative
0,899	0,014	Mucomembranous protector
MECHANISMS		
0,899	0,014	Mucomembranous protector
0,878	0,001	Sodium/bile acid cotransporter inhibitor
0,884	0,021	Membrane integrity agonist

0,884	0,021	Antiseborrheic
0,769	0,008	2,6-Dihydroxypyridine 3-monooxygenase inhibitor
0,763	0,030	CC chemokine 2 receptor antagonist