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## ***In Silico* Screening Major Spice Phytochemicals for their Novel Biological Activity and Pharmacological Fitness**

Riju A\*, Sithara K, Suja S. Nair, Shamina A and Santhosh J. Eapen

Bioinformatics Centre, Indian Institute of Spices Research, Calicut, Kerala 673 012

\*Corresponding author: Riju A, Bioinformatics Centre, Indian Institute of Spices Research, Calicut, Kerala 673 012, Tel: 04952731566; E-mail: [riju.aikkal@spices.res.in](mailto:riju.aikkal@spices.res.in)

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### **Abstract**

Spices have been known for ages as effective therapeutic food. The power of spices to impart biological activity is now slowly reemerging as an area of interest. We have screened 328 compounds present in five major spices namely, cinnamon (*Cinnamomum verum*), nutmeg (*Myristica fragrans*), garcinia (*Garcinia cambogia*), allspice (*Pimenta dioica*) and black pepper (*Piper nigrum* L.) for their biological activity as promising therapeutic compounds. Out of 328 compounds analyzed, ascorbic acid, nonaldehyde, delphinidin, malabaricone-B, malabaricone-C, isoquercitrin, quercitrin,  $\alpha$ -bisabolol, cis-nerolidol,  $\gamma$ -eudesmol, hexan-1-ol and n-octanal were reported as non-carcinogenic and non-mutagenic phytochemicals. Biological activity such as antiinflammatory, antioxidant, antiviral (HIV), antitoxic, free radical scavenging, cardioprotectant, hepatoprotectant, antitussive, antihemorrhagic etc. were reported for these compounds. Drug likeness of the compounds were checked with WDI rule and Lipinski's rule of 5. Since the drug research starts with identification of a 'lead molecule' with required biological activity, wide range of biological actions along with tox free findings may be efficiently used to develop lead candidate for human health benefits. The results of the study have been developed as a database. This can be accessed through [www.spices.res.in/passcom](http://www.spices.res.in/passcom).

**Keywords:** Phytochemicals; Biological activity; Drug likeness; *In silico* ADMET

### **Introduction**

A spice is a dried seed, fruit, root, bark or vegetative substance used in nutritionally insignificant quantities as a food additive for the purpose of flavoring, and sometimes as a preservative by killing or preventing the growth of harmful bacteria. Many of these substances are also used for other purposes, such as medicine, religious, rituals, cosmetics, perfumery or as vegetables. Spices in general are carminative. The indigenous system of medicine has given an extra special place to spices because of their unique medicinal properties. The power of spices to impart biological activity is now slowly reemerging as an area of interest.

The use of computational tools in the prediction of ADME/Tox properties of compounds is growing rapidly in drug discovery as the benefits they provide in high throughput and early application in drug design are real-

ized. Since 1960's, experience in medicinal chemistry has shown that the rigorous application of quantitative structure-activity relationship (QSAR) methods to homogeneous classes of chemicals inducing the same type of biological activity permits formulation of efficient quantitative models. These QSAR models contribute both to the elucidation of the action mechanisms and to the prediction of the biological activity of yet untested chemicals (Hansch, 1990). The use of QSAR methods has been exported from medicinal chemistry, where they presently constitute a basic building block in the design of new drugs, to the study of biological activities, including toxicity.

Numerous examples exist of drugs being withdrawn because of unacceptable toxicity in clinical trials and even after reaching the market-place. If these expensive fail-

ures can be identified and eliminated early in the drug discovery process, there is considerable scope for improving the efficiency and cost effectiveness of the industry. The maxim 'Fail early, fail fast, fail cheaply' is now firmly embedded in the minds of all drug discovery research managers. Since a typical drug takes 10–12 years, and costs up to US\$500 million, to reach the market, it is important to discover its potential toxicity at an early stage. With the advent of cheminformatics tools and accuracy in predicting the toxicity *in silico*, the cost has reduced dramatically.

## Materials and Methods

A total of 328 compounds present in five major spices cinnamon (*Cinnamomum verum*), nutmeg (*Myristica fragrans*), garcinia (*Garcinia cambogia*), allspice (*Pimenta dioica* L.) and black pepper (*Piper nigrum* L.) were screened for their biological activity for use as promising therapeutic compounds. The structure of these chemical compounds were obtained from PubChem (<http://pubchem.ncbi.nlm.nih.gov/>) and ChemSpider (<http://www.chemspider.com/>) and each chemical compound was drawn with chemical drawing tools such as ACD/ChemSketch and saved in the '.mol' file format. The biological activities of the compounds were predicted individually with the help of PASS (Predicted Activity Spectrum for Substances) server (<http://195.178.207.233/PASS/>). ADME/T (Absorption Distribution Metabolism Excretion and Toxicity) properties were analyzed through computational methods such as PreADMET server (<http://preadmet.bmdrc.org/>) and Discoverygate database browser (<https://www.discoverygate.com>). Drug likeness of the compounds was tested with WDI rule and Lipinski's rule of 5.

## Results and Discussion

Biological activity is one of the most important characteristics of a chemical compound reflecting its interaction with living organisms. Three hundred and twenty eight compounds present in five major spices selected for this study have been listed in Table 1. The biological activities of each compound were predicted individually with the help of PASS (Predicted Activity Spectrum for Substances) server (Filimonov and Poroikov, 1996). ADME/T (Absorption Distribution Metabolism Excretion and Toxicity) properties were analyzed through computational methods such as PreADMET server and Discoverygate database browser. The server predicted mutagenicity to *Salmonella strains* - TA98, TA100 and TA1535 which are often used in Ames test (Ames et al., 1972) and the results were calculated both with consideration of metabo-

lite (Metabolic activation by rat liver 10% homogenate, +S9) and without consideration of metabolite (no metabolic activation, -S9). The actual value of the prediction result is "positive" or "negative". The carcinogenicity was predicted based on the result from its model, which is built from the data of NTP (National Toxicology Program) and US FDA. Of the 328 compounds only 12 compounds were non-mutagenic and non-carcinogenic, all others showed toxicity either as mutagen or carcinogen. The 12 non-toxic compounds are ascorbic-acid, nonaldehyde, delphinidin, malabaricone-b, malabaricone-c, isoquercitrin, quercitrin,  $\alpha$ -bisabolol, cis-nerolidol,  $\gamma$ -eudesmol, hexan-1-ol and n-octanal. The healing activity of malabaricone B and malabaricone C, the major antioxidant constituents of the spice *Myristica malabarica* against the indomethacin-induced gastric ulceration in mice was reported earlier (Banerjee et al., 2008).  $\alpha$ -Bisabolol has antibacterial and antifungal activities, an indication of its defensive functions in plants (Mitova et al., 2003). It has promising activity against gram-negative and gram-positive bacteria.  $\alpha$ -Bisabolol has long been used in cosmetics for its anti-inflammatory, healing and soothing and anti-microbial properties.  $\alpha$ -Bisabolol is well suited for use in skin care preparations and can be useful in both sensitive skin and child/ baby products as a soothing agent. Delphinidin possesses antioxidant, anti-inflammatory, and antiangiogenic properties and is reported as a novel agent against human prostate cancer (PCa) (Hafeez et al., 2008).  $\alpha$ -Bisabolol, was found to have a strong time- and dose-dependent cytotoxic effect on human and rat glioma cells (Elisabetta et al., 2004). Quercetrin and isoquercitrin are effective eosinophilic inflammation suppressors, suggesting a potential for treating allergies (Rogerio et al., 2007). Apart from these we have identified compounds with biological activities such as antioxidant, antiviral (HIV), antitoxic, free radical scavenging, cardioprotectant, hepatoprotectant, antitussive, antihemorrhagic, immunostimulant etc. Important predicted activities of each compound is list in Table 2. Drug likeness of the compounds were checked by WDI rule and Lipinski's rule of 5. Since drug research starts with identification of a 'lead molecule' with required biological activity, a wide range of biological actions along with tox free findings may be efficiently used to develop lead candidates for human health benefits. The effects described herein, as well as those observed by others investigators, together with the broad spectrum of the biological effects of these substances, strongly suggest that the compounds mentioned above have various therapeutic implications. The results of the study have been made as a database. This can be accessed through [www.spices.res.in/passcom](http://www.spices.res.in/passcom).

Sl No	Generic name	Lipinski rule	Lead like rule	Ames test	Carcinogenicity (Mouse)	Carcinogenicity (Rat)
1	(-)-Epicatechin	Suitable	Suitable *	mutagen	negative	negative
2	(-)-Hydroxycitric acid	Suitable	Violated	mutagen	negative	positive
3	(+)-Alpha-phellandrene	Suitable	Violated	mutagen	positive	positive
4	(+)-Beta-pinene	Suitable	Suitable *	mutagen	negative	positive
5	(+)-Borneol	Suitable	Suitable *	mutagen	negative	positive
6	(+)-Limonene	Suitable	Violated	mutagen	negative	positive
7	(+)-Linalool	Suitable	Suitable *	mutagen	negative	negative
8	(E,E)-farnesol	Suitable	Suitable *	non- mutagen	positive	negative
9	(E)-beta-ocimene	Suitable	Violated	mutagen	positive	positive
10	(E)-cinnamaldehyde	Suitable	Suitable *	mutagen	negative	negative
11	(E)-cinnamyl-acetate	Suitable	Suitable *	mutagen	negative	positive
12	(E)-cinnamyl-alcohol	Suitable	Suitable *	mutagen	negative	negative
13	(E)-methyl-cinnamate	Suitable	Suitable *	mutagen	negative	negative
14	(E)-methyl-isoeugenol	Suitable	Suitable *	mutagen	positive	positive
15	(Z)-beta-ocimene	Suitable	Violated	mutagen	positive	positive
16	(Z)-cinnamaldehyde	Suitable	Suitable *	mutagen	negative	negative
17	(Z)-cinnamyl-acetate	Suitable	Suitable *	mutagen	negative	positive
18	(Z)-methyl-isoeugenol	Suitable	Suitable *	mutagen	positive	positive
19	(Z,e)-alpha-farnesene	Suitable	Violated	mutagen	positive	positive
20	1,8-cineole	Suitable	Suitable *	mutagen	positive	positive
21	1-terpinen-4-ol	Suitable	Suitable *	mutagen	positive	negative
22	2-methoxy-cinnamaldehyde	Suitable	Suitable *	mutagen	negative	positive
23	2-methyl butyricacid	Suitable	Suitable *	mutagen	positive	positive
24	2-methyl pentanoicacid(2-methylvalericacid)	Suitable	Violated	mutagen	negative	positive
25	2-methyl-butanol	Suitable	Violated	mutagen	positive	negative
26	2-methyl-butyl-acetate	Suitable	Suitable *	non-mutagen	positive	positive
27	2-phenylacetaldehyde	Suitable	Suitable *	mutagen	negative	negative
28	2-phenylethanol	Suitable	Suitable *	mutagen	positive	negative
29	2-phenylethyl-benzoate	Suitable	Violated	mutagen	negative	negative
30	2-phenylethyl-propionate	Suitable	Suitable *	mutagen	negative	negative
31	2-undecanone	Suitable	Violated	non-mutagen	positive	negative
32	2-vinylphenol	Suitable	Suitable *	mutagen	negative	negative
33	3-phenylpropanal	Suitable	Suitable *	mutagen	negative	negative
34	Acetic-acid	Suitable	Violated	non-mutagen	negative	positive
35	Acetone	Suitable	Violated	mutagen	negative	negative
36	Acetyl-eugenol	Suitable	Suitable *	mutagen	positive	positive
37	Allo-aromadendrene	Suitable	Violated	mutagen	negative	positive
38	Alpha-bergamotene	Suitable	Violated	non -mutagen	positive	positive
39	<b>Alpha-bisabolol</b>	<b>Suitable</b>	<b>Violated</b>	<b>non-mutagen</b>	<b>negative</b>	<b>negative</b>
40	Alpha-cadinene	Suitable	Violated	mutagen	positive	positive
41	Alpha-cis-bergamotene	Suitable	Violated	non-mutagen	positive	positive
42	Alpha-copaene	Suitable	Violated	non-mutagen	negative	positive
43	Alpha-cubebene	Suitable	Violated	non-mutagen	negative	positive
44	Alpha-farnesene	Suitable	Violated	mutagen	positive	positive
45	Alpha-guaiene	Suitable	Violated	mutagen	negative	positive
46	Alpha-gurjunene	Suitable	violated	non-mutagen	negative	positive
47	Alpha-humulene	Suitable	Violated	non-mutagen	positive	positive
48	Alpha-muurolene	Suitable	Violated	mutagen	positive	positive
49	Alpha-p-dimethyl-styrene	Suitable	Violated	mutagen	negative	negative
50	Alpha-phellandrene	Suitable	Violated	mutagen	positive	positive
51	Alpha-pinene	Suitable	Suitable *	mutagen	negative	positive

52	Alpha-santalene	Suitable	Violated	non-mutagen	negative	Positive
53	Alpha-selinene	Suitable	Violated	mutagen	negative	positive
54	Alpha-terpeneol	Suitable	Suitable *	mutagen	negative	negative
55	Alpha-terpenyl acetate	Suitable	Suitable *	mutagen	positive	negative
56	Alpha-terpinene	Suitable	Violated	mutagen	positive	positive
57	Alpha-terpineol	Suitable	Suitable *	mutagen	negative	negative
58	Alpha-thujene	Suitable	Suitable *	mutagen	negative	positive
59	Alpha-trans-bergamotene	Suitable	Violated	non-mutagen	positive	positive
60	Alpha-ylangene	Suitable	Violated	non- mutagen	negative	positive
61	Anisole	Suitable	Suitable *	mutagen	positive	negative
62	Ar-curcumene	Suitable	Violated	mutagen	positive	positive
63	Aromadendrene	Suitable	Violated	mutagen	negative	positive
64	Ascorbic-acid	Suitable	Violated	non- mutagen	negative	negative
65	Benzaldehyde	Suitable	Suitable *	mutagen	negative	negative
66	Benzoic acid	Suitable	Violated	mutagen	negative	negative
67	Benzyl-acetate	Suitable	Suitable *	mutagen	negative	negative
68	Benzyl-alcohol	Suitable	Suitable *	mutagen	negative	negative
69	Benzyl-benzoate	Suitable	Violated	mutagen	positive	negative
70	Beta-bisabolene	Suitable	Violated	mutagen	negative	positive
71	Beta-bisabolol	Suitable	Violated	non-mutagen	positive	negative
72	Beta-carotene	Violated	Violated	non- mutagen	positive	positive
73	Beta-caryophyllene	Suitable	Suitable *	mutagen	negative	positive
74	Beta-caryophyllene alcohol	Suitable	Violated	mutagen	negative	positive
75	Beta-caryophyllene-oxide	Suitable	Violated	mutagen	positive	positive
76	Beta-copaene	Suitable	Violated	mutagen	negative	positive
77	Beta-cubebene	Suitable	Violated	mutagen	negative	positive
78	Beta-elemene	Suitable	Violated	mutagen	negative	positive
79	Beta-farnesene	Suitable	Violated	non-mutagen	positive	positive
80	Beta-humulene	Suitable	Violated	mutagen	positive	positive
81	Beta-phellandrene	Suitable	Violated	mutagen	negative	positive
82	Beta-pinene	Suitable	Suitable *	mutagen	negative	positive
83	Beta-selinene	Suitable	Violated	mutagen	negative	positive
84	Beta-sitosterol	Suitable	Violated	non- mutagen	positive	negative
85	Beta-terpineol	Suitable	Violated	mutagen	negative	negative
86	Borneol	Suitable	Suitable *	mutagen	negative	positive
87	Borneol-acetate	Suitable	Suitable *	mutagen	negative	positive
88	Bulnesol	Suitable	Violated	mutagen	negative	negative
89	Butyric acid	Suitable	Violated	mutagen	negative	negative
90	Caffeic-acid	Suitable	Violated	mutagen	negative	positive
91	Calamenene	Suitable	Violated	mutagen	positive	negative
92	Calcium-oxalate	Failed	Failed	mutagen	out of range	out of range
93	Campesterol	Suitable	Violated	non- mutagen	positive	negative
94	Camphene	Suitable	Suitable *	mutagen	negative	positive
95	Camphor	Suitable	Suitable *	mutagen	negative	positive
96	Caprylic-acid	Suitable	Suitable *	mutagen	negative	positive
97	Car-3-ene	Suitable	Suitable *	mutagen	negative	positive

98	Carvacrol	Suitable	Violated	mutagen	negative	Negative
99	Carvone	Suitable	Suitable *	mutagen	negative	positive
100	Caryophyllene	Suitable	Violated	mutagen	negative	positive
101	Caryophyllene oxide	Suitable	Violated	mutagen	positive	positive
102	Caryophyllene-alcohol	Suitable	violated	mutagen	negative	positive
103	Cerotic-acid	Suitable	Violated	non -mutagen	negative	positive
104	Cerotinic-acid	Suitable	Violated	non -mutagen	negative	positive
105	Chavicol	Suitable	Suitable *	mutagen	positive	negative
106	Cineole	Suitable	Suitable *	mutagen	positive	positive
107	Cinnamaldehyde	Suitable	Suitable *	mutagen	negative	negative
108	Cinnamic acid	Suitable	Violated	mutagen	negative	negative
109	Cinnamic-acid-ethyl-ester	Suitable	Suitable *	mutagen	negative	negative
110	Cinnamic-acid-methyl-ester	Suitable	Suitable *	mutagen	negative	negative
111	Cinnamic-alcohol	Suitable	Suitable *	mutagen	negative	negative
112	Cinnamyl-acetate	Suitable	Suitable *	mutagen	negative	negative
113	Cinnamyl-alcohol	Suitable	Suitable *	mutagen	negative	negative
114	Cis-beta-ocimene	Suitable	Violated	mutagen	positive	positive
115	Cis-carveol	Suitable	Suitable *	mutagen	positive	negative
116	Cis-cinnamaldehyde	Suitable	Suitable *	mutagen	negative	negative
117	Cis-isoelemicin	Suitable	Suitable *	mutagen	positive	positive
118	Cis-linalol-oxide	Suitable	Suitable *	mutagen	positive	positive
119	Cis-nerolidol	Suitable	Violated	non-mutagen	negative	negative
120	Cis-ocimene	Suitable	Violated	mutagen	positive	positive
121	Cis-p-2-menthen-1-ol	Suitable	Suitable *	mutagen	negative	negative
122	Cis-piperitol	suitable	Suitable *	mutagen	positive	negative
123	Cis-sabinene hydrate	Suitable	Suitable *	mutagen	negative	positive
124	Citirc acid	Suitable	Violated	mutagen	negative	positive
125	Citronellal	Suitable	Suitable *	mutagen	positive	negative
126	Citronellol	Suitable	Violated	non-mutagen	positive	negative
127	Citronellol-acetate	Suitable	Violated	non -mutagen	positive	positive
128	Coniferaldehyde	Suitable	Suitable *	mutagen	negative	positive
129	Copaene	Suitable	Violated	non-mutagen	negative	positive
130	Coumarin	Suitable	Suitable *	mutagen	positive	positive
131	Cryptone	Suitable	Suitable *	mutagen	negative	negative
132	Cubebol	Suitable	Suitable *	non-mutagen	positive	positive
133	Cumene	Suitable	Violated	mutagen	positive	negative
134	Cuminaldehyde	Suitable	Suitable *	mutagen	negative	negative
135	Cyanidin	Failed	Failed	mutagen	negative	negative
136	Cyclosativene	Suitable	Violated	mutagen	negative	positive
137	Cymene	Suitable	Violated	mutagen	positive	negative
138	D-alpha-pinene	Suitable	Suitable *	mutagen	negative	positive
139	D-borneol	Suitable	Suitable *	mutagen	negative	positive
140	Dehydrodiisoeugenol	Suitable	Violated	mutagen	negative	positive
141	Delphinidin	Failed	Failed	non -mutagen	negative	negative
142	Delta-3-carene	Suitable	Suitable *	mutagen	negative	positive
143	Delta-cadinene	Suitable	Violated	mutagen	positive	positive

144	Delta-elemene	Suitable	Violated	mutagen	negative	Positive
145	Delta-selinene	Suitable	Violated	non-mutagen	positive	positive
146	Dihydrocarveol	Suitable	Suitable *	mutagen	negative	negative
147	Dihydrocarvone	Suitable	Suitable *	mutagen	negative	positive
148	Dihydrocinnamaldehyde	Suitable	Suitable *	mutagen	negative	negative
149	Dipentene	Suitable	Violated	mutagen	negative	positive
150	DL-limonene	Suitable	Violated	mutagen	negative	positive
151	Docosane	Suitable	Violated	non-mutagen	positive	positive
152	Dodecane	Suitable	Violated	non-mutagen	negative	positive
153	Eicosane	Suitable	Violated	non-mutagen	negative	positive
154	Elemene	Suitable	Violated	mutagen	negative	positive
155	Elemicin	Suitable	Suitable *	mutagen	positive	positive
156	Elemol	Suitable	Violated	non-mutagen	negative	positive
157	Epi-cubenol	Suitable	Violated	mutagen	positive	negative
158	Epiglobulol	Suitable	Violated	non-mutagen	negative	positive
159	Estragole	Suitable	Suitable *	mutagen	positive	negative
160	Ethyl-benzoate	Suitable	Suitable *	mutagen	negative	negative
161	Ethyl-cinnamate	Suitable	Suitable *	mutagen	positive	negative
162	Eugenol	Suitable	Suitable *	mutagen	positive	positive
163	Eugenol-acetate	Suitable	Suitable *	mutagen	positive	positive
164	Eugenol-methyl-ether	Suitable	Suitable *	mutagen	positive	positive
165	Farnesol	Suitable	Violated	non- mutagen	positive	negative
166	Fenchone	Suitable	Suitable *	mutagen	negative	positive
167	Fenchyl-alcohol	Suitable	Suitable *	mutagen	negative	positive
168	Formic-acid	Suitable	Violated	mutagen	negative	positive
169	Furfural	Suitable	Violated	mutagen	positive	positive
170	Furfuraldehyde	Suitable	Violated	mutagen	positive	positive
171	Furfurol	Suitable	Violated	mutagen	positive	positive
172	Gambogic-acid	Violated	Violated	non-mutagen	positive	negative
173	Gamma-cadinene	Suitable	Violated	mutagen	negative	positive
174	Gamma-eudesmol	Suitable	Violated	non-mutagen	negative	negative
175	Gamma-humulene	Suitable	Violated	mutagen	positive	positive
176	Gamma-murolene	Suitable	Violated	mutagen	negative	positive
177	Gamma-terpinene	Suitable	Violated	mutagen	positive	positive
178	Gamma-terpineol	Suitable	Suitable *	mutagen	negative	negative
179	Garcinol	Violated	Violated	mutagen	positive	negative
180	Gentisic-acid	Suitable	Violated	mutagen	negative	positive
181	Geranial	Suitable	Violated	mutagen	positive	positive
182	Geraniol	Suitable	Violated	mutagen	positive	negative
183	Geraniol-acetate	Suitable	Violated	non- mutagen	positive	positive
184	Geranyl-acetate	Suitable	Violated	non- mutagen	positive	positive
185	Germacrene D	Suitable	Violated	mutagen	positive	positive
186	Globulol	Suitable	Violated	non-mutagen	negative	positive
187	Glyceryl-trimyrystate	Violated	Violated	non-mutagen	positive	positive
188	Guaiacin	Violated	Violated	non-mutagen	positive	negative
189	Hedycaryol	Suitable	Violated	non-mutagen	negative	positive

190	Heptadecane	Suitable	Violated	non-mutagen	negative	Positive
191	Heptadecanoic-acid	Suitable	Violated	non-mutagen	negative	positive
192	Heptanal	Suitable	Suitable *	mutagen	negative	negative
193	Hexadecane	Suitable	Violated	non-mutagen	negative	positive
194	Hexan-1-ol	Suitable	Suitable *	non- mutagen	negative	negative
195	Hexanoic acid(caproic acid)	Suitable	Violated	mutagen	negative	positive
196	Humulene	Suitable	Violated	non- mutagen	positive	positive
197	Humulene-epoxide	Suitable	Violated	mutagen	positive	positive
198	Iso caryophyllene	Suitable	Violated	mutagen	negative	positive
199	Iso elemicin	Suitable	Suitable *	mutagen	positive	positive
200	Iso pinocampnone	Suitable	Suitable *	mutagen	negative	negative
201	Isoborneol	Suitable	Suitable *	mutagen	negative	positive
202	Isocaryophyllene	Suitable	Violated	mutagen	negative	positive
203	Isoelemicin	Suitable	Suitable *	mutagen	positive	positive
204	Isoeugenol	Suitable	Suitable *	mutagen	negative	positive
205	Isoeugenol-methyl-ether	Suitable	Suitable *	mutagen	positive	positive
206	Isoquercitrin	Violated	Violated	non-mutagen	negative	negative
207	Isovaleraldehyde	Suitable	Violated	mutagen	negative	negative
208	Kaempferol	Suitable	Suitable *	mutagen	negative	positive
209	Lauric-acid	Suitable	Violated	mutagen	negative	positive
210	Ledene	Suitable	Violated	non-mutagen	negative	positive
211	Ledol	Suitable	Violated	non-mutagen	positive	positive
212	Licarin-a	Suitable	Violated	mutagen	negative	positive
213	Licarin-b	Suitable	Violated	mutagen	negative	positive
214	Limonene	Suitable	Violated	mutagen	negative	positive
215	Linalool	Suitable	Suitable *	mutagen	negative	positive
216	Linalool-acetate	Suitable	Violated	mutagen	positive	positive
217	Linoleic-acid	Suitable	Violated	mutagen	positive	positive
218	Malabaricone-b	Suitable	Violated	non-mutagen	negative	negative
219	Malabaricone-c	Suitable	Violated	non-mutagen	negative	negative
220	Malic-acid	Suitable	Violated	mutagen	negative	positive
221	Mannitol	Suitable	Violated	mutagen	negative	negative
222	Methoxyeugenol	Suitable	Violated	mutagen	positive	positive
223	Methyl carvacrol	Suitable	Violated	mutagen	positive	negative
224	Methyl citronellate	Suitable	Violated	non-mutagen	positive	positive
225	Methyl eugenol	Suitable	Suitable *	mutagen	positive	positive
226	Methyl geranate	Suitable	Violated	mutagen	positive	positive
227	Methyl heptanoate	Suitable	Suitable *	mutagen	positive	positive
228	Methyl heptenone	Suitable	Suitable *	mutagen	negative	negative
229	Methyl octanoate	Suitable	Suitable *	mutagen	positive	positive
230	Methyl-benzoate	Suitable	Suitable *	mutagen	negative	negative
231	Methyl-chavicol	Suitable	Suitable *	mutagen	positive	negative
232	Methyl-cinnamate	Suitable	Suitable *	mutagen	negative	negative
233	Methyl-eugenol	Suitable	suitable *	mutagen	positive	positive
234	Methyl-isoegenol	Suitable	Suitable *	mutagen	positive	positive
235	Methyl-n-amylketone	Suitable	Suitable *	mutagen	negative	negative



236	Methyl-vinyl-ketone	Suitable	Suitable *	mutagen	negative	Positive
237	M-methyl acetophenone	Suitable	Suitable *	mutagen	negative	negative
238	Myrcene	Suitable	Violated	mutagen	negative	positive
239	Myristic-acid	Suitable	Violated	non- mutagen	negative	positive
240	Myristicin	Suitable	Suitable *	mutagen	positive	positive
241	Myrtenal	Suitable	Suitable *	mutagen	negative	negative
242	Myrtenol	Suitable	Suitable *	mutagen	negative	negative
243	N-butyrophenone	Suitable	Suitable*	mutagen	negative	negative
244	Nerol	Suitable	Violated	mutagen	positive	negative
245	Nerol-acetate	Suitable	Violated	non -mutagen	positive	positive
246	Niacin	Suitable	Violated	mutagen	negative	negative
247	N-nonadecane	Suitable	Violated	non-mutagen	negative	positive
248	N-nonane	Suitable	Violated	non-mutagen	positive	positive
249	<b>N-octanal</b>	<b>Suitable</b>	<b>Suitable *</b>	<b>non- mutagen</b>	<b>negative</b>	<b>negative</b>
250	Nonadecane	suitable	Violated	non-mutagen	negative	positive
251	N-tridecane	Suitable	Violated	non-mutagen	negative	positive
252	Octadecane	Suitable	Violated	non-mutagen	negative	positive
253	Octanoic-acid	Suitable	Suitable *	mutagen	negative	positive
254	Octanol	Suitable	Suitable*	non-mutagen	positive	negative
255	Oleanolic-acid	Suitable	Violated	non-mutagen	positive	positive
256	Oleic-acid	Suitable	Violated	mutagen	negative	positive
257	O-methoxycinnamaldehyde	Suitable	Suitable *	mutagen	negative	positive
258	Oxalic-acid	Suitable	Violated	mutagen	negative	positive
259	Palmitic-acid	Suitable	Violated	non-mutagen	negative	positive
260	P-coumaric-acid	Suitable	Violated	mutagen	negative	positive
261	P-cymene	Suitable	Violated	mutagen	positive	negative
262	P-cymene-8-ol	Suitable	Suitable *	mutagen	negative	negative
263	<b>N-Nonaldehyde</b>	<b>Suitable</b>	<b>Violated</b>	<b>non- mutagen</b>	<b>negative</b>	<b>negative</b>
264	Pentadecane	Suitable	Violated	non-mutagen	negative	positive
265	Pentadecanoic-acid	Suitable	Violated	non -mutagen	negative	positive
266	Pentanol	Suitable	Violated	non-mutagen	positive	negative
267	Phellandral	Suitable	Suitable *	mutagen	positive	negative
268	Phellandrene	Suitable	Violated	mutagen	positive	positive
269	Phenyl aceticacid	Suitable	Violated	mutagen	negative	negative
270	Phenyl-ethyl-alcohol	Suitable	Suitable *	mutagen	positive	negative
271	Phenylpropyl-acetate	Suitable	Suitable *	mutagen	negative	negative
272	Pinocamphone	Suitable	Suitable*	mutagen	negative	negative
273	Pinol	Suitable	Suitable *	mutagen	positive	negative
274	Piperidine	Suitable	Violated	mutagen	positive	positive
275	Piperitone	Suitable	Suitable *	mutagen	positive	positive
276	Piperonal	Suitable	Suitable *	mutagen	negative	positive
277	Piperonic acid	Suitable	Violated	mutagen	negative	positive
278	P-methyl acetophenone	Suitable	Suitable *	mutagen	negative	negative
279	Proanthocyanidin	Violated	Violated	non- mutagen	negative	positive
280	Proanthocyanidin-a-2	Violated	Violated	non- mutagen	negative	positive
281	Proanthocyanidin-b2	Violated	Violated	non- mutagen	negative	positive

282	Proanthocyanidin-b5	Violated	Violated	non- mutagen	negative	Positive
283	Proanthocyanidin-c1	Violated	Violated	non- mutagen	negative	positive
284	Proanthocyanidins	Violated	violated	non-mutagen	negative	positive
285	Quercetin	Suitable	Suitable*	mutagen	negative	positive
286	Quercitrin	Violated	Violated	non-mutagen	negative	negative
287	Riboflavin	Suitable	Violated	mutagen	negative	negative
288	Sabinene	Suitable	Suitable *	mutagen	negative	positive
289	Safrole	Suitable	Suitable*	mutagen	positive	positive
290	Salicylates	Suitable	Violated	mutagen	negative	negative
291	Sarisan	Suitable	Suitable *	mutagen	positive	positive
292	Sclareol	Suitable	Violated	mutagen	negative	positive
293	Sesquiterpenes	Suitable	Violated	non- mutagen	positive	negative
294	Spathulenol	Suitable	Violated	mutagen	positive	positive
295	Stearic-acid	Suitable	Violated	non -mutagen	negative	positive
296	Stigmasterol	Suitable	Violated	non- mutagen	positive	positive
297	Succinic-acid	Suitable	Violated	mutagen	negative	positive
298	Tannins	Violated	Violated	mutagen	negative	negative
299	Tartaric-acid	Suitable	Violated	mutagen	negative	positive
300	Terpinen-4-ol	Suitable	Suitable *	mutagen	negative	negative
301	Terpineol	Suitable	Suitable*	mutagen	negative	negative
302	Terpinolene	Suitable	Violated	mutagen	positive	positive
303	Tetracosane	Suitable	Violated	non-mutagen	positive	positive
304	Tetradecane	Suitable	Violated	non-mutagen	negative	positive
305	Thiamin	Suitable	Violated	mutagen	negative	negative
306	T-muurolol	Suitable	Violated	mutagen	negative	negative
307	Toluene	Suitable	Violated	mutagen	negative	negative
308	Trans-2-hexenal	Suitable	Violated	mutagen	negative	negative
309	Trans-anethole	Suitable	Suitable *	mutagen	positive	negative
310	Trans-beta-ocimene	Suitable	Violated	mutagen	positive	positive
311	Trans-carveol	Suitable	Suitable *	mutagen	positive	negative
312	Trans-cinnamaldehyde	Suitable	Suitable*	mutagen	negative	negative
313	Trans-cinnamic-acid	Suitable	Violated	mutagen	negative	negative
314	Trans-linalol-oxide	Suitable	Suitable *	mutagen	positive	negative
315	Trans-linalool-oxide	Suitable	Suitable *	mutagen	positive	positive
316	Trans-ocimene	Suitable	Violated	mutagen	positive	positive
317	Trans-pinocarveol	Suitable	Suitable *	mutagen	negative	negative
318	Trans-piperitol	Suitable	Suitable *	mutagen	positive	negative
319	Tricosane	Suitable	Violated	non-mutagen	positive	positive
320	Tridecane	Suitable	Violated	non-mutagen	negative	positive
321	Tridecanoic-acid	Suitable	Violated	non -mutagen	negative	positive
322	Trimyristin	Violated	Violated	non -mutagen	positive	positive
323	Undecane	Suitable	Violated	non-mutagen	negative	positive
324	Valeraldehyde	Suitable	Violated	mutagen	negative	negative
325	Vanillin	Suitable	Suitable*	mutagen	negative	positive
326	Viridifloral	Suitable	Violated	non-mutagen	negative	positive
327	Zingiberene	Suitable	Violated	mutagen	positive	positive
328	Zonarene	Suitable	Violated	mutagen	positive	positive

\*suitable if its binding affinity is greater than 0.1 microM.

**Table 1:** Druglikeness and Toxicity prediction of 328 compounds from 5 spices.

SI No	Compound Name	Predicted Biological Effects
1	Ascorbic acid	Antiviral (Herpes, Influenza, Hepatitis), Antiprotozoal, Antibacterial, Antitoxic, Antipruritic, Hypolipemic, Antidiabetic, Antiinflammatory, Antineoplastic, Antiparasitic, Antiischemic, Antioxidant, Antianginal
2	$\alpha$ -Bisabolol	Antiviral, Antiprotozoal, Antitussive, Antibacterial, Antitoxic, Hypolipemic, Antiinflammatory, Antidiabetic
3	N-Nonaldehyde	Antiviral (Herpes, Influenza, Hepatitis, Adenovirus, HIV), Antiprotozoal, Antiinflammatory, Antineoplastic, Antiinfertility, Antihelmintic
4	Delphinidin	Antiviral (Herpes, Hepatitis, HIV), Antiprotozoal, Antibacterial, Antipruritic, Antiinflammatory
5	Malabaricone-B	Antiviral (Herpes, Hepatitis, HIV), Antitoxic, Antipruritic, Antiinflammatory, Antineoplastic
6	Malabaricone-C	Antiviral (Herpes, Hepatitis, HIV), Antitoxic, Antipruritic, Antidiabetic, Cardiotonic, Antiinflammatory
7	Isoquercitrin,	Antiviral (Herpes, Hepatitis, HIV), Antibacterial, Antiprotozoal, Antifungal, Antitoxic, Antipruritic
8	Quercitrin,	Antiviral (Herpes, Influenza, HIV), Antibacterial, Antiprotozoal, Antitoxic, Antipruritic, Antiinflammatory, Antineoplastic, Antiischemic, Hemostatic
9	cis-Nerolidol	Antiviral (Herpes, Influenza, HIV), Antiprotozoal, Antibacterial, Antitoxic, Hypolipemic, Antiinflammatory, Antineoplastic
10	$\gamma$ -Eudesmol,	Antiviral (Herpes), Antiprotozoal, Antineoplastic, Antibacterial, Antitussive, Autoimmune disorders treatment
11	Hexan-1-ol	Antiviral (Herpes, Influenza, Hepatitis, Adenovirus, HIV), Antiprotozoal, Antibacterial, Antitoxic, Antipruritic, Antiinflammatory, Cardiotonic, Antineoplastic
12	n-Octanal	Antiviral (Herpes, Influenza, Hepatitis, Adenovirus, HIV), Antiprotozoal, Antitoxic, Antiinflammatory, Antineoplastic

**Table 2:** List of non toxic compounds having biological activity predicted by *in silico* method.

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