SUPPLEMENTARY DATA

Table S1
Active phytochemical compounds of *Syzygium cumini*.

S.No	Indian medicinal plant	Plant part	Phytochemical name
1.	Syzygium cumini	fruit	Malvidin 3-laminaribioside
2.	Syzygium cumini	fruit	Delphinidin 3-gentiobioside
3.	Syzygium cumini	fruit	Petunidin 3-gentiobioside
4.	Syzygium cumini	fruit	Flavylium
5.	Syzygium cumini	fruit	Myrcene
6.	Syzygium cumini	fruit	Citric acid
7.	Syzygium cumini	fruit	Dihydrocarvyl acetate
8.	Syzygium cumini	fruit	Geranyl butyrate
9.	Syzygium cumini	fruit	Palmitic acid
10.	Syzygium cumini	fruit	Widdrol
11.	Syzygium cumini	fruit	Oxalic acid
12.	Syzygium cumini	fruit	gamma-Decalactone
13.	Syzygium cumini	fruit	4-Carvomenthenol
14.	Syzygium cumini	fruit	Terpinolene
15.	Syzygium cumini	fruit	cis-beta-Farnesene
16.	Syzygium cumini	fruit	Humulene
17.	Syzygium cumini	fruit	Oleanolic acid
18.	Syzygium cumini	fruit	Gallic acid
19.	Syzygium cumini	fruit	Linalool
20.	Syzygium cumini	fruit	alpha-Pinene
21.	Syzygium cumini	fruit	beta-Pinene
22.	Syzygium cumini	fruit	alpha-Terpineol
23.	Syzygium cumini	fruit	delta-Cadinol
24.	Syzygium cumini	fruit	(Z)-beta-Ocimene
25.	Syzygium cumini	fruit	(-)-Globulol
26.	Syzygium cumini	fruit	beta-Caryophyllene
27.	Syzygium cumini	fruit	(E)-beta-ocimene
28.	Syzygium cumini	fruit	Bornyl acetate
29.	Syzygium cumini	fruit	cis-Nerolidol
30.	Syzygium cumini	fruit	6-Epi-beta-bisabolol
31.	Syzygium cumini	fruit	Ledol
32.	Syzygium cumini	fruit	cis-Dihydrocarvone

Table S2
Pharmacokinetic properties of the 32 phytochemical constituents identified in *Syzygium cumini*.

Phytochemical compounds	Molecular weight (g/mol)	H-bond acceptors	H-bond donors	XLOGP3	Lipinski violations	Bioavailability Score
Malvidin 3-laminaribioside	655.58	17	10	-1.16	3	0.17
Delphinidin 3-gentiobioside	627.52	17	12	-2.36	3	0.17
Petunidin 3-gentiobioside	641.55	17	11	-2.04	3	0.17
Flavylium	207.25	1	0	3.51	0	0.55
Myrcene	136.23	0	0	4.17	0	0.55
Citric acid	192.12	7	4	-1.72	0	0.56
Dihydrocarvyl acetate	196.29	2	0	3.78	0	0.55
Geranyl butyrate	224.34	2	0	4.87	0	0.55
Palmitic acid	256.42	2	1	7.17	1	0.85
Widdrol	222.37	1	1	4.08	0	0.55
Oxalic acid	90.03	4	2	-0.25	0	0.85
gamma-Decalactone	170.25	2	0	2.72	0	0.55
4-Carvomenthenol	154.25	1	1	3.26	0	0.55
Terpinolene	136.23	0	0	4.47	0	0.55
cis-beta-Farnesene	204.35	0	0	6.03	1	0.55
Humulene	204.35	0	0	4.55	1	0.55
Oleanolic acid	456.7	3	2	7.49	1	0.85
Gallic acid	170.12	5	4	0.7	0	0.56
Linalool	154.25	1	1	2.97	0	0.55
alpha-Pinene	136.23	0	0	4.48	1	0.55
beta-Pinene	136.23	0	0	4.16	1	0.55
alpha-Terpineol	154.25	1	1	3.39	0	0.55
delta-Cadinol	222.37	1	1	3.34	0	0.55
(Z)-beta-Ocimene	136.23	0	0	4.26	0	0.55
(-)-Globulol	222.37	1	1	3.74	0	0.55
beta-Caryophyllene	204.35	0	0	4.38	1	0.55
(E)-beta-ocimene	136.23	0	0	4.26	0	0.55
Bornyl acetate	196.29	2	0	4.3	0	0.55
cis-Nerolidol	222.37	1	1	4.83	0	0.55
6-Epi-beta-bisabolol	222.37	1	1	5.04	0	0.55
Ledol	222.37	1	1	3.74	0	0.55
cis-Dihydrocarvone	152.23	1	0	2.85	0	0.55

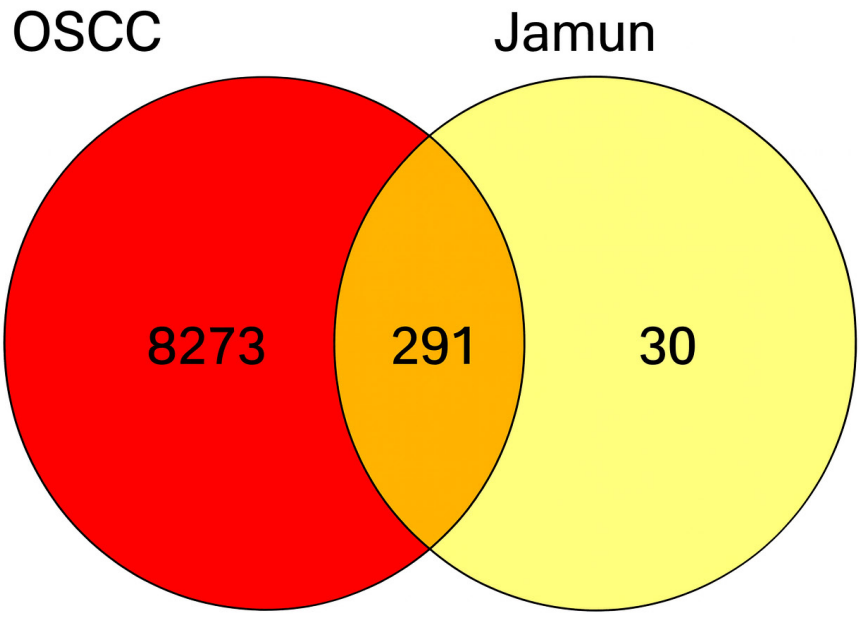

Figure S1

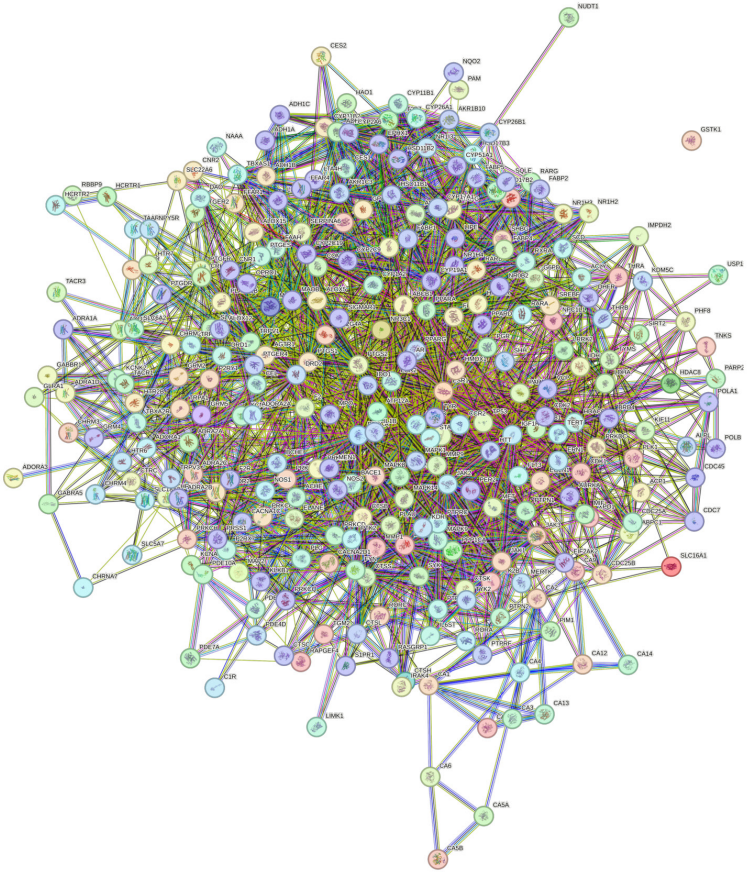

Figure S2