

Supplementary Table 4: All queried Ayurvedic INPs from the PUBLIC COMPARE portal

INP name	Ayurvedic Herb/Species Name	NSC number
Curcumin-difluorinated (CDF)	Turmeric/ <i>Curcuma longa</i>	752571
Di-O-Adamantoylcurcumin	Turmeric/ <i>Curcuma longa</i>	742024
Di-O-(2-Thienoyl)curcumin	Turmeric/ <i>Curcuma longa</i>	742023
Curcumin tri trithiadiazolaminoethylcarbonate	Turmeric/ <i>Curcuma longa</i>	742022
Curcumin tri adamantylaminoethylcarbonate	Turmeric/ <i>Curcuma longa</i>	742021
Ethoxycurcumin trithiadiazolaminomethylcarbonte	Turmeric/ <i>Curcuma longa</i>	742020
Ethoxycurcumin tribenzimidazolmethylcarbonte	Turmeric/ <i>Curcuma longa</i>	742019
Cucurbitacin-L-2-O-.beta.-D-glucopyranoside	Gourd/ <i>Cucurbitaceae</i>	710355
Curcumenol	Turmeric/ <i>Curcuma longa</i>	682343
Cucurbitacin E 2-O-glucoside	Gourd/ <i>Cucurbitaceae</i>	680118
B820585K273-F221 11-Deoxocucurbitacin I	Gourd/ <i>Cucurbitaceae</i>	605109
CUCURBITACIN I	Gourd/ <i>Cucurbitaceae</i>	521777
CUCURBITACIN D	Gourd/ <i>Cucurbitaceae</i>	521776
CUCURBITACIN E	Gourd/ <i>Cucurbitaceae</i>	521775
CUCURBITACIN B, 3 -EPI-ISO-	Gourd/ <i>Cucurbitaceae</i>	359240
16-Epicucurbitacin B	Gourd/ <i>Cucurbitaceae</i>	350002
CUCURBITACIN GLYCOSIDE DERIV B820585K205	Gourd/ <i>Cucurbitaceae</i>	337579
CUCURBITACIN GLYCOSIDE DERIV B820585K203	Gourd/ <i>Cucurbitaceae</i>	337578
CUCURBITACIN D	Gourd/ <i>Cucurbitaceae</i>	308606
CUCURBITACIN Q-1	Gourd/ <i>Cucurbitaceae</i>	306687
ISOCUCURBITACIN D, 3-EPI-	Gourd/ <i>Cucurbitaceae</i>	305982
ISOCUCURBITACIN D	Gourd/ <i>Cucurbitaceae</i>	305981
Cucurbitacin I, 2-glucoside	Gourd/ <i>Cucurbitaceae</i>	184734
Cucurbitacin B	Gourd/ <i>Cucurbitaceae</i>	144154
CUCURBITACIN D DEHYDROEPIRHAMNOSIDE	Gourd/ <i>Cucurbitaceae</i>	144153
Cucurbitacin Q	Gourd/ <i>Cucurbitaceae</i>	135075
CUCURBITACIN P	Gourd/ <i>Cucurbitaceae</i>	135074
Cucurbitacine (i)	Gourd/ <i>Cucurbitaceae</i>	112167
Cucurbitacin K	Gourd/ <i>Cucurbitaceae</i>	112166
Cucurbitacin J	Gourd/ <i>Cucurbitaceae</i>	112165
Tetrahydrocucurbitacin I	Gourd/ <i>Cucurbitaceae</i>	112164
Cucurbitacin B, dihydro-	Gourd/ <i>Cucurbitaceae</i>	106401
Isocucurbitacin B	Gourd/ <i>Cucurbitaceae</i>	106400
Cucurbitacine E	Gourd/ <i>Cucurbitaceae</i>	106399
Cucurbitacin C	Gourd/ <i>Cucurbitaceae</i>	94744

Cucurbitacin A	Gourd/Cucurbitaceae	94743
CUCURBITACIN B	Gourd/Cucurbitaceae	49451
Curcuma	Turmeric/Curcuma longa	32982
Curcumoid	Turmeric/Curcuma longa	26727
Oroxylon indicum (alc. extract - leaf,stem,fruit)	Shyonaka- Root bark/Oroxylum indicum	20362
Rauwolfia tetraphylla (hot alc. extract - leaf,flowers)	Sarpagandha/Rauwolfia serpentina	14897
7,12-Dimethylbenz[a]anthracene	Ashoka tree/Saraca indica	408823
Heterophylline (Rauwolfia)	Sarpagandha/Rauwolfia serpentina	72136
Rauwolfia	Sarpagandha/Rauwolfia serpentina	15627
Rauwolfia serpentina (alkaloidal, extract of)	Sarpagandha/Rauwolfia serpentina	15625
Elagic Acid	Pomegranate flower/ Punicoideae	656272
Piperlonguminine	Pippali/Piperaceae	125178
Hypophyllanthin	Phyllanthus	619044
Phyllanthin	Phyllanthus	619043
Phyllanthostatin A B680433K421	Phyllanthus	618898
Beta.-D-Lactosyl-1-amidophyllanthocin	Phyllanthus	615436
Beta.-D-Cellobiosyl-1-amidophyllanthocin	Phyllanthus	615435
PHYLLANTHOSIDE, S4,S4'-DIACETATE	Phyllanthus	349989
PHYLLANTHOSIDE S3-DESACETYL	Phyllanthus	349988
PHYLLANTHOSIDE, S3,S4'-DIACETATE	Phyllanthus	349987
PHYLLANTHOSTATIN 3 AGLYCON	Phyllanthus	349984
METHYLESTER		
PHYLLANTHOSE (DISACCHARIDE FROM PHYLLANTHOSIDE)	Phyllanthus	348102
PHYLLANTHOSTATIN 1,S3'-DESACETYL	Phyllanthus	348101
PHYLLANTHOSIDE PERACETATE	Phyllanthus	345396
PHYLLANTHOCIN	Phyllanthus	345395
PHYLLANTHOSIDE, DIDESACETYL	Phyllanthus	342734
PHYLLANTHOSIDE, S3'-DESACETYL-	Phyllanthus	342443
Phyllanthastatin 1	Phyllanthus	332596
Phyllanthostatin 3	Phyllanthus	332189
From plant Phyllanthus brasiliensis	Phyllanthus	330498
Phyllanthastatin 2	Phyllanthus	329098
PHYLLANTHOSIDE	Phyllanthus	328426
PHYLLANTHOSIDE, CRUDE	Phyllanthus	318507
Phyllanthoside	Phyllanthus	266492
Saffron	Oils, saffron/Crocus Sativus	407300
AZADIRACHTIN	Neem/ Azadirachta indica	368675
Leurosine	Madagascar periwinkle/Catharanthus roseus	90636
SYMPLOCOSIN, HEXAHYDRATE	Lodhra/Symplocos Racemosa	35608

Extract from Glycyrrhiza shiheziensis plant	Licorice/ Glycyrrhiza	637466
Extract from Glycyrrhiza alaensis plant	Licorice/ Glycyrrhiza	637465
Extract from Glycyrrhiza inflata plant	Licorice/ Glycyrrhiza	637464
Extract from Glycyrrhiza macrophylla plant	Licorice/ Glycyrrhiza	637463
Glycyrrhizin	Licorice/ Glycyrrhiza	234419
Glycyrrhizin	Licorice/ Glycyrrhiza	167409
Glycyrrhizic acid monosodium salt	Licorice/ Glycyrrhiza	163964
Glycyrrhizinic acid	Licorice/ Glycyrrhiza	35348
Glycyrrhizinic acid, ammonium salt (1:1)	Licorice/ Glycyrrhiza	2800
Gloriosine	Kalapikilangu/Gloriosa superba	403142
Buddhist Bauhinia	Kachnar/Bauhinia	20436
Marmelosin	Bael fruit/Aegle marmelos	402949
Symplocos paniculata (alc. extract - leaf)	Sapphire Berry/Symplocos paniculata	19238
Terminalia chebula myrobalans ext.	Haritaki/ Terminalia chebula	11099
Commiphora, polysaccharide from	Guggal/ Commiphora	407678
Unbleached ginger - Zingiber officinale (Zingiberaceae)	Ginger/Zingiberaceae	745202
Zingiberone	Ginger/Zingiberaceae	15335
Embelin	False black pepper/Embelia Ribus	91874
Isobromodeoxytopsentin	Elephant's foot/Elephantopus scaber	713185
Daturaolone	Angel's Trumpet/Datura	705537
DATURALACTONE	Angel's Trumpet/Datura	285115
Citral	Lemongrass/Cymbopogon citrates	6170
CUCURBITACIN F	Gourd/Cucurbitaceae	251680
Lupeol	Three leaves caper/Crataeva nurvala	90487
Fagarasterol (stem bark)	Three leaves caper/Crataeva nurvala	90487
Diethyl p-trifluoromethyl-.alpha.-phosphonocinnamionitrile	Cinnamon/Cinnamomum	648749
Diethyl m-phenoxy-.alpha.-phosphonocinnamionitrile	Cinnamon/Cinnamomum	648748
p-Phenoxy-diethylphosphonocinnamionitrile	Cinnamon/Cinnamomum	648747
o-Fluoro-.alpha.-benzoyl cinnamionitrile	Cinnamon/Cinnamomum	643772
o-Bromo-.alpha.-benzoyl cinnamionitrile	Cinnamon/Cinnamomum	643769
o-Methoxy-.alpha.-benzoylcinnamionitrile	Cinnamon/Cinnamomum	643764
3-Methoxy-4-benzoyloxy-.alpha.-benzoylcinnamionitrile	Cinnamon/Cinnamomum	643190
3,5-Dimethoxy-.alpha.-phenylcinnamionitrile	Cinnamon/Cinnamomum	643185
3-Methoxy-4-hydroxy-.alpha.-benzoylcinnamionitrile	Cinnamon/Cinnamomum	643183
3,4,5-Trimethoxy-.alpha.-benzoyl cinnamionitrile	Cinnamon/Cinnamomum	643181
Diethyl 3,4-methylenedioxy-.alpha.-phosphono cinnamionitrile	Cinnamon/Cinnamomum	643169

3,4-Methylenedioxy-.alpha.-benzoyl cinnamitrile	Cinnamon/Cinnamonum	643167
3-Bromo-4-dimethylamino-.alpha.-benzoyl cinnamitrile	Cinnamon/Cinnamonum	643160
p-Acetoxy-.alpha.-diethylphosphono-cinnamitrile	Cinnamon/Cinnamonum	643033
m-Phenoxy-.alpha.-phenylcinnamitrile	Cinnamon/Cinnamonum	643032
Alpha.-Phenyl-2,5-dimethoxy-.alpha.-cinnamitrile	Cinnamon/Cinnamonum	643023
Hydrocinnamitrile, .alpha.,3-dichloro-2-methyl- 8th C.I.	Cinnamon/Cinnamonum	239071
Cinnamitrile, p-(dimethylamino)- 8th C.I.	Cinnamon/Cinnamonum	122722
3-Phenylcinnamitrile	Cinnamon/Cinnamonum	120378
Hydrocinnamitrile, p-cyano- 8th C.I.	Cinnamon/Cinnamonum	117833
(E)-Cinnamitrile	Cinnamon/Cinnamonum	77496
Cinnamitrile, 3,4-dimethoxy- 8th C.I.	Cinnamon/Cinnamonum	51968
CINNAMONITRILE	Cinnamon/Cinnamonum	49137
Alpha.,.beta.-Diphenylcinnamitrile	Cinnamon/Cinnamonum	42900
Cinnamitrile	Cinnamon/Cinnamonum	42118
Cinnamonfern	Cinnamon/Cinnamonum	17993
Hydrocinnamitrile	Cinnamon/Cinnamonum	16936
Alpha.-Phenylcinnamitrile	Cinnamon/Cinnamonum	12489
Acetocinnamone	Cinnamon/Cinnamonum	5605
Hydrocinnamitrile, .beta.-oxo-	Cinnamon/Cinnamonum	4713
Alpha.-Phenylcinnamitrile	Cinnamon/Cinnamonum	2018
Alpha.-Cyanocinnamitrile	Cinnamon/Cinnamonum	490
Cichoriin aglucon	Cichory/ Asteraceae	26428
Statice limonium (Plumbaginaceae), water extract	Chitraka/Plumbago zeylanica	179851
Statice sinuata (Plumbaginaceae), methanol extract	Chitraka/Plumbago zeylanica	179850
Plumbagin	Chitraka/Plumbago zeylanica	688284
Plumbagin, 3-bromo:	Chitraka/Plumbago zeylanica	621605
CHLOROPLUMBAGIN	Chitraka/Plumbago zeylanica	362426
PLUMBAGIN	Chitraka/Plumbago zeylanica	236613
Calotropin	Arka/Calotropis Gigantea	143925
Calendulaglycoside D-6'-O-methyl ester	Marigold/Calendula	731922
Calendulaglycoside D2	Marigold/Calendula	731921
Calendulaglycoside B-6'-O-butyl ester	Marigold/Calendula	731920
Calendulaglycoside A-6'-O-butyl ester	Marigold/Calendula	731919
Calendulaglycoside C	Marigold/Calendula	731918
Calendulaglycoside B	Marigold/Calendula	731917
Calendulaglycoside A	Marigold/Calendula	731916
Faradione, from Calendula	Marigold/Calendula	277277
Calendula acids	Marigold/Calendula	119126
Butein	Palasha/Butea monosperma	652892

Isolated from Asteraceae plants	Asteraceae	603929
Achilleol A	Biranjaspaha/ Achillea millefolium	710351
DEHYDROACHILLIN	Biranjaspaha/ Achillea millefolium	180034
Achillin	Biranjaspaha/ Achillea millefolium	156236
Achillea millefolium (chloroform extract)	Biranjaspaha/ Achillea millefolium	18444
Achillea millefolium plant chloroform extract	Biranjaspaha/ Achillea millefolium	17263
Guamachil Apes-earring	Biranjaspaha/ Achillea millefolium	14900
Achilleic acid	Biranjaspaha/ Achillea millefolium	7616
Phyllanthus emblica (alc. extract - leaf,fruit)	Bhumi amalaka/Phyllanthus	20426
Terminalia bellenca (hot alcohol extract- leaf, stem, fruit) Terminalia	Bhibhitaki/ Terminalia bellenca	20331
Nimbolide	Neem/Azadirachta indica	309909
WITHANIA SOMNIFERA	Aswagandha/Withania Somnifera	329512
Common Saraca	Asoka/Saraca Asoca	20482
Terminalia chebula (alc. extract - leaf, inflor.)	Arjuna/ Arjuna Terminalia	18003
Ricinusol	Argan Fruits/Argania spinosa	360316
Ricinus communis	Argan Fruits/Argania spinosa	15384
Andrographis Extract	Kalmegh/Andrographis Paniculata	383468
Myricetin	Neem/Azadirachta indica	407290
Barbaloin	Aloe vera (Aloe)/Asphodeloideae	227189
Vasicine	Adhatoda vasica	28595
Perchlorate of an alkaloid from Rutaceae	Aegle marmelos	342730
Alkaloid from Rutaceae found in Cameroon	Aegle marmelos	342729
Bulbophyllanthrone	Bulbophyllum	708791
Rubia tenuifolia water extract	odoratissimum/ORCHIDACEAE	
Rubia tenuifolia chloroform ext.	Indian madder/ Rubia tenuifolia	179855
Tylophorine	Indian madder/ Rubia tenuifolia	179854
Tylophorine	Tylophora asthmatica	717335
Cryptoleurine	Tylophora asthmatica	76387
Limonene	Tylophora	19912
Limonene	Citrus peels/Anethum graveolens	21446
Caffeic acid	Citrus peels/Anethum graveolens	844
Gallocatechin (Bark Extract)	Honey, coffee	57197
Gedunin	Arjuna/ Arjuna Terminalia	674038
Coumestrol	Neem/Azadirachta indica	113497
Alizarin	Red clover/Trifolium pratense	22842
Quercetin	Indian madder/Rubia cordifolia	7212
Catechin	Phyllanthus	9219
Reservatol	Green tea	2819
Piceatannol	Darakchasava/Vinis vinifera	327430
	Darakchasava/Vinis vinifera	365798

All-trans beta carotene	Mahua/Madhuca indica	62794
Phenethyl Isothiocyanate	Radish/Raphanas sativus	87868
Beta-Sitosterol	Vajradanti/BARLERIA PRIONITIS	8096
Paeoniflorin	Elephant foot yam/ Amorphophallus paeoniifolius	178886

The column **Ayurvedic Herb/Species Name** shows the taxonomic origin for the sources of Ayurvedic compounds. For those compounds that originate from multiple source organisms, only selected examples of source organisms are listed.