



Supplementary Fig.1 The degree distribution of species in the species-metabolite bipartite graph. The x-axis represents the number of metabolites belonging to one species and the y-axis represents the frequency of such species.

Supplementary Table 1. The predicted unrecorded plant-metabolite relations, involving 524 metabolites and 117 plants.

metabolite	plant
Gibberellin A4	<i>Citrus limon</i> ; <i>Phaseolus lunatus</i> ; <i>Nicotiana tabacum</i> ; <i>Lupinus luteus</i>
Methyl salicylate	<i>Citrus limon</i> ; <i>Citrus aurantifolia</i> ; <i>Citrus paradisi</i> ; <i>Citrus aurantium</i>
Cyclohexane	<i>Citrus limon</i> ; <i>Citrus aurantium</i> ; <i>Artemisia annua</i> ; <i>Artemisia capillaris</i> ; <i>Centaurea sessilis</i> ; <i>Zingiber officinale</i>
o-Isopropenyl toluene	<i>Citrus limon</i> ; <i>Citrus aurantifolia</i> ; <i>Citrus paradisi</i> ; <i>Citrus sinensis</i> ; <i>Citrus aurantium</i>
Jasmonic acid	<i>Citrus limon</i>
10'-Apoviolaaxanthal	<i>Citrus limon</i>
alpha-trans-Bergamotene	<i>Citrus limon</i>
Citral	<i>Citrus aurantifolia</i> ; <i>Citrus paradisi</i> ; <i>Citrus reticulata</i>
Benzeneacetaldehyde	<i>Citrus aurantifolia</i> ; <i>Citrus paradisi</i> ; <i>Citrus aurantium</i>
Methyl epijasmone	<i>Citrus aurantifolia</i> ; <i>Citrus sinensis</i>
Salvigenin	<i>Citrus aurantifolia</i> ; <i>Citrus sinensis</i> ; <i>Citrus aurantium</i>
Rhoifolin	<i>Citrus paradisi</i>
Isopropanol	<i>Citrus paradisi</i> ; <i>Citrus reticulata</i>
Isoscutellarein 7,8-dimethyl ether	<i>Citrus sinensis</i>
Isoscutellarein 7,8,4'-trimethyl ether	<i>Citrus sinensis</i>
Gibberellin A53	<i>Citrus sinensis</i> ; <i>Lathyrus odoratus</i> ; <i>Phaseolus lunatus</i> ; <i>Phaseolus coccineus</i> ; <i>Hordeum vulgare</i> ; <i>Nicotiana tabacum</i>
Violaxanthin	<i>Citrus sinensis</i>
Gibberellin A81	<i>Citrus reticulata</i>
Gibberellin A9	<i>Citrus reticulata</i>
6-Demethoxytangeritin	<i>Citrus reticulata</i>
Tetramethylscutellarein	<i>Citrus reticulata</i>
Apigenin 7-rutinoside	<i>Citrus aurantium</i>
Caryophyllene oxide	<i>Houttuynia emeiensis</i>
Capillaridin E	<i>Artemisia annua</i> ; <i>Rhaponticum carthamoides</i>
Limonene	<i>Artemisia annua</i> ; <i>Artemisia capillaris</i> ; <i>Artemisia annua L.cultivar Jwarharti</i>
Cyclosativene	<i>Artemisia annua</i>
2-Nonanone	<i>Artemisia annua</i>
Kaempferol	<i>Artemisia capillaris</i> ; <i>Sedum sarmentosum</i> ; <i>Medicago sativa</i> ; <i>Cryptomeria japonica</i>
Salicylic acid	<i>Artemisia capillaris</i>
Apigenin	<i>Artemisia capillaris</i>
Octanal	<i>Artemisia capillaris</i>
Rhamnocitrin	<i>Rhaponticum carthamoides</i>
Genkwanin	<i>Rhaponticum carthamoides</i>
p-Cymene	<i>Rhaponticum carthamoides</i>
Hexahydrofarnesyl acetone	<i>Artemisia annua L.cultivar Jwarharti</i>

Caprylic acid	<i>Centaurea sessilis</i>
Isophytol	<i>Centaurea sessilis; Anthemis aciphylla</i>
Phytol	<i>Centaurea sessilis; Anthemis aciphylla</i>
Bicyclogermacren	<i>Centaurea sessilis</i>
(2E)-Octenal	<i>Centaurea sessilis</i>
R-(+)-trans-Verbenol	<i>Centaurea sessilis</i>
2-Pentylfuran	<i>Anthemis aciphylla</i>
Isovaleraldehyde	<i>Alphina galanga</i>
alpha-Thujene	<i>Leptospermum scoparium</i>
Neryl acetate	<i>Leptospermum scoparium</i>
6,9-Guaiadiene	<i>Piper arboreum</i>
Geraniol	<i>Piper arboreum</i>
Germacrene D	<i>Piper fimbriatum</i>
Ampelopsin 7-glucoside	<i>Pseudotsuga menziesii</i>
Indole-3-carboxylic acid	<i>Pseudotsuga menziesii; Picea abies; Lycopersicon esculentum</i>
Gibberellin A9	<i>Pinus sylvestris; Lathyrus odoratus; Brassica napus; Hordeum vulgare</i>
Gibberellin A1	<i>Pinus sylvestris; Lycopersicon esculentum; Lupinus luteus</i>
Gibberellin A7	<i>Pinus sylvestris</i>
Indole-3-acetic acid	<i>Pinus sylvestris; Brassica rapa</i>
Methyl indole-3-acetate	<i>Pinus sylvestris</i>
Syringetin 3-(6"-acetylglucoside)	<i>Pinus sylvestris</i>
Laricitrin 3-(6"-acetylglucoside)	<i>Pinus sylvestris</i>
Taxifolin 3'-glucoside	<i>Picea abies</i>
Isorhamnetin 3-(6"- acetylgalactoside)	<i>Picea abies</i>
Gibberellin A20	<i>Prunus persica; Lycopersicon esculentum</i>
Afzelechin	<i>Prunus avium</i>
Gibberellin A44	<i>Prunus avium; Hordeum vulgare</i>
Gibberellin A30	<i>Prunus avium</i>
Chrysin	<i>Prunus avium</i>
Peonidin 3-rhamnoside	<i>Pisum sativum</i>
Gibberellin A97	<i>Lathyrus odoratus; Zea mays; Oryza sativa</i>
Gibberellin A51	<i>Lathyrus odoratus; Hordeum vulgare</i>
Gibberellin A12	<i>Lathyrus odoratus; Triticum aestivum; Brassica napus</i>
Gibberellin A24	<i>Lathyrus odoratus; Brassica napus; Hordeum vulgare</i>
Gibberellin A44	<i>Lathyrus odoratus</i>
Isosojagol	<i>Phaseolus lunatus</i>
Isoferreirin	<i>Phaseolus lunatus; Phaseolus vulgaris</i>
7,4'-Dihydroxy-5,2'- dimethoxyisoflavanone	<i>Phaseolus lunatus; Phaseolus vulgaris</i>
5-Deoxykievitol	<i>Phaseolus vulgaris</i>

(-)-Glycinol	<i>Phaseolus vulgaris</i>
Psoralidin	<i>Phaseolus coccineus</i>
Gibberellin A19	<i>Phaseolus coccineus</i> ; <i>Lycopersicon esculentum</i>
Gibberellin A37	<i>Phaseolus coccineus</i>
Gibberellin A14	<i>Triticum aestivum</i>
Gibberellin A25	<i>Zea mays</i> ; <i>Brassica napus</i>
Neoglucobrassicin	<i>Raphanus sativus</i> ; <i>Armoracia lapathifolia</i>
Gibberellin A53	<i>Raphanus sativus</i>
Gibberellin A40	<i>Brassica napus</i>
Gibberellin A34	<i>Hordeum vulgare</i>
Gibberellin A8	<i>Oryza sativa</i>
Fisetin 3-methyl ether	<i>Robinia pseudoacacia</i>
Garbanzol	<i>Robinia pseudoacacia</i>
Butin	<i>Robinia pseudoacacia</i>
Gallocatechin	<i>Colophospermum mopane</i>
(+)-Gallocatechin	<i>Colophospermum mopane</i>
Dihydrorobinetin	<i>Acacia mearnsii</i>
Dihydroquercetin	<i>Acacia mearnsii</i>
Liquiritigenin	<i>Acacia mearnsii</i>
(-)-Epicatechin	<i>Acacia mearnsii</i>
ent-Epifisetinidol	<i>Acacia mearnsii</i>
Kaempferide	<i>Rhodiola sachalinensis</i> ; <i>Sinocrassula indica</i>
Sinocrassoside C1	<i>Rhodiola sachalinensis</i>
Rhodionin	<i>Sinocrassula indica</i>
Rhodosin	<i>Sinocrassula indica</i>
Nicotinic acid	<i>Lycopersicon esculentum</i>
9-Ribosyl-cis-zeatin	<i>Lycopersicon esculentum</i>
Indole-3-acetonitrile	<i>Nicotiana tabacum</i> ; <i>Solanum tuberosum</i>
Trigonelline	<i>Nicotiana tabacum</i>
Phytuberin	<i>Nicotiana tabacum</i>
(-)-Phytuberin	<i>Nicotiana tabacum</i>
1-Caffeoyl-beta-D-glucose	<i>Nicotiana tabacum</i>
Desacetylphytuberin	<i>Solanum tuberosum</i>
9-Ribosyl-trans-zeatin	<i>Solanum tuberosum</i>
Prunetin	<i>Glycyrrhiza uralensis</i> ; <i>Medicago sativa</i> ; <i>Clitoria ternatea</i> ; <i>Melilotus messanensis</i> ; <i>Glycyrrhiza pallidiflora</i> ; <i>Dalbergia odorifera</i>
Licoisoflavone A	<i>Glycyrrhiza uralensis</i> ; <i>Glycyrrhiza inflata</i>
Glabridin	<i>Glycyrrhiza uralensis</i>
Topazolin	<i>Glycyrrhiza uralensis</i>
Isoderrone	<i>Glycyrrhiza uralensis</i> ; <i>Glycyrrhiza aspera</i>
Licoflavone B	<i>Glycyrrhiza uralensis</i>

3'-Dimethylallylkievitone	<i>Glycyrrhiza uralensis</i>
Wighteone	<i>Glycyrrhiza uralensis; Glycyrrhiza aspera; Lupinus luteus; Derris scandens</i>
Hydroxywighteone	<i>Glycyrrhiza uralensis; Glycyrrhiza aspera; Lupinus albus; Erythrina variegata</i>
Licopyranocoumarin	<i>Glycyrrhiza aspera; Glycyrrhiza inflata</i>
Kanzonol W	<i>Glycyrrhiza aspera</i>
Licuroside	<i>Glycyrrhiza aspera; Glycyrrhiza inflata</i>
Neoisoliquiritigenin	<i>Glycyrrhiza aspera; Glycyrrhiza inflata</i>
1-O-Methylglycyrol	<i>Glycyrrhiza aspera; Glycyrrhiza glabra</i>
Kanzonol P	<i>Glycyrrhiza aspera; Glycyrrhiza glabra</i>
Neoliquiritin	<i>Glycyrrhiza aspera; Glycyrrhiza glabra; Glycyrrhiza inflata</i>
Licoricone	<i>Glycyrrhiza aspera; Glycyrrhiza glabra; Glycyrrhiza inflata</i>
Licicesaponin A3	<i>Glycyrrhiza aspera; Glycyrrhiza glabra</i>
Licicesaponin G2	<i>Glycyrrhiza aspera; Glycyrrhiza glabra</i>
Licicesaponin C2	<i>Glycyrrhiza aspera; Glycyrrhiza glabra; Glycyrrhiza inflata</i>
Licicesaponin E2	<i>Glycyrrhiza aspera; Glycyrrhiza glabra; Glycyrrhiza inflata</i>
Licoflavonol	<i>Glycyrrhiza aspera</i>
Gancaonin Q	<i>Glycyrrhiza aspera; Glycyrrhiza inflata</i>
Glisoflavanone	<i>Glycyrrhiza aspera</i>
Kanzonol I	<i>Glycyrrhiza aspera; Glycyrrhiza glabra</i>
Glycyrrhizol A	<i>Glycyrrhiza aspera</i>
Licoriphenone	<i>Glycyrrhiza aspera</i>
Licofuranocoumarin	<i>Glycyrrhiza glabra; Glycyrrhiza inflata</i>
Glyasperin L	<i>Glycyrrhiza glabra; Glycyrrhiza inflata</i>
Licocoumarone	<i>Glycyrrhiza glabra; Glycyrrhiza inflata</i>
Glyinflanin E	<i>Glycyrrhiza glabra</i>
Glyinflanin F	<i>Glycyrrhiza glabra</i>
Gancaonin A	<i>Glycyrrhiza glabra</i>
Semilicoisoflavone B	<i>Glycyrrhiza inflata</i>
Licoagrochalcone D	<i>Glycyrrhiza inflata</i>
Pratensol	<i>Lupinus luteus; Derris scandens; Clitoria ternatea; Melilotus messanensis; Glycyrrhiza pallidiflora; Dalbergia odorifera</i>
Indicanin E	<i>Lupinus luteus; Lupinus albus; Derris scandens</i>
Derrisoflavone B	<i>Lupinus luteus; Lupinus albus</i>
Lupinisol A	<i>Lupinus luteus</i>
Lupalbigenin	<i>Lupinus luteus</i>
Derrisoflavone F	<i>Lupinus luteus; Lupinus albus</i>
Lupinalbin B	<i>Lupinus luteus</i>
Lupinalbin G	<i>Lupinus luteus</i>
Laburnetin	<i>Lupinus luteus; Lupinus albus</i>
3'-Methylorobol	<i>Lupinus luteus; Lupinus albus</i>
Genistein	<i>Lupinus albus; Melilotus messanensis; Glycyrrhiza pallidiflora; Dalbergia odorifera</i>

Isoprunetin	<i>Lupinus albus; Derris scandens</i>
Scanderone	<i>Lupinus albus</i>
Chandalone	<i>Lupinus albus</i>
Ulexone A	<i>Lupinus albus</i>
Isolupalbigenin	<i>Lupinus albus; Derris scandens</i>
Gibberellin A18	<i>Lupinus albus</i>
Gibberellin A23	<i>Lupinus albus</i>
Lupinol C	<i>Lupinus albus</i>
Scandalenol	<i>Lupinus albus; Erythrina variegata</i>
Lupisoflavone	<i>Derris scandens</i>
Alpinumisoflavone	<i>Derris scandens</i>
Derrone	<i>Derris scandens; Erythrina variegata</i>
Angustone B	<i>Derris scandens</i>
Angustone C	<i>Derris scandens</i>
Lupinisolone A	<i>Derris scandens</i>
Lupinisoflavone H	<i>Derris scandens</i>
Lupinifolin	<i>Derris scandens</i>
Barpisoiflavone C	<i>Erythrina variegata</i>
Erysenegalensein K	<i>Erythrina variegata</i>
8-Prenylluteone	<i>Erythrina variegata</i>
Robustic acid	<i>Erythrina variegata; Erythrina senegalensis</i>
Eturunagarone	<i>Erythrina variegata; Erythrina senegalensis</i>
Bidwillon B	<i>Erythrina senegalensis</i>
Lonchocarpic acid	<i>Erythrina senegalensis</i>
Lonchocarpenin	<i>Erythrina senegalensis</i>
Scandenin	<i>Erythrina senegalensis</i>
Euchretin E	<i>Euchresta japonica</i>
Euchretin D	<i>Euchresta japonica</i>
Euchretin M	<i>Euchresta japonica</i>
Cytisine	<i>Euchresta japonica; Sophora flavescens; Maackia amurensis</i>
Formononetin	<i>Euchresta formosana</i>
Secundiflorol I	<i>Euchresta formosana; Sophora flavescens; Maackia amurensis</i>
Kushenin	<i>Euchresta formosana; Maackia amurensis; Sophora secundiflora; Sophora japonica; Glycyrrhiza pallidiflora</i>
Euchrenone a4	<i>Euchresta formosana</i>
Amorilin	<i>Euchresta formosana</i>
(-)-N-Methyleytisine	<i>Euchresta formosana</i>
Daidzein	<i>Sophora flavescens; Maackia amurensis; Melilotus messanensis; Glycyrrhiza pallidiflora; Dalbergia odorifera</i>
Thermopsine	<i>Sophora flavescens; Maackia amurensis</i>
(-)-6alpha-Hydroxylupanine	<i>Sophora flavescens; Sophora secundiflora</i>

(-)-6alpha-methoxylupanine	<i>Sophora flavescens</i> ; <i>Sophora secundiflora</i>
Pratensein	<i>Maackia amurensis</i>
Mamanine	<i>Maackia amurensis</i> ; <i>Sophora secundiflora</i>
5,6-Dehydrolupanine	<i>Maackia amurensis</i>
Argentine	<i>Maackia amurensis</i>
Maackiain	<i>Sophora secundiflora</i>
(-)-12,12'-Methylenedicytisine	<i>Sophora secundiflora</i>
Soyasapogenol E	<i>Medicago sativa</i> ; <i>Trifolium pratense</i>
Xenognosin B	<i>Medicago sativa</i> ; <i>Clitoria ternatea</i> ; <i>Trifolium pratense</i> ; <i>Sophora japonica</i> ; <i>Melilotus messanensis</i>
Vestitone	<i>Medicago sativa</i>
Anhydroglycinol	<i>Medicago sativa</i> ; <i>Trifolium pratense</i> ; <i>Melilotus messanensis</i>
Lespedezol A1	<i>Medicago sativa</i> ; <i>Trifolium pratense</i> ; <i>Melilotus messanensis</i>
6a-Hydroxymedicarpin	<i>Medicago sativa</i> ; <i>Glycyrrhiza pallidiflora</i> ; <i>Dalbergia odorifera</i>
Sophorophenolone	<i>Medicago sativa</i>
Delphinidine	<i>Medicago sativa</i> ; <i>Trifolium pratense</i> ; <i>Sophora japonica</i> ; <i>Melilotus messanensis</i>
Quercetin	<i>Medicago sativa</i> ; <i>Clitoria ternatea</i> ; <i>Melilotus messanensis</i>
Lespedezol G1	<i>Medicago sativa</i>
Licoagroside C	<i>Medicago sativa</i>
Pratol	<i>Medicago sativa</i> ; <i>Glycyrrhiza pallidiflora</i>
Licoagroside E	<i>Medicago sativa</i>
7,4'-Di-O-methylaidizein	<i>Medicago sativa</i> ; <i>Trifolium pratense</i> ; <i>Melilotus messanensis</i> ; <i>Glycyrrhiza pallidiflora</i> ; <i>Dalbergia odorifera</i>
Licodione 2'-methyl ether	<i>Medicago sativa</i>
Tricin	<i>Clitoria ternatea</i> ; <i>Trifolium pratense</i>
Myricetin	<i>Clitoria ternatea</i> ; <i>Trifolium pratense</i> ; <i>Sophora japonica</i>
Irisolidone	<i>Trifolium pratense</i> ; <i>Glycyrrhiza pallidiflora</i>
Erythrinin C	<i>Trifolium pratense</i> ; <i>Sophora japonica</i>
Licoagroisoflavone	<i>Trifolium pratense</i> ; <i>Sophora japonica</i>
Kushenin	<i>Trifolium pratense</i>
Tectoridin	<i>Trifolium pratense</i>
Sophojaponicin	<i>Trifolium pratense</i> ; <i>Glycyrrhiza pallidiflora</i>
7,3'-Dimethylorobol	<i>Trifolium pratense</i>
Irisolidone 7-O-beta-D-glucoside	<i>Trifolium pratense</i>
(-)-Maackiain	<i>Trifolium pratense</i> ; <i>Lespedeza homoloba</i>
Irilone	<i>Sophora japonica</i> ; <i>Glycyrrhiza pallidiflora</i>
Isokaempferide	<i>Sophora japonica</i>
Trifoliol	<i>Sophora japonica</i>
Trifolirhizin	<i>Sophora japonica</i>
Irilone 4'-O-glucoside	<i>Sophora japonica</i>
(+)-6a-Hydroxymaackiain	<i>Sophora japonica</i> ; <i>Lespedeza homoloba</i> ; <i>Glycyrrhiza pallidiflora</i>

Coumestrol	<i>Lespedeza homoloba</i>
Bolusanthin III	<i>Lespedeza homoloba</i>
9-O-Methylcoumestrol	<i>Lespedeza homoloba</i>
5'-Methoxysativan	<i>Lespedeza homoloba</i>
Sativanone	<i>Melilotus messanensis</i>
2-Methoxymedicarpin	<i>Melilotus messanensis</i>
Coumestrin	<i>Glycyrrhiza pallidiflora</i>
Haginin D	<i>Glycyrrhiza pallidiflora</i>
Lespedezol F1	<i>Glycyrrhiza pallidiflora</i>
2'-Methoxyisoliquiritigenin	<i>Glycyrrhiza pallidiflora</i>
Echinatin	<i>Dalbergia odorifera</i>
Glypallichalcone	<i>Dalbergia odorifera</i>
Melilotocarpan B	<i>Dalbergia odorifera</i>
Cryptopine	<i>Corydalis claviculata; Corydalis solida</i>
Allocryptopine	<i>Corydalis claviculata; Papaver somniferum</i>
Rhoeadine	<i>Corydalis claviculata</i>
Norribasine	<i>Papaver somniferum</i>
Ribasine	<i>Papaver somniferum</i>
Sinoacutine	<i>Papaver somniferum</i>
alpha-Hydrastine	<i>Papaver somniferum</i>
Noscapine	<i>Corydalis solida</i>
Narcotoline	<i>Corydalis solida</i>
Salutaridine	<i>Corydalis solida</i>
Oxocularicine	<i>Corydalis solida</i>
Glaziovine	<i>Annona cherimola; Cocculus laurifolius; Artabotrys uncinatus</i>
Calycinine	<i>Annona cherimola</i>
Juzirine	<i>Annona cherimola</i>
Pronuciferine	<i>Xylopiya parviflora; Stephania cepharantha Hayata</i>
Annocherine A	<i>Xylopiya parviflora</i>
Annocherine B	<i>Xylopiya parviflora</i>
Michelalbine	<i>Xylopiya parviflora</i>
Micheline A	<i>Xylopiya parviflora</i>
14-Episinomenine	<i>Cocculus laurifolius; Stephania cepharantha</i>
Cephamonine	<i>Stephania cepharantha</i>
Aknadilactam	<i>Stephania cepharantha</i>
Stephodeline	<i>Stephania cepharantha</i>
Tannagine	<i>Stephania cepharantha</i>
Aknadinine	<i>Stephania cepharantha</i>
Juziphine	<i>Stephania cepharantha</i>
N-Methylasimilobine	<i>Stephania cepharantha</i>
Coclaurine	<i>Stephania cepharantha Hayata</i>

Anonaine	<i>Stephania cepharantha</i> Hayata
Aknadicine	<i>Stephania cepharantha</i> Hayata
Cucoline	<i>Stephania cepharantha</i> Hayata
Oblongine	<i>Stephania cepharantha</i> Hayata
1-Methoxybrassinin	<i>Brassica oleracea</i>
Glucoviorylin	<i>Brassica oleracea</i> ; <i>Brassica rapa</i> ; <i>Hesperis matronalis</i>
Glucolepidiin	<i>Brassica oleracea</i> ; <i>Brassica rapa</i> ; <i>Hesperis matronalis</i>
Caulilexin C	<i>Brassica oleracea</i>
Brassicinal B	<i>Brassica oleracea</i>
Benzylglucosinolate	<i>Brassica oleracea</i> ; <i>Brassica rapa</i> ; <i>Hesperis matronalis</i>
Glucocheirolin	<i>Brassica oleracea</i> ; <i>Brassica rapa</i> ; <i>Hesperis matronalis</i>
Spirobrassinin	<i>Brassica oleracea</i>
3-Hydroxybutyl glucosinolate	<i>Brassica oleracea</i> ; <i>Brassica rapa</i> ; <i>Hesperis matronalis</i>
4-Methoxyglucobrassicin	<i>Brassica oleracea</i>
Sinigrin	<i>Brassica rapa</i> ; <i>Hesperis matronalis</i>
Methyl anthranilate	<i>Brassica rapa</i>
Glucoberteroin	<i>Brassica rapa</i>
1-Methoxyspirobrassinin	<i>Brassica rapa</i>
Glucosinalbate	<i>Armoracia lapathifolia</i>
Glucosalysin	<i>Armoracia lapathifolia</i>
Glucohesperin	<i>Armoracia lapathifolia</i>
Glucouiberin	<i>Hesperis matronalis</i>
Glucobrassicinapin	<i>Hesperis matronalis</i>
Glucosquereillin	<i>Hesperis matronalis</i>
2-Methoxybenzyl glucosinolate	<i>Hesperis matronalis</i>
Alstolactone	<i>Alstonia macrophylla</i>
Isoalstonisine	<i>Alstonia macrophylla</i>
Normacusine B	<i>Alstonia macrophylla</i>
N(4)-Demethylalstonerinal	<i>Alstonia macrophylla</i> ; <i>Alstonia angustifolia</i>
Cathafoline N(4)-oxide	<i>Alstonia macrophylla</i>
Alstophyllal	<i>Alstonia angustifolia</i> ; <i>Alstonia angustifolia</i> var. <i>latifolia</i>
Macrocarpine A	<i>Alstonia angustifolia</i> ; <i>Alstonia angustifolia</i> var. <i>latifolia</i>
Macrocarpine B	<i>Alstonia angustifolia</i> ; <i>Alstonia angustifolia</i> var. <i>latifolia</i>
Alstohentine	<i>Alstonia angustifolia</i> ; <i>Alstonia angustifolia</i> var. <i>latifolia</i>
Alstonisine	<i>Alstonia angustifolia</i>
Alstomaline	<i>Alstonia angustifolia</i> ; <i>Alstonia angustifolia</i> var. <i>latifolia</i>
N1-Demethylalstophylline	<i>Alstonia angustifolia</i> ; <i>Alstonia angustifolia</i> var. <i>latifolia</i>
(-)-Vincamajine	<i>Alstonia angustifolia</i> var. <i>latifolia</i>
Isopongaflavone	<i>Pongamia pinnata</i> ; <i>Tephrosia purpurea</i>
Pongaglabol methyl ether	<i>Pongamia pinnata</i> ; <i>Tephrosia purpurea</i>
Kanjone	<i>Pongamia pinnata</i> ; <i>Tephrosia purpurea</i>

Lanceolatin B	<i>Pongamia pinnata</i>
Glabranin	<i>Pongamia pinnata</i>
Purpurenone	<i>Millettia pinnata</i>
O-Methylpongamol	<i>Millettia pinnata</i>
Purpuritenin B	<i>Millettia pinnata</i>
Pinnatin	<i>Millettia pinnata</i>
Piscisoflavone D	<i>Millettia pinnata</i>
Praecansone B	<i>Millettia pinnata</i>
Ovalichromene B	<i>Millettia pinnata</i>
Piscisoflavone A	<i>Neorautanenia amboensis</i>
Millettone	<i>Neorautanenia amboensis</i>
Pongachalcone I	<i>Tephrosia purpurea</i>
Pongapinnol D	<i>Tephrosia purpurea</i>
Karanjachromene	<i>Tephrosia purpurea</i>
Dihydroamorphigenin	<i>Tephrosia purpurea; Piscidia erythrina</i>
Dalpanol	<i>Tephrosia purpurea; Piscidia erythrina</i>
Amorphigenol	<i>Tephrosia purpurea; Piscidia erythrina</i>
Amorphigenin	<i>Tephrosia purpurea; Piscidia erythrina</i>
Jamaicin	<i>Tephrosia purpurea; Amorpha fruticosa</i>
Ichthyone	<i>Tephrosia purpurea; Amorpha fruticosa</i>
Dehydromillettone	<i>Tephrosia purpurea; Amorpha fruticosa</i>
3-O-Demethylamorphigenin	<i>Tephrosia purpurea; Piscidia erythrina</i>
Rotenone	<i>Amorpha fruticosa</i>
Candidone	<i>Piscidia erythrina</i>
Dehydrodeguelin	<i>Piscidia erythrina</i>
Ambofuranol	<i>Piscidia erythrina</i>
Neorautenanol	<i>Piscidia erythrina</i>
Isopongachromene	<i>Piscidia erythrina</i>
Blestrianol A	<i>Gymnadenia conopsea</i>
Blestrin A	<i>Gymnadenia conopsea</i>
Blestrin B	<i>Gymnadenia conopsea</i>
Blestrin C	<i>Gymnadenia conopsea</i>
Blestrin D	<i>Gymnadenia conopsea</i>
Isoarundinin-II	<i>Gymnadenia conopsea</i>
Bulbocodin C	<i>Bletilla striata</i>
Bulbocodin D	<i>Bletilla striata</i>
Gymconopin C	<i>Bletilla striata</i>
Bulbocol	<i>Bletilla striata</i>
Gymconopin D	<i>Bletilla striata</i>
12-Methylferruginol	<i>Taiwania cryptomerioides</i>
Pisiferal	<i>Taiwania cryptomerioides</i>

(-)-Nortrachelogenin	<i>Taiwania cryptomerioides; Cryptomeria japonica</i>
Matairesinol	<i>Chamaecyparis formosensis</i>
Cryptomeridiol	<i>Chamaecyparis formosensis</i>
Cubeb camphor	<i>Chamaecyparis formosensis</i>
Epicubebol	<i>Chamaecyparis formosensis</i>
Diphyllin	<i>Chamaecyparis formosensis</i>
Sandaracopimarinal	<i>Chamaecyparis formosensis</i>
Sugiol	<i>Chamaecyparis formosensis</i>
3,7,4'-Tri-O-methylkaempferol	<i>Chamaecyparis formosensis</i>
19-Hydroxyferruginol	<i>Chamaecyparis formosensis</i>
Pisiferanol	<i>Cryptomeria japonica</i>
Pisiferol	<i>Cryptomeria japonica</i>
Chaenocephalol	<i>Cryptomeria japonica</i>
(-)-Pluviatolide	<i>Cryptomeria japonica</i>
12-O-Methylpisiferanol	<i>Cryptomeria japonica</i>
alpha-Cadinol	<i>Cryptomeria japonica</i>
Sugiol methyl ether	<i>Cryptomeria japonica</i>
(+)-beta-Cyclocostunolide	<i>Artemisia spp.</i>
Arbusculin C	<i>Saussurea lappa</i>
Nortetraphyllicine	<i>Tabernaemontana coffeoides</i>
Vincamine	<i>Kopsia dasyrachis</i>
Ajmalicine	<i>Kopsia dasyrachis; Rauwolfia vomitoria</i>
Sarpagine	<i>Catharanthus roseus</i>
Alstonine	<i>Catharanthus roseus</i>
(+)-Isoeburnamine	<i>Catharanthus roseus</i>
(+)-Eburnamonine	<i>Catharanthus roseus</i>
14,15-Dihydroxyvincadifformine	<i>Catharanthus roseus</i>
Serpentine	<i>Rauwolfia vomitoria</i>
10-O-Methylsarpagine	<i>Rauwolfia vomitoria</i>
Dulcisxanthone B	<i>Garcinia mangostana</i>
Cowaxanthone D	<i>Garcinia mangostana</i>
Isonormangostin	<i>Garcinia mangostana</i>
Normangostin	<i>Garcinia dulcis</i>
Garcinone C	<i>Garcinia dulcis</i>
Mangostenone D	<i>Garcinia dulcis</i>
Mangostenone E	<i>Garcinia dulcis</i>
Tovophyllin B	<i>Garcinia dulcis</i>
Arborinine	<i>Severinia buxifolia</i>
Xanthoxyletin	<i>Ruta graveolens</i>
Clausamine A	<i>Ruta graveolens</i>
1,2,3-Trihydroxyacridone	<i>Ruta graveolens</i>

Bergapten	<i>Clausena excavata</i>
Psoralen	<i>Clausena excavata</i>
Rutacridone	<i>Clausena excavata</i>
Isoscopoletin	<i>Zanthoxylum simulans</i>
N-Methylflindersine	<i>Zanthoxylum simulans</i>
(-)-5-Methoxybalanophonin	<i>Zanthoxylum simulans</i>
beta-Sitosterone	<i>Zanthoxylum integrifoliolum</i>
Sepesteonol	<i>Zanthoxylum integrifoliolum</i>
Zanthobungeanine	<i>Zanthoxylum integrifoliolum</i>
Flindersine	<i>Zanthoxylum integrifoliolum</i>
Scopoletin	<i>Broussonetia papyrifera</i>
Sanggenon L	<i>Broussonetia papyrifera</i>
Gemichalcone B	<i>Broussonetia papyrifera</i>
Gemichalcone C	<i>Broussonetia papyrifera</i>
Artocommunol CA	<i>Morus alba</i>
Artocommunol CE	<i>Morus alba</i>
Marmesin	<i>Morus alba</i>
Dihydrocycloartomunin	<i>Morus alba</i>
Dihydroisocycloartomunin	<i>Morus alba</i>
Cycloartomunin	<i>Morus alba</i>
Artochamin D	<i>Morus alba</i>
Brousoflavonol A	<i>Morus alba</i>
(-)-Cycloartocarpin	<i>Morus alba</i>
Morusin	<i>Artocarpus communis</i>
Sanggenon M	<i>Artocarpus communis</i>
Cyclomulberrin	<i>Artocarpus communis</i>
Sanggenon A	<i>Artocarpus communis</i>
Mulberrin	<i>Artocarpus communis</i>
Demethoxyisogemichalcone C	<i>Artocarpus communis</i>
Isogemichalcone C	<i>Artocarpus communis</i>
Calystegin B2	<i>Lycium chinense</i>
Atropine	<i>Lycium chinense</i>
Calystegine B4	<i>Mandragora autumnalis</i>
Baccatin V	<i>Taxus cuspidata; Taxus brevifolia; Taxus wallichiana; Taxus chinensis; Taxus mairei; Taxus yunnanensis</i>
Taxol D	<i>Taxus cuspidata; Taxus chinensis; Taxus yunnanensis</i>
Dantaxusin D	<i>Taxus cuspidata; Taxus baccata; Taxus chinensis; Taxus mairei</i>
9-Deacetyltaxininine	<i>Taxus cuspidata; Taxus chinensis; Taxus mairei; Taxus yunnanensis</i>
Taxchin B	<i>Taxus cuspidata; Taxus baccata; Taxus mairei; Taxus yunnanensis</i>
Taxinine B	<i>Taxus cuspidata; Taxus chinensis</i>
Taxine I	<i>Taxus cuspidata; Taxus chinensis</i>

Taxumairol A	<i>Taxus cuspidata; Taxus baccata; Taxus chinensis</i>
Taxchinin H	<i>Taxus cuspidata; Taxus brevifolia</i>
Taxol B	<i>Taxus cuspidata</i>
Dantaxusin A	<i>Taxus cuspidata; Taxus baccata; Taxus chinensis; Taxus mairei</i>
Taxayuntin E	<i>Taxus cuspidata; Taxus chinensis</i>
Taxayuntin F	<i>Taxus cuspidata</i>
Taxchinin A	<i>Taxus cuspidata</i>
Taxchinin D	<i>Taxus cuspidata; Taxus baccata; Taxus wallichiana</i>
Taxchinin C	<i>Taxus cuspidata; Taxus brevifolia; Taxus yunnanensis</i>
Taxchinin K	<i>Taxus cuspidata; Taxus brevifolia; Taxus yunnanensis</i>
Taxayuntin H	<i>Taxus cuspidata; Taxus brevifolia; Taxus baccata; Taxus wallichiana; Taxus mairei</i>
Baccatin IV	<i>Taxus cuspidata; Taxus yunnanensis</i>
Taxamairin B	<i>Taxus cuspidata</i>
Dantaxusin C	<i>Taxus cuspidata; Taxus baccata; Taxus mairei</i>
Taxinine A	<i>Taxus cuspidata</i>
7-Deacetylcandensene	<i>Taxus cuspidata; Taxus baccata</i>
Chinentaxunine	<i>Taxus cuspidata</i>
N-Methyltaxol C	<i>Taxus cuspidata; Taxus chinensis; Taxus yunnanensis</i>
14beta-benzoyloxybaccatin IV	<i>Taxus cuspidata; Taxus baccata; Taxus mairei</i>
5-Decinamoyltaxuspine D	<i>Taxus cuspidata; Taxus yunnanensis</i>
5-Cinnamoyltaxicin I triacetate	<i>Taxus cuspidata; Taxus chinensis; Taxus mairei; Taxus yunnanensis</i>
5-epi-Canadensene	<i>Taxus cuspidata; Taxus chinensis; Taxus mairei</i>
7,2'-Bisdeacetoxyaustroscopicatine	<i>Taxus cuspidata</i>
Taxuspinanane I	<i>Taxus brevifolia; Taxus baccata; Taxus wallichiana; Taxus chinensis; Taxus mairei; Taxus yunnanensis</i>
Ormosin VI	<i>Taxus brevifolia; Taxus mairei</i>
Taxchinin B	<i>Taxus brevifolia; Taxus wallichiana</i>
Taxuspine V	<i>Taxus brevifolia; Taxus mairei</i>
14beta-Hydroxytaxusin	<i>Taxus brevifolia; Taxus baccata; Taxus wallichiana</i>
Epitaxol	<i>Taxus baccata; Taxus wallichiana; Taxus chinensis; Taxus mairei; Taxus yunnanensis</i>
Taxachitriene A	<i>Taxus baccata</i>
Taxachitriene B	<i>Taxus baccata</i>
Taxuspine S	<i>Taxus baccata; Taxus chinensis; Taxus mairei</i>
Taxezopidine L	<i>Taxus baccata; Taxus mairei</i>
Taxol C	<i>Taxus baccata</i>
Taxuspinanane A	<i>Taxus baccata; Taxus chinensis; Taxus yunnanensis</i>
Taxinine E	<i>Taxus baccata; Taxus chinensis</i>
Taxuspine Z	<i>Taxus baccata; Taxus wallichiana</i>
Taxezopidine E	<i>Taxus baccata</i>
Taxuspine X	<i>Taxus baccata</i>
Taxezopidine F	<i>Taxus baccata; Taxus yunnanensis</i>

Taxuyunnanine C	<i>Taxus baccata</i>
Taxuspinanane B	<i>Taxus baccata; Taxus wallichiana; Taxus chinensis</i>
Ponasterone A	<i>Taxus baccata; Taxus chinensis</i>
Decinnamoyltaxinine E	<i>Taxus baccata</i>
Taxezopidine H	<i>Taxus baccata; Taxus mairei</i>
Taxuspine D	<i>Taxus baccata; Taxus mairei</i>
Taxin B	<i>Taxus baccata</i>
Taxuspine U	<i>Taxus baccata; Taxus mairei</i>
5-Deacetyltaxachitriene B	<i>Taxus baccata</i>
2-Deacetyltaxachitriene A	<i>Taxus baccata</i>
Taxuspine A	<i>Taxus wallichiana; Taxus chinensis</i>
Taxuspine P	<i>Taxus wallichiana; Taxus yunnanensis</i>
Isolariciresinol	<i>Taxus wallichiana; Taxus yunnanensis</i>
Taxuspine T	<i>Taxus chinensis; Taxus mairei</i>
Taxine II	<i>Taxus chinensis</i>
Taxuspine B	<i>Taxus chinensis; Taxus mairei</i>
Taxuspine E	<i>Taxus chinensis; Taxus yunnanensis</i>
Taxayuntin J	<i>Taxus chinensis; Taxus mairei</i>
Taxumairol F	<i>Taxus chinensis; Taxus yunnanensis</i>
Deaminoacyltaxine A	<i>Taxus chinensis; Taxus mairei; Taxus yunnanensis</i>
Isotaxine B	<i>Taxus chinensis; Taxus yunnanensis</i>
Taxinine H	<i>Taxus chinensis; Taxus mairei</i>
Dantaxusin B	<i>Taxus chinensis; Taxus mairei</i>
Taxayuntin A	<i>Taxus chinensis</i>
2-Deacetyldecinamoyltaxinine E	<i>Taxus chinensis; Taxus mairei</i>
Taxuyunnanine N	<i>Taxus mairei</i>
10-Deacetyltaxol A	<i>Taxus mairei</i>
13-Deacetoxybaccatin I	<i>Taxus mairei; Taxus yunnanensis</i>
Taxumairol V	<i>Taxus yunnanensis</i>
Taxchinin I	<i>Taxus yunnanensis</i>
Methyl pyroglutamate	<i>Panax notoginseng</i>
Ginsenoside Rh7	<i>Panax notoginseng; Panax pseudo-ginseng var. notoginseng</i>
Ginsenoyne E	<i>Panax ginseng; Panax pseudo-ginseng var. notoginseng</i>
Notoginsenoside	<i>Panax ginseng</i>
Panaxydol	<i>Panax pseudo-ginseng var. notoginseng</i>
Ginsenoside Re	<i>Panax pseudo-ginseng var. notoginseng</i>
Aristolactam IIIa	<i>Aristolochia elegans</i>
Aristolochate I	<i>Aristolochia elegans</i>
Aristolactam I	<i>Aristolochia elegans</i>
Methyl aristolochate	<i>Aristolochia elegans</i>
Aristolochate C	<i>Aristolochia elegans</i>

Aristolochic acid I	<i>Aristolochia heterophylla</i>
4-Hydroxybenzoic acid	<i>Aristolochia heterophylla</i>
O-Methylflavinantine	<i>Artabotrys uncinatus</i>
Pallidine	<i>Artabotrys uncinatus</i>
Norpallidine	<i>Artabotrys uncinatus</i>
Lysicamine	<i>Artabotrys uncinatus</i>
Flavinantine	<i>Annona purpurea</i>