

APPENDIX 1

1. THE 69 PLANTS AND EVIDENCE OF THEIR USE IN ALOPECIA

Plant name	Family	Reference of use in alopecia/hair loss
<i>Acacia concinna</i>	Fabaceae	Agrawal, S.S., Ahmad, M. and Mazhar, M., Therapeutic Potential of Some Medicinal Plants in Alopecia.
<i>Albizia julibrissin</i>	Fabaceae	Lee, J.Y., Im, K.R., Jung, T.K., Lee, M.H. and Yoon, K.S., 2012. Medicinal herbal complex extract with potential for hair growth-promoting activity. <i>Journal of the Society of Cosmetic Scientists of Korea</i> , 38(4), pp.277-287.
<i>Allium cepa</i>	Amaryllidaceae	Singh, R., Tripathi, S., Gupta, D. and Pujari, N.M., 2022. Evaluation of Pharmacognostical Properties And Hair Growth Promoting Activity Of <i>Allium cepa</i> . <i>Journal of Pharmaceutical Negative Results</i> , pp.3768-3773.
<i>Allium sativum</i>	Amaryllidaceae	Bassino, E., Gasparri, F. and Munaron, L., 2020. Protective role of nutritional plants containing flavonoids in hair follicle disruption: A review. <i>International Journal of Molecular Sciences</i> , 21(2), p.523.
<i>Aloe vera</i>	Asphodelaceae	Rathi, V., Rathi, J., Tamizharasi, S. and Pathak, A., 2008. Plants used for hair growth promotion: A review. <i>Pharmacognosy Reviews</i> , 2(3), p.185.
<i>Alpinia zerumbet</i>	Zingiberaceae	Taira, N., Nguyen, B.C.Q. and Tawata, S., 2017. Hair growth promoting and anticancer effects of p21-activated kinase 1 (PAK1) inhibitors isolated from different parts of <i>Alpinia zerumbet</i> . <i>Molecules</i> , 22(1), p.132.
<i>Ammi majus</i>	Apiaceae	Bhagavathula, A.S., Al-Khatib, A.J.M., Elnour, A.A., Al Kalbani, N.M. and Shehab, A., 2015. <i>Ammi Visnaga</i> in treatment of urolithiasis and hypertriglyceridemia. <i>Pharmacognosy research</i> , 7(4), p.397.
<i>Andrographis paniculata</i>	Acanthaceae	Kumar, N., Rungseevijitprapa, W., Narkkhong, N.A., Suttajit, M. and Chaiyasut, C., 2012. 5 α -reductase inhibition and hair growth promotion of some Thai plants traditionally used for hair treatment. <i>Journal of ethnopharmacology</i> , 139(3), pp.765-771.
<i>Angelica dahurica</i>	Apiaceae	Leem, J., Jung, W., Kim, Y., Kim, B. and Kim, K., 2018. Exploring the combination and modular characteristics of herbs for alopecia treatment in traditional Chinese medicine: an association rule mining and network analysis study. <i>BMC complementary and alternative medicine</i> , 18(1), pp.1-13.
<i>Angelica gigas</i>	Apiaceae	Lee, Y.G. and Kim, J.K., 2004. The study of the oriental medicine extract on the hair growth Effect: I. The effect of the mixture extract of <i>Polygoni multiflori Radix</i> , <i>Angelicae gigantis Radix</i> and <i>Lycii Fructus</i> on the hair growth. <i>The Korea Journal of Herbology</i> , 19(2), pp.83-83.
<i>Angelica sinensis</i>	Apiaceae	Leem, J., Jung, W., Kim, Y., Kim, B. and Kim, K., 2018. Exploring the combination and modular characteristics of herbs for alopecia treatment in traditional Chinese medicine: an association rule mining and network analysis study. <i>BMC complementary and alternative medicine</i> , 18(1), pp.1-13.
<i>Artemisia abrotanum</i>	Asteraceae	Ekiert, H., Knut, E., Świątkowska, J., Klin, P., Rzepiela, A., Tomczyk, M. and Szopa, A., 2021. <i>Artemisia abrotanum</i> L.(Southern Wormwood)—History, Current Knowledge on the Chemistry, Biological Activity, Traditional Use and Possible New Pharmaceutical and Cosmetological Applications. <i>Molecules</i> , 26(9), p.2503.
<i>Averrhoa carambola</i>	Oxalidaceae	Kumar, N., Rungseevijitprapa, W., Narkkhong, N.A., Suttajit, M. and Chaiyasut, C., 2012. 5 α -reductase inhibition and hair growth

		promotion of some Thai plants traditionally used for hair treatment. Journal of ethnopharmacology, 139(3), pp.765-771.
<i>Avicennia marina</i>	Acanthaceae	Jain, R., Monthakantirat, O., Tengamnuay, P. and De-Eknamkul, W., 2014. Avicequinone C isolated from <i>Avicennia marina</i> exhibits 5 α -reductase-type 1 inhibitory activity using an androgenic alopecia relevant cell-based assay system. <i>Molecules</i> , 19(5), pp.6809-6821.
<i>Azadirachta indica</i>	Meliaceae	Uchegbu, M., Okoli, I., Esonu, B. and Iloeje, M., 2011. The growing importance of neem (<i>Azadirachta indica</i> A. Juss) in agriculture, industry, medicine and Environment: A review. <i>Research Journal of Medicinal Plant</i> , 5(3), pp.230-245.
<i>Bidens tripartita</i>	Asteraceae	Jellin, J.M., Batz, F. and Hitchens, K., 2004. Natural medicines comprehensive database. Therapeutic Research Faculty.
<i>Camellia sinensis</i>	Theaceae	Dhariwala, M.Y. and Ravikumar, P., 2019. An overview of herbal alternatives in androgenetic alopecia. <i>Journal of cosmetic dermatology</i> , 18(4), pp.966-975.
<i>Carthamus tinctorius</i>	Asteraceae	Kumar, N., Rungseevijitprapa, W., Narkkhong, N.A., Suttajit, M. and Chaiyasut, C., 2012. 5 α -reductase inhibition and hair growth promotion of some Thai plants traditionally used for hair treatment. <i>Journal of ethnopharmacology</i> , 139(3), pp.765-771.
<i>Cedrus deodara</i>	Pinaceae	Chaudhary, A., Kaur, P., Singh, B. and Pathania, V., 2009. Chemical composition of hydrodistilled and solvent volatiles extracted from woodchips of Himalayan <i>Cedrus deodara</i> (Roxb.) Loud. <i>Natural product communications</i> , 4(9), p.1934578X0900400920.
<i>Chrysanthemum morifolium</i>	Asteraceae	Wiart, C., 2007. <i>Ethnopharmacology of medicinal plants: Asia and the Pacific</i> . Springer Science & Business Media.
<i>Chrysanthemum zawadskii</i>	Asteraceae	Li, Z., Li, J., Gu, L., Begum, S., Wang, Y., Sun, B., Lee, M. and Sung, C., 2014. <i>Chrysanthemum zawadskii</i> extract induces hair growth by stimulating the proliferation and differentiation of hair matrix. <i>International Journal of Molecular Medicine</i> , 34(1), pp.130-136.
<i>Clitoria ternatea</i>	Fabaceae	Kumar, N., Rungseevijitprapa, W., Narkkhong, N.A., Suttajit, M. and Chaiyasut, C., 2012. 5 α -reductase inhibition and hair growth promotion of some Thai plants traditionally used for hair treatment. <i>Journal of ethnopharmacology</i> , 139(3), pp.765-771.
<i>Cnidium officinale</i>	Apiaceae	Lee, J.Y., Im, K.R., Jung, T.K., Lee, M.H. and Yoon, K.S., 2012. Medicinal herbal complex extract with potential for hair growth-promoting activity. <i>Journal of the Society of Cosmetic Scientists of Korea</i> , 38(4), pp.277-287.
<i>Coffea arabica</i>	Rubiaceae	Bassino, E., Gasparri, F. and Munaron, L., 2020. Protective role of nutritional plants containing flavonoids in hair follicle disruption: A review. <i>International Journal of Molecular Sciences</i> , 21(2), p.523.
<i>Corydalis turtschaninovii</i>	Papaveraceae	WO2022055218 - COMPOSITION FOR PREVENTING OR TREATING HAIR LOSS, COMPRISING EXTRACT OF CORYDALIS YANHUSUO. https://patentscope.wipo.int/search/en/detail.jsf?docId=WO2022055218
<i>Cullen corylifolium</i>	Fabaceae	Khushboo, P.S., Jadhav, V.M., Kadam, V.J. and Sathe, N.S., 2010. <i>Psoralea corylifolia</i> Linn.—“Kushtanashini”. <i>Pharmacognosy reviews</i> , 4(7), p.69.
<i>Curcuma longa</i>	Zingiberaceae	Vaughn, A.R., Branum, A. and Sivamani, R.K., 2016. Effects of turmeric (<i>Curcuma longa</i>) on skin health: a systematic review of the clinical evidence. <i>Phytotherapy Research</i> , 30(8), pp.1243-1264.
<i>Cuscuta reflexa</i>	Convolvulaceae	Patni, P., Varghese, D., Balekar, N. and Jain, D.K., 2006. Formulation and evaluation of herbal hair oil for alopecia management. <i>Planta indica</i> , 2(3), pp.27-30.

<i>Cynomorium songaricum</i>	Cynomoriaceae	Zhang, X., Gu, C., Ahmad, B. and Huang, L., 2017. Optimization of extract method for <i>Cynomorium songaricum</i> Rupr. by response surface methodology. <i>Journal of analytical methods in chemistry</i> , 2017.
<i>Eclipta prostrata</i>	Asteraceae	Agrawal, S.S., Ahmad, M. and Mazhar, M., Therapeutic Potential of Some Medicinal Plants in Alopecia.
<i>Illicium anisatum</i>	Schisandraceae	Damodaran, R.G. and Gupta, R., 2011. Hair loss and the applied techniques for identification of novel hair growth promoters for hair re-growth. <i>Pharmacognosy Journal</i> , 3(22), pp.1-5.
<i>Impatiens balsamina</i>	Balsaminaceae	Zheng, Y., Hu, Y., Liu, K., Lu, Y. and Zhou, X., 2019. Therapeutic effect of <i>Impatiens balsamina</i> , <i>Lawsonia inermis</i> L. and Henna on androgenetic alopecia in mice. <i>Nan Fang yi ke da xue xue bao= Journal of Southern Medical University</i> , 39(11), pp.1376-1380.
<i>Jatropha gossypifolia</i>	Euphorbiaceae	Ajose, F.O., 2007. Some Nigerian plants of dermatologic importance. <i>International Journal of Dermatology</i> , 46, pp.48-55.
<i>Larrea divaricata</i>	Zygophyllaceae	Davicino, R., Martino, R. and Anesini, C., 2011. <i>Larrea divaricata</i> Cav.: Scientific evidence showing its beneficial effects and its wide potential application. <i>Boletín Latinoamericano y del Caribe de Plantas Medicinales y Aromáticas</i> , 10(2), pp.92-103.
<i>Lawsonia inermis</i>	Lythraceae	Alzweiri, M., Al Sarhan, A., Mansi, K., Hudaib, M. and Aburjai, T., 2011. Ethnopharmacological survey of medicinal herbs in Jordan, the Northern Badia region. <i>Journal of Ethnopharmacology</i> , 137(1), pp.27-35.
<i>Leonurus sibiricus</i>	Lamiaceae	Lee, J.Y., Im, K.R., Jung, T.K., Lee, M.H. and Yoon, K.S., 2012. Medicinal herbal complex extract with potential for hair growth-promoting activity. <i>Journal of the Society of Cosmetic Scientists of Korea</i> , 38(4), pp.277-287.
<i>Ligusticum sinense</i>	Apiaceae	Leem, J., Jung, W., Kim, Y., Kim, B. and Kim, K., 2018. Exploring the combination and modular characteristics of herbs for alopecia treatment in traditional Chinese medicine: an association rule mining and network analysis study. <i>BMC complementary and alternative medicine</i> , 18(1), pp.1-13.
<i>Ligustrum lucidum</i>	Oleaceae	Leem, J., Jung, W., Kim, Y., Kim, B. and Kim, K., 2018. Exploring the combination and modular characteristics of herbs for alopecia treatment in traditional Chinese medicine: an association rule mining and network analysis study. <i>BMC complementary and alternative medicine</i> , 18(1), pp.1-13.
<i>Lycium chinense</i>	Solanaceae	Seo, S.R., Kang, G., Ha, J.W. and Kim, J.C., 2013. In vivo hair growth-promoting efficacies of herbal extracts and their cubosomal suspensions. <i>Journal of Industrial and Engineering Chemistry</i> , 19(4), pp.1331-1339.
<i>Lycopersicon esculentum</i>	Solanaceae	Choi, J.S., Jung, S.K., Jeon, M.H., Moon, J.N., Moon, W.S., Ji, Y.H., Choi, I.S. and Son, W., 2013. Effects of <i>Lycopersicon esculentum</i> extract on hair growth and alopecia prevention. <i>Journal of cosmetic science</i> , 64(6), pp.429-443.
<i>Mimosa pudica</i>	Fabaceae	Patro, G., Bhattamisra, S.K., Mohanty, B.K. and Sahoo, H.B., 2016. In vitro and in vivo antioxidant evaluation and estimation of total phenolic, flavonoidal content of <i>Mimosa pudica</i> L. <i>Pharmacognosy research</i> , 8(1), p.22.
<i>Morus alba</i>	Moraceae	Li, X., Zhou, Y., Xu, M., Fu, K., Wang, Z., Sun, M. and Cao, M., 2020. Data mining on varieties, therapeutic uses and medicinal characteristics of Traditional Chinese Medicine preparations for treating hair loss. <i>Tropical Journal of Pharmaceutical Research</i> , 19(11), pp.2461-2475.
<i>Nerium oleander</i>	Apocynaceae	Chaudhary, K., Prasad, D.N. and Sandhu, B.S., 2015. Preliminary pharmacognostic and phytochemical studies on <i>Nerium oleander</i>

		Linn.(White cultivar). Journal of Pharmacognosy and Phytochemistry, 4(1).
<i>Ocimum sanctum</i>	Lamiaceae	Bind, N. and Maury, S., 2022. REVIEW ON HERBAL HAIR OIL FOR PREVENT HAIR LOSS.
<i>Oryza sativa</i>	Poaceae	Choi, J.S., Jeon, M.H., Moon, W.S., Moon, J.N., Cheon, E.J., Kim, J.W., Jung, S.K., Ji, Y.H., Son, S.W. and Kim, M.R., 2014. In vivo hair growth-promoting effect of rice bran extract prepared by supercritical carbon dioxide fluid. Biological and Pharmaceutical Bulletin, 37(1), pp.44-53.
<i>Panax ginseng</i>	Araliaceae	Bassino, E., Gasparri, F. and Munaron, L., 2020. Protective role of nutritional plants containing flavonoids in hair follicle disruption: A review. International Journal of Molecular Sciences, 21(2), p.523.
<i>Platyclus orientalis</i>	Cupressaceae	Zhang, Y., Han, L., Chen, S.S., Guan, J., Qu, F.Z. and Zhao, Y.Q., 2016. Hair growth promoting activity of cedrol isolated from the leaves of <i>Platyclus orientalis</i> . Biomedicine & Pharmacotherapy, 83, pp.641-647.
<i>Prunus persica</i>	Rosaceae	Lee, J.Y., Im, K.R., Jung, T.K., Lee, M.H. and Yoon, K.S., 2012. Medicinal herbal complex extract with potential for hair growth-promoting activity. Journal of the Society of Cosmetic Scientists of Korea, 38(4), pp.277-287.
<i>Pueraria thomsonii</i>	Fabaceae	Dawid-Pac, R., Urbanska, M., Deboz, I. and Nowak, G., 2014. Plants as potential active components in treatment of androgenetic alopecia. Herba polonica, 60(1).
<i>Rehmannia glutinosa</i>	Orobanchaceae	Li, X., Zhou, Y., Xu, M., Fu, K., Wang, Z., Sun, M. and Cao, M., 2020. Data mining on varieties, therapeutic uses and medicinal characteristics of Traditional Chinese Medicine preparations for treating hair loss. Tropical Journal of Pharmaceutical Research, 19(11), pp.2461-2475.
<i>Rhinacanthus nasutus</i>	Acanthaceae	Kumar, N., Rungseevijitprapa, W., Narkkhong, N.A., Suttajit, M. and Chaiyasut, C., 2012. 5 α -reductase inhibition and hair growth promotion of some Thai plants traditionally used for hair treatment. Journal of ethnopharmacology, 139(3), pp.765-771.
<i>Rubus coreanus</i>	Rosaceae	Kim, P.S., Kim, H.T., Roh, S.S. and Hwang, C.Y., 2004. Effect of Danguibohyultangami-bang on the alopecia and hair growth stimulation. The Journal of Korean Medicine Ophthalmology and Otolaryngology and Dermatology, 17(3), pp.38-60.
<i>Salvia miltiorrhiza</i>	Lamiaceae	Li, X., Zhou, Y., Xu, M., Fu, K., Wang, Z., Sun, M. and Cao, M., 2020. Data mining on varieties, therapeutic uses and medicinal characteristics of Traditional Chinese Medicine preparations for treating hair loss. Tropical Journal of Pharmaceutical Research, 19(11), pp.2461-2475.
<i>Salvia rosmarinus</i>	Lamiaceae	de Macedo, L.M., Santos, É.M.D., Militão, L., Tundisi, L.L., Ataide, J.A., Souto, E.B. and Mazzola, P.G., 2020. Rosemary (<i>Rosmarinus officinalis</i> L., syn <i>Salvia rosmarinus</i> Spenn.) and its topical applications: a review. Plants, 9(5), p.651.
<i>Sapindus rarak</i>	Sapindaceae	Kumar, N., Rungseevijitprapa, W., Narkkhong, N.A., Suttajit, M. and Chaiyasut, C., 2012. 5 α -reductase inhibition and hair growth promotion of some Thai plants traditionally used for hair treatment. Journal of ethnopharmacology, 139(3), pp.765-771.
<i>Scutellaria baicalensis</i>	Lamiaceae	Herman, A. and Herman, A.P., 2016. Mechanism of action of herbs and their active constituents used in hair loss treatment. Fitoterapia, 114, pp.18-25.
<i>Serenoa repens</i>	Arecaceae	Chatterjee, S. and Agrawala, S.K., 2003. Saw palmetto (<i>Serenoa repens</i>) in androgenic alopecia An effective phytotherapy.

<i>Sesamum indicum</i>	Pedaliaceae	Gupta, A., Malviya, R., Singh, T.P. and Sharma, P.K., 2010. Indian medicinal plants used in hair care cosmetics: a short review. <i>Pharmacognosy Journal</i> , 2(10), pp.361-364.
<i>Solanum nigrum</i>	Solanaceae	Mukhopadhyay, G., Sarkar, S., Kundu, S., Kundu, S., Sarkar, P., Sarkar, S., Sengupta, R., Kumar, C., Mitra, S., Jain, D. and Sodani, A., 2018. Ethno-pharmacological activity of <i>Solanum nigrum</i> .
<i>Sophora flavescens</i>	Fabaceae	Roh, S.S., Kim, C.D., Lee, M.H., Hwang, S.L., Rang, M.J. and Yoon, Y.K., 2002. The hair growth promoting effect of <i>Sophora flavescens</i> extract and its molecular regulation. <i>Journal of dermatological science</i> , 30(1), pp.43-49.
<i>Tamus communis</i>	Dioscoreaceae	Slavova, I., Tomova, T., Kusovska, S., Chukova, Y. and Argirova, M., 2022. Phytochemical Constituents and Pharmacological Potential of <i>Tamus communis</i> Rhizomes. <i>Molecules</i> , 27(6), p.1851.
<i>Terminalia bellirica</i>	Combretaceae	Kumari, S., Joshi, A.B., Gurav, S., Bhandarkar, A.V., Agarwal, A., Deepak, M. and Gururaj, G.M., 2017. A pharmacognostic, phytochemical and pharmacological review of <i>Terminalia bellerica</i> . <i>Journal of Pharmacognosy and Phytochemistry</i> , 6(5), pp.368-376.
<i>Terminalia chebula</i>	Combretaceae	Sharma, R., Kumar, S. and Jain, S., 2021. An Ayurveda approach to Androgenetic Alopecia (Khalitya)-A Case Study. <i>Journal of Ayurveda and Integrated Medical Sciences</i> , 6(01), pp.341-346.
<i>Thuja occidentalis</i>	Cupressaceae	Park, W.S., Lee, C.H., Lee, B.G. and Chang, I.S., 2003. The extract of <i>Thuja occidentalis</i> semen inhibited 5 α -reductase and androchronogenetic alopecia of B6CBAF1/j hybrid mouse. <i>Journal of dermatological science</i> , 31(2), pp.91-98.
<i>Trichosanthes cucumerina</i>	Cucurbitaceae	Kumar, N., Rungseevijitprapa, W., Narkkhong, N.A., Suttajit, M. and Chaiyasut, C., 2012. 5 α -reductase inhibition and hair growth promotion of some Thai plants traditionally used for hair treatment. <i>Journal of ethnopharmacology</i> , 139(3), pp.765-771.
<i>Trifolium pratense</i>	Fabaceae	Zgonc Škulj, A., Poljšak, N., Kočevar Glavač, N. and Kreft, S., 2020. Herbal preparations for the treatment of hair loss. <i>Archives of dermatological research</i> , 312(6), pp.395-406.
<i>Viscum album</i>	Viscaceae	Kleszken, E., Timar, A.V., Memete, A.R., Miere, F. and Vicas, S.I., 2022. On Overview Of Bioactive Compounds, Biological And Pharmacological Effects Of Mistletoe (<i>Viscum Album</i> L). <i>Pharmacophore</i> , 13(1), pp.10-26.
<i>Zingiber officinale</i>	Zingiberaceae	Kumar, N., Rungseevijitprapa, W., Narkkhong, N.A., Suttajit, M. and Chaiyasut, C., 2012. 5 α -reductase inhibition and hair growth promotion of some Thai plants traditionally used for hair treatment. <i>Journal of ethnopharmacology</i> , 139(3), pp.765-771.
<i>Ziziphus jujuba</i>	Rhamnaceae	Yoon, J.I., Al-Reza, S.M. and Kang, S.C., 2010. Hair growth promoting effect of <i>Zizyphus jujuba</i> essential oil. <i>Food and chemical toxicology</i> , 48(5), pp.1350-1354.

2. SPECIMEN OF THE PLANTS-PHYTOCHEMICALS DATABASE

Plant	Phytochemical	PubChe mCID	PMID	Other Reference
<i>Acacia concinna</i>	oxalic acid	971		https://www.thieme-connect.com/products/ejournals/abstract/10.1055/s-0028-1099805

<i>Acacia concinna</i>	nicotine	89594		https://www.thieme-connect.com/products/ejournals/abstract/10.1055/s-0028-1099805
<i>Acacia concinna</i>	kinmoonoside A	1010881 24	11141 109	
<i>Acacia concinna</i>	kinmoonoside B	1010881 25	11141 109	
<i>Acacia concinna</i>	kinmoonoside C	1010881 26	11141 109	
<i>Acacia concinna</i>	tartaric acid	875		https://www.thieme-connect.com/products/ejournals/abstract/10.1055/s-0028-1099805
<i>Acacia concinna</i>	citric acid	311		https://www.thieme-connect.com/products/ejournals/abstract/10.1055/s-0028-1099805
<i>Acacia concinna</i>	succinic acid	1110		https://www.thieme-connect.com/products/ejournals/abstract/10.1055/s-0028-1099805
<i>Acacia concinna</i>	ascorbic acid	5467006 7		https://www.thieme-connect.com/products/ejournals/abstract/10.1055/s-0028-1099805
<i>Acacia concinna</i>	calycotomine	606033		https://www.thieme-connect.com/products/ejournals/abstract/10.1055/s-0028-1099805
<i>Acacia concinna</i>	rutin	5280805		https://www.thieme-connect.com/products/ejournals/abstract/10.1055/s-0028-1099805
<i>Albizia julibrissin</i>	p-hydroxybenzaldehyde	126	25282 893	
<i>Albizia julibrissin</i>	gallic acid	370	25282 893	
<i>Albizia julibrissin</i>	palmitic acid	985	25282 893	
<i>Albizia julibrissin</i>	vanillin	1183	25282 893	
<i>Albizia julibrissin</i>	stearic acid	5281	25282 893	
<i>Albizia julibrissin</i>	uridine	6029	25282 893	
<i>Albizia julibrissin</i>	2-furoic acid	6919	25282 893	
<i>Albizia julibrissin</i>	indole-3-carboxaldehyde	10256	25282 893	
<i>Albizia julibrissin</i>	2,3-dihydroxypropyl hexadecanoate	14900	25282 893	
<i>Albizia julibrissin</i>	indole-3-carboxylic acid	69867	22223 384	
<i>Albizia julibrissin</i>	3-ethoxy4-hydroxy-benzoic acid	95085	25282 893	

<i>Albizia julibrissin</i>	3,3'-dithiodipropanoic acid	95116	22223 384
<i>Albizia julibrissin</i>	5-(hydroxymethyl)-2-furaldehyde	237332	25282 893

3. EXAMPLE OF RESULTS OF APPLYING TOOL SERVICE 1

3A. QUERY MESH TERMS

1	x ("alopecia"[MeSH Terms] OR "alopecia"[All Fields] OR ("androgenetic"[All Fields] AND "alopecia"[All Fields]) OR "androgenetic alopecia"[All Fields]) AND ("plant s"[All Fields] OR "planted"[All Fields] OR "planting"[All Fields] OR "plantings"[All Fields] OR "plants"[MeSH Terms] OR "plants"[All Fields] OR "plant"[All Fields]) AND 1950/01/01:2021/12/31[Date - Entry]
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3B. SPECIMEN OF THE ARTICLES RETRIEVED WITH TOOL SERVICE 1 FOR ANDROGENETIC ALOPECIA PLANTS

	PMID	Title	Abstract
1	34959442	Modulation of Hair Growth Promoting Effect by Natural Products.	A large number of people suffer from alopecia or hair loss worldwide. Drug-based therapies using minoxidil and finasteride for the treatment of alopecia are available but they have shown various side effects in patients. Thus, the use of new therapeutic approaches using bioactive products to reduce the risk of anti-hair-loss medications has been emphasized. Natural products have been used since ancient times and have been proven safe with few side effects. Several studies have demonstrated the use of plants and their extracts to promote hair growth. Moreover, commercial products based on these natural ingredients have been developed for the treatment of alopecia. Several clinical animal and cell-based studies have been conducted to determine the anti-alopecia effects of plant-derived biochemicals. This review is a collective study of phytochemicals with anti-alopecia effects focusing mainly on the mechanisms underlying their hair-growth-promoting effects.

2	34921844	Dermatopathy caused by Tephrosia noctiflora intoxication in cattle.	An outbreak of a disease characterized by emaciation dermatitis with erythema alopecia foul-smelling exudation crusting hyperpigmentation lichenification and edema of fore- and hindlimbs chest and dewlap is described affecting cattle in the State of Alagoas Northeastern Brazil. Microscopically the main lesions were characterized by diffuse dermatitis with infiltration of lymphocytes histiocytes parakeratotic hyperkeratosis and acanthosis. The plant Tephrosia noctiflora which exhibited signs of consumption infested the grazing areas of cattle. To test its toxicity T. noctiflora was harvested dried in the shade crushed and sourced at a concentration of 50% mixed with commercial food for three guinea pigs. The main clinical signs in guinea pigs included weight loss and multifocal moderate to severe areas of alopecia diffuse erythema of the skin vaginal edema and hematuria. Microscopically lymphocytic and histiocytic dermatitis parakeratotic hyperkeratosis and acanthosis were noted in guinea pigs. This experiment confirms that T. noctiflora is the cause of outbreaks of dermatitis observed in cattle grazing in areas infested by this plant.
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APPENDIX 2

1. SPECIMEN OF THE ARTICLES USED FOR TEXT-MINING

1. Endocrine. 2017 Jul;57(1):9-17. doi: 10.1007/s12020-017-1280-y. Epub 2017 Mar 28.

Androgenetic alopecia: a review.

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PURPOSE: Androgenetic alopecia, commonly known as male pattern baldness, is the most common type of progressive hair loss disorder in men. The aim of this paper is to review recent advances in understanding the pathophysiology and molecular mechanism of androgenetic alopecia.

METHODS: Using the PubMed database, we conducted a systematic review of the literature, selecting studies published from 1916 to 2016.

RESULTS: The occurrence and development of androgenetic alopecia depends on the interaction of endocrine factors and genetic predisposition. Androgenetic

alopecia is characterized by progressive hair follicular miniaturization, caused by the actions of androgens on the epithelial cells of genetically susceptible hair follicles in androgen-dependent areas. Although the exact pathogenesis of androgenetic alopecia remains to be clarified, research has shown that it is a polygenetic condition. Numerous studies have unequivocally identified two major genetic risk loci for androgenetic alopecia, on the X-chromosome AR/EDA2R locus and the chromosome 20p11 locus.

CONCLUSIONS: Candidate gene and genome-wide association studies have reported that single-nucleotide polymorphisms at different genomic loci are associated with androgenetic alopecia development. A number of genes determine the predisposition for androgenetic alopecia in a polygenic fashion. However, further studies are needed before the specific genetic factors of this polygenic condition can be fully explained.

DOI: 10.1007/s12020-017-1280-y

PMID: 28349362 [Indexed for MEDLINE]

2. J Cosmet Dermatol. 2021 Dec;20(12):3759-3781. doi: 10.1111/jocd.14537. Epub 2021 Nov 6.

Treatment options for androgenetic alopecia: Efficacy, side effects, compliance, financial considerations, and ethics.

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BACKGROUND: Androgenetic alopecia (AGA) is the most common form of hair loss consisting of a characteristic receding frontal hairline in men and diffuse hair thinning in women, with frontal hairline retention, and can impact an individual's quality of life. The condition is primarily mediated by 5-alpha-reductase and dihydrotestosterone (DHT) which causes hair follicles to undergo miniaturization and shortening of successive anagen cycles. Although a variety of medical, surgical, light-based and nutraceutical treatment options are available to slow or reverse the progression of AGA, it can be challenging to select appropriate therapies for this chronic condition.

AIMS: To highlight treatment options for androgenetic alopecia taking into consideration the efficacy, side effect profiles, practicality of treatment (compliance), and costs to help clinicians offer ethically appropriate treatment

regimens to their patients.

MATERIALS AND METHODS: A literature search was conducted using electronic databases (Medline, PubMed, Embase, CINAHL, EBSCO) and textbooks, in addition to the authors' and other practitioners' clinical experiences in treating androgenetic alopecia, and the findings are presented here.

RESULTS: Although topical minoxidil, oral finasteride, and low-level light therapy are the only FDA-approved therapies to treat AGA, they are just a fraction of the treatment options available, including other oral and topical modalities, hormonal therapies, nutraceuticals, PRP and exosome treatments, and hair transplantation.

DISCUSSION: Androgenetic alopecia therapy remains challenging as treatment selection involves ethical, evidence-based decision-making and consideration of each individual patient's needs, compliance, budget, extent of hair loss, and aesthetic goals, independent of potential financial benefits to the practitioners.

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DOI: 10.1111/jocd.14537

PMCID: PMC9298335

PMID: 34741573 [Indexed for MEDLINE]

Conflict of interest statement: Dr. Ablon is an investigator for Nutrafol and Viviscal.

2. SPECIMEN OF THE CSV FILE CONTAINING TEXT-MINED CHEMICALS CO-MENTIONED WITH AGA IN PUBMED ARTICLES

	CHEMICALS
1	dihydrotestosterone>MESH:D013196
2	DHT>MESH:D013196
3	minoxidil>MESH:D008914
4	finasteride>MESH:D018120
5	Dutasteride>MESH:D000068538
6	testosterone>MESH:D013739
7	4-azasteroid>-
8	Finasteride>MESH:D018120
9	dutasteride>MESH:D000068538

3. SPECIMEN OF THE CSV FILE CONTAINING TEXT-MINED DISEASES CO-MENTIONED WITH AGA IN PUBMED ARTICLES

	DISEASES
1	hair loss disorder>MESH:D000505
2	anxiety>MESH:D001007

3	depression>MESH:D000275
4	Endocrinological diseases>MESH:D004700
5	hyperandrogenism>MESH:D017588
6	polycystic ovarian syndrome>MESH:D011085
7	PCOS>MESH:D011085
8	hyperprolactinemia>MESH:D002640
9	adrenal hyperplasia>MESH:D000312
10	ovarian and adrenal tumours>MESH:D010051

4. SPECIMEN OF THE CSV FILE CONTAINING TEXT-MINED GENES CO-MENTIONED WITH AGA IN PUBMED ARTICLES

	GENES
1	PRP>5621
2	Platelet-Rich Plasma>722
3	PRP>722
4	Platelet-rich plasma>722
5	platelet-rich plasma>722
6	VEGF>7422
7	vascular endothelial growth factor>7422
8	prostaglandin D2 receptor>5729
9	androgen receptor>367
10	beta-catenin>1499
11	Dkk-1>22943
12	AR>367

5. SPECIMEN OF THE CSV FILE CONTAINING TEXT-MINED SPECIES CO-MENTIONED WITH AGA IN PUBMED ARTICLES

	SPECIES
1	men>9606
2	women>9606
3	patients>9606
4	patient>9606
5	saw palmetto>4722
6	rosemary>39367
7	humans>9606
8	children>9606
9	severe acute respiratory syndrome coronavirus 2>2697049
10	SARS-CoV-2>2697049

6. SPECIMEN OF THE CSV FILE CONTAINING TEXT-MINED WORDS CO-MENTIONED WITH AGA IN PUBMED ARTICLES

	WORDS	FREQUENCY
26631	hair	11783
13454	alopecia	9795
37404	patients	5911
31929	loss	3882
46782	treatment	3784
42355	scalp	3241
47672	university	2621
29179	information	2364
41408	results	2343
44713	study	2292
20915	dermatology	2275

7. SPECIMEN OF THE CSV FILE CONTAINING THE PMIDS OF THE PUBMED ARTICLES ON AGA

	PMID
1	28349362
2	34741573
3	28294070
4	35044013
5	24566563
6	29595184
7	28396101
8	31677111
9	31415838
10	23974579

APPENDIX 3

1. SPECIMEN OF THE GENES ASSOCIATED WITH AGA FROM 9 GWAS (LOWEST P-VALUES)

THE	REGION	REPORTED GENE(S)	SNPS	P-VALUE
27182965	Xq12	EDA2R, AR	rs200644307	1.00E-247
30573740	Xq12	OPHN1	rs1475417	4.00E-178
28196072	Xq12	AR	rs12558842	5.00E-178
28196072	Xq12	EDA2R, HEPH	rs73221556	5.00E-178
28196072	Xq12	OPHN1	rs5919427	5.00E-178
29146897	20p11.22	PAX1	rs11087368	1.00E-105
22693459	Xq12	AR	rs2497938	2.00E-91
27182965	20p11.22	FOXA2, PAX1	rs201563	3.00E-81
28196072	7p21.1	HDAC9	rs71530654	5.00E-70

2. SPECIMEN OF TWO ENTRIES IN THE GWAS CATALOG

DATE.ADDED.TO.CATALOG	13/12/2011	12/1/2018
PUBMEDID	22032556	29146897
FIRST.AUTHOR	Brockschmidt FF	Pirastu N
DATE	27/10/2011	17/11/2017
JOURNAL	Br J Dermatol	Nat Commun
LINK	www.ncbi.nlm.nih.gov/pubmed/22032556	www.ncbi.nlm.nih.gov/pubmed/29146897
STUDY	Susceptibility variants on chromosome 7p21.1 suggest HDAC9 as a new candidate gene for male-pattern baldness.	GWAS for male-pattern baldness identifies 71 susceptibility loci explaining 38% of the risk.
DISEASE.TRAIT	Male-pattern baldness	Male-pattern baldness
INITIAL.SAMPLE.SIZE	581 European ancestry male cases, 617 European ancestry male controls	25,662 British ancestry cases, 17,928 British ancestry controls
REPLICATION.SAMPLE.SIZE	461 European ancestry male cases, 151 European ancestry male controls	13,367 European ancestry cases, 11,851 European ancestry controls, 3,436 cases, 2,435 controls
REGION	Xq12	1p36.22
CHR_ID	X	1
CHR_POS	67343176	10980328
REPORTED.GENE.S.	AR, EDA2R	DFFA
MAPPED_GENE	RNU6-394P - AL049641.1	C1orf127
UPSTREAM_GENE_ID	ENSG00000222667	
DOWNSTREAM_GENE_ID	ENSG00000226280	
SNP_GENE_IDS		ENSG00000175262
UPSTREAM_GENE_DISTANCE	666812	NA
DOWNSTREAM_GENE_DISTANCE	30397	NA
STRONGEST.SNP.RISK.ALLELE	rs2497938-?	rs7542354-G
SNPS	rs2497938	rs7542354
MERGED	0	0
SNP_ID_CURRENT	2497938	7542354
CONTEXT	intergenic_variant	intron_variant
INTERGENIC	1	0
RISK.ALLELE.FREQUENCY	NR	NR
P.VALUE	3.00E-22	6.00E-49
PVALUE_MLOG	21.52287875	48.22184875
P.VALUE..TEXT.		
OR.or.BETA	6.5	0.249395
X95..CI..TEXT.	[4.30-9.82]	[0.22-0.28] unit decrease

PLATFORM..SNPS.PASSING.QC.	Illumina [560387]	Affymetrix [27512692] (imputed)
CNV	N	N
MAPPED_TRAIT	androgenetic alopecia	androgenetic alopecia
MAPPED_TRAIT_URI	http://www.ebi.ac.uk/efo/EFO_0004191	http://www.ebi.ac.uk/efo/EFO_0004191
STUDY.ACCESSION	GCST001297	GCST005116
GENOTYPING.TECHNOLOGY	Genome-wide genotyping array	Genome-wide genotyping array

APPENDIX 4

1. THE TEXT FILE CONTAINING THE IDS AND TITLES OF THE 9 USPTO PATENTS FOUND FOR ANDROGENETIC ALOPECIA

1 10,143,639 Use of adelmidrol and other topical or oral cannabinomimetic or aliamide mast cell inhibitors to treat dermatoheliosis, seborrheic keratoses, and androgenetic alopecia

2 9,855,204 Methods and compositions for treating androgenetic alopecia

3 9,561,224 Methods and compositions for treating androgenetic alopecia

4 8,758,993 Systems and methods for predicting response to anti-androgen therapy for the treatment of androgenetic alopecia

5 8,691,518 Systems and methods for predicting response to minoxidil for the treatment of androgenetic alopecia

6 8,067,470 Linoleic acid preparations for the topical treatment of male and female pattern androgenetic alopecia, age-related alopecia, and keratosis pilaris

7 6,953,571 Cosmetic or pharmaceutical composition for topical use to prevent or differ androgenetic alopecia

8 6,281,241 Use of melatonin for the treatment of androgenetic alopecia

9 5,094,857 Treatment of acne or androgenetic alopecia by topical administration of ethisterone

2. SNAPSHOT OF THE PDF FILE OF PATENT US10143639



US010143639B2

(12) **United States Patent**
McDaniel

(10) **Patent No.:** **US 10,143,639 B2**

(45) **Date of Patent:** **Dec. 4, 2018**

(54) **USE OF ADELMIIDROL AND OTHER TOPICAL OR ORAL CANNABINOMIMETIC OR ALLAMIDE MAST CELL INHIBITORS TO TREAT DERMATOHELIOSIS, SEBORRHEIC KERATOSES, AND ANDROGENETIC ALOPECIA**

(58) **Field of Classification Search**
None
See application file for complete search history.

(56) **References Cited**

U.S. PATENT DOCUMENTS

(71) Applicant: **William Robert McDaniel**, Franklin, TN (US)

2003/0049220 A1* 3/2003 Bailey A61K 8/34
424/70.1
2015/0057269 A1* 2/2015 Della Valle A61K 45/06
514/228.8

(72) Inventor: **William Robert McDaniel**, Franklin, TN (US)

* cited by examiner

(*) Notice: Subject to any disclaimer, the term of this patent is extended or adjusted under 35 U.S.C. 154(b) by 31 days.

Primary Examiner — Kortney L. Klinkel

(21) Appl. No.: **15/466,821**

(57) **ABSTRACT**

A method of correcting the visible and microscopic signs of Dermatoheliosis (chronic ultraviolet light-damaged human skin) and its various clinical manifestations (wrinkling, sagging, fragility, melasma, Poikiloderma of Civatte, solar lentigines, and senile purpura) and also Androgenetic Alopecia and Seborrheic Keratoses consists of the administra-

(22) Filed: **Mar. 22, 2017**

(65) **Prior Publication Data**

APPENDIX 5

1. ENTRIES FOR TWO OF THE CLINICAL TRIALS ON AGA

nctID	NCT03694067	NCT02591355
studyTitle	Androgenetic Alopecia and the JAK-STAT Pathway	Evaluate the Clinical Effectiveness of RegenKit Platelet-rich Plasma (PRP) in Androgenetic Alopecia Treatment
recruitment	NA	NA
studyResults	No Results Available	No Results Available
conditions	Androgenetic Alopecia	Androgenetic Alopecia
interventionTypes	Other	Device
interventions	Punch skin biopsy	Autologous Platelet Rich Plasma Saline solution injection
outcomeMeasures	Different in STAT3 Correlating STAT3 with severity	Evaluate the changes in hair density of androgenetic alopecia Evaluate the changes of hair diameter and hair shedding in androgenetic alopecia
leadSponsor	Cairo University	Regen Lab SA
allSponsors	Cairo University	Regen Lab SA RegenLab USA LLC
gender	Male	All
ageGroups	Adult Older Adult	Adult
minAge	18 Years	18 Years
maxAge	NA	60 Years
phases	NA	Not Applicable

enrollment	25	80
funders	Other	Industry
studyType	Observational	Interventional
studyDesigns	Observational Model: Case-Control Time Perspective: Retrospective	Allocation: Randomized Intervention Model: Single Group Assignment Masking: Double (Participant, Investigator) Primary Purpose: Treatment
otherIDs	Atm567	RL 03
startDate	15-Oct-18	6-Sep-17
primaryCompleteDate	1-Dec-19	18-Nov-19
completeDate	1-Dec-19	18-Nov-19
firstPostedDate	3-Oct-18	29-Oct-15
lastUpdatedDate	28-Jan-20	24-Dec-19
startYear	2018	2017
primaryCompleteYear	2019	2019
completeYear	2019	2019
firstPostedYear	2018	2015
lastUpdatedYear	2020	2019
locations	Cairo University, Cairo, Egypt	Axis Clinical Trials, Los Angeles, California, United States NYU Dermatologic Associates, New York, New York, United States
studyURL	https://ClinicalTrials.gov/show/NCT03694067	https://ClinicalTrials.gov/show/NCT02591355

2. SPECIMEN OF THE CSV ON CLINICAL TRIALS BY PARTICIPANTS AGE

CT	AGE OF PARTICIPANTS
1	Adult Older Adult
2	Adult
3	Adult
4	Adult
5	Adult
6	Adult
7	Adult Older Adult
8	Adult
9	Adult
10	Adult Older Adult

3. SPECIMEN OF THE CSV ON CLINICAL TRIALS BY PARTICIPANTS SEX

CT	SEX OF PARTICIPANTS
1	Male
2	All

3	Male
4	All
5	All
6	Male
7	All
8	Male
9	Male
10	Male

4. SPECIMEN OF THE CSV ON CLINICAL TRIALS BY TYPE OF INTERVENTION

CT	INTERVENTION TYPE
1	Other
2	Device
3	Drug
4	Device Drug
5	Drug
6	NA
7	Biological
8	Drug Other
9	Drug
10	Device Procedure

5. SPECIMEN OF THE CSV ON CLINICAL TRIALS BY PHASE OF THE TRIAL

CT	PHASE OF THE TRIAL
1	NA
2	Not Applicable
3	Phase 3
4	Phase 2
5	Phase 2
6	NA
7	Not Applicable
8	Phase 1
9	Phase 4
10	Not Applicable

6. CSV ON CLINICAL TRIALS BY STUDY TYPE

	STUDY TYPE	FREQUENCY
1	Interventional	133
2	Observational	18

APPENDIX 6

1. THE IDS OF PUBCHEM ASSAY RELATED TO ANDROGENETIC ALOPECIA

	PUBCHEM ASSAY IDS		PUBCHEM ASSAY IDS		PUBCHEM ASSAY IDS		PUBCHEM ASSAY IDS
1	389974	11	389984	21	454521	31	454531
2	389975	12	389985	22	454522	32	454532
3	389976	13	454513	23	454523	33	454533
4	389977	14	454514	24	454524	34	454534
5	389978	15	454515	25	454525	35	454535
6	389979	16	454516	26	454526	36	454536
7	389980	17	454517	27	454527	37	454537
8	389981	18	454518	28	454528	38	454538
9	389982	19	454519	29	454529	39	454539
10	389983	20	454520	30	454530	40	454540
						41	1258958

2. THE RESULTS OF PUBCHEM ASSAY 389974

SID	CID	ACTIVITY OUTCOME	ACTIVITY SCORE	ACTIVITY URL	ASSAYDATA COMMENT	Stand ard Value	Stand ard Type	S t a n d a r d R e l a t i o n	Sta nda rd Val ue	Sta nda rd Uni ts
1031 6843 7	1329 81	Active	NA	NA	NA	0.016	IC50	=	16	nM
1035 3787 1	2418 0647	Active	NA	NA	NA	0.039 9	IC50	=	39. 9	nM
1035 5143 9	1173 8282	Active	NA	NA	NA	0.02	IC50	=	20	nM
1035 5488 6	1160 9033	Active	NA	NA	NA	0.06	IC50	=	60	nM
1036 4555 8	2509 3227	Active	NA	NA	NA	0.037	IC50	=	37	nM

1036 4555 9	2509 3228	Unspecified	NA	NA	NA	3	IC50	>	300 0	nM
1036 4556 0	2509 3229	Active	NA	NA	NA	0.026	IC50	=	26	nM
1036 4556 1	2509 3230	Active	NA	NA	NA	1.599	IC50	=	159 9	nM
1036 4567 5	2509 3231	Active	NA	NA	NA	0.037	IC50	=	37	nM

APPENDIX 7

1. COMMON NAMES FOR THE 69 PLANTS

Plant Name	Indicative common names
<i>Acacia concinna</i>	
<i>Albizia julibrissin</i>	silktree, mimosa, powderpuff tree
<i>Allium cepa</i>	onion, globe onion, garden onion
<i>Allium sativum</i>	cultivated garlic
<i>Aloe vera</i>	Barbados aloe, Indian aloe, Mediterranean aloe
<i>Alpinia zerumbet</i>	shellplant, shellflower, shell ginger
<i>Ammi majus</i>	large bullwort, Bishopsweed, Lace Flower
<i>Andrographis paniculata</i>	Kalmegh,
<i>Angelica dahurica</i>	Dahuriankarhunputki
<i>Angelica gigas</i>	Giant Angelic
<i>Angelica sinensis</i>	Dong quai, Women's Ginseng
<i>Artemisia abrotanum</i>	southernwood, Abrotano
<i>Averrhoa carambola</i>	carambola, star fruit
<i>Avicennia marina</i>	gray mangrove
<i>Azadirachta indica</i>	neem, Neem Tree
<i>Bidens tripartita</i>	three-lobed beggarticks, Trifid Bur-marigold
<i>Platyclusus orientalis</i>	
<i>Carthamus tinctorius</i>	safflower, Fake Saffron

<i>Cedrus deodara</i>	Deodar cedar, Himalayan Cedar
<i>Chrysanthemum morifolium</i>	florist's daisy
<i>Chrysanthemum zawadskii</i>	
<i>Clitoria ternatea</i>	Asian pigeonwings
<i>Ligusticum officinale</i>	
<i>Coffea arabica</i>	Arabian coffee
<i>Corydalis turtschaninowii</i>	
<i>Curcuma longa</i>	common turmeric
<i>Cuscuta reflexa</i>	giant dodder
<i>Cynomorium coccineum</i> ssp. <i>Songaricum</i>	
<i>Eclipta prostrata</i>	false daisy
<i>Camellia sinensis</i>	tea, Tea plant
<i>Illicium anisatum</i>	Japanase star anise
<i>Impatiens balsamina</i>	garden balsam
<i>Jatropha gossypifolia</i>	bellyache bush
<i>Panax ginseng</i>	
<i>Larrea divaricata</i>	jarilla
<i>Lawsonia inermis</i>	henna
<i>Leonurus sibiricus</i>	honeyweed
<i>Ligusticum sinense</i>	
<i>Ligustrum lucidum</i>	glossy privet, tree privet
<i>Lycium chinense</i>	
<i>Lycopersicon esculentum</i>	garden tomato
<i>Mimosa pudica</i>	shameplant, sensitive plant
<i>Morus alba</i>	white mulberry
<i>Nerium oleander</i>	oleander
<i>Ocimum tenniflorum</i>	holy basil
<i>Oryza sativa</i>	rice
<i>Phyllanthus emblica</i>	
<i>Prunus persica</i>	nectarine, peach

<i>Cullen corylifolium</i>	Malaysian scurfpea
<i>Pueraria montana</i> var. <i>chinensis</i>	
<i>Rehmannia glutinosa</i>	
<i>Rhinacanthus nasutus</i>	
<i>Rosmarinus officinalis</i>	rosemary
<i>Rubus coreanus</i>	
<i>Salvia miltiorrhiza</i>	
<i>Sapindus rarak</i>	
<i>Scutellaria baicalensis</i>	Baikal skullcup
<i>Serenoa repens</i>	saw palmetto
<i>Sesamum indicum</i>	sesame
<i>Solanum americanum</i>	black nightshade
<i>Sophora flavescens</i>	
<i>Dioscorea communis</i>	Black bryony
<i>Terminalia bellirica</i>	
<i>Terminalia chebula</i>	
<i>Thuja occidentalis</i>	Eastern Arborvitae, eastern white cedar
<i>Trichosanthes cucumerina</i>	snakegourd
<i>Trifolium pratense</i>	red clover
<i>Viscum album</i>	European mistletoe
<i>Wedelia chinensis</i>	
<i>Zingiber officinale</i>	ginger
<i>Zizyphus jujuba</i>	Jujube, red date

2. SYNONYMS OF THE 69 PLANTS

Plant Name	Synonyms
Acacia concinna	Mimosa rugata Lam. Acacia concinna (Willd.) DC. Mimosa concinna Willd. Acacia quisumbingii Merr. Acacia rugata (Lam.) Merr. Acacia hooperiana Acacia concinna var. rugata (Benth.) Baker Acacia hooperiana var. glabriuscula Miq. Acacia hooperiana Miq. Acacia hooperiana var. subcuneata Miq. Acacia philippinarium Benth. Acacia poilanei Gagnep. Acacia polycephala DC. Guilandina microphylla DC. Nygae sylvarum-minimae Rumph.
Albizia julibrissin	Mimosa julibrissin (Durazz.) Scop. Mimosa julibrissin Acacia julibrissin (Durazz.) Willd. Acacia julibrissin Sericandra julibrissin (Durazz.) Raf. Sericandra julibrissin Feuilleea julibrissin (Durazz.) Kuntze Feuilleea julibrissin Acacia nemu Willd. Acacia nemu Albizia nemu (Willd.) Benth. Albizia nemu Mimosa speciosa Thunb. Mimosa speciosa Albizzia julibrissin Durazz. Albizzia julibrissin Albizia julibrissin Durazz. Albizia julibrissin
Allium cepa	Allium salota Dostál Allium salota Allium cepa var. aggregatum G. Don Allium cepa aggregatum Allium cepa var. multiplicans Bailey Allium cepa multiplicans Allium cepa var. proliferum (Moench) Regel Allium cepa proliferum Allium cepa var. solaninum Alef. Allium cepa solaninum Kepa esculenta Raf. Kepa esculenta Porrum cepa (L.) Rchb. Porrum cepa Cepa rubra P. Renault Cepa rubra Cepa vulgaris Garsault Cepa vulgaris Cepa esculenta Gray Cepa esculenta Cepa alba P. Renault Cepa alba Allium ascalonicum var. sterile Allium ascalonicum sterile Allium ascalonicum var. fertile Allium ascalonicum fertile Ascalonicum sativum P. Renault Ascalonicum sativum Allium ascalonicum var. condensum Allium ascalonicum condensum Cepa pallens P. Renault Cepa pallens Allium ascalonicum f. rotterianum Allium ascalonicum rotterianum Allium cepa var. flandricum Allium cepa flandricum Allium cepa var. rosum Allium cepa rosum Allium cepa var. multiplicans Allium cepa var. solaninum Allium cepa var. aggregatum Allium cepa var. tripolitanum Allium cepa tripolitanum Allium cepa var. bifolium Allium cepa bifolium Allium cepa var. sanguineum Allium cepa sanguineum Allium cepa var. jamesii Allium cepa jamesii Allium cepa var. globosum Allium cepa globosum Allium cepa var. anglicum Allium cepa anglicum Allium cepa var. portanum Allium cepa portanum Allium cepa var. crinides Allium cepa crinides Allium cepa var. lisboanum Allium cepa lisboanum Allium cepa var. hispanicum Allium cepa hispanicum Allium cepa var. luteum Allium cepa luteum Allium cepa var. praecox Allium cepa praecox Allium cepa var. argenteum Allium cepa argenteum Allium cepa var. viviparum Allium cepa viviparum Allium pauciflorum Willd. ex Ledeb. Allium pauciflorum Allium aobanum Araki Allium aobanum Allium napus Pall. ex Kunth Allium napus Allium cepaeum St.-Lag. Allium cepaeum Allium commune Noronha Allium commune Allium cumaria Buch.-Ham. ex Wall. Allium cumaria Allium angolense Baker Allium angolense Allium esculentum Salisb. Allium esculentum Allium cepa L. Allium cepa Allium cepa var. cepa L. Allium cepa cepa Allium cepa var.

	<p>viviparum (Metz) Mansf. Allium cepa var. multiplicans L.H.Bailey Allium cepa var. bulbiferum Regel Allium cepa bulbiferum</p>
<p>Allium sativum</p>	<p>Allium pekinense Prokhanov Allium pekinense Allium sativum subsp. subrotundum Allium sativum subrotundum Allium sativum subsp. controversum Allium sativum controversum Allium scorodoprasum subsp. viviparum Allium scorodoprasum viviparum Allium sativum subsp. asiae-mediae Allium sativum asiae-mediae Allium sativum f. asiae-mediae Allium sativum f. sagittatum Allium sativum sagittatum Allium sativum f. vulgare Allium sativum vulgare Porrum sativum (L.) Rchb. Porrum sativum Porrum ophioscorodon (Link) Rchb. Porrum ophioscorodon Allium sativum var. controversum Allium scorodoprasum var. viviparum Allium sativum f. pekinense Allium sativum pekinense Allium sativum var. pekinense Allium sativum var. subrotundum Allium arenarium Sadler ex Rchb. Allium arenarium Allium sativum subsp. ophioscorodon Allium sativum ophioscorodon Allium pekinense Prokh. Allium longicuspis Regel Allium longicuspis Allium sativum var. ophioscorodon Allium controversum Schrad. ex Willd. Allium controversum Allium ophioscorodon Link Allium ophioscorodon Allium sativum L. Allium sativum Allium sativa</p>

Aloe vera	Aloe vera (L.) Burm. f. Aloe vera Aloe barbadensis Aloe barbadensis Mill. Aloe vulgaris Lam. (1783) Aloe vera L. Aloe vera Mill., 1768 Aloe vera (L.) Burm.f., 1768 Aloe barbadensis Mill., 1768 Aloe elongata Murr., 1789 Aloe flava Pers., 1805 Aloe perfoliata var. vera L., 1753 Aloe vulgaris Lam., 1783 Aloe vera Burm. f.
Alpinia zerumbet	Alpinia zerumbet (Pers.) Burt & R. M. Sm. Alpinia zerumbet Alpinia speciosa K. Schum. (1903) Alpinia speciosa Renealmia spectabilis Catimbium speciosum (Wendl.) Holtt., 1950 Catimbium speciosum Costus zerumbet Pers., 1805 Costus zerumbet Zerumbet speciosum Wendl., 1798 Zerumbet speciosum Alpinia speciosa K. Schum. Languas speciosa Small Languas speciosa Alpinia schumanniana
Ammi majus	Apium ammi Crantz Apium ammi Ammi glaucifolium L. Ammi glaucifolium Ammi cicutaefolium Willd. ex Spreng. Ammi cicutaefolium Carum majus (L.) Koso-Pol. Carum majus Ammi majus var. glaucifolium (L.) Noulet Ammi majus glaucifolium Selinum ammoides E.H.L. Krause Selinum ammoides Ammi majus L. Ammi majus
Andrographis paniculata	Andrographis paniculata (Burm. f.) Wall. ex Nees Andrographis paniculata Justicia paniculata Andrographis paniculata (Burm. f.) Nees Justicia salviiflora Justicia paniculata Rose Justicia salviiflora C.B. Clarke
Angelica dahurica	Angelica dahurica Angelica dahurica (Fischer ex Hoffmann) Benth & J. D. Hooker ex Franchet & Savatier Angelica dahurica Maxim. Angelica dahurica Fisch. ex Hoffm. Angelica dahurica (Fisch. ex Hoffm.) Franch. & Sav.
Angelica gigas	Angelica gigas Angelica gigas Nakai Angelica gigas Nakai, 1917
Angelica sinensis	Angelica polymorpha var. sinensis Oliv. Angelica sinensis (Oliv.) Diels Angelica polymorpha subsp. sinensis
Artemisia abrotanum	Artemisia procera Willd. Artemisia procera Artemisia herbacea hort. wratisl. ex Besser Artemisia herbacea Artemisia altissima Ehrh. ex DC. Artemisia altissima Artemisia paniculata Lam. Artemisia paniculata Artemisia elegans Fisch. ex Ledeb. Artemisia elegans Artemisia herbacea DC. Artemisia elatior Klokov Artemisia elatior Artemisia herbacea Ehrh. ex Willd. Artemisia anethifolia Fisch. ex DC. Artemisia anethifolia Artemisia sabulosa Steven ex DC. Artemisia sabulosa Artemisia foeniculacea Steven ex DC. Artemisia foeniculacea Artemisia proceriformis Krasch. Artemisia proceriformis Artemisia tenuissima Spreng. ex Besser Artemisia tenuissima Artemisia abrotanum L. Artemisia abrotanum
Averrhoa carambola	Averrhoa carambola L. Averrhoa carambola Averrhoa carambola Linnaeus Averrhoa carambola L. (1753) Averrhoa carambola L., 1753 Averrhoa acutangula Stokes, 1812 Averrhoa pentandra Blanco, 1837 Connaropsis philippica Villar, 1880 Sarcotheca philippica (Villar) H. Hallier, 1911

Avicennia marina	Sceura marina Forssk. Sceura marina Avicennia officinalis sensu Klotzsch. Avicennia officinalis L. Avicennia officinalis officinalis Avicennia obovata Avicennia intermedia Griff. Avicennia intermedia Avicennia mindanaense Elmer Avicennia mindanaense Avicennia balanophora Stapf & Moldenke ex Moldenke Avicennia balanophora Avicennia marina (Forssk.) Vierh. Avicennia marina Avicennia alba Blume Avicennia alba Avicennia officinalis L. Avicennia officinalis Avicennia marina subsp. australasica (Walp.) J. Everett Avicennia marina australasica
Azadirachta indica	Azadirachta indica Adr. Juss. Azadirachta indica Melia indica Melia azadirachta L., 1753 Melia azadirachta Melia azadirachta L.
Bidens tripartita	Bidens acuta (Wieg.) Britt. Bidens acuta Bidens comosa (Gray) Wieg. Bidens comosa Bidens shimadai Hayata Bidens shimadai Bidens tripartita var. shimadai (Hayata) Yamam. Bidens tripartita shimadai Bidens trifoliata Gueldenst. ex Ledeb. Bidens trifoliata Bidens tripartita f. integra (Peterm.) Koch ex Beck Bidens tripartita integra Bidens tripartita f. pumila (Retz.) Roth ex Beck Bidens tripartita pumila Bidens tripartita f. tripartita Bidens tripartita tripartita Bidens tripartita subsp. eutripartita Briq. & Chev. Bidens tripartita eutripartita Bidens tripartita f. stolonifera Bolzon Bidens tripartita stolonifera Bidens tripartita f. minima (Lej.) Larss. Bidens tripartita minima Bidens orientalis Velen. Bidens orientalis Bidens acuta (Wiegand) Britton Bidens comosus Bidens tripartitus Bidens tripartita L. Bidens tripartita
Camellia sinensis	Camellia sinensis (Linnaeus) Kuntze Camellia sinensis Camellia sinensis (L.) Kuntze Camellia sinensis (L.) O. Kuntze Camellia sinensis L. Kuntze. L. Kuntze. Thea sinensis Sims Sims Thea sinensis Thea sinensis L. (1753) Thea sinensis L., 1753 Camellia sinensis Kuntze
Carthamus tinctorius	Centaurea carthamus E.H.L.Krause Centaurea carthamus Calcitrapa tinctoria Carthamus tinctorius var. tinctorius Carthamus tinctorius tinctorius Carthamus tinctorius var. albus Alef. Carthamus tinctorius albus Carthamus tinctorius var. flavus Alef. Carthamus tinctorius flavus Carthamus tinctorius var. typicus Schweinf. Carthamus tinctorius typicus Carthamus tinctorius var. spinosus Kitam. Carthamus tinctorius spinosus Carthamus tinctorius var. croceus Alef. Carthamus tinctorius croceus Carthamus glaber Burm.f. Carthamus glaber Carduus tinctorius (L.) Falk Carduus tinctorius Carduus tinctorius Ehrh. Carthamus tinctorius L. Carthamus tinctorius Carthamnus tinctorius Cathamus tinctorius L. Cathamus tinctorius
Cedrus deodara	Cedrus deodara (Roxburgh) G. Don Cedrus deodara Cedrus deodara (Roxb.) G. Don f. Cedrus deodora (Roxb. ex Lambert) (1830) Cedrus deodora Cedrus deodara (Roxb.) G. Don Cedrus deodara (Lamb.) G. Don Cedrus deodara G. Don Cedrus deodara G. Don f.
Chrysanthemum morifolium	Chrysanthemum morifolium Ramat. Chrysanthemum morifolium Chrysanthemum morifolium Ramat. (1792) Anthemis grandiflora Host, 1831 Anthemis grandiflora Ramat., 1792 Anthemis stipulacea Moench, 1802 Chrysanthemum hortorum W. Mill., 1914 Chrysanthemum morifolium Ramat., 1792 Chrysanthemum stipulaceum W. Wight, 1909 Chrysanthemum hortorum W. Mill ex L.H. Bailey

Chrysanthemum zawadskii	Chrysanthemum zawadskii subsp. naktongense (Nakai) Y. N. Lee Chrysanthemum zawadskii subsp. lucidum (Nakai) Y. N. Lee Chrysanthemum zawadskii var. leiophyllum (Nakai) Y.N.Lee Chrysanthemum zawadskii subsp. yezoense Y.N.Lee
Clitoria ternatea	Clitoria ternatea L. Clitoria albiflora Mattei Clitoria ternatensium Crantz Clitoria parviflora Raf. Clitoria ternatea Clitoria bracteata Poir. Clitoria pilosula Wall. Clitoria ternatea Linn. Clitoria ternatea L. (1753) Clitoria ternatea Linnaeus
Coffea arabica	Coffea arabica var. murta Coffea arabica murta Coffea arabica var. longistipulata Coffea arabica longistipulata Coffea arabica var. amarella Coffea arabica amarella Coffea corymbulosa Bertol. Coffea corymbulosa Coffea arabica f. abyssinica Coffea arabica abyssinica Coffea arabica var. polysperma Coffea arabica polysperma Coffea arabica var. pubescens Coffea arabica pubescens Coffea arabica var. sundana Coffea arabica sundana Coffea moka Heynh. Coffea moka Coffea arabica var. columnaris Coffea arabica columnaris Coffea arabica var. angustifolia Coffea arabica angustifolia Coffea arabica var. latifolia Coffea arabica latifolia Coffea arabica var. purpurascens Coffea arabica purpurascens Coffea arabica var. bullata Coffea arabica bullata Coffea arabica var. variegata Coffea arabica variegata Coffea arabica var. pendula Coffea arabica pendula Coffea arabica var. monosperma Coffea arabica monosperma Coffea arabica var. straminea Coffea arabica straminea Coffea arabica var. culta Coffea arabica culta Coffea arabica var. myrtifolia Coffea arabica myrtifolia Coffea arabica var. brevistipulata Coffea arabica brevistipulata Coffea laurifolia Salisb. Coffea laurifolia Coffea sundana Miq. Coffea sundana Coffea vulgaris Moench. Coffea vulgaris Coffea arabica var. typica Coffea arabica typica Coffea arabica var. bourbon Coffea arabica bourbon Coffea arabica var. erecta Coffea arabica erecta Coffea arabica var. mokka Coffea arabica mokka Coffea arabica var. maragotype Coffea arabica maragotype Coffea bourbonica Pharm. ex Wehmer Coffea bourbonica Coffea arabica var. rotundifolia Coffea arabica rotundifolia Coffea arabica var. cultoides Coffea arabica cultoides Coffea arabica L. Coffea arabica
Cullen corylifolium	Cullen corylifolia (L.) Medik. Psoralea corylifolia L. Psoralea corylifolia Cullen corylifolium Cullen corylifolia Cullen corylifolium (L.) Medik. Trifolium unifolium Forssk. Psoralea patersoniae Schonland Cullen corylifolium Medik. Psoralea corylifolia Linn.
Curcuma longa	Curcuma longa L. Curcuma longa Curcuma domestica Curcuma domestica Valetton Amomum curcuma Jacq. Kua domestica Medik. Curcuma brog Valetton Curcuma ochrorhiza Valetton Curcuma soloensis Valetton Curcuma longa Linnaeus Curcuma longa L. (1753) Stissera curcuma Giseke Curcuma longa L., 1753 Curcuma domestica L. Curcuma domestica Valetton, 1918
Cuscuta reflexa	Cuscuta reflexa Roxb. Cuscuta reflexa Cuscuta gigantea Cuscuta gigantea Griff. Cuscuta gigantea Griffith Cuscuta reflexa Roxburgh Cuscuta reflexa Decne.

Cynomorium songaricum	Cynomorium songaricum Cynomorium songaricum Rupr. Cynomorium songaricum Ruprecht Cynomorium coccineum subsp. songaricum (Rupr.) J.Leonard, 1986 Cynomorium songaricum Rupr., 1869
Eclipta prostrata	Eclipta prostrata (L.) L. Eclipta alba (L.) Hassk. Eclipta erecta L. Eclipta prostrata Eclipta alba Eclipta erecta Eclipta prostrata L. Eclipta marginata Boiss. Amellus carolinianus Walter Wiborgia oblongifolia Hook. Eclipta zippeliana Verbesina pseudoacmella L. Eclipta prostrata (Linnaeus) Linnaeus Eclipta alba Hassk Hassk Eclipta prostrata DC. (1848) Eclipta prostrata (L.) Hassak Eclipta prostrata (L.) L., 1771 Cotula alba L. Eclipta adpressa Moench, 1802 Eclipta alba (L.) Hassk., 1848 Eclipta dichotoma Raf., 1836 Eclipta erecta L., 1771 Eclipta flexuosa Raf., 1836 Eclipta nutans Raf., 1836 Eclipta parviflora Wall., 1829 Eclipta pumila Raf., 1836 Eclipta simplex Raf., 1836 Eclipta strumosa Salisb., 1796 Eclipta sulcata Raf., 1836 Eclipta tinctoria Raf., 1836 Anthemis cotula-foetida Crantz, 1766 Chamaemelum foetidum Haller ex Baumg., 1816 Eclipta zippeliana Blume, 1826 Verbesina alba L., 1753 Verbesina conyzoides Trew, 1763 Verbesina prostrata L., 1753
Illicium anisatum	Illicium anisatum L. Illicium anisatum Illicium anisatum L., 1759
Impatiens balsamina	Impatiens balsamina L. Impatiens balsamina Impatiens balsamina L., 1753 Impatiens balsamina Linnaeus Impatiens balsamina L. (1753)
Jatropha gossypifolia	Adenoropium gossypifolium Jatropha elegans (Pohl) Klotzsch Jatropha elegans Manihot gossypifolia (L.) Crantz Manihot gossypifolia Adenoropium gossypifolium (L.) Pohl Adenoropium gossypifolium Jatropha gossypifolia var. typica Jatropha gossypifolia typica Jatropha gossypifolia L. Jatropha gossypifolia Jatropha gossypifolia L. Jatropha gossypifolia Jatropha gossifolia Jatropha gossypifolia
Larrea divaricata	Larrea tridentata (DC.) Coville var. tridentata Larrea tridentata var. tridentata Larrea glutinosa Engelm. Larrea glutinosa Larrea divaricata Larrea divaricata Cav. (1800) Larrea divaricata Cav. Covillea tridentata
Lawsonia inermis	Lawsonia inermis Linnaeus Lawsonia inermis L. Lawsonia alba Lam. Lawsonia spinosa L. Rotanthea combretoides Baker Lawsonia speciosa L. Lawsonia indica Alkanna spinosa Gaertn. Leea alba
Leonurus sibiricus	Leonurus sibiricus L. Leonurus sibiricus Leonurus artemisia Leonurus sibiricus Linnaeus Leonurus sibiricus L. L. Leonurus sibiricus L. (1753) Leonurus sibiricus L., 1753
Ligusticum sinense	Ligusticum chuanxiong Ligusticum sinense Oliv. Ligusticum chuanxiong Ligusticum chuanxiong hort. ex S.H.Qiu et al.
Ligustrum lucidum	Esquirolia sinensis H. Lév. Esquirolia sinensis Ligustrum esquirolii H. Lév. Ligustrum esquirolii Ligustrum lucidum var. esquirolii (H. Lév.) H. Lév. Ligustrum lucidum esquirolii Ligustrum lucidum W. T. Aiton Ligustrum lucidum
Lycopersicon esculentum	Lycopersicon esculentum subsp. galenii (Mill.) Luckwill, 1943
Mimosa pudica	Mimosa pudica Linn. Mimosa pudica Mimosa pudica L. Mimosa pudica L. (1753) Mimosa pudica L., 1753 Mimosa pudica var. Mimosa tetrandra Humb. & Bonpl. ex Willd., 1806 Mimosa tetrandra Mimosa unijuga Duchass. & Walp., 1850 Mimosa unijuga Mimosa pudica Linnaeus Mimosa pudica Mill.

Morus alba	Morus alba var. multicaulis (Perr.) Loudon Morus alba multicaulis Morus alba var. tatarica (L.) Ser. Morus alba tatarica Morus tatarica L. Morus tatarica Morus atropurpurea Roxb. Morus atropurpurea Morus australis Poir. Morus australis Morus indica L. Morus indica Morus intermedia Perr. Morus intermedia Morus multicaulis Perr. Morus multicaulis Morus alba L. Morus alba Morus sinensis Hort. ex Loudon Morus sinensis
Nerium oleander	Nerium oleander Linnaeus Nerium oleander Nerium oleander L. Nerium indicum Nerium oleander L. L. Nerium odorum (Soland.) (1789) Nerium odorum Nerium indicum Mill. Nerium oleander L. (1753) Nerium oleander L., 1753 Nerium odoratum Lam., 1792 Nerium odoratum Nerium odorum Salisb., 1796 Nerium odorum Sol., 1789 Nerium verecundum Salisb., 1796 Nerium verecundum Nerium indicum Mill., 1768 Nerium odorum Sol. ex Aiton
Ocimum sanctum	Ocimum sanctum var. hirsutum Hook.
Oryza sativa	Oryza sativa L. Oryza sativa var. fatua Prain Oryza glutinosa Lour. Oryza sativa subsp. indica Kato Oryza communissima Lour. Oryza montana Lour. Oryza praecox Lour. Oryza formosana Masam. & Suzuki Oryza elongata (Desv.) Steud. Oryza perennis Moench Oryza rubribarbis (Desv.) Steud. Oryza aristata Blanco Oryza nepalensis G. Don ex Steud. Oryza palustris Salisb. Oryza repens Buch.-Ham. ex Steud. Oryza sativa f. spontanea Oryza sativa subsp. indica Oryza sativa subsp. japonica Oryza sativa var. elongata Desv. Oryza sativa var. rubribarbis Desv. Oryza sativa aus Oryza denudata Steud. Oryza mutica Steud. Oryza marginata Steud. Oryza pumila Steud. Oryza sorghoidea Steud. Oryza pubescens Steud. Oryza elongata Steud. Oryza segetalis Russell ex Steud. Oryza parviflora P.Beauv. Oryza sativa var. formosana Oryza sativa var. savannae Oryza sativa var. rubribarbis Oryza sativa var. plena Oryza sativa indica (misnomer)
Panax ginseng	Panax ginseng Aralia ginseng Panax quinquefolius var. ginseng Panax quinquefolius ginseng Aralia quinquefolia var. ginseng Aralia quinquefolia ginseng Panax schin-seng var. coraiensis Panax schin-seng coraiensis Panax verus Oken Panax verus Panax schinseng Nees Panax schinseng
Phyllanthus emblica	Phyllanthus emblica L. Phyllanthus emblica Emblica officinalis Phyllanthus emblica Linnaeus Phyllanthus emblica L. (1753) Phyllanthus emblica L., 1753
Platyclusus orientalis	Thuja orientalis L. 1753 Thuja orientalis Biota orientalis (L.) Endl. 1847 Biota orientalis Platyclusus stricta Spach 1841 Platyclusus stricta Thuja orientalis var. aurea (Carriere) Rehder Thuja orientalis aurea Thuja orientalis L. Thuja chengii Bordères & Gaussen Thuja chengii Thuja orientalis var. argyi Lévl. & Lemée Thuja orientalis argyi Platyclusus orientalis (L.) Franco Platyclusus orientalis Platyclusus orientalis flagelliformis Biota orientalis (L.) Endl. Thuja orientalis var. aurea (Carrière) Rehder
Prunus persica	Prunus persica

Pueraria thomsonii	Pueraria thomsonii Benth. Pueraria thomsonii Pueraria montana chinensis Pueraria montana thomsonii Pueraria montana var. chinensis (Ohwi) Sanjappa & Pradeep Pueraria montana var. chinensis Pueraria montana var. thomsonii Pueraria montana var. chinensis (Ohwi) Maesen & S.M. Almeida ex Sanjappa & Pradeep Pueraria montana var. chinensis (Ohwi) Maesen & S. M. Almeida ex Sanjappa & Pradeep
Rehmannia glutinosa	Rehmannia glutinosa Rehmannia glutinosa (Gaertn.) Steud. Rehmannia glutinosa (Gaertn.) Libosch. ex Fisch. & C.A. Mey. Rehmannia glutinosa (Gaertner) Liboschitz ex Fischer & C. A. Meyer Rehmannia glutinosa Libosch. ex Fisch. & C.A. Mey.
Rhinacanthus nasutus	Justicia nasuta L. Rhinacanthus communis Nees Rhinacanthus nasutus (L.) Kuntze Rhinacanthus nasuta Rhinacanthus nasutus (L.) Lindau
Rubus coreanus	Rubus coreanus Miq. Rubus tokkura Siebold Rubus coreana
Salvia miltiorrhiza	Salvia miltiorrhiza Bunge Salvia anomala Vaniot Salvia pogonocalyx Hance Salvia miltiorrhiza f. alba C.Y.Wu & H.W.Li Salvia miltiorrhiza Salvia mihiorrhiza
Salvia rosmarinus	Salvia rosmarinus Schleid., 1857
Sapindus rarak	Sapindus rarak Sapindus rarak DC. Sapindus rarak Candolle
Scutellaria baicalensis	Scutellaria baicalensis Georgi Scutellaria macrantha Fisch. Scutellaria lanceolaria Miq.
Serenoa repens	Serenoa repens (Bartr.) Small Serenoa repens Serenoa serrulata Serenoa repens (W. Bartram) Small Serenoa repens (Bartram) J.K.Small Serenoa repens (Bartram) Small Serenoa repens (W. Bartram) Small, 1926 Serenoa repens (W.Bartram) Small (1926)
Sesamum indicum	Sesamum orientale Linn. Sesamum orientale Sesamum indicum Linnaeus Sesamum indicum Sesamum orientale L. Sesamum indicum L. 1753 Sesamum indicum L. Sesamum orientale L., 1753 Sesamum oleiferum Moench, 1802 Sesamum oleiferum Sesamum orientale Linnaeus
Solanum nigrum	Solanum nigrum L. subsp. nigrum Solanum nigrum ssp. nigrum Solanum nigrum subsp. nigrum Solanum nigrum var nigrum Solanum nigrum subsp. nigrum L. Solanum nigrum f. nigrum
Sophora flavescens	Sophora angustifolia Siebold & Zucc. Sophora flavescens var. angustifolia (Siebold & Zucc.) Kitag. Sophora flavescens subsp. angustifolia (Siebold & Zucc.)Yakovlev Sophora tetragonocarpa Hayata Sophora macrosperma DC. Sophora angustifolia var. stenophylla Makino & Nemoto Sophora flavescens fo. angustifolia (Siebold & Zucc.) Yakovlev Sophora flavescens var. stenophylla Hayata Sophora falvescens Sophora flavescens Aiton subspecies angustifolia (Siebold & Zucc.)Yakovlev Sophora flavescens Aiton variety angustifolia (Siebold & Zucc.) Kitag.
Tamus communis	Tamus communis
Terminalia bellirica	Terminalia bellirica (Gaertner) Roxb. Terminalia bellirica Terminalia bellirica (Gaertn.) Roxb. Terminalia eichleri Alwan & Stace Terminalia belerica Terminalia bellerica Terminalia bellirica (Gaertner) Roxburgh Terminalia bellirica (Gaertn.) Roxb., 1798 Myrobalanus bellirica Gaertn., 1791

Terminalia chebula	Terminalia chebula Retzius Terminalia chebula Terminalia chebula (Gaertn.) Retz. Terminalia chebula (Gaertner) Retz. Terminalia chebula Retz.
Thuja occidentalis	Thuja occidentalis var. fastigiata H. Jaeger Thuja occidentalis fastigiata Thuja occidentalis var. nigra L. H. Bailey Thuja occidentalis nigra Thuja occidentalis var. pyramidalis Zederb. Thuja occidentalis pyramidalis Cupressus arborvitae Targ. Tozz. Cupressus arborvitae Thuja obtusa Moench Thuja obtusa Thuja procera Salisb. Thuja procera Thuja odorata Marshall Thuja odorata Thuja occidentalis L. Thuja occidentalis
Trichosanthes cucumerina	Trichosanthes cucumerina Linn. Trichosanthes cucumerina Trichosanthes cucumerina L. Trichosanthes cucumerina L. (1753) Trichosanthes cucumerina Linnaeus
Trifolium pratense	Trifolium pratense
Viscum album	Viscum polycoccon Houtt. Viscum polycoccon Viscum album var. mali Tubeuf Viscum album mali Viscum album L. Viscum album
Wedelia chinensis	Wedelia chinensis Wedelia chinensis (Osbeck) Merr. Wedelia calendulacea Rich. Wedelia calendulacea Less.
Zingiber officinale	Amomum zingiber L. Amomum zingiber Zingiber zingiber (L.) Karst. Zingiber zingiber Curcuma longifolia Wall Curcuma longifolia Zingiber aromaticum Noronha Zingiber aromaticum Zingiber majus Rumph. Zingiber majus Zingiber missionis Wall Zingiber missionis Zingiber zingiber (L.) H. Karst. Amomum angustifolium Salisb. Amomum angustifolium Amomum zinziba Hill Amomum zinziba Zingiber officinale var. cholmondeleyi Zingiber officinale cholmondeleyi Zingiber cholmondeleyi (F.M.Bailey) K.Schum. Zingiber cholmondeleyi Zingiber officinale var. rubrum Zingiber officinale rubrum Zingiber officinale f. macrorhizonum Zingiber officinale macrorhizonum Zingiber officinale f. rubens Zingiber officinale rubens Zingiber officinale var. macrorhizonum Zingiber officinale var. sichuanense Zingiber officinale sichuanense Zingiber officinale var. rubens Zingiber officinale Roscoe Zingiber officinale
Ziziphus jujuba Mill.	Ziziphus zizyphus (L.) Karst. Zizyphus jujuba Ziziphus zizyphus Ziziphus jujuba Ziziphus jujuba Mill. Ziziphus sativa Ziziphus vulgaris Lam. Ziziphus jujuba Miller Zizyphus jujuba Mill. Zizyphus jujuba Mill. () Ziziphus jujuba Lamk. Ziziphus jujuba Lam. Ziziphus jujuba Mill., 1768 Rhamnus zizyphus L., 1753 Ziziphus sativa Gaertn., 1788 Ziziphus vulgaris Lam., 1789 Ziziphus zizyphus (L.) H.Karst, 1882 Ziziphus zizyphus (L.) Meikle, 1977 Rhamnus jujuba L., 1753 Ziziphus jujuba (L.) Lam., 1789 Ziziphus jujuba (L.) Kirkbride, Joseph H. Wiersema, John H. Ziziphus zizyphus Meikle Zizyphus zizyphus H. Karst.

3. TAXONOMY OF THE 69 PLANTS

Plant	Taxonomy
Acacia concinna	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae rosids fabids Fabales Fabaceae Caesalpinioideae mimosoid clade Acacieae Acacia
Albizia julibrissin	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae rosids fabids Fabales Fabaceae Caesalpinioideae mimosoid clade Ingeae Albizia
Allium cepa	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae Liliopsida Petrosaviidae Asparagales Amaryllidaceae Allioideae Allieae Allium
Allium sativum	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae Liliopsida Petrosaviidae Asparagales Amaryllidaceae Allioideae Allieae Allium
Aloe vera	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae Liliopsida Petrosaviidae Asparagales Asphodelaceae Asphodeloideae Aloe
Alpinia zerumbet	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae Liliopsida Petrosaviidae commelinids Zingiberales Zingiberaceae Alpinia
Ammi majus	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids campanulids Apiales Apiineae Apiaceae Apioideae apioid superclade Apieae Ammi
Andrographis paniculata	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids lamiids Lamiales Acanthaceae Acanthoideae Ruellieae Andrographinae Andrographis
Angelica dahurica	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids campanulids Apiales Apiineae Apiaceae Apioideae apioid superclade Selineae Angelica
Angelica gigas	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids campanulids Apiales Apiineae Apiaceae Apioideae apioid superclade Selineae Angelica
Angelica sinensis	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids campanulids Apiales Apiineae Apiaceae Apioideae apioid superclade Selineae Angelica
Artemisia abrotanum	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids campanulids Asterales Asteraceae Asteroideae Anthemideae Artemisiinae Artemisia

Averrhoa carambola	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae rosids fabids Oxalidales Oxalidaceae Averrhoa
Avicennia marina	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids lamiids Lamiales Acanthaceae Avicennioideae Avicennia
Azadirachta indica	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae rosids malvids Sapindales Meliaceae Azadirachta
Bidens tripartita	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids campanulids Asterales Asteraceae Asteroideae Heliantheae alliance Coreopsideae Bidens
Platyclusus orientalis	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Acrogymnospermae Pinidae Cupressales Cupressaceae Platyclusus
Carthamus tinctorius	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids campanulids Asterales Asteraceae Carduoideae Cardueae Centaureinae Carthamus
Cedrus deodara	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Acrogymnospermae Pinidae Pinales Pinaceae Cedrus
Chrysanthemum morifolium	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids campanulids Asterales Asteraceae Asteroideae Anthemideae Artemisiinae Chrysanthemum
Chrysanthemum zawadskii	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids campanulids Asterales Asteraceae Asteroideae Anthemideae Artemisiinae Chrysanthemum
Clitoria ternatea	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae rosids fabids Fabales Fabaceae Papilionoideae Phaseoleae Clitoria
Ligusticum officinale	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids campanulids Apiales Apiineae Apiaceae Apioideae apiooid superclade Selineae Cnidium
Coffea arabica	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids lamiids Gentianales Rubiaceae Ixoroideae Gardenieae complex Bertiereae - Coffeaeae clade Coffeaeae Coffea
Corydalis turtschaninowii	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons early-diverging eudicotyledons Ranunculales Papaveraceae Fumarioideae Corydalis

Curcuma longa	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae Liliopsida Petrosaviidae commelinids Zingiberales Zingiberaceae Curcuma
Cuscuta reflexa	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids lamiids Solanales Convolvulaceae Cuscutae Cuscuta Monogynella
Cynomorium coccineum ssp. Songaricum	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae Saxifragales Cynomoriaceae Cynomorium
Eclipta prostrata	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids campanulids Asterales Asteraceae Asteroideae Heliantheae alliance Heliantheae Eclipta
Camellia sinensis	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids Ericales Theaceae Camellia
Illicium anisatum	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta basal Magnoliophyta Austrobaileyales Schisandraceae Illicium
Impatiens balsamina	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids Ericales Balsaminaceae Impatiens Impatiens Impatiens sect. Uniflorae
Jatropha gossypifolia	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae rosids fabids Malpighiales Euphorbiaceae Crotonoideae Jatropeae Jatropha
Panax ginseng	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids campanulids Apiales Apiineae Araliaceae Panax
Larrea divaricata	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae rosids fabids Zygophyllales Zygophyllaceae Larreoideae Larrea
Lawsonia inermis	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae rosids malvids Myrtales Lythraceae Lawsonia
Leonurus sibiricus	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids lamiids Lamiales Lamiaceae Lamiodeae Leonureae Leonurus
Ligusticum sinense	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids campanulids Apiales Apiineae Apiaceae Apioideae Acronema clade Ligusticum

Ligustrum lucidum	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids lamiids Lamiales Oleaceae Oleaceae Ligustrum
Lycium chinense	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids lamiids Solanales Solanaceae Solanoideae Lychieae Lycium
Lycopersicon esculentum	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids lamiids Solanales Solanaceae Solanoideae Solaneae Solanum Lycopersicon
Mimosa pudica	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae rosids fabids Fabales Fabaceae Caesalpinioideae mimosoid clade Mimoseae Mimosa
Morus alba	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae rosids fabids Rosales Moraceae Morus
Nerium oleander	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids lamiids Gentianales Apocynaceae Apocynoideae Nerieae Neriinae Nerium
Ocimum tenniflorum	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids lamiids Lamiales Lamiaceae Nepetoideae Ocimeae Ocimum
Oryza sativa	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae Liliopsida Petrosaviidae commelinids Poales Poaceae BOP clade Oryzoideae Oryzeae Oryzinae Oryza
Phyllanthus emblica	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae rosids fabids Malpighiales Phyllanthaceae Phyllanthoideae Phyllanthae Phyllanthus
Prunus persica	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae rosids fabids Rosales Rosaceae Maloideae Amygdaleae Prunus
Cullen corylifolium	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae rosids fabids Fabales Fabaceae Papilionoideae Psoraleae Cullen
Pueraria montana var. chinensis	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae rosids fabids Fabales Fabaceae Papilionoideae Phaseoleae Pueraria Pueraria montana
Rehmannia glutinosa	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids lamiids Lamiales Orobanchaceae Orobanchaceae incertae sedis Rehmannia
Rhinacanthus nasutus	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids lamiids Lamiales Acanthaceae Acanthoideae Ruellieae Justiciinae Rhinacanthus

Rosmarinus officinalis	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids lamiids Lamiales Lamiaceae Nepetoideae Mentheae Salvia Rosmarinus
Rubus coreanus	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae rosids fabids Rosales Rosaceae Rosoideae Rosoideae unplaced Rubus
Salvia miltiorrhiza	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids lamiids Lamiales Lamiaceae Nepetoideae Mentheae Salvia
Sapindus rarak	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae rosids malvids Sapindales Sapindaceae Sapindus
Scutellaria baicalensis	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids lamiids Lamiales Lamiaceae Scutellarioideae Scutellaria
Serenoa repens	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae Liliopsida Petrosaviidae commelinids Arecales Areaceae Coryphoideae Livistoneae Livistoneae incertae sedis Serenoa
Sesamum indicum	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids lamiids Lamiales Pedaliaceae Sesamum
Solanum americanum	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids lamiids Solanales Solanaceae Solanoideae Solaneae Solanum
Sophora flavescens	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae rosids fabids Fabales Fabaceae Papilionoideae Sophoreae Sophora
Dioscorea communis	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae Liliopsida Petrosaviidae Dioscoreales Dioscoreaceae Dioscorea
Terminalia bellirica	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae rosids malvids Myrtales Combretaceae Terminalia
Terminalia chebula	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae rosids malvids Myrtales Combretaceae Terminalia
Thuja occidentalis	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Acrogymnospermae Pinidae Cupressales Cupressaceae Thuja
Trichosanthes cucumerina	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae rosids fabids Cucurbitales Cucurbitaceae Sicyoeae Trichosanthes

Trifolium pratense	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae rosids fabids Fabales Fabaceae Papilionoideae Trifolieae Trifolium
Viscum album	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae Santalales Viscaceae Viscum
Wedelia chinensis	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae asterids campanulids Asterales Asteraceae Asteroideae Heliantheae alliance Heliantheae Wedelia
Zingiber officinale	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae Liliopsida Petrosaviidae commelinids Zingiberales Zingiberaceae Zingiber
Zizyphus jujuba	cellular organisms Eukaryota Viridiplantae Streptophyta Streptophytina Embryophyta Tracheophyta Euphyllophyta Spermatophyta Magnoliophyta Mesangiospermae eudicotyledons Gunneridae Pentapetalae rosids fabids Rosales Rhamnaceae Paliureae Ziziphus

4. THE INPUT FILE USED FOR THE CORRECTION OF PLANT NAMES

Full Name	Genus	Species	Var	Intraspecific
Acacia concinna	Acacia	concinna		
Albizia julibrissin	Albizia	julibrissin		
Allium cepa	Allium	cepa		
Allium sativum	Allium	sativum		
Aloe vera	Aloe	vera		
Alpinia zerumbet	Alpinia	zerumbet		
Ammi majus	Ammi	majus		
Andrographis paniculata	Andrographis	paniculata		
Angelica dahurica	Angelica	dahurica		
Angelica gigas	Angelica	gigas		
Angelica sinensis	Angelica	sinensis		
Artemisia abrotanum	Artemisia	abrotanum		
Averrhoa carambola	Averrhoa	carambola		
Avicennia marina	Avicennia	marina		
Azadirachta indica	Azadirachta	indica		
Bidens tripartita	Bidens	tripartita		
Camellia sinensis	Camellia	sinensis		
Carthamus tinctorius	Carthamus	tinctorius		
Cedrus deodara	Cedrus	deodara		
Chrysanthemum morifolium	Chrysanthemum	morifolium		
Chrysanthemum zawadskii	Chrysanthemum	zawadskii		
Clitoria ternatea	Clitoria	ternatea		
Cnidium officinale	Cnidium	officinale		

Coffea arabica	Coffea	arabica		
Corydalis turtschaninovii	Corydalis	turtschaninovii		
Cullen corylifolium	Cullen	corylifolium		
Curcuma longa	Curcuma	longa		
Cuscuta reflexa	Cuscuta	reflexa		
Cynomorium songaricum	Cynomorium	songaricum		
Eclipta prostrata	Eclipta	prostrata		
Illicium anisatum	Illicium	anisatum		
Impatiens balsamina	Impatiens	balsamina		
Jatropha gossypifolia	Jatropha	gossypifolia		
Larrea divaricata	Larrea	divaricata		
Lawsonia inermis	Lawsonia	inermis		
Leonurus sibiricus	Leonurus	sibiricus		
Ligusticum sinense	Ligusticum	sinense		
Ligustrum lucidum	Ligustrum	lucidum		
Lycium chinense	Lycium	chinense		
Lycopersicon esculentum	Lycopersicon	esculentum		
Mimosa pudica	Mimosa	pudica		
Morus alba	Morus	alba		
Nerium oleander	Nerium	oleander		
Ocimum sanctum	Ocimum	sanctum		
Oryza sativa	Oryza	sativa		
Panax ginseng	Panax	ginseng		
Platyclusus orientalis	Platyclusus	orientalis		
Prunus persica	Prunus	persica		
Pueraria thomsonii	Pueraria	thomsonii		
Rehmannia glutinosa	Rehmannia	glutinosa		
Rhinacanthus nasutus	Rhinacanthus	nasutus		
Rubus coreanus	Rubus	coreanus		
Salvia miltiorrhiza	Salvia	miltiorrhiza		
Salvia rosmarinus	Salvia	rosmarinus		
Sapindus rarak	Sapindus	rarak		
Scutellaria baicalensis	Scutellaria	baicalensis		
Serenoa repens	Serenoa	repens		
Sesamum indicum	Sesamum	indicum		
Solanum nigrum	Solanum	nigrum		
Sophora flavescens	Sophora	flavescens		
Tamus communis	Tamus	communis		
Terminalia bellirica	Terminalia	bellirica		
Terminalia chebula	Terminalia	chebula		
Thuja occidentalis	Thuja	occidentalis		
Trichosanthes cucumerina	Trichosanthes	cucumerina		
Trifolium pratense	Trifolium	pratense		
Viscum album	Viscum	album		
Zingiber officinale	Zingiber	officinale		
Ziziphus jujuba	Ziziphus	jujuba		

5. CORRECTION OF THE PLANTS NAME TO THE ACCEPTED NAME

	Taxon	Genus	Species	Taxonomic status	New.Genus	New.Species	New.Taxonomic.status
1	Acacia concinna	Acacia	concinna	Accepted	Acacia	concinna	Accepted
2	Albizia julibrissin	Albizia	julibrissin	Accepted	Albizia	julibrissin	Accepted
3	Allium cepa	Allium	cepa	Accepted	Allium	cepa	Accepted
4	Allium sativum	Allium	sativum	Accepted	Allium	sativum	Accepted
5	Aloe vera	Aloe	vera	Accepted	Aloe	vera	Accepted
6	Alpinia zerumbet	Alpinia	zerumbet	Accepted	Alpinia	zerumbet	Accepted
7	Ammi majus	Ammi	majus	Accepted	Ammi	majus	Accepted
8	Andrographis paniculata	Andrographis	paniculata	Accepted	Andrographis	paniculata	Accepted
9	Angelica dahurica	Angelica	dahurica	Accepted	Angelica	dahurica	Accepted
10	Angelica gigas	Angelica	gigas	Accepted	Angelica	gigas	Accepted
11	Angelica sinensis	Angelica	sinensis	Accepted	Angelica	sinensis	Accepted
12	Artemisia abrotanum	Artemisia	abrotanum	Accepted	Artemisia	abrotanum	Accepted
13	Averrhoa carambola	Averrhoa	carambola	Accepted	Averrhoa	carambola	Accepted
14	Avicennia marina	Avicennia	marina	Accepted	Avicennia	marina	Accepted
15	Azadirachta indica	Azadirachta	indica	Accepted	Azadirachta	indica	Accepted
16	Bidens tripartita	Bidens	tripartita	Accepted	Bidens	tripartita	Accepted
17	Camellia sinensis	Camellia	sinensis	Accepted	Camellia	sinensis	Accepted
18	Carthamus tinctorius	Carthamus	tinctorius	Accepted	Carthamus	tinctorius	Accepted
19	Cedrus deodara	Cedrus	deodara	Accepted	Cedrus	deodara	Accepted
20	Chrysanthemum morifolium	Chrysanthemum	morifolium	Accepted	Chrysanthemum	morifolium	Accepted
21	Chrysanthemum zawadskii	Chrysanthemum	zawadskii	Accepted	Chrysanthemum	zawadskii	Accepted

2 2	Clitoria ternatea	Clitoria	ternatea	Accepted	Clitoria	ternatea	Accepted
2 3	Cnidium officinale	Cnidium	officinale	Synonym	Ligusticum	officinale	Unresolved
2 4	Coffea arabica	Coffea	arabica	Accepted	Coffea	arabica	Accepted
2 5	Corydalis turtschani novii	Corydalis	turtschan inovii	Accepted	Corydalis	turtschan inovii	Accepted
2 6	Cullen corylifoliu m	Cullen	corylifoliu m	Accepted	Cullen	corylifoliu m	Accepted
2 7	Curcuma longa	Curcuma	longa	Accepted	Curcuma	longa	Accepted
2 8	Cuscuta reflexa	Cuscuta	reflexa	Accepted	Cuscuta	reflexa	Accepted
2 9	Cynomoriu m songaricu m	Cynomoriu m	songaricu m	Synonym	Cynomoriu m	coccineu m	Accepted
3 0	Eclipta prostrata	Eclipta	prostrata	Accepted	Eclipta	prostrata	Accepted
3 1	Illicium anisatum	Illicium	anisatum	Unresolved	Illicium	anisatum	Unresolved
3 2	Impatiens balsamina	Impatiens	balsamin a	Accepted	Impatiens	balsamin a	Accepted
3 3	Jatropha gossypiifol ia	Jatropha	gossypiifo lia	Accepted	Jatropha	gossypiifo lia	Accepted
3 4	Larrea divaricata	Larrea	divaricata	Accepted	Larrea	divaricata	Accepted
3 5	Lawsonia inermis	Lawsonia	inermis	Accepted	Lawsonia	inermis	Accepted
3 6	Leonurus sibiricus	Leonurus	sibiricus	Accepted	Leonurus	sibiricus	Accepted
3 7	Ligusticum sinense	Ligusticum	sinense	Accepted	Ligusticum	sinense	Accepted
3 8	Ligustrum lucidum	Ligustrum	lucidum	Accepted	Ligustrum	lucidum	Accepted
3 9	Lycium chinense	Lycium	chinense	Accepted	Lycium	chinense	Accepted
4 0	Lycopersic on esculentu m	Lycopersic on	esculentu m	Accepted	Lycopersic on	esculentu m	Accepted
4 1	Mimosa pudica	Mimosa	pudica	Accepted	Mimosa	pudica	Accepted
4 2	Morus alba	Morus	alba	Accepted	Morus	alba	Accepted
4 3	Nerium oleander	Nerium	oleander	Accepted	Nerium	oleander	Accepted

44	Ocimum sanctum	Ocimum	sanctum	Synonym	Ocimum	tenuiflorum	Accepted
45	Oryza sativa	Oryza	sativa	Accepted	Oryza	sativa	Accepted
46	Panax ginseng	Panax	ginseng	Accepted	Panax	ginseng	Accepted
47	Platyclus orientalis	Platyclus	orientalis	Accepted	Platyclus	orientalis	Accepted
48	Prunus persica	Prunus	persica	Accepted	Prunus	persica	Accepted
49	Pueraria thomsonii	Pueraria	thomsonii	Synonym	Pueraria	montana	Accepted
50	Rehmannia glutinosa	Rehmannia	glutinosa	Accepted	Rehmannia	glutinosa	Accepted
51	Rhinacanthus nasutus	Rhinacanthus	nasutus	Accepted	Rhinacanthus	nasutus	Accepted
52	Rubus coreanus	Rubus	coreanus	Accepted	Rubus	coreanus	Accepted
53	Salvia miltiorrhiza	Salvia	miltiorrhiza	Accepted	Salvia	miltiorrhiza	Accepted
54	Salvia rosmarinus	Salvia	rosmarinus	Synonym	Rosmarinus	officinalis	Accepted
55	Sapindus rarak	Sapindus	rarak	Accepted	Sapindus	rarak	Accepted
56	Scutellaria baicalensis	Scutellaria	baicalensis	Accepted	Scutellaria	baicalensis	Accepted
57	Serenoa repens	Serenoa	repens	Accepted	Serenoa	repens	Accepted
58	Sesamum indicum	Sesamum	indicum	Accepted	Sesamum	indicum	Accepted
59	Solanum nigrum	Solanum	nigrum	Synonym	Solanum	americanum	Accepted
60	Sophora flavescens	Sophora	flavescens	Accepted	Sophora	flavescens	Accepted
61	Tamus communis	Tamus	communis	Synonym	Dioscorea	communis	Accepted
62	Terminalia bellirica	Terminalia	bellirica	Accepted	Terminalia	bellirica	Accepted
63	Terminalia chebula	Terminalia	chebula	Accepted	Terminalia	chebula	Accepted
64	Thuja occidentalis	Thuja	occidentalis	Accepted	Thuja	occidentalis	Accepted
65	Trichosanthes cucumerina	Trichosanthes	cucumerina	Accepted	Trichosanthes	cucumerina	Accepted

6	Trifolium pratense	Trifolium	pratense	Accepted	Trifolium	pratense	Accepted
6	Viscum album	Viscum	album	Accepted	Viscum	album	Accepted
6	Zingiber officinale	Zingiber	officinale	Accepted	Zingiber	officinale	Accepted
6	Ziziphus jujuba	Ziziphus	jujuba	Accepted	Ziziphus	jujuba	Accepted

APPENDIX 8

1. SPECIMEN OF THE FASTA FILE OF THE PLANTS

>|Acacia_concinna|

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TGCTCCTCCTTTTCATTTATTAAGGCTCTTTCTTTATGAGTATTGTAATTGGAATAGTCTTACTCAA
AAAAACAGGATTTCTACTTTTTCAAAAAGTAATCCAAGATTTTTCTGTTCTTATATAATTTTTATGTAT
GTGAATACGAATCCATCTTTCTTTTCTCCGTAACAAATCTTCTATTTACGATTAACATCTTCTGGAGT
CTTTTTGAACGAATCTATTTCTATGCAAAAATAGAACATTTTTTAGAAGTCTTTGATAAGGATTTTCC
GTCCACCCTACGGTTCTTCAAGGACCCTTTCATTCATTATGTTAGATATCAAGGAAAATCCATTCTGGC
TTCAAAGAATACGCCTTTTTGATGAAAAAATGGAAATACTATCTTATCCATTTATGGCAATGTCATTT
TTTTGTTGGTCTCAACCAGGAAAGATCCATATAAACCAATTATCCGAGCATTCAATTTCTTTTTGGG
CTATTTTTCAAATGTGCGGCTAAATCCTTCAGTGGTACGGAGTCAAATGTTGGAAAAGTCATTTATAA
TGAAAATCTTATGAAAAGCTTGATACAATAATTCCAATTGTTCTCTAATTAGATCATTGGCTCAA
GCAAGATTTTGAATCTATTAGGACATCCATTAGTAAGCCGGTCTGGGCCGATTCATCCGATTTTGA
TATTATTGAACGATTTTTGCAGATATGCAGAA
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>|Albizia_julibrissin|

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AAACCTTCGATACTGGGTGAAAGATGCCTCCTCCTTTTCATTTATTAAGGCTCTTTCTTTATGAGTATT
GTAATTGGAATAGTCTGATTACTCAAAAAAAGGATTTCTACTTTTTCAAAAAGTAATCCAAGATTT
CTCCTGTTCTATATAATTTTTATGTATGTGAATACGAATCCATCTTTCTTTTCTCCGTAACAAATCTTC
TATTTACGATTAACATCTTCTGGAGTCTTTTTGAACGAATCTATTTCTATGCAAAAATAGAACATTTT
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AGATATCAAGGAAAATCCATTCTAGCTTCAAAGAATACGCCCTTTTTGATGAAAAAATGGAAATACTA
TCTTATCCATTTATGGCAATGTCATTTTTTTGTTTGGTCTCAACCAGGAAAGATCCATATAAACCAATT
ATCCGAGCATTCAATTTGACTTTTTGGGCTATTTTTCAAATGTGCGGCTAAATCCTTCAGTGGTACGGA
GTCAAATGTTGGAAAAGTCATTTATAATGGAAAATCTTCTGAAAAGCTTGATACAATAATTCCAATT
ATTCCTAATTAGATCATTGGCTAAAGCAAAATTTTGAATGTATTAGGACATCCATTAGTAAGCC
GGTCTGGGCCGATTCATCCGATTTTGTATTATTGATCGATTTTTGCAGATATGCAGAGATCTCTCTCA
TTATTACAACGGATCTCAAAAAAAGAGTTTGTATCGAATCAAATATATACTTCGGCTTTCTTGTAT
TAAACTTTGG
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2. SPECIMEN OF THE MULTIPLE SEQUENCE ALIGNMENT OF THE PLANTS

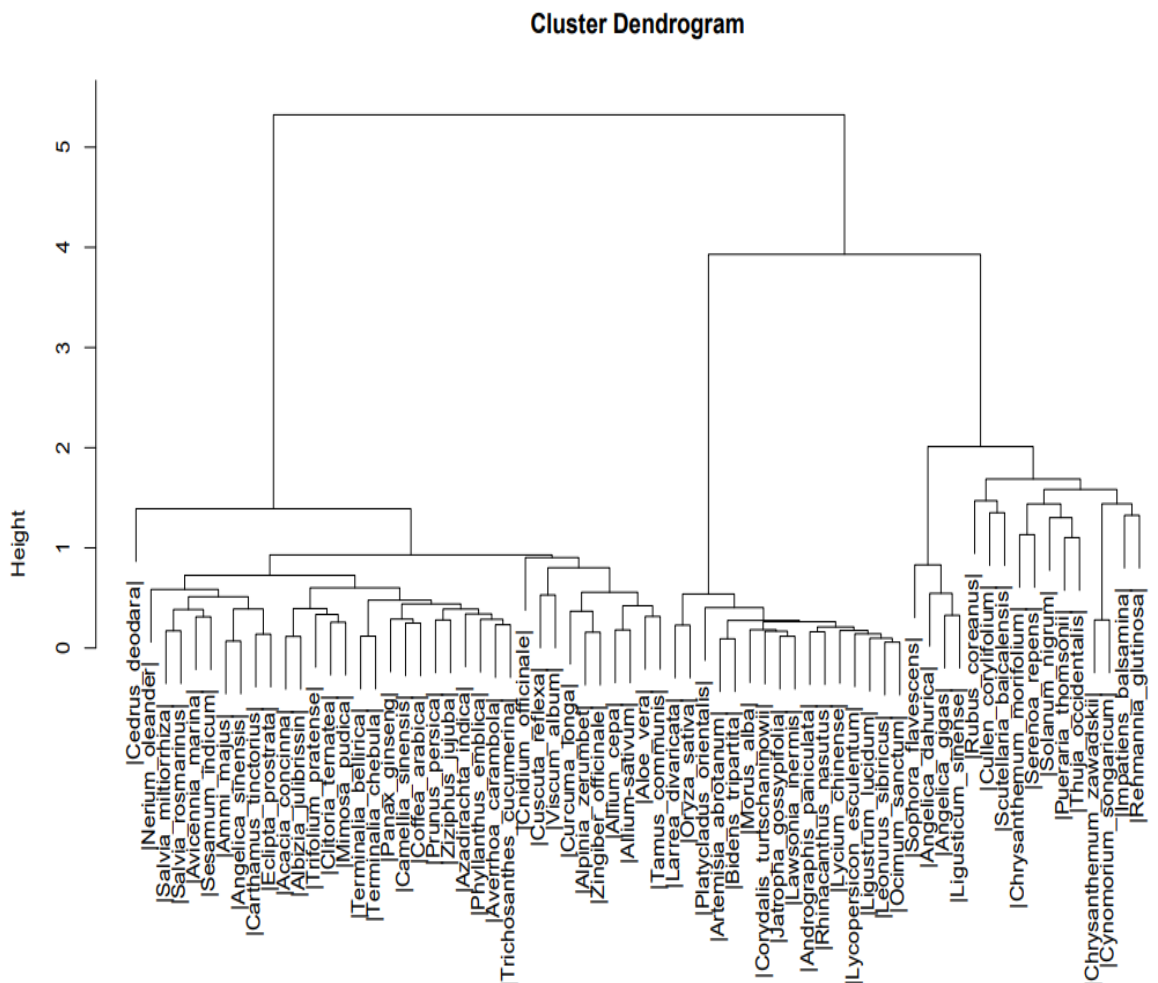
>|Acacia_concinna|

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TCC-----ACCTATGGTCTTCAAG-----
-----GACCTTTCATTATTATGTTAGATATCAAGGAAAATCCATTC
TAGCT-----TCAAAGAATACGCC-----TTTTTGATGAAAAATGGAATACTAT
CTTATCCATTTATGGCAATGT-----CATTTTTTGTGGTCTCAACCAGGAAA
GATCCATATAAACCAATTATCCGAGCATTATTGACTTTTTGGGCTATTTTTCAAATGTGCGG-----

-----CTAAAT
CCTTCAGTGGTACGGAGTCAAATGTTGGAAAAGTCATTATAATGGAAAATCTTCTGAAAAAG-----
-CTTGATAC
AATAATTCCAATTATTCCTCTAATTAGATCATTGGCT-----
AAAGCAAATTTTGTAAATGTAT
TAGGACATCCCATTAGT-----
AAGCCGGTCTGGGCCGATTTCATCCGATTTTGATATTATTGATCGATTTTTGCAGATA
TGCAGAGATCTCTCATTATTACAACGGATCCTCAAAAAAAGAGTTTGTATCGAATCAAATATAT
ACTTCGGCTTTC
TTGTATTAATAACTTTGG-----

3. THE PHYLOGENY DIAGRAM



APPENDIX 9

FREQUENCY OF PHYTOCHEMICALS OCCURRENCE IN THE 69 PLANTS

	Name of Phytochemical	Pubchem CID	Found in # alopecia plants	Plant names
CM P 1	beta-sitosterol	222284	17	<i>Cynomorium songaricum, Curcuma longa, Tamus communis, Panax ginseng, Morus alba, Viscum album, Sophora flavescens, Lycium chinense, Eclipta prostrata, Rubus coreanus, Zingiber officinale, Ligusticum sinense, Solanum nigrum, Sesamum indicum, Salvia miltiorrhiza, Angelica dahurica, Carthamus tinctorius</i>
CM P 2	palmitic acid	985	16	<i>Cynomorium songaricum, Terminalia chebula, Carthamus tinctorius, Oryza sativa, Zingiber officinale, Cnidium officinale, Viscum album, Panax ginseng, Curcuma longa, Eclipta prostrata, Ziziphus jujuba, Bidens tripartita, Lycium chinense, Chrysanthemum zawadskii, Andrographis paniculata, Albizia julibrissin</i>
CM P 3	ferulic acid	445858	15	<i>Zingiber officinale, Cnidium officinale, Angelica sinensis, Salvia miltiorrhiza, Allium sativum, Ligusticum sinense, Rubus coreanus, Solanum nigrum, Ziziphus jujuba, Scutellaria baicalensis, Lycium chinense, Carthamus tinctorius, Chrysanthemum morifolium, Sesamum indicum, Morus alba</i>
CM P 4	quercetin	5280343	15	<i>Carthamus tinctorius, Allium cepa, Chrysanthemum morifolium, Oryza sativa, Platycladus orientalis, Cnidium officinale, Allium sativum, Solanum nigrum, Zingiber officinale, Albizia julibrissin, Cynomorium songaricum, Ziziphus jujuba, Morus alba, Rubus coreanus, Cuscuta reflexa</i>
CM P 5	linoleic acid	5280450	14	<i>Prunus persica, Terminalia chebula, Carthamus tinctorius, Zingiber officinale, Cnidium officinale, Cullen corylifolium, Viscum album, Ziziphus jujuba, Ligusticum sinense, Eclipta prostrata, Ligustrum lucidum, Curcuma longa, Panax ginseng, Albizia julibrissin</i>
CM P 6	stearic acid	5281	12	<i>Eclipta prostrata, Ziziphus jujuba, Carthamus tinctorius, Ziziphus jujuba, Rubus coreanus, Zingiber officinale, Cynomorium songaricum, Lycium chinense, Panax ginseng, Terminalia chebula, Curcuma longa, Albizia julibrissin</i>
CM P 7	vanillic acid	8468	12	<i>Cnidium officinale, Oryza sativa, Salvia miltiorrhiza, Allium sativum, Rubus coreanus, Lycium chinense, Solanum nigrum, Zingiber officinale, Sesamum indicum, Morus alba, Ziziphus jujuba, Carthamus tinctorius</i>
CM P 8	chlorogenic acid	1794427	12	<i>Chrysanthemum morifolium, Cnidium officinale, Salvia miltiorrhiza, Morus alba, Lycium chinense, Ziziphus jujuba, Solanum nigrum, Scutellaria baicalensis, Rubus coreanus, Andrographis paniculata, Eclipta prostrata, Cuscuta reflexa</i>
CM P 9	kaempferol	5280863	12	<i>Carthamus tinctorius, Allium cepa, Allium sativum, Camellia sinensis, Chrysanthemum morifolium, Solanum nigrum, Zingiber officinale, Rubus coreanus, Albizia julibrissin, Morus alba, Panax ginseng, Cuscuta reflexa</i>
CM P 10	protocatechuic acid	72	11	<i>Salvia miltiorrhiza, Oryza sativa, Allium cepa, Cnidium officinale, Allium sativum, Rubus coreanus, Ziziphus jujuba, Solanum nigrum, Chrysanthemum morifolium, Morus alba, Cynomorium songaricum</i>
CM	gallic acid	370	11	<i>Terminalia chebula, Cnidium officinale, Rubus coreanus, Zingiber officinale, Ziziphus jujuba, Solanum nigrum, Cynomorium songaricum, Morus alba, Terminalia bellirica, Carthamus tinctorius, Albizia julibrissin</i>

P 1 1				
C M P 1 2	caffeic acid	689 043	10	<i>Salvia miltiorrhiza, Cnidium officinale, Allium sativum, Rubus coreanus, Lycium chinense, Ziziphus jujuba, Solanum nigrum, Morus alba, Carthamus tinctorius, Chrysanthemum morifolium</i>
C M P 1 3	apigenin	528 044 3	10	<i>Chrysanthemum morifolium, Andrographis paniculata, Ocimum sanctum, Cnidium officinale, Solanum nigrum, Albizia julibrissin, Lycium chinense, Scutellaria baicalensis, Eclipta prostrata, Larrea divaricata</i>
C M P 1 4	rutin	528 080 5	10	<i>Carthamus tinctorius, Clitoria ternatea, Platycladus orientalis, Morus alba, Lycium chinense, Solanum nigrum, Zingiber officinale, Ziziphus jujuba, Rubus coreanus, Chrysanthemum morifolium</i>
C M P 1 5	beta-elemene	985 909 4	9	<i>Zingiber officinale, Ligusticum sinense, Platycladus orientalis, Panax ginseng, Curcuma longa, Bidens tripartita, Angelica dahurica, Chrysanthemum zawadskii, Chrysanthemum morifolium</i>
C M P 1 6	alpha-pinen e	665 4	8	<i>Zingiber officinale, Bidens tripartita, Curcuma longa, Platycladus orientalis, Cnidium officinale, Panax ginseng, Chrysanthemum zawadskii, Chrysanthemum morifolium</i>
C M P 1 7	beta-terpinene	746 1	8	<i>Zingiber officinale, Cnidium officinale, Platycladus orientalis, Curcuma longa, Chrysanthemum zawadskii, Chrysanthemum morifolium, Cnidium officinale, Angelica dahurica</i>
C M P 1 8	beta-myrcene	312 53	8	<i>Zingiber officinale, Platycladus orientalis, Curcuma longa, Bidens tripartita, Angelica dahurica, Panax ginseng, Chrysanthemum zawadskii, Chrysanthemum morifolium</i>
C M P 1 9	oleic acid	445 639	8	<i>Prunus persica, Terminalia chebula, Ziziphus jujuba, Zingiber officinale, Ligustrum lucidum, Carthamus tinctorius, Panax ginseng, Curcuma longa</i>
C M P 2 0	p-coumaric acid	154 910 6	8	<i>Albizia julibrissin, Lycium chinense, Allium sativum, Rubus coreanus, Solanum nigrum, Ziziphus jujuba, Morus alba, Carthamus tinctorius</i>
C M P	alpha-caryophyllene	528 152 0	8	<i>Zingiber officinale, Cnidium officinale, Platycladus orientalis, Panax ginseng, Eclipta prostrata, Ziziphus jujuba, Curcuma longa, Bidens tripartita</i>

2 1				
C M P 2 2	p- hydro xyben zoic acid	135	7	<i>Solanum nigrum, Allium sativum, Rubus coreanus, Carthamus tinctorius, Ziziphus jujuba, Chrysanthemum morifolium, Morus alba</i>
C M P 2 3	benzal dehyd e	240	7	<i>Ziziphus jujuba, Terminalia chebula, Panax ginseng, Bidens tripartita, Curcuma longa, Lycium chinense, Chrysanthemum morifolium</i>
C M P 2 4	vanilli n	118 3	7	<i>Zingiber officinale, Cnidium officinale, Angelica sinensis, Sesamum indicum, Curcuma longa, Panax ginseng, Albizia julibrissin</i>
C M P 2 5	arachi dic acid	104 67	7	<i>Ziziphus jujuba, Cynomorium songaricum, Panax ginseng, Cnidium officinale, Lycium chinense, Terminalia chebula, Curcuma longa</i>
C M P 2 6	olean olic acid	104 94	7	<i>Ligustrum lucidum, Viscum album, Panax ginseng, Rubus coreanus, Ziziphus jujuba, Cuscuta reflexa, Viscum album</i>
C M P 2 7	alpha- thujen e	178 68	7	<i>Panax ginseng, Zingiber officinale, Chrysanthemum morifolium, Platycladus orientalis, Bidens tripartita, Curcuma longa, Chrysanthemum zawadskii</i>
C M P 2 8	alpha- curcu mene	921 39	7	<i>Curcuma longa, Zingiber officinale, Ligusticum sinense, Cnidium officinale, Chrysanthemum morifolium, Platycladus orientalis, Bidens tripartita</i>
C M P 2 9	luteoli n	528 044 5	7	<i>Terminalia chebula, Chrysanthemum morifolium, Andrographis paniculata, Ocimum sanctum, Solanum nigrum, Albizia julibrissin, Eclipta prostrata</i>
C M P 3 0	myrist ic acid	110 05	6	<i>Ziziphus jujuba, Zingiber officinale, Cynomorium songaricum, Terminalia chebula, Lycium chinense, Panax ginseng</i>
C M P	adeno sine	609 61	6	<i>Solanum nigrum, Carthamus tinctorius, Angelica dahurica, Sesamum indicum, Corydalis turtschaninovii, Ziziphus jujuba</i>

3 1				
C M P 3 2	ursolic acid	649 45	6	<i>Viscum album, Cynomorium songaricum, Ligustrum lucidum, Rubus coreanus, Ziziphus jujuba, Salvia miltiorrhiza</i>
C M P 3 3	palmit oleic acid	445 638	6	<i>Ziziphus jujuba, Zingiber officinale, Cynomorium songaricum, Panax ginseng, Curcuma longa, Andrographis paniculata</i>
C M P 3 4	pinocavone	100 120 81	6	<i>Bidens tripartita, Curcuma longa, Zingiber officinale, Chrysanthemum morifolium, Chrysanthemum zawadskii, Panax Ginseng</i>

MCS-SYSTEM STRUCTURAL SIMILARITY BETWEEN THE PHYTOCHEMICALS

The screenshot displays an Excel spreadsheet titled "MCS-MATRIX - Excel (Product Activation failed)". The spreadsheet contains a similarity matrix for 38 phytochemicals, labeled CMP1 through CMP38. The matrix is a lower triangular grid of numerical values, where each cell represents the structural similarity between two compounds. The values range from 0.0 to 1.0. The diagonal elements are all 1.0, indicating 100% similarity of a compound to itself. The matrix is symmetric, meaning the similarity between compound A and B is the same as between B and A. The spreadsheet interface includes the Microsoft Excel ribbon with various tabs like File, Home, Insert, Page Layout, Formulas, Data, Review, View, Developer, and Tell me what you want to do... The ribbon also shows various toolbars for editing, formatting, and data analysis.

APPLICATION OF LIPINSKI RULE OF FIVE ON THE PHYTOCHEMICALS

PHYTOCHEMICAL	LIPINSKI FAILURES
1	0
2	0
3	0
4	0
5	2
6	0
7	2
8	0
9	0
10	0
11	2
12	1
13	2
14	0
15	0
16	0
17	1
18	1
19	1
20	2
21	2
22	0
23	0
24	0
25	1
26	0
27	0
28	0
29	2
30	2
31	0
32	1
33	1
34	0

SNAPSHOT OF LIU ALERTS RESULTS

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z	AA	AB	AC	AD	AE	AF	AG	AH	AI	
1		CMP1	CMP2	CMP3	CMP4	CMP5	CMP6	CMP7	CMP8	CMP9	CMP10	CMP11	CMP12	CMP13	CMP14	CMP15	CMP16	CMP17	CMP18	CMP19	CMP20	CMP21	CMP22	CMP23	CMP24	CMP25	CMP26	CMP27	CMP28	CMP29	CMP30	CMP31	CMP32	CMP33	CMP34	
2	Liu1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	Liu2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	Liu3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	Liu4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6	Liu5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
7	Liu7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	Liu8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	2
9	Liu9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10	Liu10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
11	Liu11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12	Liu12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
13																																				

SNAPSHOT OF MADDEN ALERTS RESULTS

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z	AA	AB	AC	AD	AE	AF	AG	AH	AI		
1		CMP1	CMP2	CMP3	CMP4	CMP5	CMP6	CMP7	CMP8	CMP9	CMP10	CMP11	CMP12	CMP13	CMP14	CMP15	CMP16	CMP17	CMP18	CMP19	CMP20	CMP21	CMP22	CMP23	CMP24	CMP25	CMP26	CMP27	CMP28	CMP29	CMP30	CMP31	CMP32	CMP33	CMP34		
2	Madden1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
3	Madden2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
4	Madden3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	Madden4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6	Madden5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
7	Madden6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	Madden7	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9	Madden8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10	Madden11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
11	Madden12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12	Madden13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
13	Madden14	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
14	Madden15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
15	Madden16	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
16	Madden17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
17																																					

SNAPSHOT OF WALTER & MURCKO RESULTS

Walter&MurckoRESULTS - Excel (Product Activation Faile...)

File Home Insert Page Layout Formulas Data Review View Developer Tell me what you want to do...

Clipboard Font Alignment Number Conditional Formatting Styles Cells Editing

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W	X	Y	Z	AA	AB	AC	AD	AE	AF	AG	AH	AI	
1		DMP1	DMP2	DMP3	DMP4	DMP5	DMP6	DMP7	DMP8	DMP9	DMP10	DMP11	DMP12	DMP13	DMP14	DMP15	DMP16	DMP17	DMP18	DMP19	DMP20	DMP21	DMP22	DMP23	DMP24	DMP25	DMP26	DMP27	DMP28	DMP29	DMP30	DMP31	DMP32	DMP33	DMP34	
2	Waters0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
3	Waters1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
4	Waters2	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
5	Waters3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
6	Waters4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
7	Waters5	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
8	Waters6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
9	Waters7	0	0	0	0	14	0	18	0	0	0	0	22	0	10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
10	Waters8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
11	Waters9	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
12	Waters10	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
13	Waters11	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

DESCRIPTION OF CDK MOLECULAR DESCRIPTORS CLASSES

Class	Description
AcidicGroupCountDescriptor	Returns the number of acidic groups.
ALOGPDescriptor	This class calculates ALOGP (Ghose-Crippen LogKow) and the Ghose-Crippen molar refractivity [Ghose, A.K. and Crippen, G.M. , <i>Atomic physicochemical parameters for three-dimensional structure-directed quantitative structure-activity relationships. 1. Partition coefficients as a measure of hydrophobicity</i> , Journal of Computational Chemistry, 1986, 7:565-577, doi:10.1002/jcc.540070419, Ghose, A.K. and Crippen, G.M. , <i>Atomic physicochemical parameters for three-dimensional-structure-directed quantitative structure-activity relationships. 2. Modeling dispersive and hydrophobic interactions</i> , Journal of Chemical Information and Computer Science, 1987, 27:21-35, doi:10.1021/ci00053a005].
AminoAcidCountDescriptor	Class that returns the number of each amino acid in an atom container.
APolDescriptor	Sum of the atomic polarizabilities (including implicit hydrogens).
AromaticAtomsCountDescriptor	Class that returns the number of aromatic atoms in an atom container.
AromaticBondsCountDescriptor	This Class contains a method that returns the number of aromatic atoms in an AtomContainer.
AtomCountDescriptor	IDescriptor based on the number of atoms of a certain element type.
AutocorrelationDescriptorCharge	This class calculates ATS autocorrelation descriptor, where the weight equal to the charges.
AutocorrelationDescriptorMass	This class calculates ATS autocorrelation descriptor, where the weight equal to the scaled atomic mass [Moreau G. and Broto P., <i>The autocorrelation of a topological structure: A new molecular descriptor</i> , Nouveau Journal de Chimie, 1980, ? :359-360].
AutocorrelationDescriptorPolarizability	This class calculates ATS autocorrelation descriptor, where the weight equal to the charges.
BasicGroupCountDescriptor	Returns the number of basic groups.

BCUTDescriptor	Eigenvalue based descriptor noted for its utility in chemical diversity.
BondCountDescriptor	IDescriptor based on the number of bonds of a certain bond order.
BPolDescriptor	Sum of the absolute value of the difference between atomic polarizabilities of all bonded atoms in the molecule (including implicit hydrogens) with polarizabilities taken from http://www.sunysccc.edu/academic/mst/ptable/p-table2.htm This descriptor assumes 2-centered bonds.
CarbonTypesDescriptor	Topological descriptor characterizing the carbon connectivity.
ChiChainDescriptor	Evaluates chi chain descriptors.
ChiClusterDescriptor	Evaluates chi cluster descriptors.
ChiPathClusterDescriptor	Evaluates chi path cluster descriptors.
ChiPathDescriptor	Evaluates chi path descriptors.
CPSADescriptor	Calculates 29 Charged Partial Surface Area (CPSA) descriptors.
EccentricConnectivityIndexDescriptor	A topological descriptor combining distance and adjacency information.
FMFDescriptor	An implementation of the FMF descriptor characterizing complexity of a molecule.
FractionalPSADescriptor	Polar surface area expressed as a ratio to molecular size.
FragmentComplexityDescriptor	Class that returns the complexity of a system.
GravitationalIndexDescriptor	IDescriptor characterizing the mass distribution of the molecule.
HBondAcceptorCountDescriptor	This descriptor calculates the number of hydrogen bond acceptors using a slightly simplified version of the PHACIR atom types.
HBondDonorCountDescriptor	This descriptor calculates the number of hydrogen bond donors using a slightly simplified version of the PHACIR atom types.
HybridizationRatioDescriptor	IMolecularDescriptor that reports the fraction of sp ³ carbons to sp ² carbons.
IPMolecularLearningDescriptor	Deprecated
KappaShapeIndicesDescriptor	Kier and Hall kappa molecular shape indices compare the molecular graph with minimal and maximal molecular graphs; a description is given at: http://www.chemcomp.com/Journal_of_CCG/Features/descr.htm#KH : "they are intended to capture different aspects of molecular shape.
KierHallSmartsDescriptor	A fragment count descriptor that uses e-state fragments.
LargestChainDescriptor	Class that returns the number of atoms in the largest chain.
LargestPiSystemDescriptor	Class that returns the number of atoms in the largest pi system.
LengthOverBreadthDescriptor	Evaluates length over breadth descriptors.
LongestAliphaticChainDescriptor	Class that returns the number of atoms in the longest aliphatic chain.
MannholdLogPDescriptor	Prediction of logP based on the number of carbon and hetero atoms.
MDEDescriptor	Calculates the Molecular Distance Edge descriptor described in [Liu, S. and Cao, C. and Li, Z. , <i>Approach to Estimation and Prediction for Normal Boiling Point (NBP) of Alkanes Based on a Novel Molecular Distance Edge (MDE) Vector, lambda</i> , Journal of Chemical Information and Computer Sciences, 1998, 38:387-394].
MomentOfInertiaDescriptor	A descriptor that calculates the moment of inertia and radius of gyration.
PetitjeanNumberDescriptor	According to the Petitjean definition, the eccentricity of a vertex corresponds to the distance from that vertex to the most remote vertex in the graph.

PetitjeanShapeIndexDescriptor	Evaluates the Petitjean shape indices, These original Petitjean number was described by Petitjean ([Petitjean, M. , <i>Applications of the radius-diameter diagram to the classification of topological and geometrical shapes of chemical compounds</i> , Journal of Chemical Information and Computer Science, 1992, 32:331-337]) and considered the molecular graph.
RotatableBondsCountDescriptor	The number of rotatable bonds is given by the SMARTS specified by Daylight on SMARTS tutorial
RuleOfFiveDescriptor	This Class contains a method that returns the number failures of the Lipinski's Rule Of 5.
SmallRingDescriptor	Small ring descriptors: these are based on enumeration of all the small rings (sizes 3 to 9) in a molecule, which can be obtained quickly and deterministically.
TPSADescriptor	Calculation of topological polar surface area based on fragment contributions (TPSA) [Ertl, P. and Rohde, B. and Selzer, P., Fast Calculation of Molecular Polar Surface Area as a Sum of Fragment-Based Contributions and Its Application to the Prediction of Drug Transport Properties, J. Med. Chem., 2000, 43:3714-3717, doi:10.1021/jm000942e].
VABCDescriptor	Volume descriptor using the method implemented in the VABCVolume class.
VAdjMaDescriptor	Vertex adjacency information (magnitude): $1 + \log_2 m$ where m is the number of heavy-heavy bonds.
WeightDescriptor	IDescriptor based on the weight of atoms of a certain element type.
WeightedPathDescriptor	Evaluates the weighted path descriptors.
WHIMDescriptor	Holistic descriptors described by Todeschini et al [Todeschini, R. and Gramatica, P., <i>New 3D Molecular Descriptors: The WHIM theory and QAR Applications</i> , Persepectives in Drug Discovery and Design, 1998, ? :355-380].
WienerNumbersDescriptor	This descriptor calculates the Wiener numbers.
XLogPDescriptor	Prediction of logP based on the atom-type method called XLogP.
ZagrebIndexDescriptor	Zagreb index: the sum of the squares of atom degree over all heavy atoms i.

TRANSLATION OF PHYTOCHEMICALS TO KEGG IDS

C00230	protocatechuic acid
C00156	p-hydroxybenzoic acid
C00193	benzaldehyde
C01424	gallic acid
C00249	palmitic acid
C00755	vanillin
C01530	stearic acid
C09880	alpha-pinene
C09898	beta-terpinene
C06672	vanillic acid
C06425	arachidic acid
C17148	oleanolic acid
C06424	myristic acid
C21702	alpha-thujene

C06074	beta-myrcene
C00212	adenosine
C08988	ursolic acid
C09649	alpha-curcumene
C01753	beta-sitosterol
C08362	palmitoleic acid
C00712	oleic acid
C01494	ferulic acid
C01197	caffeic acid
C00811	p-coumaric acid
C00852	chlorogenic acid
C00389	quercetin
C01477	apigenin
C01514	luteolin
C01595	linoleic acid
C05625	rutin
C05903	kaempferol
C09629	alpha-caryophyllene
C17094	beta-elemene
C09884	pinocarvone

SPECIMEN OF THE TRANSLATION OF DRUGS TO KEGG IDS

D00038	Benzoic acid	Antifungal, Antiseptic
D02277	Sodium benzoate	A16AX11
D05576	Potassium benzoate	Pharmaceutic aid (preservative)
D02907	Aminobenzoate sodium	D02BA01
D02906	Aminobenzoate potassium	D02BA01 D11AX23
D02458	Methylparaben sodium	Pharmaceutic aid (antimicrobial preservative)
D01400	Methylparaben	Pharmaceutic aid (antifungal preservative)
D02456	p-Aminobenzoic acid	D02BA01- Ultraviolet screen
D01647	Ethylparaben	Pharmaceutic aid (antifungal preservative)
D10929	Ethylparaben sodium	Pharmaceutic aid (antifungal preservative)
D02314	Benzaldehyde	Pharmaceutic aid (flavor)
D00077	Benzyl alcohol	P03AX06
D03470	o-Phthalaldehyde	Disinfectant
D01470	Phenylpropanol	Pharmaceutic aid (flavor, solvent)
D02816	Alkyl (C12-15) benzoate	Pharmaceutic aid (emollient)
D04951	Metacresol	Antifungal, Antiseptic (topical)
D00045	Adenosine	C01EB10
D06298	Vidarabine	J05AB03 S01AD06
D00406	Vidarabine monohydrate	J06AB03 S01AD06

D07966	Fludarabine	L01BB05
D01678	Thioinosine	Antineoplastic, Antimetabolite
D00054	Inosine	D06BB05 G01AX02 S01XA10
D01370	Cladribine	L01BB04 L04AA40
D03546	Clofarabine	L01BB06
D04759	Lodensine	Antiviral, Reverse transcriptase inhibitor

SPECIMEN FROM SIMCOMP ANALYSIS: THE MOST SIGNIFICANT SIMILARITIES OF PHYTOCHEMICALS AND DRUGS

PHYTOCHEMICAL KEGG ID	DRUG KEGG ID	TANIMOTO COEFFICIENT
C00249	D05875	0.884817
C00249	D00119	0.88481
C00712	D00119	0.95876
C00712	D05875	0.95876
C01530	D05875	1
C01530	D00119	1
C01595	D00119	0.919192
C01595	D05875	0.91919
C06424	D05875	0.780105
C06424	D00119	0.780105
C06425	D00119	0.818182
C06425	D05875	0.818182
C08632	D05875	0.764706
C08632	D00119	0.764706
C00249	D02315	0.8
C00712	D02315	1
C01530	D02315	0.95876
C01595	D02315	0.95876
C06425	D02315	0.785714
C08632	D02315	0.884817
C00156	D00038	0.881188
C00156	D02277	0.881188
C00156	D05576	0.881188
C00193	D05576	0.808511
C00193	D00038	0.808511
C00193	D02277	0.80851
C00230	D00038	0.785714
C00230	D02277	0.78571

APPENDIX 10

SNAPSHOT OF ADR CASES FOR THE DRUG DUTASTERIDE

	A	B	C	D	E	F	G	H
1		X1	X1.1	Therapeutic.response	Therapeutic.and.nontherapeutic.responses	Therapeutic.and.nontherapeutic.effects	Genrl	X187
2	814956	1	1	Dyspnoea	Breathing abnormalities	Respiratory disorders NEC	Resp	6918296
3	814957	2	1	Dyspnoea	Breathing abnormalities	Respiratory disorders NEC	Resp	6918296
4	814958	2	2	Wheezing	Bronchospasm and obstruction	Bronchial disorders (excl neoplasms)	Resp	6918296
5	814959	3	1	Diarrhoea	Diarrhoea (excl infective)	Gastrointestinal motility and defaecation disorders NEC	Gastr	6918296
6	814960	3	2	Dizziness	Neurological signs and symptoms NEC	Neurological disorders NEC	Nerv	6918296
7	814961	3	3	Feeling of body temperature	Feelings and sensations NEC	General system disorders NEC	Genrl	6918296
8	814962	3	4	Headache	Headaches NEC	Headaches	Nerv	6918296
9	814963	4	1	Hair disorder	Pilar disorders NEC	Skin appendage conditions	Skin	6918296
10	814964	4	2	Headache	Headaches NEC	Headaches	Nerv	6918296
11	814965	4	3	Insomnia	Disturbances in initiating and maintaining sleep	Sleep disorders and disturbances	Psych	6918296
12	814966	4	4	Mood swings	Fluctuating mood symptoms	Mood disorders and disturbances NEC	Psych	6918296
13	814967	4	5	Palpitations	Cardiac signs and symptoms NEC	Cardiac disorder signs and symptoms	Card	6918296
14	814968	5	1	Arrhythmia	Rate and rhythm disorders NEC	Cardiac arrhythmias	Card	6918296
15	814969	5	2	Circulatory collapse	Circulatory collapse and shock	Decreased and nonspecific blood pressure	Vasc	6918296
16	814970	5	3	Seizure	Seizures and seizure disorders NEC	Seizures (incl subtypes)	Nerv	6918296
17	814971	6	1	Rash	Rashes, eruptions and exanths NEC	Epidermal and dermal conditions	Skin	6918296
18	814972	7	1	Abortion spontaneous	Abortions spontaneous	Abortions and stillbirth	Preg	6918296
19	814973	8	1	Pelvic pain	Reproductive tract signs and symptoms NEC	Reproductive tract disorders NEC	Repro	6918296
20	814974	9	1	Confusional state	Confusion and disorientation	Deliria (incl confusion)	Psych	6918296
21	814975	9	2	Hallucination	Perception disturbances	Disturbances in thinking and perception	Psych	6918296
22	814976	10	1	Abdominal pain lower	Gastrointestinal and abdominal pains (excl oral)	Gastrointestinal signs and symptoms	Gastr	6918296
23	814977	10	2	Dysuria	Bladder and urethral symptoms	Urinary tract signs and symptoms	Renal	6918296

SNAPSHOT OF THE DRUG-DRUG INTERACTIONS OF FINASTERIDE

	A	B	C	D
1		DRUG1.CID	DRUG2.CID	INTERACTION.CLASS
2	171307	57363	11540687	CYP induction: CYP3A4
3	171308	57363	444795	Enzyme: CYP2C9 / CYP inhibition: CYP2C9
4	171309	57363	2375	Enzyme: CYP3A4
5	171310	57363	5757	Enzyme: CYP3A4
6	171311	57363	60934	Enzyme: CYP3A4
7	171312	57363	64142	Enzyme: CYP3A4
8	171313	57363	158550	Enzyme: CYP3A4
9	171314	57363	441325	Enzyme: CYP3A4
10	171315	57363	15527165	Enzyme: CYP3A4
11	171316	57363	23674889	Enzyme: CYP3A4
12	171317	57363	23679632	Enzyme: CYP3A4
13	171318	57363	92042797	Enzyme: CYP3A4
14	171319	57363	3672	Enzyme: CYP3A4 / CYP inhibition: CYP3A4
15	171320	57363	65329	Enzyme: CYP3A4 / CYP inhibition: CYP3A4
16	171321	57363	129228	Enzyme: CYP3A4 / CYP inhibition: CYP3A4

DRUGS CAUSING ALOPECIA AS A SIDE EFFECT

STITCH CID	Drug Name	ATC	Frequency of SE
CID100004594	Omeprazole	A02BC01	Uncommon
CID100002099	Alosetron	A03AE01	Rare
CID100000247	Betaine	A16AA06	Uncommon
CID100004171	Metoprolol	C07AB02	Rare
CID100003937	Lisinopril	C09AA03	Rare
CID100003339	Fenofibrate	C10AB05	Rare
CID100003365	Fluconazole	D01AC15, J02AC01, J01RA07	Rare
CID100002749	Ciclopirox	D01AE14, G01AX12	Rare
CID100002284	Baclofen	D06BB03, D06BB55, S01AD03	Uncommon
CID100005372	Tacrolimus	D11AH01, L04AD02	Common
CID100002443	Bromocriptine	G02CB01, N04BC01	Uncommon
CID100000450	Estradiol	G03AC03	Uncommon
CID100000699	Estrogen	G03C	Common
CID100216416	Lasofixifene	G03XC03	Uncommon
CID100054373	Octreotide	H01CB02	Common
CID100071616	Voriconazole	J02AC03	Common
CID100002022	Acyclovir	J05AB01	Uncommon
CID100060613	Cidofovir	J05AB12	Very Common
CID100060787	Saquinavir	J05AE01	Common
CID100148192	Atazanavir	J05AE08	Uncommon
CID100003877	Lamivudine	J05AF05	Common
CID100005064	Ribavirin	J05AP01	Very Common
CID110324367	Boceprevir	J05AP03	Very Common
CID145375808	Sofosbuvir	J05AP08, J05AP51, J05AP55, J05AP56	Common
CID100004053	Melphalan	L01AA03	Very Common
CID100005394	Temozolomide	L01AX03	Common
CID100005394	Temozolomide	L01AX03	Very Common
CID100119182	Clofarabine	L01BB06	Common
CID100003461	Gemcitabine	L01BC05	Common
CID100001805	5-Azacytidine	L01BC07	Common
CID100004666	Paclitaxel	L01CD01, L01CD03	Very Common
CID100001690	Doxorubicin	L01DB01	Very Common
CID100004609	Oxaliplatin	L01XA03	Very Common
CID100005291	Imatinib	L01XE01	Common
CID100123631	Gefitinib	L01XE02	Common
CID100208908	Lapatinib	L01XE07	Very Common
CID100644241	Nilotinib	L01XE08	Common
CID106442177	Everolimus	L01XE10, L04AA18	Common
CID144462760	Dabrafenib	L01XE23	Very Common
CID100003657	Hydroxyurea	L01XX05	Uncommon
CID100005515	Topotecan	L01XX17	Very Common
CID100003902	Letrozole	L02BG04	Common
CID100060198	Exemestane	L02BG06	Common
CID105479141	Mifamurtide	L03AX15	Common

CID100003899	Leflunomide	L04AA13	Common
CID100002265	Azathioprine	L04AX01	Rare
CID100216326	Lenalidomide	L04AX04	Common
CID100004440	Naratriptan	N02CC02	Rare
CID100077993	Eletriptan	N02CC06	Rare
CID100002554	Carbamazepine	N03AF01	Rare
CID100034312	Oxcarbazepine	N03AF02	Common
CID100005514	Topiramate	N03AX11	Rare
CID100003388	Fluphenazine	N05AB02	Uncommon
CID100060853	Ziprasidone	N05AE04	Rare
CID100002771	Citalopram	N06AB04	Uncommon
CID100004691	Paroxetine	N06AB05	Uncommon
CID100005203	Sertraline	N06AB06	Uncommon
CID100003404	Fluvoxamine	N06AB08	Rare
CID100005656	Venlafaxine	N06AX16	Uncommon
CID100004158	Methylphenidate	N06BA04	Common

OFF-TARGETS ALOPECIA AS A SIDE-EFFECT

ChemicalName	CasRN	GeneSymbol	Organism
Cidofovir	113852-37-2	CASP3	Homo sapiens
Ribavirin	36791-04-5	CASP3	Homo sapiens
Melphalan	148-82-3	CASP3	Homo sapiens
Temozolomide	85622-93-1	CASP3	Homo sapiens
Paclitaxel		CASP3	Homo sapiens
Oxaliplatin		CASP3	Homo sapiens
Lapatinib		CASP3	Homo sapiens
Topotecan	123948-87-8	CASP3	Homo sapiens
Doxorubicin	23214-92-8	CASP3	Homo sapiens
Cidofovir	113852-37-2	BCL2	Homo sapiens
Melphalan	148-82-3	BCL2	Homo sapiens
Temozolomide	85622-93-1	BCL2	Homo sapiens
Paclitaxel		BCL2	Homo sapiens
Oxaliplatin		BCL2	Homo sapiens

Lapatinib		BCL2	Homo sapiens
Topotecan	123948-87-8	BCL2	Homo sapiens
Doxorubicin	23214-92-8	BCL2	Homo sapiens
Cidofovir	113852-37-2	BAX	Homo sapiens
Melphalan	148-82-3	BAX	Homo sapiens
Temozolomide	85622-93-1	BAX	Homo sapiens
Paclitaxel		BAX	Homo sapiens
Oxaliplatin		BAX	Homo sapiens
Lapatinib		BAX	Homo sapiens
Topotecan	123948-87-8	BAX	Homo sapiens
Doxorubicin	23214-92-8	BAX	Homo sapiens

SNAPSHOT OF DRUGS THAT WERE REPORTED TO CAUSE ALOPECIA AS AN ADR IN MHRA'S YELLOW CARD SCHEME

	A	B	C	D	E	F	G	Formula Bar	I
1	1366502	54	1	Alopecia	Alopecias	Skin appen	Skin	N	13109
2	1366531	65	2	Alopecia	Alopecias	Skin appen	Skin	N	13109
3	1366543	73	2	Alopecia	Alopecias	Skin appen	Skin	N	13109
4	1366559	83	1	Alopecia	Alopecias	Skin appen	Skin	N	13109
5	1366597	104	1	Alopecia	Alopecias	Skin appen	Skin	N	13109
6	1366652	134	1	Alopecia	Alopecias	Skin appen	Skin	N	13109
7	1366729	179	1	Alopecia	Alopecias	Skin appen	Skin	N	13109
8	1366861	255	1	Alopecia	Alopecias	Skin appen	Skin	N	13109
9	1366880	267	1	Alopecia	Alopecias	Skin appen	Skin	N	13109
10	1366884	271	1	Alopecia	Alopecias	Skin appen	Skin	N	13109
11	1366912	284	1	Alopecia	Alopecias	Skin appen	Skin	N	13109
12	1366966	311	1	Alopecia	Alopecias	Skin appen	Skin	N	13109
13	1366979	319	1	Alopecia	Alopecias	Skin appen	Skin	N	13109
14	1366980	320	1	Alopecia	Alopecias	Skin appen	Skin	N	13109
15	1366987	325	2	Alopecia	Alopecias	Skin appen	Skin	N	13109
16	1367031	353	1	Alopecia	Alopecias	Skin appen	Skin	N	13109
17	1367036	356	1	Alopecia	Alopecias	Skin appen	Skin	N	13109
18	1367095	388	1	Alopecia	Alopecias	Skin appen	Skin	N	13109
19	1367097	389	2	Alopecia	Alopecias	Skin appen	Skin	N	13109
20	1367148	416	1	Alopecia	Alopecias	Skin appen	Skin	N	13109
21	1367184	431	1	Alopecia	Alopecias	Skin appen	Skin	N	13109
22	1367211	444	1	Alopecia	Alopecias	Skin appen	Skin	N	13109
23	1367234	458	2	Alopecia	Alopecias	Skin appen	Skin	N	13109
24	1367266	477	1	Alopecia	Alopecias	Skin appen	Skin	N	13109
25	1367273	481	1	Alopecia	Alopecias	Skin appen	Skin	N	13109
26	1367288	488	1	Alopecia	Alopecias	Skin appen	Skin	N	13109
27	1367308	494	1	Alopecia	Alopecias	Skin appen	Skin	N	13109

OFF-TARGETS ALOPECIA AS AN ADR

Chemical Name	CasRN	Gene	Organism
levonorgestrel	797-63-7	PGR	Homo sapiens
ethinyl estradiol	57-63-6	PGR	Homo sapiens
norethisterone	68-22-4	PGR	Homo sapiens
etonogestrel		PGR	Homo sapiens
estradiol	50-28-2	PGR	Homo sapiens
desogestrel	54024-22-5	PGR	Homo sapiens
danazol	17230-88-5	PGR	Homo sapiens
tibolone		PGR	Homo sapiens

levonorgestrel	797-63-7	ESR1	Homo sapiens
ethinyl estradiol	57-63-6	ESR1	Homo sapiens
norethisterone	68-22-4	ESR1	Homo sapiens
estradiol	50-28-2	ESR1	Homo sapiens
danazol	17230-88-5	ESR1	Homo sapiens
tibolone		ESR1	Homo sapiens
norgestrel	6533-00-2	ESR1	Homo sapiens
levonorgestrel	797-63-7	AR	Homo sapiens
ethinyl estradiol	57-63-6	AR	Homo sapiens
norethisterone	68-22-4	AR	Homo sapiens
estradiol	50-28-2	AR	Homo sapiens
danazol	17230-88-5	AR	Homo sapiens
norgestrel	6533-00-2	AR	Homo sapiens

APPENDIX 11

PART OF THE GENE INFO PROVIDED FOR GENE AKT1

	V1	V2
ENTRY2	207	207
NAME2	AKT1, AKT, CWS6, PKB, PKB-ALPHA, PRKBA, RAC, RAC-ALPHA	AKT1, AKT, CWS6, PKB, PKB-ALPHA, PRKBA, RAC, RAC-ALPHA
ORGANISM 2	Homo sapiens (human)	Homo sapiens (human)
PATHWAY2	EGFR tyrosine kinase inhibitor resistance	Endocrine resistance
BRITE2	KEGG Orthology (KO) [BR:hsa00001]	09130 Environmental Information Processing
STRUCTURE 2	PDB: 1UNQ 1UNR 1H10 4GV1 1UNP 3QKL 2UZR 2UVM 4EKL 3CQW 3MVH	PDB:6NPZ 6CCY 4EJN 3QKM 3CQU 6S9W 6HHG 6HHJ 3QKK 6BUU 2UZS

AA SEQUENCE INFO FOR AKT1

A	MSDVAIVKEGWLHKRGEYIKTWRPRYFLLKNDGTFIGYKERPQDQVDQREAPLNNFSVAQCQLMKTERPRP
K	NTFIIRCLQWTTVIERTFHVETPEEREWTTAIQTVADGLKKQEEEEEMDFRSGSPSDNSGAEEMEVSLAKPK
T	HRVTMNEFEYLKLLGKGTFGKVLVKEKATGRYYAMKILKKEVIVAKDEVAHTLTENRVLQNSRHPFLTALKY
1	SFQTHDRLCFVMEYANGGELFFHLSRERVFSEDRARFYGAEIVSALDYHSEKNVVYRDLKLENLMLDKDGH IKITDFGLCKEIKDGATMKTFCGTPEYLAPEVLEDNDYGRAVDWWGLGVVMYEMMCGRLPFYNQDHEK LFELILMEEIRFPRTLGPPEAKSLLSGLLKKDPKQRLGGGSEDAKEIMQHRFFAGIVWQHVVYEKLSPPFKPQV TSETDTRYFDEEFTAQMITITPPDQDDSMECVDSERRPHFPQFSYSASGTA

NUCLEOTIDE SEQUENCE INFO FOR AKT1

A	ATGAGCGACGTGGCTATTGTGAAGGAGGGTTGGCTGCACAAACGAGGGGAGTACATCAAGACCTGGC
K	GGCCACGCTACTTCTCCTCAAGAATGATGGCACCTCATTGGCTACAAGGAGCGGCCGAGGATGTG
T	GACCAACGTGAGGCTCCCCTCAACAACCTTCTGTGGCGCAGTGCCAGCTGATGAAGACGGAGCGGCC
1	CCGGCCCAACACCTTCATCATCCGCTGCCTGCAGTGGACCACTGTCATCGAACGCACCTTCCATGTGGA GACTCCTGAGGAGCGGGAGGAGTGGACAACCGCCATCCAGACTGTGGCTGACGGCCTCAAGAAGCAG GAGGAGGAGGAGATGGACTTCCGGTCCGGCTCACCCAGTGACAACCTCAGGGGCTGAAGAGATGGAG GTGTCCCTGGCCAAGCCCAAGCACCGCGTGACCATGAACGAGTTTGAGTACCTGAAGCTGCTGGGCAA GGGCACTTTCGGCAAGGTGATCCTGGTGAAGGAGAAGGCCACAGGCCGCTACTACGCCATGAAGATC CTCAAGAAGGAAGTCATCGTGGCCAAGGACGAGGTGGCCACACACTCACCGAGAACCGCGTCTGC AGAACTCCAGGCACCCCTCCTCACAGCCCTGAAGTACTCTTCCAGACCCACGACCGCCTCTGCTTGT CATGGAGTACGCCAACGGGGGCGAGCTGTTCTCCACCTGTCCCGGAGCGTGTGTTCTCCGAGGACC GGGCCCCGTTCTATGGCGCTGAGATTGTGTCAGCCCTGGACTACCTGCACTCGGAGAAGAAGCTGGTG TACCGGGACCTCAAGCTGGAGAACCTCATGCTGGACAAGGACGGGCACATTAAGATCACAGACTTCG GGCTGTGCAAGGAGGGGATCAAGGACGGTGCCACCATGAAGACCTTTTGCGGCACACCTGAGTACCT GGCCCCGAGGTGCTGGAGGACAATGACTACGGCCGTGCAGTGGACTGGTGGGGGCTGGGCGTGGT CATGTACGAGATGATGTGCGGTGCCTGCCCTTCTACAACCAGGACCATGAGAAGCTTTTTGAGCTCAT CCTCATGGAGGAGATCCGCTTCCGCGCACGCTTGGTCCCGAGGCCAAGTCTTGTTCAGGGCTGCT CAAGAAGGACCCCAAGCAGAGGCTTGGCGGGGGCTCCGAGGACGCCAAGGAGATCATGCAGCATCG CTTCTTTGCCGGTATCGTGTGGCAGCACGTGTACGAGAAGAAGCTCAGCCCACCTTCAAGCCCCAGG TCACGTCGGAGACTGACACCAGGATTTTGTGAGGAGTTCACGGCCCAGATGATCACCATCACACCA CCTGACCAAGATGACAGCATGGAGTGTGTGGACAGCGAGCGCAGGCCCACTTCCCCAGTTCTCTTA CTCGGCCAGCGGCACGGCCTGA

APPENDIX 12

TRANSLATIONS OF THE 48 GENES

	From_UniProtKB_AC_ID	To_KEGG_ID	To_EGGNOG_ID	To_ENSEMBL_ID	To_GENENAME
1	P31749	hsa:207	KOG0690	ENSG00000142208	AKT1
2	Q9H161	hsa:60529	KOG0490	ENSG00000052850	ALX4
3	P10275	hsa:367	KOG3575	ENSG00000169083	AR

4	P10415	hsa:596	KOG4728	ENSG000001717 91	BCL2
5	O60885	hsa:23476	KOG1474	ENSG000001418 67	BRD4
6	P24385	hsa:595	KOG0656	ENSG000001100 92	CCND1
7	P06850	hsa:1392	ENOG502S25G	ENSG000001475 71	CRH
8	P35222	hsa:1499	KOG4203	ENSG000001680 36	CTNNB1
9	O94907	hsa:22943	KOG1218	ENSG000001079 84	DKK1
1 0	Q86SJ6	hsa:14740 9	KOG3594	ENSG000001750 65	DSG4
1 1	Q9UH73	hsa:1879	KOG3836	ENSG000001643 30	EBF1
1 2	Q9UNE0	hsa:10913	ENOG502QRV5	ENSG000001359 60	EDAR
1 3	P12034	hsa:2250	KOG3885	ENSG000001386 75	FGF5
1 4	P21781	hsa:2252	KOG3885	ENSG000001402 85	FGF7
1 5	Q9UKV0	hsa:9734	KOG1343	ENSG000000480 52	HDAC9
1 6	O43593	hsa:55806	KOG1356	ENSG000001684 53	HR
1 7	P05019	hsa:3479	ENOG502RCAB	ENSG000000174 27	IGF1
1 8	P01308	hsa:3630	ENOG502S5P5	ENSG000002546 47	INS
1 9	Q15306	hsa:3662	ENOG502QUE4	ENSG000001372 65	IRF4
2 0	P07288	hsa:354	KOG3627	ENSG000001425 15	KLK3
2 1	Q7RTS7	hsa:12139 1	ENOG502RNQG	ENSG000001704 84	KRT74
2 2	O95678	hsa:9119	ENOG502RTYA	ENSG000001704 54	KRT75
2 3	o43790	hsa:3892	ENOG502RTZU	ENSG000001704 42	KRT86
2 4	Q9BXB1	hsa:55366	KOG0619, KOG2087	ENSG000002052 13	LGR4
2 5	Q8WWY8	hsa:20087 9	ENOG502QUQT	ENSG000001638 98	LIPH
2 6	P43657	hsa:10161	ENOG502QSC2	ENSG000001396 79	LPAR6
2 7	P48449	hsa:4047	KOG0497	ENSG000001602 85	LSS

28	P10636	hsa:4137	KOG2418	ENSG0000018668, ENSG0000027756, ENSG00000276155	MAPT
29	P42898	hsa:4524	KOG0564	ENSG0000017700	MTHFR
30	P19838	hsa:4790	KOG0504	ENSG00000109320	NFKB1
31	P46531	hsa:4851	KOG1217	ENSG00000148400	NOTCH1
32	Q13635	hsa:5727	KOG1935	ENSG00000185920	PTCH1
33	P35354	hsa:5743	KOG2408	ENSG00000073756	PTGS2
34	Q04206	hsa:5970	ENOG502QT4Z	ENSG00000173039	RELA
35	Q01196	hsa:861	KOG3982	ENSG00000159216	RUNX1
36	P04278	hsa:6462	KOG3927	ENSG00000129214	SHBG
37	Q15465	hsa:6469	KOG3638	ENSG00000164690	SHH
38	Q13485	hsa:4089	KOG3701	ENSG00000141646	SMAD4
39	O95863	hsa:6615	KOG2462	ENSG00000124216	SNAI1
40	P48436	hsa:6662	KOG0527	ENSG00000125398	SOX9
41	P31213	hsa:6716	KOG1638	ENSG00000277893	SRD5A2
42	P61812	hsa:7042	KOG3900	ENSG00000092969	TGFB2
43	P01375	hsa:7124	ENOG502S4K8	ENSG00000204490, ENSG00000206439, ENSG00000228321, ENSG00000228849, ENSG00000230108, ENSG00000223952, ENSG00000232810	TNF
44	Q9H3D4	hsa:8626	ENOG502QQ48	ENSG00000073282	TP63

4				ENSG00000233608, ENSG00000288335	
5	Q8WVJ9	hsa:117581	KOG4447		TWIST2
4				ENSG00000111424	
6	P11473	hsa:7421	KOG3575		VDR
4				ENSG00000135925	
7	Q9GZT5	hsa:80326	KOG3913		WNT10A
4				ENSG00000169884	
8	O00744	hsa:7480	KOG3913		WNT10B

APPENDIX 13

SPECIMEN OF THE BINDING AFFINITY FOR TARGET AKT1

Monomer id	smiles	affinity _type	affinity
2579	<chem>CN[C@@H]1C[C@H]2O[C@@](C)([C@@H]1OC)n1c3cccc3c3c4CNC(=O)c4c4c5cccc5n2c4c13 r </chem>	IC50	1.2
2579	<chem>CN[C@@H]1C[C@H]2O[C@@](C)([C@@H]1OC)n1c3cccc3c3c4CNC(=O)c4c4c5cccc5n2c4c13 r </chem>	IC50	1.5
2579	<chem>CN[C@@H]1C[C@H]2O[C@@](C)([C@@H]1OC)n1c3cccc3c3c4CNC(=O)c4c4c5cccc5n2c4c13 r </chem>	Kd	2
8727	<chem>N[C@]1(C[C@](O)(C1)C1CC1)c1ccc(cc1)-c1nc2ccc3nnc(C4NCNN4)n3c2cc1-c1cccc1 r,wU:3.3,wD:3.6,1.0,(13.13,-7.57,,11.8,-6.8,,12.89,-5.71,,11.8,-4.62,,11.03,-3.29,,10.71,-5.71,,12.57,-3.29,,13.9,-2.52,,12.57,-1.75,,10.46,-7.57,,10.46,-9.11,,9.13,-9.88,,7.8,-9.11,,7.8,-7.57,,9.13,-6.8,,6.46,-9.88,,5.13,-9.11,,3.8,-9.88,,2.46,-9.11,,1.13,-9.88,,1.13,-11.42,,-0.2,-12.45,,.61,-13.86,,2.14,-13.7,,3.23,-14.79,,4.76,-14.63,,5.39,-16.03,,4.24,-17.06,,2.91,-16.29,,2.46,-12.19,,3.8,-11.42,,5.13,-12.19,,6.46,-11.42,,7.8,-12.19,,7.8,-13.73,,9.13,-14.5,,10.46,-13.73,,10.46,-12.19,,9.13,-11.42,) </chem>	IC50	0.7

APPENDIX 14

PART OF THE GO TERMS FOR GENE AKT1

Gene	ID	GO term
AKT1	GO:0004672	protein kinase activity
AKT1	GO:0016772	transferase activity, transferring phosphorus-containing groups
AKT1	GO:0016301	kinase activity
AKT1	GO:0016740	transferase activity
AKT1	GO:0003824	catalytic activity
AKT1	GO:0016773	phosphotransferase activity, alcohol group as acceptor
AKT1	GO:0005488	binding
AKT1	GO:1901363	heterocyclic compound binding
AKT1	GO:0097159	organic cyclic compound binding
AKT1	GO:0043167	ion binding
AKT1	GO:0000166	nucleotide binding
AKT1	GO:0043168	anion binding
AKT1	GO:1901265	nucleoside phosphate binding
AKT1	GO:0032549	ribonucleoside binding
AKT1	GO:0017076	purine nucleotide binding
AKT1	GO:0005524	ATP binding
AKT1	GO:0032559	adenyl ribonucleotide binding
AKT1	GO:0032555	purine ribonucleotide binding
AKT1	GO:0032550	purine ribonucleoside binding
AKT1	GO:0032553	ribonucleotide binding

APPENDIX 15

GENES RELATED TO AGA ACCORDING TO DISGENET

	uniprotid	gene_symbol	score	disease_name
1	P10275	AR	0.5	Alopecia, Male Pattern
2	P31213	SRD5A2	0.42	Androgenetic Alopecia
3	P31213	SRD5A2	0.41	Alopecia, Male Pattern
4	P10275	AR	0.4	Androgenetic Alopecia
5	Q92887	ABCC2	0.3	Androgenetic Alopecia
6	P06850	CRH	0.3	Androgenetic Alopecia
7	P09874	PARP1	0.3	Androgenetic Alopecia

8	O60885	BRD4	0.3	Androgenetic Alopecia
9	P61586	RHOA	0.3	Androgenetic Alopecia
10	P42898	MTHFR	0.3	Androgenetic Alopecia
11	Q8IUH4	ZDHHC13	0.3	Androgenetic Alopecia
12	P10644	PRKAR1A	0.3	Androgenetic Alopecia
13	O43593	HR	0.3	Androgenetic Alopecia
14	Q8IYB8	SUPV3L1	0.3	Androgenetic Alopecia
15	P11473	VDR	0.3	Androgenetic Alopecia
16	P26651	ZFP36	0.3	Androgenetic Alopecia
17	O00220	TNFRSF10A	0.3	Androgenetic Alopecia
18	Q92887	ABCC2	0.3	Alopecia, Male Pattern
19	P06850	CRH	0.3	Alopecia, Male Pattern
20	P09874	PARP1	0.3	Alopecia, Male Pattern
21	O60885	BRD4	0.3	Alopecia, Male Pattern
22	P61586	RHOA	0.3	Alopecia, Male Pattern
23	P42898	MTHFR	0.3	Alopecia, Male Pattern
24	Q8IUH4	ZDHHC13	0.3	Alopecia, Male Pattern
25	P10644	PRKAR1A	0.3	Alopecia, Male Pattern
26	O43593	HR	0.3	Alopecia, Male Pattern
27	Q8IYB8	SUPV3L1	0.3	Alopecia, Male Pattern
28	P11473	VDR	0.3	Alopecia, Male Pattern
29	P26651	ZFP36	0.3	Alopecia, Male Pattern
30	O00220	TNFRSF10A	0.3	Alopecia, Male Pattern

COMMON GENES BETWEEN DISGENET DISEASE NETWORKS AND THE 48 GENES

O M I M ID	Disease	Genes implicated/DISGENET	Common genes with OUR CHOSEN GENES
10 92 00	Androgenetic alopecia	AR,SRD5A2,ABCC2,CRH,PARP1,BRD4,RHOA,MTHFR,ZDHHC13,PRKAR1A,HR,SUPV3L1,VDR,ZFP36,TNFRSF10A	AR,SRD5A2,CRH,BRD4,MTHFR,HR,VDR
60 53 89	Hypotrichosis 1	ADCC1,LPAR6,LIPH,LSS,RPL21,SNRPE,DSG4	LPAR6,LIPH,LSS,DSG4
14 65 20	Hypotrichosis 2	CDSN,KRT74	KRT74
61 39 81	Hypotrichosis 3	KRT74	KRT74
14 65 50	Hypotrichosis 4	HR	HR
60 79 03	Hypotrichosis 6	DSG4	DSG4
60 43 79	Hypotrichosis 7	LIPH	LIPH
27 81 50	Hypotrichosis 8	LPAR6	LPAR6
61 50 59	Hypotrichosis 11	SNRPE	
61 58 85	Hypotrichosis 12	RPL21	
61 58 96	Hypotrichosis 13	KRT71	
61 82 75	Hypotrichosis 14	LSS	LSS
20 36 55	Alopecia universalis	HR	HR
20 95 00	Atrichia with papular lesions	HR	HR
60 06 28	Loose anagen hair syndrome	KRT75	KRT75

60 00 82	Benign prostatic hyperplasia	KLK3,SRD5A2,FGF7,PRL	KLK3,SRD5A2,FGF7
17 68 07	Prostate cancer		AR,CTNNB1,CCND1,KLK3,AKT1,BRD4,IGF1,MTHFR,PTGS2,BCL2,SHBG,SRD5A2,VDR,WNT10B
12 58 53	Type 2 Diabetes Mellitus		INS,BCL2,TNF,SHBG,NFKB1,RELA

APPENDIX 16

AGA DRUGS AND THEIR METABOLIC FATE

PubChem.CID	METABOLISM.ENZYME.AND.TRANSPORTERS	Relation	PMID
4201	Sulphotransferase	Substrate	1349030
4201	Sulphotransferase	Substrate	8423770
4201	Sulphotransferase	Substrate	2390100
4201	Sulphotransferase	Substrate	9566733
4201	Sulphotransferase	Substrate	9037254
4201	Sulphotransferase	Substrate	2230218
4201	Sulphotransferase	Substrate	3480782
4201	Sulphotransferase	Substrate	6958263
4201	Sulphotransferase	Substrate	7755612
57363	3A4	Substrate	11996015
57363	3A4	Substrate	8654202
57363	GST	Inhibitor	19077407
6918296	3A5	Substrate	34690761

PHYTOCHEMICALS AND THEIR METABOLIC FATE

ChemicalName	CasRN	GeneSymbol	Organism
Quercetin	117-39-5	CYP11B1	Homo sapiens
Apigenin	520-36-5	CYP11B1	Homo sapiens
Apigenin	520-36-5	CYP17A1	Homo sapiens
Quercetin	117-39-5	CYP19A1	Homo sapiens
Apigenin	520-36-5	CYP19A1	Homo sapiens
ferulic acid	1135-24-6	CYP1A1	Homo sapiens

Quercetin	117-39-5	CYP1A1	Homo sapiens
Linoleic Acid	2197-37-7	CYP1A1	Homo sapiens
kaempferol	520-18-3	CYP1A1	Homo sapiens
Apigenin	520-36-5	CYP1A1	Homo sapiens
Rutin	153-18-4	CYP1A1	Homo sapiens
alpha-pinene	80-56-8	CYP1A1	Homo sapiens
beta-myrcene	123-35-3	CYP1A1	Homo sapiens
Oleic Acid	112-80-1	CYP1A1	Homo sapiens
p-coumaric acid		CYP1A1	Homo sapiens
vanillin	121-33-5	CYP1A1	Homo sapiens
Luteolin	491-70-3	CYP1A1	Homo sapiens
ferulic acid	1135-24-6	CYP1A2	Homo sapiens
Quercetin	117-39-5	CYP1A2	Homo sapiens
Linoleic Acid	2197-37-7	CYP1A2	Homo sapiens
kaempferol	520-18-3	CYP1A2	Homo sapiens
Apigenin	520-36-5	CYP1A2	Homo sapiens
Oleic Acid	112-80-1	CYP1A2	Homo sapiens
p-coumaric acid		CYP1A2	Homo sapiens
Oleanolic Acid	508-02-1	CYP1A2	Homo sapiens
Luteolin	491-70-3	CYP1A2	Homo sapiens
Quercetin	117-39-5	CYP1B1	Homo sapiens
kaempferol	520-18-3	CYP1B1	Homo sapiens
Apigenin	520-36-5	CYP1B1	Homo sapiens
Rutin	153-18-4	CYP1B1	Homo sapiens
Luteolin	491-70-3	CYP1B1	Homo sapiens
Gallic Acid	149-91-7	CYP20A1	Homo sapiens

Apigenin	520-36-5	CYP21A2	Homo sapiens
Palmitic Acid	57-10-3	CYP24A1	Homo sapiens
Quercetin	117-39-5	CYP24A1	Homo sapiens
Oleic Acid	112-80-1	CYP24A1	Homo sapiens
Palmitic Acid	57-10-3	CYP26A1	Homo sapiens
Oleic Acid	112-80-1	CYP26A1	Homo sapiens
Palmitic Acid	57-10-3	CYP26B1	Homo sapiens
Oleic Acid	112-80-1	CYP26B1	Homo sapiens
Quercetin	117-39-5	CYP27B1	Homo sapiens
Quercetin	117-39-5	CYP2A6	Homo sapiens
Linoleic Acid	2197-37-7	CYP2A6	Homo sapiens
stearic acid	57-11-4	CYP2A6	Homo sapiens
Oleic Acid	112-80-1	CYP2A6	Homo sapiens
benzaldehyde	100-52-7	CYP2A6	Homo sapiens
vanillin	121-33-5	CYP2A6	Homo sapiens
Oleic Acid	112-80-1	CYP2B6	Homo sapiens
Quercetin	117-39-5	CYP2B7P	Homo sapiens
Quercetin	117-39-5	CYP2C19	Homo sapiens
Linoleic Acid	2197-37-7	CYP2C19	Homo sapiens
Luteolin	491-70-3	CYP2C19	Homo sapiens
ursolic acid	77-52-1	CYP2C19	Homo sapiens
Quercetin	117-39-5	CYP2C8	Homo sapiens
Quercetin	117-39-5	CYP2C9	Homo sapiens
Linoleic Acid	2197-37-7	CYP2C9	Homo sapiens
kaempferol	520-18-3	CYP2C9	Homo sapiens
Apigenin	520-36-5	CYP2C9	Homo sapiens
Luteolin	491-70-3	CYP2C9	Homo sapiens

Quercetin	117-39-5	CYP2D6	Homo sapiens
Quercetin	117-39-5	CYP2E1	Homo sapiens
Linoleic Acid	2197-37-7	CYP2E1	Homo sapiens
stearic acid	57-11-4	CYP2E1	Homo sapiens
Apigenin	520-36-5	CYP2E1	Homo sapiens
Oleic Acid	112-80-1	CYP2E1	Homo sapiens
Quercetin	117-39-5	CYP2J2	Homo sapiens
Quercetin	117-39-5	CYP2S1	Homo sapiens
Quercetin	117-39-5	CYP3A4	Homo sapiens
Linoleic Acid	2197-37-7	CYP3A4	Homo sapiens
stearic acid	57-11-4	CYP3A4	Homo sapiens
kaempferol	520-18-3	CYP3A4	Homo sapiens
Apigenin	520-36-5	CYP3A4	Homo sapiens
Oleic Acid	112-80-1	CYP3A4	Homo sapiens
Oleanolic Acid	508-02-1	CYP3A4	Homo sapiens
Luteolin	491-70-3	CYP3A4	Homo sapiens
Quercetin	117-39-5	CYP3A5	Homo sapiens
Luteolin	491-70-3	CYP3A5	Homo sapiens
Oleic Acid	112-80-1	CYP4A11	Homo sapiens
alpha-pinene	80-56-8	CYP4B1	Homo sapiens
Quercetin	117-39-5	CYP4F11	Homo sapiens
gamma-terpinene	99-85-4	CYP4F8	Homo sapiens
Myristic Acid	544-63-8	CYP4Z1	Homo sapiens
Quercetin	117-39-5	CYP51A1	Homo sapiens
Quercetin	117-39-5	CYP8B1	Homo sapiens
Quercetin	117-39-5	SULT1A1	Homo sapiens

Gallic Acid	149-91-7	SULT1A1	Homo sapiens
caffeic acid	331-39-5	SULT1A1	Homo sapiens
Apigenin	520-36-5	SULT1A1	Homo sapiens
p-coumaric acid		SULT1A1	Homo sapiens
4-hydroxybenzoic acid	99-96-7	SULT1A1	Homo sapiens
Quercetin	117-39-5	SULT1A2	Homo sapiens
caffeic acid	331-39-5	SULT1A2	Homo sapiens
Quercetin	117-39-5	SULT1A3	Homo sapiens
caffeic acid	331-39-5	SULT1A3	Homo sapiens
Quercetin	117-39-5	SULT1C1	Homo sapiens
Quercetin	117-39-5	SULT1C2	Homo sapiens
caffeic acid	331-39-5	SULT1C2	Homo sapiens
Quercetin	117-39-5	SULT1E1	Homo sapiens
Apigenin	520-36-5	SULT1E1	Homo sapiens
Quercetin	117-39-5	SULT2A1	Homo sapiens
Quercetin	117-39-5	UGT1A1	Homo sapiens
kaempferol	520-18-3	UGT1A1	Homo sapiens
Apigenin	520-36-5	UGT1A1	Homo sapiens
Luteolin	491-70-3	UGT1A1	Homo sapiens
ferulic acid	1135-24-6	UGT1A10	Homo sapiens
Quercetin	117-39-5	UGT1A10	Homo sapiens
Vanillic Acid	121-34-6	UGT1A10	Homo sapiens
Chlorogenic Acid	327-97-9	UGT1A10	Homo sapiens
kaempferol	520-18-3	UGT1A10	Homo sapiens
caffeic acid	331-39-5	UGT1A10	Homo sapiens

Apigenin	520-36-5	UGT1A10	Homo sapiens
vanillin	121-33-5	UGT1A10	Homo sapiens
ferulic acid	1135-24-6	UGT1A3	Homo sapiens
Quercetin	117-39-5	UGT1A3	Homo sapiens
Vanillic Acid	121-34-6	UGT1A3	Homo sapiens
Chlorogenic Acid	327-97-9	UGT1A3	Homo sapiens
kaempferol	520-18-3	UGT1A3	Homo sapiens
caffeic acid	331-39-5	UGT1A3	Homo sapiens
vanillin	121-33-5	UGT1A3	Homo sapiens
Luteolin	491-70-3	UGT1A3	Homo sapiens
Quercetin	117-39-5	UGT1A6	Homo sapiens
ferulic acid	1135-24-6	UGT1A7	Homo sapiens
Quercetin	117-39-5	UGT1A7	Homo sapiens
Vanillic Acid	121-34-6	UGT1A7	Homo sapiens
Chlorogenic Acid	327-97-9	UGT1A7	Homo sapiens
kaempferol	520-18-3	UGT1A7	Homo sapiens
caffeic acid	331-39-5	UGT1A7	Homo sapiens
Apigenin	520-36-5	UGT1A7	Homo sapiens
vanillin	121-33-5	UGT1A7	Homo sapiens
ferulic acid	1135-24-6	UGT1A8	Homo sapiens
Quercetin	117-39-5	UGT1A8	Homo sapiens
Vanillic Acid	121-34-6	UGT1A8	Homo sapiens
Chlorogenic Acid	327-97-9	UGT1A8	Homo sapiens
kaempferol	520-18-3	UGT1A8	Homo sapiens
caffeic acid	331-39-5	UGT1A8	Homo sapiens

Apigenin	520-36-5	UGT1A8	Homo sapiens
vanillin	121-33-5	UGT1A8	Homo sapiens
Quercetin	117-39-5	UGT1A9	Homo sapiens
kaempferol	520-18-3	UGT1A9	Homo sapiens
Apigenin	520-36-5	UGT1A9	Homo sapiens
Quercetin	117-39-5	UGT2A3	Homo sapiens
Quercetin	117-39-5	UGT2B15	Homo sapiens
Apigenin	520-36-5	UGT2B15	Homo sapiens
Quercetin	117-39-5	UGT2B4	Homo sapiens
Quercetin	117-39-5	UGT2B7	Homo sapiens
kaempferol	520-18-3	UGT2B7	Homo sapiens
Palmitic Acid	57-10-3	GSTA1	Homo sapiens
Quercetin	117-39-5	GSTA1	Homo sapiens
Linoleic Acid	2197-37-7	GSTA1	Homo sapiens
kaempferol	520-18-3	GSTA1	Homo sapiens
Oleic Acid	112-80-1	GSTA1	Homo sapiens
Quercetin	117-39-5	GSTA4	Homo sapiens
Quercetin	117-39-5	GSTK1	Homo sapiens
Quercetin	117-39-5	GSTM2	Homo sapiens
kaempferol	520-18-3	GSTM2	Homo sapiens
Quercetin	117-39-5	GSTM4	Homo sapiens
Quercetin	117-39-5	GSTM5	Homo sapiens
Quercetin	117-39-5	GSTO2	Homo sapiens
Quercetin	117-39-5	GSTP1	Homo sapiens
kaempferol	520-18-3	GSTP1	Homo sapiens

Quercetin	117-39-5	GSTT1	Homo sapiens
Quercetin	117-39-5	GSTZ1	Homo sapiens
Quercetin	117-39-5	ABCC4	Homo sapiens
Quercetin	117-39-5	SLCO1A2	Homo sapiens
Quercetin	117-39-5	SLCO1B1	Homo sapiens
kaempferol	520-18-3	SLCO1B1	Homo sapiens
Apigenin	520-36-5	SLCO1B1	Homo sapiens
Rutin	153-18-4	SLCO1B1	Homo sapiens
Luteolin	491-70-3	SLCO1B1	Homo sapiens
Quercetin	117-39-5	SLCO1B3	Homo sapiens
kaempferol	520-18-3	SLCO1B3	Homo sapiens
Apigenin	520-36-5	SLCO1B3	Homo sapiens
Rutin	153-18-4	SLCO1B3	Homo sapiens
Quercetin	117-39-5	SLCO2A1	Homo sapiens
Quercetin	117-39-5	SLCO2B1	Homo sapiens
Rutin	153-18-4	SLCO2B1	Homo sapiens
Quercetin	117-39-5	SLCO4A1	Homo sapiens
Quercetin	117-39-5	SLCO4C1	Homo sapiens
Quercetin	117-39-5	SLCO5A1	Homo sapiens

MOLECULAR DOCKING OF 5 PHYTOCHEMICALS TO SULT1A1

ChemicalName	PubChem CID	Binding affinity(Kcal/mol)
p-hydroxybenzoic acid	135	-4.3
apigenin	5280443	-6
caffeic acid	689043	-4.6
gallic acid	370	-4.2

p-coumaric acid	637542	-5.1
minoxidil	4201	-5
tretinoin	444795	-5.7

APPENDIX 17

BINDING SITE (AMINOACIDS AND THEIR POSITION) OF ANDROGEN RECEPTOR

1	LEU 701 (A)
2	LEU 704 (A)
3	ASN 705 (A)
4	LEU 707 (A)
5	GLY 708 (A)
6	GLN 711 (A)
7	TRP 741 (A)
8	MET 742 (A)
9	MET 745 (A)
10	VAL 746 (A)
11	MET 749 (A)
12	ARG 752 (A)
13	PHE 764 (A)
14	MET 780 (A)
15	MET 787 (A)
16	GLU 793 (A)
17	TRP 796 (A)
18	LEU 797 (A)
19	TYR 857 (A)
20	GLN 858 (A)
21	LYS 861 (A)

22	LEU 873 (A)
23	PHE 876 (A)
24	THR 877 (A)
25	LEU 880 (A)
26	PHE 891 (A)
27	MET 895 (A)
28	ILE 899 (A)

MOLECULAR DOCKING OF DRUGS TO ANDROGEN RECEPTOR

Name of Drug	Pubchem CID	PyRx Binding affinity (Kcal/mol)
minoxidil	4201	-7.2
finasteride	57363	-7.7
dutasteride	6918296	-9
bimatoprost	5311027	-5.9
biotin	171548	-6.1
carpronium chloride	2582	-4.7
alfatradiol	68570	-7.7

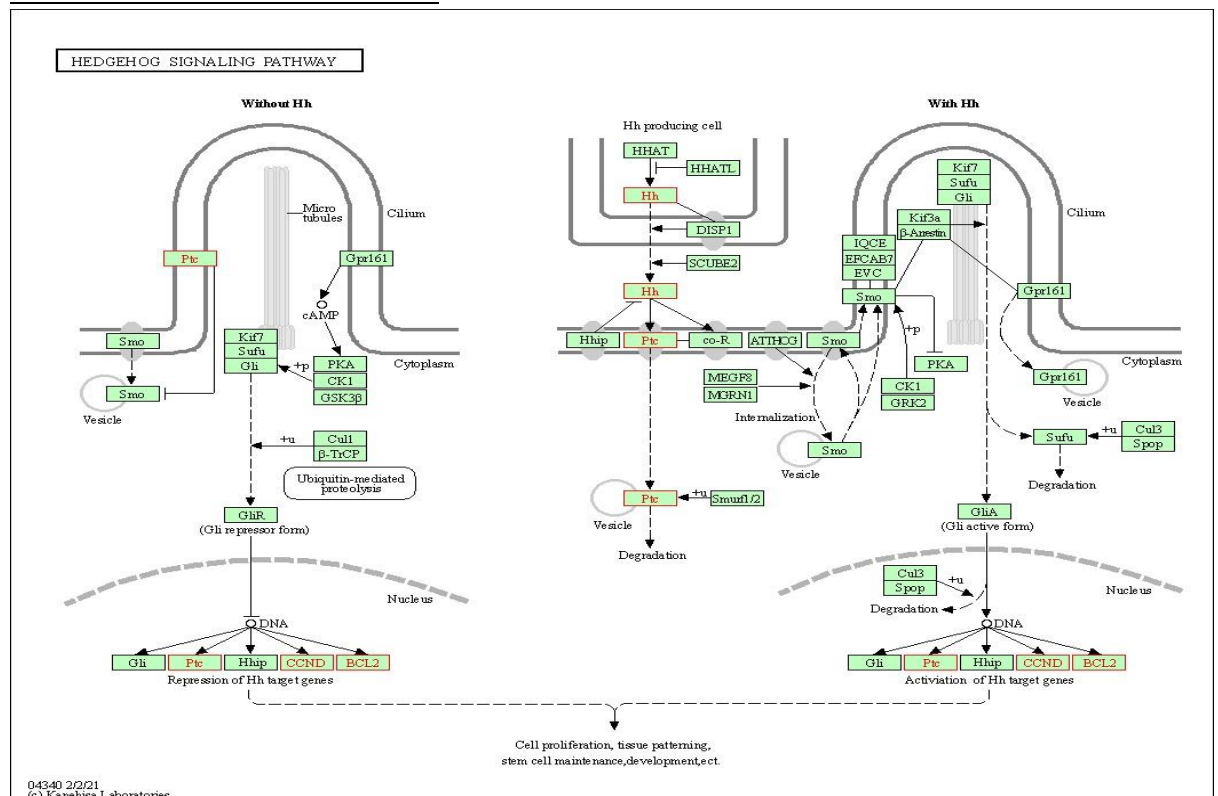
MOLECULAR DOCKING OF ALL PHYTOCHEMICALS TO ANDROGEN RECEPTOR

Name of Phytochemical	Pubchem CID	PyRx Binding affinity (Kcal/mol)
apigenin	5280443	-9.9
kaempferol	5280863	-9.6
quercetin	5280343	-9.1
beta-sitosterol	222284	-8.4
chlorogenic acid	1794427	-7.9
rutin	5280805	-7.9
adenosine	60961	-7.8
luteolin	5280445	-7.7
oleanolic acid	10494	-7.6
ursolic acid	64945	-7.6
alpha-curcumene	92139	-7.3
alpha-caryophyllene	5281520	-7
caffeic acid	689043	-6.9
p-coumaric acid	1549106	-6.8
oleic acid	445639	-6.7

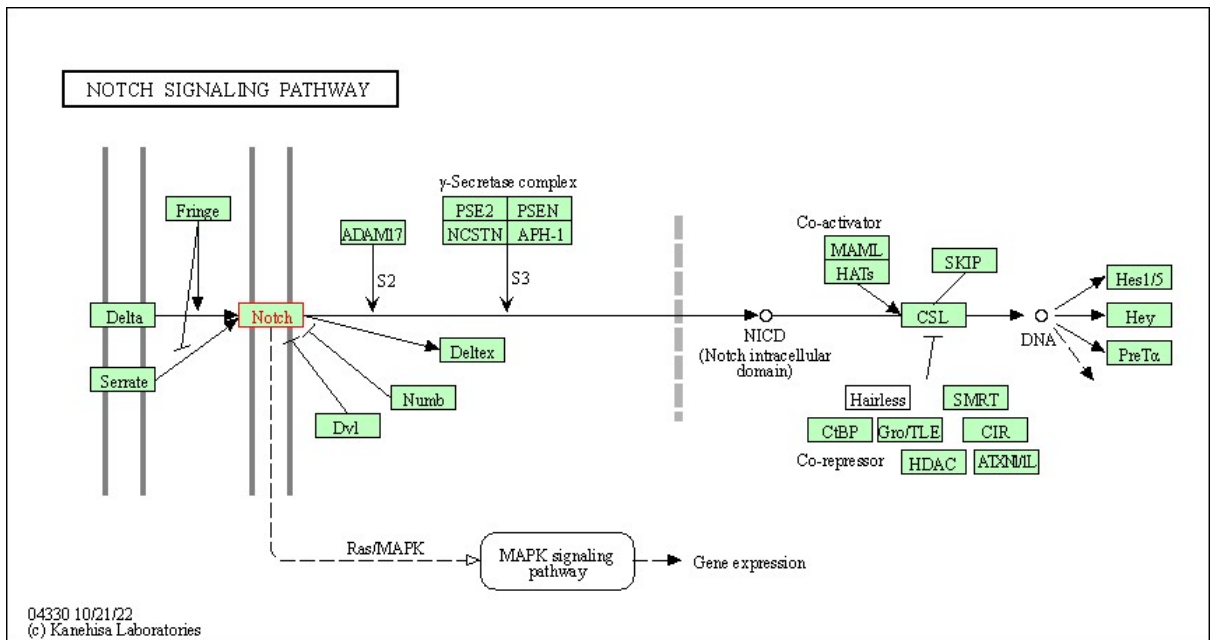
vanillic acid	8468	-6.6
gallic acid	370	-6.5
protocatechuic acid	72	-6.4
beta-terpinene	7461	-6.4
ferulic acid	445858	-6.4
stearic acid	5281	-6.3
p-hydroxybenzoic acid	135	-6.2
pinocarvone	10012081	-6.2
alpha-thujene	17868	-6.1
vanillin	1183	-6
linoleic acid	5280450	-5.9
alpha-pinene	6654	-5.6
palmitoleic acid	445638	-5.5
benzaldehyde	240	-5.4
beta-elemene	9859094	-5.4
arachidic acid	10467	-5.2
beta-myrcene	31253	-4.9
palmitic acid	985	-4.7
myristic acid	11005	-4.6

APPENDIX 18

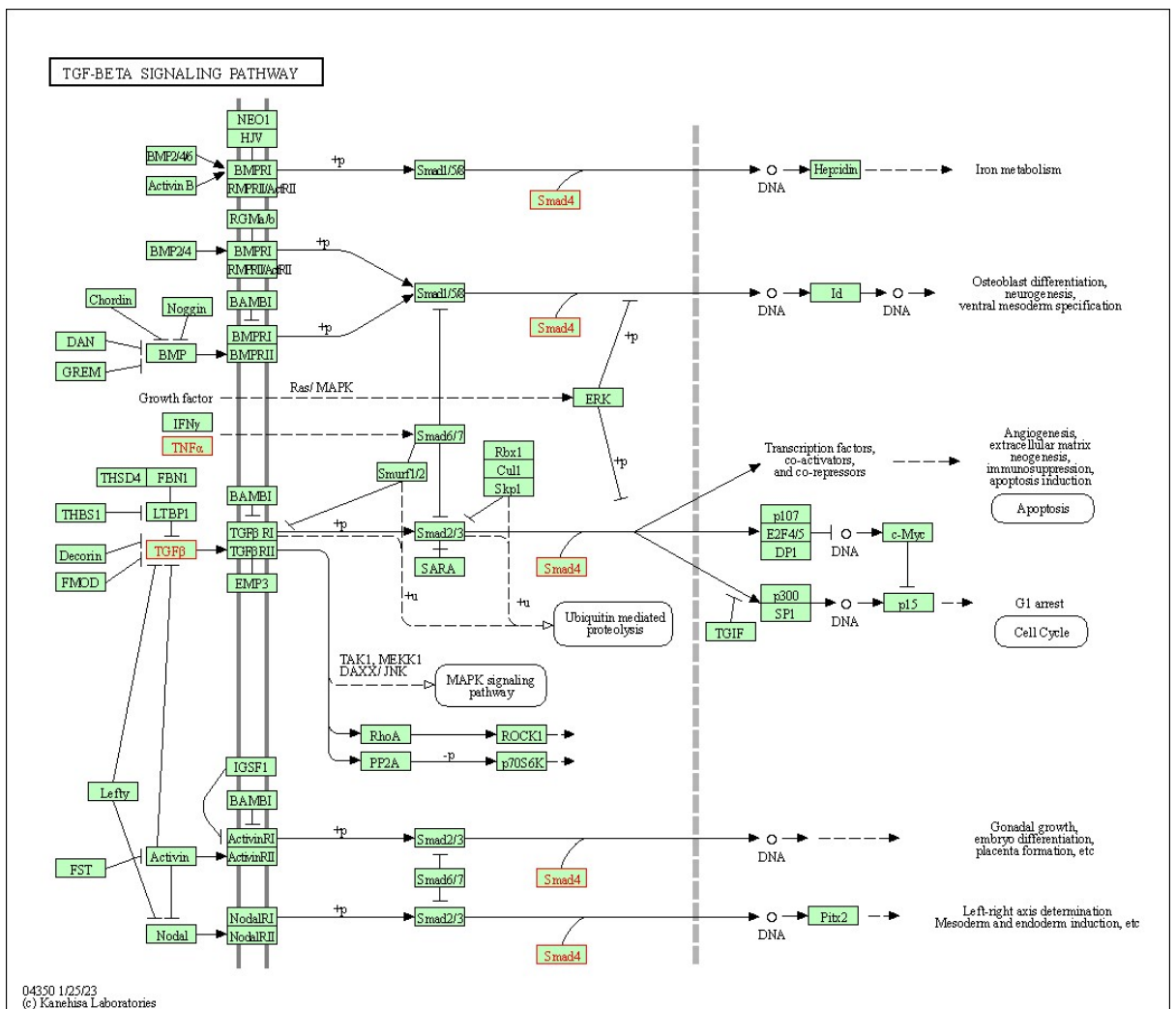
HEDGEHOG SIGNALLING PATHWAY



NOTCH SIGNALLING PATHWAY



TGF-BETA SIGNALLING PATHWAY



APPENDIX 19

INPUT FILE FOR PANEV CONTAINING THE 48 GENES

ensembl_gene_id	entrezgene	external_gene_name
ENSG00000142208	207	AKT1
ENSG00000052850	60529	ALX4
ENSG00000169083	367	AR
ENSG00000171791	596	BCL2
ENSG00000141867	23476	BRD4
ENSG00000110092	595	CCND1
ENSG00000147571	1392	CRH
ENSG00000168036	1499	CTNNB1
ENSG00000107984	22943	DKK1
ENSG00000175065	147409	DSG4
ENSG00000164330	1879	EBF1
ENSG00000135960	10913	EDAR
ENSG00000138675	2250	FGF5
ENSG00000140285	2252	FGF7
ENSG00000048052	9734	HDAC9
ENSG00000168453	55806	HR
ENSG00000017427	3479	IGF1
ENSG00000254647	3630	INS
ENSG00000137265	3662	IRF4
ENSG00000142515	354	KLK3
ENSG00000170484	121391	KRT74
ENSG00000170454	9119	KRT75
ENSG00000170442	3892	KRT86
ENSG00000205213	55366	LGR4
ENSG00000163898	200879	LIPH
ENSG00000139679	10161	LPAR6
ENSG00000160285	4047	LSS
ENSG00000186868	4137	MAPT
ENSG00000177000	4524	MTHFR
ENSG00000109320	4790	NFKB1
ENSG00000148400	4851	NOTCH1
ENSG00000185920	5727	PTCH1
ENSG00000073756	5743	PTGS2
ENSG00000173039	5970	RELA
ENSG00000159216	861	RUNX1
ENSG00000129214	6462	SHBG
ENSG00000164690	6469	SHH
ENSG00000141646	4089	SMAD4
ENSG00000124216	6615	SNAI1
ENSG00000125398	6662	SOX9
ENSG00000277893	6716	SRD5A2
ENSG00000092969	7042	TGFB2
ENSG00000204490	7124	TNF

ENSG00000073282 8626 TP63
 ENSG00000233608 117581 TWIST2
 ENSG00000111424 7421 VDR
 ENSG00000135925 80326 WNT10A
 ENSG00000169884 7480 WNT10B

1L GENES

ensemblgene	entrezgene	gene_name	path_description	path_ID
ENSG00000168036	1499	CTNNB1	Wnt signaling pathway	path:hsa04310
ENSG00000107984	22943	DKK1	Wnt signaling pathway	path:hsa04310
ENSG00000141646	4089	SMAD4	Wnt signaling pathway	path:hsa04310
ENSG00000135925	80326	WNT10A	Wnt signaling pathway	path:hsa04310
ENSG00000205213	55366	LGR4	Wnt signaling pathway	path:hsa04310
ENSG00000110092	595	CCND1	Wnt signaling pathway	path:hsa04310
ENSG00000169884	7480	WNT10B	Wnt signaling pathway	path:hsa04310
ENSG00000148400	4851	NOTCH1	Notch signaling pathway	path:hsa04330
ENSG00000185920	5727	PTCH1	Hedgehog signaling pathway	path:hsa04340
ENSG00000171791	596	BCL2	Hedgehog signaling pathway	path:hsa04340
ENSG00000164690	6469	SHH	Hedgehog signaling pathway	path:hsa04340
ENSG00000110092	595	CCND1	Hedgehog signaling pathway	path:hsa04340

2L GENES

ensemblgene	entrezgene	gene_name	path_description	path_ID
ENSG00000140285	2252	FGF7	MAPK signaling pathway	path:hsa04010
ENSG00000138675	2250	FGF5	MAPK signaling pathway	path:hsa04010
ENSG00000186868	4137	MAPT	MAPK signaling pathway	path:hsa04010
ENSG00000173039	5970	RELA	MAPK signaling pathway	path:hsa04010
ENSG00000017427	3479	IGF1	MAPK signaling pathway	path:hsa04010
ENSG00000142208	207	AKT1	MAPK signaling pathway	path:hsa04010
ENSG00000204490	7124	TNF	MAPK signaling pathway	path:hsa04010
ENSG00000254647	3630	INS	MAPK signaling pathway	path:hsa04010
ENSG00000109320	4790	NFKB1	MAPK signaling pathway	path:hsa04010
ENSG00000092969	7042	TGFB2	MAPK signaling pathway	path:hsa04010
ENSG00000092969	7042	TGFB2	Cell cycle	path:hsa04110
ENSG00000110092	595	CCND1	Cell cycle	path:hsa04110
ENSG00000141646	4089	SMAD4	Cell cycle	path:hsa04110
ENSG00000171791	596	BCL2	p53 signaling pathway	path:hsa04115
ENSG00000017427	3479	IGF1	p53 signaling pathway	path:hsa04115
ENSG00000110092	595	CCND1	p53 signaling pathway	path:hsa04115

ENSG00000141646	4089	SMAD4	TGF-beta signaling pathway	path:hsa04350
ENSG00000092969	7042	TGFB2	TGF-beta signaling pathway	path:hsa04350
ENSG00000204490	7124	TNF	TGF-beta signaling pathway	path:hsa04350
ENSG00000168036	1499	CTNNB1	Focal adhesion	path:hsa04510
ENSG00000017427	3479	IGF1	Focal adhesion	path:hsa04510
ENSG00000110092	595	CCND1	Focal adhesion	path:hsa04510
ENSG00000142208	207	AKT1	Focal adhesion	path:hsa04510
ENSG00000171791	596	BCL2	Focal adhesion	path:hsa04510
ENSG00000124216	6615	SNAI1	Adherens junction	path:hsa04520
ENSG00000168036	1499	CTNNB1	Adherens junction	path:hsa04520
ENSG00000141646	4089	SMAD4	Adherens junction	path:hsa04520
ENSG00000173039	5970	RELA	Alzheimer disease	path:hsa05010
ENSG00000109320	4790	NFKB1	Alzheimer disease	path:hsa05010
ENSG00000107984	22943	DKK1	Alzheimer disease	path:hsa05010
ENSG00000168036	1499	CTNNB1	Alzheimer disease	path:hsa05010
ENSG00000169884	7480	WNT10B	Alzheimer disease	path:hsa05010
ENSG00000254647	3630	INS	Alzheimer disease	path:hsa05010
ENSG00000142208	207	AKT1	Alzheimer disease	path:hsa05010
ENSG00000186868	4137	MAPT	Alzheimer disease	path:hsa05010
ENSG00000135925	80326	WNT10A	Alzheimer disease	path:hsa05010
ENSG00000073756	5743	PTGS2	Alzheimer disease	path:hsa05010
ENSG00000204490	7124	TNF	Alzheimer disease	path:hsa05010

APPENDIX 20

PART OF THE CTD DATA ON AGA GENES TARGETED BY THE PHYTOCHEMICALS

ChemicalName	CasRN	DiseaseName	InferenceGeneSymbol
10,11-dihydro-5H-dibenzo(a,d)cycloheptene		Alopecia	AR
10-methoxy-2,2-dimethyl-2,6-dihydropyrano(3,2-c)quinolin-5-one		Alopecia	PARP1
10-nitro-oleic acid		Alopecia	PARP1
10-(octyloxy)decyl-2-(trimethylammonium)ethyl phosphate		Alopecia	PARP1
1,12-benzoperylene	191-24-2	Alopecia	PARP1
1,1-bis(3'-indolyl)-1-(4-hydroxyphenyl)methane		Alopecia	PARP1
1,1-bis(4-hydroxyphenyl)cyclohexane		Alopecia	AR
11-ketotestosterone	53187-98-7	Alopecia	AR
1,2,3,6,7,8-hexachlorodibenzodioxin	57653-85-7	Alopecia	AR
1,24,25-trihydroxyvitamin D3	50648-94-7	Alopecia	VDR
1,24-dihydroxyvitamin D2	124043-51-2	Alopecia	VDR
1,2,5,6-dibenzanthracene	53-70-3	Alopecia	AR

1,2,5,6-dibenzanthracene	53-70-3	Alopecia	MTHFR
(1,2,5,6-tetrahydropyridin-4-yl)methylphosphinic acid		Alopecia	PARP1
1,25-dihydroxy-16-ene-vitamin D3	124409-58-1	Alopecia	VDR
1,25-dihydroxy-26,27-dimethylcholecalciferol	97473-92-2	Alopecia	VDR
1,25-dihydroxyergocalciferol	55248-15-2	Alopecia	VDR
1,25-dihydroxyvitamin D	66772-14-3	Alopecia	VDR
1,25(OH)2-16-ene-23-yne-26,27-hexafluoro-19-nor-D3		Alopecia	VDR
1,2-bis(2-aminophenoxy)ethane-N,N,N',N'-tetraacetic acid	85233-19-8	Alopecia	PARP1

PART OF THE GENE ONTOLOGIES FOR HAIR PROCESSES

X..GOName	GOID	DiseaseName	InferenceGeneSymbols
anagen	GO:0042640	Abdominal Pain	
anagen	GO:0042640	Abnormalities, Drug-Induced	
anagen	GO:0042640	Abnormalities, Multiple	
anagen	GO:0042640	Abnormalities, Severe Teratoid	
anagen	GO:0042640	Acidosis, Renal Tubular	
anagen	GO:0042640	Acute Kidney Injury	
anagen	GO:0042640	Adams Oliver syndrome	NOTCH1
anagen	GO:0042640	Adenocarcinoma	AKT1 PTGS2
anagen	GO:0042640	Adenocarcinoma Of Esophagus	PTGS2
anagen	GO:0042640	Adenomatosis, Pulmonary	
anagen	GO:0042640	Adenomatous Polyposis Coli	AKT1 PTGS2
anagen	GO:0042640	Adrenal Gland Neoplasms	PTGS2
anagen	GO:0042640	Agranulocytosis	
anagen	GO:0042640	Albuminuria	PTGS2
anagen	GO:0042640	Alkalosis	
anagen	GO:0042640	Alopecia	

anagen	GO:0042 640	Alzheimer Disease	PSEN1 PSEN2
anagen	GO:0042 640	Alzheimer Disease, Familial, 3, with Spastic Paraparesis and Apraxia	PSEN1
anagen	GO:0042 640	Alzheimer disease type 4	PSEN2
anagen	GO:0042 640	Amenorrhea	
anagen	GO:0042 640	Amphetamine-Related Disorders	AKT1
anagen	GO:0042 640	Amyloid Neuropathies	PSEN1
anagen	GO:0042 640	Amyloidosis	PSEN1
anagen	GO:0042 640	Amyotrophic Lateral Sclerosis	PTGS2

APPENDIX 21

SMILES OF THE 34 PHYTOCHEMICALS

adenosine	<chem>C1=NC(=C2C(=N1)N(C=N2)[C@H]3[C@@H]([C@@H]([C@H](O3)CO)O)O)N</chem>
alpha-caryophyllene	<chem>CC1=CCC(C=CCC(=CCC1)C)(C)C</chem>
alpha-curcumene	<chem>CC1=CC=C(C=C1)C(C)CCC=C(C)C</chem>
alpha-pinene	<chem>CC1=CCC2CC1C2(C)C</chem>
alpha-thujene	<chem>CC1=CCC2(C1C2)C(C)C</chem>
apigenin	<chem>C1=CC(=CC=C1C2=CC(=O)C3=C(C=C(C=C3O2)O)O)O</chem>
arachidic acid	<chem>CCCCCCCCCCCCCCCCCCCC(=O)O</chem>
benzaldehyde	<chem>C1=CC=C(C=C1)C=O</chem>
beta-elemene	<chem>CC(=C)[C@@H]1CC[C@@]([C@@H](C1)C(=C)C)(C)C=C</chem>
beta-myrcene	<chem>CC(=CCCC(=C)C=C)C</chem>
beta-sitosterol	<chem>CC[C@H](CC[C@@H](C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@@H](C4)O)C)C)C(C)C</chem>

beta-terpine ne	<chem>CC(C)C1=CCC(=C)CC1</chem>
caffeic acid	<chem>C1=CC(=C(C=C1/C=C/C(=O)O)O)O</chem>
chlorog enic acid	<chem>C1[C@H]([C@H]([C@@H](C[C@@]1(C(=O)O)O)OC(=O)/C=C/C2=CC(=C(C=C2)O)O)O)O</chem>
ferulic acid	<chem>COC1=C(C=CC(=C1)C=CC(=O)O)O</chem>
gallic acid	<chem>C1=C(C=C(C(=C1O)O)O)C(=O)O</chem>
kaempferol	<chem>C1=CC(=CC=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O</chem>
linoleic acid	<chem>CCCCC/C=C\C/C=C\CCCCCCCC(=O)O</chem>
luteolin	<chem>C1=CC(=C(C=C1C2=CC(=O)C3=C(C=C(C=C3O2)O)O)O)O</chem>
myristic acid	<chem>CCCCCCCCCCCCCCCC(=O)O</chem>
oleanolic acid	<chem>C[C@]12CC[C@@H](C([C@@H]1CC[C@@]3([C@@H]2CC=C4[C@]3(CC[C@@]5([C@H]4CC(CC5)(C)C)C(=O)O)C)C)C)C)O</chem>
oleic acid	<chem>CCCCCCCCC=CCCCCCCCC(=O)O</chem>
palmitic acid	<chem>CCCCCCCCCCCCCCCCC(=O)O</chem>
palmitoleic acid	<chem>CCCCCCC=CCCCCCCCC(=O)O</chem>
p-coumaric acid	<chem>C1=CC(=CC=C1/C=C/C(=O)O)O</chem>
p-hydroxybenzoic acid	<chem>C1=CC(=CC=C1C(=O)O)O</chem>
pinocarvone	<chem>CC1(C2CC1C(=C)C(=O)C2)C</chem>
protocatechuic acid	<chem>C1=CC(=C(C=C1C(=O)O)O)O</chem>
quercetin	<chem>C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O)O</chem>
rutin	<chem>C[C@H]1[C@@H]([C@H]([C@H]([C@@H](O1)OC[C@@H]2[C@H]([C@@H]([C@H]([C@@H](O2)OC3=C(OC4=CC(=CC(=C4C3=O)O)O)C5=CC(=C(C=C5)O)O)O)O)O)O)O</chem>
stearic acid	<chem>CCCCCCCCCCCCCCCCC(=O)O</chem>
ursolic acid	<chem>C[C@@H]1CC[C@@]2(CC[C@@]3(C(=CC[C@H]4[C@]3(CC[C@@H]5[C@@]4(CC[C@@H](C5(C)C)O)C)C)[C@@H]2[C@H]1C)C(=O)O</chem>
vanillic acid	<chem>COC1=C(C=CC(=C1)C(=O)O)O</chem>
vanillin	<chem>COC1=C(C=CC(=C1)C=O)O</chem>

IMPORTANT MOLECULAR DESCRIPTORS FOR THE RF MODEL

Descriptor	Description	Class
BCUTc-1h	nlow highest partial charge weighted BCUTS	2D
piPC6	Conventional bond order ID number of order 6 (ln(1+x))	2D
MDEC-23	Molecular distance edge between all secondary and tertiary carbons	2D
MLFER_L	Solute gas-hexadecane partition coefficient	2D
AATSC1p	Average centered Broto-Moreau autocorrelation - lag 1 / weighted by polarizabilities	2D
SdssC	Sum of atom-type E-State: =C<	2D
maxwHBa	Maximum E-States for weak Hydrogen Bond acceptors	2D
SP-6	Simple path, order 6	2D
GATS1p	Geary autocorrelation - lag 1 / weighted by polarizabilities	2D
VE1_Dzv	Coefficient sum of the last eigenvector from Barysz matrix / weighted by van der Waals volumes	2D
VP-5	Valence path, order 5	2D
SP-7	Simple path, order 7	2D
maxaaSC	Maximum atom-type E-State: :C:-	2D
maxaaCH	Maximum atom-type E-State: :CH:	2D
MWC4	Molecular walk count of order 4 (ln(1+x))	2D
BCUTp-1h	nlow highest polarizability weighted BCUTS	2D
GATS8c	Geary autocorrelation - lag 8 / weighted by charges	2D
VPC-5	Valence path cluster, order 5	2D
SpMax2_Bhp	Largest absolute eigenvalue of Burden modified matrix - n 2 / weighted by relative polarizabilities	2D
piPC9	Conventional bond order ID number of order 9 (ln(1+x))	2D
TpiPC	Total conventional bond order (up to order 10) (ln(1+x))	2D
piPC10	Conventional bond order ID number of order 10 (ln(1+x))	2D
GATS1c	Geary autocorrelation - lag 1 / weighted by charges	2D
MATS3s	Moran autocorrelation - lag 3 / weighted by I-state	2D
ETA_Alpha	Sum of alpha values of all non-hydrogen vertices of a molecule	2D
AATSC1i	Average centered Broto-Moreau autocorrelation - lag 1 / weighted by first ionization potential	2D
GATS5e	Geary autocorrelation - lag 5 / weighted by Sanderson electronegativities	2D
SpMax2_Bhv	Largest absolute eigenvalue of Burden modified matrix - n 2 / weighted by relative van der Waals volumes	2D
SpMin2_Bhi	Smallest absolute eigenvalue of Burden modified matrix - n 2 / weighted by relative first ionization potential	2D