Flavonoid Production Predictions

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Author Note

This senior thesis is submitted as partial fulfillment of the graduation requirements for Kettering University for the purpose of obtaining a Bachelor of Science in Computer Science. Any conclusions drawn or opinions expressed within this thesis are my own and are not representative of the position and values held by Kettering University and any other individuals involved with this culminating undergraduate experience.

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Abstract

This project is focused on both theoretical predictions and experimental results of research concerning biosynthesis of select flavonoids: genistein, cyanidin, butein, isoliquiritigenin, catechin, epicatechin, epigallocatechin, gallocatechin, eriodictyol, naringenin, kaempferol, myricetin, quercetin, apigenin, and luteolin. The theoretical predictions are the result of code written in the Python programming language by utilizing data from the Kyoto Encyclopedia of Genes and Genomes (KEGG). The experimental data was collected by conducting a database and literature, involving different methods of data acquisition and processing. The results of the comparisons yielded somewhat mixed results, as there was a significant number of results from the literature and database search that both agreed and disagreed with the programmatic predictions. The comparisons for kaempferol and naringenin were very promising as the predictions for both had at least 40 experimental confirmations and zero experimental disagreements. This means that the species predicted for these compounds would be the best basis for designing tests for determining the phytochemical composition of selected species. The comparisons for cyanidin, eriodictyol, and quercetin were less promising. The predictions for eriodictyol had no experimental disagreements but only a small amount of experimental agreements, while the predictions for cyanidin and quercetin each had two experimental disagreements, which may require an additional literature search focused entirely on said compounds in order to better gauge the program accuracy.

Keywords: anthocyanidins, biosynthesis, chalcones, flavan-3-ols, flavonoids, flavonols, flavanones, flavones, isoflavonoids, python, scripting.

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Introduction

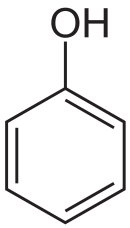
Background

Flavonoids

Flavonoids are a class of polyphenolic compounds, meaning that phenols are a defining part of their structure as well as a contributing factor of their beneficial activities. Phenol is a relatively simple compound as shown in Figures 1 and 2, yet is very useful due to its antimicrobial properties, making it a key ingredient in slimicides as well as a competent disinfectant and antiseptic (National Center for Biotechnology Information, 2021).

Figure 1

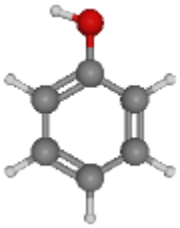
2D structure of phenol.



From the Wikipedia entry for phenol (NEUROtiker, 2007).

Figure 2

3D structure of phenol



From the PubChem entry for phenol (National Center for Biotechnology Information, 2021).

The defining characteristic that distinguishes flavonoids from other polyphenols is its characteristic 15-carbon skeleton. This simple skeleton consists of phenolic A and B

rings, that typically have an accompanying OH group, and an additional C ring as shown in Figure 3.

Figure 3

Basic flavonoid structure.

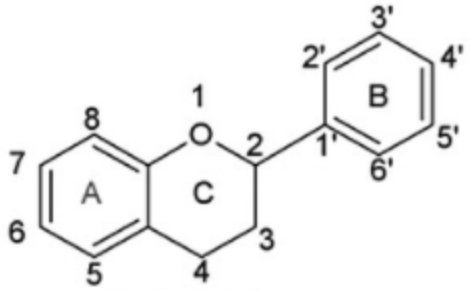
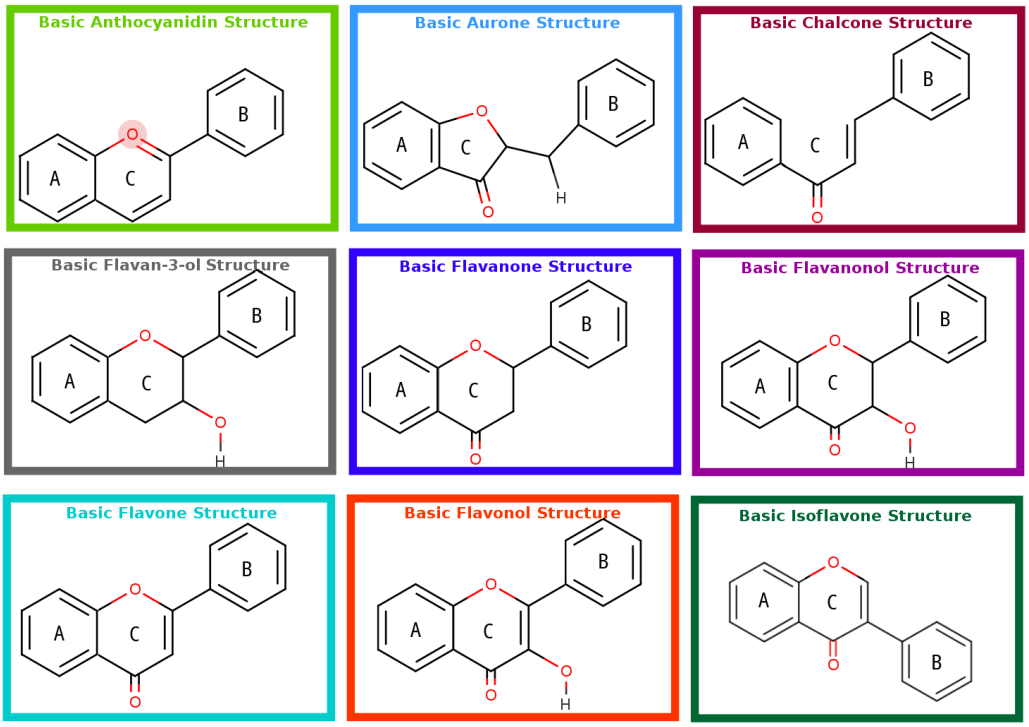


Image adapted from Panche et al., 2016

Since flavonoids are such a large class of compounds, it is helpful to break these compounds down into different subclasses. These subclasses are determined by the specific modifications of the C ring, which can be seen in the diagrams of each subclass' skeleton, shown in Figure 4.

Figure 4

Diagram of differing flavonoid structures.



Flavonoids are a highly diverse and extensive class of *secondary metabolites*, beneficial compounds that are not essential for reproduction and development (LibreTexts, 2021), and can be produced in most of the parts of a living plant (leaves, roots, flowers, etc.) (Dias et al., 2021). Since they are so diverse in their structures and distributions, it would then follow that their functional properties and availability would vary as well. For instance, anthocyanidins can provide red, blue, and purple pigmentation (Tuladhar et al., 2021) while flavones can provide white pigmentation or co-pigmentation (Hostetler et al., 2017), which means that a plant's coloration could tie into the availability of select flavonoids. While pigments can be beneficial for attracting pollinators, flavonoids also can also play a part in tactical and protective advantages, including: UV protection, chemical signaling and antifungal activities (Robertson, 2021).

The helpful benefits of flavonoids are not exclusive to the plant world though.

Humans greatly benefit from the antioxidant properties of the compounds as they are extremely common amongst the plants which play a part in the human diet (Panche, et al., 2016). The antioxidant properties of flavonoids are common across the large class of compounds, yet the medicinal potential does not stop there as several different beneficial properties have been recorded to date such as antibacterial (Xie et al., 2015), antiviral (Lalani & Poh, 2021) and anti-inflammatory (Panche, et al., 2016) activities. This potential is what makes flavonoids so interesting and promising, resulting in an abundance of ongoing research for the purpose of discovering new activities and medicinal applications.

Kyoto Encyclopedia of Genes and Genomes (KEGG)

KEGG (https://www.genome.jp.kegg/) is a freely accessible database resource, sponsored by the Kanehisa Laboratories of the Institute of Chemical Research of Kyoto University. It contains and has access to large amounts of information that is relevant for understanding the biological systems of animals, plants, fungi, protists, bacteria, and archaea, including: enzymes, proteins, pathways, genes and entire genomes. Since the database is a culmination of work that dates back to 1995 and is focused on connecting current knowledge and high throughput computing, the data that is available is extensive and is stored in an extremely interconnected fashion. That is, an entry in KEGG will have its own unique identifiers, along with the identifiers of associated entries such as genes, compounds or reactions, which makes the process of accessing specific information much easier.

Genes and Genomes

Genes are a part of living organisms and are the vehicle through which traits are passed down from parent to offspring (National Library of Medicine, 2021) and are responsible for providing the instructions for making essential macromolecules, like proteins. They are able to do this due to a special molecular building-block: *deoxyribonucleic acid* (DNA). DNA is a molecule which carries genetic information and instructions by using unique sequences of specific chemical bases (National Human Genome Research Institute) and is what allows for genes to code for specific proteins. A single gene only has so much influence over an organism however, and are but a smaller part of a collective referred to as a genome. An organism's genome is the entirety of its genetic information which determines how an organism forms, grows and functions. Due to the advancements in technology, entire genomes of numerous organisms have been sequenced. In other words, their chemically-coded instructions have been determined, which has been an essential step in better understanding the underlying biological mechanisms of organisms, and has become incredibly valuable knowledge in the context of agriculture and medicine. In the context of this project though, genes and genomes are significant because they allow for a more comprehensive understanding of flavonoid biosynthesis, which relies on the analysis of the specific genes that code for the enzymes that are essential to this process.

Proteins, Enzymes and EC Numbers

Proteins are another important class of organic macromolecules, which are large and complex molecules found in organisms. They are constructed by structures within a

cell called ribosomes, which takes in a copied piece of DNA, in the form of a messenger ribonucleic acid (mRNA) molecule (Bartee et al., 2016), and using those instructions, then assembles a specific sequence of amino acids (National Human Genome Research Institute). Though they provide a wide range of purposes, the most relevant proteins in this context are ones that act as catalysts, or rather, chemicals that increase the rate of essential chemical reactions without being consumed in the process (National Human Genome Research Institute). These proteins are referred to as enzymes and are an essential group of molecules that regulates an organism's biological functions. There are seven different types of enzymes commonly referred to that are grouped based on their functions and/or associated reactions: *oxidoreductases* catalyze oxidation-reduction reactions; *transferases* catalyze the transfer of molecules' functional group(s); *hydrolases* break chemical bonds with water; *lyases* catalyze bond-breaking without oxidation or hydrolysis; *isomerases* rearrange the structure of molecules; *ligases* create chemical bonds between molecules (Chou & Elrod, 2003); and *translocases* aid in moving a molecule other than itself (Zhang & He, 2019).

The classification of enzymes is more complex than sorting enzymes into seven -different groups, which is where the *enzyme commission* (EC) number becomes very helpful. EC numbers are used for classifying enzymes and take the format x.x.x.x, where the number in each position is associated with specific identifiers that are determined by the enzyme and its associated reaction(s) (Hu et al. 2012). The first digit corresponds with an enzyme's class: (1) oxidoreductase, (2) transferase, (3) hydrolase, (4) lyase, (5) isomerase, (6) ligase, and (7) translocases (Tipton & McDonald). The second digit refers

to the type of compound(s) involved, the third digit relays more information regarding the reaction type, and the final digit is a serial number used for identifying enzymes within their respective classifications. For example, as shown the enzyme database ExplorEnz's webpage (https://www.enzyme-database.org/class.php), the EC number for hydroxycinnamoyl-CoA reductase is EC 1.3.1.117 because: it is an oxidoreductase (1.x.x.x) that acts on the CH-CH group of donors (1.3.x.x) with NAD^+ or $NADP^+$ as an acceptor (1.3.1.x) and has a serial number of 117 (1.3.1.117) (McDonald et al., 2009). EC numbers are an important portion of this project as they are included in the KEGG database entries for a gene, if the gene happens to code for one or more enzymes, and is extracted by parsing within the program.

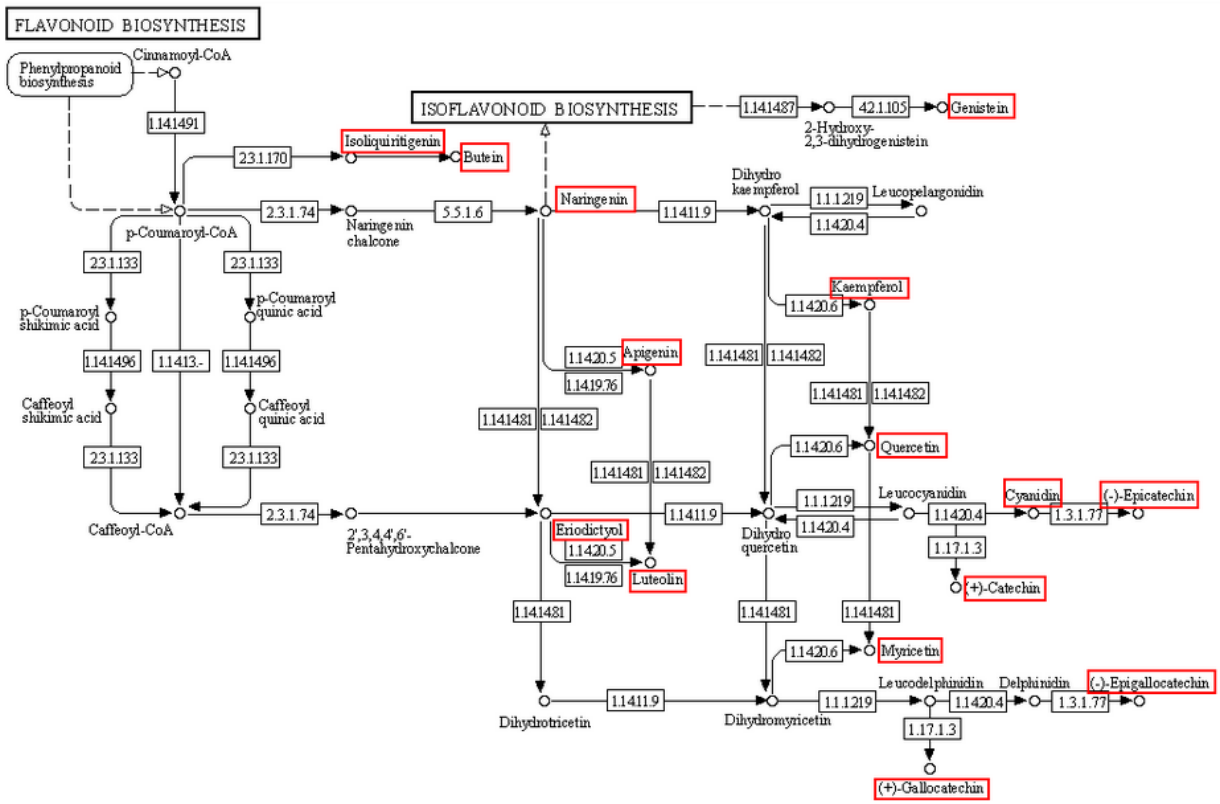
Biological Pathways and Flavonoid Biosynthesis

A *biological pathway* is a specific chain of molecular events within a cell that result in changes to the cell or lead to the production of one or more compounds (National Human Genome Research Institute, 2020). *Biosynthesis*, also referred to as *anabolism*, is a type of biological pathway that results in a product that is produced by enzyme-catalyzed reactions involving simpler precursor compounds (Biology Online, 2021). Numerous different pathways have been understood to date and are represented by diagrams referred to as pathway maps, which visualize the steps of a pathway. KEGG has a collection of pathway maps which use arrows to indicate the progression of reactions along with the pathways relevant precursors, products and enzymes and these maps have been an essential reference in better understanding flavonoid biosynthesis because their database entries also include the known associated genes and enzymes. The maps

provided by KEGG are generalized, as in they are not representative of a specific organism and are made by utilizing information from numerous organisms in order to cover a wider range of reactions. Flavonoid biosynthesis requires the products of phenylpropanoid biosynthesis as precursor compounds and then ultimately ends up with the production of select compounds that feed into additional pathways: isoflavonoid biosynthesis, flavone biosynthesis, flavonol biosynthesis, and anthocyanin biosynthesis. Figure 5 shows a modified pathway map of KEGG's flavonoid biosynthesis (Kanehisa Laboratories, 2019) where it has been connected to the isoflavonoid map (Kanehisa Laboratories, 2021) to include genistein. Additionally, the compounds that do not serve as precursors or intermediates to the flavonoids in the data set have been removed for the sake of simplicity.

Figure 5

Simplified combination of the flavonoid and isoflavonoid biosynthesis pathways. The flavonoids of interest are boxed in red. Figure was made using modified maps accessed from KEGG (Kanehisa Laboratories 2019 & 2021) .



Python

Python is a very popular multi-purpose programming language that is utilized across a wide range of fields. The language has an emphasis on code readability by enforcing levels of indentation in order to create clearly structured and nested code. This emphasis on indentation along with the numerous handy built-in functions (that could take several lines to implement in other programming languages) makes Python easier to learn for those with little to no formal programming experience, making it a popular choice for writing programs relating to the natural sciences. As a result, a multitude of individuals have developed different libraries for the purpose of scientific programming,

which only furthers the benefits of the language.

Python is also an ideal choice for this project because of the Bioservices (Cokelaer et al., 2013) library for Python. It is a free collection of code relating to biology and bioinformatics and is extremely diverse in its utility, which includes easy programmatic access of the data hosted by KEGG.

Purpose and Nature

The data regarding the flavonoid composition of different plants can be considered lacking due to a bias or favoritism towards testing culinary or medicinal plants, as well as a bias which favors certain flavonoids. For instance, butein was first reportedly isolated in 1904 (Perkin & Hummel, 1904) and cyanidin does not appear to have any reference in literature until 1913 (Willstätter & Everest, 1913), yet when either compound is searched in Google scholar, as of December 2021 there are about 58,600 results for cyanidin and only around 13,900 results for butein. Many of the first results are regarding medical studies and applications though, yet one could anticipate that the usage in these applications could inspire more investigation into source organisms. The purpose of this project is to programmatically predict biosynthesis in specific species of plants. The predictions serve to inspire future testing of the chemical contents of said plants by using a method such as high-performance liquid chromatography (HPLC) in the efforts to find traces of select flavonoids. This would help to fill in the gap of missing data relating to the plants in the data set and compounds they are not yet experimentally known to synthesize. Additionally, this project consists of a literature and database search for the purpose of comparing the predictions to existing data and to analyze and comment

on the available data in the databases.

Flavonoids in the Data Set

The flavonoids of interest belong to seven different classes: isoflavonoids (genistein), anthocyanidins (cyanidin), chalcones (butein and isoliquiritigenin), flavan-3-ols ((+)-catechin, (-)-epicatechin, (-)-epigallocatechin and (+)-gallocatechin), flavanones ((-)-eriodictyol and (-)-naringenin), flavones (apigenin and luteolin), and flavonols (kaempferol , myricetin, and quercetin). The structures for each of the compounds can be seen in Figure 6. It should be noted that references to the flavan-3-ols and flavanones will omit the +/- as the project is not concerned with more than one of the compounds' stereoisomers, which are compounds that are almost identical but differ in their orientation of atoms (Reusch, 2013).

Figure 6

Chemical structures of the flavonoids in the data set.

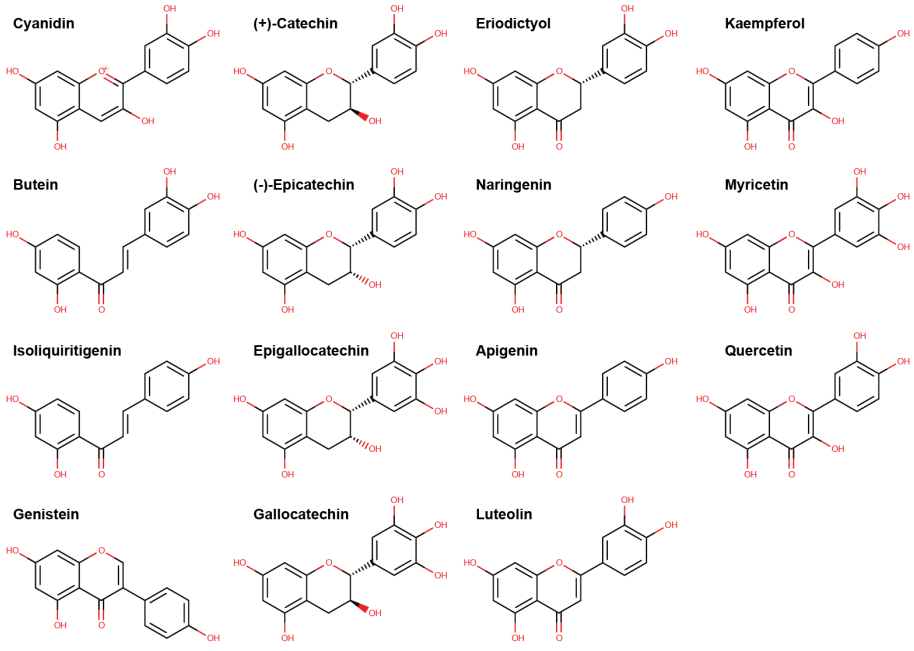


Image created by Dr. Veronica Moorman.

Plants in the Data Set

There are 105 species within the project data set, which belong to 43 different plant families. The dataset had been determined by the available genomic data for plants provided by KEGG at the time of official project work (October 2020). The majority of these species (90) fall under the classification of flowering land plants. Green algae, red algae, mosses and club mosses make up the remainder of the data set. Table 1 lists the species of the data set, which have been sorted by select taxonomic classifications in order to serve as a visual aid of the species distribution. The taxonomic information was collected from four different online sources: UniProt (Velankar et al., 2013), the NCBI Taxonomy Browser (Schoch et al., 2020), Integrated Taxonomic Information System (ITIS, 2021), and AlgaeBase (Guiry & Guiry, 2022).

Table 1

List of the plants in the data set which includes the designated codes assigned by KEGG.

				Family	*Species*	KEGG Code
Red Algae				Cyanidiaceae	*Cyanidioschyzon merolae*	cme
					Galdieria sulphuraria	gsl
				Gigartinaceae	*Chondrus crispus (carrageen moss)*	ccp
Green Algae				Bathycoccaceae	*Bathycoccus prasinos*	bpg
					Ostreococcus lucimarinus	olu
					Ostreococcus tauri	ota
				Chlamydomonadaceae	*Chlamydomonas reinhardtii*	cre
				Chlorellaceae	*Auxenochlorella protothecoides*	apro
					Chlorella variabilis	cvr
				Coccomyxaceae	*Coccomyxa subellipsoidea*	csl
				Mamiellaceae	*Micromonas commoda*	mis
					Micromonas pusilla	mpp
				Selenastraceae	*Monoraphidium neglectum*	mng
				Volvocaceae	*Volvox carteri f. nagariensis*	vcn
Land Plants	**Non-vascular Plants**			Funariaceae	*Physcomitrium patens (spreading earth moss)*	ppp
	Vascular Plants	**Seedless**		Selaginellaceae	*Selaginella moellendorffii (spikemoss)*	smo
		Flowering Plants	**Basal Angiosperms**	Amborellaceae	*Amborella trichopoda (primitive flowering shrub)*	atr
			Monocots	Arecaceae	*Elaeis guineensis (African oil palm)*	egu
					Phoenix dactylifera (date palm)	pda
				Asparagaceae	*Asparagus officinalis (garden*	aof

		asparagus)	
	Musaceae	*Musa acuminata (wild Malaysian banana)*	mus
	Orchidaceae	*Dendrobium catenatum (chained dendrobium)*	dct
		Phalaenopsis equestris (moth orchid)	peq
	Poaceae	*Aegilops tauschii (wheat D)*	ats
		Brachypodium distachyon (purple false brome)	bdi
		Oryza brachyantha (malo sina)	obr
		Oryza sativa subsp. japonica (Japanese rice)	osa/dosa
		Setaria italica (foxtail millet)	sita
		Sorghum bicolor (sorghum)	sbi
		Zea mays (maize)	zma
	Amaranthaceae	*Beta vulgaris (sugar beet)*	bvg
		Spinacia oleracea (spinach)	soe
	Apiaceae	*Daucus carota (carrot)*	dcr
	Asteraceae	*Cynara cardunculus var. scolymus (artichoke)*	ccav
		Helianthus annuus (common sunflower)	han
		Lactuca sativa (garden lettuce)	lsv
	Bombacaceae	*Durio zibethinus (durian)*	dzi
	Chenopodiaceae	*Chenopodium quinoa (quinoa)*	cqi
	Convolvulaceae	*Ipomoea nil (Japanese morning glory)*	ini
	Cucurbitaceae	*Cucumis melo (muskmelon)*	cmo
		Cucumis sativus (cucumber)	csv
		Cucurbita maxima (winter squash)	cmax
		Cucurbita moschata (crookneck pumpkin)	cmos
		Cucurbita pepo subsp. pepo (vegetable marrow)	cpep
		Momordica charantia (bitter melon)	mcha
Eudicots	Euphorbiaceae	*Hevea brasiliensis (rubber tree)*	hbr
		Jatropha curcas (Barbados nut)	jcu
		Manihot esculenta (cassava)	mesc
		Ricinus communis (castor bean)	rcu
	Fabaceae	*Arachis duranensis (peanut diploid ancestor)*	adu
		Arachis ipaensis (peanut diploid ancestor)	aip
		Cajanus cajan (pigeon pea)	ccaj
		Cicer arietinum (chickpea)	cam
		Glycine max (soybean)	gmx
		Glycine soja (wild soybean)	gsj
		Lotus japonicus (birdsfoot trefoil)	lja
		Lupinus angustifolius (narrow-leaved blue lupine)	lang
		Medicago truncatula (barrel medic)	mtr
		Phaseolus vulgaris (common bean)	pvu
		Vigna angularis (adzuki bean)	var
		Vigna radiata (mung bean)	vra
		Vigna unguiculata (cowpea)	vun
		Quercus suber (cork oak)	qsu

Juglandaceae	*Juglans regia (English walnut)*	jre
Malvaceae	*Gossypium arboreum (tree cotton)*	gab
	Gossypium hirsutum (upland cotton)	ghi
	Gossypium raimondii (Peruvian cotton)	gra
	Theobroma cacao (cacao)	tcc
Myrtaceae	*Eucalyptus grandis (rose gum)*	egr
Oleaceae	*Olea europaea var. sylvestris (wild olive)*	oeu
Papaveraceae	*Papaver somniferum (opium poppy)*	psom
Pedaliaceae	*Sesamum indicum (sesame)*	sind
Rhamnaceae	*Ziziphus jujuba (Chinese jujube)*	zju
Rosaceae	*Fragaria vesca (woodland strawberry)*	fve
	Malus domestica (apple)	mdm
	Prunus avium (sweet cherry)	pavi
	Prunus mume (Japanese apricot)	pmum
	Prunus persica (peach)	pper
	Pyrus x bretschneideri (Chinese white pear)	pxb
	Rosa chinensis (China rose)	rcn
Rutaceae	*Citrus clementina (mandarin orange)*	cic
Rutaceae	*Citrus sinensis (Valencia orange)*	cit
Salicaceae	*Populus euphratica (Euphrates poplar)*	peu
	Populus trichocarpa (black cottonwood)	pop
Solanaceae	*Capsicum annuum (cayenne pepper)*	cann
	Nicotiana attenuata (coyote tobacco)	nau
	Nicotiana sylvestris (woodland tobacco)	nsy
	Nicotiana tabacum (common tobacco)	nta
	Nicotiana tomentosiformis (wild tobacco)	nto
	Solanum lycopersicum (tomato)	sly
	Solanum pennellii (wild tomato)	spen
	Solanum tuberosum (potato)	sot
Vitaceae	*Vitis vinifera (wine grape)*	vvi
Brassicaceae	*Arabidopsis lyrata (lyrate rockcress)*	aly
	Arabidopsis thaliana (thale cress)	ath
	Brassica napus (rapeseed)	bna
	Brassica oleracea (wild cabbage)	boa
	Brassica rapa (field mustard)	brp
	Camelina sativa (false flax)	csat
	Capsella rubella (pink shepherd's-purse)	crb
	Eutrema salsugineum (saltwater cress)	eus
	Raphanus sativus (radish)	rsz
Caricaceae	*Carica papaya (papaya)*	cpap
Cleomaceae	*Tarenaya hassleriana (spider flower)*	thj
Nelumbonaceae	*Nelumbo nucifera (sacred lotus)*	nnu

It should be noted that for the sake of simplicity, there will be shortened names that will be used to refer to certain plants within relevant figures and tables since the data

set does not contain more than one variety, cultivar, etc. for any given species. The shortened names are listed in Table 2. It also should be noted that there were two entries for *Oryza sativa subsp. japonica* due to the differences in the sources of the sequenced genomes, and for simplicity, the results from the predictions are condensed into one entry.

Table 2

Shortened plant names.

Scientific Name	Shortened Name
Cucurbita pepo subsp. pepo	Cucurbita pepo
Cynara cardunculus var. scolymus	Cynara cardunculus
Olea europaea var. sylvestris	Olea europaea
Oryza sativa subsp. japonica	Oryza sativa
Pyrus x bretschneideri	Pyrus x
Volvox carteri f. nagariensis	Volvox carteri

Literature and Database Search

The literature and database search was a process of obtaining as much data as possible relating to the plants in the dataset and the synthesis of the flavonoids in the data set. Specifically, this search was focused primarily on finding plant-compound pairs, i.e. determining which of the plants in the data set are already known to synthesize the flavonoids in the data set. The motivation of conducting this search is based on the purely theoretical nature of the code. Any of the experimental data relating to the phytochemical contents of select plants that has been collected for this project is useful to compare against the programmatic predictions in order to provide a gauge of the accuracy of the program.

Conclusions and Recommendations

Conclusions

Overall, there are undoubtedly further database and literature searches that will be necessary, as the data becomes available, in order to get a better grasp on the competency of the program as there are enough disagreements between the experimental and theoretical data to create doubt, yet there are also an abundance of agreements that do not completely dismiss the program as dysfunctional. Many of these disagreements come from either one single data source or are the results of studies that focus on culinary and other heavily cultivated (and thus potentially genetically modified) plants. This should not dismiss the validity of the data in its entirety however - it just means that these disagreements could be more likely to be resolved through further investigation of literature. Despite the number of experimental disagreements, there were enough experimental confirmations of the predictions which indicates that the program is at the very least directionally correct In terms of designing experiments in order to confirm or deny predictions made by the code, naringenin and kaempferol would serve as ideal candidates as there was a relatively large set of species that were both predicted and experimentally confirmed to synthesize the compounds. Experimenting with cyanidin, eriodictyol and quercetin would most likely be of some benefit for gauging the accuracy of the code as the experimental data agreed to a point where, at the very least, additional experimentation could address uncertainties in accuracy.

Recommendations for Future Work

Since the data set of species has been solidified since October of 2020 and

reflected the available genome sequences available through KEGG, the data set of plants used in this project is now limited as the number of species with accessible sequences has increased. The database now provides information for an additional 21 species (Table 3) of plants, which provides an opportunity for updating the data files for the code, and for conducting additional literature and database searches.

Table 3

The new species available from KEGG.

		Family	*Species*	KEGG Code
Flowering Plants	**Basal Angiosperms**	Nymphaeaceae	*Nymphaea colorata*	ncol
	Monocots	Poaceae	*Panicum hallii (Hall's panicgrass)*	phai
			Panicum virgatum (switchgrass)	pvir
			Triticum aestivum (bread wheat)	taes
			Triticum dicoccoides (wild emmer wheat)	tdc
	Eudicots	Anacardiaceae	*Mangifera indica (mango)*	minc
		Anacardiaceae	*Pistacia vera (pistachio)*	pvy
		Asteraceae	*Erigeron canadensis (horseweed)*	ecad
		Celastraceae	*Tripterygium wilfordii (thunder duke vine)*	twl
		Convolvulaceae	*Ipomoea triloba (trilobed morning glory)*	itr
		Cucurbitaceae	*Benincasa hispida (wax gourd)*	bhj
		Fabaceae	*Abrus precatorius (Indian licorice)*	aprc
		Fabaceae	*Arachis hypogaea (peanut)*	ahf
		Fagaceae	*Quercus lobata (valley oak)*	qlo
		Lamiaceae	*Salvia splendens (scarlet sage)*	sspl
		Moraceae	*Morus notabilis (mulberry species)*	mnt
		Phrymaceae	*Erythranthe guttata (spotted monkey flower)*	egt
		Proteaceae	*Macadamia integrifolia (macadamia nut)*	ming
		Rosaceae	*Prunus dulcis (almond)*	pdul
		Salicaceae	*Populus alba (white poplar)*	palz
		Vitaceae	*Vitis riparia (riverbank grape)*	vri

Additionally, it is recommended to extend the literature and database search to include the compounds from Table 4, in order to compare the new data to the predictions generated for these new compounds. The prediction code has been written for these compounds after the completion of the main project and is accessible through GitHub at *https://github.com/mbagg4152/pfpy* and can be found in the appendix. Since the basis of the program was already established it did not take long to update it to accommodate the new compounds. However, there was not enough time to conduct an updated literature

and database search as the process is extremely time consuming and the new list of compounds is much larger than the working set from this project.

Table 4

Additional compounds, sorted by classification.

Classification	Compound
Dihydrochalcones	Phloretin
Flavan 3-ols	Afzelechin
	Epiafzelechin
Flavan 4-ols	Apiforol
	Luteoforol
Flavanones	Butin
	Dihydrotricetin
	Hesperetin
	Liquiritigenin
	Pinocembrin
Flavones	Chrysin
	Galangin
	Tricetin
Flavononols	Ampelopsin (Dihydromyricetin)
	Dihydrokaempferol
	Fustin (2, 3-Dihydrofisetin)
	Garbonzol
	Pinobanksin
	Taxifolin (Dihydroquercetin)
Isoflavanones	2-Hydroxy-2, 3-dihydrogenistein
	2, 6, 7, 4'-Tetrahydroxyisoflavanone
	2, 7, 4'-Trihydroxyisoflavanone
	6, 7, 4'-Trihydroxyflavanone
Isoflavones	6-Hydroxydaidzein
	7-4'-dihydroxyflavone
	Daidzein
Leucoanthocyanidins (Flavan 3, 4-diols)	Leucocyanidin
	Leucodelphinidin
	Leucopelargonidin

Another opportunity for future work lies in utilizing specific data that the code has already collected in order to analyze the genes and associated enzymes and flavonoids for the plants in the data set. This could be used to lead to a better

understanding of the evolution of flavonoids, along with their distributions across different plant species.

Additionally, there is an opportunity to conduct a literature and database search for compounds similar to the flavonoids in the data set. This could potentially include defining a strict definition for the similar compound and/or selecting specific similar compounds. Currently, the data that has been collected was collected while searching for data for the flavonoids in the data set and includes data from compounds that either derive from or have one of the flavonoids as a component. The data collected to date can be found at the beginning of the appendix in Tables 70-83.

The final recommendation is to test specific plants from the data sets for the purpose of comparing the predictions for isoliquiritigenin, butein, kaempferol, naringenin, cyanidin, eriodictyol and quercetin. It would be beneficial to test plants from Asteraceae and Fabaceae as there is existing data which confirms butein synthesis in these families, and more importantly there are species from these families within the dataset used for this project. If the data set is expanded to include all available KEGG species, it may be beneficial to also work with *Pistacia vera*, as it belongs to Anacardiaceae, which also contains plants confirmed to synthesize butein (Nara Institute of Science and Technology). Additionally, it would be advantageous to test for isoliquiritigenin in these same species because (1) it is lacking experimental confirmations (albeit not to the same extent as butein), and (2) the KEGG flavonoid biosynthesis map appears to imply the reaction that transforms isoliquiritigenin to butein is bi-directional (Figure 7).

Testing kaempferol and naringenin would be greatly beneficial, and testing cyanidin, eriodictyol and quercetin could be of some benefit, given the predictions of the program and the comparisons made against experimentally known data, which will be covered later in the paper. If an experiment was conducted in order to focus on these five compounds, then it would be suggested that the initial subjects belong to *Fabaceae*. Each compound is predicted to be synthesized by most of the species of the dataset that belong to this family. Additionally, there is experimental data that shows that there are members of this family that have been known to synthesize each of these five compounds.

Figure 7

The KEGG entry for the reaction associated with isoliquiritigenin and butein.

Entry	R07994 Reaction
Definition	Isoliquiritigenin <=> Butein
Equation	C08650 <=> C08578
	 C08650 C08578
Comment	chalcone 3-hydroxylase
Reaction class	RC00046 C08578_C08650
Pathway	rn00941 Flavonoid biosynthesis

From "KEGG REACTION: R07994" (Kanehisa Labs).

Methods

The bulk of the work for this project consisted of working on a program written in Python 3 and conducting literature and database searches. The most important goal of the program is to make the predictions regarding the flavonoid production in certain plant species.

The program was written using the standard distribution of Python, version 3.8.5. The program relies on additional library modules in order to function properly. Most of these modules are part of the Python standard library (The Python Software Foundation): datetime, json, os, re, sys, threading, and urllib. The final module needed for the program is Bioservices (version 1.7.11 was used for this project) and is the only external source which needs to be installed using the pip3 package manager. Bioservices is an extensive Python library and a crucial component of the program, meaning that it must be installed on a machine in order for the code to be able to execute and make its predictions. The program also requires JSON (JavaScript object notation) input files, which have been created specifically for this project. They serve as a better method of storing larger pieces of data compared to simply storing them as variables in the program, which takes out excess clutter from the code and makes data modification simpler. They look visually similar to the lists and dictionaries (key-value pairs) that are used in Python, which made the transition from hard-coded values (used in the previous project program versions) to JSON files extremely simple.

The literature and database searches were conducted as a way to gather as much information as possible in order to comment on the ranges of available data, but more

importantly to compare experimentally known results with results predicted by the program. Much of the data referenced in the project comes from the databases, with additional information that has been collected from smaller sources and will be discussed further in the following subsections.

Prediction Program Utilizing Data from KEGG

Initialization

The initialization of the program is quite simple and focuses primarily on setting up the structure of directories for output and initializing key variables and constants. Many of the constants used are stored in JSON files in order to make the process of updating these values much simpler and to make the code more readable. Most of these values take the form of simple lists or dictionaries. The former is used for gathering data by using iteration while the latter is used for making the program output more human readable by using the keys to acquire the value that is to be printed. Some of the data used includes lists of the pathway and species codes, along with dictionaries that use these codes as the keys with the values being the actual name associated with the code. For example, *Arabidopsis thaliana* has a KEGG code of *"ath"* so the dictionary entry for this organism would be *"ath": "Arabidopsis thaliana"*.

The most important values used within the program are contained within the list of organism-pathway codes, which are used to gather the core information that will be used throughout the program. As with any database, KEGG too has its own unique identifiers for all of the information that is stored and made publicly available. The codes for the organisms are a set of three to four alphabetic characters while the pathway codes

are numeric strings. Conveniently, if an organism has genes that are involved in any given biological pathway, then the name and identifiers of these genes can be found by concatenating the organism and pathway codes.

The organism and pathway codes are held separately for the purpose of saving time and avoiding human error, as manually checking the names for each organism-pathway code would be extremely time consuming and tedious. The organism-pathway codes are generated iteratively by creating five new organism-pathway codes for each existing organism code, one for each of the biological pathways relating to this project as shown in Figures 8 and 9.

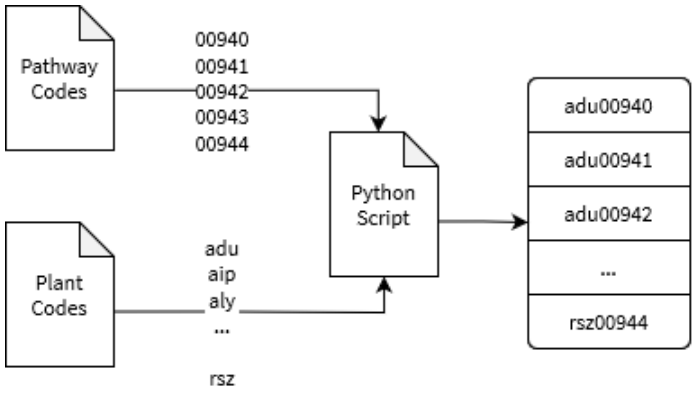
Figure 8

The code for generating organism-pathway pairs.

```
# Combines plant and pathway codes.
plant_pathways = [i + j for i in plant_list for j in path_map_list]
```

Figure 9

Visualization of organism-pathway code creation.



Once this is complete, a list of plant objects are created using the KEGG codes and their corresponding scientific names, which are python objects created specifically to store collections of information associated with each species as shown in Figure 10.

Figure 10

The process of creating the new plant objects.

```
for key in plant_dict:
    # Call constructor to make new plant.
    tmp_plant = Plant(code=key, name=plant_dict[key])
    # Add to list if not present. Prevents duplicates.
    if not tmp_plant.is_in(plant_objects): plant_objects.append(tmp_plant)
```

Retrieving and Parsing Gene Data from KEGG

The list of organism-pathway codes created during initialization is first broken down into a collection of smaller lists. This is because the acquisition stage takes advantage of multithreading which greatly decreases the overall runtime of the program. Gathering the information for each organism-pathway code is a standalone process, which is what makes the usage of multithreading possible. Figure 11 highlights one of the implementations of multithreading in the program. Here, when each thread is created, a list will be passed as a parameter to the function that gathers the data.

Figure 11

Portion of the code responsible for creating the threads.

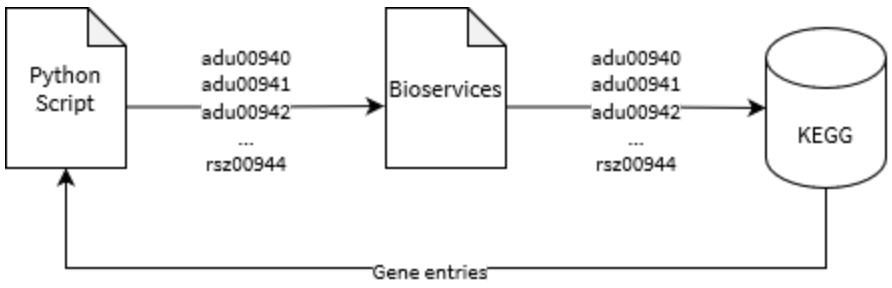
```
# A thread is made for each sub-list which then passes each sub-list
# as a parameter to the pathway parser.
for sub_list in sub_lists:
    thread = threading.Thread(target=path_parse, args=(sub_list,))
    thread.start()
    threads.append(thread)
```

The function path_parse utilizes a very helpful library called bioservices which provides a multitude of functions for gathering and processing information from KEGG. When the function receives the list of organism-pathway codes, it iterates over the list,

sending each code to KEGG. It then will return either an associated entry or an error message if the organism in question does not have any genes associated with the given pathway. Figure 12 visualizes this step of the program as the code consists of different sub-steps of tedious processing.

Figure 12

Visualization of data retrieval from KEGG.



Once a valid entry is gathered, it is then parsed to gather the gene's KEGG ID, orthology, associated compound name, and most importantly the EC (enzyme commission) numbers. The EC numbers are added to a list belonging to the corresponding plant object that had been created earlier. This information alongside the organism's code and name as well as the pathway code are written to output files for easier reference.

Making Predictions

After the entries have been processed and each organisms' list of EC numbers has been appropriately updated, the program can move onto predicting the organism-compound pairs.This is done by first iterating through the list of plant objects and then for each individual plant object, the program then iterates through the list of flavonoid objects, which contains the chemical's name and a shortened code. This code

corresponds with the name of its respective function that is used for making its predictions and is used to trigger said function call.

The idea behind the functions used for making each compounds' predictions are the same in nature: each flavonoid has a set of enzymes that are necessary for its production and are represented by EC numbers which means that the prediction can be handled by using a combination of logical ANDs and ORs. The logical operations were used because each step of synthesizing a compound may require one specific enzyme or may require one enzyme from a set of enzymes, then these steps must be chained together in order to get to a final product. These operations were set up by referencing KEGG's pathway maps and are necessary to check if the enzymes required to synthesize a given flavonoid are present in a plant's list, i.e., the plant has a specific set of genes that code for the required enzymes. For the sake of simplicity, two small utility functions have been created which are then used to run the logical operations when there are two or more elements that are to be checked as part of the overall logic flow, shown in Figure 13.

Figure 13

The logical functions that return true or false depending on the required enzymes and the input list.

```
# returns true if at least 1 arg is in the list
def or_in(items, *args):
    for a in args:
        if a in items:
            return True
    return False

# returns true only if all args are in the list
def and_in(items, *args):
    for a in args:
        if a not in items:
            return False  # all values must be present
    return True
```

In addition to the logical utility functions, some prediction functions can be simplified by using the output of another flavonoid's function due the structure of the biological pathways. For example, as shown in Figure 14, naringenin requires one more enzyme than its precursor naringenin chalcone which then in turn allows for a simpler logical function as seen in Figure 15. This means that the function that predicts naringenin only needs to call the function which predicts naringenin chalcone and then determine if a plant has genes that code for the additional enzyme, instead of checking the presence of numerous enzymes in one line of code.

Figure 14

Logic for predicting naringenin, derived from KEGG pathway diagrams.

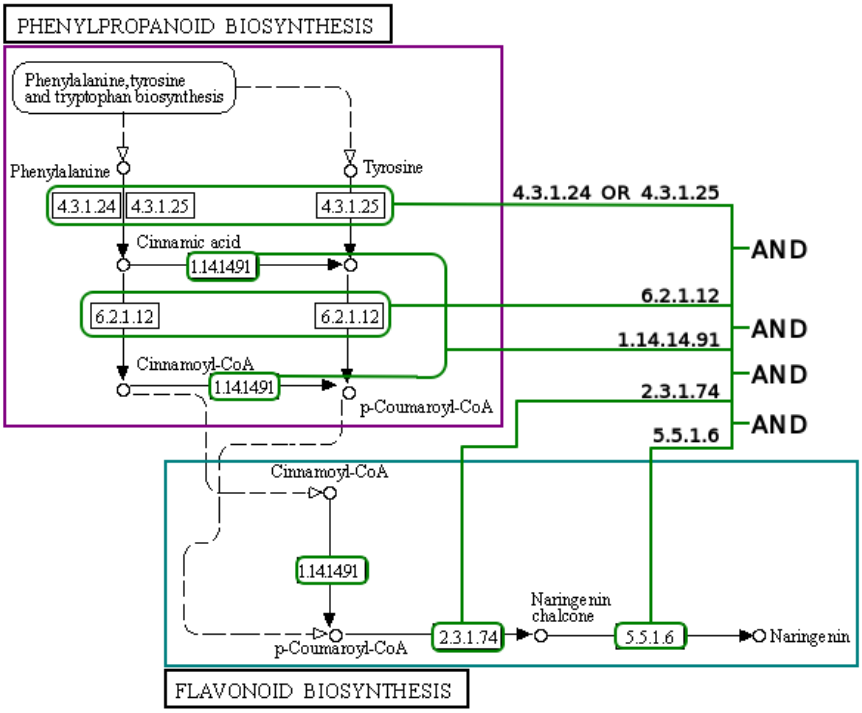


Figure 15

The prediction functions for naringenin chalcone and naringenin.

```
def narc(e):  # naringenin chalcone || new
   return wca(e) and (E09 in e)

def nar(e):  # naringenin || mh thesis
   return narc(e) and (E10 in e)
```

Additional Code Functionality

Once the predictions have been made, the program will continue to complete two other tasks which have been deemed to be important in future research planned by Dr. Moorman. While this code does not affect the predictions in any way, it relies on different steps taken in the prediction process and is too significant of a part of the script to neglect entirely.

Right after the predictions have been completed, the program then moves on to look at the list of EC numbers for each plant that had been built by parsing the gene entries from KEGG. When building the list, duplicates were not removed so the program was able to count the occurrence of each EC number associated with each plant, which is helpful for determining the number of a plant's genes that code for the same enzymes. Once this is done, the results are output into a tab delimited file where each row contains the plant name, the EC numbers and their counts.

After the EC number counts have been written to files, the program then shifts focus to grab the nucleotide sequences for each single gene that had been processed previously. The sequences are also hosted by KEGG but unlike gathering the gene entries, gathering the sequences had to be done differently due to bioservices not providing any functions relating to this specifically. Instead, the program uses DBGET URLs for accessing and downloading the sequences. DBGET is a database retrieval method implemented by KEGG which allows for easier data access since the URLs have a set format and are able to be built programmatically.

This portion of the code also utilizes multithreading as the number of genes from the selected list of organisms is roughly 24,000, which would take an extended amount of time to process if the program was written to only use a single thread. The function that handles the downloads and processing of these entries also saves each page as a local text file, which makes the execution time much faster if a user wishes to run the program multiple times. Each entry that is accessed is in the form of a simple HTML web page which is then parsed using regular expressions in order to extract the nucleotide

sequence. Once a sequence has been gathered, the program then takes the key organism and gene identifiers and then uses these values to output the sequences in FASTA format. After every sequence is gathered and processed they are then sorted into collections based on associated EC numbers, which are then used to produce a set of FASTA files that, for each unique enzyme, contain the set of genes that code for them.

Literature and Database Search

The literature and database search was centered around finding and collecting data associated with the plants from the working data set. The data used in this project primarily consists of data from various articles and journals and data gathered from large databases. Some sources referenced were collected by Jordan Wilson for his work on this project and his thesis *Computational Analysis of Flavonoid Pathways from Various Plant Species*, while others were found by utilizing different online resources such as Google Scholar and PubChem. The databases referenced for data collection are:

1. NPASS (Natural Product Activity and Species Source database) (Zeng et al., 2018), available at http://bidd.group/NPASS/search.php;
2. KNApSAcK (Afendi et al., 2012), available at http://www.knapsackfamily.com/knapsack_core/top.php;
3. USDA Database for the Flavonoid Content of Selected Foods (Haytowitz et al., 2018), available at https://www.ars.usda.gov/ARSUserFiles/80400535/Data/Flav/Flav3.3.pdf;
4. Microbiome Analysis for Patients (Lassesen Consulting, LLC), available at https://www.microbiomeprescription.com/Library/Flavonoids;

5. IMPPAT (Indian Medicinal Plants Phytochemistry and Therapeutics) (Mohanraj et al., 2018), available at https://cb.imsc.res.in/imppat/home;
6. Dr. Duke's Phytochemical and Ethnobotanical Databases at NAL (U.S. Department of Agriculture, Agricultural Research Service, 1992-2016), available at https://phytochem.nal.usda.gov/phytochem/search/list;
7. and NAPRALERT (NAtural PRoducts ALERT) (Loub et al., 1985), previously available at https://napralert.org/ but is unavailable as of January 2022.

Each database referenced in this project is available in different formats and accessible through different interfaces, meaning that data was collected both manually and programmatically. The data from NPASS and KNApSAcK were collected programmatically, while the remainder of the databases were accessed manually.

The data from NPASS was available to be exported as tab delimited text files, which then went through different levels of processing using regular expressions. This was done in order to create the appropriate JSON dictionaries consisting of the compound and organism IDs matched with their names. It should be noted that these values were collected on the basis of string matching, so there were additional codes collected as the names of some of the selected flavonoids were a substring in the names of additional flavonoids. In addition to creating the JSON data, a script was written for the purpose of processing the NPASS data. The script would use the collection of the specific NPASS codes that were collected previously in order to extract any pair from the NPASS data file that contained a selected organism and compound code. The selected pairs were then output and pasted into excel.

Accessing KNApSAcK was a simpler process given that the database is set up such that URLs can be generated in a formulaic fashion, which was extremely beneficial in creating the parsing script. For each plant in the data set, the program would create a KNApSAcK URL using its scientific name and then would download the corresponding HTML page. Once this was completed, the HTML files were then parsed one at a time using regular expressions, which would extract the compound names for each plant and would then complete a string search which would then determine if a compound and its corresponding plant could be saved as a matching pair. If the pair contains a flavonoid from the data set, then that specific pair is selected to be saved to an output file. This output file can then be pasted into excel and then filtered or searched to get a list of specific compounds. This could be done in the code, but it was preferable to finish this portion in excel so that the matches could be filtered by compound and pasted into their appropriate columns in the sheet used for storing the KNApSAcK data.

The remaining databases (USDA, Microbiome, IMPPAT, Dr. Duke's and NAPRALERT) were presented in ways that did not make them ideal candidates for simple parsing scripts. All of the remaining databases, except for the USDA database, were searched by using the host website's search functionality. The USDA database was accessed in PDF format so it was simply read through for finding matches. As each piece of data was collected, it had been added to a spreadsheet in order to keep track of the sources that stated whether a given plant is known to synthesize any of the compounds from the data set.

It should also be noted that the data from Microbiome is the result of theoretical

predictions as well but should nonetheless still offer useful data for comparison and is grouped into the category of experimentally known data for the sake of simplicity. Almost none of the exact matches referenced can be attributed solely to Microbiome, as there is almost always one accompanying match from another database or literary source.

Database Comparisons

Each database was created by different types of organizations (government agencies, academic groups, etc.) in order to serve different purposes, as described in the discussion. The difference in the purpose and nature of these databases means that the accessible data varies in their records on different organisms, compounds and their relationships. The data is also skewed towards specific organisms and compounds due to the differing levels of interest and perceived usefulness and as such, there were noticeable differences in the number and types of missing plants. This was found by keeping track of different database statistics in a spreadsheet. For each source, there is a list of compounds and organisms from the project lists that were missing. In addition to keeping track of the missing entries, the number of exact compound-organism matches were recorded to then determine how much each database was able to contribute. It should be noted that for each database, there was an attempt to search for each single plant and flavonoid from the dataset. For the programmatically searched databases, there was a manual search conducted to confirm the list of missing items as reported by the program.

Supplemental Sources

Any other sources recorded and used for comparisons are simply a collection of smaller sources (i.e. academic papers, single studies, etc.).

Comparisons Between the Literature and Program Output

This information relies entirely on data stored in and operations done on spreadsheets. In the main spreadsheet where these comparisons are made, there is a column which contains the name of each plant and additional columns which track if each plant is experimentally known or predicted to synthesize a compound.

For the experimentally known portion of data, the cell which corresponds with a specific plant and compound will be marked or blank, which is determined by attempting to find the plant name in specific named ranges which are named by compound and literature source. Then the appropriate letter code will be placed in the specific cell so long as a match is made. Keeping track of the predictions is far simpler. It is set up in a similar way to the experimentally known portion, but simply marks with an ‘x’ if there is a match for any given cell.

Using the aforementioned data, one can then use the values of those cells to then take count of the occurrences of a plant being experimentally known to synthesize a compound, a plant being predicted to be capable of synthesizing a compound, or a combination thereof. This can be used to put the outcome of the program into perspective.

Results

Predictions

The predictions listed in this section are the output of the project program which has been designed to, on a theoretical basis, predict if any of the 105 selected species could be capable of synthesizing any of the 15 selected flavonoids. A summary of the number of species predicted to synthesize each flavonoid can be seen in Table 5.

Table 5

Number of species predicted to synthesize each flavonoid.

Compound	Number of Species
Genistein	9
Cyanidin	76
Butein	90
Isoliquiritigenin	90
Catechin	58
Epicatechin	65
Epigallocatechin	43
Gallocatechin	42
Eriodictyol	89
Naringenin	90
Kaempferol	84
Myricetin	47
Quercetin	83
Apigenin	37
Luteolin	37

Isoflavonoid

There are nine species that have been predicted to be capable of synthesizing genistein (Table 6), all of which belong to the legume family, Fabaceae.

Table 6

Plants predicted to synthesize genistein.

1. Cajanus cajan	*4. Glycine soja*	*7. Vigna angularis*
2. Cicer arietinum	*5. Lupinus angustifolius*	*8. Vigna radiata*
3. Glycine max	*6. Phaseolus vulgaris*	*9. Vigna unguiculata*

Anthocyanidin

There are 76 species which were predicted to synthesize cyanidin (Table 7), all of which are angiosperms of varying genera.

Table 7

Plants predicted to synthesize cyanidin.

1. Aegilops tauschii	*27. Gossypium arboreum*	*52. Phoenix dactylifera*
2. Amborella trichopoda	*28. Gossypium hirsutum*	*53. Populus euphratica*
3. Arabidopsis lyrata	*29. Gossypium raimondii*	*54. Populus trichocarpa*
4. Arabidopsis thaliana	*30. Helianthus annuus*	*55. Prunus avium*
5. Arachis duranensis	*31. Hevea brasiliensis*	*56. Prunus mume*
6. Asparagus officinalis	*32. Ipomoea nil*	*57. Prunus persica*
7. Beta vulgaris	*33. Jatropha curcas*	*58. Pyrus x*
8. Brassica napus	*34. Juglans regia*	*59. Quercus suber*
9. Brassica oleracea	*35. Lotus japonicus*	*60. Raphanus sativus*
10. Brassica rapa	*36. Lupinus angustifolius*	*61. Ricinus communis*
11. Camelina sativa	*37. Malus domestica*	*62. Rosa chinensis*
12. Capsicum annuum	*38. Manihot esculenta*	*63. Sesamum indicum*
13. Carica papaya	*39. Medicago truncatula*	*64. Setaria italica*
14. Chenopodium quinoa	*40. Musa acuminata*	*65. Solanum lycopersicum*
15. Cicer arietinum	*41. Nelumbo nucifera*	*66. Solanum pennellii*
16. Citrus clementina	*42. Nicotiana attenuata*	*67. Solanum tuberosum*
17. Citrus sinensis	*43. Nicotiana sylvestris*	*68. Spinacia oleracea*
18. Cynara cardunculus	*44. Nicotiana tabacum*	*69. Tarenaya hassleriana*
19. Daucus carota	*45. Nicotiana tomentosiformis*	*70. Theobroma cacao*
20. Dendrobium catenatum	*46. Olea europaea*	*71. Vigna angularis*
21. Durio zibethinus	*47. Oryza brachyantha*	*72. Vigna radiata*
22. Elaeis guineensis	*48. Oryza sativa*	*73. Vigna unguiculata*
23. Eucalyptus grandis	*49. Papaver somniferum*	*74. Vitis vinifera*
24. Eutrema salsugineum	*50. Phalaenopsis equestris*	*75. Zea mays*
25. Glycine max	*51. Phaseolus vulgaris*	*76. Ziziphus jujuba*
26. Glycine soja		

Chalcones

There are 90 species which were predicted to synthesize both butein and isoliquiritigenin (Table 8), the majority of which are angiosperms. The only exceptions were the Byrophite *Physcomitrium patens* and the Lycophyte *Selaginella moellendorffii,* which are far removed from flowering plants as they both reproduce using spores instead

of seeds (Rensing et al., 2020; Wallheimer, 2011).

Table 8

Plants predicted to synthesize the chalcones of the data set.

1. Aegilops tauschii	*31. Eucalyptus grandis*	*61. Phalaenopsis equestris*
2. Amborella trichopoda	*32. Eutrema salsugineum*	*62. Phaseolus vulgaris*
3. Arabidopsis lyrata	*33. Fragaria vesca*	*63. Phoenix dactylifera*
4. Arabidopsis thaliana	*34. Glycine max*	*64. Physcomitrium patens**
5. Arachis duranensis	*35. Glycine soja*	*65. Populus euphratica*
6. Arachis ipaensis	*36. Gossypium arboreum*	*66. Populus trichocarpa*
7. Asparagus officinalis	*37. Gossypium hirsutum*	*67. Prunus avium*
8. Beta vulgaris	*38. Gossypium raimondii*	*68. Prunus mume*
9. Brachypodium distachyon	*39. Helianthus annuus*	*69. Prunus persica*
10. Brassica napus	*40. Hevea brasiliensis*	*70. Pyrus x*
11. Brassica oleracea	*41. Ipomoea nil*	*71. Quercus suber*
12. Brassica rapa	*42. Jatropha curcas*	*72. Raphanus sativus*
13. Cajanus cajan	*43. Juglans regia*	*73. Ricinus communis*
14. Camelina sativa	*44. Lactuca sativa*	*74. Rosa chinensis*
15. Capsicum annuum	*45. Lotus japonicus*	*75. Selaginella moellendorffii**
16. Carica papaya	*46. Lupinus angustifolius*	*76. Sesamum indicum*
17. Chenopodium quinoa	*47. Malus domestica*	*77. Setaria italica*
18. Cicer arietinum	*48. Manihot esculenta*	*78. Solanum lycopersicum*
19. Citrus clementina	*49. Medicago truncatula*	*79. Solanum pennellii*
20. Citrus sinensis	*50. Momordica charantia*	*80. Solanum tuberosum*
21. Cucumis melo	*51. Musa acuminata*	*81. Sorghum bicolor*
22. Cucumis sativus	*52. Nelumbo nucifera*	*82. Spinacia oleracea*
23. Cucurbita maxima	*53. Nicotiana attenuata*	*83. Tarenaya hassleriana*
24. Cucurbita moschata	*54. Nicotiana sylvestris*	*84. Theobroma cacao*
25. Cucurbita pepo	*55. Nicotiana tabacum*	*85. Vigna angularis*
26. Cynara cardunculus	*56. Nicotiana tomentosiformis*	*86. Vigna radiata*
27. Daucus carota	*57. Olea europaea*	*87. Vigna unguiculata*
28. Dendrobium catenatum	*58. Oryza brachyantha*	*88. Vitis vinifera*
29. Durio zibethinus	*59. Oryza sativa*	*89. Zea mays*
30. Elaeis guineensis	*60. Papaver somniferum*	*90. Ziziphus jujuba*

** Bryophyte (non-flowering).*

Flavan-3-ols

The entirety of the species predicted to synthesize the flavan-3-ols were a diverse set of angiosperms. There are 58 predicted species for catechin (Table 9), 65 for epicatechin (Table 10), 43 for epigallocatechin (Table 11), and 42 for gallocatechin (Table 12). There were 40 species that were predicted to synthesize all four of these compounds,

which can be seen in Table 13. The differences in the prediction sets can be attributed to the presence or absence of specific enzymes: flavonoid 3',5'-hydroxylase (EC:1.14.14.81) is needed to synthesize gallocatechin and epigallocatechin; leucoanthocyanidin reductase (EC:1.17.1.3) is needed to synthesize catechin and gallocatechin; and anthocyanidin reductase (EC:1.3.1.77) is needed to synthesize epicatechin and epigallocatechin.

Table 9

Plants predicted to synthesize catechin.

1. Aegilops tauschii	*21. Hevea brasiliensis*	*40. Phoenix dactylifera*
2. Amborella trichopoda	*22. Jatropha curcas*	*41. Populus euphratica*
3. Arachis duranensis	*23. Juglans regia*	*42. Populus trichocarpa*
4. Asparagus officinalis	*24. Lotus japonicus*	*43. Prunus avium*
5. Beta vulgaris	*25. Lupinus angustifolius*	*44. Prunus mume*
6. Brachypodium distachyon	*26. Malus domestica*	*45. Prunus persica*
7. Carica papaya	*27. Manihot esculenta*	*46. Pyrus x*
8. Chenopodium quinoa	*28. Medicago truncatula*	*47. Quercus suber*
9. Cicer arietinum	*29. Musa acuminata*	*48. Ricinus communis*
10. Citrus clementina	*30. Nelumbo nucifera*	*49. Rosa chinensis*
11. Citrus sinensis	*31. Nicotiana attenuata*	*50. Solanum pennellii*
12. Durio zibethinus	*32. Nicotiana sylvestris*	*51. Solanum tuberosum*
13. Elaeis guineensis	*33. Nicotiana tabacum*	*52. Spinacia oleracea*
14. Eucalyptus grandis	*34. Nicotiana tomentosiformis*	*53. Theobroma cacao*
15. Glycine max	*35. Olea europaea*	*54. Vigna angularis*
16. Glycine soja	*36. Oryza brachyantha*	*55. Vigna radiata*
17. Gossypium arboreum	*37. Oryza sativa*	*56. Vigna unguiculata*
18. Gossypium hirsutum	*38. Papaver somniferum*	*57. Vitis vinifera*
19. Gossypium raimondii	*39. Phaseolus vulgaris*	*58. Ziziphus jujuba*
20. Helianthus annuus		

Table 10

Plants predicted to synthesize epicatechin.

1. Aegilops tauschii	*23. Gossypium arboreum*	*45. Populus euphratica*
2. Amborella trichopoda	*24. Gossypium hirsutum*	*46. Populus trichocarpa*
3. Arabidopsis lyrata	*25. Gossypium raimondii*	*47. Prunus avium*
4. Arabidopsis thaliana	*26. Hevea brasiliensis*	*48. Prunus mume*
5. Arachis duranensis	*27. Jatropha curcas*	*49. Prunus persica*
6. Asparagus officinalis	*28. Juglans regia*	*50. Pyrus x*
7. Beta vulgaris	*29. Lotus japonicus*	*51. Quercus suber*
8. Brassica napus	*30. Lupinus angustifolius*	*52. Raphanus sativus*
9. Brassica oleracea	*31. Malus domestica*	*53. Ricinus communis*

10. Brassica rapa
11. Camelina sativa
12. Carica papaya
13. Chenopodium quinoa
14. Cicer arietinum
15. Citrus clementina
16. Citrus sinensis
17. Durio zibethinus
18. Elaeis guineensis
19. Eucalyptus grandis
20. Eutrema salsugineum
21. Glycine max
22. Glycine soja
32. Manihot esculenta
33. Medicago truncatula
34. Musa acuminata
35. Nelumbo nucifera
36. Nicotiana attenuata
37. Nicotiana sylvestris
38. Nicotiana tabacum
39. Nicotiana tomentosiformis
40. Oryza brachyantha
41. Oryza sativa
42. Papaver somniferum
43. Phaseolus vulgaris
44. Phoenix dactylifera
54. Rosa chinensis
55. Setaria italica
56. Solanum lycopersicum
57. Solanum pennellii
58. Solanum tuberosum
59. Tarenaya hassleriana
60. Theobroma cacao
61. Vigna angularis
62. Vigna radiata
63. Vigna unguiculata
64. Zea mays
65. Ziziphus jujuba

Table 11

Plants predicted to synthesize epigallocatechin.

1. Aegilops tauschii
2. Carica papaya
3. Cicer arietinum
4. Citrus clementina
5. Citrus sinensis
6. Durio zibethinus
7. Elaeis guineensis
8. Eucalyptus grandis
9. Glycine max
10. Glycine soja
11. Gossypium arboreum
12. Gossypium hirsutum
13. Gossypium raimondii
14. Hevea brasiliensis
15. Jatropha curcas
16. Juglans regia
17. Lotus japonicus
18. Lupinus angustifolius
19. Manihot esculenta
20. Medicago truncatula
21. Musa acuminata
22. Nelumbo nucifera
23. Nicotiana attenuata
24. Nicotiana sylvestris
25. Nicotiana tabacum
26. Nicotiana tomentosiformis
27. Oryza brachyantha
28. Oryza sativa
29. Phaseolus vulgaris
30. Phoenix dactylifera
31. Populus euphratica
32. Populus trichocarpa
33. Quercus suber
34. Setaria italica
35. Solanum lycopersicum
36. Solanum pennellii
37. Solanum tuberosum
38. Theobroma cacao
39. Vigna angularis
40. Vigna radiata
41. Vigna unguiculata
42. Zea mays
43. Ziziphus jujuba

Table 12

Plants predicted to synthesize gallocatechin.

1. Aegilops tauschii
2. Brachypodium distachyon
3. Carica papaya
4. Cicer arietinum
5. Citrus clementina
6. Citrus sinensis
7. Durio zibethinus
8. Elaeis guineensis
9. Eucalyptus grandis
15. Hevea brasiliensis
16. Jatropha curcas
17. Juglans regia
18. Lotus japonicus
19. Lupinus angustifolius
20. Manihot esculenta
21. Medicago truncatula
22. Musa acuminata
23. Nelumbo nucifera
29. Oryza sativa
30. Phaseolus vulgaris
31. Phoenix dactylifera
32. Populus euphratica
33. Populus trichocarpa
34. Quercus suber
35. Solanum pennellii
36. Solanum tuberosum
37. Theobroma cacao

10. Glycine max	*24. Nicotiana attenuata*	*38. Vigna angularis*
11. Glycine soja	*25. Nicotiana sylvestris*	*39. Vigna radiata*
12. Gossypium arboreum	*26. Nicotiana tabacum*	*40. Vigna unguiculata*
13. Gossypium hirsutum	*27. Nicotiana tomentosiformis*	*41. Vitis vinifera*
14. Gossypium raimondii	*28. Oryza brachyantha*	*42. Ziziphus jujuba*

Table 13

Species predicted to synthesize the flavan-3-ols from the data set.

1. Aegilops tauschii	*15. Jatropha curcas*	*28. Oryza sativa japonica*
2. Carica papaya	*16. Juglans regia*	*29. Phaseolus vulgaris*
3. Cicer arietinum	*17. Lotus japonicus*	*30. Phoenix dactylifera*
4. Citrus clementina	*18. Lupinus angustifolius*	*31. Populus euphratica*
5. Citrus sinensis	*19. Manihot esculenta*	*32. Populus trichocarpa*
6. Durio zibethinus	*20. Medicago truncatula*	*33. Quercus suber*
7. Elaeis guineensis	*21. Musa acuminata*	*34. Solanum pennellii*
8. Eucalyptus grandis	*22. Nelumbo nucifera*	*35. Solanum tuberosum*
9. Glycine max	*23. Nicotiana attenuata*	*36. Theobroma cacao*
10. Glycine soja	*24. Nicotiana sylvestris*	*37. Vigna angularis*
11. Gossypium arboreum	*25. Nicotiana tabacum*	*38. Vigna radiata*
12. Gossypium hirsutum	*26. Nicotiana tomentosiformis*	*39. Vigna unguiculata*
13. Gossypium raimondii	*27. Oryza brachyantha*	*40. Ziziphus jujuba*
14. Hevea brasiliensis		

Flavanones

There are 89 predicted species for eriodictyol and 90 for naringenin (Table 14). The predicted species for both compounds were exactly the same, with the exception of *Momordica charantia*, which was predicted to synthesize naringenin but not eriodictyol. This difference is caused by *M. charantia* not being able to produce specific enzymes (Figure 16), as per the data supplied by KEGG. All of the associated species are classified as angiosperms, with the exceptions of *P. patens* and *S. moellendorffii.*

Table 14

Plants predicted to synthesize the flavanones in the data set.

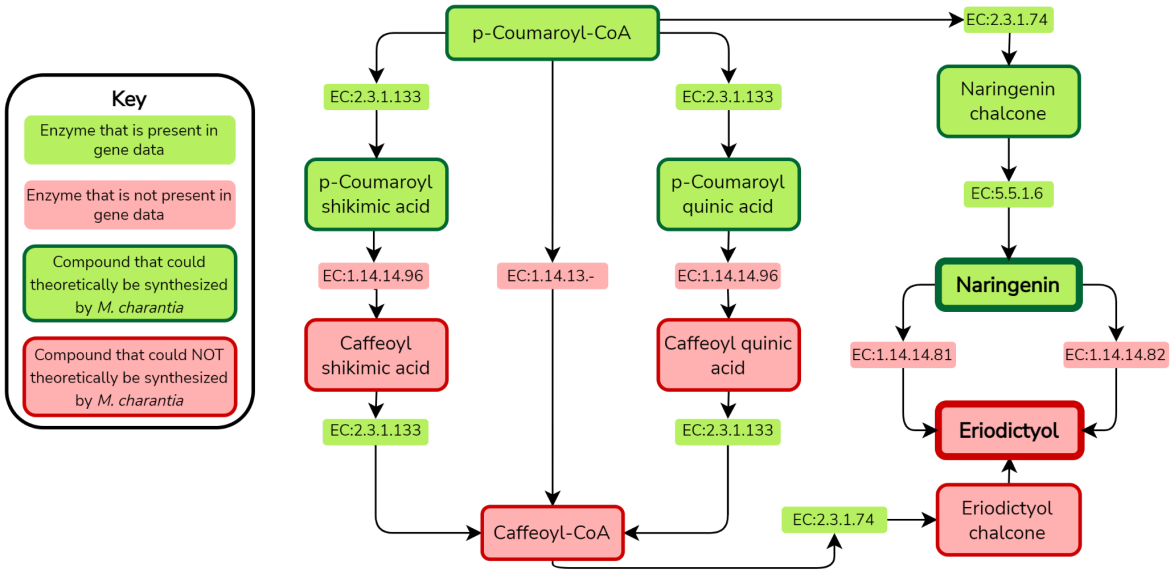
1. Aegilops tauschii	*31. Eucalyptus grandis*	*61. Phalaenopsis equestris*
2. Amborella trichopoda	*32. Eutrema salsugineum*	*62. Phaseolus vulgaris*
3. Arabidopsis lyrata	*33. Fragaria vesca*	*63. Phoenix dactylifera*

4. Arabidopsis thaliana
5. Arachis duranensis
6. Arachis ipaensis
7. Asparagus officinalis
8. Beta vulgaris
9. Brachypodium distachyon
10. Brassica napus
11. Brassica oleracea
12. Brassica rapa
13. Cajanus cajan
14. Camelina sativa
15. Capsicum annuum
16. Carica papaya
17. Chenopodium quinoa
18. Cicer arietinum
19. Citrus clementina
20. Citrus sinensis
21. Cucumis melo
22. Cucumis sativus
23. Cucurbita maxima
24. Cucurbita moschata
25. Cucurbita pepo
26. Cynara cardunculus
27. Daucus carota
28. Dendrobium catenatum
29. Durio zibethinus
30. Elaeis guineensis
34. Glycine max
35. Glycine soja
36. Gossypium arboreum
37. Gossypium hirsutum
38. Gossypium raimondii
39. Helianthus annuus
40. Hevea brasiliensis
41. Ipomoea nil
42. Jatropha curcas
43. Juglans regia
44. Lactuca sativa
45. Lotus japonicus
46. Lupinus angustifolius
47. Malus domestica
48. Manihot esculenta
49. Medicago truncatula
50. Momordica charantia **
51. Musa acuminata
52. Nelumbo nucifera
53. Nicotiana attenuata
54. Nicotiana sylvestris
55. Nicotiana tabacum
56. Nicotiana tomentosiformis
57. Olea europaea
58. Oryza brachyantha
59. Oryza sativa
60. Papaver somniferum
64. Physcomitrium patens *
65. Populus euphratica
66. Populus trichocarpa
67. Prunus avium
68. Prunus mume
69. Prunus persica
70. Pyrus x
71. Quercus suber
72. Raphanus sativus
73. Ricinus communis
74. Rosa chinensis
75. Selaginella moellendorffii *
76. Sesamum indicum
77. Setaria italica
78. Solanum lycopersicum
79. Solanum pennellii
80. Solanum tuberosum
81. Sorghum bicolor
82. Spinacia oleracea
83. Tarenaya hassleriana
84. Theobroma cacao
85. Vigna angularis
86. Vigna radiata
87. Vigna unguiculata
88. Vitis vinifera
89. Zea mays
90. Ziziphus jujuba

** Bryophyte (non-flowering).*
*** Predicted to synthesize naringenin only.*

Figure 16

Key enzymes that are produced by M. charantia in the context of eriodictyol and naringenin synthesis.



Flavonols

There are 84 predicted angiosperm species for kaempferol (Table 15), 47 for myricetin (Table 16), and 83 for quercetin (Table 17). All of the species predicted to synthesize myricetin were also predicted to synthesize kaempferol and quercetin. There were 37 species predicted to synthesize kaempferol and quercetin (but not myricetin) because each plant was missing genes that code for flavonoid 3', 5'-hydroxylase (EC:1.14.14.81) which is needed to synthesize myricetin. The set of species predicted to synthesize kaempferol and quercetin were almost identical, with the exception of *M. charantia* which was predicted to synthesize kaempferol but not quercetin. This is because *M. charantia* was missing the genes that code for flavonoid 3',5'-hydroxylase or flavonoid 3'-monooxygenase (EC:1.14.14.82), which are needed to synthesize quercetin from kaempferol or dihydrokaempferol. Additionally, *M. charantia* does have genes that

code for naringenin 3-dioxygenase (EC:1.14.11.9) and flavonol synthase (EC:1.14.20.6), which are needed to go from eriodictyol to dihydroquercetin to quercetin, but would not work as *M. charantia* was not predicted to synthesize eriodictyol.

Table 15

Plants predicted to synthesize kaempferol .

1. Aegilops tauschii	*29. Eucalyptus grandis*	*57. Papaver somniferum*
2. Amborella trichopoda	*30. Eutrema salsugineum*	*58. Phalaenopsis equestris*
3. Arabidopsis lyrata	*31. Fragaria vesca*	*59. Phaseolus vulgaris*
4. Arabidopsis thaliana	*32. Glycine max*	*60. Phoenix dactylifera*
5. Arachis duranensis	*33. Glycine soja*	*61. Populus euphratica*
6. Arachis ipaensis	*34. Gossypium arboreum*	*62. Populus trichocarpa*
7. Asparagus officinalis	*35. Gossypium hirsutum*	*63. Prunus avium*
8. Beta vulgaris	*36. Gossypium raimondii*	*64. Prunus mume*
9. Brachypodium distachyon	*37. Helianthus annuus*	*65. Prunus persica*
10. Brassica napus	*38. Hevea brasiliensis*	*66. Pyrus x*
11. Brassica oleracea	*39. Ipomoea nil*	*67. Quercus suber*
12. Brassica rapa	*40. Jatropha curcas*	*68. Raphanus sativus*
13. Camelina sativa	*41. Juglans regia*	*69. Ricinus communis*
14. Capsicum annuum	*42. Lactuca sativa*	*70. Rosa chinensis*
15. Carica papaya	*43. Lotus japonicus*	*71. Sesamum indicum*
16. Chenopodium quinoa	*44. Lupinus angustifolius*	*72. Setaria italica*
17. Cicer arietinum	*45. Malus domestica*	*73. Solanum lycopersicum*
18. Citrus clementina	*46. Manihot esculenta*	*74. Solanum pennellii*
19. Citrus sinensis	*47. Medicago truncatula*	*75. Solanum tuberosum*
20. Cucumis melo	*48. Momordica charantia*	*76. Spinacia oleracea*
21. Cucumis sativus	*49. Musa acuminata*	*77. Tarenaya hassleriana*
22. Cucurbita maxima	*50. Nelumbo nucifera*	*78. Theobroma cacao*
23. Cucurbita moschata	*51. Nicotiana attenuata*	*79. Vigna angularis*
24. Cucurbita pepo	*52. Nicotiana sylvestris*	*80. Vigna radiata*
25. Cynara cardunculus	*53. Nicotiana tabacum*	*81. Vigna unguiculata*
26. Daucus carota	*54. Nicotiana tomentosiformis*	*82. Vitis vinifera*
27. Durio zibethinus	*55. Olea europaea*	*83. Zea mays*
28. Elaeis guineensis	*56. Oryza sativa*	*84. Ziziphus jujuba*

Table 16

Plants predicted to synthesize myricetin.

1. Aegilops tauschii	*17. Jatropha curcas*	*33. Phoenix dactylifera*
2. Brachypodium distachyon	*18. Juglans regia*	*34. Populus euphratica*
3. Capsicum annuum	*19. Lotus japonicus*	*35. Populus trichocarpa*
4. Carica papaya	*20. Lupinus angustifolius*	*36. Quercus suber*
5. Cicer arietinum	*21. Manihot esculenta*	*37. Setaria italica*
6. Citrus clementina	*22. Medicago truncatula*	*38. Solanum lycopersicum*
7. Citrus sinensis	*23. Musa acuminata*	*39. Solanum pennellii*

8. Durio zibethinus
9. Elaeis guineensis
10. Eucalyptus grandis
11. Glycine max
12. Glycine soja
13. Gossypium arboreum
14. Gossypium hirsutum
15. Gossypium raimondii
16. Hevea brasiliensis
24. Nelumbo nucifera
25. Nicotiana attenuata
26. Nicotiana sylvestris
27. Nicotiana tabacum
28. Nicotiana tomentosiformis
29. Oryza sativa
30. Oryza brachyantha
31. Phalaenopsis equestris
32. Phaseolus vulgaris
40. Solanum tuberosum
41. Theobroma cacao
42. Vigna angularis
43. Vigna radiata
44. Vigna unguiculata
45. Vitis vinifera
46. Zea mays
47. Ziziphus jujuba

Table 17

Plants predicted to synthesize quercetin.

1. Aegilops tauschii
2. Amborella trichopoda
3. Arabidopsis lyrata
4. Arabidopsis thaliana
5. Arachis duranensis
6. Arachis ipaensis
7. Asparagus officinalis
8. Beta vulgaris
9. Brachypodium distachyon
10. Brassica napus
11. Brassica oleracea
12. Brassica rapa
13. Camelina sativa
14. Capsicum annuum
15. Carica papaya
16. Chenopodium quinoa
17. Cicer arietinum
18. Citrus clementina
19. Citrus sinensis
20. Cucumis melo
21. Cucumis sativus
22. Cucurbita maxima
23. Cucurbita moschata
24. Cucurbita pepo
25. Cynara cardunculus
26. Daucus carota
27. Durio zibethinus
28. Elaeis guineensis
29. Eucalyptus grandis
30. Eutrema salsugineum
31. Fragaria vesca
32. Glycine max
33. Glycine soja
34. Gossypium arboreum
35. Gossypium hirsutum
36. Gossypium raimondii
37. Helianthus annuus
38. Hevea brasiliensis
39. Ipomoea nil
40. Jatropha curcas
41. Juglans regia
42. Lactuca sativa
43. Lotus japonicus
44. Lupinus angustifolius
45. Malus domestica
46. Manihot esculenta
47. Medicago truncatula
48. Musa acuminata
49. Nelumbo nucifera
50. Nicotiana attenuata
51. Nicotiana sylvestris
52. Nicotiana tabacum
53. Nicotiana tomentosiformis
54. Olea europaea
55. Oryza sativa
56. Papaver somniferum
57. Phalaenopsis equestris
58. Phaseolus vulgaris
59. Phoenix dactylifera
60. Populus euphratica
61. Populus trichocarpa
62. Prunus avium
63. Prunus mume
64. Prunus persica
65. Pyrus x
66. Quercus suber
67. Raphanus sativus
68. Ricinus communis
69. Rosa chinensis
70. Sesamum indicum
71. Setaria italica
72. Solanum lycopersicum
73. Solanum pennellii
74. Solanum tuberosum
75. Spinacia oleracea
76. Tarenaya hassleriana
77. Theobroma cacao
78. Vigna angularis
79. Vigna radiata
80. Vigna unguiculata
81. Vitis vinifera
82. Zea mays
83. Ziziphus jujuba

Flavones

There are 37 species that were predicted to synthesize both apigenin and luteolin

(Table 18), with the entirety of the list of associated compounds consisting of angiosperms.

Table 18

Plants predicted to synthesize the flavones from the data set.

1. Aegilops tauschii	*14. Glycine soja*	*26. Oryza sativa*
2. Arachis duranensis	*15. Gossypium arboreum*	*27. Phaseolus vulgaris*
3. Arachis ipaensis	*16. Gossypium hirsutum*	*28. Populus euphratica*
4. Brachypodium distachyon	*17. Gossypium raimondii*	*29. Populus trichocarpa*
5. Cajanus cajan	*18. Helianthus annuus*	*30. Ricinus communis*
6. Cicer arietinum	*19. Hevea brasiliensis*	*31. Sesamum indicum*
7. Citrus clementina	*20. Lactuca sativa*	*32. Setaria italica*
8. Citrus sinensis	*21. Lupinus angustifolius*	*33. Sorghum bicolor*
9. Cynara cardunculus	*22. Manihot esculenta*	*34. Theobroma cacao*
10. Daucus carota	*23. Medicago truncatula*	*35. Vigna angularis*
11. Durio zibethinus	*24. Olea europaea*	*36. Vigna unguiculata*
12. Eucalyptus grandis	*25. Oryza brachyantha*	*37. Zea mays*
13. Glycine max		

Literature and Database search

The literature and database search was conducted in order to find documentation that would provide exact matches for organism-compound pairs from the data set in order to be used later for comparisons against the predictions. A summary of these results can be found in Table 19.

Table 19

Number of species known to synthesize each flavonoid.

Compound	Unique Exact Matches
Genistein	17
Cyanidin	27
Butein	1
Isoliquiritigenin	5
Catechin	48
Epicatechin	38
Epigallocatechin	10
Gallocatechin	10
Eriodictyol	11
Naringenin	44
Kaempferol	49

Myricetin	19
Quercetin	59
Apigenin	30
Luteolin	36

Isoflavonoid

There are 17 different species that are experimentally known to synthesize Genistein (Table 20).

Table 20

Plants known to produce Genistein.

1. Amborella trichopoda [3]	*7. Glycine max* [D, K, N, P, T]	*13. Spinacia oleracea* [2]
2. Arabidopsis thaliana [K]	*8. Gossypium hirsutum* [1]	*14. Vigna angularis* [D, K]
3. Beta vulgaris [N]	*9. Lupinus angustifolius* [N]	*15. Vigna radiata* [D, K, N, T]
4. Brassica oleracea [K]	*10. Medicago truncatula* [K]	*16. Vigna unguiculata* [D, T]
5. Cajanus cajan [D, K, N]	*11. Phaseolus vulgaris* [K, D, A]	*17. Zea mays* [K]
6. Cicer arietinum [D, K, N]	*12. Prunus avium* [T]	

Sources:(D) Dr. Duke; (K) KNApSAcK; (N) NAPRALERT; (P) NPASS; (T) IMPPAT; (1) (1) Nix et al., 2017; (2) Singh, 2016; (3) Wu et al., 2019.

Anthocyanidin

There are 27 different species experimentally known to synthesize cyanidin (Table 21).

Table 21

Plants known to produce cyanidin.

1. Arabidopsis thaliana [K]	*10. Juglans regia* [U]	*19. Prunus avium* [U, K, M]
2. Brassica oleracea [K, T]	*11. Lactuca sativa* [T]	*20. Prunus persica* [U]
3. Capsicum annuum [K]	*12. Lotus japonicus* [P]	*21. Raphanus sativus* [K]
4. Carica papaya [T]	*13. Malus domestica* [U, M, D]	*22. Solanum tuberosum* [K]
5. Daucus carota [K]	*14. Medicago truncatula* [K]	*23. Theobroma cacao* [D]
6. Fragaria vesca [P]	*15. Olea europaea* [N]	*24. Vigna angularis* [K]
7. Glycine max [P]	*16. Papaver somniferum* [N]	*25. Vigna unguiculata* [T]
8. Gossypium hirsutum [1]	*17. Phaseolus vulgaris* [U]	*26. Vitis vinifera* [K, M, T, D, N]
9. Ipomoea nil [N]	*18. Phoenix dactylifera* [U, M]	*27. Zea mays* [K, T, D, A]

Sources: (D) Dr. Duke; (K) KNApSAcK; (M) Microbiome; (N) NAPRALERT; (P) NPASS; (T) IMPPAT; (U) USDA; (1) Nix et al., 2017.

Chalcones

There is only one species (*Glycine soja*) known to synthesize butein and this information was collected from NPASS. There are five species known to synthesize isoliquiritigenin (Table 22).

Table 22

Plants known to produce isoliquiritigenin.

1. *Arabidopsis thaliana* [K]
2. *Cicer arietinum* [K, P]
3. *Glycine max* [D, K, P]
4. *Helianthus annuus* [D]
5. *Medicago truncatula* [K]

Sources: (D) Dr. Duke; (K) KNApSAcK; (P) NPASS.

Flavan-3-ols

There are 48 species known to synthesize catechin (Table 23), 38 species known to synthesize Epcatechin (Table 24), 10 species known to synthesize epigallocatechin (Table 25), and 10 species known to synthesize gallocatechin (Table 26).

Table 23

Plants known to produce catechin.

1. *Aegilops tauschii* [3]
2. *Amborella trichopoda* [23]
3. *Arabidopsis thaliana* [K]
4. *Asparagus officinalis* [K]
5. *Beta vulgaris* [6]
6. *Brassica rapa* [12]
7. *Camelina sativa* [20]
8. *Capsicum annuum* [7]
9. *Carica papaya* [4]
10. *Chenopodium quinoa* [8]
11. *Cicer arietinum* [16]
12. *Citrus sinensis* [15]
13. *Cucumis melo* [21]
14. *Cucumis sativus* [24]
15. *Cucurbita pepo* [14]
17. *Elaeis guineensis* [11]
18. *Eucalyptus grandis* [17]
19. *Fragaria vesca* [N]
20. *Glycine max* [D]
21. *Gossypium hirsutum* [N]
22. *Jatropha curcas* [10]
23. *Juglans regia* [N]
24. *Malus domestica* [D, U]
25. *Manihot esculenta* [2]
26. *Medicago truncatula* [K]
27. *Momordica charantia* [K]
28. *Musa acuminata* [K]
29. *Nelumbo nucifera* [N, P]
30. *Nicotiana tabacum* [18]
31. *Olea europaea* [D]
33. *Phaseolus vulgaris* [N, U]
34. *Phoenix dactylifera* [N]
35. *Populus trichocarpa* [22]
36. *Prunus avium* [K, M, N, U]
37. *Prunus mume* [M, P]
38. *Prunus persica* [K, M, U]
39. *Pyrus x* [26]
40. *Sesamum indicum* [25]
41. *Solanum tuberosum* [1]
42. *Sorghum bicolor* [N]
43. *Spinacia oleracea* [19]
44. *Theobroma cacao* [K, N, U]
45. *Vigna angularis* [K, P]
46. *Vigna radiata* [5]
47. *Vitis vinifera* [D, K, M, N, P, U]

16. Durio zibethinus [9]
32. Oryza sativa [12]
48. Ziziphus jujuba [K, M, N, P, U]

Sources: (D) Dr. Duke; (K) KNApSAcK; (M) Microbiome; (N) NAPRALERT; (P) NPASS; (U) USDA; (1) Akyol et al., 2016; (2) Buschmann et al., 2000; (3) Dong-Dong et al., 2015; (4) Duru & Duru, 2019; (5) Gan et al., 2016; (6) Georgiev et al., 2010; (7) Ghasemnezhad et al., 2010; (8) Hemalatha et al., 2016; (9) Ho & Bhat, 2015; (10) Igbinosa et al., 2011; (11) Jaffri et al., 2011; (12) Kim et al., 2015; (13) Kim et al., 2017; (14) Kostecka-Gugała et al., 2020; (15) Liew et al., 2018; (16) Quintero-Soto et al., 2018; (17) Santos et al., 2013; (18) Shimoda et al., 2007; (19) Singh, 2016; (20) Terpinc et al., 2012; (21) Tsanova-Savova et al., 2015; (22) Wang et al., 2013; (23) Wu et al., 2019; (24) Xu et al., 2019; (25) Zeb et al., 2017; (26) Zhai et al., 2014.

Table 24

Plants known to produce epicatechin.

1. Amborella trichopoda [14]
2. Arabidopsis thaliana [K]
3. Beta vulgaris [6]
4. Brassica napus [2]
5. Capsicum annuum [4]
6. Carica papaya [11]
7. Cucumis melo [M, U]
8. Durio zibethinus [7]
9. Elaeis guineensis [1]
10. Eucalyptus grandis [12]
11. Fragaria vesca [N]
12. Glycine max [N, T]
13. Gossypium hirsutum [10]
14. Juglans regia [15]
15. Malus domestica [D, M, U]
16. Medicago truncatula [K]
17. Momordica charantia [K]
18. Musa acuminata [K]
19. Nelumbo nucifera [T]
20. Nicotiana sylvestris [P]
21. Nicotiana tabacum [3]
22. Phaseolus vulgaris [U]
23. Phoenix dactylifera [N]
24. Populus trichocarpa [13]
25. Prunus avium [K, M, U]
26. Prunus mume [P]
27. Prunus persica [U]
28. Pyrus x [17]
29. Ricinus communis [N]
30. Sesamum indicum [16]
31. Solanum tuberosum [K, T]
32. Sorghum bicolor [8]
33. Spinacia oleracea [9]
34. Theobroma cacao [D, K, M, N, P, T, U]
35. Vigna angularis [P]
36. Vigna radiata [5]
37. Vitis vinifera [D, K, M, N, P, T, U]
38. Ziziphus jujuba [N, P, U]

Sources: (D) Dr. Duke; (K) KNApSAcK; (M) Microbiome; (N) NAPRALERT; (P) NPASS; (T) IMPPAT; (U) USDA; (1) Ahmad et al., 2018; (2) Auger et al., 2010; (3) Chen et al., 2013; (4) di Sotto et al., 2018; (5) Ganesan & Xu, 2018 ; (6) Georgiev et al., 2010; (7) Liu et al., 2013; (8) Luo et al., 2018; (9) Singh, 2016; (10) Nix et al., 2017; (11) Oboh et al., 2013; (12) Santos et al., 2012; (13) Wang et al., 2013; (14) Wu et al., 2019; (15) Yan et al., 2019; (16) Zeb et al., 2017; (17) Zhai et al., 2014.

Table 25

Plants known to produce epigallocatechin.

1. Citrus sinensis [2]
2. Cucumis melo [M, U]
3. Gossypium hirsutum [N]
4. Malus domestica [U]
5. Phaseolus vulgaris [1]
6. Prunus avium [M, U]
7. Prunus persica [M, U]
8. Theobroma cacao [D, N]
9. Vitis vinifera [D, N]
10. Ziziphus jujuba [N]

Sources: (D) Dr. Duke; (M) Microbiome; (N) NAPRALERT; (U) USDA; (1) Ganesan & Xu, 2017; (2) Liew et al., 2018.

Table 26

Plants known to produce gallocatechin.

1. Gossypium hirsutum [2]	5. Phaseolus vulgaris [1]	8. Vigna radiata [K]
2. Juglans regia [T]	6. Theobroma cacao [N]	9. Vitis vinifera [D, K, N, P, T]
3. Medicago truncatula [K]	7. Vigna angularis [K]	10. Ziziphus jujuba [N]
4. Nelumbo nucifera [N, T]		

Sources: (D) Dr. Duke; (K) KNApSAcK; (N) NAPRALERT; (P) NPASS; (T) IMPPAT; (1) Ganesan & Xu, 2017; (2) Nix et al., 2017.

Flavanones

There are 11 species known to synthesize eriodictyol (Table 27) and 44 species known to synthesize naringenin (Table 28).

Table 27

Plants known to produce eriodictyol.

1. Amborella trichopoda [6]	5. Malus domestica [7]	9. Theobroma cacao [1]
2. Eucalyptus grandis [3]	6. Prunus avium [4]	10. Vigna radiata [5]
3. Glycine soja [P]	7. Prunus persica [N]	11. Ziziphus jujuba [N]
4. Gossypium hirsutum [2]	8. Sorghum bicolor [N]	

Sources: (N) NAPRALERT; (P) NPASS; (1) Gallego et al., 2019; (2) Nix et al., 2017; (3) Santos et al., 2013; (4) Sanz et al., 2010; (5) Tang et al., 2014 (6) Wu et al., 2019; (7) Yıldırım et al., 2015.

Table 28

Plants known to produce naringenin.

1. Amborella trichopoda [18]	16. Daucus carota [K]	31. Prunus avium [D, K, N]
2. Arabidopsis thaliana [K]	17. Dendrobium catenatum [P]	32. Prunus mume [K, N, P]
3. Asparagus officinalis [K]	18. Eucalyptus grandis [12]	33. Prunus persica [K, N, T]
4. Brachypodium distachyon [7]	19. Fragaria vesca [3]	34. Raphanus sativus [K]
5. Brassica napus [10]	20. Glycine max [D, K, N, T]	35. Selaginella moellendorffii [20]
6. Brassica oleracea [K, T]	21. Gossypium hirsutum [8]	36. Solanum lycopersicum [D]
7. Brassica rapa [16]	22. Juglans regia [19]	37. Solanum tuberosum [17]
8. Cajanus cajan [8]	23. Medicago truncatula [K]	38. Sorghum bicolor [N]
9. Capsicum annuum [K]	24. Momordica charantia [K]	39. Spinacia oleracea [13]
10. Carica papaya [K]	25. Musa acuminata [K]	40. Theobroma cacao [K]
11. Chenopodium quinoa [4]	26. Nelumbo nucifera [15]	41. Vigna angularis [N]
12. Cicer arietinum [N]	27. Olea europaea [14]	42. Vigna radiata [D]

13. *Citrus sinensis* [D, N, P, U]
14. *Cucumis melo* [6]
15. *Cynara cardunculus* [D, U]
28. *Oryza sativa* [5]
29. *Phaseolus vulgaris* [2]
30. *Phoenix dactylifera* [1]
43. *Vitis vinifera* [11]
44. *Zea mays* [K, T]

Sources: (D) Dr. Duke; (K) KNApSAcK; (N) NAPRALERT; (P) NPASS; (T) IMPPAT; (U) USDA; (1) El-Kholy et al., 2019; (2) Ganesan & Xu, 2017; (3) Gasperotti et al., 2015; (4) Hemalatha et al., 2016; (5) Kim et al., 2017; (6) Mallek-Ayadi et al., 2017; (7) Napoleão et al., 2017; (8) Nix et al., 2015; (9) Nix et al., 2017; (10) Pei et al., 2012; (11) Perestrelo et al., 2012; (12) Santos et al., 2017; (13) Singh, 2016; (14) Tamasi et al., 2019; (15) Tang et al., 2017; (16) Thiruvengadam & Chung, 2015; (17) Valiñas et al., 2017; (18) Wu et al., 2019; (19) Yan et al., 2019; (20) Yobi et al., 2012.

Flavonols

There are 49 different species known to synthesize kaempferol (Table 29), 19 species known to synthesize myricetin (Table 30), and there are 59 species known to synthesize quercetin (Table 31).

Table 29

Plants known to produce kaempferol .

1. *Arabidopsis thaliana* [K, N, T]
2. *Asparagus officinalis* [D, K, M, T, U]
3. *Beta vulgaris* [N, P]
4. *Brassica napus* [N]
5. *Brassica oleracea* [D, K, M, N, T, U]
6. *Brassica rapa* [U]
7. *Capsicum annuum* [K, M, U]
8. *Carica papaya* [K, M, U]
9. *Chenopodium quinoa* [N]
10. *Cicer arietinum* [N, T]
11. *Citrus sinensis* [M, N, U]
12. *Cucumis melo* [M, U]
13. *Cucumis sativus* [M, N, T, U]
14. *Cucurbita maxima* [N]
15. *Cucurbita pepo* [D]
16. *Daucus carota* [D, M, N, T, U]
17. *Elaeis guineensis* [4]
18. *Fragaria vesca* [1]
19. *Glycine max* [D, K, M, N, T, U]
20. *Gossypium hirsutum* [3]
21. *Hevea brasiliensis* [N]
22. *Juglans regia* [D]
23. *Lactuca sativa* [D, N]
24. *Lotus japonicus* [P]
25. *Lupinus angustifolius* [N]
26. *Malus domestica* [D, M, U]
27. *Medicago truncatula* [K, N]
28. *Momordica charantia* [K]
29. *Musa acuminata* [K, N]
30. *Nelumbo nucifera* [D, M, N, P, T, U]
31. *Nicotiana tabacum* [D, N]
32. *Olea europaea* [N]
33. *Oryza sativa* [2]
34. *Papaver somniferum* [N, T]
35. *Phaseolus vulgaris* [N, U]
36. *Prunus avium* [D, M, N, U]
37. *Prunus persica* [K, M, N, T, U]
38. *Raphanus sativus* [K, M, N, U]
39. *Ricinus communis* [D]
40. *Rosa chinensis* [N, P]
41. *Solanum lycopersicum* [D, K]
42. *Solanum tuberosum* [D, M, N, U]
43. *Spinacia oleracea* [D, M, N, U]
44. *Theobroma cacao* [D, N]
45. *Vigna radiata* [D, M, N, U]
46. *Vigna unguiculata* [T]
47. *Vitis vinifera* [D, M, N, U]
48. *Zea mays* [K, T]
49. *Ziziphus jujuba* [N]

Sources: (D) Dr. Duke; (K) KNApSAcK; (M) Microbiome; (N) NAPRALERT; (P) NPASS; (T) IMPPAT; (U) USDA; (1) Gasperotti et al., 2015; (2) Kim et al., 2017; (3) Nix et al., 2017; (4) Zhou et al., 2019.

Table 30

Plants known to produce myricetin.

1. *Asparagus officinalis* [K]
2. *Brassica rapa* [U]
3. *Capsicum annuum* [D, N, U]
4. *Carica papaya* [M, U]
5. *Citrus sinensis* [D, M, N, U]
6. *Daucus carota* [D, M, N, U]
7. *Gossypium hirsutum* [2]
8. *Juglans regia* [4]
9. *Lotus japonicus* [P]
10. *Malus domestica* [3]
11. *Medicago truncatula* [K, N]
12. *Nelumbo nucifera* [M, P, T, U]
13. *Phaseolus vulgaris* [U]
14. *Prunus avium* [M, U]
15. *Solanum tuberosum* [D, N]
16. *Spinacia oleracea* [M, U]
17. *Vigna radiata* [1]
18. *Vigna unguiculata* [T]
19. *Vitis vinifera* [D, M, N, P, U]

Sources: (D) Dr. Duke; (K) KNApSAcK; (M) Microbiome; (N) NAPRALERT; (P) NPASS; (T) IMPPAT; (U) USDA; (1) Ganesan & Xu, 2018; (2) Nix et al., 2017; (3) Petkovska et al., 2017; (4) Yan et al., 2019.

Table 31

Plants known to produce quercetin.

1. *Amborella trichopoda* [7]
2. *Arabidopsis thaliana* [K, T]
3. *Asparagus officinalis* [D, K, M, T, U]
4. *Beta vulgaris* [D, M, N, P, U]
5. *Brassica napus* [N]
6. *Brassica oleracea* [D, K, M, N, U]
7. *Brassica rapa* [U]
8. *Cajanus cajan* [4]
9. *Camelina sativa* [6]
10. *Capsicum annuum* [D, K, M, P, U]
11. *Carica papaya* [K, N]
12. *Chenopodium quinoa* [N]
13. *Cicer arietinum* [N, T]
14. *Citrus sinensis* [D, M, N, P, U]
15. *Cucumis melo* [M, U]
16. *Cucumis sativus* [M, N, U]
17. *Cucurbita maxima* [N]
18. *Cucurbita pepo* [D]
19. *Cynara cardunculus* [D]
20. *Daucus carota* [D, M, N, T, U]
21. *Fragaria vesca* [2]
22. *Glycine max* [D, M, N, U]
23. *Gossypium arboreum* [N]
24. *Gossypium hirsutum* [5]
25. *Helianthus annuus* [D, N]
26. *Hevea brasiliensis* [N]
27. *Jatropha curcas* [3]
28. *Juglans regia* [D, N]
29. *Lactuca sativa* [D, N, T]
30. *Lotus japonicus* [P]
31. *Lupinus angustifolius* [N]
32. *Malus domestica* [D, M, U]
33. *Manihot esculenta* [N]
34. *Medicago truncatula* [K, N]
35. *Momordica charantia* [K]
36. *Musa acuminata* [K, M, N]
37. *Nelumbo nucifera* [D, M, P, U]
38. *Nicotiana tabacum* [D, N]
39. *Olea europaea* [D, N]
40. *Papaver somniferum* [N, T]
41. *Phaseolus vulgaris* [N, T, U]
42. *Phoenix dactylifera* [D, N, U]
43. *Prunus avium* [D, K, M, N, U]
44. *Prunus mume* [P]
45. *Prunus persica* [M, N, U]
46. *Quercus suber* [N, P]
47. *Raphanus sativus* [K, N]
48. *Ricinus communis* [D, N]
49. *Rosa chinensis* [N, P]
50. *Solanum lycopersicum* [1]
51. *Solanum tuberosum* [D, M, N, U]
52. *Spinacia oleracea* [D, M, N, U]
53. *Theobroma cacao* [D, N, U]
54. *Vigna angularis* [P]
55. *Vigna radiata* [D, M, N, U]
56. *Vigna unguiculata* [M, N, U]
57. *Vitis vinifera* [D, M, N, P, U]
58. *Zea mays* [D, K]
59. *Ziziphus jujuba* [M, P, U]

Sources: (D) Dr. Duke; (K) KNApSAcK; (M) Microbiome; (N) NAPRALERT; (P) NPASS; (T) IMPPAT; (U) USDA; (1) Bhandari & Lee, 2016; (2) Gasperotti et al., 2015; (3) Igbinosa et al., 2011; (4) Nix et al., 2015; (5) Nix et al., 2017; (6) Terpinc et al., 2012; (7) Wu et al., 2019.

Flavones

There are 30 species known to synthesize apigenin (Table 32), and 36 species known to synthesize luteolin (Table 33).

Table 32

Plants known to produce apigenin.

1. Asparagus officinalis [K]	*11. Cucurbita pepo* [1]	*21. Olea europaea* [D, N, T]
2. Beta vulgaris [4]	*12. Cynara cardunculus* [D, U]	*22. Phaseolus vulgaris* [D]
3. Brassica oleracea [K, M]	*13. Daucus carota* [D, K, N, T]	*23. Phoenix dactylifera* [D, N]
4. Brassica rapa [U]	*14. Fragaria vesca* [P]	*24. Populus trichocarpa* [N]
5. Cajanus cajan [N]	*15. Glycine max* [N, P]	*25. Prunus avium* [K]
6. Capsicum annuum [T]	*16. Jatropha curcas* [D, N]	*26. Raphanus sativus* [K]
7. Carica papaya [M, U]	*17. Juglans regia* [D, M]	*27. Ricinus communis* [T]
8. Chenopodium quinoa [2]	*18. Lactuca sativa* [N]	*28. Sorghum bicolor* [N]
9. Citrus sinensis [3]	*19. Lupinus angustifolius* [N]	*29. Theobroma cacao* [K]
10. Cucurbita moschata [P]	*20. Medicago truncatula* [K]	*30. Zea mays* [D, K, N]

Sources: (D) Dr. Duke; (K) KNApSAcK; (M) Microbiome; (N) NAPRALERT; (P) NPASS; (T) IMPPAT; (U) USDA; (1) Akomolafe et al., 2016; (2) Hemalatha et al., 2016; (3) Liew et al., 2018; (4) Silva et al., 2020.

Table 33

Plants known to produce luteolin.

1. Amborella trichopoda [7]	*13. Cucurbita moschata* [U]	*25. Olea europaea* [D, M,, N, U]
2. Asparagus officinalis [K]	*14. Cucurbita pepo* [1]	*26. Phaseolus vulgaris* [D, U]
3. Beta vulgaris [M, U]	*15. Cynara cardunculus* [D, U]	*27. Phoenix dactylifera* [4]
4. Brassica napus [5]	*16. Daucus carota* [D, K, M, N, T, U]	*28. Raphanus sativus* [K]
5. Brassica oleracea [K, M, T, U]	*17. Fragaria vesca* [P]	*29. Setaria italica* [N]
6. Brassica rapa [U]	*18. Helianthus annuus* [D, N]	*30. Solanum lycopersicum* [2]
7. Cajanus cajan [N]	*19. Lactuca sativa* [D, N]	*31. Solanum tuberosum* [N]
8. Capsicum annuum [D, K, M, N, P, T, U]	*20. Lupinus angustifolius* [N]	*32. Sorghum bicolor* [6]
9. Carica papaya [M, U]	*21. Malus domestica* [D, M, U]	*33. Spinacia oleracea* [M, U]
10. Chenopodium quinoa [4]	*22. Medicago truncatula* [K]	*34. Theobroma cacao* [D, K]
11. Citrus sinensis [M, N, U]	*23. Momordica charantia* [T]	*35. Vitis vinifera* [D, M, N]
12. Cucumis melo [M, U]	*24. Nelumbo nucifera* [D, M, P, T, U]	*36. Zea mays* [K, N]

Sources: (D) Dr. Duke; (K) KNApSAcK; (M) Microbiome; (N) NAPRALERT; (P) NPASS; (T) IMPPAT; (U) USDA; (1) Akomolafe et al., 2016; (2) Bhandari & Lee, 2016; (3) Hemalatha et al., 2016; (4) Khallouki et al., 2018; (5) Pei et al., 2012; (6) Svensson et al., 2010; (7) Wu et al., 2019.

Database Comparisons

NAPRALERT contained the greatest number of exact plant-compound matches, and only the USDA, IMPPAT, and Microbiome were missing data for flavonoids from the data set, as shown in Table 34. After looking at the species which were present in each database, it was then possible to create Figures 17 and 18 by editing figures generated by UpSet (Lex et al., 2014). As can be seen in Figure 17, KNApSAck, NPASS, and NAPRALERT, in this order, had the most species from the dataset. Additionally, there are 10 that have no records in any of the databases, and 22 species that had records in all of the databases. This information can be seen in Figure 18, which shows the number of overlaps in species data amongst the databases. The darkened dots indicates species' presence in a database: the first row indicates that there are 22 species in all of the databases, the second row shows there are 10 missing from all databases, and the third row indicates there are 10 species with associated records in KNApSAcK, NPASS and NAPRALERT only.

Table 34

Notable information about the databases.

Database	Accessed	Exact Matches	Missing Plants	Missing Compounds
NPASS	April 2021	45	25	N/A
KNApSAcK	June 2021	107	24	N/A
NAPRALERT	May 2021	147	27	N/A
Dr. Duke	June 2021	98	46	N/A
IMPPAT	June 2021	52	60	Epigallocatechin Isoliquiritigenin
USDA	June 2021	98	70	Butein Genistein

				Isoliquiritigenin
Microbiome	June 2021	76	77	Isoliquiritigenin

Figure 17

Number of plants from the dataset that are present in each database.

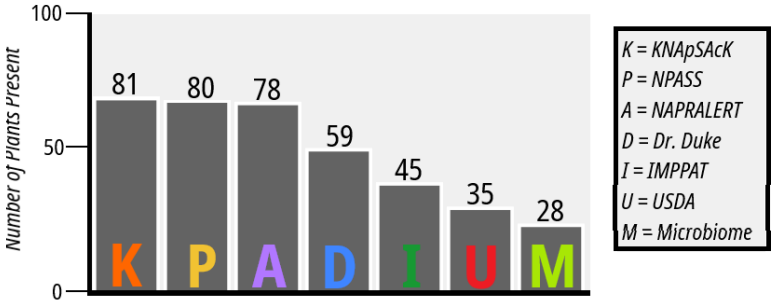
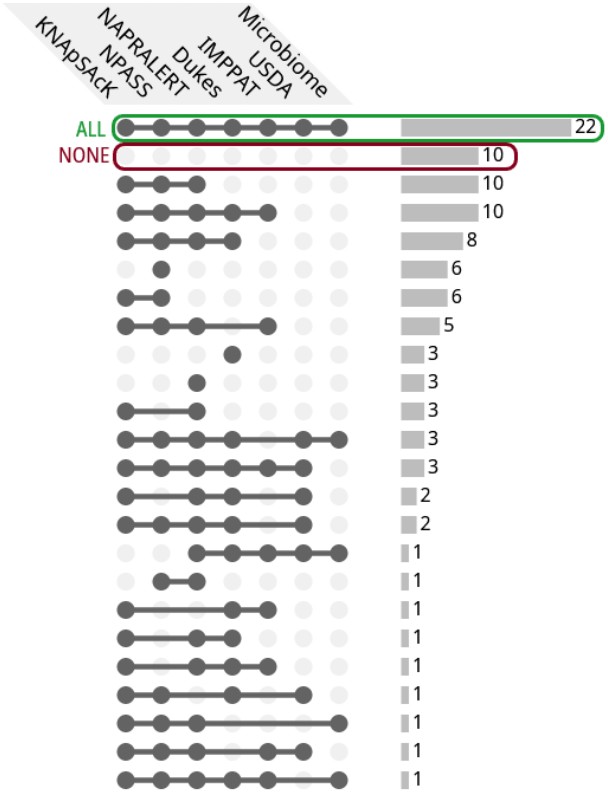


Figure 18

Grouping of the databases by overlapping the presence of each specific species.



Discussion

Databases

As mentioned earlier, KNApSAck, NPASS, and NAPRALERT were the databases with the fewest missing species, with NAPRALERT and KNApSAcK having the most and second most exact pairs, respectively. This follows accordingly with important claims from each of these databases, as they seemingly aim to be more generalized and extensive. NAPRALERT reports that data is pulled from research and reports that cover a range of topics which include: medically relevant activities, activities that affect plant growth, ethnomedical plants, and natural insecticides (Loub, et al., 1985). KNApSAcK states that data is pulled from numerous sources, especially those with data relating to biological pathways, and on their search engine (NAIST Comparative Genomics Laboratory, 2021), it is stated to have 57,906 metabolite entries and 137,333 metabolite-species pairs as of their most recent update in August 2021. NPASS states that their 25,041 source organisms include plants, microbes and marine species from differing Kingdoms, and that there are records for 35,032 different natural products (Zeng et al., 2018).

The list of species found in all of the databases referenced in this project (Table 35) are influenced by the nature of Dr. Duke's database, the USDA database, IMPPAT and Microbiome, which are mostly concerned with data relating to culinary and/or traditional medicinal applications. The species consist almost entirely of primarily culinary plants, except for Nelumbo nucifera, which has a long history of both culinary and traditional medicinal applications (Board of Trustees of the Royal Botanic Gardens,

Kew).

Table 35

List of species present in all the databases, as of the first half of 2021.

1. Asparagus officinalis	*7. Citrus sinensis*	*13. Nelumbo nucifera*	*19. Spinacia oleracea*
2. Beta vulgaris	*8. Cucumis melo*	*14. Phaseolus vulgaris*	*20. Vigna radiata*
3. Brassica oleracea	*9. Cucumis sativus*	*15. Prunus avium*	*21. Vigna unguiculata*
4. Capsicum annuum	*10. Daucus carota*	*16. Prunus persica*	*22. Vitis vinifera*
5. Carica papaya	*11. Glycine max*	*17. Raphanus sativus*	
6. Cicer arietinum	*12. Juglans regia*	*18. Solanum tuberosum*	

The list of species missing from each database (Table 36) makes sense in the context of the information provided by the databases, diverse and specialized alike. While some provide more diverse data than others, there is only so much available information that is available for acquisition, which could provide an explanation as to why half of these species (*M. commoda, M. neglectum, O. lucimarinus, O. tauri, and V. carteri f. nagariensis*) are green algae. The remaining species do not appear to have any culinary or medicinal applications, which also offers a better understanding of their absence. Though it should be noted that each of the non-algae species listed have been subjects of interest relating to genomes sequencing: *A. tauschii* and the evolution of hexaploid wheat (Dvorak et al., 1998); Genome analysis of diploid the ancestors of *A. hypogea* (peanut), *A. duranensis* and *A. ipaensis* (Bertioli et al., 2016); Studies of self-compatibility and incompatibility by analyzing *C. rubella* (Slotte et al., 2013); Comparing genomes of *Brassicaceae* to sister family *Cleomaceae* by sequencing the genome of *T. hassleriana* (Cheng et al., 2013).

Table 36

List of species missing from all databases, as of the first half of 2021.

1. Aegilops tauschii	*5. Micromonas commoda*	*8. Ostreococcus tauri*
2. Arachis duranensis	*6. Monoraphidium neglectum*	*9. Tarenaya hassleriana*

3. Arachis ipaensis *7. Ostreococcus lucimarinus* *10. Volvox carteri*
4. Capsella rubella

Overall, the databases seemed to be most effective at providing data relating to culinary plants, while also providing information on a decent number of traditional medicinal species, with the exception of the USDA database as it was specifically concerned with the flavonoid content in food items. The focus on these types of plants is in no way surprising as medicine and the contents of the human diet are heavily intertwined with the collective interest of extending and improving human life.

While the more diverse and extensive databases provided a wider range of plant species, the information on species of algae were lacking as the data collected is somewhat telling of the focus of research from which is reported. Research regarding phytochemicals has been a long, ongoing endeavor which was seemingly more focused on land plants, especially earlier in the time span which could have been affected by something as simple as the accessibility of subjects or perhaps believing that there was nothing noteworthy about pond scum.

Comparisons of Experimental Data and Program Output

The experimentation and research relating to flavonoid biosynthesis has biases in terms of the flavonoids and plants chosen for the subject of study, which leads to an uneven distribution of experimentally known data. As a result, there are programmatically predicted organism-compound pairs that do not have any sort of representations within the data gathered during the literature and database search, which is kept in mind when comparing data. In addition to the predicted pairs without matching

experimental data, it is also important to look at the pairs which are experimentally reported but have no predicted counterparts.

At the time of writing, there are some potential reasons that could offer an explanation for the data that is experimentally known but not predicted:

1. There is some issue in the code and/or input files which has remained consistent and undetected to date and thus has negatively impacted the predictions.
2. There could be some missing context in designing the logic for the prediction functions, which could potentially have a significant impact on the outcome.
3. There could be issues that could arise from the assembled pathways from KEGG, especially if there is a popularized or standardized usage of a specific strain, such as the "Grandsen" strain of *P. patens* (Rensing et al., 2020).
4. Some sources used dried plant matter for testing, which is important to note as the drying process can impact the chemical composition of a plant (di Cesare et al., 2003).
5. Some plants, especially commonly edible plants, can have numerous cultivars, varieties, and subspecies, such as *Brassica oleracea*. There could be compositions unique to different sub-groups and as a result, if these sub-groups are not considered or reported then there could be some unanticipated errors.
6. KEGG's flavonoid biosynthesis map involves specific stereoisomers, while the sources have had mentions of both stereoisomers of the flavan-3-ols.
7. There could be some type of unknown or undocumented convergence of biosynthetic capabilities between different lineages.

8. As the disclaimer from Dr. Duke's database states, "To err is human", which sets the expectation of some degree of error in the collected data.

Isoflavonoid

Of the nine species of plants predicted to synthesize genistein, eight of them are experimentally known to do so (Table 37). *Glycine soja* is the only species predicted to synthesize genistein without an experimental confirmation. Additionally, there are nine species which are only experimentally known to synthesize genistein (Table 38), though there is only one data source for each of these exact pairs. Therefore, at this point, there could be issues with the program or the data that has been collected. Additionally, some of the disagreements between the experimentally known data and the predictions could be attributed to the mass cultivation and *Beta vulgaris*, *Brassica oleracea*, *Prunus avium*, *Spinacia oleracea*, and *Zea mays*.

Table 37

Plants predicted and experimentally known to synthesize genistein

1. Cajanus cajan	*4. Lupinus angustifolius*	*7. Vigna radiata*
2. Cicer arietinum	*5. Phaseolus vulgaris*	*8. Vigna unguiculata*
3. Glycine max	*6. Vigna angularis*	

Table 38

Plants experimentally known to synthesize genistein but were not predicted.

1. Amborella trichopoda	*4. Brassica oleracea*	*7. Prunus avium*
2. Arabidopsis thaliana	*5. Gossypium hirsutum*	*8. Spinacia oleracea*
3. Beta vulgaris	*6. Medicago truncatula*	*9. Zea mays*

Anthocyanidin

Of the 76 species predicted to synthesize cyanidin, 25 of them were experimentally known to synthesize cyanidin (Table 39), while the remaining 51 species

currently have no corresponding data (Table 40). There were only two species that were experimentally known but not predicted to synthesize cyanidin: *Fragaria vesca* and *Lactuca sativa*. Given that there is a small number of disagreements and that these disagreements could be attributed to the heavy cultivation and selective breeding of these species, the predictions for cyanidin could be useful in designing experiments for testing phytochemical contents in the selected species.

Table 39

Plants predicted and experimentally known to synthesize cyanidin.

1. Arabidopsis thaliana	*10. Lotus japonicus*	*18. Prunus persica*
2. Brassica oleracea	*11. Malus domestica*	*19. Raphanus sativus*
3. Capsicum annuum	*12. Medicago truncatula*	*20. Solanum tuberosum*
4. Carica papaya	*13. Olea europaea*	*21. Theobroma cacao*
5. Daucus carota	*14. Papaver somniferum*	*22. Vigna angularis*
6. Glycine max	*15. Phaseolus vulgaris*	*23. Vigna unguiculata*
7. Gossypium hirsutum	*16. Phoenix dactylifera*	*24. Vitis vinifera*
8. Ipomoea nil	*17. Prunus avium*	*25. Zea mays*
9. Juglans regia		

Table 40

Plants predicted to synthesize cyanidin but not yet found experimentally.

1. Aegilops tauschii	*18. Eucalyptus grandis*	*35. Oryza sativa*
2. Amborella trichopoda	*19. Eutrema salsugineum*	*36. Phalaenopsis equestris*
3. Arabidopsis lyrata	*20. Glycine soja*	*37. Populus euphratica*
4. Arachis duranensis	*21. Gossypium arboreum*	*38. Populus trichocarpa*
5. Asparagus officinalis	*22. Gossypium raimondii*	*39. Prunus mume*
6. Beta vulgaris	*23. Helianthus annuus*	*40. Pyrus x*
7. Brassica napus	*24. Hevea brasiliensis*	*41. Quercus suber*
8. Brassica rapa	*25. Jatropha curcas*	*42. Ricinus communis*
9. Camelina sativa	*26. Lupinus angustifolius*	*43. Rosa chinensis*
10. Chenopodium quinoa	*27. Manihot esculenta*	*44. Sesamum indicum*
11. Cicer arietinum	*28. Musa acuminata*	*45. Setaria italica*
12. Citrus clementina	*29. Nelumbo nucifera*	*46. Solanum lycopersicum*
13. Citrus sinensis	*30. Nicotiana attenuata*	*47. Solanum pennellii*
14. Cynara cardunculus	*31. Nicotiana sylvestris*	*48. Spinacia oleracea*
15. Dendrobium catenatum	*32. Nicotiana tabacum*	*49. Tarenaya hassleriana*
16. Durio zibethinus	*33. Nicotiana tomentosiformis*	*50. Vigna radiata*
17. Elaeis guineensis	*34. Oryza brachyantha*	*51. Ziziphus jujuba*

Chalcones

G. soja is the only species that was experimentally known and predicted to synthesize butein. While it is good that the only experimental confirmation from the dataset is also predicted, it is difficult to determine the accuracy of these predictions from such a small data set.

The entirety of the plants that were experimentally known to synthesize isoliquiritigenin were also predicted in the program (Table 41). While it is slightly promising to find data that confirms a number of these predictions, it would be more advantageous to find more experimental data before coming to a solid conclusion regarding the accuracy of the predictions for isoliquiritigenin.

Table 41

Plants predicted and experimentally known to synthesize isoliquiritigenin.

1. Arabidopsis thaliana	*3. Glycine max*	*5. Medicago truncatula*
2. Cicer arietinum	*4. Helianthus annuus*	

Flavan-3-ols

Of the 58 species predicted to synthesize catechin, there were 37 of these which were also experimentally known to synthesize catechin (Table 42). The species that were predicted but have no corresponding experimental data can be found in Table 43. However there were 11 species which have been experimentally known to synthesize catechin but were not predicted by the program. The number of predicted results with experimental confirmations does look promising in terms of program accuracy, though it may require further investigation of the species in Table 44 to better understand the discrepancies before finding more confidence with the predictions for catechin. Each

experimental disagreement had only one corresponding data source, which could potentially be indicative of isolated incidents of catechin synthesis in a specific variety or cultivar which may have not been specified in the documented experimental results.

Table 42

Plants predicted and experimentally known to synthesize catechin.

1. Aegilops tauschii	*14. Jatropha curcas*	*26. Populus trichocarpa*
2. Amborella trichopoda	*15. Juglans regia*	*27. Prunus avium*
3. Asparagus officinalis	*16. Malus domestica*	*28. Prunus mume*
4. Beta vulgaris	*17. Manihot esculenta*	*29. Prunus persica*
5. Carica papaya	*18. Medicago truncatula*	*30. Pyrus x*
6. Chenopodium quinoa	*19. Musa acuminata*	*31. Solanum tuberosum*
7. Cicer arietinum	*20. Nelumbo nucifera*	*32. Spinacia oleracea*
8. Citrus sinensis	*21. Nicotiana tabacum*	*33. Theobroma cacao*
9. Durio zibethinus	*22. Olea europaea*	*34. Vigna angularis*
10. Elaeis guineensis	*23. Oryza sativa*	*35. Vigna radiata*
11. Eucalyptus grandis	*24. Phaseolus vulgaris*	*36. Vitis vinifera*
12. Glycine max	*25. Phoenix dactylifera*	*37. Ziziphus jujuba*
13. Gossypium hirsutum		

Table 43

Plants predicted to synthesize catechin but not yet found experimentally.

1. Arachis duranensis	*8. Hevea brasiliensis*	*15. Papaver somniferum*
2. Brachypodium distachyon	*9. Lotus japonicus*	*16. Populus euphratica*
3. Citrus clementina	*10. Lupinus angustifolius*	*17. Quercus suber*
4. Glycine soja	*11. Nicotiana attenuata*	*18. Ricinus communis*
5. Gossypium arboreum	*12. Nicotiana sylvestris*	*19. Rosa chinensis*
6. Gossypium raimondii	*13. Nicotiana tomentosiformis*	*20. Solanum pennellii*
7. Helianthus annuus	*14. Oryza brachyantha*	*21. Vigna unguiculata*

Table 44

Plants experimentally known to synthesize catechin but were not predicted.

1. Arabidopsis thaliana	*5. Cucumis melo*	*9. Momordica charantia*
2. Brassica rapa	*6. Cucumis sativus*	*10. Sesamum indicum*
3. Camelina sativa	*7. Cucurbita pepo*	*11. Sorghum bicolor*
4. Capsicum annuum	*8. Fragaria vesca*	

Of the species that were predicted to synthesize epicatechin, there are 30 species which provide experimental confirmation (Table 45) and 35 which do not (Table 46). There were also eight species which were experimentally known to synthesize epicatechin but were not predicted (Table 47). There too should be investigation into these species before drawing any further conclusions, as the entirety of these species are culinary and thus have been subject to selective breeding and genetic variation.

Table 45

Plants predicted and experimentally known to synthesize epicatechin.

1. Amborella trichopoda	*11. Juglans regia*	*21. Prunus avium*
2. Arabidopsis thaliana	*12. Malus domestica*	*22. Prunus mume*
3. Beta vulgaris	*13. Medicago truncatula*	*23. Prunus persica*
4. Brassica napus	*14. Musa acuminata*	*24. Pyrus x*
5. Carica papaya	*15. Nelumbo nucifera*	*25. Ricinus communis*
6. Durio zibethinus	*16. Nicotiana sylvestris*	*26. Solanum tuberosum*
7. Elaeis guineensis	*17. Nicotiana tabacum*	*27. Theobroma cacao*
8. Eucalyptus grandis	*18. Phaseolus vulgaris*	*28. Vigna angularis*
9. Glycine max	*19. Phoenix dactylifera*	*29. Vigna radiata*
10. Gossypium hirsutum	*20. Populus trichocarpa*	*30. Ziziphus jujuba*

Table 46

Plants predicted to synthesize epicatechin but not yet found experimentally.

1. Aegilops tauschii	*13. Glycine soja*	*25. Papaver somniferum*
2. Arabidopsis lyrata	*14. Gossypium arboreum*	*26. Populus euphratica*
3. Arachis duranensis	*15. Gossypium raimondii*	*27. Quercus suber*
4. Asparagus officinalis	*16. Hevea brasiliensis*	*28. Raphanus sativus*
5. Brassica oleracea	*17. Jatropha curcas*	*29. Rosa chinensis*
6. Brassica rapa	*18. Lotus japonicus*	*30. Setaria italica*
7. Camelina sativa	*19. Lupinus angustifolius*	*31. Solanum lycopersicum*
8. Chenopodium quinoa	*20. Manihot esculenta*	*32. Solanum pennellii*
9. Cicer arietinum	*21. Nicotiana attenuata*	*33. Tarenaya hassleriana*
10. Citrus clementina	*22. Nicotiana tomentosiformis*	*34. Vigna unguiculata*
11. Citrus sinensis	*23. Oryza brachyantha*	*35. Zea mays*
12. Eutrema salsugineum	*24. Oryza sativa*	

Table 47

Plants experimentally known to synthesize epicatechin but were not predicted.

1. Capsicum annuum	*4. Momordica charantia*	*7. Spinacia oleracea*
2. Cucumis melo	*5. Sesamum indicum*	*8. Vitis vinifera*

3. Fragaria vesca *6. Sorghum bicolor*

Of the species predicted to synthesize epigallocatechin, there are only five experimentally known to synthesize the compound (Table 48), while the remaining 38 species are not yet known to do so (Table 49). There were five species of plants that were experimentally known to synthesize epigallocatechin but were not predicted (Table 50), which is concerning when compared to the number of experimental confirmations. Most likely these disagreements could be attributed to the usage of different cultivars in testing as these species are all culinary plants, but more research will need to be done in order to confirm or deny these disagreements before making any further judgments of the predictions for epigallocatechin.

Table 48

Plants predicted and experimentally known to synthesize epigallocatechin.

1. Citrus sinensis *3. Phaseolus vulgaris* *5. Ziziphus jujuba*
2. Gossypium hirsutum *4. Theobroma cacao*

Table 49

Plants predicted to synthesize epigallocatechin but not yet found experimentally.

1. Aegilops tauschii
2. Carica papaya
3. Cicer arietinum
4. Citrus clementina
5. Durio zibethinus
6. Elaeis guineensis
7. Eucalyptus grandis
8. Glycine max
9. Glycine soja
10. Gossypium arboreum
11. Gossypium raimondii
12. Hevea brasiliensis
13. Jatropha curcas
14. Juglans regia
15. Lotus japonicus
16. Lupinus angustifolius
17. Manihot esculenta
18. Medicago truncatula
19. Musa acuminata
20. Nelumbo nucifera
21. Nicotiana attenuata
22. Nicotiana sylvestris
23. Nicotiana tabacum
24. Nicotiana tomentosiformis
25. Oryza brachyantha
26. Oryza sativa
27. Phoenix dactylifera
28. Populus euphratica
29. Populus trichocarpa
30. Quercus suber
31. Setaria italica
32. Solanum lycopersicum
33. Solanum pennellii
34. Solanum tuberosum
35. Vigna angularis
36. Vigna radiata
37. Vigna unguiculata
38. Zea mays

Table 50

Plants experimentally known to synthesize epigallocatechin but were not predicted.

1. Cucumis melo	*3. Prunus avium*	*5. Vitis vinifera*
2. Malus domestica	*4. Prunus persica*	

Of the species predicted to synthesize gallocatechin, 10 species are known to synthesize the compound (Table 51), while the remaining 32 species have not yet been recorded to do so (Table 52). The lack of only experimentally known results is promising in terms of analyzing the accuracy of the predictions, though it is suggested that more experimental data should be collected as available before designing experiments based on the predictions for gallocatechin.

Table 51

Plants predicted and experimentally known to synthesize gallocatechin.

1. Gossypium hirsutum	*5. Phaseolus vulgaris*	*8. Vigna radiata*
2. Juglans regia	*6. Theobroma cacao*	*9. Vitis vinifera*
3. Medicago truncatula	*7. Vigna angularis*	*10. Ziziphus jujuba*
4. Nelumbo nucifera		

Table 52

Plants predicted to synthesize gallocatechin but not yet found experimentally.

1. Aegilops tauschii	*12. Gossypium arboreum*	*23. Nicotiana tomentosiformis*
2. Brachypodium distachyon	*13. Gossypium raimondii*	*24. Oryza brachyantha*
3. Carica papaya	*14. Hevea brasiliensis*	*25. Oryza sativa*
4. Cicer arietinum	*15. Jatropha curcas*	*26. Phoenix dactylifera*
5. Citrus clementina	*16. Lotus japonicus*	*27. Populus euphratica*
6. Citrus sinensis	*17. Lupinus angustifolius*	*28. Populus trichocarpa*
7. Durio zibethinus	*18. Manihot esculenta*	*29. Quercus suber*
8. Elaeis guineensis	*19. Musa acuminata*	*30. Solanum pennellii*
9. Eucalyptus grandis	*20. Nicotiana attenuata*	*31. Solanum tuberosum*
10. Glycine max	*21. Nicotiana sylvestris*	*32. Vigna unguiculata*
11. Glycine soja	*22. Nicotiana tabacum*	

Flavanones

Of the species predicted to synthesize eriodictyol, 11 species are known to

synthesize the compound (Table 53), while the remaining 78 species have not yet been recorded to do so (Table 54).The lack of experimental disagreements looks promising in the context of the predictions, though, the number of confirmations are still small compared to the overall set of predicted species meaning that more literature is needed before labeling the predictions for eriodictyol as accurate.

Table 53

Plants predicted and experimentally known to synthesize eriodictyol.

1. Amborella trichopoda	*5. Malus domestica*	*9. Theobroma cacao*
2. Eucalyptus grandis	*6. Prunus avium*	*10. Vigna radiata*
3. Glycine soja	*7. Prunus persica*	*11. Ziziphus jujuba*
4. Gossypium hirsutum	*8. Sorghum bicolor*	

Table 54

Plants predicted to synthesize eriodictyol but not yet found experimentally.

1. Aegilops tauschii	*27. Dendrobium catenatum*	*53. Oryza sativa*
2. Arabidopsis lyrata	*28. Durio zibethinus*	*54. Papaver somniferum*
3. Arabidopsis thaliana	*29. Elaeis guineensis*	*55. Phalaenopsis equestris*
4. Arachis duranensis	*30. Eutrema salsugineum*	*56. Phaseolus vulgaris*
5. Arachis ipaensis	*31. Fragaria vesca*	*57. Phoenix dactylifera*
6. Asparagus officinalis	*32. Glycine max*	*58. Physcomitrium patens*
7. Beta vulgaris	*33. Gossypium arboreum*	*59. Populus euphratica*
8. Brachypodium distachyon	*34. Gossypium raimondii*	*60. Populus trichocarpa*
9. Brassica napus	*35. Helianthus annuus*	*61. Prunus mume*
10. Brassica oleracea	*36. Hevea brasiliensis*	*62. Pyrus x*
11. Brassica rapa	*37. Ipomoea nil*	*63. Quercus suber*
12. Cajanus cajan	*38. Jatropha curcas*	*64. Raphanus sativus*
13. Camelina sativa	*39. Juglans regia*	*65. Ricinus communis*
14. Capsicum annuum	*40. Lactuca sativa*	*66. Rosa chinensis*
15. Carica papaya	*41. Lotus japonicus*	*67. Selaginella moellendorffii*
16. Chenopodium quinoa	*42. Lupinus angustifolius*	*68. Sesamum indicum*
17. Cicer arietinum	*43. Manihot esculenta*	*69. Setaria italica*
18. Citrus clementina	*44. Medicago truncatula*	*70. Solanum lycopersicum*
19. Citrus sinensis	*45. Musa acuminata*	*71. Solanum pennellii*
20. Cucumis melo	*46. Nelumbo nucifera*	*72. Solanum tuberosum*
21. Cucumis sativus	*47. Nicotiana attenuata*	*73. Spinacia oleracea*
22. Cucurbita maxima	*48. Nicotiana sylvestris*	*74. Tarenaya hassleriana*
23. Cucurbita moschata	*49. Nicotiana tabacum*	*75. Vigna angularis*
24. Cucurbita pepo	*50. Nicotiana tomentosiformis*	*76. Vigna unguiculata*
25. Cynara cardunculus	*51. Olea europaea*	*77. Vitis vinifera*
26. Daucus carota	*52. Oryza brachyantha*	*78. Zea mays*

Of the 90 species predicted to synthesize naringenin, 44 species are known to synthesize the compound (Table 55), while the remaining 46 species have not yet been recorded to do so (Table 56). Due to the absence of species that were experimentally known but not predicted and the comparably larger amount of experimental confirmations for the predicted species, these predictions could provide a better basis for research in comparison to the other flavonoids.

Table 55

Plants predicted and experimentally known to synthesize naringenin.

1. Amborella trichopoda	*16. Daucus carota*	*31. Prunus avium*
2. Arabidopsis thaliana	*17. Dendrobium catenatum*	*32. Prunus mume*
3. Asparagus officinalis	*18. Eucalyptus grandis*	*33. Prunus persica*
4. Brachypodium distachyon	*19. Fragaria vesca*	*34. Raphanus sativus*
5. Brassica napus	*20. Glycine max*	*35. Selaginella moellendorffii*
6. Brassica oleracea	*21. Gossypium hirsutum*	*36. Solanum lycopersicum*
7. Brassica rapa	*22. Juglans regia*	*37. Solanum tuberosum*
8. Cajanus cajan	*23. Medicago truncatula*	*38. Sorghum bicolor*
9. Capsicum annuum	*24. Momordica charantia*	*39. Spinacia oleracea*
10. Carica papaya	*25. Musa acuminata*	*40. Theobroma cacao*
11. Chenopodium quinoa	*26. Nelumbo nucifera*	*41. Vigna angularis*
12. Cicer arietinum	*27. Olea europaea*	*42. Vigna radiata*
13. Citrus sinensis	*28. Oryza sativa*	*43. Vitis vinifera*
14. Cucumis melo	*29. Phaseolus vulgaris*	*44. Zea mays*
15. Cynara cardunculus	*30. Phoenix dactylifera*	

Table 56

Plants predicted to synthesize naringenin but not yet found experimentally.

1. Aegilops tauschii	*17. Gossypium raimondii*	*32. Papaver somniferum*
2. Arabidopsis lyrata	*18. Helianthus annuus*	*33. Phalaenopsis equestris*
3. Arachis duranensis	*19. Hevea brasiliensis*	*34. Physcomitrium patens*
4. Arachis ipaensis	*20. Ipomoea nil*	*35. Populus euphratica*
5. Beta vulgaris	*21. Jatropha curcas*	*36. Populus trichocarpa*
6. Camelina sativa	*22. Lactuca sativa*	*37. Pyrus x*
7. Citrus clementina	*23. Lotus japonicus*	*38. Quercus suber*
8. Cucumis sativus	*24. Lupinus angustifolius*	*39. Ricinus communis*
9. Cucurbita maxima	*25. Malus domestica*	*40. Rosa chinensis*
10. Cucurbita moschata	*26. Manihot esculenta*	*41. Sesamum indicum*
11. Cucurbita pepo	*27. Nicotiana attenuata*	*42. Setaria italica*

12. Durio zibethinus
13. Elaeis guineensis
14. Eutrema salsugineum
15. Glycine soja
16. Gossypium arboreum
28. Nicotiana sylvestris
29. Nicotiana tabacum
30. Nicotiana tomentosiformis
31. Oryza brachyantha
43. Solanum pennellii
44. Tarenaya hassleriana
45. Vigna unguiculata
46. Ziziphus jujuba

Flavonols

Of the 84 species predicted to synthesize kaempferol, 49 species are known to synthesize the compound (Table 57), while the remaining 35 species have not yet been recorded to do so (Table 58). Similar to naringenin, the large number of experimental confirmations and the lack of disagreements between the experimental and theoretical data makes these predictions ideal to use as a basis for experimentation.

Table 57

Plants predicted and experimentally known to synthesize kaempferol .

1. Arabidopsis thaliana
2. Asparagus officinalis
3. Beta vulgaris
4. Brassica napus
5. Brassica oleracea
6. Brassica rapa
7. Capsicum annuum
8. Carica papaya
9. Chenopodium quinoa
10. Cicer arietinum
11. Citrus sinensis
12. Cucumis melo
13. Cucumis sativus
14. Cucurbita maxima
15. Cucurbita pepo
16. Daucus carota
17. Elaeis guineensis
18. Fragaria vesca
19. Glycine max
20. Gossypium hirsutum
21. Hevea brasiliensis
22. Juglans regia
23. Lactuca sativa
24. Lotus japonicus
25. Lupinus angustifolius
26. Malus domestica
27. Medicago truncatula
28. Momordica charantia
29. Musa acuminata
30. Nelumbo nucifera
31. Nicotiana tabacum
32. Olea europaea
33. Oryza sativa
34. Papaver somniferum
35. Phaseolus vulgaris
36. Prunus avium
37. Prunus persica
38. Raphanus sativus
39. Ricinus communis
40. Rosa chinensis
41. Solanum lycopersicum
42. Solanum tuberosum
43. Spinacia oleracea
44. Theobroma cacao
45. Vigna radiata
46. Vigna unguiculata
47. Vitis vinifera
48. Zea mays
49. Ziziphus jujuba

Table 58

Plants predicted to synthesize kaempferol but not yet found experimentally.

1. Aegilops tauschii
2. Amborella trichopoda
3. Arabidopsis lyrata
4. Arachis duranensis
13. Eutrema salsugineum
14. Glycine soja
15. Gossypium arboreum
16. Gossypium raimondii
25. Phoenix dactylifera
26. Populus euphratica
27. Populus trichocarpa
28. Prunus mume

5. Arachis ipaensis
6. Brachypodium distachyon
7. Camelina sativa
8. Citrus clementina
9. Cucurbita moschata
10. Cynara cardunculus
11. Durio zibethinus
12. Eucalyptus grandis
17. Helianthus annuus
18. Ipomoea nil
19. Jatropha curcas
20. Manihot esculenta
21. Nicotiana attenuata
22. Nicotiana sylvestris
23. Nicotiana tomentosiformis
24. Phalaenopsis equestris
29. Pyrus x
30. Quercus suber
31. Sesamum indicum
32. Setaria italica
33. Solanum pennellii
34. Tarenaya hassleriana
35. Vigna angularis

Of the 47 species predicted to synthesize myricetin, 13 species are known to synthesize the compound (Table 59), while the remaining 34 species have not yet been recorded to do so (Table 60). However, there are six species experimentally known to synthesize myricetin but were not predicted by the program (Table 61). It is promising that the list of disagreements consists entirely of culinary plants, but further investigation is necessary before completely dismissing the data as inaccurately reported data from specific cultivars. Currently, the limited and conflicting nature of the data do not indicate that the predictions for myricetin are correct, so the predictions should not be used as a basis for experimentation.

Table 59

Plants predicted and experimentally known to synthesize myricetin.

1. Capsicum annuum
2. Carica papaya
3. Citrus sinensis
4. Gossypium hirsutum
5. Juglans regia
6. Lotus japonicus
7. Medicago truncatula
8. Nelumbo nucifera
9. Phaseolus vulgaris
10. Solanum tuberosum
11. Vigna radiata
12. Vigna unguiculata
13. Vitis vinifera

Table 60

Plants predicted to synthesize myricetin but not yet found experimentally.

1. Aegilops tauschii
2. Brachypodium distachyon
3. Cicer arietinum
4. Citrus clementina
5. Durio zibethinus
6. Elaeis guineensis
7. Eucalyptus grandis
13. Jatropha curcas
14. Lupinus angustifolius
15. Manihot esculenta
16. Musa acuminata
17. Nicotiana attenuata
18. Nicotiana sylvestris
19. Nicotiana tabacum
24. Phoenix dactylifera
25. Populus euphratica
26. Populus trichocarpa
27. Quercus suber
28. Setaria italica
29. Solanum lycopersicum
30. Solanum pennellii

8. Glycine max	*20. Nicotiana tomentosiformis*	*31. Theobroma cacao*
9. Glycine soja	*21. Oryza brachyantha*	*32. Vigna angularis*
10. Gossypium arboreum	*22. Oryza sativa*	*33. Zea mays*
11. Gossypium raimondii	*23. Phalaenopsis equestris*	*34. Ziziphus jujuba*
12. Hevea brasiliensis		

Table 61

Plants experimentally known to synthesize myricetin but were not predicted.

1. Asparagus officinalis	*3. Daucus carota*	*5. Prunus avium*
2. Brassica rapa	*4. Malus domestica*	*6. Spinacia oleracea*

Of the 83 species predicted to synthesize Quercetin, 57 species are known to synthesize the compound (Table 62), while the remaining 26 species have not yet been recorded to do so (Table 63). There were two species *C. cajan* and *M. charantia* that were experimentally known to synthesize quercetin but were not predicted. Although there are two species which offer some disagreement, they are culinary plants and thus have different cultivars that can affect phytochemical composition. The sheer amount of available literature combined with the largest set of experimental confirmations for the predictions makes quercetin, at the very least, worth the investigation in order to better address the disagreements.

Table 62

Plants predicted and experimentally known to synthesize quercetin.

1. Amborella trichopoda	*20. Fragaria vesca*	*39. Phaseolus vulgaris*
2. Arabidopsis thaliana	*21. Glycine max*	*40. Phoenix dactylifera*
3. Asparagus officinalis	*22. Gossypium arboreum*	*41. Prunus avium*
4. Beta vulgaris	*23. Gossypium hirsutum*	*42. Prunus mume*
5. Brassica napus	*24. Helianthus annuus*	*43. Prunus persica*
6. Brassica oleracea	*25. Hevea brasiliensis*	*44. Quercus suber*
7. Brassica rapa	*26. Jatropha curcas*	*45. Raphanus sativus*
8. Camelina sativa	*27. Juglans regia*	*46. Ricinus communis*
9. Capsicum annuum	*28. Lactuca sativa*	*47. Rosa chinensis*
10. Carica papaya	*29. Lotus japonicus*	*48. Solanum lycopersicum*
11. Chenopodium quinoa	*30. Lupinus angustifolius*	*49. Solanum tuberosum*
12. Cicer arietinum	*31. Malus domestica*	*50. Spinacia oleracea*

13. Citrus sinensis	*32. Manihot esculenta*	*51. Theobroma cacao*
14. Cucumis melo	*33. Medicago truncatula*	*52. Vigna angularis*
15. Cucumis sativus	*34. Musa acuminata*	*53. Vigna radiata*
16. Cucurbita maxima	*35. Nelumbo nucifera*	*54. Vigna unguiculata*
17. Cucurbita pepo	*36. Nicotiana tabacum*	*55. Vitis vinifera*
18. Cynara cardunculus	*37. Olea europaea*	*56. Zea mays*
19. Daucus carota	*38. Papaver somniferum*	*57. Ziziphus jujuba*

Table 63

Plants predicted to synthesize quercetin but not yet found experimentally.

1. Aegilops tauschii	*10. Eucalyptus grandis*	*19. Phalaenopsis equestris*
2. Arabidopsis lyrata	*11. Eutrema salsugineum*	*20. Populus euphratica*
3. Arachis duranensis	*12. Glycine soja*	*21. Populus trichocarpa*
4. Arachis ipaensis	*13. Gossypium raimondii*	*22. Pyrus x*
5. Brachypodium distachyon	*14. Ipomoea nil*	*23. Sesamum indicum*
6. Citrus clementina	*15. Nicotiana attenuata*	*24. Setaria italica*
7. Cucurbita moschata	*16. Nicotiana sylvestris*	*25. Solanum pennellii*
8. Durio zibethinus	*17. Nicotiana tomentosiformis*	*26. Tarenaya hassleriana*
9. Elaeis guineensis	*18. Oryza sativa*	

Flavones

Of the 37 species predicted to synthesize apigenin, 15 species are known to synthesize the compound (Table 64), while the remaining 22 species have not yet been recorded to do so (Table 65). Additionally there were 15 species that were only experimentally known to synthesize apigenin (Table 66), which does not instill much confidence in the accuracy of these predictions. All of the disagreements, besides Jatropha curcas, are commonly known culinary plants which then means an additional investigation should be conducted regarding the cultivars utilized in the experiments before investigating the logic of the program.

Table 64

Plants predicted and experimentally known to synthesize apigenin.

1. Cajanus cajan	*6. Lactuca sativa*	*11. Populus trichocarpa*
2. Citrus sinensis	*7. Lupinus angustifolius*	*12. Ricinus communis*

3. Cynara cardunculus	*8. Medicago truncatula*	*13. Sorghum bicolor*
4. Daucus carota	*9. Olea europaea*	*14. Theobroma cacao*
5. Glycine max	*10. Phaseolus vulgaris*	*15. Zea mays*

Table 65

Plants predicted to synthesize apigenin but not yet found experimentally.

1. Aegilops tauschii	*9. Glycine soja*	*16. Oryza brachyantha*
2. Arachis duranensis	*10. Gossypium arboreum*	*17. Oryza sativa*
3. Arachis ipaensis	*11. Gossypium hirsutum*	*18. Populus euphratica*
4. Brachypodium distachyon	*12. Gossypium raimondii*	*19. Sesamum indicum*
5. Cicer arietinum	*13. Helianthus annuus*	*20. Setaria italica*
6. Citrus clementina	*14. Hevea brasiliensis*	*21. Vigna angularis*
7. Durio zibethinus	*15. Manihot esculenta*	*22. Vigna unguiculata*
8. Eucalyptus grandis		

Table 66

Plants experimentally known to synthesize apigenin but were not predicted.

1. Asparagus officinalis	*6. Carica papaya*	*11. Jatropha curcas*
2. Beta vulgaris	*7. Chenopodium quinoa*	*12. Juglans regia*
3. Brassica oleracea	*8. Cucurbita moschata*	*13. Phoenix dactylifera*
4. Brassica rapa	*9. Cucurbita pepo*	*14. Prunus avium*
5. Capsicum annuum	*10. Fragaria vesca*	*15. Raphanus sativus*

Of the 37 species predicted to synthesize luteolin, 14 species are known to synthesize the compound (Table 67), while the remaining 23 species have not yet been recorded to do so (Table 68). Unfortunately, there were 22 species that were experimentally known to synthesize luteolin but were not predicted (Table 69), which needs to be further investigated due to most of the plants having a long history of cultivation.

Table 67

Plants predicted and experimentally known to synthesize luteolin.

1. Cajanus cajan	*6. Lactuca sativa*	*11. Setaria italica*
2. Citrus sinensis	*7. Lupinus angustifolius*	*12. Sorghum bicolor*
3. Cynara cardunculus	*8. Medicago truncatula*	*13. Theobroma cacao*

4. Daucus carota
5. Helianthus annuus
9. Olea europaea
10. Phaseolus vulgaris
14. Zea mays

Table 68

Plants predicted to synthesize luteolin but not yet found experimentally.

1. Aegilops tauschii
2. Arachis duranensis
3. Arachis ipaensis
4. Brachypodium distachyon
5. Cicer arietinum
6. Citrus clementina
7. Durio zibethinus
8. Eucalyptus grandis
9. Glycine max
10. Glycine soja
11. Gossypium arboreum
12. Gossypium hirsutum
13. Gossypium raimondii
14. Hevea brasiliensis
15. Manihot esculenta
16. Oryza brachyantha
17. Oryza sativa
18. Populus euphratica
19. Populus trichocarpa
20. Ricinus communis
21. Sesamum indicum
22. Vigna angularis
23. Vigna unguiculata

Table 69

Plants experimentally known to synthesize luteolin but were not predicted.

1. Amborella trichopoda
2. Asparagus officinalis
3. Beta vulgaris
4. Brassica napus
5. Brassica oleracea
6. Brassica rapa
7. Capsicum annuum
8. Carica papaya
9. Chenopodium quinoa
10. Cucumis melo
11. Cucurbita moschata
12. Cucurbita pepo
13. Fragaria vesca
14. Malus domestica
15. Momordica charantia
16. Nelumbo nucifera
17. Phoenix dactylifera
18. Raphanus sativus
19. Solanum lycopersicum
20. Solanum tuberosum
21. Spinacia oleracea
22. Vitis vinifera

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Appendix

Similar Compounds

Isoflavonoids

Table 70

Similar and derivative compounds of genistein synthesized by plants in the data set.

Compound Name(s)	Species	Source(s)
1. 2'-Hydroxygenistein	Cajanus cajan	K, T
	Lupinus angustifolius	K, N
	Phaseolus vulgaris	K, N, T
	Vigna angularis	K, N
	Vigna radiata	T, N
	Vigna unguiculata	T
2. 4'-Methylgenistein Biochanin A	Cicer arietinum	K, P
	Glycine max	K
	Phaseolus vulgaris	2
3. Genistein 7-O-β-D-glucoside Genistin	Glycine max	K, P
	Lupinus angustifolius	1
	Medicago truncatula	K
	Raphanus sativus	K
4. Genistein 7-O-β-D-glucoside 6''-O-malonate	Glycine max	K
	Medicago truncatula	K
5. Genistein 7-O-glucosyl-glucoside	Lupinus angustifolius	D
6. Genistein apiofuranosyl diglycoside	Lupinus angustifolius	1
7. Genistein apiofuranosyl glycoside	Lupinus angustifolius	1
8. Genistin 6''-O-acetate	Glycine max	K
9. Genistin 6''-O-malonate Malonylgenistin	Glycine max	N
10. Hidroxygenistein 7-glucoside	Lupinus angustifolius	1
11. Hidroxygenistein 7-acetylglucoside	Lupinus angustifolius	1
12. Hydroxygenistein	Vigna angularis	D
	Vigna radiata	D
13. Isogenistein 7-O-glucoside	Cajanus cajan	D
14. Methylgenistein	Glycine max	D

Sources: (D) Dr. Duke; (K) KNApSAcK; (N) NAPRALERT; (P) NPASS; (T) IMPPAT; (1) Dueñas et al., 2009; (2) Ganesan & Xu, 2017

Anthocyanidins

Table 71

Similar and derivative compounds of cyanidin synthesized by plants in the data set.

Compound Name(s)	Species	Source(s)
1. Cyanidin 3-(3'',6''-dimalonylglucoside)	Zea mays	K, N
2. Cyanidin 3-(4''-acetylglucoside)	Citrus sinensis	K
3. Cyanidin 3-(6''-acetylglucoside)	Vitis vinifera	K
4. Cyanidin 3-(6''-caffeyl-6'''-feruly-lsophoroside)-5-glucoside	Raphanus sativus	K
5. Cyanidin 3-(6''-malonylglucoside)	Citrus sinensis	K

		Lactuca sativa	K
		Zea mays	K, N
6.	Cyanidin 3-(6'',6'''-disinapylsophoroside)-5-glucoside	Brassica oleracea	K
7.	Cyanidin 3-(sinapoyl-xylosyl-glucosyl)-galactoside	Daucus carota	N
8.	Cyanidin 3-[6-(3-glucosylcaffeyl)glucoside]-5-glucoside	Ipomoea nil	K
9.	Cyanidin 3-[6''-(4-glucosyl-p-coumaryl)sophoroside]-5-glucoside	Brassica oleracea	K
10.	Cyanidin 3-[6''-(4-glucosylcaffeyl)sophoroside]-5-glucoside	Ipomoea nil	K
11.	Cyanidin 3-acetyl-glucoside Cyanidin 3-O-acetyl-glucoside	Vitis vinifera	N
12.	Cyanidin 3-arabinoside	Malus domestica Theobroma cacao	D K
13.	Cyanidin 3-coyumaroyl-glucoside	Vitis vinifera	N
14.	Cyanidin 3-dimalonyl-glucoside	Zea mays	D, N
15.	Cyanidin 3-galactoside Cyanidin 3-O-galactoside Cyanidin 3-O-β-D-galactopyranoside Idaein	Daucus carota Fragaria vesca Glycine max Theobroma cacao Vitis vinifera Zea mays	K, N 2 P D, K D D, N
16.	Cyanidin 3-galactoside p-coumaric acid ester	Zea mays	D
17.	Cyanidin 3-glucogalactoside	Daucus carota	N
18.	Cyanidin 3-glucoside Cyanidin 3-O-glucoside Cyanidin 3-O-β-D-glucoside Cyanidin 3-monoglucoside Chrysanthemin Kuromanin	Amborella trichopoda Asparagus officinalis Citrus sinensis Fragaria vesca Olea europaea Phaseolus vulgaris Vigna radiata Vitis vinifera	3 D K 2 D 1 D D, P
19.	Cyanidin 3-glucosyl-rutinoside Cyanidin 3-O-β-D-glucosyl-rutinoside	Olea europaea Prunus avium	N N
20.	Cyanidin 3-lathyroside	Daucus carota	K
21.	Cyanidin 3-malonyl-glucoside	Helianthus annuus	N
22.	Cyanidin 3-malonyl-xyloside	Helianthus annuus	N
23.	Cyanidin 3-O-(6-O-para-coumaroyl)-glucoside	Vitis vinifera	N
24.	Cyanidin 3-O-[2-O-(2-O-(sinapoyl)-bata-D-xylopyranosyl) 6-O-(4-O-(β-D-glucopyranosyl)-p-coumaroyl-bata-D-glucopyranoside] 5-O-[6-O-(malonyl) bata-D-glucopyranoside]	Arabidopsis thaliana	K
25.	Cyanidin 3-O-[2''-O-(2'''-O-(sinapoyl) xylosyl) 6''-O-(p-coumaroyl) glucoside] 5-O-glucoside	Arabidopsis thaliana	K
26.	Cyanidin 3-O-[2''-O-(2'''-O-(sinapoyl) xylosyl) 6''-O-(p-O-(glucosyl) p-coumaroyl) glucoside] 5-O-glucoside	Arabidopsis thaliana	K
27.	Cyanidin 3-O-[2''-O-(xylosyl) 6''-O-(p-O-(glucosyl) p-coumaroyl) glucoside] 5-O-[6'''-O-(malonyl) glucoside]	Arabidopsis thaliana	K
28.	Cyanidin 3-O-[2''-O-(xylosyl) glucoside] 5-O-(6'''-O-malonyl) glucoside	Arabidopsis thaliana	K
29.	Cyanidin 3-O-[2''-O-(xylosyl)-6''-O-(p-O-(glucosyl)-p-coumaroyl) glucoside] 5-O-glucoside	Arabidopsis thaliana	K
30.	Cyanidin 3-O-[6-O-(malonyl)-β-D-glucopyranoside]-7,3'-di-O-[6-O-(sinapyl)-β-D-glucopyranoside]	Phalaenopsis equestris	K
31.	Cyanidin 3-O-[β-D-glucopyranoside]-7,3'-di-O-[6-O-(sinapyl)-β-D-glucopyranoside]	Phalaenopsis equestris	K
32.	Cyanidin 3-rhamnosyl-glucosyl-glucoside	Asparagus officinalis	N
33.	Cyanidin 3-rhamnosyl-glucoside	Asparagus officinalis	D

34. Cyanidin 3-rutinoside	Olea europaea	D, N
Cyanidin 3-O-β-D-rutinoside	Prunus avium	N
35. Cyanidin 3-sambubioside-5-glucoside	Arabidopsis thaliana	K
36. Cyanidin 3-sophoroside-5-glucoside	Brassica oleracea	K, N
Cyanidin 3-O-sophoroside-5-O-glucoside	Raphanus sativus	N
Cyanidin 3-sophorobiose-5-O-β-D-glucoside		
37. Cyanidin 3-xyloside	Helianthus annuus	K, N
38. Cyanidin 3,5-digalactoside	Daucus carota	N
39. Cyanidin 3,5-diglucoside	Asparagus officinalis	D
Cyanidin 3,5-O-diglucoside	Brassica oleracea	N
Cyanin	Fragaria vesca	P
	Malus domestica	D
40. Cyanidin 7-arabinoside	Malus domestica	D
41. Cyanidin chloride	Glycine max	P
42. Leucocyanidin	Amborella trichopoda	3
	Arabidopsis thaliana	N
	Brassica napus	K
	Capsicum annuum	K
	Gossypium hirsutum	N
	Medicago truncatula	K
	Momordica charantia	K
	Nelumbo nucifera	K
	Phaseolus vulgaris	K
	Prunus avium	K
	Ziziphus jujuba	N

Sources: (D) Dr. Duke; (K) KNApSAcK; (N) NAPRALERT; (P) NPASS; (1) Ganesan & Xu, 2017; (2) Gasperotti et al., 2015; (3) Wu et al., 2019

Chalcones

Table 72

Similar and derivative compounds of isoliquiritigenin synthesized by plants in the data set.

Compound Name	Species	Source(s)
1. Isoliquiritin	Cicer arietinum	P
2. Liquirtigenin	Glycine soja	P
3. Neoisoliquiritigenin	Glycine max	K

Sources: (K) KNApSAcK; (P) NPASS

Flavan-3-ols

Table 73

Similar and derivative compounds of catechin synthesized by plants in the data set.

Compound Name(s)	Species	Source(s)
1. (+)-Gallocatechin-(4α->8)-(+)-catechin	Nelumbo nucifera	N
2. Catechin (4α->6)-catechin	Nelumbo nucifera	P
Procyanidin B6	Vitis vinifera	N, P
3. Catechin (4α->6)-epicatechin	Nelumbo nucifera	P
Procyanidin B8	Vitis vinifera	N, P
4. Catechin (4α->8)-catechin	Fragaria vesca	1
Procyanidin B3	Nelumbo nucifera	P

		Vitis vinifera	N, P
5.	Catechin (4α->8)-catechin-(4α->8)-catechin Procyanidin C2	Vitis vinifera	N
6.	Catechin (4α->8)-epicatechin Procyanidin B4	Nelumbo nucifera Theobroma cacao Vitis vinifera	P N P
7.	Catechin (4α->8)-epicatechin-3-O-gallate	Vitis vinifera	K
8.	Catechin 3'-O-gallate	Ziziphus jujuba	N
9.	Catechin 7-O-β-D-glucopyranoside	Vigna angularis	K, N
10.	Catechin gallate	Lotus japonicus Vigna angularis Vitis vinifera	P N P
11.	Epicatechin (4β->6)-catechin Procyanidin B7	Theobroma cacao Vitis vinifera	N P
12.	Epicatechin (4β->8)-catechin Procyanidin B1	Amborella trichopoda Fragaria vesca Nelumbo nucifera Theobroma cacao Vigna angularis Vitis vinifera	2 N, 1 P N, P P N, P
13.	Epicatechin (4β->8)-epicatechin-(4β->8)-catechin Procyanidin T2	Vitis vinifera	N

Sources: (K) KNApSAcK; (N) NAPRALERT; (P) NPASS; (1) Gasperotti et al., 2015; (2) Wu et al., 2019

Table 74

Similar and derivative compounds of epicatechin synthesized by plants in the data set.

Compound Name(s)		**Species**	**Source(s)**
1.	[Epicatechin (4β->8)]2-epicatechin Procyanidin C1	Theobroma cacao Vitis vinifera	N, P P
2.	9,10-Dihydro-8-hydroxy-10-methyl-8H-pyrano[2,3-h]epicatechin	Lupinus angustifolius	K
3.	Catechin (4α->8)-catechin-(4α->8)-catechin Procyanidin C2	Vitis vinifera	N
4.	Catechin (4α->8)-epicatechin Procyanidin B4	Theobroma cacao Vitis vinifera	N P
5.	Catechin-(4α->6)-epicatechin Procyanidin B8	Vitis vinifera	N
6.	Epicatechin (4β->6)-epicatechin Procyanidin B5	Fragaria vesca Nicotiana sylvestris Theobroma cacao Vitis vinifera	N P N, P N, P
7.	Epicatechin (4β->6)catechin Procyanidin B7	Theobroma cacao Vitis vinifera	P N
8.	Epicatechin (4β->8)-catechin Procyanidin B1	Fragaria vesca Nelumbo nucifera Theobroma cacao Vigna angularis Vitis vinifera	N P N P N, P
9.	Epicatechin (4β->8)-epicatechin Procyanidin B2	Fragaria vesca Nelumbo nucifera Nicotiana sylvestris Theobroma cacao Vitis vinifera Ziziphus jujuba	N P P N, P N, P P
10.	Epicatechin (4β->8)-epicatechin-(4β->6)-epicatechin	Vitis vinifera	P

11. Epicatechin (4β->8)-epicatechin-(4β->8)-catechin Procyanidin T2	Vitis vinifera	N
12. Epicatechin (6'->8)-epicatechin	Vitis vinifera	N
13. Epicatechin 3-gallate	Citrus sinensis Malus domestica Prunus avium Prunus persica Vitis vinifera	M M, U M, U U D, M, U
14. Epicatechin 3-O-gallate	Prunus persica Theobroma cacao Vitis vinifera Ziziphus jujuba	N N K N
15. Epicatechin 8-C-β-D-galactopyranoside	Theobroma cacao	N
16. Epicatechin 8-C-β-D-galactoside	Theobroma cacao	K
17. Epicatechin gallate	Lotus japonicus Vitis vinifera Zea mays	P P, T T
18. Epicatechin pentaacetate	Prunus persica	P

Sources: (D) Dr. Duke; (K) KNApSAcK; (M) Microbiome; (N) NAPRALERT; (P) NPASS; (T) IMPPAT; (U) USDA

Table 75

Similar and derivative compounds of epigallocatechin synthesized by plants in the data set.

Compound Name		Species	Source(s)
1.	Epigallocatechin 3-gallate Epigallocatechin 3-O-gallate	Citrus sinensis Malus domestica Phoenix dactylifera Prunus persica Vitis vinifera	M M, U M M, U M, N
2.	Epigallocatechin gallate	Lotus japonicus Vitis vinifera	P K

Sources: (K) KNApSAcK; (M) Microbiome; (N) NAPRALERT; (P) NPASS; (U) USDA

Table 76

Similar and derivative compounds of gallocatechin synthesized by plants in the data set.

Compound Name	Species	Source(s)
1. Gallocatechin 3-O-gallate	Vitis vinifera	K, N
2. (+)-Gallocatechin-(4α->8)-(+)-catechin	Nelumbo nucifera	N

Sources: (K) KNApSAcK; (N) NAPRALERT

Flavanones

Table 77

Similar and derivative compounds of eriodictyol synthesized by plants in the data set.

Compound Name(s)	Species	Source
1. Eriodictyol 5-O-β-glucoside	Sorghum bicolor	N
2. Eriodictyol 7-O-glucoside Eriodictyol 7-O-β-D-glucoside	Amborella trichopoda Prunus avium	Wu N
3. Eriodictyol-7-O-rutinoside Eriocitrin	Citrus sinensis	P

Sources: (N) NAPRALERT; (P) NPASS; (1) Wu et al., 2019

Table 78

Similar and derivative compounds of naringenin synthesized by plants in the data set.

	Compound Name(s)	Species	Source(s)
1.	(2R) Naringenin 5-O-β-D-glucopyranoside	Prunus persica	P
2.	2-hydroxynaringenin	Zea mays	K
3.	6-prenylnaringenin	Raphanus sativus	K
4.	6,8-di-C-glucopyranosylnaringenin	Ziziphus jujuba	K
5.	6,8-diprenylnaringenin Lonchocarpol A Senegalensein	Glycine max	K
6.	Naringenin 4',7-dimethyl ether	Cajanus cajan	N
7.	Naringenin 7-(2-p-coumaroylglucoside)	Ricinus communis	K
8.	Naringenin 7-methyl ether Naringenin 7-O-methyl ether 7-O-Methylnaringenin Sakuranetin	Daucus carota Glycine max Phaseolus vulgaris Prunus avium	D P 2 K
9.	Naringenin 7-O-glucoside Naringenin 7-O-β-D-glucoside Prunin	Amborella trichopoda Cynara cardunculus Phaseolus vulgaris Prunus persica Solanum lycopersicum Theobroma cacao Vitis vinifera	4 D 2 K K K P
10.	Naringenin 7-O-neohesperidoside Naringin	Amborella trichopoda Citrus sinensis Phaseolus vulgaris Prunus mume Solanum tuberosum Theobroma cacao	4 D 2 P K 1
11.	Naringenin 7-rutinoside Naringenin 7-O-rutinoside Narirutin	Citrus sinensis Cynara cardunculus Phaseolus vulgaris	D, K, P, T D, K 2
12.	Naringenin chalcone	Arabidopsis thaliana Asparagus officinalis Capsicum annuum Daucus carota Ipomoea nil Medicago truncatula Momordica charantia Solanum lycopersicum Vitis vinifera	K K K K N K K K K
13.	Naringenin hexoside	Sorghum bicolor Theobroma cacao	3 1

Sources: (D) Dr. Duke; (K) KNApSAcK; (N) NAPRALERT; (P) NPASS; (T) IMPPAT; (1) Gallego et al., 2019; (2) Ganesan & Xu, 2017; (3) Luo et al., 2018;(4) Wu et al., 2019

Flavonols

Table 79

Similar and derivative compounds of kaempferol synthesized by plants in the data set.

Compound Name(s)	Species	Source(s)

1.	3,6-Dimethoxy Kaempferol	Beta vulgaris	P
2.	Dihydrokaempferol Aromadendrin	Fragaria vesca Glycine soja Momordica charantia	4 P K
3.	Dihydrokaempferol 7-O-β-D-glucoside	Ipomoea nil	N
4.	Kaempferol 3-(2''-p-coumarylglucoside) 2''-p-coumarylastragalin	Quercus suber	K
5.	Kaempferol 3-(2''-sinapylglucoside)-7-sophoroside	Brassica napus	K
6.	Kaempferol 3-(2'',3''-diacetyl-4''-(Z)-p-coumaryl-6''-(E)-p-coumarylglucoside)	Quercus suber	K
7.	Kaempferol 3-(2'''-(E)-caffeoylglucosyl)-(1->2)-glucoside-7-cellobioside	Brassica oleracea	K
8.	Kaempferol 3-(2'''-(E)-caffeylsophoroside)-7-glucoside	Brassica oleracea	K
9.	Kaempferol 3-(2'''-(E)-p-coumarylsophoroside)-7-glucoside	Brassica oleracea	K
10.	Kaempferol 3-(2G-glucosylrutinoside) Kaempferol 3-(6'''-rhamnosyl-2'''-glucosyl-glucoside)	Prunus avium	K
11.	Kaempferol 3-(3'',4''-diacetyl-2'',6''-di-(E)-p-coumarylglucoside)	Quercus suber	K
12.	Kaempferol 3-(4''-acetyl-6''-p-coumarylglucoside)	Quercus suber	K
13.	Kaempferol 3-(6''-acetylglucosyl)-(1->3)-galactoside Ricinitin	Ricinus communis	K
14.	Kaempferol 3-[2'''-(E)-ferulylsophoroside]-7-glucoside	Brassica oleracea	K
15.	Kaempferol 3-apiosyl-(1->2)-glucoside	Cicer arietinum	K
16.	Kaempferol 3-feruloyl-sophoroside	Brassica napus Brassica oleracea Brassica rapa	N N N
17.	Kaempferol 3-galactoside-7-rhamnoside	Arabidopsis thaliana	K
18.	Kaempferol 3-galactosyl-7-diglucoside	Prunus persica	N
19.	Kaempferol 3-gentiobioside Kaempferol 3-O-gentiobioside Kaempferol 3-O-β-D-gentiobioside	Glycine max	K, N
20.	Kaempferol 3-gentiobioside-7-rhamnoside Kaempferol 3-glucoside-(1->6)-glucoside-7-α-L-rhamnoside	Arabidopsis thaliana	K
21.	Kaempferol 3-glucoside Kaempferol 3-O-β-D-glucoside Kaempferol 3-O-β-D-glucopyranoside Astragalin	Cicer arietinum Daucus carota Fragaria vesca Glycine max Lotus japonicus Nelumbo nucifera Nicotiana tabacum Phaseolus vulgaris Rosa chinensis Spinacia oleracea Vitis vinifera	T D 4 D K P, T D 3 P D D, P
22.	Kaempferol 3-glucosyl-7-arabinoside	Raphanus sativus	N
23.	Kaempferol 3-glucosyl-7-diglucoside	Prunus persica	N
24.	Kaempferol 3-glucuronide Kaempferol-3-β-D-glucuronide Kaempferol 3-O-β-D-glucuronide	Fragaria vesca Nelumbo nucifera Phaseolus vulgaris Vigna radiata	4 D, N, T K, T K, N
25.	Kaempferol 3-neohesperidoside Kaempferol 3-O-β-D-neohesperidoside	Glycine max	N
26.	Kaempferol 3-O-(2,6-di-O-α-L-rhamnopyranosyl)-β-D-galactopyranoside Mauritianin	Chenopodium quinoa	K
27.	Kaempferol 3-O-(2'',6''-di-(E)-p-coumaroyl)-β-glucopyranoside	Quercus suber	P

28.	Kaempferol 3-O-(3'',4"-diacetyl-2",6"-di-(E)-p-coumaroyl)-glucoside	Quercus suber	P
29.	Kaempferol 3-O-[α-L-rhamnopyranosyl(1->2)-β-D-glucopyranosyl]-7-O-α-L-rhamnopyranoside	Arabidopsis thaliana	N
30.	Kaempferol 3-O-D-galactoside	Nelumbo nucifera	P, N
	Kaempferol 3-O-α-L-galactoside	Nicotiana tabacum	2
	Kaempferol 3-O-β-D-galactoside	Prunus persica	N
	Kaempferol 3-O-β-D-galactopyranoside	Zea mays	N
	Trifolin		
31.	Kaempferol 3-O-digalactopyranoside	Glycine max	N
32.	Kaempferol 3-O-diglucopyranoside	Glycine max	N
33.	Kaempferol 3-O-glucosyl-gentiobioside	Glycine max	N
34.	Kaempferol 3-O-glucosyl-rutinoside	Glycine max	N
35.	Kaempferol 3-O-neohesperidoside	Glycine max	N
		Gossypium hirsutum	N
36.	Kaempferol 3-O-rhamnosyl-gentiobioside	Glycine max	N
37.	Kaempferol 3-O-rhamnosyl-rutinoside	Glycine max	N
38.	Kaempferol 3-O-robinobioside	Nelumbo nucifera	P
39.	Kaempferol 3-O-robinoside-7-O-rhamnoside	Amborella	6
	Robinin	trichopoda	D
		Nelumbo nucifera	D
		Vigna radiata	
40.	Kaempferol 3-O-rutinoside	Nelumbo nucifera	P
	Kaempferol 3-O-β-rutinoside	Phaseolus vulgaris	3
	Kaempferol 3-O-(α-L-rhamnopyranosyl(1->6)-β-D-glucopyranoside	Prunus mume	7
		Ricinus communis	D, K
	Nicotiflorin	Ziziphus jujuba	P
	Nicotifloroside		
41.	Kaempferol 3-O-sophoroside	Brassica napus	N
	Kaempferol 3-O-β-sophoroside	Brassica oleracea	N
	Kaempferol 3-O-β-D-sophoroside	Brassica rapa	N
	Sophoraflavonoloside	Glycine max	K, N
		Solanum tuberosum	D
		Vigna angularis	N
		Vigna radiata	N
42.	Kaempferol 3-O-sophoroside-7-O-β-D-glucopyranoside	Brassica rapa	K
43.	Kaempferol 3-O-α-L-rhamnopyranosyl (1->6)-β-D-glucopyranoside	Nelumbo nucifera	N
44.	Kaempferol 3-O-β-D-diglucoside	Prunus persica	N
45.	Kaempferol 3-O-β-D-glucopyranoside-7-O-α-L-rhamnopyranoside	Arabidopsis thaliana	N
46.	Kaempferol 3-O-β-D-glucopyranosyl-7-O-α-L-rhamnopyranoside	Arabidopsis thaliana	N
47.	Kaempferol 3-O-β-D-glucuronopyranosyl methyl ester	Nelumbo nucifera	N
48.	Kaempferol 3-O-β-D-glycoside	Nicotiana tabacum	2
49.	Kaempferol 3-O-β-D-xylopyranoside	Ricinus communis	D, N
50.	Kaempferol 3-rhamnoglucoside	Nicotiana tabacum	N
	Kaempferol 3-O-rhamnoglucoside	Phoenix dactylifera	5
51.	Kaempferol 3-rhamnoside	Raphanus sativus	K
	Kaempferol 3-O-rhamnoside	Rosa chinensis	P
	Kaempferol 3-O-α-rhamnoside		
	Kaempferol 3-O-α-L-rhamnopyranoside		
	Afzelin		
52.	Kaempferol 3-rutinosyl-4'-diglucoside	Prunus avium	N
53.	Kaempferol 3-sinapoyl-sophoroside	Brassica napus	N
		Brassica oleracea	N

	Brassica rapa	N
54. Kaempferol 3-sophoroside-7-cellobioside	Brassica oleracea	K
55. Kaempferol 3-sophoroside-7-glucoside	Brassica napus Brassica oleracea Brassica rapa	N N N
56. Kaempferol 3-sophoroside-7-rhamnoside	Solanum tuberosum	K
57. Kaempferol 3-sophoroside-rhamnoside	Solanum tuberosum	D
58. Kaempferol 3-sophorotrioside-7-rhamnoside	Solanum tuberosum	K
59. Kaempferol 3-triglucoside-7-rhamnoside	Solanum tuberosum	D
60. Kaempferol 3-xyloside	Ricinus communis	K
61. Kaempferol 3-β-D-glucuronopyranoside	Phaseolus vulgaris	N
62. Kaempferol 3,4'-diglucoside Kaempferol 3,4'-di-O-β-D-glucopyranoside	Prunus avium	K
63. Kaempferol 3,4'-dimethyl ether	Arabidopsis thaliana	N
64. Kaempferol 3,7-diglucoside Kaempferol 3,7-di-O-β-D-glucoside Kaempferol 3,7-O-β-D-diglucopyranoside Kaempferol 3,7-di-O-β-D-glucopyranoside	Arabidopsis thaliana Brassica napus Brassica rapa	P N N
65. Kaempferol 3,7-dirhamnoside Kaempferitrin	Arabidopsis thaliana Lotus japonicus Raphanus sativus	D, P K K
66. Kaempferol 4'-methyl ether Kaempferide	Populus trichocarpa Raphanus sativus	N N
67. Kaempferol 7-glucoside Kaempferol 7-O-glucoside Populnin	Cicer arietinum Vitis vinifera	T D
68. Kaempferol 7-O-rutinoside	Prunus mume	7
69. Kaempferol 7-O-β-d-glucopyranoside	Nelumbo nucifera	P
70. Kaempferol 7-rhamnoside Kaempferol 7-O-rhamnoside Kaempferol 7-O-α-L-rhamnopyranoside	Phaseolus vulgaris Vigna angularis Vigna radiata	K N N
71. Kaempferol 7-α-L-arabinoside	Raphanus sativus	K
72. Kaempferol 7,4'-dimethoxy ether	Raphanus sativus	N
73. Kaempferol sinapoyl-trihexoside	Brassica napus	1

Sources: (D) Dr. Duke; (K) KNApSAcK; (N) NAPRALERT; (P) NPASS; (T) IMPPAT; (1) Auger et al., 2010; (2) Chen et al., 2013; (3) Ganesan & Xu, 2017; (4) Gasperotti et al., 2015; (5) Khallouki et al., 2018; (6) Wu et al., 2019 ; (7) Zhang et al., 2015.

Table 80

Similar and derivative compounds of myricetin synthesized by plants in the data set.

Compound Name(s)	Species	Source(s)
1. 3'-O-Methylmyricetin Laricitrin	Medicago truncatula	K
2. Dihydromyricetin Ampelopsin	Capsicum annuum	K
3. Myricetin 3-glucoside Myricetin 3-O-glucoside Myricetin 3-O-β-D-glucoside Myricetin 3-O-β-D-glucopyranoside Isomyricitrin	Nelumbo nucifera Phaseolus vulgaris Vitis vinifera	P K, 1 N
4. Myricetin 3-glucuronide	Nelumbo nucifera	P

	Myricetin 3-O-β-D-glucuronide	Vitis vinifera	N
5.	Myricetin 3-O-rhamnoside	Phaseolus vulgaris	1
6.	Myricetin 3-O-β-D-galactopyranoside	Nelumbo nucifera Vitis vinifera	P P
7.	Myricetin 3',5'-dimethyl ether Syringetin	Nelumbo nucifera	P
8.	Syringetin 3-O-glucoside Syringetin 3-O-β-D-glucopyranoside	Nelumbo nucifera	N, P

Sources: (K) KNApSAcK; (N) NAPRALERT; (P) NPASS; (1) Ganesan & Xu, 2017

Table 81

Similar and derivative compounds of quercetin synthesized by plants in the data set.

Compound Name(s)		**Species**	**Source(s)**
1.	Dihydroquercetin Taxifolin Distylin	Asparagus officinalis Capsicum annuum Daucus carota Fragaria vesca Glycine soja Medicago truncatula Momordica charantia Nelumbo nucifera Nicotiana tabacum Olea europaea Prunus avium Zea mays	K K K 5 P K K P 2 6 K K
2.	Dihydroquercetin 3-O-rhamnoside Taxifolin 3-O-rhamnoside	Phoenix dactylifera	7
3.	Isorhamnetin 3-galactoside Isorhamnetin 3-O-galactoside	Beta vulgaris Phaseolus vulgaris Prunus mume	P K 10
4.	Isorhamnetin 3-glucoside Isorhamnetin 3-O-glucoside	Amborella trichopoda Brassica napus Fragaria vesca Nelumbo nucifera Phoenix dactylifera Quercus suber	9 1 5 P 7 P
5.	Isorhamnetin 3-O-neohesperidoside	Prunus mume	10
6.	Isorhamnetin 3-O-rhamnoglucoside	Phoenix dactylifera	7
7.	Isorhamnetin 3-O-rhamnoside	Prunus mume	K, P
8.	Isorhamnetin 3-O-rutinoside	Amborella trichopoda Prunus mume	9 10
9.	Isorhamnetin 7-O-rutinoside	Prunus mume	10
10.	Isorhamnetin dihexoside	Brassica napus	1
11.	Isorhamnetin hexoside-sulfate	Brassica napus	1
12.	Isorhamnetin sinapoyl-trihexoside	Brassica napus	1
13.	Quercetin 3-(2'''-(E)-caffeylsophoroside]-7-glucoside	Brassica oleracea	K
14.	Quercetin 3-(6''-malonylglucoside)-7-glucoside	Lactuca sativa	K
15.	Quercetin 3-[2'''-(E)-feruloylsophoroside]-7-glucoside	Brassica oleracea	K
16.	Quercetin 3-2G-rhamnosylrutinoside Manghaslin	Glycine max	K
17.	Quercetin 3-acetylglucoside	Fragaria vesca	5
18.	Quercetin 3-arabinoside	Juglans regia	D
19.	Quercetin 3-D-xyloside Quercetin 3-O-xyloside	Malus domestica	D

20.	Quercetin 3-diglucoside	Nicotiana tabacum	D
	Quercetin 3-O-diglucoside	Prunus persica	N
	Quercetin 3-O-β-D-diglucoside	Ziziphus jujuba	N
21.	Quercetin 3-galactoside	Juglans regia	D
	Quercetin 3-O-galactoside	Malus domestica	D
	Quercetin 3-β-galactoside	Musa acuminata	K
	Quercetin 3-O-β-D-galactoside	Nelumbo nucifera	K, P
	Quercetin 3-O-galactopyranoside	Nicotiana tabacum	2
	Quercetin 3-β-galactopyranoside	Phaseolus vulgaris	4
	Quercetin 3-O-β-D-galactopyranoside	Phoenix dactylifera	7
	Hyperin	Rosa chinensis	P
	Hyperoside	Theobroma cacao	K
		Ziziphus jujuba	P
22.	Quercetin 3-gentiobioside	Glycine max	K
		Papaver somniferum	D, K, N
23.	Quercetin 3-glucoside	Asparagus officinalis	P
	Quercetin 3-O-glucoside	Brassica napus	1
	Quercetin 3-O-β-glucoside	Cicer arietinum	T
	Quercetin 3-O-β-D-glucoside	Daucus carota	D
	Quercetin 3-O-β-D-glucopyranoside	Fragaria vesca	5
	Isoquercetin	Glycine max	D
	Isoquercitrin	Gossypium hirsutum	K, N
	Hirsutrin	Juglans regia	T
		Lactuca sativa	T
		Lotus japonicus	K
		Momordica charantia	K
		Musa acuminata	K
		Nelumbo nucifera	K, P, T
		Nicotiana tabacum	D
		Papaver somniferum	D
		Phaseolus vulgaris	T, 4
		Phoenix dactylifera	7
		Prunus mume	P, 10
		Quercus suber	P
		Ricinus communis	D, K, T
		Rosa chinensis	P
		Solanum tuberosum	D, K
		Theobroma cacao	T
		Vigna radiata	D
		Vitis vinifera	P
		Ziziphus jujuba	P
24.	Quercetin 3-glucosilarabinoside	Fragaria vesca	5
25.	Quercetin 3-glucuronide	Fragaria vesca	5
	Quercetin 3-O-glucuronide	Nelumbo nucifera	D
	Miquelianin	Phaseolus vulgaris	D
		Vitis vinifera	N
26.	Quercetin 3-methyl ether	Beta vulgaris	P
	3-O-methylquercetin	Carica papaya	P
27.	Quercetin 3-O-(2,6-di-α-L-rhamnopyranosyl)-β-D-galactopyranoside	Chenopodium quinoa	N
28.	Quercetin 3-O-[6''-O-rhamnosyl-glucoside] 7-O-rhamnoside	Arabidopsis thaliana	K
29.	Quercetin 3-O-glucosyl-galactoside	Juglans regia	N
		Ziziphus jujuba	N
30.	Quercetin 3-O-methyl-ether	Phaseolus vulgaris	D
31.	Quercetin 3-O-neohesperidoside	Glycine max	K
		Gossypium hirsutum	N
		Prunus mume	K, N, P
		Zea mays	K
32.	Quercetin 3-O-rhamnosyl(1->6)-galactoside	Prunus mume	N
33.	Quercetin 3-O-rutinoside	Asparagus officinalis	D, K, P

	Rutin	Carica papaya	K
		Citrus sinensis	D
		Cucumis melo	D, P
		Cynara cardunculus	D
		Glycine max	D
		Lotus japonicus	P
		Malus domestica	D
		Momordica charantia	K
		Musa acuminata	K
		Nelumbo nucifera	D
		Nicotiana tabacum	D, P
		Olea europaea	D, 6
		Phaseolus vulgaris	4
		Phoenix dactylifera	D, 7
		Prunus mume	K
		Ricinus communis	D
		Solanum lycopersicum	K D, K
		Solanum tuberosum	D
		Spinacia oleracea	D
		Theobroma cacao	P
		Vigna angularis	D
		Vigna radiata	D
		Vitis vinifera	D, K, P
		Ziziphus jujuba	
34.	Quercetin 3-O-α-L-arabinopyranoside Guaijaverin Guajavarin	Theobroma cacao	N
35.	Quercetin 3-O-α-L-rhamnopyranosyl-7-O-β-D-glucopyranoside	Capsicum annuum	N
36.	Quercetin 3-O-α-L-rhamnosyl-glucoside	Manihot esculenta	N
37.	Quercetin 3-O-β-D-2-glucosyl-rutinoside	Glycine max	D
38.	Quercetin 3-O-β-D-glucopyranosyl-7-O-α-L-rhamnopyranoside	Arabidopsis thaliana	K
39.	Quercetin 3-O-β-D-xylopyranoside Reynoutrin	Malus domestica Ricinus communis	D D, K
40.	Quercetin 3-O-β-robinoside 7-O-α-L-rhamnopyranoside	Phaseolus vulgaris	D
41.	Quercetin 3-rhamnoglucoside	Malus domestica	D
42.	Quercetin 3-rhamnoside Quercetin 3-O-rhamnoside Quercetin 3-O-rhamnopyranoside Quercitrin	Arabidopsis thaliana Capsicum annuum Daucus carota Glycine max Juglans regia Malus domestica Nicotiana tabacum Olea europaea Raphanus sativus Ricinus communis Rosa chinensis Solanum lycopersicum Solanum tuberosum Spinacia oleracea	T K, P D D D D D D, 6 K D P K D D
43.	Quercetin 3-rhamnoside-7-glucoside	Capsicum annuum	K
44.	Quercetin 3-rhamnosyl-(1->6)-(2''-acetylglucoside)	Prunus avium Prunus mume	K K
45.	Quercetin 3-rutinoside-4'-glucoside	Prunus avium	K
46.	Quercetin 3-rutinoside-7-glucoside	Nicotiana tabacum	K
47.	Quercetin 3-sophoroside Quercetin 3-O-sophoroside	Brassica oleracea Glycine max	N K, N

	Quercetin 3-O-β-D-sophoroside Baimaside	Vigna radiata	K, N
48.	Quercetin 3-sophoroside-7-glucoside	Brassica napus Brassica oleracea	K K
49.	Quercetin 3,3'-diglucoside	Zea mays	K
50.	Quercetin 3,3'-dimethyl ether	Nicotiana tabacum	D
51.	Quercetin 3,4-diglucoside	Fragaria vesca	5
52.	Quercetin 3,4'-diglucoside	Solanum lycopersicum	P
53.	Quercetin 3,4'-dimethyl ether 3',4'-Dimethoxyquercetin Dillenetin	Vigna unguiculata	N
54.	Quercetin 3,5,3',4'-tetramethyl ether	Gossypium hirsutum	K
55.	Quercetin 3,5,7,4'-tetramethyl ether	Gossypium hirsutum	K
56.	Quercetin 3,7-di-O-α-L-rhamnopyranoside	Arabidopsis thaliana	K
57.	Quercetin 3,7-diglucoside Quercetin 3,7-di-O-β-D-glucoside Quercetin 3,7-O-β-diglucopyranoside Quercetin 3,7-di-O-β-D-glucopyranoside 7-O-β-D-glucopyranosyl-quercetin-3-O-β-D-glucopyranoside	Brassica napus Brassica rapa Solanum lycopersicum Zea mays	N N, P P D, K, P
58.	Quercetin 3,7-dimethyl ether 5-glucoside	Zea mays	K
59.	Quercetin 3'-glucoside	Gossypium arboreum Gossypium hirsutum Helianthus annuus	K K D
60.	Quercetin 3'-methyl ether 3'-O-Methylquercetin Isorhamnetin	Amborella trichopoda Brassica oleracea Cicer arietinum Lotus japonicus Nelumbo nucifera Nicotiana tabacum Prunus avium Prunus mume Raphanus sativus	9 K K, T P P D M 10 K
61.	Quercetin 4-O-β-D-glucoside	Ipomoea nil	N
62.	Quercetin 4'-methyl ether 4'-Methoxyquercetin Tamarixetin	Raphanus sativus	K
63.	Quercetin 4'-O-β-D-glucopyranoside Spiraeoside		
64.	Quercetin 7-methyl ether 7-Methoxyquercetin 7-O-Methxyl quercetin Rhamnose Rhamnetin	Sesamum indicum	P
65.	Quercetin 7-O-glucoside	Olea europaea	6
66.	Quercetin 7-O-β-D-glucoside Quercimeritrin	Helianthus annuus	D
67.	Quercetin 7,4'-di-O-β-D-glucopyranoside	Solanum lycopersicum	P
68.	Quercetin dihexoside	Brassica napus	1
69.	Quercetin glucuronide	Phaseolus vulgaris Rosa chinensis Vitis vinifera	P P P
70.	Quercetin hexoside	Beta vulgaris Theobroma cacao	8 3

Sources: (D) Dr. Duke; (K) KNApSAcK; (M) Microbiome; (N) NAPRALERT; (P) NPASS; (T) IMPPAT; (1) Auger et al., 2010; (2) Chen et al., 2013; (3) Gallego et al., 2019; (4) Ganesan & Xu, 2017; (5) Gasperotti et al., 2013; (6) Hashmi et al., 2015; (7) Khallouki et al., 2018; (8) Vissers et al., 2017; (9) Wu et al., 2019; (10) Zhang et al., 2015

Flavones

Table 82

Similar and derivative compounds of apigenin synthesized by plants in the data set.

	Compound Name(s)	Species	Source(s)
1.	6-Hydroxyapigenin Scutellarin	Fragaria vesca	P
2.	Apigenin 4'-methyl ether Acacetin	Populus trichocarpa	N
3.	Apigenin 4'-O-rhamnosyl-glucoside	Olea europaea	N
4.	Apigenin 4'-O-β-D-glucoside	Daucus carota	D, N
5.	Apigenin 4',7-diglucoside	Cynara cardunculus	D
6.	Apigenin 5-O-β-D-glucoside	Daucus carota	N
7.	Apigenin 6-C-glucoside Isovitexin	Cucumis sativus Jatropha curcas Nelumbo nucifera Theobroma cacao Vigna angularis Vigna radiata Zea mays Ziziphus jujuba	K D P K P K K P
8.	Apigenin 6-C-α-L-arabinopyranoside-8-C-β-D-glucopyranoside Isoschaftoside	Capsicum annuum Nelumbo nucifera	K P
9.	Apigenin 6-C-β-D-glucopyranosyl-8-C-α-L-arabinopyranoside Schaftoside	Capsicum annuum	N
10.	Apigenin 6,8-di-C-glucoside Vicenin II	Cucumis sativus Fragaria vesca Medicago truncatula Olea europaea Ziziphus jujuba	K P K 4 P
11.	Apigenin 7-apioglucoside Apiin	Capsicum annuum Lupinus angustifolius	D 1
12.	Apigenin 7-di-O-xyloside Apigenin 7-di-O-β-D-xyloside	Olea europaea	D, N
13.	Apigenin 7-galactomannoside	Daucus carota	N
14.	Apigenin 7-glucoside Apigenin 7-O-glucoside Apigenin 7-O-β-D-glucoside Apigenin 7-O-β-D-glucopyranoside Apigetrin Cosmosiin	Asparagus officinalis Capsicum annuum Cynara cardunculus Daucus carota Fragaria vesca Olea europaea Phaseolus vulgaris Theobroma cacao	K K D D, K P D, 4 3 D, K
15.	Apigenin 7-glycoside	Cucumis melo	6
16.	Apigenin 7-methyl-glucuronide	Cynara cardunculus	N
17.	Apigenin 7-neohesperidoside	Lupinus angustifolius	1
18.	Apigenin 7-O-(6''-O-para-coumaroyl-	Cucumis sativus	N

	glucoside)		
19.	Apigenin 7-O-apiofuranosyl(1->2)-β-D-glucoside	Lactuca sativa	N
20.	Apigenin 7-O-α-L-rhamno-glucoside	Citrus sinensis	N
21.	Apigenin 7-O-β-D-galactomannoside	Daucus carota	D
22.	Apigenin 7-O-β-D-glucosyl-6-C-glucoside	Cucurbita pepo	N
23.	Apigenin 7-rutinoside Apigenin 7-O-rutinoside Apigenin 7-O-β-D-rutinoside Isorhoifolin	Cynara cardunculus Daucus carota Olea europaea	D D, K 4
24.	Apigenin 7,4'-dimethyl ether	Populus trichocarpa	N
25.	Apigenin 8-C-glucoside Vitexin	Beta vulgaris Cucumis sativus Glycine max Jatropha curcas Nelumbo nucifera Theobroma cacao Vigna angularis Vigna radiata Ziziphus jujuba	P K D, K D P D, K P K P
26.	Apigenin 8-C-glucoside-2'-rhamnoside Vitexin 2'-O-rhamnoside	Glycine max	D
27.	Apigenin C-diglucoside	Phoenix dactylifera	5
28.	Apigenin di-C-glycoside	Lupinus angustifolius	N
29.	Apigenin hexoside	Theobroma cacao	2
30.	Apigenin trimethyl ether	Citrus sinensis	N
31.	Apigeninidin	Sorghum bicolor Zea mays	K N
32.	Trimethylapigenin	Citrus sinensis	P

Sources: (D) Dr. Duke; (K) KNApSAcK; (N) NAPRALERT; (P) NPASS; (1) Dueñas et al., 2009; (2) Gallego et al., 2019; (3) Ganesan & Xu, 2017; (4) Hashmi et al., 2015; (5) Khallouki et al., 2018; (6) Mallek-Ayadi et al., 2017.

Table 83

Similar and derivative compounds of luteolin synthesized by plants in the data set.

Compound Name(s)		**Species**	**Source(s)**
1.	2''-O-α-L-rhamnosyl-6-C-fucosyl-3'-methoxyluteolin	Zea mays	N
2.	2''-O-α-L-rhamnosyl-6-C-fucosyl-luteolin	Zea mays	N
3.	2''-O-α-L-rhamnosyl-6-C-quinovosyl-luteolin	Zea mays	N
4.	Luteolin 3'-methyl ether Chrysoeriol	Amborella trichopoda Fragaria vesca Olea europaea Phoenix dactylifera Zea mays Ziziphus jujuba	6 P 3 4 K P
5.	Luteolin 3'-methyl ether 7-O-glucoside Chrysoeriol 7-O-glucoside	Olea europaea Phoenix dactylifera	3 4
6.	Luteolin 3'-methyl ether 7-O-rhamnoglucoside Chrysoeriol 7-O-rhamnoglucoside	Phoenix dactylifera	4
7.	Luteolin 3'-O-β-D-glucoside	Cynara cardunculus	D

8.	Luteolin 4-β-D-glucoside	Cynara cardunculus	D
9.	Luteolin 4'-glucoside	Cynara cardunculus	D
	Luteolin 4'-O-glucoside	Daucus carota	D
	Luteolin 4'-β-D-glucoside	Olea europaea	D, N
	Luteolin 4'-O-β-D-glucoside		
	Luteolin 4'-O-β-D-glucopyranoside		
	Juncein		
10.	Luteolin 4'-methyl ether	Amborella trichopoda	6
	4'-Methylluteolin	Nelumbo nucifera	P
	Diosmetin	Olea europaea	3
11.	Luteolin 4'-sulfate	Daucus carota	K, T
12.	Luteolin 4',7-diglucoside	Cynara cardunculus	D
13.	Luteolin 5-glucoside	Olea europaea	D
14.	Luteolin 6-C-glucoside	Nelumbo nucifera	P
	Luteolin 6-C-β-D-glucopyranoside		
	Homoorientin		
	Isoorientin		
15.	Luteolin 7-gentiobioside	Cynara cardunculus	D
16.	Luteolin 7-glucoside	Cajanus cajan	D
	Luteolin 7-O-glucoside	Capsicum annuum	D, P
	Luteolin 7-O-β-D-glucoside	Cynara cardunculus	D
	Cynaroside	Fragaria vesca	P
	Glucoluteolin	Lupinus angustifolius	1
	Luteoloside	Nelumbo nucifera	D, P
		Olea europaea	D, 3
		Prunus mume	P
		Theobroma cacao	D
17.	Luteolin 7-glycoside	Cucumis melo	5
18.	Luteolin 7-O-(2-apiofuranosyl-4-glucopyranosyl-6-malonyl) glucopyranoside	Capsicum annuum	K
19.	Luteolin 7-O-(6''-malonylglucoside)	Daucus carota	K
20.	Luteolin 7-O-glucuronic acid	Fragaria vesca	P
21.	Luteolin 7-O-rhamnoglucoside	Phoenix dactylifera	4
22.	Luteolin 7-O-β-glucuronide	Daucus carota	D, K, N
	Luteolin 7-O-β-D-glucuronide		
23.	Luteolin 7-rutinoside	Cynara cardunculus	D
	Luteolin 7-O-rutinoside	Daucus carota	D, K
	Luteolin 7-O-β-rutinoside	Olea europaea	3
	Luteolin 7-O-β-D-rutinoside	Phoenix dactylifera	D, N
24.	Luteolin 7-β-rutinoside	Cynara cardunculus	D
25.	Luteolin 7,4-O-diglucoside	Olea europaea	3
26.	Luteolin 8-C-glucoside	Beta vulgaris	P
	Luteolin 8-C-β-D-glucopyranoside	Capsicum annuum	P
	Lutexin	Cucumis melo	K
	Orientin	Nelumbo nucifera	P
		Theobroma cacao	K
27.	Luteolin glucopyranosyl acetate	Lupinus angustifolius	1
28.	Luteolin hexoside	Theobroma cacao	2

Sources: (D) Dr. Duke; (K) KNApSAcK; (N) NAPRALERT; (P) NPASS; (T) IMPPAT; (1) Dueñas et al., 2009; (2) Gallego et al., 2019; (3) Hashmi et al., 2015; (4) Khallouki et al., 2018; (5) Mallek-Ayadi et al., 2017; (6) Wu et al., 2019

GitHub

All of the files are hosted on GitHub at https://github.com/mbagg4152/pfpy/tree/master/projects/mh/. The README for the repository can be found here: https://github.com/mbagg4152/pfpy#readme.

Script Files

Main file: keggv3.py

```
# custom project library imports
from flib.fconstants import *
from flib.data_types import *
import flib.prediction_logic as predict

# other library imports
from urllib import request
from urllib.error import HTTPError, URLError
import datetime
import sys
import threading

sys.path.append(os.getcwd().replace(os.sep + 'flavonoid', ''))
from sharedlib.regexlines import *

try:
  import bioservices
  from bioservices.kegg import KEGG
except ImportError as e:
  print('Program needs bioservices in order to work. In the terminal, try:\n'
        '`pip3 install bioservices` or `pip install bioservices`')
  print(e)
  exit(1)

####################
# Global Variables #
####################
init_time = datetime.datetime.now()  # get time of program execution
kegg = KEGG()  # used to access KEGG's functions from bioservices

# The lists are used for processing/accessing data as well as making output files.
all_genes = []
ec_collections = []
pathgenes = []
plant_matrix = []
plant_objects = []
plant_pathways = []

# The locks are to protect the values of the global variables when using multithreading.
lock_ec = threading.Lock()
lock_gene = threading.Lock()
lock_kegg = threading.Lock()
```

```
lock_plant = threading.Lock()
lock_dbget = threading.Lock()

# These will hold the file path values for the programs outputs and current
# and project directory.
path_chem = ''
path_cwd = ''
path_fasta = ''
path_gene = ''
path_main = ''
path_raw_gene = ''
path_raw_fasta = ''

thread_lim = 5  # The max number of processor threads to be used by program.


def main():
  """
  This is the main function of the file which calls specific functions in order when
  running and displays the total run time at the end of the code execution.
  """
  setup()
  get_parse_pathway_genes()
  flavonoid_predictions()
  make_plant_ec_counts()
  build_nt_fasta_by_ec()

  runtime = datetime.datetime.now() - init_time
  print('\nRun time: ' + str(runtime))


def setup():
  """
  This is the initial setup function for the program. If the user supplies a directory
  name in the command line args, then that name will be used when outputting the data.
  If no name is supplied, then the data is outputted to the directory named data. This
  function also creates the list of pathway and plant codes based on the KEGG codes
  that can be found in the JSON files. After making the list, it creates a list of plant
  objects that will be used throughout the program.
  """

  # Make sure global values can be used and updated
  global path_chem
  global path_cwd
  global path_fasta
  global path_gene
  global path_main
  global path_raw_gene
  global plant_objects
  global plant_pathways
  global path_raw_fasta

  # Check if user supplied directory name as a commandline argument.
  # if not, default to 'data'
  opt_dir_name = ''
  if len(sys.argv) > 1:  # Alternate directory name supplied by user
     opt_dir_name = sys.argv[1]  # Get directory name
```

```
    else:
        print('No directory name supplied, defaulting to `data`. '
              'Supply name using `python3 keggv2.py dir_name`')
        opt_dir_name = 'data'

    # Update the global path values based on user decision
    path_cwd = os.getcwd() + SEP
    path_main = path_cwd + opt_dir_name
    path_chem = path_main + DIR_CHEM
    path_fasta = path_main + DIR_FASTA
    path_gene = path_main + DIR_GENE
    path_raw_gene = path_main + DIR_RGENE
    path_raw_fasta = path_main + DIR_RFASTA

    #  Initialize the output directories if they don't exist
    init_dir(path_main)
    init_dir(path_gene)
    init_dir(path_fasta)
    init_dir(path_chem)
    init_dir(path_raw_gene)
    init_dir(path_raw_fasta)

    # Combines plant and pathway codes.
    plant_pathways = [i + j for i in plant_list for j in path_map_list]

    # Go through the list of plants and create a Plant object which will store
    # related predictions.
    for key in plant_dict:
        # Call constructor to make new plant.
        tmp_plant = Plant(code=key, name=plant_dict[key])

        # Add to list if not present. Prevents duplicates.
        if not tmp_plant.is_in(plant_objects):
            plant_objects.append(tmp_plant)


def get_parse_pathway_genes():
    """
    This function breaks the list of plant pathways into different lists in order for
    different data to be processed at the same time using multithreading. Once all of
    the threads have finished, then the list of genes by path will be looped through
    in order to create both the gene data output files for each pathway and for the
    master file that contains all of the gene information.
    """
    global path_gene
    global plant_objects
    global plant_pathways
    global thread_lim

    # Chunk up the list of plant-pathway codes.
    sub_lists = list_partition(plant_pathways, thread_lim)
    threads = []  # Will be used to keep track of and kill off threads.

    # A thread is made for each sub-list which then passes each sub-list as a parameter
    # to the pathway parser.
    for sub_list in sub_lists:
        thread = threading.Thread(target=path_parse, args=(sub_list,))
```

```
            thread.start()
            threads.append(thread)

        for thread in threads: thread.join()  # Wait for each thread to die before continuing.

        master_output = ''  # Data for the master file which holds all gathered gene data.
        for item in pathgenes:
            tmp_file = path_gene + SEP + item.path + '.csv'
            tmp_output = ''  # Data for current gene's output file.
            for gene in item.genes:
                # Get the formatted string of gene information for the current and master files.
                tmp_output += gene.simple() + '\n'
                master_output += gene.simple() + '\n'
            write_append(tmp_file, tmp_output, write_over=True)
        write_append(path_main + SEP + 'MasterList.csv', master_output, write_over=True)


    def path_parse(paths):
        """
        Given a pathway for a specific plant, the program then passes it to KEGG where it
        retrieves the appropriate entry. The EC number, KO number and each GENE entry are
        parsed from the data sent back by KEGG and then are appropriately saved by updating
        the plant objects.
        """
        for path in paths:
            global pathgenes
            global plant_objects

            print(path)  # Not necessary, but is nice for a gauge of progress.

            with lock_kegg:
                raw = ''

                # Look for local raw gene file to save time by preventing the call to kegg.get().
                try:
                    with open(path_raw_gene + SEP + path + '.csv', 'r') as tmp_read:
                        raw = tmp_read.read()
                        tmp_read.close()

                # No local raw gene data file found so the data must be downloaded.
                except FileNotFoundError:
                    raw = kegg.get(path)
                    with open(path_raw_gene + SEP + path + '.csv', 'w') as tmp_get:
                        try: tmp_get.write(raw)

                        # Error should only ever occur for plant-pathway codes that don't exist.
                        except TypeError: pass
                        tmp_get.close()

                gene_entry = {}
                if isinstance(raw, str):
                    if len(raw) > 0:  # Don't bother parsing the empty entries.
                        kegg_entry = kegg.parse(raw)  # Parses kegg entry into dictionary.
                        gene_entry = kegg_entry.get(GKY)  # Get data from dictionary w/ key `GENE`.

            # If gene_entry is not empty, the statement will succeed. Otherwise ignore blanks.
            if gene_entry:
```

```
plant_code = ''.join(re.split(RE_ALPH, path))  # Plant code is alpha-only.
plant_name = plant_dict.get(plant_code)

with lock_gene:
   pathgenes.append(PathGene(path=path))  # Make new PathGene  & add to list.

for key in gene_entry:
   tmp_entry = gene_entry[key]
   try:
      # Get all EC nums from entry using regular expressions
      ec_nums = re.findall(RE_EC, tmp_entry)

      # Remove unwanted characters and format each EC num.
      for i in range(0, len(ec_nums)):
         item = multi_replace(ec_nums[i], [('[', ''), (']', ''),
                                           (':', ''), (' ', '')])
         ec_nums[i] = 'EC:' + item

      # Find and process the orthology ID.
      orthology = multi_replace(quick_fetch(RE_KO, tmp_entry),
                                [('[', ''), (']', '')])

      # Remove EC & KO in order to get compound name.
      name = re.sub(RE_KO, '', (re.sub(RE_EC, '', tmp_entry)))

      # Call Gene constructor and pass in the parsed values.
      tmp_gene = Gene(gene_id=key, plant=plant_name, ec_nums=ec_nums,
                      path=path, ortho=orthology, compound=name,
                      plant_code=plant_code)
      with lock_gene:
         for pathgene in pathgenes:  # Update list of genes for current path.
            if pathgene.path == path: pathgene.genes.append(tmp_gene)

      with lock_plant:
         for index, plant in enumerate(plant_objects):
            if plant.name == tmp_gene.plant:
               tmp_plant = plant

               # Add to list of plant genes if not present.
               if not tmp_gene.is_in(tmp_plant.genes):
                  tmp_plant.genes.append(tmp_gene)

               # Add to list of all genes if not present.
               if not tmp_gene.is_in(all_genes):
                  all_genes.append(tmp_gene)

               # Update the plant's EC nums. Dupes preferred
               # (for the master count matrix).
               tmp_plant.ec_nums.extend(ec_nums)

               # Update the plant list with the new/additional info
               # for current plant.
               plant_objects[index] = plant

   except IndexError:
      pass  # There was nothing found using regular expressions.
```

```
def flavonoid_predictions():
  """
  This is the function that goes through each plant, looks at the list of EC numbers
  then applies a function in order to determine whether or not the plant has the
  required EC numbers needed to synthesize each compound.
  """

  global plant_objects
  output_list = ''  # Master list of all flavonoids and predicted plants.
  output_yn = ''  # Master list of all flavonoids & a Y/N based on predicted status
  plant_ec_output = ''  # For outputting each plant & EC numbers from their gene entries.
  plant_names = 'Name\n'  # Each plant's name, used in the first line of the Y/N output.

  for plant in plant_objects:
     unique_nums = []
     plant_ec_output += '\n' + plant.name + '\t'
     plant_names = plant_names + plant.name + '\n'

     # Go through the plant's EC nums and add each EC number to the output once.
     for num in plant.ec_nums:
        if num not in unique_nums:
           plant_ec_output += num + '\t'  # Add EC number to the output
           unique_nums.append(num)  # Ensures EC num isn't added to output again.

     for chem_data in flav_data_lists:  # Make the call to the prediction functions.
        if predict.flav_check(getattr(predict, chem_data.code.lower()), unique_nums):
          # Add the name of the plant, if predicted.
          chem_data.plants.append(plant.name)

  # Create the formatted strings for the output prediction file.
  output_yn = plant_names.replace('\n', '\t')
  for key in flav_data_lists:
     save_file([key.plants], key.file_name, path_chem, sep='\n')

     output_list = output_list + '\n' + key.code

     for plant in key.plants:
        output_list = output_list + '\t' + plant

     output_yn = output_yn + '\n' + key.code

     for item in plant_objects:
        if item.name in key.plants:
           output_yn = output_yn + '\tY'
        else:
           output_yn = output_yn + '\tN'

     item_count = len(key.plants)
     print(key.label + ' predicted in ' + str(item_count) + ' organisms.')
  write_append(path_chem+SEP+'_plant-ec-nums.tsv', plant_ec_output, write_over=True)
  write_append(path_chem+SEP+'_predictions_list.tsv', output_list, write_over=True)
  write_append(path_chem+SEP+'_predictions_yn.tsv', output_yn, write_over=True)


def make_plant_ec_counts():
  """
```

```
    This function creates and outputs a 'matrix' relating to each species and EC number
    by running the fill_matrix function on multiple threads. For each gene entry
    containing a specific EC number, the program will increase the counter and display
    it at the end next to the appropriate EC number.
    """
    global plant_objects
    for plant in plant_objects:
        fill_count_matrix(plant)  # Update master matrix using the info from each plant.

    out = ''  # Output string for the master EC count matrix.
    for plant in plant_matrix:
        out += plant.name + ':\t'
        for count in plant.ec_counts:
            # Update with EC num & its occurrence.
            out += str(count.number) + ' (' + str(count.count) + ')\t'
        out += '\n'

    write_append(path_main + SEP + 'MasterECCountMatrix.tsv', out, write_over=True)


def fill_count_matrix(plant):
    """
    This function builds the ec counts for each list.
    """
    global plant_objects
    tmp_plant = plant

    for num in tmp_plant.ec_nums:
        if tmp_plant.has_ec_count(num):
            tmp_plant.incr_ec_count(num)  # Increment EC number's count.
        else:  # Need to create count object for current EC number.
            tmp_count = EcCounts(number=num, count=1)
            plant.ec_counts.append(tmp_count)

    with lock_plant:  # Update the count matrix.
        plant_matrix.append(tmp_plant)


def build_nt_fasta_by_ec():
    """
    This function uses multithreading and the information gathered from running
    run_path_parse in order to get the FASTA/DNA sequence for each of the gene entries
    that were found. As before, the program parses the list after all threads are done
    and then created a FASTA file for each EC number and created the Master FASTA file.
    """

    # Chunk up the list of all plant genes.
    sub_lists = list_partition(all_genes, thread_lim)
    threads = []  # For keeping track of each thread.
    print('getting data for ' + str(len(all_genes)) + ' genes')

    for sub_list in sub_lists:  # Make new thread for each sublist & pass to build_fasta().
        thread = threading.Thread(target=build_fasta, args=(sub_list,))
        thread.start()
        threads.append(thread)

    for thread in threads: thread.join()  # Don't continue until all threads are done.
```

```
    print('Starting to gather data for FASTA files ... ')
    master_fasta = path_main + SEP + 'MasterFASTA.fasta'
    master_output = ''
    for item in ec_collections:  # just to make sure file is cleared before populating
        item.ec_name = item.ec_name.replace('.', '-').replace(':', '')
        tmp_file_path = path_fasta + SEP + item.ec_name + '.fasta'
        write_append(tmp_file_path, '', write_over=True)

    for item in ec_collections:
        item.ec_name = item.ec_name.replace('.', '-').replace(':', '')
        tmp_file_path = path_fasta + SEP + item.ec_name + '.fasta'
        tmp_output = ''

for entry in item.ec_entries:
            # add to string to be printed into specific EC file
            tmp_output += entry.simple() + '\n'

            # add to string to be printed into master FASTA
            master_output += entry.simple() + '\n'

        # write the file for current EC number
        write_append(tmp_file_path, tmp_output, write_over=False)


    # write the master FASTA file
    write_append(master_fasta, master_output, write_over=True)
    print('Done making the FASTA files.')


def build_fasta(genes):
    """
    This function uses the plant code and gene id in order to find the matching FASTA
    sequence using the appropriate dbget url. The pages are saved into memory as HTML
    and are parsed in order to extract the important information from the web page.
    After parsing, the FASTA sequences are added to EcFastaCollection objects in order
    to maintain proper association when writing all of the sequences out to files.
    """
    global ec_collections
    for gene in genes:
        # using the plant code and gene id create a string formatted as code:gene
        combined = gene.plant_code.strip() + ':' + \
                   gene.gene_id.replace('(RAP-DB) ', '').strip()

        # append code-gene string to the end of the dbget incomplete URL
        db_url = URL_DBGET + combined
        url_data = ''
        with lock_dbget:
            tmp_code = gene.plant_code
            tmp_id = gene.gene_id
            try:  # Look for local raw fasta file to save time by not having to download.
                with open(path_raw_fasta + SEP + tmp_code + tmp_id + TF, 'r') as tmp_read:
                    url_data = tmp_read.read()
                    tmp_read.close()

            # No local raw fasta data file found so the data must be downloaded.
            except FileNotFoundError:
```

```
            try:
               # read the html from the dbget url
               with request.urlopen(db_url) as db_site:
                  url_data = db_site.read().decode('utf-8')

               with open(path_raw_fasta+SEP+tmp_code+tmp_id+TF, 'w') as tmp_get:
                  tmp_get.write(url_data)
                  tmp_get.close()

            except (HTTPError, URLError) as url_http_err:
               print('Something went wrong with error ' + url_http_err)
               continue

         # get the header of the FASTA entry using regular expressions,
         # &gt;  is the HTML representation of >
         fasta_header = ''.join(re.findall(RE_NT_HEAD, url_data)).replace('&gt; ', '>')+\
                        ' {' + plant_dict[gene.plant_code.strip()] + '}'

         # get the DNA sequence body using regular expressions
         fasta_body = ''.join(re.findall(RE_NT_SEQ, url_data))

         full_fasta_entry = fasta_header + '\n' + fasta_body  # create FASTA entry string

         tmp_entry = FastaEcEntry(plant=plant_dict.get(gene.plant_code),
                                  gene=gene.gene_id, dna=full_fasta_entry)
         with lock_ec:
            for g in gene.ec_nums:
               tmp_ec = EcFastaCollection(ec_num=g, ec_entries=[tmp_entry])
               ec_collections.append(tmp_ec)


if __name__ == '__main__':
  main()
```

Library file: data_types.py

```
# custom project library import
from flib.fconstants import *


class Flav:
  """
  This class holds the data for each flavonoid. The objects are initialized with their
  file name and label and only later in the program, their empty list of plants will
  be filled.
  ------------------------------------------------------------------------------------
  ATTRIBUTES
  self.label: string that contains the flavonoids name
  self.plants: list of plants predicted to produce the flavonoid
  self.file_name: string that holds the flavonoids output file name
  ------------------------------------------------------------------------------------
  FUNCTIONS
  __init__: constructor for the object
  __eq__: defines equality of the object
  is_in: determines if an identical or nearly identical object is already in the list
  """
```

```
    def __init__(self, label: str, plants: [str], file_name: str, code=''):
        self.plants = plants
        self.label = label
        self.file_name = file_name
        self.code = code

    def __eq__(self, other):
        return self.plants == other.plants and \
               self.label == other.label and \
               self.file_name == other.file_name

    def is_in(self, items):
        for item in items:
            if self == item: return True
        return False


class Plant:
    """
    This object holds information about each plant used in the program. The plant objects
    are initialized with their scientific name and their code and then have different
    information added later.
    ---------------------------------------------------------------------------
    ATTRIBUTES
    self.name: scientific name of the plant
    self.code: KEGG code for the plant
    self.genes: the gene entries for the plant
    self.ec_nums: the EC numbers parsed from the plants gene entries
    self.flavonoids: the list of flavonoids that the plant could potentially produce
    self.ec_counts: list of objects that hold the number of times each EC number appears
    ---------------------------------------------------------------------------
    FUNCTIONS
    __init__: constructor for the object
    __eq__: defines equality of the object
    is_in: determines if an identical or nearly identical object is already in the list
    has_ec_count: used to determine whether or not a specific EC number is already in the
                  list of EC counts
    incr_ec_count: used to increase the count for the EC count objects.
    """

    def __init__(self, name=None, code=None, genes=None, ec_nums=None, flavonoids=None,
                 ec_counts=None):
        self.name = name if name is not None else ' '
        self.code = code if code is not None else ' '
        self.genes = genes if genes is not None else []
        self.ec_nums = ec_nums if ec_nums is not None else []
        self.flavonoids = flavonoids if flavonoids is not None else []
        self.ec_counts = ec_counts if ec_counts is not None else []

    def __eq__(self, other):
        return self.name == other.name and \
               self.code == other.code and \
               self.genes == other.genes and \
               self.ec_nums == other.ec_nums and \
               self.flavonoids == other.flavonoids

    def is_in(self, items):
```

```
        for item in items:
            if self == item: return True
        return False

    def simple(self):
        gstr = ''
        for gene in self.genes: gstr += gene.no_plant() + ' || '
        return self.name + ', ' + self.code + ', ' + gstr + ', ' + \
               str(self.ec_nums) + ', ' + str(self.flavonoids)

    def has_ec_count(self, ec_number):
        for ec in self.ec_counts:
            if ec.number == ec_number: return True
        return False

    def incr_ec_count(self, ec_number):
        for ec in self.ec_counts:
            if ec.number == ec_number:
                ec.count += 1


class PathGene:
    """
    This object is used to hold Gene objects in a way such that they are sorted by the
    pathway from which they were found.
    ---------------------------------------------------------------------------------
    ATTRIBUTES
    self.path: the pathway that resulted in the gene entry
    self.genes: the list of gene entries from this pathway
    ---------------------------------------------------------------------------------
    FUNCTIONS
    __init__: constructor for the object
    __eq__: defines equality of the object
    is_in: determines if an identical or nearly identical object is already in the list
    """

    def __init__(self, path=None, genes=None):
        self.path = path if path is not None else ' '
        self.genes = genes if genes is not None else []

    def __eq__(self, other):
        return self.path == other.path and \
               self.genes == other.genes

    def is_in(self, items):
        for item in items:
            if self == item: return True
        return False


class Gene:
    """
    This object holds data gathered from KEGG for each plant's pathway (like aip00491).
    ---------------------------------------------------------------------------------
    ATTRIBUTES
    self.gene_id: the ID of the gene from a plant
    self.plant: the scientific name of the plant that has this gene
```

```
    self.plant_code: the KEGG code for the plant
    self.compound: the compound name listed in the entry
    self.ec_nums: the list of EC numbers found in the entry
    self.ortho: the KEGG orthology code for the compound
    self.path: the pathway where the gene was found
    ---------------------------------------------------------------------------
    FUNCTIONS
    __init__: constructor for the object
    __eq__: defines equality of the object
    is_in: determines if an identical or nearly identical object is already in the list
    simple: returns a formatted string that contains information from the object
    no_plant: same as simple, but without including the plant name
    """

    def __init__(self, gene_id=None, plant=None, compound=None, ec_nums=None,
                 ortho=None, path=None, plant_code=None):
        self.gene_id = gene_id if gene_id is not None else ' '
        self.plant = plant if plant is not None else ' '
        self.plant_code = plant_code if plant_code is not None else ' '
        self.compound = compound if compound is not None else ' '
        self.ec_nums = ec_nums if ec_nums is not None else []
        self.ortho = ortho if ortho is not None else ' '
        self.path = path if path is not None else ' '

    def __eq__(self, other):
        return self.gene_id == other.gene_id and \
               self.plant_code == other.plant_code and \
               self.ec_nums == other.ec_nums

    def is_in(self, items):
        for item in items:
            if self == item: return True
        return False

    def simple(self):
        return self.plant + ', ' + self.gene_id + ', ' + self.compound + ', ' + \
               str(self.ec_nums) + ', ' + self.ortho

    def no_plant(self):
        return self.gene_id + ', ' + self.compound + ', ' + self.ec_nums + ', ' + self.ortho


class EcFastaCollection:
    """
    This object is used to hold the associated FASTA entries for any given EC number.
    ---------------------------------------------------------------------------
    ATTRIBUTES
    self.ec_name: the EC number & name used when writing the file
    self.ec_entries: the list of associated FASTA entries (FastaEcEntry objects)
    ---------------------------------------------------------------------------
    FUNCTIONS
    __init__: constructor for the object
    __eq__: defines equality of the object
    is_in: determines if an identical or nearly identical object is already in the list
    """

    def __init__(self, ec_num=None, ec_entries=None):
```

```
        self.ec_name = ec_num if ec_num is not None else ' '
        self.ec_entries = ec_entries if ec_entries is not None else []

    def __eq__(self, other):
        return self.ec_name == other.ec_name and \
               self.ec_entries == other.ec_entries

    def is_in(self, items):
        for item in items:
            if self == item: return True
        return False


class EcCounts:
    """
    This object is a property of the Plant object and is used to hold each EC number and
    the number of times it occurs in gene entries of a given plant.
    ---------------------------------------------------------------------------------------
    ATTRIBUTES
    self.number: the EC number
    self.count: number of times that the EC number shows up in gene entries.
    ---------------------------------------------------------------------------------------
    FUNCTIONS
    __init__: constructor for the object
    """

    def __init__(self, number=None, count=None):
        self.number = number if number is not None else ' '
        self.count = count if number is not None else 0


class FastaEcEntry:
    """
    This object is a property of EcFastaCollection and contains the information for a
    specific FASTA entry.
    ---------------------------------------------------------------------------------------
    ATTRIBUTES
    self.gene_id: the gene ID associated with the sequence
    self.plant: the plant that the gene is from
    self.dna_seq: the dna sequence/FASTA entry for the specific gene
    ---------------------------------------------------------------------------------------
    FUNCTIONS
    __init__: constructor for the object
    __eq__: defines equality of the object
    is_in: determines if an identical or nearly identical object is already in the list
    simple: returns a formatted string
    """

    def __init__(self, gene=None, dna=None, plant=None):
        self.gene_id = gene if gene is not None else ' '
        self.dna_seq = dna if dna is not None else ' '
        self.plant = plant if dna is not None else ' '

    def __eq__(self, other):
        return self.gene_id == other.gene_id and \
               self.dna_seq == other.dna_seq and \
               self.plant == other.plant
```

```
  def is_in(self, items):
     for item in items:
        if self == item: return True
     return False

  def simple(self):
     return self.dna_seq
```

Library file: fconstants.py

```
# custom project library imports
from flib.futil import *
from flib.data_types import Flav

# other imports
import os
import sys

SEP = os.sep  # get the right slash. / for linux & mac, \ for windows

# misc strings
CSV = '.csv'
GDATA = 'Gene_data_'
JKEY = 'obj'
NIX = ''
NL = '\n'
SP = ' '
TF = '.txt'
URL_DBGET = 'https://www.kegg.jp/dbget-bin/www_bget?-f+-n+n+'

# output directories
DIR_CHEM = SEP + 'Chemical_Data'
DIR_FASTA = SEP + 'FASTA_Data'
DIR_GENE = SEP + 'Gene_Data'
DIR_RGENE = DIR_GENE + SEP + 'Raw_Gene'
DIR_RFASTA = DIR_FASTA + SEP + 'Raw_FASTA'

# pathways for the json data  (and the name of the json object used in all files)
JSON_DIR = '..' + SEP + 'json_data' + SEP
DIR_FJSON = 'fjson' + SEP

JSON_FLAVS = DIR_FJSON + 'flav_names.json'
JSON_FLAV_REL = DIR_FJSON + 'flav_related.json'
JSON_FLAV_SYN = DIR_FJSON + 'flav_syns.json'
JSON_PATH_DICT = DIR_FJSON + 'path_codes_names.json'
JSON_PATH_LIST = DIR_FJSON + 'path_codes.json'
JSON_PLANT_DICT = DIR_FJSON + 'plant_names_codes.json'
JSON_PLANT_DICT_COMMON = DIR_FJSON + 'plant_names_codes_plus.json'
JSON_PLANT_LIST = DIR_FJSON + 'plant_codes.json'
JSON_TST_MED = DIR_FJSON + 'test_med.json'
JSON_TST_SHORT = DIR_FJSON + 'test_short.json'
JSON_TST_SINGLE = DIR_FJSON + 'test_single.json'
JSON_FLAV_NAMES = DIR_FJSON + 'flav_info.json'

# lists and dictionaries made from JSON files
flav_list = get_json_data(JSON_FLAVS, JKEY)  # list of flavonoids of interest (FOI)
```

```
flav_names_info = get_json_data(JSON_FLAV_NAMES)
flav_relatives = get_json_data(JSON_FLAV_REL)  # relatives of FOI
flav_synonyms = get_json_data(JSON_FLAV_SYN)  # synonyms for FOI
path_map_dict = get_json_data(JSON_PATH_DICT, JKEY)  # pathway names and codes
path_map_list = get_json_data(JSON_PATH_LIST, JKEY)  # pathway codes
plant_dict_common = get_json_data(JSON_PLANT_DICT_COMMON, JKEY)  # common & sci. names
plant_dict_reg = get_json_data(JSON_PLANT_DICT, JKEY)  # scientific names and plant codes
plant_full_list = get_json_data(JSON_PLANT_LIST, JKEY)  # full list of plant codes
test_med = get_json_data(JSON_TST_MED, JKEY)  # testing list of plant codes
test_short = get_json_data(JSON_TST_SHORT, JKEY)  # testing list of plant codes
test_single = get_json_data(JSON_TST_SINGLE, JKEY)  # testing list of plant codes

plant_dict = plant_dict_reg  # variable exists for ease of value change when testing
plant_list = plant_full_list  # variable exists for ease of value change when testing

flav_data_lists = []
for k in flav_names_info:
  info = flav_names_info.get(k)
  tmp_flav = Flav(k, [], info.get('file'), info.get('code'))
  flav_data_lists.append(tmp_flav)

# keys for accessing dictionaries
EKY = 'EC'
GKY = 'GENE'
NKY = 'NTSEQ'
OKY = 'ORTHOLOGY'
PKY = 'PLANT'

README = SEP + 'ReadMe.txt'

# EC numbers
E01 = 'EC:4.3.1.24'
E02 = 'EC:4.3.1.25'
E03 = 'EC:1.14.14.91'
E04 = 'EC:6.2.1.12'
E05 = 'EC:2.3.1.170'
E06 = 'EC:2.3.1.133'
E07 = 'EC:1.14.14.96'
E08 = 'EC:1.14.13•—'
E09 = 'EC:2.3.1.74'
E10 = 'EC:5.5.1.6'
E11 = 'EC:1.14.20.5'
E12 = 'EC:1.14.19.76'
E13 = 'EC:1.14.14.81'
E14 = 'EC:1.14.14.82'
E15 = 'EC:1.14.11.9'
E16 = 'EC:1.14.20.6'
E17_1 = 'EC:1.1.1.219'
E17_2 = 'EC:1.1.1.234'
E17_FULL = 'EC:1.1.1.219 1.1.1.234'
E18 = 'EC:1.14.20.4'
E19 = 'EC:1.3.1.77'
E20 = 'EC:1.17.1.3'
E21 = 'EC:1.14.14.87'
E22 = 'EC:4.2.1.105'
E23 = 'EC:2.4.1.357'
E24 = 'EC:1.3.1.117'
```

```
E_DEC = 'EC:2.3.1.70'
E_GGT = 'EC:2.4.1.74'
E_SOA = 'EC:2.3.1.30'
E_V1G = 'EC:2.4.1.136'
```

Library file: futil.py

```
import json
import os
import re

SEP = os.sep  # get the right slash. / for linux, \ for windows
JKEY = 'obj'


def get_json_data(file_name, key=None):
  """
  This function uses the python JSON library in order to parse JSON files into usable
  python objects. Can return lists or dictionaries, depending on the JSON file's
  structure.
  """

  if key is None: key = JKEY
  data = ''
  try:
     with open(file_name) as jsonFile:
        data = json.load(jsonFile)
  except FileNotFoundError:
     file_name = '..' + SEP + file_name
     with open(file_name) as jsonFile:
        data = json.load(jsonFile)
  return data[key]


def remove_dupes(dupe_list):
  """
  removes duplicate elements
  """
  unique_list = []  # creates an empty list
  for item in dupe_list:
     # adds item to empty list if it's not already in the list
     if item not in unique_list: unique_list.append(item)
  return unique_list


def unique_element_list(list_name, index):
  """
  find unique EC numbers so have a generic function and run it
  be careful as there are cases of one less item - use "last" to fix that problem here
  """
  original_index = index
  element_list = []

  # assigns the string "last" to the very last list in the list of lists
  for i in list_name:
     # finds unique EC num not in the list & adds it to the list
     if original_index == 'last': index = len(i) - 1
```

```
            if i[int(index)] not in element_list: element_list.append(i[int(index)])
        return element_list


    def list_partition(seq, num):
        """
        This function takes in a list and then splits it into as many parts as specified
        by parameter num
        """
        avg = len(seq) / float(num)
        out = []
        last = 0.0
        while last < len(seq):
            out.append(seq[int(last):int(last + avg)])
            last += avg

        return out


    def write_readme(main_dir, readme, init_time, fasta_path, gene_path):
        """
        Creates the ReadMe file
        """
        print('- creating README ... ')
        with open(main_dir + readme, 'w') as readme_doc:
            readme_doc.write("KEGG_v1p1.py\n")
            readme_doc.write(init_time.strftime("%m-%d-%Y") + "\n")
            readme_doc.write(main_dir + "\n")
            readme_doc.write('This script creates a series of files related to the genes ' +
                             'associated with plant flavonoids from various species of ' +
                             'plants. This script first creates the MasterCount and ' +
                             'MasterList files;   the MasterCount counts the number genes ' +
                             'each plant species have that correspond with each EC number;  ' +
                             'while the MasterList lists every gene with number for each ' +
                             'plant specie. These are located in ' + os.getcwd() + '. The ' +
                             'script also creates files that only contains the genes of a ' +
                             'single plant species biochemical pathway which are located in ' +
                            gene_path + '. The script also creates a Master FASTA files ' +
                             'which contains the DNA sequence of each gene and FASTA files ' +
                             'organized by EC number, these are located in ' + fasta_path)
            readme_doc.close()


    def save_file(lists_to_write, output_dir, current, sep=', '):
        """
        This function takes a list or list of lists and then writes its contents to a file.
        """
        os.chdir(current)

        writedoc = open(output_dir, 'w')  # open file to be written
        for line in lists_to_write:
            for item in line:
                item = str(item).replace('\n', '')  # removes the new lines in each list of list
                if item == '':
                    writedoc.write('-')  # if the list in the list of list is empty writes a dash
                else:
                    writedoc.write(item)  # write the entry in the list of lists to the file
```

```
            writedoc.write(sep)  # tab delimited;  use "," for csv files
      writedoc.write('\n')
      writedoc.close()


def write_append(path, content, write_over=None, skip=None):
      """
      This function takes a filename and the contents to be written to a file. If the
      file doesn't exist, it is created then written to. If it does exist, then it is
      appended to. The optional arg write_over is used for when the file exists and the
      content needs to be written over.
      """
      try:
         file = open(path, 'x')
         file.close()
         file = open(path, 'w')
         file.write(content)
         file.close()
      except FileExistsError:
         if write_over:
            file = open(path, 'w')
            file.write(content)
            file.close()
         elif skip:
            pass
         else:
            file = open(path, 'a')
            file.write(content)
            file.close()


def is_http_error(msg):
      """
      Checks if a string is an HTTP error.
      """
      if str(msg).strip() in HTTP_ERRS:
         return False
      else:
         return True


def init_dir(dir_path):
      """
      Initializes directories for keggv2.py
      """
      # replaced WindowsError with OSError for more general usage.
      # try to make data directories and handle any errors
      try:
         os.mkdir(dir_path)
      except OSError:
         pass


def quick_fetch(pattern, line):
      """
      Fetch one item from re.findall and return as a string.
      """
```

```
  out = ''
  try:
     out = re.findall(pattern, line)[0]
  except IndexError:
     out = ''
  return out


def multi_replace(line, pairs):
  """
  This function makes multiple string replacements.
  """
  for pair in pairs: line = line.replace(pair[0], pair[1])
  return line


def skin(line):
  """
  Simple function that removes ALL whitespace from a string
  """
  return ''.join(line.split()).strip()
```

Library file: prediction_logic.py

```
# custom project library imports
from flib.fconstants import *

# take the label, which is the same as the function name & then call the function.
def flav_check(label, ec_list):
  try:
     res = label(ec_list)
  except KeyError:
     res = False
  return res

# returns true if at least 1 arg is in the list
def or_in(items, *args):
  for a in args:
     if a in items:
        return True
  return False

# returns true only if all args are in the list
def and_in(items, *args):
  for a in args:
     if a not in items:
        return False  # all values must be present
  return True

# The prediction functions. There is one for numerous compounds not being predicted
# as they are precursors to the compounds of interest, which makes the predictions
# a little more readable. Function names are either the 3 letter code assigned
# to a specific compound by the Protein Data Bank (PDB) or are alternative codes
# for compounds that either do not have a PDB code or do not have a variable-friendly
# PDB code (for example, the PDB code for Epicatechin cannot be used because it is
# 28E and the python interpreter does not allow functions to start with a number)
# Function order is determined by a compounds requirements as functions cannot
```

```
# be called before they are written.

def tca(e):  # cinnamic acid || precursor
  return or_in(e, E01, E02)

def hc4(e):  # p-coumaric acid || precursor
  return tca(e) and (E03 in e)

def nca(e):  # cinnamoyl-coa || precursor
  return tca(e) and (E04 in e)

def pich(e):  # pinocembrin chalcone || new
  return nca(e) and (E09 in e)

def pino(e):  # pinocembrin || new
  return pich(e) and (E10 in e)

def chsn(e):  # chrysin || new
  return pino(e) and (E11 in e)

def pban(e):  # pinobanksin || new
  return pino(e) and (E15 in e)

def galn(e):  # galangin || new
  return pban(e) and (E16 in e)

def wca(e):  # p-coumaroyl-coa || precursor
  return (nca(e) and (E03 in e)) or (hc4(e) and (E04 in e))

def g50(e):  # phloretin || new
  return wca(e) and (and_in(e, E24, E09))

def narc(e):  # naringenin chalcone || new
  return wca(e) and (E09 in e)

def nar(e):  # naringenin || mh thesis
  return narc(e) and (E10 in e)

def dgen(e):  # 2-Hydroxy-2,3-dihydrogenistein || new
  return nar(e) and (E21 in e)

def hesp(e):  # hesperetin || new
  return nar(e)

def apif(e):  # apiforol || new
  return nar(e) and (or_in(e, E17_1, E17_FULL, E17_2))

def agi(e):  # apigenin || mh thesis
  return nar(e) and or_in(e, E11, E12)

def lu2(e):  # luteolin || mh thesis
  return agi(e) and (or_in(e, E13, E14))

def fca(e):  # caffeoyl-coa || precursor
  return wca(e) and (and_in(e, E06, E07) or (E08 in e))

def erdc(e):  # eriodictyol chalcone || new
```

```
  return (nar(e) and or_in(e, E13, E14)) or (fca(e) and (E09 in e))

def erd(e):  # eriodictyol  || mh thesis || same as erch for now
  return erdc(e)

def lutf(e):  # luteoforol || new
  return erd(e) and (or_in(e, E17_1, E17_FULL, E17_2))

def dtri(e):  # dihydrotricetin || new
  return erd(e) and (E13 in e)

def myf(e):  # tricetin || new
  return lutf(e) and (E13 in e) or (dtri(e) and (E11 in e))

def dkam(e):  # dihydrokaempferol || new
  return nar(e) and (E15 in e)

def lpel(e):  # leucopelargonidin || new
  return dkam(e) and (E17_1 in e)

def pelr(e):  # pelargonidin || new
  return lpel(e) and (E18 in e)

def ezel(e):  # epiafzelechin || new
  return pelr(e) and (E19 in e)

def azel(e):  # afzelechin || new
  return lpel(e) and (E20 in e)

def kmp(e):  # kaempferol ||  mh thesis
  return dkam(e) and (E16 in e)

def dque(e):  # dihydroquercetin || new
  return (dkam(e) and or_in(e, E13, E14)) or (erd(e) and (E15 in e))

def lcyn(e):  # leucocyanidin || new
  return dque(e) and or_in(e, E17_1, E17_FULL)

def que(e):  # quercetin || mh thesis
  return (kmp(e) and or_in(e, E13, E14)) or (dque(e) and (E16 in e))

def kxn(e):  # catechin || mh thesis
  return lcyn(e) and (E20 in e)

def hwb(e):  # cyanidin || mh thesis
  return lcyn(e) and (E18 in e)

def ec(e):  # epicatechin || mh thesis
  return hwb(e) and (E19 in e)

def dmyr(e):  # dihydromyricetin || new
  return (dque(e) and (E13 in e)) or (erd(e) and and_in(e, E13, E15))

def myc(e):  # myricetin ||  mh thesis
  return (dmyr(e) and (E16 in e)) or (que(e) and (E13 in e))

def ldel(e):  # leucodelphinidin || new
```

```
  return dmyr(e) and or_in(e, E17_1, E17_FULL)

def dlm(e):  # delphinidin || new
  return ldel(e) and (E18 in e)

def gc(e):  # gallocatechin || mh thesis
  return ldel(e) and (E20 in e)

def egt(e):  # epigallocatechin || mh thesis
  return dlm(e) and (E19 in e)

def gen(e):  # genistein || mh thesis
  return nar(e) and and_in(e, E21, E22)

def bun(e):  # butein || mh thesis
  return wca(e) and (or_in(e, E05, E09))

def butn(e):  # butin || new
  return bun(e) and (E10 in e)

def hcc(e):  # isoliquiritigenin || mh thesis
  return bun(e)

def dfv(e):  # liquiritigenin || new
  return hcc(e) and (E10 in e)

def gban(e):  # garbanzol || new
  return dfv(e) and (E15 in e)

def fstn(e):  # dihydrofisetin || new
  return (gban(e) and (E14 in e)) or (butn(e) and (E15 in e))

def df74(e):  # 7,4'-dihydroxyflavone || new
  return dfv(e) and (or_in(e, E11, E12))

def tiso(e):  # 2,7,4'-Trihydroxyisoflavanone || new
  return dfv(e) and (E21 in e)

def daid(e):  # daidzein || new
  return tiso(e) and (E22 in e)

def tnon(e):  # 6,7,4'-Trihydroxyflavanone || new
  return dfv(e) and (E08 in e)

def tet2(e):  # 2,6,7,4'-Tetrahydroxyisoflavanone || new
  return tnon(e) and (E21 in e)

def hdai(e):  # 6-Hydroxydaidzein || new
  return tet2(e)

def ggt(e):  # Glycosaminoglycan galactosyltransferase || enzyme
  return E_GGT in e

def dec(e):  # Deleted entry || enzyme
  return E_DEC in e

def soa(e):  # Serine O-acetyltransferase || enzyme
```

```
  return E_SOA in e

def v1g(e):  # vanillate 1-glucosyltransferase || enzyme
  return E_V1G in e
```

Data files

flav_names.json

```
{
 "obj": [
   "Apigenin", "Butein", "Catechin", "Cyanidin", "Epicatechin", "Epigallocatechin",
   "Eriocitrin", "Eriodictyol", "Gallocatechin", "Genistein", "Isoliquiritigenin",
   "Kaempferol", "Luteolin", "Myricetin", "Naringenin", "Quercetin"
 ]
}
```

flav_info.json

```
{
 "obj": {
   "2,6,7,4'-Tetrahydroxyisoflavanone": {
     "code": "TET2",
     "file": "TET2_2-6-7-4-tetrahydroxyisoflavanone.csv"
   },
   "2,7,4'-Trihydroxyisoflavanone": {
     "code": "TISO",
     "file": "TISO_2-7-4-trihydroxyisoflavanone.csv"
   },
   "2-Hydroxy-2,3-dihydrogenistein": {
     "code": "DGEN",
     "file": "DGEN_2-hydroxy-2-3-dihydrogenistein.csv"
   },
   "6,7,4'-Trihydroxyflavanone": {
     "code": "TNON",
     "file": "TNON_6-7-4-trihydroxyflavanone.csv"
   },
   "6-Hydroxydaidzein": {"code": "HDAI", "file": "HDAI_6-hydroxydaidzein.csv"},
   "7,4'-Dihydroxyflavone": {"code": "DF74", "file": "DF74_7-4-dihydroxyflavone.csv"},
   "Afzelechin": {"code": "AZEL", "file": "AZEL_afzelechin.csv"},
   "Apiforol": {"code": "APIF", "file": "APIF_apiforol.csv"},
   "Apigenin": {"code": "AGI", "file": "AGI_apigenin.csv"},
   "Butein": {"code": "BUN", "file": "BUN_butein.csv"},
   "Butin": {"code": "BUTN", "file": "BUTN_butin.csv"},
   "Catechin": {"code": "KXN", "file": "KXN_catechin.csv"},
   "Chrysin": {"code": "CHSN", "file": "CHSN_chrysin.csv"},
   "Cyanidin": {"code": "HWB", "file": "HWB_cyanidin.csv"},
   "Daidzein": {"code": "DAID", "file": "DAID_daidzein.csv"},
   "Delphinidin": {"code": "DLM", "file": "DLM_delphinidin.csv"},
   "Dihydrofisetin": {"code": "FSTN", "file": "FSTN_dihydrofisetin.csv"},
   "Dihydrokaempferol": {"code": "DKAM", "file": "DKAM_dihydrokaempferol.csv"},
   "Dihydromyricetin": {"code": "DMYR", "file": "DMYR_dihydromyricetin.csv"},
   "Dihydroquercetin": {"code": "DQUE", "file": "DQUE_dihydroquercetin.csv"},
   "Dihydrotricetin": {"code": "DTRI", "file": "DTRI_dihydrotricetin.csv"},
   "Enzyme Deleted entry": {"code": "DEC", "file": "EC_2-3-1-70.csv"},
   "Enzyme Glycosaminoglycan galactosyltransferase": {
     "code": "GGT",
```

```
    "file": "EC_2-4-1-74.csv"
   },
   "Enzyme Serine O-acetyltransferase": {"code": "SOA", "file": "EC_2-3-1-30.csv"},
   "Enzyme Vanillate 1-glucosyltransferase": {"code": "V1G", "file": "EC_2-4-1-136.csv"},
   "Epiafzelechin": {"code": "EZEL", "file": "EZEL_epiafzelechin.csv"},
   "Epicatechin": {"code": "EC", "file": "EC_epicatechin.csv"},
   "Epigallocatechin": {"code": "EGT", "file": "EGT_epigallocatechin.csv"},
   "Eriodictyol Chalcone": {"code": "ERDC", "file": "ERDC_eriodictyol-chalcone.csv"},
   "Eriodictyol": {"code": "ERD", "file": "ERD_eriodictyol.csv"},
   "Galangin": {"code": "GALN", "file": "GALN_galangin.csv"},
   "Gallocatechin": {"code": "GC", "file": "GC_gallocatechin.csv"},
   "Garbanzol": {"code": "GBAN", "file": "GBAN_garbanzol.csv"},
   "Genistein": {"code": "GEN", "file": "GEN_genistein.csv"},
   "Hesperetin": {"code": "HESP", "file": "HESP_hesperetin.csv"},
   "Isoliquiritigenin": {"code": "HCC", "file": "HCC_isoliquiritigenin.csv"},
   "Kaempferol": {"code": "KMP", "file": "KMP_kaempferol.csv"},
   "Leucocyanidin": {"code": "LCYN", "file": "LCYN_leucocyanidin.csv"},
   "Leucodelphinidin": {"code": "LDEL", "file": "LDEL_leucodelphinidin.csv"},
   "Leucopelargonidin": {"code": "LPEL", "file": "LPEL_leucopelargonidin.csv"},
   "Liquiritigenin": {"code": "DFV", "file": "DFV_liquiritigenin.csv"},
   "Luteoforol": {"code": "LUTF", "file": "LUTF_luteoforol.csv"},
   "Luteolin": {"code": "LU2", "file": "LU2_luteolin.csv"},
   "Myricetin": {"code": "MYC", "file": "MYC_myricetin.csv"},
   "Naringenin Chalcone": {"code": "NARC", "file": "NARC_naringenin-chalcone.csv"},
   "Naringenin": {"code": "NAR", "file": "NAR_naringenin.csv"},
   "Pelargonidin": {"code": "PELR", "file": "PELR_pelargonidin.csv"},
   "Phloretin": {"code": "G50", "file": "G50_phloretin.csv"},
   "Pinobanksin": {"code": "PBAN", "file": "PBAN_pinobanksin.csv"},
   "Pinocembrin chalcone": {"code": "PICH", "file": "PICH_pinocembrin_chalcone.csv"},
   "Pinocembrin": {"code": "PINO", "file": "PINO_pinocembrin.csv"},
   "Quercetin": {"code": "QUE", "file": "QUE_quercetin.csv"},
   "Tricetin": {"code": "MYF", "file": "MYF_tricetin.csv"}
 }
}
```


plant_codes.json


```
{
 "obj": [
   "adu", "aip", "aly", "aof", "apro", "ath", "atr", "ats", "bdi", "bna", "boe", "bpg",
   "brp", "bvg", "cam", "cann", "ccaj", "ccav", "ccp", "cic", "cit", "cmax", "cme",
   "cmo", "cmos", "cpap", "cpep", "cqi", "crb", "cre", "csat", "csl", "csv", "cvr",
   "dcr", "dct", "dzi", "egr", "egu", "eus", "fve", "gab", "ghi", "gmx", "gra", "gsj",
   "gsl", "han", "hbr", "ini", "jcu", "jre", "lang", "lja", "lsv", "mcha", "mdm", "mesc",
   "mis", "mng", "mpp", "mtr", "mus", "nau", "nnu", "nsy", "nta", "nto", "obr", "oeu",
   "olu", "dosa", "osa", "ota", "pavi", "pda", "peq", "peu", "pmum", "pop", "pper",
   "ppp", "psom", "pvu", "pxb", "qsu", "rcn", "rcu", "sbi", "sind", "sita", "sly", "smo",
   "soe", "sot", "spen", "tcc", "thj", "var", "vcn", "vra", "vun", "vvi", "zju", "zma",
   "rsz"
 ]
}
```


plant_names_codes.json


```
{
 "obj": {
```

```
   "ats": "Aegilops tauschii", "atr": "Amborella trichopoda",
   "aly": "Arabidopsis lyrata", "ath": "Arabidopsis thaliana",
   "adu": "Arachis duranensis", "aip": "Arachis ipaensis",
   "aof": "Asparagus officinalis", "apro": "Auxenochlorella protothecoides",
   "bpg": "Bathycoccus prasinos", "bvg": "Beta vulgaris",
   "bdi": "Brachypodium distachyon", "bna": "Brassica napus", "boe": "Brassica oleracea",
   "brp": "Brassica rapa", "ccaj": "Cajanus cajan", "csat": "Camelina sativa",
   "crb": "Capsella rubella", "cann": "Capsicum annuum", "cpap": "Carica papaya",
   "cqi": "Chenopodium quinoa", "cre": "Chlamydomonas reinhardtii",
   "cvr": "Chlorella variabilis", "ccp": "Chondrus crispus", "cam": "Cicer arietinum",
   "cic": "Citrus clementina", "cit": "Citrus sinensis",
   "csl": "Coccomyxa subellipsoidea", "cmo": "Cucumis melo", "csv": "Cucumis sativus",
   "cmax": "Cucurbita maxima", "cmos": "Cucurbita moschata",
   "cpep": "Cucurbita pepo subsp. pepo", "cme": "Cyanidioschyzon merolae",
   "ccav": "Cynara cardunculus var. scolymus", "dcr": "Daucus carota",
   "dct": "Dendrobium catenatum", "dzi": "Durio zibethinus", "egu": "Elaeis guineensis",
   "egr": "Eucalyptus grandis", "eus": "Eutrema salsugineum", "fve": "Fragaria vesca",
   "gsl": "Galdieria sulphuraria", "gmx": "Glycine max", "gab": "Gossypium arboreum",
   "ghi": "Gossypium hirsutum", "gra": "Gossypium raimondii", "han": "Helianthus annuus",
   "hbr": "Hevea brasiliensis", "ini": "Ipomoea nil", "jcu": "Jatropha curcas",
   "jre": "Juglans regia", "lsv": "Lactuca sativa", "lja": "Lotus japonicus",
   "lang": "Lupinus angustifolius", "mdm": "Malus domestica",
   "mesc": "Manihot esculenta", "mis": "Micromonas commoda", "mpp": "Micromonas pusilla",
   "mcha": "Momordica charantia", "mng": "Monoraphidium neglectum",
   "mus": "Musa acuminata", "nnu": "Nelumbo nucifera", "nau": "Nicotiana attenuata",
   "nsy": "Nicotiana sylvestris", "nta": "Nicotiana tabacum",
   "nto": "Nicotiana tomentosiformis", "oeu": "Olea europaea v. sylvestris",
   "obr": "Oryza brachyantha", "dosa": "Oryza sativa japonica RAPDB",
   "osa": "Oryza sativa japonica RefSeq", "olu": "Ostreococcus lucimarinus",
   "ota": "Ostreococcus tauri", "psom": "Papaver somniferum",
   "peq": "Phalaenopsis equestris", "pvu": "Phaseolus vulgaris",
   "pda": "Phoenix dactylifera", "ppp": "Physcomitrium patens subsp. Patens",
   "pop": "Populus trichocarpa", "peu": "Populus euphratica", "pavi": "Prunus avium",
   "pmum": "Prunus mume", "pper": "Prunus persica", "pxb": "Pyrus x bretschneideri",
   "qsu": "Quercus suber", "rcu": "Ricinus communis",
   "smo": "Selaginella moellendorffii", "sind": "Sesamum indicum",
   "sita": "Setaria italica", "sly": "Solanum lycopersicum", "spen": "Solanum pennellii",
   "sot": "Solanum tuberosum", "sbi": "Sorghum bicolor", "soe": "Spinacia oleracea",
   "thj": "Tarenaya hassleriana", "tcc": "Theobroma cacao", "var": "Vigna angularis",
   "vra": "Vigna radiata", "vvi": "Vitis vinifera",
   "vcn": "Volvox carteri f. nagariensis", "zma": "Zea mays", "zju": "Ziziphus jujuba",
   "gsj": "Glycine soja", "mtr": "Medicago truncatula", "rcn": "Rosa chinensis",
   "vun": "Vigna unguiculata", "rsz": "Raphanus sativus"
 }
}
```


path_codes.json


```
{
 "obj": ["00940", "00941", "00942", "00943","00944"]
}
```


path_codes_names.json


```
{
 "obj": {
```

```
    "00940": "phenylpropanoids",
    "00941": "flavonoids",
    "00942": "anthocyanins",
    "00943": "isoflavonoids",
    "00944": "flavones/flavonols",
    "00945": "stilbenoids"
  }
}
```


Additional JSON files

There are some additional JSON files not listed here as they do not play a direct role in code functionality and can be found on the project GitHub.