

## PROCEEDING

# Construction of a novel database for flavonoids

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**Abstract:** Flavonoids are polyphenolic compounds that exist ubiquitously in foods of plant origin. Flavonoids show various interesting biological activities, such as removal of oxygen radical, anti-cancer action, improvement of high blood pressure, antibacterial, antibiotic and anti-allergy actions. So far, over 4000 structurally unique flavonoids have been isolated from plant sources. Recently, databases of chemicals have been utilized in to help chemical and biological researches, however the comprehensive database of flavonoids with information about structural, biological and physicochemical properties not yet available. We have constructed the integrated database of flavonoids for nutrition research. *J. Med. Invest.* 52 Suppl. : 291-292, November, 2005

**Keywords :** biological activity, database, flavonoid, nutrition research, physicochemical property, structure

## FLAVONOIDS

Flavonoids are the building blocks of polyphenol compounds that can be found in various foods. They commonly have a generic structure consisting of two aromatic rings (A and B rings) linked by 3 carbons that are usually in an oxygenated heterocycle ring (C ring). Differences in the generic structure of the heterocycle C ring classify them as flavones, flavonols, flavanones, flavanols, isoflavonoids, and anthocyanidins, as shown in Figure 1.

It is considered that hundreds of milligrams are taken as for person's intake in a day. For flavonoids, many activities, such as removal of oxygen radical, anti-cancer action, improvement of high blood pressure, antibacterial, antibiotic, and anti-allergy actions, have been found in recent years. Over 4000 structurally unique flavonoids have been identified in plant sources (1-4). Recently, various databases of chemicals were compiled to help biological and/or chemical research works (5, 6),

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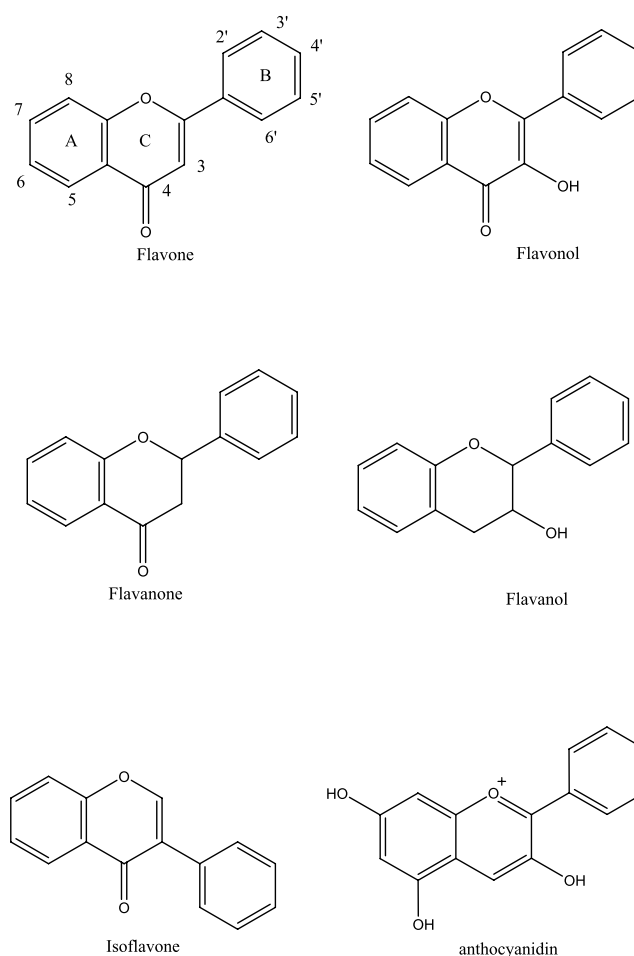


Figure 1. Structures classification of flavonoids

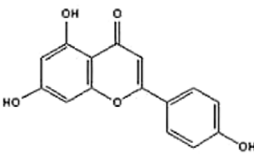
<b>MOL_ID</b>	20	<b>Structure</b>	
<b>Formula</b>	C <sub>15</sub> H <sub>10</sub> O <sub>5</sub>	<b>MolWeight</b>	270.2369
<b>analchem_ID</b>	MDDR_20	<b>MDDR_anal_active_ID</b>	21466
<b>MDDR_anal_active2_ID</b>	21466	<b>Active_index</b>	09210 75000 75845 7837
<b>Active_Class</b>	Nootropic Agent Antineoplastic Chemoprotective Ornithine Decarboxylase Inhibitor	<b>Phase</b>	Preclinical
<b>ACTION</b>	ACTION - Potential cancer chemopreventive agent, a nontoxic and nonmutagenic plant flavonoid that dose-dependently inhibited (1 to 20 μmol) TPA-induced epidermal ornithine decarboxylase, when applied topically in senescent mice it also prevented the development of skin tumorigenesis initiated by DMBA and promoted by TPA, and showed a tendency to decrease conversion of papillomas to carcinomas.	<b>name</b>	Apigenin : 4',5,7-Trihydroxyflavone 5,7-Dihydroxy-2-(4-hydroxy-phenyl)-1-benzopyran-4-one Apigenin
<b>lit_type</b>	Antitumor Activity	<b>ClogP</b>	2.91000008583069
<b>lit_title</b>	1) Inhibitory effect of apigenin, a plant flavonoid, on epidermal ornithine decarboxylase and skin tumor promotion in mice 2) Studies on inhibitors of skin tumor promotion (IV) Inhibitory effects of flavonoids of Epstein-Barr virus activation. II. 3) Studies on inhibitors of skin tumor promotion (IV) Inhibitory effects of flavonoids on Epstein-Barr virus activation (I).	<b>lit_ref</b>	1) Wei, H. et al. Cancer Res 1990, 50(3): 499-502. 2) Konoshima, T. et al. Jpn J Pharmacogn 1989, 43(2): 135-41. 3) Konoshima, T. et al. Jpn J Pharmacogn 1988, 42(4): 343-6.
<b>Har</b>	0	<b>Hdnr</b>	3
<b>MlogP</b>	3.0199998092651	<b>Phase_year</b>	

Figure 2. Screenshot of Flavonoid database

but the comprehensive database of flavonoids with molecular structures and physicochemical parameters is not available yet.

## DATABASE FOR FLAVONOIDS

Among existing drugs, there are a huge number of compounds bearing flavonoid related skeleton. We have merged information on the flavonoids of plant origin and flavonoids used as medicine into our database. Structural and biological information about flavonoids and their structurally related compounds was extracted from USDA Flavonoid Database (7), Functional Food Factors Database (6, 8, 9), National Cancer Institute (10), MDL Screening Compound Directory (11) and MDL Drug Data Report (12). The combined database consists of about 8000 flavonoids and their structurally related compounds. Molecular physicochemical properties such as log *P* and numbers of hydrogen bonding acceptors/donors are known to be definitely important in the structure-activity relationship and drug discovery. These quantities of each compound were added into the database as additional information. A screenshot of this database is shown in Figure 2. Users can easily retrieve chemical structures, biological and physicochemical properties of desired compounds from the database by using various type of queries. This database will be open to the public as The University of Tokushima Food Database in the near future. We expect that this database will be useful for the comprehensive and deeper understanding of structure-activity relationship of food

compounds and finding of a promising food compound.

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