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RESEARCH ARTICLE

Sstructural Conformational Study of Isoflavon Derivatives in Soybean Using Semi empirical Methods

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Abstract

Isoflavon was falconoid group which was a polifenolic compound. As a member of flavonoid groups, isoflavon was a bioactive compound that contains phenolic group reported to have an ability as antioxidant and prevent free radical damage through two mechanism. The mechanism are donating hydrogen ions and directly acting as a free radical scavenger. One of the seed plants which contain isoflavon was soybean. Isoflavon derivatives in soybean are biochanin a, genistein, daidzein, equol, formononetin, dan glycitein. The compounds can be applied in medical and pharmaceutical. Generally the is of lavon derivatives in soy bean have been conducted to anti-allergic, antioxidant, dan anti cholesterol. These studies based on optimization and structural conformational to support QSAR and Molecular docking studies. In this study, semiempirical AM1 method was used for optimization all the structure. The distance of two nearby atoms affect the structure stability and the strain energy because the lower the strain energy, the more stable that compound The most stable structure for biochanin a, genwastein, daidzein, glycitein, formononetin was 40° while the most stable structure for equol was 280°.

Keywords: *Conformation, Derivatives, Energy, Isoflavon, Soybean.*

Introduction

Isoflavon was flavonoid group which was a polifenolic compound. The based chemistry structure of isoflavon almost equal with flavonoid, that consist of two benzena rings (A-ring and B-ring) which was bind to heterocyclic pyran ring (C-ring). The difference was in the B-ring orientation. B-ring in flavonoid compound was bind by the number 2 carbon (C2) in C-ring to the number 1' carbon in B-ring; hence, isoflavon was bind by the number 3 carbon (C3) in C-ring [1]. As a member of flavonoid groups, isoflavon was a bioactive compound that contains phenolic group reported to have ability as antioxidant and prevent free radical damage through two mechanism [2].

The Mechanism of Antioxidant in Flavonoid Groups Are

- By donating hydrogen ions [3]
- By directly acting as a free radical scavenger [1]

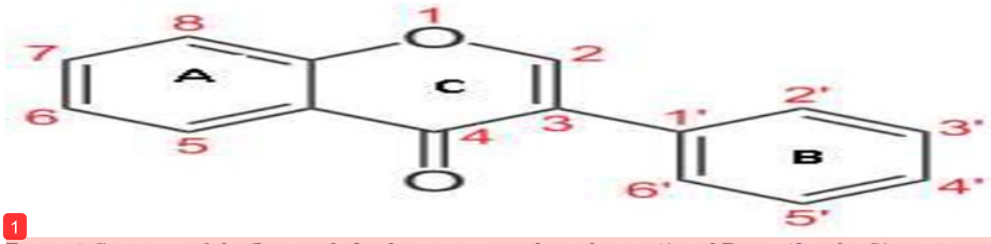

Figure 1: Structure of the flavonoids [with two aromatic benzol rings (A and B rings)] and a C3 portion cyclized with oxygen (C ring)

One of the seed plants which contain isoflavon was soybean. As we know, soy was widely used in Asia as a staple food and consumed regularly in traditional food items such as tofu, miso, natto, edamame (whole soybeans), soybean paste, and shoyu (fermented soy sauce). In soybean contain isoflavon compound that have an ability as an antioxidant that can be anti cancer. Hence, the isoflavone intake among Asians was about a factor of 100 higher than that of people in the Western world. The daily isoflavone intake among Southeast Asians ranges between 15 and 47 mg, while European consumes only between 0.15 and 1.7 mg isoflavones per day. Isoflavon derivatives in soybean are biochanin a, genwastein, daidzein, equol, formononetin, dan glycitein [4].

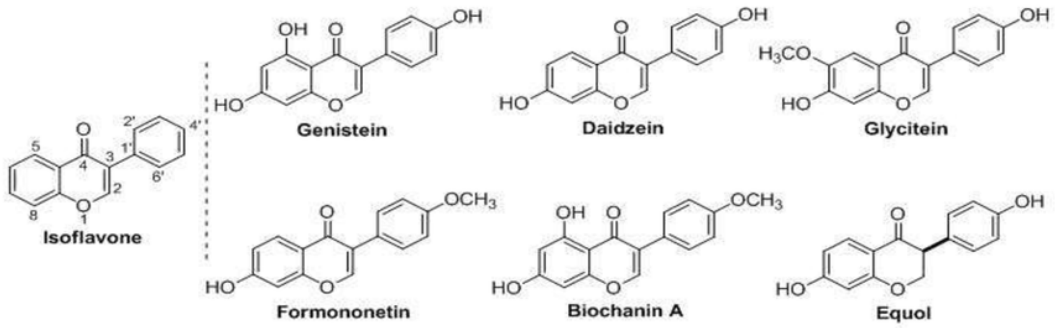

Figure 2: Structure of is flavone: geniste in, daidze in, for monometer, biochanin A, and glycitein [5].

The compounds can be applied in medical and pharmaceutical. Generally the isoflavon derivatives in soybean have been conducted to anti-allergic, antioxidant, dan anti cholesterol. Genistein has role as antioxidant, anti-angiogenik, metastasis cancer cell, protein kinase inhibitor and proliferasi inhibitor [2].

Biochanin a can prevent high cholesterol, anti-fungal, anti tumor, regulate hormonal stage in human body, anti cancer, antispasmodic, and lower lipidin blood. Daidzein can prevent and lower cancer risk, absence of tumor, cure syndrome activity, such as menopause syndrome and anti-osteoporosis. Formononetin was anti cancer (breast cancer, prostat cancer, dan colon cancer), have effect to reduce fat. Glycitein can be use for bone healthy, menopause symtomps, to reduce the stress hormones and anti inflammation that lead by cancer [3]. One of the best way to know all the function from the isoflavones derivatives through QSAR and Molecular docking.

These studies based on optimization and structural conformational to support QSAR and Molecular Docking studies [7]. The result in study can find the possibility structure of isoflavones derivatives in soybean as a cancer drugs. In this study, semiempirical AM1 method was used for optimization all the structure. Austin Model 1 or AM 1 was first introduced by Dewar when he was in the Texas University, Austin. AM1 has a specific parameters than MNDO, 14 parameters/atom. The other difference was AM 1 uses a new tribe to describe their interaction [8].

$$E_{AB} = Z_A Z_B < S_A S_A | S_B S_B > + \frac{Z_A Z_B}{R_{AB}} \sum_{i=1} [a_i^A \exp(-b_i^A (r_{AB} - c_i^A)^2) + a_i^B \exp(-b_i^B (r_{AB} - c_i^A)^2]$$

a,b and c are parameters from Gaussian function that was associated with atoms in the definition (superscript).

Experimental Section

Materials

Computer (ASUS Vivo book Flip TP410UA-DB71T 14-inch FHD Touchscreen, Intel Core i7).

Optimized Structural Conformational

Structural conformational of the optimized isoflavones derivatives was carried out with the use of an efficient progam, AM1. Hypechem was used to draw and optimization all the structure. To get the result for structural conformation, constrain variation bond angle between C(2)-C(3), C(3)-C(1'), and C(1')-C(2') each ten degree, from zero degree to three hundred and sixty degree. So, strain energy and bond length has been obtained. Make strain energy graphics to identify the stable and unstable structure from isoflavones derivatives. Calculate the bond length based on numbering of carbon atoms (IUPAC). The methodology can be expressed as following (Figure 3).

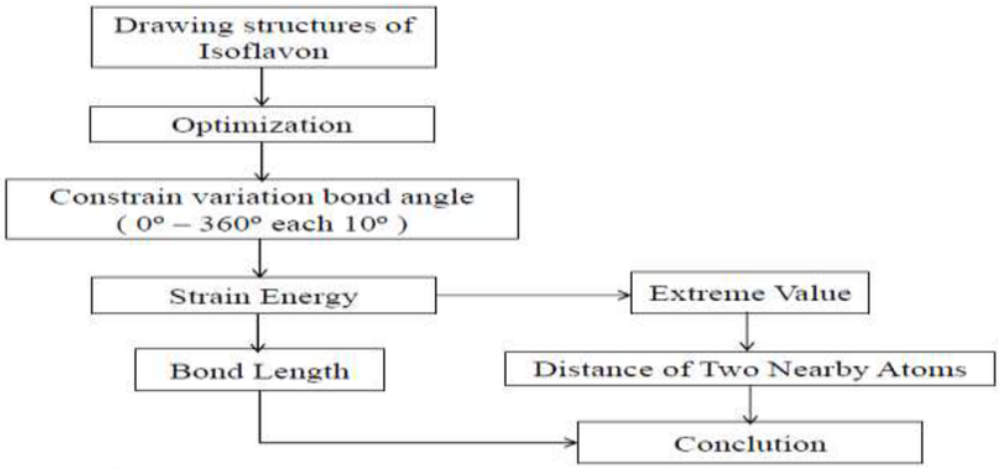

Figure 3: Methodology of structural conformational study of isoflavon derivatives

Results and Discussion

Optimization AM 1 for Isoflavon Derivatives in Soybean

The bond length result in Table 1 show the bond length between one compound and another was similar where was the difference of one compound and the other compounds was about 0,016 Å. The differences from the bond length results of one compound minus with the others and then sum all the result. The totals divide by the amount of all bond lengths. But there was a structure difference between the five isoflavons and equol, the difference was in the C(3)-C(2) bond, in which the orbital changes from sp^2 to sp^3. The bond length of equol was longer than the other structures.

Table 1: Bond Length between Each Atoms of Isoflavon Derivatives in Soybean

Atom	Bond Length (Å)					
	Genistein	Daidzein	Glycitein	Formononetin	Biochanin A	Equol
O(1)-C(2)	1,375	1,3736	1,3723	1,3738	1,3752	1,4321
C(2)-C(3)	1,3538	1,3559	1,3564	1,3559	1,3538	1,5207
C(3)-C(4)	1,4784	1,4746	1,4735	1,4745	1,2784	1,5197
C(5)-C(6)	1,4007	1,3858	1,3872	1,3858	1,4087	1,3873
C(6)-C(7)	1,4032	1,4095	1,4231	1,4049	1,4032	1,4075
C(7)-C(8)	1,4006	1,3998	1,3947	1,3997	1,4005	1,401
C(3)-C(1')	1,4597	1,4595	1,4595	1,4594	1,4596	1,495
C(1')-C(2')	1,4044	1,4019	1,4044	1,4004	1,4051	1,4019
C(2')-C(3')	1,3893	1,3915	1,3892	1,3933	1,3879	1,3907
C(3')-C(4')	1,4049	1,4018	1,405	1,3995	1,4078	1,4026
C(3')-C(4')	1,4018	1,4049	1,4017	1,4078	1,3995	1,4041
C(3')-C(4')	1,3915	1,389	1,3915	1,3876	1,3932	1,3909
C(6')-C(1')	1,4025	1,405	1,4024	1,4057	1,4011	1,3999

Conformational Study

In structural conformation study, the strain energy graphic (Figure 2) indicates the extreme values of each compound in soybean isoflavones derivatives. Biochanin a, daidzein, glycitein, formononetin, and genistein have the similar structure (Figure 2). Because of that, they have similar angle of extreme values at 40°, 80°, 140°, 180°, 220°,

dan 320°. But there was a difference extreme values in equol, the extreme values were at 80°, 140°, 280°, dan 340°. It was because there was no double bond in equol structure, which the others have [9].

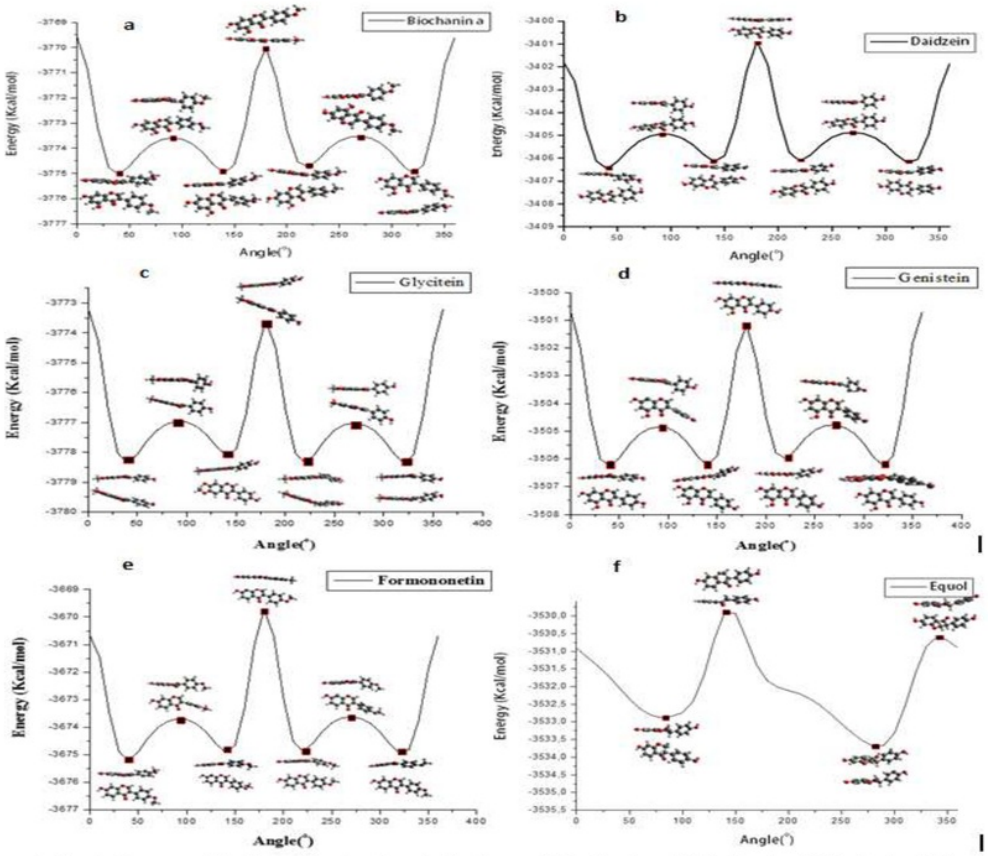

Figure 4: Strain Energy of Isoflavon Derivatives in Soybean a) Biochanin a; b) Daidzein; c) Glycitein; d) Genistein; e) Formononetin; f) Equol

Table 2: Distance of Two nearby Atoms

Angle	Atom	Distance (Å)					
		Biochanin a	Daidzein	Glycitein	Formononetin	Genistein	Equol
40°	O-H(C2')	2,281	2,282	2,281	2,281	2,281	-
	H(C2)-H(C6')	2,029	1,994	2,029	2,029	2,029	-
80°	H(C2)-H(C6')	3,278	3,280	3,278	3,2778	3,278	2,558
	O-H(C2')	3,423	3,394	3,423	3,423	3,423	1,731
140°	O-H(C6')	2,094	2,166	2,094	2,094	2,094	-
	H(C2)-H(C2')	2,004	2,007	2,004	2,004	2,004	1,730
	H(C3)-H(C2')	-	-	-	-	-	2,422
180°	O-H(C6')	1,821	1,814	1,821	1,821	1,821	-
	H(C2)-H(2')	1,706	1,675	1,706	1,706	1,706	-
190°	O-H(C6')	-	-	-	-	-	1,842
	H(C3)-H(C2')	-	-	-	-	-	2,533
220°	O-H(C6')	2,094	2,069	2,094	2,094	2,094	-
	H(C2)-H(C2')	1,959	1,953	1,959	1,959	1,959	-
260°	O-H(C6')	3,007	3,003	3,007	3,007	3,007	-
	H(C2)-H(2')	2,780	2,779	2,780	2,780	2,780	-
280°	H(C2)-H(C6')	-	-	-	-	-	1,909
	H(C3)-H(C2')	-	-	-	-	-	2,461
320°	O-H(C2')	2,128	2,107	2,129	2,129	2,129	-
	H(C2)-H(C6')	1,889	1,874	1,889	1,888	1,889	-
340°	O-H(C2')	-	-	-	-	-	1,590
	H(C2)-H(C6')	-	-	-	-	-	2,025

Table 3: Energy from Extreme Value of Isoflavon Derivatives in Soybean

Angle	Energy (kcal/mol)					
	Biochanin a	Daidzein	Glycitein	Formononetin	Genistein	Equol
40°	-3775,037	-3406,4587	-3778,365	-3675,219	-3506,286	-
80°	-3773,662	-3405,031	-3777,047	-3673,792	-3504,914	-3532,874
140°	-3774,984	3406,137	-3778,101	-3674,906	-3506,235	-3529,888
180°	-3770,012	-3400,902	-3773,596	-3669,719	-3501,186	-
220°	-3774,745	3406,125	3778,357	-3674,885	-3505,992	-
260°	-3773,551	-3404,910	-3777,070	-3673,670	-3504.804	-
280°	-	-	-	-	-	-3533,686
320°	-3774,994	-3406,192	-3778,357	-3674,953	-3506,255	-
340°	-	-	-	-	-	-3530,594

Table 2 show the distance of nearby atoms in extreme values angles each derivatives compound of isoflavon in soybean. Nearby atoms was two neighboring atoms that occur repulsion energy between that atoms. The extreme values were happened because the interaction of the two nearby atoms and make the energy higher. The lower the strain energy, the more stable that compound. From Table 3, the most minimum energy of derivatives compound of isoflavon in soybean biochanin a, daidzein, glycitein, formononetin, genistein, and equol was at 40°.

The most maximum energy from that compound at 180° because when the torsion at 180°, two nearby atoms was very close that makes the structure more unstable. Besides, equol has the minimum energy at 280° and the most maximum energy at 140°. For example in biochanin a at 40°, the nearby atoms in H (C2)-H(C2') was 2,00438 Å. The nearby atoms at 180° in O-H(C6') was 1,82086 Å and H(C2)-H(2') was 1,70648 Å. Biochanin a, daidzein, glycitein, formononetin, genistein and equal have a nearby atoms that was affect the maximum and minimum energy. Hence, this was the proof that distance of two nearby atoms affects the structure stability and strain energy.

Conclusion

The structural conformational study of derivatives compound of isoflavon in soybean was performed based on the desktop molecular modeling program by IS 1 semi empirical and selected. The distances of two nearby atoms affect the structure stability and the strain energy because the lower the strain energy, the more stable that compound.

In this study, the most stable structure for biochanin a, genistein, daidzein, glycitein, formononetin was 40° while the most stable structure for equol was 280°. From the angles, the next study can found the possibility of derivatives compound of isoflavon in soybean as a cancer drugs by molecular docking research. From that study, researchers no need to test every derivatives compound of isoflavon in soybean in laboratory and more efficient in time, money, substances, and energy.

Acknowledgements

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