COMPUTATION OF BINDING ENERGY OF BIOACTIVE CONSTITUENTS PRESENT IN CASSIA FISTULA SPECIES BY DFT APPROACH

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ABSTRACT

Bioactive compounds isolated from Cassia fistula plant were found to exhibit various pharmacological properties as revealed by the literature resources. In order to find the lead compounds among the eight pharmacological important constituents selected for our work, binding energy were computed by DFT approach using Gaussian software. B3LYP and HF method using three basis sets like STO-3G, 32-1G and 63-1G were adopted for the calculation of binding energy. Among the above constituents , Sennoside A was found to have good binding energy by both the methods. B3LYP method binding energies were found to be STO-3G (-3088.394), 32-1G(-3107.367) and 63-1G (-3124.647). Binding energy by STO-3G (-3066.066), 32-1G (-3088.914) and 63-1G (-3104.859) were observed by HF method. These results showed that among the bioactive constituents present in the cassia fistula plant, Sennoside A was found to have very good binding energy. Because of this very good binding energy, it may find as good medicine for the treatment of disease in future.

Keywords: Cassia fistula plant, DFT, B3LYP and HF.

No. of Tables: *2* ***No. of Figures:*** *8* ***No. of References:24***

INTRODUCTION

Studies of phytochemical analysis of cassia fistula species have demonstratedanthrax quinone derivative and flavanoids present in the plant are widely used for its medicinal properties. Cassia fistulaplantextract is used as an anti-periodic agent and in the treatment of rheumatism [1]. The leaf extract is found to have anti-tussiveand wound healing properties [2]. In the Indian literature, this plant has been described to be useful against skin diseases, liver troubles, tuberculous glands and for the treatment ofhaematemesis, pruritus,leucodermand diabetes [3-14]. The plant parts could be used as a therapeutic agent in the treatment ofhypercholesterolaemia [15] . The plant has a high therapeutic value and can used as anti-inflammatory, hypoglycemic, antipyretic, analgesic, anti- ulcer and laxative agent [16]. Leaves and flowers are both purgative like the pulp. Ashes from burnt pods mixed with little salt are used with honey taking 3- 4 times to relieve cough.Flowers and pods are used as, febrifugal, biliousness andastringent. The ethanolic extract of pods show antifertility activity in female albino rats. The roots are used in fever, heart diseases, chest pain, joint pain, migraine, biliousness, and also applied in blood poisoning, anthrax ,antidysentric, leprosy and antidiabetic, for the removal of abdominal obstruction and blood dysentery. The extract of the root lowered the blood sugar level up to 30 % [17,18,19,20]. The bark possess tonic andantidysentricproperties, skin complaints, the powder or decoction of the bark is administeredin leprosy, jaundice, syphilis and heart diseases[21]. In our present work, binding energies of eightconstituents has beencomputatedusing the B3LYP and HF methods by DFT approach.

MATERIALS & METHODS

Thebioactiveconstituents present in the Cassia fistula plant were selected for ourwork as given below in figure.1-8 [22].

Methods

DFT APPROACH

The structures of the constituents like Catechin, Fistulicacid, Kaempferol, Rhein, Physcion, Rhein-8-glucoside, ProcyanidinB2 and SennosideA were drawn in Gauss View 5.0 The binding energieswere calculated byB3LYP and HF methods using STO-3G, 3-21G, 6-31G basissets [23,24&25]. The binding energy of the above compounds predicted by B3LYP and HF methods were given in**Table- 1 & Table- 2**

RESULT ANDDISCUSSION

DFT calculation: B3LYP method

The binding energy calculated by STO-3G basis set were -1090.608, -941.280, -1015.450, -1014.247, -974.506, -1616.099, -2033.321 and -3083.394a.u.forCatechin,Fistulicacid,Kaempferol,Rhein,Physcion, Rhein-8-glucoside, Procyanidin B2 andSennoside A compounds. Sennoside A was found to be to have good binding energy as -3083.394 a.u.Sennoside A have -3107.369a.u good binding energy compared to the other constituents binding energy, which were found to be -1099.005, -948.376, -1023.174, -1021.998, 984.376, -1628.638 and -2048.825 by 3-21G basis sets.Thebinding energies of the

above compoundscalculated by 6-31G basis sets were found to be -1104.773,-953.367,-1028.548,-1027.374,-986.636,-1637.184 and -2059.539a.u..From the above datait was concluded thatSennosideAwas found to have a good binding energy as -3123.647a.u. among theother bioactive constituents.

HF method

STO-3G

Among the bioactive compounds,Sennoside A have good binding energy as -3066.066a.u andtheotherconstituentswere found to be -1084.594,-935.926,-1009.783,-1008.594,-980.131,-1607.212 and -2021.731a.u.

3-21G

Sennoside A havegood binding energy as -3088.914 comparedto other bioactive constituents which were found to be -1092.623,-942.736,-1017.196,-1016.039,-987.468,-942.738,-1619.171and-2036.566a.u.

6-31G

The binding energies observed using 6-31G basis sets for the aboveconstituentswere found to be -1098.275,-947.636,-1022.466,-1021.317,-992.656,-953.374,-1627.543,-2036.566and -3104.859a.u. From these data it was found thatSennoside Awas found to be more stable among other compounds.

CONCLUSION

The binding energy of eight bioactive constituents were calculated byB3LYP and HF method using STO-3G, 3-21G and 6-31G.The B3LYP methodrevealed thatsennoside Awas found to have goodbindingenergy(-3123.647) and compared to other bioactive constituents -1104.773, -953.367, -1028.548, -1027.374, -986.636, -953.374, -1637.184 and -2059.539a.u. The HF methods of calculation of binding energies of showed that sennoside A was found to be good binding energy as-3104.859compared to other bioactive compounds-1098.275,-947.636,-1022.466,-1021.317,-992.656,-953.374,-1627.543 and-2036.56a.u.The above computation of binding energy showed that among the eight bioactive compounds selected for the above work,sennoside A was found to have agood binding energy.

Figures:

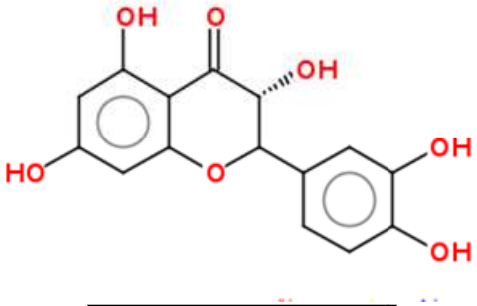

Figure. 1 Catechin

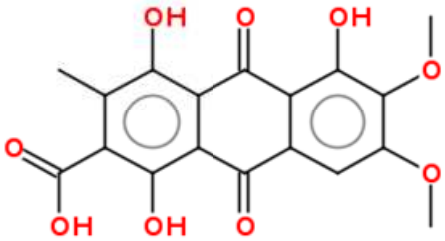

Figure. 2 Fistulicacid

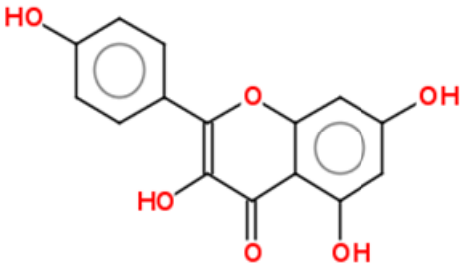

Figure. 3 Kaemferol

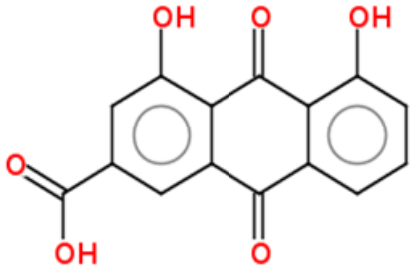

Figure. 4 Rhein

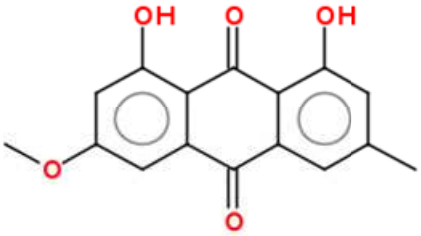

Figure. 5Physcion

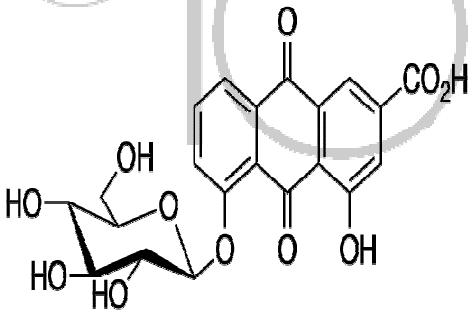

Figure. 6 Rhein-8-glucoside

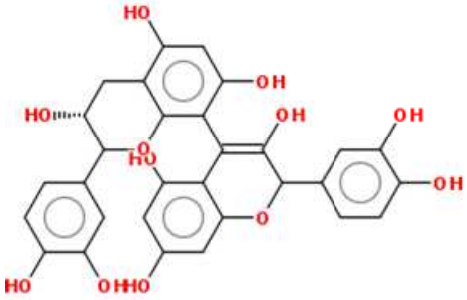

Figure. 7 Procyanidin B2

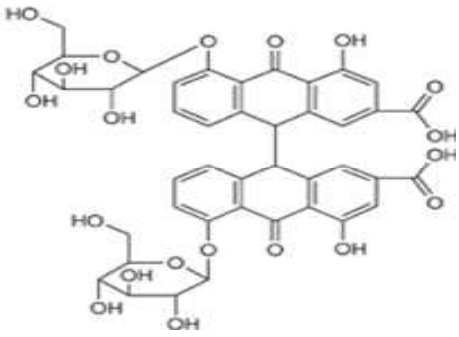

Figure. 8Sennoside A

Table 1:*Binding energy of compounds in B3LYP method*

S.No	Compounds name	Basis sets		
		STO-3G	3-21G	6-31G
1	Catechin	-1090.608	-1099.005	-1104.773
2	Fistulic acid	-941.280	-948.376	-953.367
3	Kaempferol	-1015.450	-1023.174	-1028.548
4	Rhein	-1014.247	-1021.998	-1027.374
5	Physcion	-974.506	-984.376	-986.636
6	Rhein-8-glucoside	-1616.099	-1628.638	-1637.184
7	Procyanidin B2	-2033.321	-2048.825	-2059.539
8	Sennoside A	-3083.394	-3107.369	-3123.647

Table 2:*Binding energy of compounds in HF method*

S.No	Compounds Name	Basis sets		
		STO-3G	3-21G	6-31G
1	Catechin	-1084.594	-1092.623	-1098.275
2	Fistulic acid	-935.926	-942.736	-947.636
3	Kaempferol	-1009.783	-1017.196	-1022.466
4	Rhein	-1008.594	-1016.039	-1021.317
5	Physcion	-980.131	-987.468	-992.656
6	Rhein-8-glucoside	-1607.212	-1619.171	-1627.543
7	Procyanidin B2	-2021.731	-2036.566	-2036.566
8	Sennoside A	-3066.066	-3088.914	-3104.859

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