DFT CALCULATIONS AND INSILICO DRUG ACTIVITY PREDICTIONS FOR FEW BIOACTIVE COMPOUNDS

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ABSTRACT

The bioactive compounds isolated from many plants articles collected the compounds like andrographolide, arjungenin, arjunicacid, Gossypin, Phyllanthin, Silymarin and Sitosterol.The present study make an effort to investigate DFT calculations for the determination of binding energy were bring out by using the Gaussian software. DFT were performed at B3LYP and HF methods using three basis sets like STO-3G, 3-21G, 6-31G. The DFT calculations of binding energy showed that gossypin was established to be more stable among other selected seven compounds.

KEYWORDS: Medicinal Plants compounds DFT, B3LYP and HF.

No: of Tables : 2 **No: of Figures: 6** **No: of References : 8**

INTRODUCTION

Andrographis paniculata plant belongs to Acanthaceae family[1]. The leaves and the root of A. Paniculata are used in medicine as Anti -cancer, astringent, diuretic, emmenagogue, gastric tonic, carminative.Andrographis paniculata plant parts are used to cure fever, cold, laryngitis ,disorders of liver, colic pain, loss of appetite,dysentry, cholera, piles, and gonnorhoea, diabetes, influenza, anti-malarial, anti-bacterial, filaricidal, bronchitis, swellings and itches, herpes, sore throat, hepatitis,snake bite[1].Terminalia Arjuna plant belongs to combretaceae family commonly known as Arjuna or Arjun. The leaves and the bark of T.arjuna are used in medicine as astringent. demulcent, expectorant, cardiotonic, styptic, antidysenteric, urinary astringent, aphrodisiac, anti-dysentric, lithotriptic, antipyretic.Terminalia arjuna plant parts are used to cure Asthma, diabetes, cough, tumour, excessive respiration, ulcers,spermatorrhoea, leucorrhoea, inflammation and skin disorders, obesity, hypertension and hyperglycemia, biliousness, sores and an antidote to poison, hepatic, congenital, venereal and viral diseases, cardiac ailments. leaves of Terminalia were used as anti microbial and antifungal activity, hypolipidemic, hypocholesteremic, anticoagulant, antihypertensive, antithrombotic,antiviral, antifungal and antibacterial agent.leaves soaked in water over night used in burning sensation and dyspepsia[2,3].Hibiscus vitifolia plant belongs to Malvaceae family commonly known as 'Dhakto Kalo Bhendo' . The roots of H.vitifolia plant are used in medicine as astringent, urinary disinfectant, sedative, analgesic, neuro muscular block properties.Hibiscus vitifolia plant parts are used to cure antiinflammatory, anti-pyretic, antifungal, hypoglycemic. The plant root extract possess potent protective action against anti-tubercular drug induced hepatotoxicity . They are also used in the treatment of pulsating anterior fontanelle in babies, in kidney problems. The seeds are considered as stimulant and anti-spasmodic. Aqueous extracts of root showed hepatotoxicity activity[4]. Phyllanthus amarus plant belongs to Euphorbiaceae family commonly known as Jangli amli .The leaves of P.amarus are used in medicine as antiviral, antihyperglycemic, antioxidant and hepatoprotective . Phyllanthus amarus plant parts are used to cure anticancerous, antimicrobial. antiinflammatory, antihepatotoxic, antilithic, analgesic, hypotensive, antispasmodic, antiviral, antibacterial, diuretic, antimutagenic and hypoglycemic properties.Treatment of flu, dropsy, diabetes, jaundice, gall and bladder calculus, liver disease. Hypocholesteremic. Antifungal .Radioprotective activities. Extract of the plant is known to inhibit gastric carcinogenesis[5].Swertia chirata plant belongs to Gentianaceae family commonly known as Chiravata.The S. chirayita roots are used in medicine as antipyretic, anthelminitic, antiperiodic, cathartic and in asthma and leucorrhoea in Ayurveda and as harsh, analeptic, stomachic, mitigate inflammation, relaxing

to pregnant uterus and never ending fevers .Swertia chirata plant parts are used to cure diarrhea, never ending fever, anemia, liver function disorders and bronchial asthma.It is a remedy for ulcers, Gastrointestinal diseases, skin diseases, cough, hiccup, liver and Kidney diseases, Neurological disorders ,and urinogenital tract disorders.[6].

EXPERIMENTAL METHODS

Materials

The bioactive constituents present in the few plant were selected for our literature work as given below in figure-I to figure-VIII [7].

Methods

DFT Calculation DFT calculations were carried out using Gaussian software 05. Binding energies of the Andro grapholide , Arjungenin , Arjunic acid, Gossypin , Phyllanthin , Silymarin, Sitosterol compounds were calculated by B3LYP and HF methods using STO-3G, 3-21G, 6-31G basis sets[14]. The structures of these compounds were drawn in Gauss View 5.0. The drawn chemical structure become visible as given below The bioactive constituents present in the few plant were selected for our literature work as given below in figure-I to figure-VIII [7].

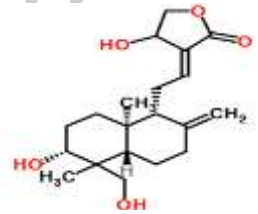

Figure- I Andrographolide

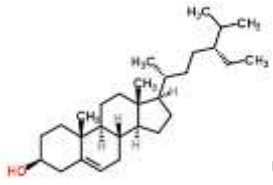

Figure-II Silymarin

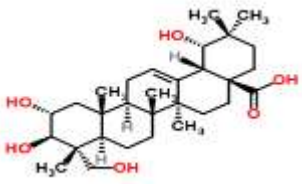

Figure-IIArjungenin

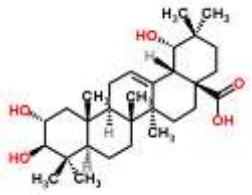

Figure-III Arjunic acid

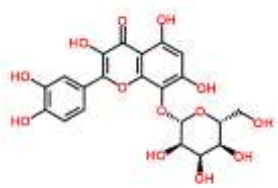

Figure-IV Gossypin

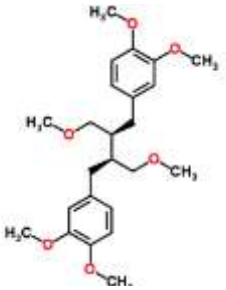

Figure-V Phyllanthin

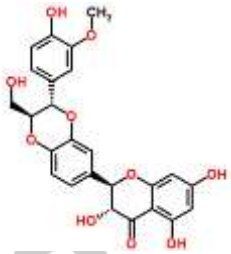

Figure-VI Sitosterol

Table- I Binding energy of compounds in B3LYP method

S.No	Compounds Name	Basis sets		
		STO-3G	3-21G	6-31G
1	Andrographolide	-1140.343	-1148.814	-1154.786
2	Arjungenin	-1600.325	-1612.229	-1620.591
3	Arjunic acid	-1526.193	-1537.446	-1545.418
4	Gossypin	-1765.005	-1778.811	-1788.139
5	Phyllanthin	-1368.374	-1378.366	-1385.539
6	Silymarin	-1695.181	-1708.054	-1716.992
7	Sitosterol	-1154.741	-1162.671	-1168.715

Table-II Binding energy of compounds in HF method

S.No	Compounds Name	Basis sets		
		STO-3G	3-21G	6-31G
1	Andrographolide	-1133.356	-1141.452	-1147.307
2	Arjungenin	-1590.357	-1601.652	-1609.844
3	Arjunic acid	-1516.540	-1527.223	-1535.036
4	Gossypin	-1755.365	-1768.516	-1777.647
5	Phyllanthin	-1360.174	-1369.709	-1376.733
6	Silymarin	-1695.181	-1708.054	-1716.992
7	Sitosterol	-1154.741	-1162.671	-1168.715

RESULT AND DISCUSSION

a) DFT calculation

i) B3LYP method The binding energy calculation by using three basis sets (STO-3G,3-21G,6-31G) listed in **Table- I** showed the following resultThe binding energies were found to be Andrographolide(-1140.343), Arjungenin(-1600.325), Arjunic acid(-1526.193), Gossypin (-1765.005), Phyllanthin(-1368.374) ,Silymarin (-1695.181), Sitosterol (-1154.741) compounds using STO-3G basis sets. From the above data it was found that Gossypin was found to have good binding energy among the other bioactive constituents.

From above compounds were found to be Gossypin have a good binding energy as -1778.811 a.u among the other bioactive constituents using 3-21G basis sets, other compounds binding energies were found to be -1148.814, -1612.229, -1537.446,-1378.366, -1708.054, -1162.671 and -1124.872 a.u . The binding energies of the above nine compounds by 6-31G basis sets were found to be -1545.418, -1154.786, -1620.591, -1385.539, -1716.992, -1168.715 and -1130.747 a.u. From the above data it was ended with the intention of gossypin was found to have a good binding energy as -1788.139 a.u. among the other bioactive constituents.

ii) HF method

In **Table – II** showed the following observations the binding energy calculated by using three basis sets STO-3G, 3-21G, 6-31G as listed above.

STO-3G source

The binding energy for the selected eight compounds were found to be -1133.356, -1590.357, -1516.540, -1755.365, -1360.174, -1695.181,-1154.741, -1116.749a.u.

and it was found that gossypin have good binding energy.

3-21G source

Gossypin was found to be (-1768.516) more stable using 3-21G basis sets other seven compounds binding energies were found to be-1141.452, -1601.652,-1527.223, -1369.709, -1708.054,-1162.671, -1124.872 a.u.

6-31G source

The binding energies observed using 6-31G basis sets for the above compounds were

-1147.307, -1609.844, -1535.036, -1777.647, -1376.733, -1716.992, -1168.715,-1130.747 a.u. From these data it was found that gossypin was found to be more stable among other compounds.

Conclusion

In the present investigation, 8 bioactive compounds from 6 medicinal plants.The eight bioactive constituents were calculated by binding energies as per the above 3 basis sources and hence gossypin was establish to be more stable than other bioactive constituents. It was observed that gossypin was found to have -1765.005, -1778.811, -1788.139 a.u by B3LYP method. The HF methods of calculation of binding energies of showed that gossypin was found to be good binding energy as -1755.365a.u. as STO-3G basis sets , -1768.516a.u. as 321-G basis sets and -1777.647a.u. as 631-G basis sets.

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