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ORIGINAL ARTICLE

Ab initio study of thermodynamic properties of Curcumin

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ABSTRACT
Curcumin, a yellow pigment present in the Indian spice turmeric (associated with curry powder), has been linked with suppression of inflammation; angiogenesis; tumor genesis; diabetes; diseases of the cardiovascular , pulmonary, and neurological systems, of skin, and of liver; loss of bone and muscle; depression; chronic fatigue; and neuropathic pain. The usefulness of curcumin is limited by its color, lack of water solubility, and comparatively low invivo bioavailability. as a result of the multiple therapeutic activities attributed to curcumin , however,there is an intense search for a "super curcumin" without these problems Computational calculations using HF and DFT (LSDA,BPV86,B3LYP) and The basis set used were{-31G(d)- 3-21G(d)- STO3G(d)} level of theory were under taken to predict the structural properties of one molecule.
Keywords: *Turmeric plant, Curcumin, frequency calculations, density functional theory (DFT)*

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INTRODUCTION

Phyto chemicals are obviously taking place substances found in plants. There has been considerable public and scientific importance in the use of phytochemicals derived from nutritional components to combat human diseases, especially the two commonest killers in the developed world, cardiovascular disease and cancer. The dried ground rhizome of the perennial herb *Curcuma longa* Linn., called turmeric in English, haldi in Hindi and ukon in Japanese, has been used in Asian medicine since the next millennium BC [1] its utility is referred to in the olden Hindu scripture, the Ayurveda. Other than its aromatic, stimulant and coloring properties in the diet, turmeric is mixed with other natural compounds such as slaked lime and has been used topically as a treatment for wounds, inflammation and tumors. In contrast to the maximum dietary consumption of 1.5 g per person per day in certain South East Asian communities, smaller quantities of turmeric tend to be used for medicinal purposes [2]Curcuma spp. include turmerin (a water-soluble peptide), necessary oils (such as turmerones, atlantones and zingiberene) and curcuminoids counting curcumin [1,7-bis-(4-hydroxy-3-methoxyphenyl)-1,6 heptadiene-3, 5-dione]. Curcuminoids can be defined as phenolic compounds derived from the roots of Curcuma spp. (Zingiberaceae). Curcumin (diferuloyl methane) is a low molecular weight polyphenol, earliest chemically characterized in 1910, that is generally regarded as the most active constituent of and comprises 2–8% of most turmeric preparations [3-4] Curcumin, 1,7-bis(4-hydroxy-3-methoxyphenyl)-1,6-heptadiene-3,5-dione, is the main yellow bioactive component of turmeric (Curcuma longa), a perennial plant of the ginger family)Zingiberaceae), which is native to tropical South Asia [5-6].It isextensively used as a spice, food preservative and coloring agent.It is a non-toxic, highly promising normal antioxidant compound having a wide series of biological applications. It is anticipated that curcumin may find applications as a novel drug in the near future to control various diseases, including anti-inflammatory activity [7-8-9] antiarthritic [10], Antiamyloid [11], hepatoprotective [12], thrombosuppressive [13], anti-HIV [14] antimicrobial [15-16] Antioxidant [17] and antitumor agent [18]In addition, Curcumin has been found to be effectual in treating the squamous cell carcinoma of head and neck, melanoma,sarcoma, leukemia, lymphoma, and the cancers of colon, breast, nervous system, lung, pancreas and ovarian [19-20]Curcumin has drawn intense interest lately due to its potential pharmaceutical importance [21–22-23-24]. Unfortunately, its poor water solubility and inadequate absorption in vivo result in low bioavailability and significantly limit its clinical application Curcumin is weakly absorbed from the gut and the quantity of curcumin that reaches tissues outside the gut is pharmacologically insignificant as per the measurements of blood plasma levels and biliary excretion. The insolubility of curcumin in water at physiological pH limits absorption, poor bioavailability, rapid metabolism, an excretion[25-26] Curcumin has been encapsulated in liposome [27] silk fibroin and chitosan [28] chitosan [29]phospholipids [30] cyclodextrin[31] silica particles [32] and polymeric nanoparticles [33-34] Curcumin molecular possesses two isomers. One is di-ketonic while another is ketoenolic [35] Modern computational chemistry methods, principally DFT, have proven to be exceptional tools for determining molecular structures [36]. All calculations have been in the gas phase, while gas phase predications are appropriate for many purposes and inadequate for describing many systems in solutions. Solvent effects on electronic structure of molecules have been investigated by many chemists and physicists to understand molecular structure, mechanism of chemical reactions in solution etc. by using quantum chemical calculations and molecular dynamics simulations. Physical properties such as geometry of molecules and charge distribution in solution often vary from those in vacuum [37].As widely used in the theoretical studies on molecular electronic structure and spectral properties, density functional theory (DFT) and time-dependent density functional theory (TDDFT) [38] are used in the simulations in this work to do high-level computational analysis of the designed compound.

COMPUTATIONAL ANALYSIS

Computational chemistry software designed to model a broad series of molecular systems under a range of conditions, performing its computations starting from the basic laws of quantum mechanics. It was primarily released in 1970. The current version Gaussian 09 is its 19th versions.

Gaussian has implemented almost all the quantum mechanical methods which include Hartree-Fock and post Hartree-Fock method and DFT method. It can be used to calculate the electronic properties, charges, molecular energy, IR, Raman, UV, NMR and other spectroscopic properties of small to media molecules.

Calculations the structure of molecule Curcumin was fully optimized with functional at the basis set using Gaussian 2003 program23 The optimized structure was used to calculate the NMR spectra at the level using the GIAO method.

In this study, charge distribution, geometry optimizations and thermodynamic properties were employed with diverse model chemistries Computational calculations using B3LYP/6-31G(d)- B3LYP/3-21G(d)- B3LYP/STO3G(d)-HF /6-31G(d)- HF/3-21G(d)- HF /STO3G(d)-LSDA/6-31G(d)- LSDA/3-21G(d)- LSDA/STO3G(d)-PVB86/6-31G(d)- PVB86/3-21G(d)-PVB86/STO3G(d)- level of theory were under taken to predict the structural properties of curcumin molecule.

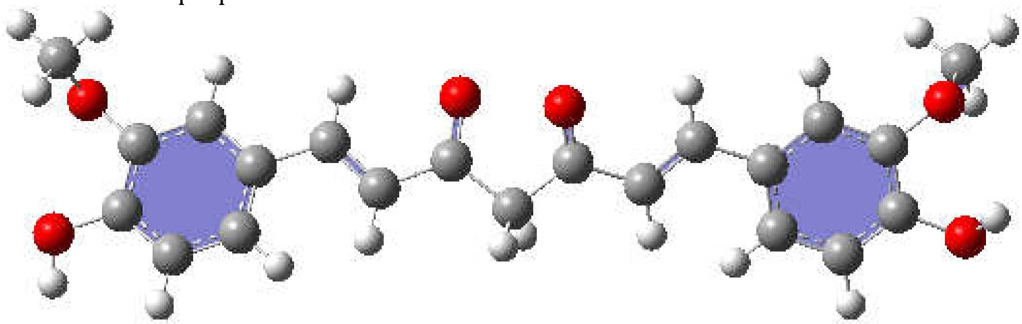

Fig 1. The Chemical structures of curcumin(1,7-bis(4-hydroxy-3-methoxyphenyl)1,6-heptadiene-3,5-dione)..

RESULTS AND DISCUSSIONS

As matter of fact, the energies and thermo chemical parameters can give valuable information about structures and relative stabilities of these systems. The relative stability of various structures of ($C_{21}H_{20}O_6$) are computed in DFT methods using b3lyp-PVB86-LSDA ,and HF levels of theory which present thermodynamic properties of ($C_{21}H_{20}O_6$) and comparison of different levels with each other's were.

The energetic information is thermodynamically favored to determine the most stable structure at finite pressure and temperature in which individual terms are referred to 298k , and the Gibbs free energy should be used To verify structural stability of our system we have optimized($C_{21}H_{20}O_6$).

Therefore, in this paper, by using ab initio calculations, we analyze the Gibbs free energy of the formation. we found that bet ween these methods , the result obtained at those of the other calculations though HF shows the best result for ($C_{21}H_{20}O_6$).systems with are the most stable one with the minimum at -4813.92Kcal/Mol .As can be seen in Table 1 ,Table 2 ,Table 3 .which display different levels of theory as a function of energy the lowest value of energy is belong to HF levels at the -5548.63K CAL/MOL for ($C_{21}H_{20}O_6$).systems which indicate that at this point our system have got the most stability.show in Figure1, Figure 2 , Figure 3.

Table1.Relative thermodynamic data for ($C_{21}H_{20}O_6$) system in Kcal/Mol and antropy incal/Mol.kelvin

BASIS SET 6-31g*						
METHOD	Zero-point correction	Zero-point Energies	ΔG	ΔH	S	ΔE
B3LYP	-6.55	-48.36	-44.45	-50.26	163.07	-48.69
LSDA	0.00	-4320.56	-4317.50	-4322.35	159.86	-5002.50
HF	-24.00	-4816.53	-4813.92	-4818.28	158.21	-5548.63
BVP86	-0.24	0.00	0.00	0.00	145.52	0.00

Table 2.Relative thermodynamic data for ($C_{21}H_{20}O_6$) system in Kcal/Mol and antropy incal/Mol .kelvin

BASIS SET	**3-21g***					
METHOD	Zero-point correction	Zero-point Energies	ΔG	ΔH	S	ΔE
B3LYP	-6.02	-52.43	-51.50	-53.46	152.46	-54.28
LSDA	0.00	-4283.49	-4282.48	-4284.77	154.27	-4959.80
HF	-21.83	-4838.83	-4836.88	-4840.91	160.09	-5577.50
BVP86	-0.43	0.00	0.00	0.00	146.57	0.00

Table 3.Relative thermodynamic data for ($C_{21}H_{20}O_6$) system in Kcal/Mol and antropy incal/Mol .kelvin

BASIS SET STO-3G*						
METHOD	Zero-point correction	Zero-point Energies	ΔG	ΔH	S	ΔE
B3LYP	-6.76	-106.59	-105.89	-106.80	126.49	-99.83
LSDA	-1.68	-5068.43	-5063.68	-5070.39	143.28	-5066.74
HF	-32.27	-5375.10	-5370.79	-5377.61	143.61	-5342.82
BVP86	0.00	0.00	0.00	0.00	123.85	0.00

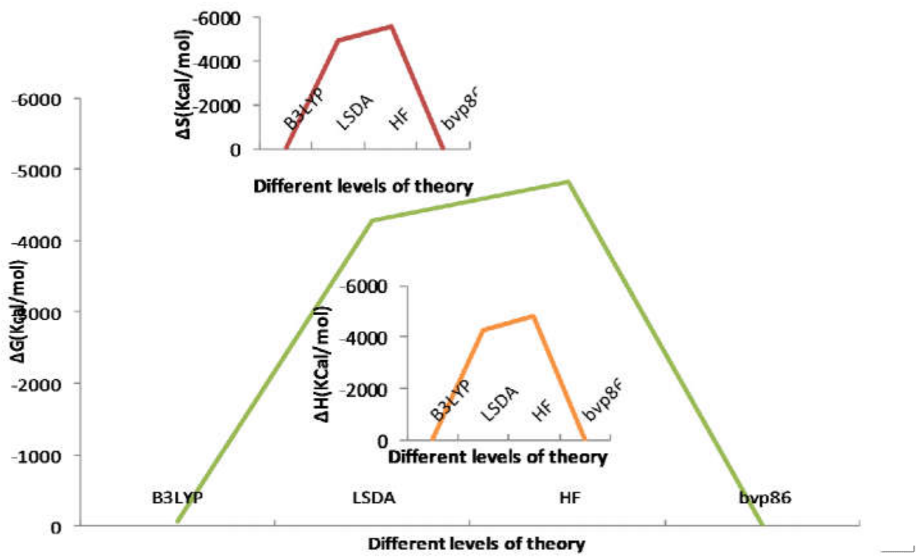

Figure 1. Different levels of theory as a function of Δ (ΔG) Δ (ΔH) Δ (ΔE) in Kcal/mol in

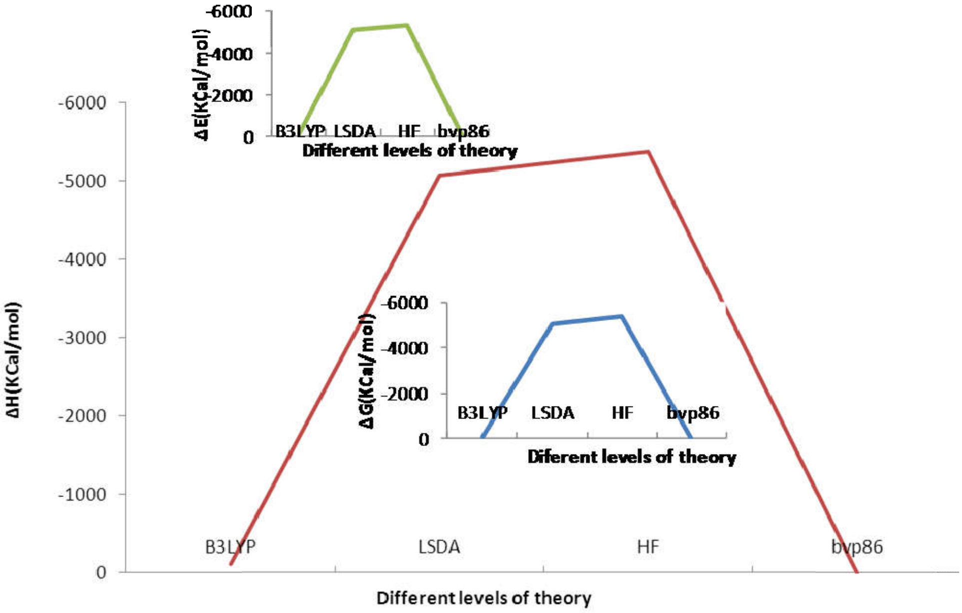

Figure 3. Different levels of theory as a function of Δ(ΔG) Δ(ΔH) Δ(ΔE) in Kcal/mol in $C_{21}H_{20}O_6$ structure

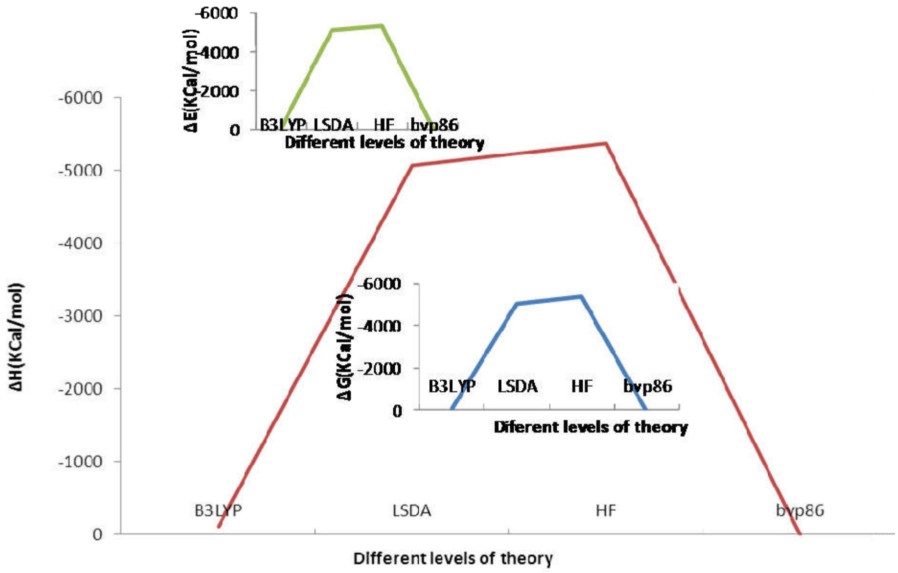

Figure 3. Different levels of theory as a function of Δ(ΔG) Δ(ΔH) Δ(ΔE) in Kcal/mol in $C_{21}H_{20}O_6$ structure

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