The Investigation Of Menthol's Bioactivity As Theoritical By Using DFT (Density Functional Theory)

Faik Gökalp

Kırıkkale University, Faculty of Education,
Department Of Primary Education, Science Education Division,
Yahşihan/Kırıkkale, Turkey
faik.gokalp@kirikkale.edu.tr

Abstract

Mints are used tradational medicine for hundred years by humankind. The important constitiuent of mint, menthol, is especially in blood is eager to give reaction as an antioksidan. To understand menthol's bioactivity in body, some thermodynamical values (gibbs free energy, dipol moment HOMO, LUMO and the difference between HOMO, LUMO) of menthol are measured by using DFT. Menthol dissolves in blood easily, reacts as antioksidant and it is more stable than in gas form. So,It is so stable as protecting from radicalic attracts.

Keywords: Mint, Menthol and DFT

1 Introduction

Menthol, the constitiuent of mint, is commonly used pharmaceutical and flovoring industries. The production of it has increased day by day [1].

Some plants are rich in phenolic compounds. For example, oregano, thyme, basil and mint. They have strong antioxidant acitivity and cell protection against to free radicals. Morever, the substances that have phenolic groups show protective activities in cancer diseases [2-4].

Mint includes over two hundred different substances such as carvone, limonene, menthone, menthol, vitamin A, C, K, some minerals (calcium,sodium,iron) and thiamine,niacin.

Natural products from medicinal plants represent a fertile ground for the development of novel anticancer agents. Essential oils from some herbs and spices have both anti-bacterial and cancer chemopreventive activities [5,6].

Essential oils from mints,one of them menthol, has antimicrobial proporties against to Paenibacillus larvae [7]. Mentha piperita has medicinal treatment effects especially cancer, diabetes, asthma,heart problems and also antibacterial, antifungal, antimicrobial du e to phenlic grroups in essential oils of it [8]. One of them is menthol.

Mint that has pharmaetucal for some diseases as anti-cancer,antimicrobial,anti-inflammatory, analgesic etc. icludes a lot of active compounds. Menthol that gives flavour and arome to the mint is one of them [9].

Treatment with menthol reduces the activity of MPO and SOD, and the protein levels of GSH, GSH-Px and GR were increased. The levels of TNF-α and IL-6 decreases and there was an increase in the level of IL-10 [10].

2 Results And Discussions

The structure of menthol found in mint, is given in Figure 1.

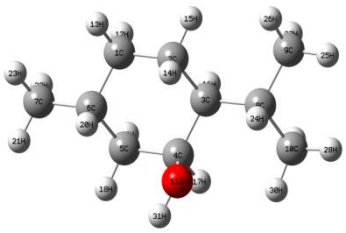

Figure 1. The structure of Menthol

Thermodynamical values releated to the menthol are given in Table 1.

Table 1. Menthol's values by Using DFT (The values are given as Hartree 1Hartree:=627.5095 kcal. mol-1)

DFT	Menthol (Blood)	Menthol (Gas)
E0	-468.3948352	-468.3753363
EZPE	0.285800	0.287595
Etot	0.298450	0.300062
Hcorr	0.299395	0.301006
Gcorr	0.247841	0.249976
E0 + EZPE	-468.109035	-468.087741
E0 + Etot	-468.096385	-468.075275
E0 + Hcorr	-468.095441	-468.074331
E0 + Gcorr	-468.146994	-468.125360
Dipol Moment	1.9158	1.2866
HOMO	-0.26985	-0.25792
LUMO	0.00034	0.06579
Δ (HOMO-LUMO)	-0.27019	-0.91582

When we compare menthol in gas and blood forms; Thee gibbs free energy in blood -468.146994 Hartree in gas, -468.125360 Hartree So,menthol in blood is higher that means it is eager to give reaction. Dipol moment of the menthol in blood is 1.9158 debye and in gas form is 1.2866 debye. Therefore we can say ıt dissolves in blood and give reaction as an antioksidan because of having phenolic group. Besides, in blood Δ (HOMO-LUMO) is -0.27019, It is lower from the gas form, -0.91582. As a result of these, Menthol dissolves in blood easily, reacts as antioksidant and more stable than in gas form. It is so stable that ıt protect from radicalic attacts.

3 References

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