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PHOTOCATALYTIC DEGRADATION OF AMOXICILLIN: A COMBINED COMPUTATIONAL APPROACH TO THE DETERMINATION OF REACTION PATHWAYS

AMOKSİSİLİNİN FOTOKATALİTİK DEGRADASYONU: HESAPSAL OLARAK REAKSİYON YOLLARININ BELİRLENMESİ

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ABSTRACT

Amoxicillin, an antibacterial drug, is a part of aminopenicillin family, which is so called broad-spectrum penicillin. In addition to many therapeutic activities, these drugs have several side effects like rash and anaphylaxis. The drug interactions occurring outside the body are categorized as physical or chemical and may occur during formulation, storage as well as while mixing ingredients.

The presence of pharmaceuticals in the aquatic environment as well as in drinking water has raised a growing concern in recent years. Among the groups of pharmaceutical compounds of greatest environmental interest are antibiotics due to their extensive use for the treatment of bacterial infections in the whole world. The most dangerous effect of antibiotics is the development of multi-resistant bacterial strains that can no longer be treated with the presently known drugs.

Calculations were carried out using the Density Functional Theory DFT/B3LYP/6-31G* levels by using COSMO as the solvation model. For this purpose, possible rections was examined estimately using Gaussian 09 package software.

Figure 1: Structure of amoxicillin.

Keywords

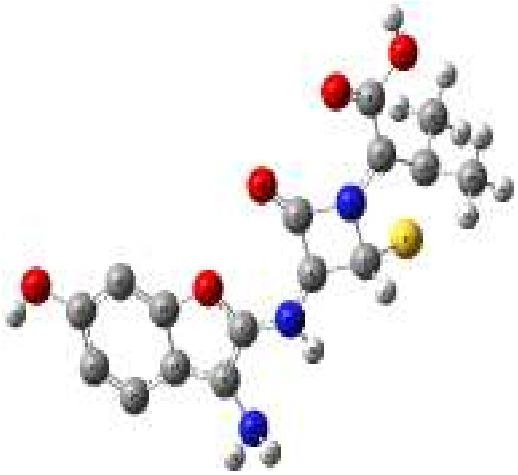
Amoxicillin, DFT, Gaussian09.

ÖZET

Amoksisilin, anti-bakteriyel bir maddedir, bu yüzden, penisilin grubundan aminopenisilin ailesinin bir parçasıdır. Birçok tedavi faaliyetlerinin yanı sıra, bu ilaçlar döküntü ve anafilaksi gibi birçok yan etkileri vardır. Vücut dışında fiziksel ya da kimyasal olarak etkileşimi vardır.

Son yıllarda içme sularında bu ilaçlara rastlanması büyük endişe yarattı. Farmasötik bileşik grupları arasında olan antibiyotikler bakteriyel enfeksiyonların tedavisi için geniş bir kullanım alanına sahiptir.

Hesaplamalar su fazında Cosmo modeli kullanarak ve gaz fazında Yoğunluk Fonksiyonel Teorisi DFT / B3LYP / 6-31G * seviyeleri kullanılarak gerçekleştirilmiştir. Bu amaçla, muhtemel reaksiyon yolları, Gauss 09 paket programı kullanılarak incelenmiştir.



Şekil 1: Amoksisilin molekülünün optimize modeli.

Anahtar Kelimeler

Amoksisilin, DFT, Gaussian 09.

Kaynaklar / References

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