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THEORETICAL CALCULATIONS OF SOME NEW N-(A,B-UNSATURATED ACYL)SULFONAMIDES AND INVESTIGATION ON CORRELATIONS WITH THOSE EXPERIMENTAL VALUES

BAZI YENİ N-(A,B-DOYMAMIŞ AÇİL)SÜLFONAMİDLERİN TEORİK HESAPLAMALARI VE BU DEĞERLERİN DENEYSEL SONUÇLARLA KARŞILAŞTIRILMASI

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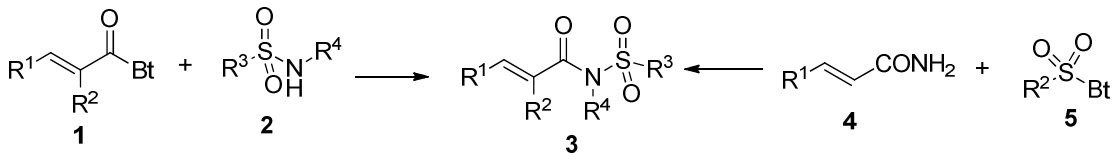
ABSTRACT

In this study, certain theoretical properties of three N-(α,β-Unsaturated acyl)sulphonamides (3) and seven reactants; Sulfonamides(2) with N-(α,β-unsaturated acyl)benzotriazoles(1) and α,β-unsaturated carboxamides(4) with sulfonylbenzotriazoles(5) (Table 1) , calculated in Gaussian09 program [1] using DFT method at B3LYP/6-311++g(d,p) level of theory.

The theoretical data was then compared with that of certain experimental results [2]

Table 1. IUPAC Nomenclature of the Studied Molecules



Molecule	IUPAC Name	Substituents		
		R^1	R^2	R^3
3a	4-Methyl-N-[(E)-3-phenyl-2- propenoyl]benzenesulfonamide	Ph	H	Tol
3b	N-[(E)-3-(2-Furyl)-2-propenoyl]-4-methylbenzenesulfonamide	Fur	H	Tol
3c	4-Methyl-N-[(E)-3-(2-thienyl)-2-propenoyl]benzenesulfonamide	Thi	H	Tol
3d	N-[(E)-3-Phenyl-2-propenoyl]methanesulfonamide	Ph	H	Me

Keywords

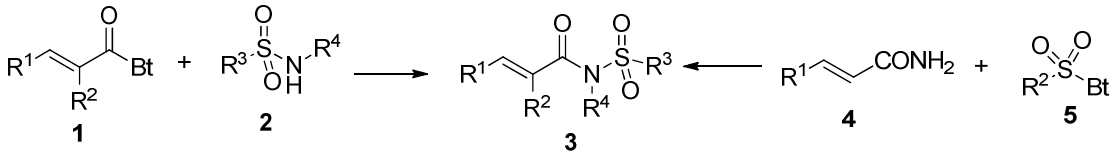
N-(α,β-unsaturated acyl)sulfonamides, Theoretical calculation, DFT.

ÖZET

Bu çalışmada, üç N-(α,β-Doymamış açil) molekülü (3) ve yedi adet Sülfonamid (2) ile N-(α,β-doymamış açil)benzotriazol (1) ve N-(α,β-doymamış Karboksiamid(4) ile sülfonilbenzotriazol reaktantlarının(5) (Tablo 1) , belirli teorik hesaplamaları Gaussian09 programı [1] kullanılarak DFT metod ile B3LYP/6-311++g(d,p) seviyesinde hesaplanmıştır.

Elde edilen teorik sonuçların önceden elde edilen deneysel verilerle karşılaştırılmaları yapılmıştır. [2]

Tablo 1. Çalışılan Moleküllerin IUPAC Adlandırılmaları.



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3c	4-Methyl-N-[(E)-3-(2-thienyl)-2-propenoyl]benzenesülfonamid	Thi	H	Tol

Anahtar Kelimeler

N-(α,β-doymamış açil)sülfonamid, Teorik hesaplama, DFT.

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Kaynaklar / References

[1] Gaussian 09. Revision B.01. Gaussian Inc.. Wallingford. CT. (2009).
[2] Alan R. Katritzky, S. Hanci, N.K. Meher, Arkivoc 2009 (iv), 115-124 , (2009).