



International Symposium on  
Multidisciplinary Studies

## V. ULUSLARARASI MULTİDİSİPLİNER ÇALIŞMALARİ SEMPOZYUMU (ISMS)

(16 - 17 Kasım 2018, Ankara/ Türkiye)

(Özet Kitabı)

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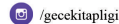
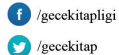
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## <sup>1</sup>H NMR kinetic and mechanistic study of the formation of amino acids derived N-allyl-2-thiohydantoins

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### Abstract

The reaction between amino acid esters and allyl isothiocyanate leading to the formation of N-allyl-2-thiohydantoin derivatives is investigated using <sup>1</sup>H NMR spectroscopy.

The reactions are carried out at ambient temperature in CDCl<sub>3</sub>, in the presence of triethylamine as a base, under *second*-order conditions with an initial molar ratio 1:1. The changes in intensities of relevant signals show that after a few days there is only one dominant product in the system.

Monitoring of the formation of thiohydantoin derivatives by <sup>1</sup>H NMR spectroscopy confirmed that the reaction occurs in two consecutive steps. The first step is formation of thiohydantoic acid which undergoes cyclization in the second step, forming the thiohydantoin nucleus. The rate constants are calculated after integration of the relevant signals of substrate and product of the cyclization.

The reactivities of the amino acid esters are compared and a conclusion is made on the basis of their affinities towards cyclization to thiohydantoins in regards to their structure relationships.

**Key words:** amino acids, thiohydantoins, kinetics, mechanism, reactivity