



III. International Turkish Congress on Molecular Spectroscopy



**AUGUST 26-29**

**Bodrum | Turkey**

**BOOK OF ABSTRACTS**



III. International Turkish Congress on Molecular Spectroscopy

**B O D R U M**  
**T U R K E Y**

AUGUST 26-29

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### **WELCOME TO TURCMOS 2017,**

On behalf of the Scientific and Organizing Committee, we would like to welcome you all to the “**International Turkish Congress on Molecular Spectroscopy (TURCMOS2017)**”. The scope of the congress is to encourage the exchange of ideas and future collaborations all around the world, introduce new techniques and instruments, and present recent developments in this field of research. In the congress, all aspects of spectroscopic methods as well as related computational and theoretical approaches will be considered. Contacts between young researchers (M.Sc. and Ph.D.) and prominent experts will be particularly stimulated, aiming at the development of future collaborations.

We would like to express our acknowledgements to Muğla Sıtkı Koçman University Rectorateship, Faculty of Fine Arts Deanship and Turkish Physics Foundation for their support.

We hope that the congress will provide you intellectual and social experience. We wish you enjoyable week in Bodrum

**Ozan ÜNSALAN**

*President*

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*Vice President*

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**Supramolecular self-assembly of new benzamide derivatives directed by intermolecular and  $\pi$ -stacking interactions: Crystal structures and Hirshfeld surface analyses**

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We have synthesized and characterized a series of closely related two thiourea derivative molecules (1 and 2), obtained by reaction of 4-R-benzoyl chloride (R: H and OCH<sub>3</sub>) with an equimolar amount of potassium thiocyanate and dibenzilamine in dry acetone (Fig. 1). The crystalline and molecular structures of synthesized compounds have been examined to understand how alter the crystal packing of the substituted different functional groups at para positions on the aromatic ring. Single-crystal X-ray analysis has revealed that molecules of the prepared compounds are assembled into supramolecular units connected via networks of similar intermolecular interactions. The packing arrangements of the compounds, however, were found to be different. We have also conducted an analysis of Hirshfeld surfaces and associated two dimensional fingerprint plots for the synthesized compounds and followed the changes of different properties on these surfaces upon systematic variation of the substituent. Hirshfeld surface analysis and decomposed fingerprint plots show that the structures are stabilized by H $\cdots$ H, H $\cdots$ S, O $\cdots$ H, N $\cdots$ H, C-H $\cdots$  $\pi$  and  $\pi\cdots\pi$  intermolecular interactions. The most significant contributions come from H $\cdots$ H and C $\cdots$ H contacts, which correspond to van der Waals interactions and the C-H $\cdots$  $\pi$  contacts, respectively.

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**Keywords:** Hirshfeld surfaces, Non-covalent interactions, Benzamide, X-ray single crystal diffraction, Synthesis.

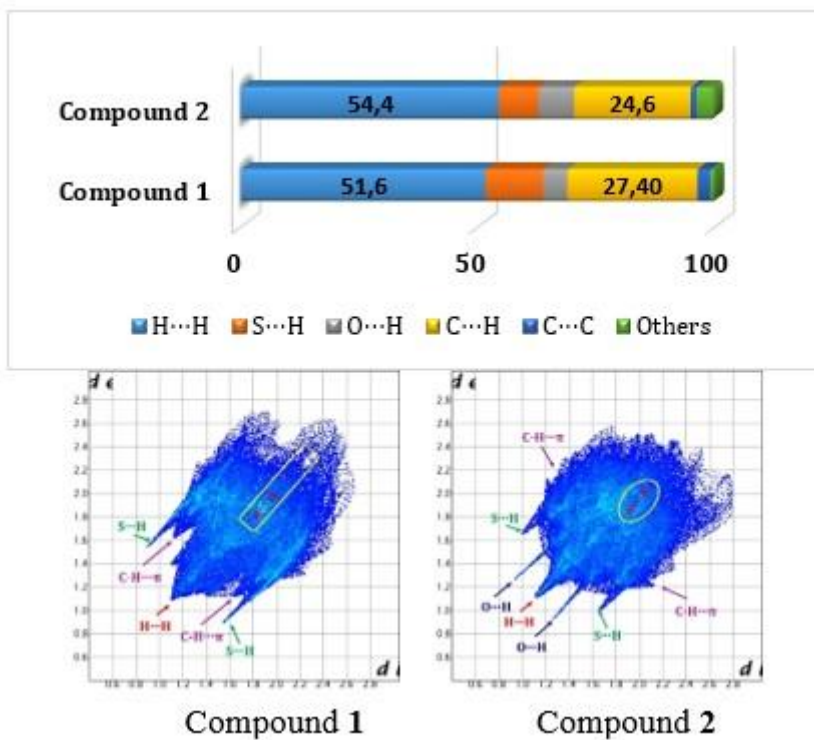


Fig. 1