



# 6th National Crystallography Meeting

17-19 May 2026 | Giresun University



Sunday, 17 May 2026 (Şehit Ömer Halisdemir Conference Hall)

10:00 - 12:00

**Registration, Opening Ceremony & Congress Opening Speeches**

12:00 - 13:30

**Visit to the Stands & Lunch**

13:30 - 14:00

**Session I (Invited Speaker)**

*Prof. Dr. Santiago GARCIA-GRANDA (University of Oviedo, Spain)*

New sustainable ceramic pigments based on solid solutions of Olivine and Diopside

*Chairs: Prof. Dr. Zehra SAYERS & Prof. Dr. Sema ÖZTÜRK YILDIRIM*

14:00 - 14:30

**Session II (Invited Speaker)**

*Prof. Dr. Zehra SAYERS (Sabancı University, Türkiye)*

Bringing the invisible into focus with synchrotron radiation

*Chairs: Prof. Dr. Metin KUL & Prof. Dr. Mehmet KABAK*

14:30 - 15:00

**Coffee Break**

15:00 - 15:30

**Session III (Invited Speaker)**

*Assoc. Prof. Dr. Cengiz ARICI (TÜBİTAK, Türkiye)*

ARDEB Programları ve Yenilikler

*Chairs: Prof. Dr. Yelda BİNGÖLALPASLAN & Prof. Dr. Gökhan ALPASLAN*

## Scientific Program – Oral Presentations (15:30 – 16:15)

*Chairs: Prof. Dr. Orhan BÜYÜKGÜNGÖR & Prof. Dr. Can ALAŞALVAR*

15:30 - 15:45

*Sultan Başak, Başak Koşar Kırca, Çiğdem Albayrak Kaştaş*

Quantum Chemical Characterization and Molecular Docking Analysis of (E)-2-[(4-Chloro-3-nitrophenylimino)methyl]-3-methoxyphenol: A Novel Schiff Base Ligand with Potential Anticancer Activity

15:45 - 16:00

*Sema Öztürk Yıldırım, Metin Kul, Ray J. Butcher*

Crystal Structure of S-2-Aminophenyl phenylcarbamothioate

16:00 - 16:15

*Onur Rauf Yılmaz, Çiğdem Albayrak Kaştaş, Canan Kazak*

A Comparison of Isomeric Schiff Bases Featuring Halogens at Different Contact Points



NanoSpek



Sunday, 17 May 2026 (Şehit Ömer Halisdemir Conference Hall)

**Scientific Program – Poster Presentations (16:15 – 17:00)**

Chairs: Prof. Dr. Birol ERTUĞRAL & Prof. Dr. Halil GÖKÇE

**Poster 1**

*Sema Öztürk Yıldırım, Zeki Büyükmumcu, Rahime Şimşek, Gökalp Çetin, Ray J. Butcher*

Synthesis and Spectroscopic Characterization and DFT Study of benzyl 4-([1,1'-biphenyl]-4-yl)-2,6,6-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate

**Poster 2**

*Rahime Şimşek, Zeki Büyükmumcu, Sema Öztürk Yıldırım, Gökalp Çetin, Cihat Şafak, Ray J. Butcher*

DFT Studies, Synthesis, Biological Activity and Crystal Structure of Tert-Butyl 4-([1,1'-Biphenyl]-4-yl)-2-Methyl-5-Oxo-1,4,5,6,7,8-Hexahydroquinoline-3-Carboxylate

**Poster 3**

*Sema Öztürk Yıldırım, Zeki Büyükmumcu, Rahime Şimşek, Gökalp Çetin, Cihat Şafak, Ray J. Butcher*

Synthesis, Structural Characterization and Density Functional Studies of ethyl 4-(biphenyl-4-yl)-2,6,6-trimethyl-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate – A non-merohedral Twinned Structure

**Poster 4**

*Gökhan Kaştaş, Çiğdem Albayrak Kaştaş, Cumhuriyet Avşar*

Structural, Catalytic, and Biological Evaluation of a Copper(II) Schiff Base Complex: bis{2-ethoxy-6-(E)-[(4-fluorophenyl)imino)methyl]phenolato-κN,κO}copper(II)·1.5H<sub>2</sub>O

**Poster 5**

*Başak Koşar Kırca, Çiğdem Albayrak Kaştaş, Gökhan Kaştaş*

Bis{2-ethoxy-6-(E)-[(4-bromophenyl)imino)methyl]phenolato-κN,κO}copper(II)

**Poster 6**

*Çiğdem Albayrak Kaştaş, Gökhan Kaştaş*

Synthesis, Structural, and Spectroscopic Characterization of a Seesaw-Geometry Schiff Base Complex: bis{2-ethoxy-6-(E)-[(4-methylphenyl)imino)methyl]phenolato-κN,κO}copper(II)·monohydrate

**Poster 7**

*Tuğba Bayın, Onur Rauf Yılmaz, Erbil Açar, Seda Nur Aygün, Canan Kazak*

Substituent-Dependent Crystal Packing in Ortho-Hydroxy Schiff Bases

**Poster 8**

*Esengül Ejder*

DFT and Molecular Docking Evaluation of a Novel Schiff Base (E)-2-(4-((2,4-dimethoxybenzylidene)amino)phenyl)ethan-1-ol: From Electronic Structure to Biological Interaction

**18:00 - 20:00**

**Social Events - Dinner**

## Monday, 18 May 2026 (Mevlana Celaledin-i Rumi Conference Hall)

09:30 - 10:00

### Session IV (Invited Speaker)

*Prof. Dr. Bill CLEGG (Newcastle University, United Kingdom)*

Refining difficult structures and workshops

*Chairs: Prof. Dr. Onur ŞAHİN & Prof. Dr. Resul SEVİNÇEK*

10:00 - 10:30

### Session V (Invited Speaker)

*Prof. Dr. Michael PROBERT (Newcastle University, United Kingdom)*

Exploring the Crystallization Field Using High-Efficiency ENaCt Methods

*Chairs: Prof. Dr. Ufuk ÇORUH ve Prof. Dr. Ümit CEYLAN*

10:30 - 11:00

### Coffee Break

11:00 - 11:30

### Session VI (Invited Speaker)

*Ph.D. Mustafa Fatih GENİŞEL (SESAME, Jordan)*

The Light of Science in the Middle East: SESAME and Research Opportunities

*Chairs: Prof. Dr. Ahmet ERDÖNMEZ & Assoc. Prof. Dr. M. HakkıYILDIRIM*

11:30 - 13:30

### Visit to the Stands & Lunch

13:30 - 14:00

### Session VII (Invited Speaker)

*Prof. Dr. Veysel Turan YILMAZ (Karadeniz Technical University, Turkey)*

Crystal structure–NMR spectra correlations: Two examples of metal complexes

*Chairs: Prof. Dr. Ersin TEMEL & Prof. Dr. Fulya Aydın TEMEL*

## Scientific Program – Oral Presentation (14:00 – 14:15)

*Chairs: Prof. Dr. Ersin TEMEL & Prof. Dr. Fulya Aydın TEMEL*

14:00 - 14:15

*Öznur Ölmez Nalcioğlu, Mine Sulak, Ayşe Gül Caniklioğlu, Bahadır Koz*

Transforming PET Bottle Waste into Multifunctional ZnO@MIL-101(Cr) Material via Moss-Mediated Synthesis: Characterization and Antimicrobial Evaluation

14:15 - 14:45

### Session VIII (Invited Speaker)

*Assoc. Prof. Dr. Santanu PATHAK (SESAME MS/XPD Beamline, Jordan)*

The MS/XPD Beamline at SESAME: Capabilities, Applications and User Opportunities

*Chairs: Prof. Dr. Veysel Turan YILMAZ & Prof. Dr. Aytaç GÜDER*

15:45 - 16:30

### Coffee Break & Poster Session

*Chairs: Prof. Dr. Serkan DEMİR & Assoc. Prof. Dr. Selbi KESKİN*

Poster 1

*Nuri Yıldırım*

Crystal and molecular structure of N-(3,5-diphenyl-4H-1,2,4-triazole-4-yl)thiophene-2-carboxamide

Poster 2

*Nuri Yıldırım*

Crystal and molecular structure of N-(3,5-di-p-tolyl-4H-1,2,4-triazol-4-yl)thiophene-2-carboxamide

## Monday, 18 May 2026 (Mevlana Celaledin-i Rumi Conference Hall)

### Poster 3

*Ceyda İÇSEL*

Crystal and molecular structure of a new binuclear silver(I) complex with bridging chlorido and 1,4- bis(diphenylphosphino)butane ligands

### Poster 4

*Murat Tekingündüz, Resul Sevinçek*

Electronic Structure Engineering of Pentagraphene via Site-Selective B and N Substitution: A First-Principles Study

### Poster 5

*Selim Adıgüzel, Resul Sevinçek*

Ti<sub>2</sub>BN Monolayer as a Novel MBene: A First-Principles Study of Stability and Electronic Structure

### Poster 6

*Hanifi Özşanlı, Gülnur Odabaş, Ufuk Çoruh*

Detailed examination of 4-[(4-Ethyl-5-phenyl-4H-1,2,4-triazol-3-yl)sulfanyl]phthalonitrile crystal packing, Hirshfeld surface analysis, and 2D fingerprint map

### Poster 7

*Berru Özkaya, Emine Berrin Poyraz, Mustafa Şanlı, Metin Yavuz, Ufuk Çoruh*

Investigation of the Crystal Structure of a 4,5-Dicyanobenzene Derivative via Hirshfeld Surface Analysis and Energy Frameworks Method

### Poster 8

*Gül Yakalı, Zeynep Türkmen Bulca, Merve İzmirli, Resul Sevinçek*

Charge Mobility Analysis of Phenanthroline Derivatives via Density Functional Theory: Role of Reorganization Energy and Charge Transfer Integrals

### Poster 9

*Merve İzmirli, Hasan Karabıyık, Gül Özkan, Resul Sevinçek, Hande Karabıyık, Muhittin Aygün*

Crystal Structure and Hirshfeld Surface Analyses of some PEPPSI Type Pd(II)NHC Complexes

**16:30 - 17:30**

**Closing Ceremony**

**19:00 - 23:00**

**Gala Dinner**

## Tuesday, 19 May 2026

**10:00 - 18:00**

**Giresun Tour**

Social program and city tour in Giresun.