

Prof. Gustavo Portalone

Since 1.11.2001: Associate Professor of General and inorganic chemistry at the Faculty of Mathematical, Physical and Life Sciences of "Sapienza" University of Rome.

1981-2001: Academic researcher.

1980-1: Winner of a scholarship in Chemistry of the British Council at the Chemical Crystallography Laboratory in Oxford (Supervisor: Prof. C. K. Prout, the late; Director Prof. D. C Hodgkin, Nobel laureate, the late).

1978-80: Fellow of the Accademia Nazionale dei Lincei - Fondazione Guido Donegani (Supervisor: Prof. A. Vaciago, the late) and member of the Gruppo di Chimica Biologica e Strutturistica Chimica (Director: Prof. Alessandro Ballio, the late).

Research scientist at the Structural Chemistry Research Group of the Hungarian Academy of Sciences (Budapest, 1983, 1986 and 1987) for chemical applications of gas electron diffraction.

Research unit manager (PRIN 1996 and 1997).

As president of the teaching committee of the Italian Crystallographic Association (AIC) he has organized and directed the annual school of Crystallography from 1994 to 1996 and edited the proceedings in three volumes.

In the period 2003-2005 he served as secretary of AIC.

Since 2007 he is responsible for the X-ray diffraction (XRD) laboratory of the Chemistry Department of "Sapienza" University of Rome.

Author or coauthor of more than 130 peer-reviewed publications (scientific papers, book chapters and books) in the field of X-ray crystallography, gas electron diffraction, high-level quantum chemical calculations of molecular interactions and a book of Chemistry at university level.

Member of the editorial board of the Journal of Chemistry, the Dataset Papers in Chemistry, the Journal of Crystallography, AIMS Materials Science, Crystals and Frontiers in Chemistry.

Referee for Crystals, Molecules, Crystal Growth & Design, Journal of Molecular Structure, Acta Crystallographica, sect B, Acta Crystallographica, sect C, Zeitschrift für Kristallographie.

2018: Guest editor of the special issue of Crystals: "Noncanonical nucleobases".

2019: Guest editor of the special issue of Crystals: "Design, Synthesis, and Structures of Modified RNA/DNA Bases".

2020: Topic editor of the special issue of Frontiers in Chemistry: "Structural Characterization and Analysis of Intercalation, Adsorption and Insertion of Chemical Species into Micro and Nanometric materials".

2021: Guest editor of the special issue of Crystals: "DNA and Small Molecular Complex Crystallization".

2021: Guest editor of the special issue of Molecules: "Halogenated Nucleic Acids".

2022: Guest editor of the special issue of Molecules: "New Trends in Supramolecular Chemistry of Nucleobases".

2022: Guest editor of the special issue of Crystals: "Crystal Engineering of API-Based Crystals with Enhanced Properties".

He teaches General and Inorganic Chemistry (bachelor's degree in Chemistry) and Structural Chemistry (master's degree in Chemistry).

The research of Portalone group lies in the field of supramolecular chemistry and focuses on the design (exploiting molecular recognition through hydrogen and halogen bonds), solid-state synthesis and structure determination of binary/ternary cocrystals of canonical and unnatural DNA/RNA nucleobases *via* the combined approach of SCXRD and PXRD, *ab initio* and molecular dynamics calculations, AFM and thermodynamic measurements. In the solid state, molecular recognition of modified nucleobases *via* hydrogen and halogen bonds has important implications in medicine (drugs against cancer), genetics (synthetic DNA; PAM recognition mechanism) and materials chemistry (DNA-based supercomputers). Public funding received in the period 1991-2021: 359430 euro.



Ministero dell'Università e della Ricerca
SEGRETARIATO GENERALE
Direzione generale delle istituzioni della formazione superiore

N: 41642

Gent.le
Gustavo PORTALONE
E-Mail: gustavo.portalone@uniroma1.it

Courtesy translation of the original document in Italian language.

We hereby certify that Gustavo PORTALONE, born in Roma (RM) on 14/11/1952 , achieved the National Scientific qualification as full professor in the Italian higher education system, in the call 2016/2018 (Ministerial Decree n. 1532/2016) for the disciplinary field of 03/B1 - Principles of chemistry and inorganic systems. (Academic Recruitment Field 03/B - Inorganic chemistry and applied technologies, according to the national classification).

The validity of the qualification is twelve years¹, starting from the 04/04/2018 and will expire on the 04/04/2030².

Rome, 20/02/2025

Il Dirigente
Dott.ssa Maria Giovanna Zilli³

¹ Termine prorogato ai sensi dell'art. 4, c. 2-bis del D.L. 28 ottobre 2024, n. 160, introdotto dalla Legge di conversione 20 dicembre 2024, n. 199, recante "Disposizioni urgenti in materia di lavoro, università, ricerca e istruzione per una migliore attuazione del Piano nazionale di ripresa e resilienza".

² The list of qualified candidates are always available on the website <https://abilitazione.mur.gov.it>, "CANDIDATI E RISULTATI" section, by clicking on the year of the session of interest, link "Risultati".

³ Firma autografa sostituita a mezzo stampa ai sensi e per gli effetti dell'art. 3, co.2, D. Lgs. n.39/1993.

Il Responsabile del procedimento: Il Dirigente Dott.ssa Maria Giovanna Zilli

Ufficio V "Stato giuridico ed economico del personale universitario"
Largo Antonio Ruberti, 1 - 00153 Roma - Tel. 06 9772 6381
PEO: dgistituzioni.ufficio5@mur.gov.it – PEC: dgistituzioni@pec.mur.gov.it

Peer-reviewed Articles

- 1 - M. Colapietro, A. Domenicano, G. Portalone:"Structural Studies of Benzene Derivatives. VII. The Structure of *p*-Aminobenzoic Acid Hydrochloride".
Acta Cryst., B36, 354 (1980).
- 2 - M. Colapietro, A. Domenicano, C. Marciante, G. Portalone:"Structural Studies of Benzene Derivatives. IX. The Structures of *p*-Fluoroaniline and *p*-Cyanoaniline Hydrochlorides".
Acta Cryst., B37, 387 (1981).
- 3 - M. Colapietro, A. Domenicano, C. Marciante, G. Portalone:"*p*-Nitroaniline revisited".
Acta Cryst., A37, 199 (1981).
- 4 - M. Colapietro, A. Domenicano, C. Marciante, G. Portalone:"Effects of Through-Conjugation on the Molecular Structure of *p*-Nitroaniline".
Z. Naturforsch., 37b, 1309 (1982).
- 5 - M. Colapietro, A. Domenicano, C. Marciante, G. Portalone:"Structural Studies of Benzene Derivatives. XI. The Structure of *p*-Toluidine Hydrochloride".
Acta Cryst., B38, 2825 (1982).
- 6 - G.B. Marini-Bettolo, M. Nicoletti, I. Messana, M. Nicoletti, M. Patamia, C. Galeffi, J.U. Oguakwa, G. Portalone, A. Vaciago:"Research on African Medicinal Plants - IV. Boonein, a new C-9 Terpenoid Lactone from Alstonia Boonei:a possible precursor in the Indole Alkaloid Biogenesis".
Tetrahedron, 39, 2, 323 (1983).
- 7 - M. Colapietro, A. Domenicano, G. Portalone, Gy. Schultz, I. Hargittai:"Molecular Structure and Ring Distortions of *p*-Dicyanobenzene in the Gas Phase and in the Crystal".
J. Mol. Struct., 112, 141 (1984).
- 8 - J. Brunvoll, M. Colapietro, A. Domenicano, C. Marciante, G. Portalone, I. Hargittai: "Molecular Structure of *p*-Methylsulphonyl Benzoic Acid and Methylphenylsulphone: Comparison of X-Ray and Electron Diffraction Results".
Z. Naturforsch., 39b, 607 (1984).
- 9 - M. Colapietro, A. Domenicano, C. Marciante, G. Portalone:"Structural Studies of Benzene Derivatives. XII. The Molecular Structure of 3,5-Dimethylbenzoic Acid in the Crystal, and a Comparison with the Gas Phase Structure of Related Molecules".
Z. Naturforsch., 39b, 1361 (1984).
- 10 - G. Portalone, Gy. Schultz, A. Domenicano, I. Hargittai:"Molecular Structure and Ring Distortions of Fluorobenzene: an Electron Diffraction Study, and a Comparison with other Experimental and *ab initio* MO Results".
J. Mol. Struct., 118, 53 (1984).
- 11 - M. Colapietro, A. Domenicano, G. Portalone, I. Torrini, I. Hargittai, Gy. Schultz:"Molecular Structure and Ring Distortions of *p*-Diisocyanobenzene in the Gaseous Phase and in the Crystal"
J. Mol. Struct., 125, 19 (1984).
- 12 - M. Colapietro, A. Domenicano, C. Marciante, G. Portalone:"Angular Ring Distortions in Benzene Derivatives: the Effect of the NO₂ and the COOH Substituents".

Acta Cryst., A40, 98 (1984).

- 13 - G. Di Maio, G. Portalone, R. Spagna, E. Vecchi, E. Zeuli:"The Molecular Structure of trans 3,6-Dimethyl-6-Phenyltetrahydro-2-Pyrone in the Crystal".
Z. fur Kristall., 175, 131 (1986).
- 14 - M. Colapietro, A. Domenicano, G. Portalone, Gy. Schultz, I. Hargittai:"Molecular Structure of *p*-Diaminobenzene in the Gaseous Phase and in the Crystal".
J. Phys. Chem., 91, 1728 (1987).
- 15 - G. Portalone, A. Domenicano, Gy. Schultz, I. Hargittai:"Molecular Structure and Ring Distortions of Cyanobenzene: an Electron Diffraction Study".
J. Mol. Struct., 160, 97 (1987).
- 16 - C.W. Bock, A. Domenicano, Ph. George, I. Hargittai, G. Portalone, Gy. Schultz: "Benzene Ring Deformation and Rotational Isomerism in Terephthalaldehyde: a Study by Electron Diffraction and Molecular Orbital Calculations".
J. Phys. Chem., 91, 6120 (1987).
- 17 - A. Domenicano, I. Hargittai, G. Portalone, Gy. Schultz:"A Gas-Phase Electron Diffraction Study of the Molecular Structure of *sym*-Trihydroxybenzene".
Z. fur Kristall., 185, 204 (1988).
- 18 - Gy. Schultz, M. Kolonitz, I. Hargittai, A. Domenicano, G. Portalone:"Molecular Structure and Ring Distortions of *p*-Dibromobenzene as determined by Electron Diffraction".
J. Mol. Struct., 176, 71 (1988).
- 19 - A. Domenicano, I. Hargittai, G. Portalone, Gy. Schultz:"Effect of Intermolecular Hydrogen Bonding on the Molecular and Electronic Structure of Hydroxybenzenes".
Acta Chem. Scand., A42, 460 (1988).
- 20 - G. Portalone, A. Domenicano, Gy. Schultz, I. Hargittai:"The Molecular Structure of *p*-Benzendithiol as determined by Electron Diffraction".
J. Mol. Struct. (Theochem), 186, 185 (1989).
- 21 - A. Domenicano, Gy. Schultz, I. Hargittai, M. Colapietro, G. Portalone, Ph. George, C.W. Bock:"Molecular Structure of Nitrobenzene in the Planar and Orthogonal Conformations: a Concerted Study by Electron Diffraction, X-Ray Crystallography and MO Calculations".
Struct. Chem., 1, 107 (1990).
- 22 - M. Colapietro, G. Pagani Zecchini, M. Paglialunga Paradisi, G. Portalone, R. Spagna, I. Torrini:"The X-Ray Molecular Structure of (3*R*,5*S*)-tetrahydro-2*H*-1,4-thiazine-3,5-dicarboxylic Acid".
Acta Cryst., A46, 185 (1990).

- 23 - F. Ramondo, G. Portalone, L. Bencivenni: "Ab initio Determination of the Equilibrium Geometry and Vibrational Frequencies of Borazine".
J. Mol. Struct. (Theochem), 236, 29 (1991).
- 24 - F. Ramondo, G. Portalone, A. Domenicano, G. Schultz, I. Hargittai: "Molecular Structure of 1,3,5-Trifluorobenzene: comparison of two Electron Diffraction Studies".
J. Mol. Struct., 269, 367 (1992).
- 25 - G. Portalone, G. Schultz, A. Domenicano, I. Hargittai: "Molecular Structure and Ring Distortions of Phenol: an Electron Diffraction Study".
Chem. Phys. Lett., 197, 482 (1992).
- 26 - G. Schultz, T. Nagy, G. Portalone, F. Ramondo, I. Hargittai, A. Domenicano: "Molecular Structure of Ethynylbenzene from Electron Diffraction and Ab initio Molecular Orbital Calculations".
Struct. Chem., 4, 183 (1993).
- 27 - G. Portalone, A. Cassetta, G. Pagani Zecchini, I. Torrini: "Structure of (3R,5R)-tetrahydro-2H-1,4-thiazine-3,5-dicarboxylic Acid Monohydrate".
Acta Cryst., C49, 976 (1993).
- 28 - K. Zhou, G. Di Maio, S. Li, G. Portalone, L. Migneco: "Stereochemical Studies on Cyclohexanone Semicarbazone Derivatives. II. Crystal and Molecular Structures of 4-Methyl-Cyclohexanone Semicarbazone and 4-Cyclohexyl-Cyclohexanone Semicarbazone".
J. Struct. Chem., 12, 43 (1993).
- 29 - F. Ramondo, G. Portalone, M. Colapietro, L. Bencivenni: "HF-SCF Study of the Ground State Geometry and Harmonic Vibrational Frequencies of Borazine Derivatives".
J. Mol. Struct. (Theochem), 283, 85 (1993).
- 30 - F. Ramondo, L. Bencivenni, G. Portalone, A. Domenicano: "Effect of Intermolecular Hydrogen Bonding on the Molecular and Electronic Structures of Imidazole and 1,2,4-Triazole: a Study by ab initio Molecular Orbital Calculations".
Struct. Chem., 5, 1 (1994).
- 31 - G. Di Maio, S. Li, G. Portalone, K. Zhou, C. Marcante, R. Spagna: "Cyclohexanone Semicarbazone and 4-tert-butyl-Cyclohexanone Semicarbazone".
Acta Cryst., C50, 635 (1994).
- 32 - F. Ramondo, L. Bencivenni, G. Portalone, A. Domenicano: "Effect of Intermolecular O-H...O Hydrogen Bonding on the Molecular Structure of Phenol: An ab initio Molecular Orbital Study".
Struct. Chem., 6, 37 (1995).
- 33 - K. Zhou, G. Di Maio, G. Portalone, S. Li: "4-Acetamidocyclohexanone Semicarbazone Dihydrate".
Acta Cryst., C51, 1844 (1995).
- 34 - K. Zhou, G. Di Maio, G. Portalone, S. Li: "Crystal and Molecular Structures of 4-Phenyl-Cyclohexanone Semicarbazone".
J. Struct. Chem., 14, 70 (1995).

35 - C. Pettinari, G. Gioia Lobbia, G. Sclavi, D. Leonesi, M. Colapietro, G. Portalone: "Synthesis and characterization of derivatives of copper(I) with N-donor ligands. I. Crystal Structure of nitrito bis(*tri-p-tolylphosphine*)copper(I)".
Polyhedron, 14, 1709 (1995).

36 - S. Bernstorff, E. Busetto, C. Gramaccioni, A. Lausi, L. Olivi, F. Zanini, A. Savoia, M. Colapietro, G. Portalone, M. Camalli, A. Pifferi, R. Spagna, L. Barba, A. Cassetta: "The Macromolecular Crystallography Beamline of Elettra".
Rev. Sci. Instrum., 55, 1661 (1995).

37 - R. Spagna, L. Barba, M. Camalli, A. Cassetta, M. Catricalà, C. Marciante, A. Pifferi, M. Colapietro, G. Portalone: "The four circle diffractometer at ELETTRA".
Acta Cryst., A52 16 (1996).

38 - A. Domenicano, G. Portalone, F. Ramondo, G. Schultz, I. Hargittai: "Molecular Structure of Aniline in the Gaseous Phase: A concerted Study by Electron Diffraction and *Ab initio* Molecular Orbital Calculations".
Struct. Chem., 7, 59 (1996).

39 - M. Bossa, M. Colapietro, G.O. Morpurgo, S. Morpurgo, G. Portalone: "X-Ray Structure and AM1 Studies of the Proton Transfer Adduct between 2,5-dihydroxy-*p*-quinone and 4 *N,N*-dimethylamino pyridine".
J. Phys. Chem. 100, 9302 (1996).

40 - C. Pettinari, F. Marchetti, R. Polimante, A. Cingolani, G. Portalone, M. Colapietro: "Synthesis and spectroscopic characterization of new Cu(I) complexes containing triaryl-, tricicloalkylphosphines and heterocyclic anionic or neutral N-donor ligands. Crystal and molecular structure of $(Cy_3P)_2(pzH)CuClO_4\cdot CH_3OH$ ($Cy =$ cyclohexyl, $pzH =$ pyrazole)".
Inorganica Chim. Acta, 249, 215 (1996).

41 - A. Domenicano, A. Arcadi, F. Ramondo, A.R. Campanelli, G. Portalone, G. Schultz, I. Hargittai: "Molecular Structure of and Large-Amplitude Substituent Motions in *p*-Diethynilbenzene: a Study by Gas Phase Electron Diffraction and Theoretical Calculations".
J. Phys. Chem., 100, 14625 (1996).

42 - G. Portalone, F. Ramondo, A. Domenicano, I. Hargittai: "Molecular Structure of Phenylsilane: a Study by Electron Diffraction and *Ab initio* Molecular Orbital Calculations".
J. Organom. Chem., 560, 183 (1998).

43 - G. Portalone, M. Colapietro, F. Ramondo, L. Bencivenni, A. Pieretti: "The Effect of Hydrogen Bonding on the Structures of Uracil and some Methyl Derivatives by Experiment and Theory".
Acta Chem. Scand., 53, 57 (1999).

44 - B. Brunetti, V. Piacente, G. Portalone: "Sublimation Enthalpies of some Methyl Derivatives of Uracil from Vapor Pressures Measurements".
J. Chem. Eng. Data, 45, 242 (2000).

45 - R. D'Amato, A. Furlani, M. Colapietro, G. Portalone, M. Casalboni, M. Falconieri, M.V. Russo: "Synthesis, characterization and optical properties of symmetrical and unsymmetrical Pt(II) and Pd(II) bisacetylides. Crystal structures of *trans*-[Pt(PPh₃)₂(C≡C-C₆H₅)(C≡C-C₆H₄NO₂)]".
J. Organom. Chem., 627, 13 (2001).

- 46 - B. Brunetti, V. Piacente, G. Portalone:"Sublimation Thermodynamics Parameters for 5-Fluorouracil and its 1-Methyl and 1,3-Dimethyl Derivatives from Vapor Pressures Measurements".
J. Chem. Eng. Data, 47, 17 (2002).
- 47 – C. Bellitto, D. Caschera, M. Colapietro, F. Federici, G. Portalone:"X-ray Single Crystal Structure and Magnetic Properties of $\text{Fe}[\text{CH}_3\text{PO}_3] \cdot \text{H}_2\text{O}$: a new Weak Ferromagnet".
Inorg. Chem., 41, 709 (2002).
- 48 - G. Portalone, P. Ballirano, A. Maras:"The crystal structure of 3-methyluracil from X-ray powder diffraction data".
J. Mol. Struct., 608, 35 (2002).
- 49 - B. Masci, M. Colapietro, G. Portalone, S. Saccheo:"1,3-bridged *p*-methyloctahomo tetraoxacalix[4]arene-biscrown-3".
Acta Cryst., C58, 345 (2002).
- 50 - E. M. Bauer, C. Bellitto, M. Colapietro, G. Portalone, G. Righini:" $\text{Cr}[(\text{H}_3\text{N}-\text{CH}_2)_2\text{PO}_3](\text{Cl}) \cdot \text{H}_2\text{O}$: X-ray Single-Crystal Structure and Magnetism of a Polar Organic-Inorganic Hybrid Chromium(II) Organophosphonate".
Inorg. Chem., 42, 6345 (2003).
- 51 - G. Portalone, M. Colapietro:"Redetermination of phenylbiguanide hydrochloride".
Acta Cryst., E60, 1165 (2004).
- 52 - G. Portalone, M. Colapietro:"First example of cocrystals of polymorphic maleic hydrazide".
J. Chem. Cryst., 34, 609 (2004).
- 53 - A. Anillo, A. Altomare, A.G.G. Moliterni, E.M. Bauer, C. Bellitto, M. Colapietro, G. Portalone, G. Righini:"Hydrothermal Synthesis, Structural Characterization and Magnetic Studies of the New Pillared Microporous Ammonium Fe(III) carboxyethylphosphonate: $[\text{NH}_4][\text{Fe}_2(\text{OH})\{\text{O}_3\text{P}(\text{CH}_2)_2\text{CO}_2\}_2]$ ".
J. Solid State Chem., 178, 306 (2005).
- 54 - C. Conti, P. Mastromarino, P. Goldoni, G. Portalone, N. Desideri:"Synthesis and anti-rhinovirus properties of Fluoro-substituted flavonoids".
Antiv. Chem. & Chemioth., 16, 267 (2005).
- 55 - G. Portalone:"*p*-Bromoanilinium chloride".
Acta Cryst., E61, 3083 (2005).
- 56- E.M Bauer, C. Bellitto, M. Colapietro, S.A. Ibrahim, M.R. Mahmoud, G. Portalone and G. Righini:" Co(II) *n*-Alkyl Phosphonates: Examples of Hybrid Organic-Inorganic Compounds".
Acta Cryst., A61, 358 (2005).
- 57 - E.M Bauer, C. Bellitto, M. Colapietro, S.A. Ibrahim, M.R. Mahmoud, G. Portalone and G. Righini:"Layered hybrid organic-inorganic Co(II) alkylphosphonates. Synthesis, crystal structure and magnetism of the first two members of the series: $[\text{Co}(\text{CH}_3\text{PO}_3)\text{H}_2\text{O}]$ and $[\text{Co}(\text{C}_2\text{H}_5\text{PO}_3)\text{H}_2\text{O}]$ ".
Solid State Chem., 179, 389 (2006).

COVER ISSUE

- 58 - G. Portalone, M. Colapietro:"Redetermination of 5-Fluorocytosine monohydrate".
Acta Cryst., E62, 1049 (2006).
- 59 - G. Portalone, M. Colapietro:"Redetermination of ammonium oxalate oxalic acid dihydrate".
Acta Cryst., E62, 4725 (2006).
- 60 - G. Portalone, M. Colapietro:"Asymmetric base pairing in the complex 5-Fluorocytosinium chloride/5-Fluorocytosine monohydrate".
J. Chem. Cryst., 37, 141 (2007).
- 61 - G. Portalone, M. Colapietro, S. Bindya, M. A. Ashok and H.S. Yathirajan:"5-[3-(Dimethyl amino)propyl]-10,11-dihydro-5H-dibenz[a, d][7]annulen-5-ol".
Acta Cryst., E63, 746 (2007).
- 62 - G. Portalone, M. Colapietro:"The 1:1 cocrystals of the proton-transfer compound dilituric acid / phenylbiguanide hydrate ".
Acta Cryst., C63, 181 (2007).
- 63 - G. Portalone, M. Colapietro:"Redetermination of isocytosine".
Acta Cryst., E63, 1869 (2007).
- 64 - G. Portalone, M. Colapietro:"The 1:1 complex of cytosine/5-Fluorouracil monohydrate revisited".
Acta Cryst., C63, 423 (2007).
- 65 - G. Portalone:"2,4-Diamino-1,3,5-triazine (Guanamine)".
Acta Cryst., E63, 3232 (2007).
- 66 - G. Portalone, M. Colapietro:"Unusual *syn* conformation of 5-formyluracil stabilized by supramolecular interactions".
Acta Cryst., C63, 650 (2007).
- 67 - M. Cametti, A. Dalla Cort, M. Colapietro, G. Portalone, L. Russo and K. Rissanen:"Evidence of the facile hydride and enolate addition to the imine bond of an Aluminum-Salophen complex".
Inorg. Chem., 46, 9057 (2007).
- 68 - G. Portalone, M. Colapietro."Hydrogen-bonded supramolecular motifs in the 1:1 monohydrated molecular adduct of acetoguanaminium chloride with acetoguanamine and in 2,4,6-triaminopyrimidinium dichloride dihydrate".
Acta Cryst., C63, 655 (2007).
- 69 - G. Portalone, M. Colapietro:"Nicotinohydrazide".
Acta Cryst., E64, 304 (2008).
- 70 - G. Portalone:"Redetermination of 5-Iodouracil".
Acta Cryst., E64, 365 (2008).
- 71 - G. Portalone, A. Cassetta, M. Colapietro and S.H. Plattner:" (3*R*,5*S*)-5(3)-Carboxy-3,4,5,6-tetrahydro-2*H*-1,4-thiazin-4-iun-3(5)-carboxylate".
Acta Cryst., E64, 636 (2008).

72 - G. Portalone:"Redetermination of orotic acid monohydrate".
Acta Cryst., E64, 656 (2008).

73 - G. Portalone:"Biguanidinium dichloride".
Acta Cryst., E64, 683 (2008).

74 - G. Portalone:"Redetermination of 3-deazauracil".
Acta Cryst., E64, 1107 (2008).

75 - G. Portalone:"Benzamidinium tetrahydropentaborate sesquihydrate".
Acta Cryst., E64, 1282 (2008).

76 - G. Portalone:"Acetoguanamine *N,N*-dimethylformamide solvate".
Acta Cryst., E64, 1685 (2008).

77 - E. M. Bauer, C. Bellitto, G. Righini, M. Colapietro, G. Portalone, M. Drillon and P. Rabu:"Comparison of the Structure and Magnetic Order in a Series of Layered Ni(II) Organophosphonates, Ni[(RPO₃)(H₂O)], (R = C₆H₅, CH₃, C₁₈H₃₇)".
Inorg. Chem., 47, 10945 (2008).

78 - G. Portalone, M. Colapietro:"Solid-phase molecular recognition of cytosine based on proton-transfer reaction".
J. Chem. Crystallogr., 39, 193 (2009).

79 - E. Viola, M.P. Donzello, S. Ciattini, G. Portalone and C. Ercolani:"Tetra-2,3-Pyrazinoporphyrazines with externally appended pyridine rings. VII. Redox Chemistry of Tetrakis 2,3-[5,6-di(2-pyridil)pyrazino]Porphyrazinato-Cobalt(II): Isolation and Characterization of solid pure Co(I), Co(II) and Co(III) complexes."
Eur. J. Inorg. Chem., 1600 (2009).

80 - G. Portalone:"Redetermination of 2,6-dimethoxybenzoic acid".
Acta Cryst., E65, 327 (2009).

81 - G. Portalone:"Redetermination of *o*-nitrobenzoic acid".
Acta Cryst., E65, 954 (2009).

82 - D. Torino, A. Mollica, F. Pinnen, F. Feliciani, G. Luente, G. Fabrizi, G. Portalone, P. Davis, J. Lai, S.-W. Ma, F. Porreca and V.J. Hruby."Synthesis and evaluation of new endomorphin-2 analogues containing (Z)-a,b-didehydro-phenylalanine (DzPhe) residues".
J. Med. Chem., 53, 4550 (2010).

83 - G. Portalone:"Supramolecular association in proton-transfer adducts containing benzamidinium cations. (I). Four molecular salts with uracil derivatives".
Acta Cryst., C66, 295 (2010).

84 - E.M. Bauer, C. Bellitto, P. Imperatori, G. Righini, M. Colapietro, G. Portalone and C. J. Gomez-Garcia: "A Novel 1D-AF Hybrid Organic-Inorganic Chromium(II) Methyl Phosphonate: Synthesis, X-ray Crystal and Molecular Structure and Magnetic Properties".
Inorg. Chem., 49, 7472 (2010).

85 - G. Portalone, S. Irrera:" Supramolecular structure of unnatural nucleobases: revised structure of (2:1) 6-methylisocytosinium dihydrogen monophosphate adduct".

J. Mol. Struct., 991, 92 (2011).

86 - G.M. Lombardo, G. Portalone, M. Colapietro, A. Rescifina and F. Punzo: "From the X-rays to a reliable "Low cost" computational structure of caffeic acid: DFT, MP2, HF and integrated molecular dynamics X-ray diffraction approach to condensed phases".

J. Mol. Struct., 994, 87 (2011).

87 - M. Habgood, S.L. Price, G. Portalone, S. Irrera: "Testing a Variety of Electronic-Structure-Based Methods for the Relative Energies of 5-Formyluracil Crystals".

J. Chem. Theor. Comp., 7, 2685 (2011)

88 - G. Portalone: "Solid-phase molecular recognition of cytosine based on proton-transfer reaction. Part II. Supramolecular architecture in the cocrystals of cytosine and its 5-fluoroderivative with 5-nitouracil".

Chem. Centr. J., 5, 51 (2011).

89 - G. Portalone: "A new polymorph of 2,6-dimethoxybenzoic acid".

Acta Cryst., E67, 3394 (2011).

90- S. Irrera, M. Habgood, G. Portalone: "Polymorph prediction and molecular modeling of 5-formyluracil".

ACS National Meeting & Exposition, 147 (2011).

91 - S. Irrera, M. Habgood, G. Portalone: "Ab initio molecular dynamics of 5-formyluracil polymorphs".

ACS National Meeting & Exposition, 302 (2011).

92 - G. Portalone: "4-Methoxybenzamidinium 2,6-dimethoxybenzoate".

Acta Cryst., E68, 268 (2012).

93 - G. M. Lombardo, G. Portalone, U. Chiacchio, A. Rescifina and F. Punzo: "Potassium caffeoate/caffeic acid co-crystal: the rat race between catecholic and carboxylic moieties in an atypical co-crystal".

Dalton Trans. 41, 14337 (2012)

94 - S. Irrera, G. Ortaggi and G. Portalone: "Supramolecular association in proton-transfer adducts containing benzamidinium cations. (II). Concomitant polymorphs of the molecular salt of 2,6-dimethoxybenzoic acid with benzamidine".

Absolute Structure Special Issue of Acta Cryst., C68, 447 (2012).

95 - S. Irrera, G. Portalone: "4-Methoxybenzamidinium chloride monohydrate".

Acta Cryst., E68, 3083(2012).

96 - S. Irrera, G. Portalone: "4-Methoxybenzamidinium hydrogen sulfate".

Acta Cryst., E68, 3244 (2012).

97 - S. Irrera, G. Portalone: "4-Methoxybenzamidinium acetate".

Acta Cryst., E68, 3277(2012).

98 - S. Irrera, G. Portalone: "4-Methoxybenzamidinium nitrate".

Acta Cryst., E68, 3334 (2012).

99 - S. Irrera, G. Portalone:"4-Methoxybenzamidinium hydrogen oxalate mono hydrate".
Acta Cryst., E68, 3350 (2012).

100 - G. Portalone:"Cytosinium orotate dihydrate".
Acta Cryst., E69, 14 (2013).

101 - S. Irrera, G. Portalone:"4-Methoxybenzamidinium bromide".
Acta Cryst., E69, 56 (2013).

102 - S. Irrera, A. Roldan, G. Portalone and N.H. De Leeuw:"The role of hydrogen bonding and proton transfer in the formation of uracil networks on the gold (100) surface: a density functional theory approach".
J. Phys. Chem. C, 117, 3949 (2013).

103 - S. Irrera, G. Portalone, N. H. De Leeuw:"Chemisorption of uracil on gold surfaces via density functional theory".
Surf. Sci., 614, 20 (2013).

104 - G. Portalone:"Benzamidinium 2-methoxybenzoate".
Acta Cryst., E69, 1114 (2013).

105 - I. Giannicchi, G. Portalone, A. Dalla Cort:"Molecular Aggregation of Novel Zn-salophen pyridin Derivatives".
Supramol. Chem., 25, 709 (2013).

106 - S. Irrera, G. Portalone:"First X-ray diffraction and quantum chemical study of proton-acceptor and proton-donor forms of 5-carboxylcytosine, the last-discovered nucleobase".
J. Mol. Struct., 1050, 140 (2013).

107 - G. Portalone:"Supramolecular association in proton-transfer adducts containing benzamidinium cations. III. Three molecular salts of 3-methoxy, 4-methoxy and 3,4,5-trimethoxybenzoic acid with benzamidine".
Acta Cryst., C70, 225 (2014).

108 - B. Brunetti, S. Irrera, G. Portalone:"Sublimation Enthalpies of 5-Haloderivatives of 1,3-Dimethyluracil".
J. Chem. Eng. Data, 60, 74 (2015).

109 - G. Portalone, J. O. Moilanen, H. M. Tuononen, Kari Rissanen:"The Role of Weak Hydrogen Bonds and Halogen Bonds in 5-Halo-1,3-dimethyluracils and their Cocrystals - A Combined Experimental and Computational Study".
Cryst. Growth Des., 16, 2631 (2016).

110 - N. R. Filipović, S. Bjelogrlić, G. Portalone, S. Pelliccia, R. Silvestri, O. Klisurić, M. Senčanski, D. Stanković, T. R. Todorović, C. D. Muller:"Pro-apoptotic and pro-differentiation induction by 8-quinolinecarboxaldehyde selenosemicarbazone and its Co(III) complex in human cancer cell lines".
MedChemComm, 7, 1604 (2016).

111 - T. R. Todorović, J. Vukašinović, G. Portalone, S. Suleiman, N. Gligorijević, S. Bjelogrlić, K. Jovanović, S. Radulović, K. Andđelković, A. Cassar, N. R. Filipović, P. Schembri-Wismayer:

"(Chalcogen)semicarbazones and their cobalt complexes differentiate HL-60 myeloid leukaemia cells and are cytotoxic towards tumor cell lines".
MedChemComm, 8, 103 (2017).

112 – I. S. Djordjević, J. Vukašinović, T. R. Todorović, N. R. Filipović, M. Rodić, A. Lolić, G. Portalone, M. Zlatović, S. Grubišić: "Synthesis, structures and electronic properties of Co(III) complexes with 2-quinolinecarboxaldehyde thio- and seleno-semicarbazone: a combined experimental and theoretical study".
J. Serb. Chem. Soc., 82, 825 (2017).

113 – S. Irrera, S. E. Ruiz-Hernandez, M. Reggente, D. Passeri, M. Natali, F. Gala, G. Zollo, M. Rossi, G. Portalone: "Self-assembling of calcium salt of the new DNA base 5-carboxylcytosine".
Appl. Surf. Sc., 407, 297 (2017).

114 - N. D. Rode, A. Arcadi, M. Chiarini, F. Marinelli, G. Portalone: "Gold-Catalyzed Synthesis of Dibenzo[1,5]diazocyne ring from β -(2-Aminophenyl)- α,β -ynones".
Adv. Synt. & Cat., 359, 3371 (2017).

115 – G. Righi, R. Pelagalli, V. Isoni, I. Tirotta, M. Marini, M. Palagri, R. Dallocchio, A. Dessì, B. Macchi, C. Frezza, G. Forte, A. Dalla Cort, G. Portalone, Paolo Bovicelli: "Synthesis of potential HIV integrase inhibitors inspired by natural polyphenol structures".
Nat. Prod. Res., 32, 1893 (2018).

116 - G. Portalone, K. Rissanen: "Multifacial Recognition in Binary and Ternary Cocrystals from 5-Halouracil and Aminoazine Derivatives".
Cryst. Growth Des., 18, 5904 (2018).

117 - O. R. Klisurić, S. J. Armaković, S. Armaković, S. Marković, T. R. Todorović, G. Portalone, N. R. Filipović: "Structural and computational study of quinoline-based chalcogen semicarbazones:"
*Acta Cryst. A*75, 566 (2019).

118 - G. Portalone: "6-Methyluracil: a redetermination of polymorph (II)".
IUCrData, 4, x190861 (2019).

119 – G. Portalone: "Site Selectivity of Halogen Oxygen Bonding in 5- and 6-Haloderivatives of Uracil".
Crystals, 9, 467 (2019).

120 – O. R. Klisurić, S. J. Armaković, S. Armaković, S. Marković, T. R. Todorović, G. Portalone, K. Novović, J. Lozo, N. R. Filipović: "Structural, biological and in-silico study of quinoline-based chalcogen semicarbazones".
J. Mol. Struct., 1203, 127482 (2020).

121 – A. Arcadi, M. Aschi, M. Chiarini, F. Marinelli, V. Marsicano, G. Portalone: "Experimental results and computational insight into sequential reactions of β -(2-aminophenyl)- α,β -ynones with aryl isocyanates/benzoyl isothiocyanate".
Org. Biomol. Chem., 18, 3177 (2020).

122 - G. Portalone: "Crystal structure and Hirshfeld surface analysis of a third polymorph of 2,6-di methoxybenzoic acid".
Acta Cryst., E76, 1823 (2020).

123 – G. Portalone: "5-Fluorocytosine/Isocytosine Monohydrate. The First Example of Isomorphic and Isostructural Co-Crystal of Pyrimidine Nucleobases". **Editor's Choice article.**
Crystals, 10, 999 (2020).

124 – A. Goulielmina, A. Bauzá, L. Gentiluomo, J. M. Cunha Rodrigues, G. Portalone, A. Frontera, K. Rissanen, R. Puttreddy: "Short X···N Halogen Bonds with Hexamethylenetetraamine as the Acceptor".

Front. Chem., 9, 623595 (2021).

125 - M. Aschi, G. Toto Brocchi, G. Portalone: "A Combined Experimental and Computational Study of Halogen and Hydrogen Bonding in Molecular Salts of 5-Bromocytosine". **Editor's Choice article.**
Molecules, 26, 3111 (2021).

PAPERS PUBLISHED IN INTERNATIONAL PEER-REVIEWED PROCEEDINGS

P1 - F. Di Rienzo, A. Domenicano, G. Portalone, A. Vaciago: "Benzene Ring Deformations in *para*-Substituted Anisoles"
Izv. Jugosl. cent. kristalogr., Suppl Vol. 11, A102 (1976).

P2 - G.B. Marini-Bettolo, C. Galeffi, I. Messana, M. Nicoletti, J.U. Oguakwa, M. Patamia, G. Portalone, K. Prout, A. Vaciago: "The Structure of Boonein, a possible Precursor in the Indole Alkaloid Biogenesis".
God. Jugosl. cent. krystalogr., Suppl. Vol. 17, S67 (1982).

GUEST EDITORSHIP

GE1 – "Noncanonical Nucleobases". *Crystals* (2018).

GE2 – "Design, Synthesis, and Structures of Modified RNA/DNA Bases". *Crystals* (2019).

GE3 – "Structural Characterization and Analysis of Intercalation, Adsorption and Insertion of Chemical Species into Micro and Nanometric materials". *Frontiers in Chemistry* (2020).

GE4 – "DNA and Small Molecular Complex Crystallization". *Crystals* (2021).

GE5 – "Halogenated Nucleic Acids". *Molecules* (2021).

GE6 – "New Trends in Supramolecular Chemistry of Nucleobases". *Molecules* (2022).

GE7 – "Crystal Engineering of API-Based Crystals with Enhanced Properties". *Crystals* (2022).

BOOK CHAPTERS

BC1 - G. Portalone: "Applicazioni dei metodi MO *ab initio* a problemi d'interesse strutturistico". *Atti della XXII Scuola A.I.C.*, Perugia 'Villa La Colombella' (1992).

BC2 – L. Campanella, G. Portalone: "I metalli e le leghe".

L. Campanella, A. Casoli, M.P. Colombini, R. Marini Bettolo, M. Matteini, M.L. Migneco, A. Montenero, L. Nodari, C. Piccioli, M. Plossi, G. Portalone, U. Russo, M. Sammartino: "*CHIMICA PER L'ARTE*", Zanichelli (2007). Cap. VI, pp. 347-409.

UNIVERSITY BOOKS

B1) L. Loreto, G. Portalone, P. Ugliengo, Eds. "*Acquisizione, valutazione ed utilizzo di dati diffrattometrici e strutturali in cristallografia*". Centro Stampa dell'Università (Pg) (1994).

B2) L. Loreto, G. Portalone, P. Ugliengo, Eds. "*Fondamenti di crescita cristallina*". Centro Stampa dell'Università (Pg) (1995).

B3) L. Loreto, G. Portalone, P. Ugliengo, Eds. "*Cristallografia strutturale e riconoscimento di specie molecolari e ioniche*". Centro Stampa dell'Università (Pg) (1996).

B4) L. Campanella, A. Casoli, M.P. Colombini, R. Marini Bettolo, M. Matteini, M.L. Migneco, A. Montenero, L. Nodari, C. Piccioli, M. Plossi, G. Portalone, U. Russo, M. Sammartino: "*CHIMICA PER L'ARTE*", Zanichelli (2007).

Finanziamenti alla ricerca ottenuti nel periodo 1991-2021: 359430 euro

Relatore/correlatore di 15 tesi di laurea magistrale

60 insegnamenti del S.S.D. CHIM/03 impartiti dal 1992 in CdL a ciclo unico, triennali e magistrali

(Fisica, Scienze Biologiche, Scienze applicate ai Beni Culturali, Chimica)

INDICATORI BIBLIOMETRICI (WOS)

H	29
Citations	2263
Papers in the last 10 years	42
Papers in the last 15 years	71
Single author	21
Corresponding author	40
First name	5
Last name	19
Authors/paper	3.20