Cruciani Gabriele
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Present position: Full professor of Organic Chemistry (CHIM/06) at the Department of Chemistry, Biology and Biotechnology, University of Perugia, and the Head of the lab of Excellence H-ECoTox, within the same Department. Deputy Rector for the Third Mission sector and Scientific Director of three SME (Molecular Discovery Ltd (UK), Molecular Horizon (IT), Montelino Therapeutics (USA)). - Director of Human Cytochrome Consortium Initiative (a consortium of Abbvie, Accelera, Astrazeneca, Novartis, Pfizer, Sanofi, Servier pharmaceutical companies collaborating to address metabolism issues in predictive human metabolism). Member of the technical scientific advisory board of several pharmaceutical companies. Professor of Molecular Design at the Bachelor Degree in Chemistry and of Cheminformatics at the Master Degree in Chemical Sciences, University of Perugia.

Education:
Degree in Chemistry, University of Perugia (1987)

Career and research experience:
1992-1993: Fellowship from the National Research Council, Italy at the Laboratory of Molecular Biophysics, Oxford University
1999-2000: Fellowship from the National Research Council, Italy at Laboratory of Pharmaceutical Chemistry, University of Lausanne
1989-2000: Researcher at UniPG
2000-2005: Associate Professor of Organic Chemistry at UniPG
2005-present: Full Professor of Organic Chemistry at UniPG

Awards:
2001: Hansch Award from QSAR and Modeling Society, Tilton (USA)
2005: Research Award from the Organic Division of the Italian Chemical Society
2009: Novartis Lectureship Award, from Novartis pharmaceutical company, Basel
2014: Gold medal Award Angelo Mangini from Italian Chemical Society
2015: Gold medal Herman Wold Award from Swedish Chemical Society
2019: Honorary Diploma of International Scientific Partnership Foundation (Russian)
He is included in the Top Italian Scientists list.

Scientific Productivity and Impact:
Publications: 190
Book: 1
Book Chapters: 52
Conference Proceedings: 27
Invited lectures at Congresses, Workshops and Research Institutions: 220
(WoK ISI) Sum of Times Cited without self-citations : 7850
(WoK ISI) Average Citations per Item: 44.3
(WoK ISI) H-index: 50
Patents: 2
- Costi M.P., Costantino L., Sammak S., Ponterini G., Ferrari S., Luciani R., Franchini S., Santucci M., Cruciani G., Carosati E., New molecules as antitumor agents, 22/01/2013 n.mi2013a000085

- Loregian A., Palù G., Muratore G., Cruciani G., Tabarrini O., New phenyl group containing compound comprising e.g. methyl 2-amino-4-(1,3-benzodioxol-5-yl)-1-(3-chloro-2-methylphenyl)-5-oxo-1,4,5,6,7,8-hexahydroquinoline-3-carboxylate is a viral RNA polymerase inhibitor, useful to treat influenza, Patent Number(s): WO2013123974-A1

Organisation of scientific meetings:
The 16th European Symposium on QSAR & MM; 10-17 September 2006, Italy
Perugia Fluorine Days: 2nd International Symposium on Organofluorine Compounds in Biomedical and Agricultural Sciences Perugia 11-15 July 2010
VI, VII and VIII European Workshop in Drug Design June 03 - 09, 2007; May 24 - 30, 2009;
May 22 - 28, 2011 - Certosa di Pontignano, Siena, Italy
Meeting of European Project LIGHTS (Ligand Interfering with HumanThymidylate Synthase) Perugia 22-23/10/2008
Meeting of European Project DEPPICT (Designing Therapeutic Protein-Protein Inhibitors for Brain Cancer Treatments), Perugia 30/03/2009
Meeting of Human Liver Consortium Project, Perugia 30/05/2012
14th Scandinavian Symposium on Chemometrics (SSC14) 17-19/06/2015, Sardegna

Refereeing activities:
National:
- Member of the Evaluation Panel of grant proposals at UniPG (2014)
International:
- Evaluation of EU proposals (2000-2008)
- Evaluator of research projects from the national research council of the Netherlands (NWO)
- Referee for a number of international journals and for EU projects (FP6, FP7)
- Life Sciences Evaluation Panel for Research Training Networks Israel 2016

Others activities:
- Scientific Board member of Epix Pharmaceutical (TelAviv and Boston).
- Scientific Board member of ABAC Therapeutics (Barcelona).
- Member of the following Editorial Boards: Journal of Computer Aided Molecular Design, QSAR and Combinatorial Sciences and Drug Discovery Today.
- Founder of Molecular Horizon srl, a Chemioinformatics italian based company in 2016.
- Founder of QSAR, Chemioinformatics and Modeling Society (QCMS) in 2017.

National and international grants (as Principal Investigator or member):
- PRIN 2000 (Proposal reference: MM05151851_002). PI Ronchi Severino (Univ. of Milan) - "Progettazione di nuovi composti antibatterici basata sulla struttura tridimensionale di enzimi della biosintesi del NAD". Role: Responsible for the PG research unit
- PRIN 2002 (Proposal reference: 2002057745_005). PI Ronchi Severino (Univ. of Milan) – "Progettazione razionale di inibitori di enzimi coinvolti nella biosintesi del NAD basata sulla struttura cristallografica tridimensionale, per lo sviluppo di nuovi farmaci antibatterici". Role: responsible for the PG research unit
- IZSUM Project (Proposal reference n.2/2011) - "Dai metodi multiresiduo ai multiclasse: sviluppo di protocolli innovativi nel campo della ricerca dei residui di farmaci veterinari negli alimenti. Role: responsible for the PG research unit
- Fondazione Cassa di Risparmio di Perugia Project 2012 - "Studio della tossicità: un metodo alternativo ai tests su animali" (02/07/2012-30/05/2014). Role: PI

- 2012-2016 CMST COST Action CM1207 – GLISTEN: GPCR-Ligand Interactions, Structures and Transmembrane Signalling: a European Research Network. Role: WG member for Italy
- Fondazione Cassa di Risparmio di Perugia Project 2017 - "Biomarkers lipidici del siero umano in relazione a patologie cardiovascolari". Role: PI
- BRiC-2019 INAIL – PI: Franco Lucarelli (University of Florence) "Valutazione ambientale e impatto sanitario di inquinanti organici emergenti quali ritardanti di fiamma bromurati, sostanze perfluoroalchiliche e inquinanti inorganici tossici in ambienti di lavoro". Role: responsible for the PG research unit
- COST2019 PI: Maria do Rosário Domingues (University of Aveiro -Portugal). LipidNET- Pan-European Network in Lipidomics and EpiLipidomics (Proposal reference: OC-2019-1-23795). MC substitute for Italy.
- Molecular Horizon srl into POR FESR 2014/2020 Umbria Region Project (Complex research & development projects). Role: scientific responsible

Main research activities, technical skills and competences in cheminformatics:
- development of in silico procedures to produce innovative fingerprints to describe chemical entities for drug design.
- Design of compounds with antiviral, antibacterial or anticancer properties
- Developing of simulation methods involving electron transfer processes focused on proteins and metalloproteins (Cytochromes, Molybdopterin-containing enzymes, Flavin Monoxigenases).
- Human metabolism and DMPK: quantification and prediction of ADMET properties (Adsorption, Distribution, Metabolism, Excretion, Toxicity).
- Development of ultra-fast methods for metabolite identification via LC-MSMS.
- Lipidomics: targeted, untargeted and MALDI advanced lipidomic procedures. Development of methods to quantify end-point effect from 3D human micro tissues (early tox effects and mechanisms of drug candidates)
- QSAR: 3D-qsar and qspr for molecular design and development.
- Xenobiotic toxicity: new methodologies in silico and in vitro for drug safety evaluation.
- prediction of organic syntheses. Prediction of nucleofilicity and elecrophilicity of molecules by ab initio methods (developed in house)
- Virtual screening: use of molecular interaction fields to produce a unique fingerprint for ligands and proteins. Water network prediction in protein cavities with applications in drug design.
- Developing of Quantitative Structure Property Relationships for small ligands (drug) and-or macromolecular structures for ligand ADME profile or macromolecule ADME-profile

Main research activities, technical skills and competences in organic synthesis:
- Synthesis of compounds as antiviral, antibacterial or anticancer properties
- Synthesis of PROTACs

Main research activities, technical skills and competences in experimental determination of ADMET properties:
- MetID via LC-MSMS: functional and mechanistic studies of metalloproteins and/or proteins involved in Phase I and II xenobiotic metabolism.
- Untargeted lipidomics: automatic identification of lipids from all different biofluid matrices. Multivariate statistical analyses on lipid fingerprints. Early toxicity prediction from experiments using three dimensional microtissues (human liver, skin, pancreas, brain).
- Forced degradation of compound for the determination of chemical stability