Roberto Nico Dallocchio

Profile: Technician

Office location: Sassari

E-mail address: robertonico.dallocchio@cnr.it

Work phone #: +39 079 2841213

Biography:

Roberto Dallocchio, born in Sassari in 1962, carries out its activities as a technician in the National Research Council (CNR) since 1984 Diplomato in chemistry, in time has acquired a great experience in computer programming, and in management of computer networks.

He mainly deals with computational modeling of biomolecules. These calculations include the use of techniques of molecular mechanics, quantum chemistry, docking, virtual screening and molecular dynamics.

His experience includes the following chemistry software: Autodock, Gaussian, Amber.

Has founded in 2001 the molecular modelling group of the ICB Institute of Sassari.

Is coauthor of numerous publications in international journals of chemistry / biology.

His computer experience led him to play different positions in the field of computer networks, such as the design of infrastructure networks of CNR in Sardinia, the management and programming of devices, such as routers, switches and firewalls (mainly Cisco devices) Currently manages the Computing Center of the CNR Research Area of Sassari, where he specialized in the management of computing servers, virtualization, NAS storage , and application oriented to web (HTML, Javascript, PHP, etc.) He gained experience in various programming languages, including C, C++, Pascal, PHP, Javascript and in the programming world of relational databases (MSQL,MySQL and PosgreSQL).

SCIENTIFIC ACTIVITIES

Skills and expertise:

Docking studies

Virtual Screening

Molecular graphics

Molecular Modeling

Molecular Dynamics

Computer and Parallel Programming

Topics:

Computational Chemistry

Medicinal Chemistry

Inorganic Chemistry

Spectroscopy

Computer Networks

Major publications

Roberto Nico Dallocchio, Alessandro Dessì, Andrea De Vito, Giovanna Delogu, Pier Andrea Serra, Giordano Madeddu
Early combination treatment with existingHIV antivirals: an effective treatment for COVID-19?
European review for medical and pharmacological sciences, 2435, (2021), Doi:10.26355/eurrev_202103_25285

Roberto Dallocchio, Barbara Sechi, Alessandro Dessì, Bezhan Chankvetadze, Sergio Cossu, Victor Mamane, Robin Weiss, Patrick Pale, Paola Peluso
Enantioseparations of polyhalogenated 4,4'-bipyridines on polysaccharide-based chiral stationary phases and molecular dynamics simulations of selector-selectand interactions
Electrophoresis (2021) ; Doi:10.1002/elps.202100049

Giuseppe Marchetti, Alessandro Dessì,Roberto Dallocchio,Ioannis Tsamesidis, Maria Carmina Pau, Francesco Michelangelo Turrini, Antonella Pantaleo
Syk Inhibitors: New Computational Insights into Their Intraerythrocytic Action in Plasmodium falciparum Malaria
International journal of molecular sciences, (2020); DOI: 0.3390/ijms21197009

P. Peluso, C. Gatti, A. Dessì, R. Dallocchio, R.Weiss, E. Aubert, P. Pale, S. Cossu, V. Mamane; Enantioseparation of fluorinated 3-(aryl)thio-4,4'-bipyridines: insights into chalcogen and p-hole bonds in high-performanceliquid chromatography; Journal Chromatography A, 2018, 1567, 119-129; DOI:10.1016/j.choroma.2018.06.060

R. Dallocchio, A. Dessì, M. Solinas, A. Arras, S. Cossu, E. Aubert, V. Mamane, P. Peluso; Halogen bond in high-performance liquid chromatography enantioseparations: Description, features and modelling; Journal Chromatography A, 2018, 1563, 71-81; DOI:10.1016/j.choroma.2018.05.061

P. Peluso, V. Mamane, R. Dallocchio, A. Dessì, R. Villano, D. Sanna, E. Aubert, P. Pale, S. Cossu; Polysaccharide-based chiral stationary phases as halogen bond acceptors: A novel strategy for detection of stereoselective σ-hole bonds in solution; Journal Separation Science 2018, 41, (6), 1247-1256; DOI:10.1002/jssc.201701206

G. Righi, R. Pelagalli, V. Isoni, I. Tirotta, M. Martini, M., Palagri, R. Dallocchio, A. Dessì, B. Macchi, C. Frezza, G. Forte, A. Dalla Cort, G. Portalone, P. Bovicelli; Synthesis, of potential HIV Integrase inhibitors inspired by polyphenol structures; Natural Product Research 2018, 32, (16) 1893-1901; DOI:10.1080/14786419.2017.1354191

R. Cadoni, N. Pala, C. Lomelino,B.P. Mahon, R. McKenna, R. Dallocchio, A. Dessì, M. Carcelli, D. Rogolino, V. Sanna, M. Rassu, C. Iaccarino, D. Vullo, C. Supuran, M. Sechi; Exploring heteroaryl-pyrazole carboxylic acids as human carbonic anhydrase XII inhibitors; ACS Medicinal Chemistry Letters 2017, 8 (9), 941–946; DOI:10.1021/acsmedchemlett.7b00229

G. Righi, R. Pelagalli, V. Isoni, I. Trotta, R. Dallocchio, A. Dessì, B.Macchi, C. Frezza, I. Rossetti, P. Bovicelli; Synthesis, molecular modelling and biological evaluation of two new chicoric acid analogs; Natural Product Research, 2017, 31 (4), 397-403; DOI:10.1080/14786419.2016.1169413

G. Pani, A. Dessì, R. Dallocchio, B. Scherm, E. Azara, G. Delogu, Q. Migheli; Natural phenolic inhibitors of trichothecene biosynthesis by the wheat fungal pathogen Fusarium culmorum: a computational insight into the structure-activity relationsh; PlosOne Open Access 2016; DOI:10.1371/journal.pone.0157316

P. Peluso, V. Mamane, E. Aubert, A. Dessì, R. Dallocchio, A.Dore, P. Pale and S. Cossu; Insights into halogen bonding-driven enantioseparations; Journal Chromatography A ,2016, 1467, 228-238; DOI: 10.1016/j.chroma.2016.06.007

N. Pala, A. Stevaert, R. Dallocchio, A. Dessì, D. Rogolino, M. Carcelli, V.Sanna, M. Sechi, L. Naesens; Virtual screening and biological validation of novel influenza virus PA enduclease inhibitors; ACS Medicinal Chemistry Letters 2015, 6 (8), pp 866-871; DOI: 10.1021/acsmedchemlett.5b00109

M.A. Dettori, D. Fabbri, M. Pisano, C. Rozzo, G. Palmieri, A. Dessì, R. Dallocchio,G. Delogu; 4-Substituted-2-Methoxyphenol: Suitable building block to prepare new bioactive natural-like hydroxylated biphenyls; Letters in Drug Design & Discovery, 2015, 12, 131-139; DOI: 10.2174/1570180811666140915222343

Keyword

Docking, Molecular Dynamics, Virtual Screening, Anti HIV, Antiviral, Paralel Computing