CURRICULUM VITAE IDONEO ALLA PUBBLICAZIONE

PERSONAL DATA

Name, Surname   Giuseppe Felice, Mangiatordi

WORK EXPERIENCE

Senior Researcher
Institute of Crystallography - National Research Council (CNR) [01/01/2023 – Current]

City: Bari
Country: Italy

Researcher
Institute of Crystallography - National Research Council (CNR) [30/11/2018 – Current]

City: Bari
Country: Italy

Researcher
Istituto tumori Giovanni Paolo II (IRCCS) - HAHNEMANN 10 - BARI [01/12/2017 – 30/11/2018]

City: Bari
Country: Italy

- Research in the field of molecular modelling (project: "Point-of-care microfluidic device for quantification of chemotherapeutic drugs in small body fluid samples by highly selective nanoparticle extraction and liquid crystaldetection" – Supervisor Prof. Silke Krol)

Post-doctoral researcher
University of Bari [16/04/2013 – 11/2017]

City: Bari
Country: Italy

- Research in the field of molecular modelling (project: "Ruolo patofisiologico della mutazione D184E in hAQP4" – Supervisor Prof. Orazio Nicolotti)

University teacher
University of Bari [01/01/2019 – 30/06/2020]

City: Bari
Country: Italy

- Responsible for the university course "*Chimica Analitica*" for graduate students in Pharmacy

University teacher

University of Bari [01/01/2017 – 30/06/2017]

City: Bari
Country: Italy

- Responsible for the university course "*Chimica Analitica ed Esercitazioni Numeriche di Laboratorio*" for graduate students in Pharmacy

Researcher

University of Modena e Reggio Emilia [19/06/2009 – 19/12/2009]

City: Modena
Country: Italy

- Research in the field of molecular modelling (project: "Computational approaches for the discovery of multi-target inhibitors for cancer therapy" – Supervisor Prof. Giulio Rastelli)

EDUCATION AND TRAINING

PhD in Physical and Analytical Chemistry (Supervisor: Prof. Carlo Adamo)

Ecole Nationale Supérieure de Chimie de Paris (ENSCP) [01/01/2010 – 31/12/2012]

Address: Paris (France)
Field(s) of study: Theoretical Chemistry, Density Functional Theory, MD simulations
Final grade: PhD (Très Honorable)

Degree (Chimica e Tecnologia Farmaceutiche)

University of Bari [01/09/2002 – 17/11/2008]

Address: Bari (Italy)
Field(s) of study: Medicinal Chemistry and Pharmaceutical Technology
Final grade: 110/110 summa cum laude

INTERNATIONAL TEACHING EXPERIENCES

Teacher of the university course "Thermostatistique et Modélisation Moléculaire"

Ecole Nationale Supérieure de Chimie de Paris (ENSCP) [01/02/2012 – 28/02/2012]

City: Paris
Country: France

Teacher at the workshop " Introduction of Gaussian: Theory and Practice "

Central Leather Research Institute [01/01/2012 – 09/01/2012]

City: Chennai
Country: India

SUPERVISION OF PHD STUDENTS

Supervisor (Tutor) of the PhD student Dr Giuseppe Lamanna (Dottorato in Scienze Chimiche e Molecolari - XXXVI corso – Università di Bari)

[01/11/2020 – Current]

Supervisor (Tutor) of the PhD student Dr Pietro Delre (Dottorato in Scienze Chimiche e Molecolari - XXXIV corso – Università di Bari)

[21/01/2019 – Current]

SUPERVISION OF STUDENTS FROM FOREIGN INSTITUTIONS

Supervisor of the student Arthur Barbault, (Université de Poitiers – France)

[14/05/2019 – 31/07/2019]

- Internship in Molecular Modelling

Supervisor of the student Zara Farooq, (Queeen Mary University of London)

- Internship in Molecular Modelling

HONOURS AND AWARDS

Abilitazione Scientifica Nazionale (ASN)

Italian Ministry of Education, University and Research [31/10/2018]

- Abilitazione Scientifica Nazionale (ASN) a Professore Associato nel settore concorsuale 03/D1, Chimica e tecnologie farmaceutiche, tossicologiche e nutraceutico-alimentari

PRINCIPAL INVESTIGATOR OF THE FOLLOWING FOUNDED PROJECTS

Project RIPARTI

[06/04/2022 – Current]

Principal Investigator of the Project " Sviluppo di una piattaforma tecnologica per contrastare il rischio di fosfolipidosi nello sviluppo pre-clinico del farmaco" - Founded by REGIONE PUGLIA with **€ 36.000,00**

Project @cnr (Call 2020)

[13/01/2022 – Current]

Principal Investigator of the Project " Development of A Technological platform for the Identification of s1R Allosteric MOdulators with potent SARS-CoV-2 antiviral activity " - Founded by CNR with **€ 80.760,00**

Project "Research in Paris 2014"

[01/02/2015 – 31/07/2015]

Principal Investigator of the project "Designing nanotube-drug complexes as efficient drug delivery systems for anticancer therapy". Founded by "Ville de Paris" with **€ 15.000,00**.

PRINCIPAL INVESTIGATOR OF THE FOLLOWING PROJECTS FOUNDED WITH CORE HOURS

- Italian SuperComputing Resource Allocation – ISCRA (B class) as Principal Investigator, (Title: Epitope for Neuromyelitis Optica autoantibody binding in human aquaporin 4: exploring the role of highly conserved TM2 residues, IscrB_epi-NMO, HP10B4VZO7)

- Italian SuperComputing Resource Allocation – ISCRA (C class) as Principal Investigator (Title "Design of carbon nanotube-drug complexes as drug delivery systems with tunable release velocity, DrugCNT", IscrC_DrugCNT, HP10CWS1PD)

- Italian SuperComputing Resource Allocation – ISCRA (B class) as Principal Investigator. (Title "Exploring molecular mechanisms in AQP4 water regulation, IscrB_WRegAQP4", IscrB_WRegAQP4, HP10BWMW76)

- Italian SuperComputing Resource Allocation – ISCRA (B class) as Principal Investigator. (Title "Simulating human-AQP4 aggregation: towards a structural characterization of the Neuromyelitis Optica epitope", IscrB_OAP-AQP4", HP10BGY23X).

BIBLIOMETRIC INDICATORS

H-index= 31; citations = 3300 - Source: Google Scholar

H-index= 28; citations = 2506 - Source: Scopus Elsevier

LIST OF n.82 PUBLICATIONS

[1] Delre, P.; Lavado, G.J.; Lamanna, G.; Saviano, M.; Roncaglioni, A.; Benfenati, E.; **Mangiatordi, G.F**.; Gadaleta, D. Ligand-based prediction of hERG-mediated cardiotoxicity based on the integration of different machine learning techniques. (2022) *Front. Pharmacol.,* 13, 951083. DOI: 10.3389/fphar.2022.951083.

[2] Spinetti, E.; Delre, P.; Saviano, M.; Siliqi, D.; Lattanzi, G.; **Mangiatordi, GF**. A Comparative Molecular Dynamics Study of Selected Point Mutations in the Shwachman-Bodian-Diamond Syndrome Protein SBDS. (2022) *Int J Mol Sci*. 23 (14), 7938. DOI: 10.3390/ijms23147938.

[3] Creanza, T. M.; Lamanna, G.; Delre, P.; Contino, M.; Corriero, N.; Saviano, M.; **Mangiatordi, G. F**.; Ancona,N. DeLA-Drug: A Deep Learning Algorithm for Automated Design of Druglike Analogues. (2022) *J.Chem.Inf.Model.*,62, 20. DOI: 10.1021/acs.jcim.2c00205.

[4] Belviso, B.D.; **Mangiatordi G.F**.; Alberga, D.; Mangini, V.; Carozzini, B.; Caliandro, R. Structural Characterization of the Full-Length Anti-CD20 Antibody Rituximab. Frontiers in Molecular Biosciences. (2022). DOI: 10.3389/fmolb.2022.823174.

[5] Creanza, T.M.; Lamanna, G.; Delre, P.; Contino, M.; Corriero, N.; Saviano, M.; **Mangiatordi, G.F**.; Ancona, N. eLA-Drug: A Deep Learning Algorithm for Automated Design of Druglike Analogue. (2022) Journal of Chemical Information and Modeling 62 (6), 1411-1424. DOI: 10.1021/acs.jcim.2c00205

[6] Gargano, E.M., Mohamed, A., Abdelsamie, A.S., **Mangiatordi, G.F**., Drzewiecka, H., Jagodziński, P.P., Mazzini, A., Van Koppen, C.J., Laschke, M.W., Nicolotti, O., Carotti, A., Marchais-Oberwinkler, S., Hartmann, R.W., Frotscher, M.17β-Hydroxysteroid Dehydrogenase Type 1 Inhibition: A Potential Treatment Option for Non-Small Cell Lung Cancer (2021) ACS Medicinal Chemistry Letters, 12 (12), pp. 1920-1924.

[7] Lee, S.H., Denora, N., Laquintana, V., **Mangiatordi, G.F**., Lopedota, A., Lopalco, A., Cutrignelli, A., Franco, M., Delre, P., Song, I.H., Kim, H.W., Kim, S.B., Park, H.S., Kim, K., Lee, S.-Y., Youn, H., Lee, B.C., Kim, S.E.
Radiosynthesis and characterization of [18F]BS224: a next-generation TSPO PET ligand insensitive to the rs6971 polymorphism (2021) European Journal of Nuclear Medicine and Molecular Imaging, 49 (1), pp. 110-124.

[8] Mansouri, K., Karmaus, A.L., Fitzpatrick, J., Patlewicz, G., Pradeep, P., Alberga, D., Alepee, N., Allen, T.E.H., Allen, D., Alves, V.M., Andrade, C.H., Auernhammer, T.R., Ballabio, D., Bell, S., Benfenati, E., Bhattacharya, S., Bastos, J.V., Boyd, S., Brown, J.B., Capuzzi, S.J., Chushak, Y., Ciallella, H., Clark, A.M., Consonni, V., Daga, P.R., Ekins, S., Farag, S., Fedorov, M., Fourches, D., Gadaleta, D., Gao, F., Gearhart, J.M., Goh, G., Goodman, J.M., Grisoni, F., Grulke, C.M., Hartung, T., Hirn, M., Karpov, P., Korotcov, A., Lavado, G.J., Lawless, M., Li, X., Luechtefeld, T., Lunghini, F., **Mangiatordi,**

G.F., Marcou, G., Marsh, D., Martin, T., Mauri, A., Muratov, E.N., Myatt, G.J., Nguyen, D.-T., Nicolotti, O., Note, R., Pande, P., Parks, A.K., Peryea, T., Polash, A.H., Rallo, R., Roncaglioni, A., Rowlands, C., Ruiz, P., Russo, D.P., Sayed, A., Sayre, R., Sheils, T., Siegel, C., Silva, A.C., Simeonov, A., Sosnin, S., Southall, N., Strickland, J., Tang, Y., Teppen, B., Tetko, I.V., Thomas, D., Tkachenko, V., Todeschini, R., Toma, C., Tripodi, I., Trisciuzzi, D., Tropsha, A., Varnek, A., Vukovic, K., Wang, Z., Wang, L., Waters, K.M., Wedlake, A.J., Wijeyesakere, S.J., Wilson, D., Xiao, Z., Yang, H., Zahoranszky-Kohalmi, G., Zakharov, A.V., Zhang, F.F., Zhang, Z., Zhao, T., Zhu, H., Zorn, K.M., Casey, W., Kleinstreuer, N.C. Erratum: Catmos: Collaborative acute toxicity modeling suite (Environ Health Perspect. 129(4):047013, 2021. 10.1289/EHP8495) (2021) Environmental Health Perspectives, 129 (10), art. no. 109001.

[9] Creanza, T.M., Delre, P., Ancona, N., Lentini, G., Saviano, M., **Mangiatordi, G.F.** Structure-Based Prediction of hERG-Related Cardiotoxicity: A Benchmark Study (2021) Journal of Chemical Information and Modeling, 61 (9), pp. 4758-4770.

[10] Di Gaetano, S., Capasso, D., Delre, P., Pirone, L., Saviano, M., Pedone, E., **Mangiatordi, G.F**. More is always better than one: The n-terminal domain of the spike protein as another emerging target for hampering the sars-cov-2 attachment to host cells (2021) International Journal of Molecular Sciences, 22 (12), art. no. 6462.

[11] Sarcina, L., **Mangiatordi, G.F.**, Torricelli, F., Bollella, P., Gounani, Z., Österbacka, R., Macchia, E., Torsi, L. Surface plasmon resonance assay for label-free and selective detection of hiv-1 p24 protein (2021) Biosensors, 11 (6), art. no. 180.

[12] Gnocchi, D., Cavalluzzi, M.M., **Mangiatordi, G.F**., Rizzi, R., Tortorella, C., Spennacchio, M., Lentini, G., Altomare, A., Sabbà, C. and Mazzocca, A. (2021), Xanthenylacetic Acid Derivatives Effectively Target Lysophosphatidic Acid Receptor 6 to Inhibit Hepatocellular Carcinoma Cell Growth. ChemMedChem 16, 1 –10.

[13] Prencipe, F., Zanfardino, A., Di Napoli, M., Rossi, F., D'errico, S., Piccialli, G., **Mangiatordi, G.F**., Saviano, M., Ronga, L., Varcamonti, M., Tesauro, D. Silver (I) n-heterocyclic carbene complexes: A winning and broad spectrum of antimicrobial properties (2021) 22 (5), art. no. 2497, pp. 1-11.

[14] Mansouri, K., Karmaus, A.L., Fitzpatrick, J., Patlewicz, G., Pradeep, P., Alberga, D., Alepee, N., Allen, T.E.H., Allen, D., Alves, V.M., Andrade, C.H., Auernhammer, T.R., Ballabio, D., Bell, S., Benfenati, E., Bhattacharya, S., Bastos, J.V., Boyd, S., Brown, J.B., Capuzzi, S.J., Chushak, Y., Ciallella, H., Clark, A.M., Consonni, V., Daga, P.R., Ekins, S., Farag, S., Fedorov, M., Fourches, D., Gadaleta, D., Gao, F., Gearhart, J.M., Goh, G., Goodman, J.M., Grisoni, F., Grulke, C.M., Hartung, T., Hirn, M., Karpov, P., Korotcov, A., Lavado, G.J., Lawless, M., Li, X., Luechtefeld, T., Lunghini, F., **Mangiatordi, G.F**., Marcou, G., Marsh, D., Martin, T., Mauri, A., Muratov, E.N., Myatt, G.J., Nguyen, D.-T., Nicolotti, O., Note, R., Pande, P., Parks, A.K., Peryea, T., Polash, A.H., Rallo, R., Roncaglioni, A., Rowlands, C., Ruiz, P., Russo, D.P., Sayed, A., Sayre, R., Sheils, T., Siegel, C., Silva, A.C., Simeonov, A., Sosnin, S., Southall, N., Strickland, J., Tang, Y., Teppen, B., Tetko, I.V., Thomas, D., Tkachenko, V., Todeschini, R., Toma, C., Tripodi, I., Trisciuzzi, D., Tropsha, A., Varnek, A., Vukovic, K., Wang, Z., Wang, L., Waters, K.M., Wedlake, A.J., Wijeyesakere, S.J., Wilson, D., Xiao, Z., Yang, H., Zahoranszky-Kohalmi, G., Zakharov, A.V., Zhang, F.F., Zhang, Z., Zhao, T., Zhu, H., Zorn, K.M., Casey, W., Kleinstreuer, N.C. CATMoS: Collaborative acute toxicity modeling suite (2021) 129 (4).

[15] **Mangiatordi, G.F**., Intranuovo, F., Delre, P., Abatematteo, F.S., Abate, C., Niso, M., Creanza, T.M., Ancona, N., Stefanachi, A., Contino, M. Cannabinoid Receptor Subtype 2 (CB2R) in a Multitarget Approach: Perspective of an Innovative Strategy in Cancer and Neurodegeneration (2020) Journal of Medicinal Chemistry, 63 (23), pp. 14448-14469.

[16] Zacheo, A., Hodek, J., Witt, D., **Mangiatordi, G.F**., Ong, Q.K., Kocabiyik, O., Depalo, N., Fanizza, E., Laquintana, V., Denora, N., Migoni, D., Barski, P., Stellacci, F., Weber, J., Krol, S. Multi-sulfonated ligands on gold nanoparticles as virucidal antiviral for Dengue virus (2020) Scientific Reports, 10 (1), art. no. 9052.

[17] Delre, P., Alberga, D., Gijsbers, A., Sánchez-Puig, N., Nicolotti, O., Saviano, M., Siliqi, D., **Mangiatordi, G.F**. Exploring the role of elongation Factor-Like 1 (EFL1) in Shwachman-Diamond syndrome through molecular dynamics (2020) Journal of Biomolecular Structure and Dynamics, 38 (17), pp. 5219-5229.

[18] Passeri, I., Trisciuzzi, D., Alberga, D., Siragusa, L., Leonetti, F., **Mangiatordi, G.F.,** Nicolotti, O., Strategies of virtual screening in medicinal chemistry (2020) Data Analytics in Medicine: Concepts, Methodologies, Tools, and Applications.

[19] Delre, P., Caporuscio, F., Saviano, M., **Mangiatordi, G.F**. Repurposing Known Drugs as Covalent and Non-covalent Inhibitors of the SARS-CoV-2 Papain-Like Protease (2020) Frontiers in Chemistry, 8, art. no. 594009.

[20] Blasi, D., Sarcina, L., Tricase, A., Stefanachi, A., Leonetti, F., Alberga, D., **Mangiatordi, G.F**., Manoli, K., Scamarcio, G., Picca, R.A., Torsi, L. Enhancing the Sensitivity of Biotinylated Surfaces by Tailoring the Design of the Mixed Self-Assembled Monolayer Synthesis (2020) ACS Omega, 5 (27), pp. 16762-16771.

[21] Spinelli, F., Giampietro, R., Stefanachi, A., Riganti, C., Kopecka, J., Abatematteo, F.S., Leonetti, F., Colabufo, N.A., **Mangiatordi, G.F**., Nicolotti, O., Perrone, M.G., Brea, J., Loza, M.I., Infantino, V., Abate, C., Contino, M.
Design and synthesis of fluorescent ligands for the detection of cannabinoid type 2 receptor (CB2R)
(2020) European Journal of Medicinal Chemistry, 188, art. no. 112037.

[22] Cavalluzzi, M.M., Imbrici, P., Gualdani, R., Stefanachi, A., **Mangiatordi, G.F**., Lentini, G., Nicolotti, O.
Human ether-à-go-go-related potassium channel: exploring SAR to improve drug design
(2020) Drug Discovery Today, 25 (2), pp. 344-366.

[23] Mansouri, K., Kleinstreuer, N., Abdelaziz, A.M., Alberga, D., Alves, V.M., Andersson, P.L., Andrade, C.H., Bai, F., Balabin, I., Ballabio, D., Benfenati, E., Bhhatarai, B., Boyer, S., Chen, J., Consonni, V., Farag, S., Fourches, D., García-Sosa, A.T., Gramatica, P., Grisoni, F., Grulke, C.M., Hong, H., Horvath, D., Hu, X., Huang, R., Jeliazkova, N., Li, J., Li, X., Liu, H., Manganelli, S., **Mangiatordi, G.F**., Maran, U., Marcou, G., Martin, T., Muratov, E., Nguyen, D.-T., Nicolotti, O., Nikolov, N.G., Norinder, U., Papa, E., Petitjean, M., Piir, G., Pogodin, P., Poroikov, V., Qiao, X., Richard, A.M., Roncaglioni, A., Ruiz, P., Rupakheti, C., Sakkiah, S., Sangion, A., Schramm, K.-W., Selvaraj, C., Shah, I., Sild, S., Sun, L., Taboureau, O., Tang, Y., Tetko, I.V., Todeschini, R., Tong, W., Trisciuzzi, D., Tropsha, A., Van Den Driessche, G., Varnek, A., Wang, Z., Wedebye, E.B., Williams, A.J., Xie, H., Zakharov, A.V., Zheng, Z., Judson, R.S.
Compara: Collaborative modeling project for androgen receptor activity
(2020) Environmental Health Perspectives, 128 (2), art. no. 027002

[24] Tondo, A.R., Caputo, L., **Mangiatordi, G.F.,** Monaci, L., Lentini, G., Logrieco, A.F., Montaruli, M., Nicolotti, O., Quintieri, L. Structure-Based Identification and Design of Angiotensin Converting Enzyme-Inhibitory Peptides from Whey Proteins
(2020) Journal of Agricultural and Food Chemistry, 68 (2), pp. 541-548.

[25] Tondo, A.R., Montaruli, M., **Mangiatordi, G.F.**, Nicolotti, O.
Early prediction of ecotoxicological side effects of pharmaceutical impurities based on open-source non-testing approaches
(2020) Methods in Pharmacology and Toxicology, pp. 235-269.

[26] Catto, M., Pisani, L., Mora, E.D.L., Belviso, B.D., **Mangiatordi, G.F**., Pinto, A., Palma, A.D., Denora, N., Caliandro, R., Colletier, J.-P., Silman, I., Nicolotti, O., Altomare, C.D.
Chiral separation, X-ray structure, and biological evaluation of a potent and reversible dual binding site ache inhibitor
(2020) ACS Medicinal Chemistry Letters, 11 (5), pp. 869-876.

[27] Montaruli, M., Alberga, D., Ciriaco, F., Trisciuzzi, D., Tondo, A.R., **Mangiatordi, G.F**., Nicolotti, O.
Accelerating drug discovery by early protein drug target prediction based on a multi-fingerprint similarity search †
(2019) Molecules, 24 (12), art. no. 2233, .

[28] Lakshminarayanan, B., Baek, S.C., Lee, J.P., Kannappan, N., **Mangiatordi, G.F**., Nicolotti, O., Subburaju, T., Kim, H., Mathew, B.
Ethoxylated Head of Chalcones as a New Class of Multi-Targeted MAO Inhibitors
(2019) ChemistrySelect, 4 (21), pp. 6614-6619.

[29] Alberga, D., Trisciuzzi, D., Mansouri, K., **Mangiatordi, G.F**., Nicolotti, O.
Prediction of Acute Oral Systemic Toxicity Using a Multifingerprint Similarity Approach
(2019) Toxicological Sciences, 167 (2), pp. 484-495.

[30] Alberga, D., Trisciuzzi D., Montaruli, M., Leonetti, F., **Mangiatordi, G.F.,** Nicolotti, O.
A New Approach for Drug Target and Bioactivity Prediction: The Multifingerprint Similarity Search Algorithm (MuSSeL)
(2019) Journal of Chemical Information and Modeling, 59 (1), pp. 586-596.

[31] Catto, M., Trisciuzzi, D., Alberga, D., **Mangiatordi, G.F.**, Nicolotti, O.
Multitarget drug design for neurodegenerative diseases
(2019) Methods in Pharmacology and Toxicology, pp. 93-105.

[32] Reeta, Baek, S.C., Lee, J.P., Rangarajan, T.M., Ayushee, Singh, R.P., Singh, M., **Mangiatordi, G.F**., Nicolotti, O., Kim, H., Mathew, B.
Ethyl acetohydroxamate incorporated chalcones: Unveiling a novel class of chalcones for multitarget monoamine oxidase-b inhibitors against alzheimer's disease
(2019) CNS and Neurological Disorders - Drug Targets, 18 (8), pp. 643-654.

[33] Macchia, E., Manoli, K., Holzer, B., Di Franco, C., Ghittorelli, M., Torricelli, F., Alberga, D., **Mangiatordi, G.F**., Palazzo, G., Scamarcio, G., Torsi, L.

Single-molecule detection with a millimetre-sized transistor (2018) Nature Communications, 9 (1), art. no. 3223.

[34] **Mangiatordi, G.F.,** Guzzo, T., Rossano, E.C., Trisciuzzi, D., Alberga, D., Fasciglione, G., Coletta, M., Topai, A., Nicolotti, O.
Design, Synthesis, and Biological Evaluation of Tetrahydro-β-carboline Derivatives as Selective Sub-Nanomolar Gelatinase Inhibitors
(2018) ChemMedChem, 13 (13), pp. 1343-1352.

[35] **Mangiatordi, G.F.**, Trisciuzzi, D., Iacobazzi, R., Denora, N., Pisani, L., Catto, M., Leonetti, F., Alberga, D., Nicolotti, O.
Automated identification of structurally heterogeneous and patentable antiproliferative hits as potential tubulin inhibitors
(2018) Chemical Biology and Drug Design, 92 (1), pp. 1161-1170.

[36] Gargano, E.M., **Mangiatordi, G.F.,** Weber, I., Goebel, C., Alberga, D., Nicolotti, O., Ruess, W., Wierlacher, S.
Persulfate Reaction in a Hair-Bleaching Formula: Unveiling the Unconventional Reactivity of 1,13-Diamino-4,7,10-Trioxatridecane
(2018) ChemistryOpen, 7 (5), pp. 319-322.

[37] Altamura, C., **Mangiatordi, G.F**., Nicolotti, O., Sahbani, D., Farinato, A., Leonetti, F., Carratù, M.R., Conte, D., Desaphy, J.-F., Imbrici, P.
Mapping ligand binding pockets in chloride ClC-1 channels through an integrated in silico and experimental approach using anthracene-9-carboxylic acid and niflumic acid
(2018) British Journal of Pharmacology, 175 (10), pp. 1770-1780.

[38] Trisciuzzi, D., Alberga, D., Leonetti, F., Novellino, E., Nicolotti, O., **Mangiatordi, G.F**.
Molecular docking for predictive toxicology
(2018) Methods in Molecular Biology, 1800, pp. 181-197.

[39] Trisciuzzi, D., Alberga, D., Mansouri, K., Judson, R., Novellino, E., **Mangiatordi, G.F.,** Nicolotti, O.
Predictive Structure-Based Toxicology Approaches to Assess the Androgenic Potential of Chemicals
(2017) Journal of Chemical Information and Modeling, 57 (11), pp. 2874-2884.

[40] Cavalluzzi, M.M., **Mangiatordi, G.F.,** Nicolotti, O., Lentini, G.
Ligand efficiency metrics in drug discovery: the pros and cons from a practical perspective
(2017) Expert Opinion on Drug Discovery, 12 (11), pp. 1087-1104.

[41] Sánchez-Rodríguez, A., Pérez-Castillo, Y., Schürer, S.C., Nicolotti, O., **Mangiatordi, G.F.,** Borges, F., Cordeiro, M.N.D.S., Tejera, E., Medina-Franco, J.L., Cruz-Monteagudo, M.
From flamingo dance to (desirable) drug discovery: a nature-inspired approach
(2017) Drug Discovery Today, 22 (10), pp. 1489-1502.

[42] Imbrici, P., Altamura, C., Gualandi, F., **Mangiatordi, G.F**., Neri, M., De Maria, G., Ferlini, A., Padovani, A., D'Adamo, M.C., Nicolotti, O., Pessia, M., Conte, D., Filosto, M., Desaphy, J.-F.
A novel KCNA1 mutation in a patient with paroxysmal ataxia, myokymia, painful contractures and metabolic dysfunctions
(2017) Molecular and Cellular Neuroscience, 83, pp. 6-12.

[43] Pocquet, L., Vologdin, N., **Mangiatordi, G.F.,** Ciofini, I., Nicolotti, O., Thorimbert, S., Salmain, M.
Supramolecular Anchoring of NCN-Pincer Palladium Complexes into a β-Barrel Protein Host: Molecular-Docking and Reactivity Insights
(2017) European Journal of Inorganic Chemistry, 2017 (30), pp. 3622-3634.

[44] Alberga, D., Trisciuzzi, D., Lattanzi, G., Bennett, J.L., Verkman, A.S., **Mangiatordi, G.F.**, Nicolotti, O.
Comparative molecular dynamics study of neuromyelitis optica-immunoglobulin G binding to aquaporin-4 extracellular domains
(2017) Biochimica et Biophysica Acta - Biomembranes, 1859 (8), pp. 1326-1334.

[45] Gissi, A., **Mangiatordi, G.F.**, Sobański, T., Netzeva, T., Nicolotti, O.
Nontest Methods for REACH Legislation
(2017) Comprehensive Medicinal Chemistry III, 1-8, pp. 472-490.

[46] **Mangiatordi, G.F**., Alberga, D., Pisani, L., Gadaleta, D., Trisciuzzi, D., Farina, R., Carotti, A., Lattanzi, G., Catto, M., Nicolotti, O.
A rational approach to elucidate human monoamine oxidase molecular selectivity
(2017) European Journal of Pharmaceutical Sciences, 101, pp. 90-99.

[47] Imbrici, P., Tricarico, D., **Mangiatordi, G.F**., Nicolotti, O., Lograno, M.D., Conte, D., Liantonio, A.

Pharmacovigilance database search discloses ClC-K channels as a novel target of the AT1 receptor blockers valsartan and olmesartan
(2017) British Journal of Pharmacology, 174 (13), pp. 1972-1983.

[48] Alberga, D., Ciofini, I., **Mangiatordi, G.F**., Pedone, A., Lattanzi, G., Roncali, J., Adamo, C.
Effects of substituents on transport properties of molecular materials for organic solar cells: A theoretical investigation
(2017) Chemistry of Materials, 29 (2), pp. 273-281.

[49] **Mangiatordi, G.F**., Trisciuzzi, D., Alberga, D., Denora, N., Iacobazzi, R.M., Gadaleta, D., Catto, M., Nicolotti, O.
Novel chemotypes targeting tubulin at the colchicine binding site and unbiasing P-glycoprotein
(2017) European Journal of Medicinal Chemistry, 139, pp. 792-803.

[50] Stefanachi, A., **Mangiatordi, G.F.**, Tardia, P., Alberga, D., Leonetti, F., Niso, M., Colabufo, N.A., Adamo, C., Nicolotti, O., Cellamare, S.
[1] Design, synthesis, biological evaluation, NMR and DFT studies of structurally simplified trimethoxy benzamides as selective P-glycoprotein inhibitors: the role of molecular flatness
(2016) Chemical Biology and Drug Design, 88 (6), pp. 820-831.

[51] Imbrici, P., Altamura, C., Camerino, G.M., **Mangiatordi, G.F**., Conte, E., Maggi, L., Brugnoni, R., Musaraj, K., Caloiero, R., Alberga, D., Marsano, R.M., Ricci, G., Siciliano, G., Nicolotti, O., Mora, M., Bernasconi, P., Desaphy, J.-F., Mantegazza, R., Camerino, D.C.
Multidisciplinary study of a new ClC-1 mutation causing myotonia congenita: A paradigm to understand and treat ion channelopathies
(2016) FASEB Journal, 30 (10), pp. 3285-3295.

[52] Gadaleta, D., **Mangiatordi G.F.,** Catto, M., Carotti A., Nicolotti, O., Applicability Domain for QSAR Models: Where Theory Meets Reality (2016) International Journal of Quantitative Structure-Property Relationships (IJQSPR) 1(1).

[53] **Mangiatordi, G.F**., Alberga, D., Altomare, C.D., Carotti, A., Catto, M., Cellamare, S., Gadaleta, D., Lattanzi, G., Leonetti, F., Pisani, L., Stefanachi, A., Trisciuzzi, D., Nicolotti, O.
Mind the Gap! A Journey towards Computational Toxicology
(2016) Molecular Informatics, pp. 294-308.

[54] Pisani, L., Farina, R., Catto, M., Iacobazzi, R.M., Nicolotti, O., Cellamare, S., **Mangiatordi, G.F.,** Denora, N., Soto-Otero, R., Siragusa, L., Altomare, C.D., Carotti, A.
Exploring Basic Tail Modifications of Coumarin-Based Dual Acetylcholinesterase-Monoamine Oxidase B Inhibitors: Identification of Water-Soluble, Brain-Permeant Neuroprotective Multitarget Agents
(2016) Journal of Medicinal Chemistry, 59 (14), pp. 6791-6806.

[55] **Mangiatordi, G.F**., Alberga, D., Trisciuzzi, D., Lattanzi, G., Nicolotti, O.
Human aquaporin-4 and molecular modeling: Historical perspective and view to the future
(2016) International Journal of Molecular Sciences, 17 (7), art. no. 1119.

[56] Mansouri, K., Abdelaziz, A., Rybacka, A., Roncaglioni, A., Tropsha, A., Varnek, A., Zakharov, A., Worth, A., Richard, A.M., Grulke, C.M., Trisciuzzi, D., Fourches, D., Horvath, D., Benfenati, E., Muratov, E., Wedebye, E.B., Grisoni, F., **Mangiatordi, G.F**., Incisivo, G.M., Hong, H., Ng, H.W., Tetko, I.V., Balabin, I., Kancherla, J., Shen, J., Burton, J., Nicklaus, M., Cassotti, M., Nikolov, N.G., Nicolotti, O., Andersson, P.L., Zang, Q., Politi, R., Beger, R.D., Todeschini, R., Huang, R., Farag, S., Rosenberg, S.A., Slavov, S., Hu, X., Judson, R.S. CERAPP: Collaborative estrogen receptor activity prediction project (2016) Environmental Health Perspectives, 124 (7), pp. 1023-1033.

[57] Macchia, E., Alberga, D., Manoli, K., **Mangiatordi, G.F.,** Magliulo, M., Palazzo, G., Giordano, F., Lattanzi, G., Torsi, L.
Organic bioelectronics probing conformational changes in surface confined proteins
(2016) Scientific Reports, 6, art. no. 28085.

[58] Alberga, D., **Mangiatordi, G.F**.
Understanding complexity of physiology by combined molecular simulations and experiments: Anion channels as a proof of concept
(2016) Journal of Physiology, 594 (11), pp. 2777-2778.

[59] Liantonio, A., Imbrici, P., Camerino, G.M., Fracchiolla, G., Carbonara, G., Giannico, D., Gradogna, A., **Mangiatordi, G.F**., Nicolotti, O., Tricarico, D., Pusch, M., Camerino, D.C.
Kidney CLC-Kchloride channels inhibitors: Structure-based studies and efficacy in hypertension and associated CLC-Kpolymorphisms
(2016) Journal of Hypertension, 34 (5), pp. 981-992.

[60] Pisani, L., Farina, R., Soto-Otero, R., Denora, N., **Mangiatordi, G.F**., Nicolotti, O., Mendez-Alvarez, E., Altomare, C.D.,

Catto, M., Carotti, A.
Searching for multi-targeting neurotherapeutics against Alzheimer's: Discovery of potent AChE-MAO B inhibitors through the decoration of the 2H-Chromen-2-one structural motif
(2016) Molecules, 21 (3), art. no. 362.

[61] **Mangiatordi, G.F**., Carotti, A., Novellino, E., Nicolotti, O. A round trip from medicinal chemistry to predictive toxicology
(2016) Methods in Molecular Biology, 1425, pp. 461-473.

[62] Madern, N., Queyriaux, N., Chevalley, A., Ghasemi, M., Nicolotti, O., Ciofini, I., **Mangiatordi, G.F**., Salmain, M.
Piano-stool d6-rhodium(III) complexes of chelating pyridine-based ligands and their papain bioconjugates for the catalysis of transfer hydrogenation of aryl ketones in aqueous medium (2015) Journal of Molecular Catalysis B: Enzymatic, 122, pp. 314-322.

[63] Kontogiorgis, C., Nicolotti, O., **Mangiatordi, G.F**., Tognolini, M., Karalaki, F., Giorgio, C., Patsilinakos, A., Carotti, A., Hadjipavlou-Litina, D., Barocelli, E.
Studies on the antiplatelet and antithrombotic profile of anti-inflammatory coumarin derivatives
(2015) Journal of Enzyme Inhibition and Medicinal Chemistry, 30 (6), pp. 925-933.

[64] Castillo-González, D., Mergny, J.-L., De Rache, A., Pérez-Machado, G., Cabrera-Pérez, M.A., Nicolotti, O., Introcaso, A., **Mangiatordi, G.F.**, Guédin, A., Bourdoncle, A., Garrigues, T., Pallardó, F., Cordeiro, M.N.D.S., Paz-Y-Miño, C., Tejera, E., Borges, F., Cruz-Monteagudo, M.
Harmonization of QSAR Best Practices and Molecular Docking Provides an Efficient Virtual Screening Tool for Discovering New G-Quadruplex Ligands
(2015) Journal of Chemical Information and Modeling, 55 (10), pp. 2094-2110.

[65] Alberga, D., **Mangiatordi, G.F**., Labat, F., Ciofini, I., Nicolotti, O., Lattanzi, G., Adamo, C.
Theoretical investigation of hole transporter materials for energy devices
(2015) Journal of Physical Chemistry C, 119 (42), pp. 23890-23898.

[66] Alberga, D., **Mangiatordi, G.F.,** Motta, A., Nicolotti, O., Lattanzi, G.
Effects of Different Self-Assembled Monolayers on Thin-Film Morphology: A Combined DFT/MD Simulation Protocol
(2015) Langmuir, 31 (39), pp. 10693-10701.

[67] Imbrici, P., Maggi, L., **Mangiatordi, G.F**., Dinardo, M.M., Altamura, C., Brugnoni, R., Alberga, D., Pinter, G.L., Ricci, G., Siciliano, G., Micheli, R., Annicchiarico, G., Lattanzi, G., Nicolotti, O., Morandi, L., Bernasconi, P., Desaphy, J.-F., Mantegazza, R., Camerino, D.C.
ClC-1 mutations in myotonia congenita patients: Insights into molecular gating mechanisms and genotype-phenotype correlation
(2015) Journal of Physiology, 593 (18), pp. 4181-4199.

[68] Alberga, D., Perrier, A., Ciofini, I., **Mangiatordi, G.F**., Lattanzi, G., Adamo, C.
Morphological and charge transport properties of amorphous and crystalline P3HT and PBTTT: Insights from theory
(2015) Physical Chemistry Chemical Physics, 17 (28), pp. 18742-18750.

[69] **Mangiatordi, G.F**., Alberga, D., Siragusa, L., Goracci, L., Lattanzi, G., Nicolotti, O.
Challenging AQP4 druggability for NMO-IgG antibody binding using molecular dynamics and molecular interaction fields
(2015) Biochimica et Biophysica Acta - Biomembranes, 1848 (7), pp. 1462-1471.

[70] Gissi, A., Lombardo, A., Roncaglioni, A., Gadaleta, D., **Mangiatordi, G.F**., Nicolotti, O., Benfenati, E.
Evaluation and comparison of benchmark QSAR models to predict a relevant REACH endpoint: The bioconcentration factor (BCF)
(2015) Environmental Research, 137, pp. 398-409.

[71] Trisciuzzi, D., Alberga, D., Mansouri, K., Judson, R., Cellamare, S., Catto, M., Carotti, A., Benfenati, E., Novellino, E., **Mangiatordi, G.F**., Nicolotti, O.
Docking-based classification models for exploratory toxicology studies on high-quality estrogenic experimental data
(2015) Future Medicinal Chemistry, 7 (14), pp. 1921-1936.

[72] Pisani, F., Mola, M.G., Simone, L., Rosito, S., Alberga, D., **Mangiatordi, G.F**., Lattanzi, G., Nicolotti, O., Frigeri, A., Svelto, M., Nicchia, G.P.
Identification of a point mutation impairing the binding between aquaporin-4 and neuromyelitis optica Autoantibodies
(2014) Journal of Biological Chemistry, 289 (44), pp. 30578-30589.

[73] Floris, M., Manganaro, A., Nicolotti, O., Medda, R., **Mangiatordi, G.F**., Benfenati, E.
A generalizable definition of chemical similarity for read-across
(2014) Journal of Cheminformatics, 6 (1), art. no. 39.

[74] Tardia, P., Stefanachi, A., Niso, M., Stolfa, D.A., **Mangiatordi, G.F**., Alberga, D., Nicolotti, O., Lattanzi, G., Carotti, A., Leonetti, F., Perrone, R., Berardi, F., Azzariti, A., Colabufo, N.A., Cellamare, S.
Trimethoxybenzanilide-based P-glycoprotein modulators: An interesting case of lipophilicity tuning by intramolecular hydrogen bonding
(2014) Journal of Medicinal Chemistry, 57 (15), pp. 6403-6418.

[75] Alberga, D., **Mangiatordi, G.F.,** Torsi, L., Lattanzi, G.
Effects of annealing and residual solvents on amorphous P3HT and PBTTT films
(2014) Journal of Physical Chemistry C, 118 (16), pp. 8641-8655.

[76] Nicolotti, O., Benfenati, E., Carotti, A., Gadaleta, D., Gissi, A., **Mangiatordi, G.F.**, Novellino, E.
REACH and in silico methods: An attractive opportunity for medicinal chemists
(2014) Drug Discovery Today, 19 (11), pp. 1757-1768.

[77] Alberga, D., Nicolotti, O., Lattanzi, G., Nicchia, G.P., Frigeri, A., Pisani, F., Benfenati, V., **Mangiatordi, G.F**.
A new gating site in human aquaporin-4: Insights from molecular dynamics simulations
(2014) Biochimica et Biophysica Acta - Biomembranes, 1838 (12), pp. 3052-3060.

[78] **Mangiatordi, G.F**., Laage, D., Adamo, C.
Backbone effects on the charge transport in poly-imidazole membranes: A theoretical study
(2013) Journal of Materials Chemistry A, 1 (26), pp. 7751-7759.

[79] **Mangiatordi, G.F**., Brémond, E., Adamo, C.
DFT and proton transfer reactions: A benchmark study on structure and kinetics
(2012) Journal of Chemical Theory and Computation, 8 (9), pp. 3082-3088.

[80] **Mangiatordi, G.F**., Butera, V., Russo, N., Laage, D., Adamo, C.
Charge transport in poly-imidazole membranes: A fresh appraisal of the Grotthuss mechanism
(2012) Physical Chemistry Chemical Physics, 14 (31), pp. 10910-10918.

[81] **Mangiatordi, G.F.,** Hermet, J., Adamo, C.
Modeling proton transfer in imidazole-like dimers: A density functional theory study
(2011) Journal of Physical Chemistry A, 115 (12), pp. 2627-2634.

[82] Del Rio, A., Barbosa, A.J.M., Caporuscio, F., **Mangiatordi, G.F**.
CoCoCo: A free suite of multiconformational chemical databases for high-throughput virtual screening purposes
(2010) Molecular BioSystems, 6 (11), pp. 2122-2128.