



PERSONAL DATA

Name, Surname	Giuseppe Felice, Mangiatordi
Address	Via Vecchia Sovereto 50, Terlizzi (BA), 70037
House number, street name, postcode, city, country	Italy
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E-mail	giuseppe.mangiatordi@ic.cnr.it
Nationality	Italian
Place and Date of birth	Terlizzi (BA), 19/07/1983

WORK EXPERIENCE

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 crystal detection" – 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, (Queen 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 – IS CRA (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 – IS CRA (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 – IS CRA (B class) as Principal Investigator. (Title “Exploring molecular mechanisms in AQP4 water regulation, IscrB_WRegAQP4”, IscrB_WRegAQP4, HP10BWMW76)
- Italian SuperComputing Resource Allocation – IS CRA (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= 25; citations = 2129 - Source: Google Scholar

H-index= 23; citations = 1569 - Source: Scopus –Elsevier

LIST OF n.79 PUBLICATIONS

[1] Belviso, B.D.; **Mangiatoridi 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.

[2] Creanza, T.M.; Lamanna, G.; Delre, P.; Contino, M.; Corriero, N.; Saviano, M.; **Mangiatoridi, 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

[3] Gargano, E.M., Mohamed, A., Abdelsamie, A.S., **Mangiatoridi, 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. 17 β -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.

[4] Lee, S.H., Denora, N., Laquintana, V., **Mangiatoridi, 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.

[5] 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., **Mangiatoridi, 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.

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

- [7] 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.
- [8] 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.
- [9] 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.
- [10] 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.
- [11] 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).
- [12] **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.
- [13] 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.
- [14] Delre, P., Alberga, D., Gijbers, 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.
- [15] 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*.
- [16] 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.
- [17] Blasi, D., Sarcina, L., Tricase, A., Stefanachi, A., Leonetti, F., Alberga, D., **Mangiatordi, G.F.**, Manoli, K., Scamarcio, G., Picca, R.A., Torsi, L. [7] 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.
- [18] 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.

- [19] 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.
- [20] 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., Bhatarai, 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., Jeliakova, 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
- [21] 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.
- [22] 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.
- [23] 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.
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- [26] 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.
- [27] 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.
- [28] 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.
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- [32] **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.
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