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Curriculum Vitae

Prof. Donatella Boschi

Personal Statement

Donatella Boschi, after two degree in Pharmacy and Chemistry and Drug Technologies (CTF), received her Ph.D. in Medicinal Chemistry in the 1993 presenting a dissertation based on studies on the α1-adrenoceptor blocking activity of analogues of prazosin. The same year (1993) she become Assistant Professor in Medicinal Chemistry at the Faculty of Pharmacy, Università del Piemonte Orientale "Amedeo Avogadro" in Novara. After moving in the 1999 to Faculty of Pharmacy, University of Turin, Department of Drug Science and Technologies at Torino, in the 2001 she became Associated Professor in the same Faculty. Her expertise is on Drug Design, in particular on use of heterocyclic chemistry to design small molecules blocking receptors as well as enzymes. Her research was directed in the development of small molecules active on cardiovascular diseases, inflammation, cancer, immunosuppression and parasitic infections.

Publications: 66 scientific articles, **2** patents, **1147** citations, **21** h-index. **Expertise**: Medicinal Chemistry, Drug Design, Synthetic Chemistry, Metabolism, Bioisosterism.

Educational activities

Since 1993 she spends her teaching duty in UniTo chemistry related Master courses. Specifically, in the present academic year she is in charge of four Courses at the DSTF (Medicinal Chemistry I, Drug Synthesis, Advanced Medicinal Chemistry, Laboratory of Advanced Medicinal Chemistry) involving more the 90 students inside 140 teaching hours over two semesters. As member of the Specialisation School of Hospital Pharmacy she is in charge of the course of Bibliographic Research.

In more then twenty years of academic research, she became skilled in training young scientist. In this sense, she has so far supervised more than 60 Master students that decided to defend their thesis under her supervision. She is responsible of Erasmus agreements with Birmingham (UK), Dublin (IRL), Tubingen (D), Dusseldorf (D), Bordeaux (F), Paris (F), Kritis (G), Valencia (E), Madrid (E), Tenerife (E), Granada (E), Sevilla (E), Geneva (CH), Louven (B), Lisboa (P) and every years she supervises more than 10 students for their didactic experiences abroad.

She coordinates the framework agreements for scientific cooperation between Università Di Torino Dipartimento Scienza e Tecnologia del Farmaco and the following international universities:

1. Universidad De Buenos Aires - Argentine,
2. Università Mayor de San Andrés - Bolivia,
3. Nirma University - India
4. Stellenbosch University - South Africa.

Research Fellowship Coordination

2014 COFINANZIATO MIUR - TORNATA XVII codice: PROG102916 Nuovi inibitori del fattore di trascrizione NFkB: researcher Dr Agnese Pippione

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2015 World Wide Style Project, Second Edition, call D.D. n. 923 18/03/2015 Dr Rodolfo Braga

2019 COFINANZIATO MIUR - I tornata 2019 codice: PROGD10249 Progettazione di nuovi inibitori della DHODH umana per la cura della leucemia mieloide acuta: Dr Stefano Sainas.

2019 Ex Post Compagnia di San Paolo. Brasil student exchanges. PhD student: J. T. Moreira Filho

2021 COFINANZIATO MIUR - I tornata 2021 codice: PROGD11200 Progettazione di nuovi inibitori della DHODH umana per la cura della leucemia mieloide acuta: Dr Stefano Sainas.

Other Experience and Professional Memberships

1997 Scientific secretariat of the First Italian Swiss Meeting in Medicinal Chemistry - Turin 23-26/9/1997.

From 1999 Member of teaching staff of the Master program titled "Chemistry and Drug Technologies" of the Faculty of Pharmacy of the Turin University.

2001 - 2015 Present in the teaching staff of the Master program titled “Pharmacy” of the Faculty of Pharmacy of the Turin University.

2001 - 2011 Member of the Scientific Board of the Doctorate School of Science and High Technology.

From 2008 International Mobility Coordinator for the Pharmacy Faculty and DSTF.

From 2010 Member of the Specialisation School of Hospital Pharmacy.

2012-2017 Vice-dean of the Master program titled "Chemistry and Drug Technologies".

From 2008 Peer Review Committee: Journal of Medicinal Chemistry, European Journal of Medicinal Chemistry, ChemMedChem, Journal of the Brazilian Chemical Society, Archivoc, Bioorganic and Medicinal Chemistry Letters, Organic & Biomolecular Chemistry.

From 2014 Reviewer for SIR project valuation for Italian Ministry of Scientific Research.

november 2020: founder of the start-up Drug Discovery and Clinic s.r.l., a University of Turin Spin-off.

november 2020- september 2021: member of the Board of Directors of DDC s.r.l. in charges as Chief Patent Officer.

october 2021-november 2022: member of the second Board of Directors of DDC s.r.l. in charges as Chief Patent Officer.

from november 2022- on going: member of the third Board of Directors of DDC s.r.l. in charges as Chief Patent Officer.

Research Support

2022-2024 MIUR per la ricerca locale dell'Università di Torino. Role: PI.

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2021 – 2023 Regione Piemonte Piano Riparti Piemonte INFRA-P2 COVID Linea B, "*SARS-CoV-2 e non solo: portare fino alla sperimentazione umana un candidato farmaco antivirale pan-coronavirus. Thinking innovative to fight the unexpected* (**SILK**)", 799958 Euro.

2022 – 2024 NATO Emerging Security Challenges Division, SPS Programme, G5937, "*Learning a lesson: fighting SARS-CoV-2 Infection and get ready for other future PandEmic scenaRios* (**VIPER**)", 320000 Euro.

2020-2024 AIRC 2019. "Dihydroorotate Dehydrogenase Inhibition to Induce Apoptosis and Differentiation in Myeloid Leukemias (DIORAMA)" (IG 2019 Id.23344) PI: Prof Giuseppe Saglio, Founded with 609.000 Euro. Role: leader of the Medicinal Chimistry Unit.

2022-2025 Erasmus+ Partner Countries (Paesi extra-UE) 2019 - KA107 International Credit Mobility approved vs Nirma University (India) – Founded with: 19.460 euro. Role: Teaching Coordinator.

2020-2023 Erasmus+ Partner Countries (Paesi extra-UE) 2020 - KA107 International Credit Mobility approved vs Bolivia- Universidad Mayor de San Andrés- 2020-2025. Founded with 33.590 euro. Project code 2017-1-IT02-KA107-036256FCH JU platform. Role: Teaching Coordinator.

2020-2022 MIUR per la ricerca locale dell'Università di Torino. Role: PI.

2018-2020 High Priority Italy- Sweden, funded by the Swedish Council and Italian Ministero degli Esteri; Founded with: 45.000 Euro/y. Role: Co-investigator.

2018-2019 Erasmus+ Partner Countries (Paesi extra-UE) 2017 - KA107 International Credit Mobility approved vs Bolivia- Universidad Mayor de San Andrés- 2018-2019. Founded with 28.800,00 euro. Project code 2017-1-IT02-KA107-036256FCH JU platform. Role: Teaching Coordinator.

2019-2021 Funding Institution: Italian Ministry of Scientific Research for University of Turin. Role: PI.

2018-2020 Funding Institution: Italian Ministry of Scientific Research for University of Turin. Role: PI.

2017-2021 Fondazione CRT. "Nuove armi contro il tumore alla prostata refrattario alle terapie attuali (NACTUS)." Totale Budget: 35 000 EUR. Role: PI.

2016-2018 Funding Institution: Italian Ministry of Scientific Research for University of Turin. Role: PI.

2015-2017 Funding Institution: Italian Ministry of Scientific Research for University of Turin. "Searching potent anti-inflammatory agents able to block the NFkB cascade". Role: PI.

2014-2016. Finanziatore: EU. FP7-2014-LIFESCIHELTH "Translational Kinase Tumour Inhibitor discovery Consortium". Local DSTF Unit budget: 482 000 EUR (Budget of the consortium 1 250 000 EUR). Ruolo: Co-investigator.

2014-2016 Funding Institution: Italian Ministry of Scientific Research for University of Turin "Study of new hydroxylated heterocycles as tools for scaffold hopping strategy in drug design". Role: Co-investigator.

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2013-2015 Funding Institution: Italian Ministry of Scientific Research for University of Turin. “Study of new hydroxyl-heterocycles as carboxylic acid bioisosters”. Role: Co-investigator.

2012-2014 Funding Institution: Italian Ministry of Scientific Research for University of Turin. “Study of compounds activity against new validated biological target for tumors”. Role: Co-investigator.

PRIN 2003: Project title: “New NO donor cardiovascular drugs”. Duration 24 months. Role: Co-investigator.

PRIN 2001: Funding Institution: Italian Ministry of Scientific Research. Project title: “NO donor hybrid as vasodilator and antiaggregant agents”. Duration 24 months. Role: Co-investigator.

PRIN 1999: Funding Institution: Italian Ministry of Scientific Research. Project title: “Nitrogen Oxides Prodrug”. Duration 24 months. Role: Co-investigator.

PRIN 1997: Funding Institution: Italian Ministry of Scientific Research. Project title: “Nitrogen Oxides Prodrug”. Duration 24 months. Role: Co-investigator.

Patents

Boschi Donatella, Giorgis Marta, Lolli Marco Lucio, Saglio Giuseppe, Martinelli Giovanni (2020). Inibitori della diidroorotato deidrogenasi umana (hDHODH) per l'uso come antivirali. 102020000027251.

Boschi Donatella, Giorgis Marta, Lolli Marco Lucio, Saglio Giuseppe, Martinelli Giovanni (2019). Novel Human Dihydroorotate Dehydrogenase (Hdhodh) Inhibitors And Their Use In Targeting Oncological Diseases Sensitive To Pyrimidine Starvation. Wo2019/234186 A1, Boschi Donatella, Giorgis Marta, Lolli Marco Lucio, Martinelli Giovanni, Saglio Giuseppe

Boschi Donatella, Giorgis Marta, Lolli Marco Lucio, Saglio Giuseppe, Martinelli Giovanni (2018). Nuovi inibitori della diidroorotato deidrogenasi umana (hDHODH) e loro uso mirato sul differenziamento mieloide. 102018000006067, Boschi Donatella, Giorgis Marta, Lolli Marco Lucio, Saglio Giuseppe, Martinelli Giovanni

Peer-reviewed Publications

Publications: 66 scientific articles, 1147 citations, 21 h-index.

1. Houshmand, M.; Vitale, N.; Orso, F.; Cignetti, A.; Molineris, I.; Gaidano, V.; Sainas, S.; Giorgis, M.; Boschi, D.; Fava, C.; Passoni, A.; Gai, M.; Geuna, M.; Sora, F.; Iurlo, A.; Abruzzese, E.; Breccia, M.; Mulas, O.; Caocci, G.; Castagnetti, F.; Taverna, D.; Oliviero, S.; Pane, F.; Lolli, M. L.; Circosta, P.; Saglio, G., Dihydroorotate dehydrogenase inhibition reveals metabolic vulnerability in chronic myeloid leukemia. *Cell Death & Disease* **2022,** *13* (6), 576.

2. Galati, S.; Sainas, S.; Giorgis, M.; Boschi, D.; Lolli, M. L.; Ortore, G.; Poli, G.; Tuccinardi, T., Identification of Human Dihydroorotate Dehydrogenase Inhibitor by a Pharmacophore-Based Virtual Screening Study. *Molecules* **2022,** *27* (12).

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3. Pippione, A. C.; Kilic-Kurt, Z.; Kovachka, S.; Sainas, S.; Rolando, B.; Denasio, E.; Pors, K.; Adinolfi, S.; Zonari, D.; Bagnati, R.; Lolli, M. L.; Spyrakis, F.; Oliaro-Bosso, S.; Boschi, D., New aldo-keto reductase 1C3 (AKR1C3) inhibitors based on the hydroxytriazole scaffold. *Eur J Med Chem* **2022,** *237*, 114366.

4. Rubin, E.; Pippione, A. C.; Boyko, M.; Einaudi, G.; Sainas, S.; Collino, M.; Cifani, C.; Lolli, M. L.; Abu-Freha, N.; Kaplanski, J.; Boschi, D.; Azab, A. N., A New NF-κB Inhibitor, MEDS-23, Reduces the Severity of Adverse Post-Ischemic Stroke Outcomes in Rats. *Brain Sciences* **2022,** *12* (1), 35.

5. Calistri, A.; Luganini, A.; Mognetti, B.; Elder, E.; Sibille, G.; Conciatori, V.; Del Vecchio, C.; Sainas, S.; Boschi, D.; Montserrat, N.; Mirazimi, A.; Lolli, M. L.; Gribaudo, G.; Parolin, C., The New Generation hDHODH Inhibitor MEDS433 Hinders the In Vitro Replication of SARS-CoV-2 and Other Human Coronaviruses. *Microorganisms* **2021,** *9* (8), 1731.

6. Sainas, S.; Giorgis, M.; Circosta, P.; Gaidano, V.; Bonanni, D.; Pippione, A. C.; Bagnati, R.; Passoni, A.; Qiu, Y.; Cojocaru, C. F.; Canepa, B.; Bona, A.; Rolando, B.; Mishina, M.; Ramondetti, C.; Buccinnà, B.; Piccinini, M.; Houshmand, M.; Cignetti, A.; Giraudo, E.; Al-Karadaghi, S.; Boschi, D.; Saglio, G.; Lolli, M. L., Targeting Acute Myelogenous Leukemia Using Potent Human Dihydroorotate Dehydrogenase Inhibitors Based on the 2-Hydroxypyrazolo[1,5-a]pyridine Scaffold: SAR of the Biphenyl Moiety. *J. Med. Chem.* **2021,** *64* (9), 5404-5428.

7. Luganini, A.; Sibille, G.; Mognetti, B.; Sainas, S.; Pippione, A. C.; Giorgis, M.; Boschi, D.; Lolli, M. L.; Gribaudo, G., Effective deploying of a novel DHODH inhibitor against herpes simplex type 1 and type 2 replication. *Antiviral Research* **2021,** *189*, 105057.

8. Peraldo-Neia, C.; Ostano, P.; Mello-Grand, M.; Guana, F.; Gregnanin, I.; Boschi, D.; Oliaro-Bosso, S.; Pippione, A. C.; Carenzo, A.; De Cecco, L.; Cavalieri, S.; Micali, A.; Perrone, F.; Averono, G.; Bagnasacco, P.; Dosdegani, R.; Masini, L.; Krengli, M.; Aluffi-Valletti, P.; Valente, G.; Chiorino, G., AKR1C3 is a biomarker and druggable target for oropharyngeal tumors. *Cell Oncol (Dordr)* **2021,** *44* (2), 357-372.

9. Gaidano, V.; Houshmand, M.; Vitale, N.; Carrà, G.; Morotti, A.; Tenace, V.; Rapelli, S.; Sainas, S.; Pippione, A. C.; Giorgis, M.; Boschi, D.; Lolli, M. L.; Cilloni, D.; Cignetti, A.; Saglio, G.; Circosta, P., The Synergism between DHODH Inhibitors and Dipyridamole Leads to Metabolic Lethality in Acute Myeloid Leukemia. *Cancers (Basel)* **2021,** *13* (5).

10. Sainas, S.; Pippione, A. C.; Boschi, D.; Lolli, M. L., Chapter Five - Hydroxyazoles as acid isosteres and their drug design applications—Part 1: Monocyclic systems. In *Advances in Heterocyclic Chemistry*, Meanwell, N. A.; Lolli, M. L., Eds. Academic Press: 2021; Vol. 134, pp 185-272.
11. Pippione, A. C.; Sainas, S.; Boschi, D.; Lolli, M. L., Chapter Six - Hydroxyazoles as acid isosteres and their drug design applications—Part 2: Bicyclic systems. In *Advances in Heterocyclic Chemistry*, Meanwell, N. A.; Lolli, M. L., Eds. Academic Press: 2021; Vol. 134, pp 273-311.

12. Sainas, S.; Pippione, A. C.; Giraudo, A.; Martina, K.; Bosca, F.; Rolando, B.; Barge, A.; Ducime, A.; Federico, A.; Grossert, S. J.; White, R. L.; Boschi, D.; Lolli, M. L., Regioselective N-Alkylation of Ethyl 4-Benzyloxy-1,2,3-triazolecarboxylate: A Useful Tool for the Synthesis of Carboxylic Acid Bioisosteres. *J. Heterocycl. Chem.* **2019,** *56* (1), 19.

13. Pippione, A. C.; Sainas, S.; Goyal, P.; Fritzson, I.; Cassiano, G. C.; Giraudo, A.; Giorgis, M.; Tavella, T. A.; Bagnati, R.; Rolando, B.; Caing-Carlsson, R.; Costa, F. T. M.; Andrade, C. H.; Al-Karadaghi, S.; Boschi, D.; Friemann, R.; Lolli, M. L., Hydroxyazole scaffold-based Plasmodium falciparum dihydroorotate dehydrogenase inhibitors: Synthesis, biological evaluation and X-ray structural studies. *Eur J Med Chem* **2019,** *163*, 266-280.

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14. Boschi, D.; Pippione, A. C.; Sainas, S.; Lolli, M. L., Dihydroorotate dehydrogenase inhibitors in anti-infective drug research. *European Journal of Medicinal Chemistry* **2019,** *183*, 111681.

15. Giraudo, A.; Krall, J.; Bavo, F.; Nielsen, B.; Kongstad, K. T.; Rolando, B.; De Blasio, R.; Gloriam, D. E.; Loftier, R.; Thiesen, L.; Harpsoe, K.; Frydenvang, K.; Boschi, D.; Wellendorph, P.; Lolli, M. L.; Jensen, A. A.; Frolund, B., Five-Membered N-Heterocyclic Scaffolds as Novel Amino Bioisosteres at gamma-Aminobutyric Acid (GABA) Type A Receptors and GABA Transporters. *J. Med. Chem.* **2019,** *62* (12), 5797-5809.

16. Santos, A. R. N.; Sheldrake, H. M.; Ibrahim, A. I. M.; Danta, C. C.; Bonanni, D.; Daga, M.; Oliaro-Bosso, S.; Boschi, D.; Lolli, M. L.; Pors, K., Exploration of 2+2+2 cyclotrimerisation methodology to prepare tetrahydroisoquinoline-based compounds with potential aldo-keto reductase 1C3 target affinity. *Medchemcomm* **2019,** *10* (8), 1476-1480.

17. Sainas, S.; Temperini, P.; Farnsworth, J. C.; Yi, F.; Mollerud, S.; Jensen, A. A.; Nielsen, B.; Passoni, A.; Kastrup, J. S.; Hansen, K. B.; Boschi, D.; Pickering, D. S.; Clausen, R. P.; Lolli, M. L., Use of the 4-Hydroxytriazole Moiety as a Bioisosteric Tool in the Development of Ionotropic Glutamate Receptor Ligands. *J. Med. Chem.* **2019,** *62* (9), 4467-4482.

18. Lolli, M. L.; Carnovale, I. M.; Pippione, A. C.; Wahlgren, W. Y.; Bonanni, D.; Marini, E.; Zonari, D.; Gallicchio, M.; Boscaro, V.; Goyal, P.; Friemann, R.; Rolando, B.; Bagnati, R.; Adinolfi, S.; Oliaro-Bosso, S.; Boschi, D., Bioisosteres of Indomethacin as Inhibitors of Aldo-Keto Reductase 1C3 (AKR1C3). *ACS Med. Chem. Lett.* **2019**.

19. Pippione, A. C.; Sainas, S.; Goyal, P.; Fritzson, I.; Cassiano, G. C.; Giraudo, A.; Giorgis, M.; Tavella, T. A.; Bagnati, R.; Rolando, B.; Caing-Carlsson, R.; Costa, F. T. M.; Andrade, C. H.; Al-Karadaghi, S.; Boschi, D.; Friemann, R.; Lolli, M. L., Hydroxyazole scaffold-based Plasmodium falciparum dihydroorotate dehydrogenase inhibitors: Synthesis, biological evaluation and X-ray structural studies. *Eur. J. Med. Chem.* **2018,** *163*, 266-280.

20. Sainas, S.; Dosio, F.; Boschi, D.; Lolli, M. L., Targeting Human Onchocerciasis: Recent Advances Beyond Ivermectin. In *Neglected Diseases: Extensive Space for Modern Drug Discovery*, Botta, M., Ed. Elsevier Academic Press Inc: San Diego, 2018; Vol. 51, pp 1-38.

21. Giraudo, A.; Krall, J.; Nielsen, B.; Sorensen, T. E.; Kongstad, K. T.; Rolando, B.; Boschi, D.; Frolund, B.; Lolli, M. L., 4-Hydroxy-1,2,3-triazole moiety as bioisostere of the carboxylic acid function: a novel scaffold to probe the orthosteric gamma-aminobutyric acid receptor binding site. *Eur. J. Med. Chem.* **2018,** *158*, 311-321.

22. Sainas, S.; Pippione, A. C.; Boschi, D.; Gaidano, V.; Circosta, P.; Cignetti, A.; Dosio, F.; Lolli, M. L., DHODH inhibitors and leukemia: an emergent interest for new myeloid differentiation agents. *Drugs Future* **2018,** *43* (11), 823-834.

23. Grossert, J. S.; Boschi, D.; Lolli, M. L.; White, R. L., Fragmentation pathways arising from protonation at different sites in aminoalkyl-substituted 3-hydroxy-1,2,5-oxadiazoles (3-hydroxyfurazans). *Rapid Commun. Mass Spectrom.* **2018,** *32* (16), 1403-1413.

24. Sainas, S.; Pippione, A. C.; Lupino, E.; Giorgis, M.; Circosta, P.; Gaidano, V.; Goyal, P.; Bonanni, D.; Rolando, B.; Cignetti, A.; Ducime, A.; Andersson, M.; Järvå, M.; Friemann, R.; Piccinini, M.; Ramondetti, C.; Buccinnà, B.; Al-Karadaghi, S.; Boschi, D.; Saglio, G.; Lolli, M. L., Targeting Myeloid Differentiation Using Potent 2-Hydroxypyrazolo[1,5-a]pyridine Scaffold-Based Human Dihydroorotate Dehydrogenase Inhibitors. *J. Med. Chem.* **2018,** *61* (14), 6034-6055.

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25. Pippione, A. C.; Sainas, S.; Federico, A.; Lupino, E.; Piccinini, M.; Kubbutat, M.; Contreras, J. M.; Morice, C.; Barge, A.; Ducime, A.; Boschi, D.; Al-Karadaghi, S.; Lolli, M. L., N-Acetyl-3-aminopyrazoles block the non-canonical NF-kB cascade by selectively inhibiting NIK. *Medchemcomm* **2018,** *9* (6), 963-968.

26. Pippione, A. C.; Carnovale, I. M.; Bonanni, D.; Sini, M.; Goyal, P.; Marini, E.; Pors, K.; Adinolfi, S.; Zonari, D.; Festuccia, C.; Wahlgren, W. Y.; Friemann, R.; Bagnati, R.; Boschi, D.; Oliaro-Bosso, S.; Lolli, M. L., Potent and selective aldo-keto reductase 1C3 (AKR1C3) inhibitors based on the benzoisoxazole moiety: application of a bioisosteric scaffold hopping approach to flufenamic acid. *Eur. J. Med. Chem.* **2018,** *150*, 930-945.

27. Lolli, M. L.; Sainas, S.; Pippione, A. C.; Giorgis, M.; Boschi, D.; Dosio, F., Use of human Dihydroorotate Dehydrogenase (hDHODH) Inhibitors in Autoimmune Diseases and New Perspectives in Cancer Therapy. *Recent. Pat. Anticancer Drug Discov.* **2018,** *13* (1), 86-105.

28. Pippione, A. C.; Boschi, D.; Pors, K.; Oliaro-Bosso, S.; Lolli, M. L., Androgen-AR axis in primary and metastatic prostate cancer: chasing steroidogenic enzymes for therapeutic intervention. *J. Cancer Metastasis Treat.* **2017,** *3* (12), 328-61.

29. Pippione, A. C.; Giraudo, A.; Bonanni, D.; Carnovale, I. M.; Marini, E.; Cena, C.; Costale, A.; Zonari, D.; Pors, K.; Sadiq, M.; Boschi, D.; Oliaro-Bosso, S.; Lolli, M. L., Hydroxytriazole derivatives as potent and selective aldo-keto reductase 1C3 (AKR1C3) inhibitors discovered by bioisosteric scaffold hopping approach. *Eur. J. Med. Chem.* **2017,** *139* (Supplement C), 936-946.

30. Pippione, A. C.; Federico, A.; Ducime, A.; Sainas, S.; Boschi, D.; Barge, A.; Lupino, E.; Piccinini, M.; Kubbutat, M.; Contreras, J.-M.; Morice, C.; Al-Karadaghi, S.; Lolli, M. L., 4-Hydroxy-N-[3,5-bis(trifluoromethyl)phenyl]-1,2,5-thiadiazole-3-carboxamide: a novel inhibitor of the canonical NF-[small kappa]B cascade. *MedChemComm* **2017,** *8*, 1850 - 1855.

31. Sainas, S.; Pippione, A. C.; Giorgis, M.; Lupino, E.; Goyal, P.; Ramondetti, C.; Buccinnà, B.; Piccinini, M.; Braga, R. C.; Andrade, C. H.; Andersson, M.; Moritzer, A.-C.; Friemann, R.; Mensa, S.; Al-Karadaghi, S.; Boschi, D.; Lolli, M. L., Design, synthesis, biological evaluation and X-ray structural studies of potent human dihydroorotate dehydrogenase inhibitors based on hydroxylated azole scaffolds. *Eur. J. Med. Chem.* **2017,** *129*, 287-302.

32. Pippione, A. C.; Dosio, F.; Ducime, A.; Federico, A.; Martina, K.; Sainas, S.; Frølund, B.; Gooyit, M.; Janda, K. D.; Boschi, D.; Lolli, M. L., Substituted 4-hydroxy-1,2,3-triazoles: synthesis, characterization and first drug design applications through bioisosteric modulation and scaffold hopping approaches. *MedChemComm* **2015,** *6* (7), 1285-1292.

33. Grossert, J. S.; Pippione, A. C.; Boschi, D.; Lolli, M. L.; White, R. L., Heterocyclic ring cleavage upon collision-induced dissociation of deprotonated 3-hydroxy-1,2,5-oxadiazoles (3-hydroxyfurazans). *J. Mass Spectrom.* **2015,** *50* (12), 1433-1437.

34. Chegaev, K.; Lazzarato, L.; Tamboli, Y.; Boschi, D.; Blangetti, M.; Scozzafava, A.; Carta, F.; Masini, E.; Fruttero, R.; Supuran, C. T.; Gasco, A., Furazan and furoxan sulfonamides are strong alpha-carbonic anhydrase inhibitors and potential antiglaucoma agents. *Bioorg. Med. Chem.* **2014,** *22* (15), 3913-3921.

35. Boschi, D.; Tosco, P.; Chandra, N.; Chaurasia, S.; Fruttero, R.; Griffin, R.; Wang, L. Z.; Gasco, A., 6-Cyclohexylmethoxy-5-(cyano-NNO-azoxy)pyrimidine-4-amine: A new scaffold endowed with potent CDK2 inhibitory activity. *Eur. J. Med. Chem.* **2013,** *68*, 333-338.

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36. Boschi, D.; Guglielmo, S.; Aiello, S.; Morace, G.; Borghi, E.; Fruttero, R., Synthesis and in vitro antimicrobial activities of new (cyano-NNO-azoxy)pyrazole derivatives. *Bioorg. Med. Chem. Lett.* **2011,** *21* (11), 3431-3434.

37. Gerace, E.; Salomone, A.; Fasano, F.; Costa, R.; Boschi, D.; Di Stilo, A.; Vincenti, M., Validation of a GC/MS method for the detection of two quinolinone-derived selective androgen receptor modulators in doping control analysis. *Anal. Bioanal. Chem.* **2011,** *400* (1), 137-144.

38. Boschi, D.; Giorgis, M.; Cena, C.; Talniya, N. C.; Di Stilo, A.; Morini, G.; Coruzzi, G.; Guaita, E.; Fruttero, R.; Gasco, A., Multitarget Drugs: Synthesis and Preliminary Pharmacological Characterization of Zileuton Analogues Endowed with Dual 5-LO Inhibitor and NO-Dependent Activities. *ChemMedChem* **2010,** *5* (9), 1444-1449.

39. Boschi, D.; Cena, C.; Di Stilo, A.; Rolando, B.; Manzini, P.; Fruttero, R.; Gasco, A., Nitrooxymethyl-Substituted Analogues of Rofecoxib: Synthesis and Pharmacological Characterization. *Chem. Biodiversity* **2010,** *7* (5), 1173-1182.

40. Bozzo, F.; Bassignana, A.; Lazzarato, L.; Boschi, D.; Gasco, A.; Bocca, C.; Miglietta, A., Novel nitro-oxy derivatives of celecoxib for the regulation of colon cancer cell growth. *Chemico-Biological Interactions* **2009,** *182* (2-3), 183-190.

41. Boschi, D.; Lazzarato, L.; Rolando, B.; Filieri, A.; Cena, C.; Di Stilo, A.; Fruttero, R.; Gasco, A., Nitrooxymethyl-Substituted Analogues of Celecoxib: Synthesis and Pharmacological Characterization. *Chem. Biodiversity* **2009,** *6* (3), 369-379.

42. Gasco, A.; Boschi, D.; Chegaev, K.; Cena, C.; Di Stilo, A.; Fruttero, R.; Lazzarato, L.; Rolando, B.; Tosco, P., Multitarget drugs: Focus on the NO-donor hybrid drugs. *Pure and Applied Chemistry* **2008,** *80* (8), 1693-1701.

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