

2015-2020 Publications

1. **Chiarelli LR**, Salina EG, Mori G, Azhikina T, Riabova O, Lepioshkin A, Grigorov A, Forbak M, Madacki J, Orena BS, Manfredi M, Gosetti F, Buzzi A, Degiacomi G, Sammartino JC, Marengo E, Korduláková J, Riccardi G, Mikušová K, Makarov V, Pasca MR. New insights into the mechanism of action of the thienopyrimidine antitubercular prodrug TP053. **ACS Infect Dis.** (2020) doi: 10.1021/acsinfecdis.9b00388
2. Costabile G, Provenzano R, Azzalin A, Scoffone VC, Chiarelli LR, Rondelli V, Grillo I, Zinn T, Lepioshkin A, Savina S, Miro A, Quaglia F, Makarov V, Coenye T, Brocca P, Riccardi G, Buroni S, Ungaro F. PEGylated mucus-penetrating nanocrystals for lung delivery of a new FtsZ inhibitor against *Burkholderia cenocepacia* infection. **Nanomedicine** (2020) 23: 102113 .
3. **Chiarelli LR**, Mori M, Beretta G, Gelain A, Pini E, Sammartino JC, Stelitano G, Barlocco D, Costantino L, Lapillo M, Poli G, Caligiuri I, Rizzolio F, Bellinzoni M, Tuccinardi T, Villa S, Meneghetti F. New insight into structure-activity of furan-based salicylate synthase (MbtI) inhibitors as potential antitubercular agents. **J Enzyme Inhib Med Chem.** (2019) 34:823-828.
4. Lightly T, Frejuk K, Groleau M, **Chiarelli LR**, Ras C, Buroni S, Déziel E, Sorensen J, Cardona S. Phenylacetyl-CoA, not phenylacetic acid, attenuates CepIR-regulated virulence in *Burkholderia cenocepacia*. **Appl Environ Microbiol.** (2019) 85:e01594-19
5. Mori M, Sammartino JC, Costantino L, Gelain A, Meneghetti F, Villa S, **Chiarelli LR**[§]. An Overview on the Potential Antimycobacterial Agents Targeting Serine/Threonine Protein Kinases from *Mycobacterium tuberculosis*. **Curr Top Med Chem.** (2019) 19:646-661 ([§]Corresponding author)
6. Sass A, Slachmuylders L, Van Acker H, Vandenbussche I, Ostyn L, Bové M, Crabbé C, **Chiarelli LR**, Buroni S, Van Nieuwerburgh F, Abatih E, Coenye T. Various evolutionary trajectories lead to loss of the tobramycin-potentiating activity of the quorum-sensing inhibitor baicalin hydrate in *Burkholderia cenocepacia* biofilms. **Antimicrob Agents Chemother.** (2019) 63(4): pii: e02092-18.
7. Buroni S, Scoffone VC, Fumagalli M, Makarov V, Cagnone M, Trespidi G, De Rossi E, Forneris F, Riccardi G, **Chiarelli LR**[§]. Investigating the mechanism of action of diketopiperazines inhibitors of the *Burkholderia cenocepacia* quorum sensing synthase CepI: a site-directed mutagenesis study. **Front. Pharmacol.** (2018) 9:836. ([§]Corresponding author)
8. **Chiarelli LR**, Mori M, Barlocco D, Beretta G, Gelain A, Pini E, Porcino M, Mori G, Stelitano G, Costantino L, Lapillo M, Bonanni D, Poli G, Tuccinardi T, Villa S, Meneghetti F. Discovery and development of novel salicylate synthase (MbtI) Furanic inhibitors as antitubercular agents. **Eur. J. Med Chem.** (2018) 155:754–763.
9. Pini E, Poli G, Tuccinardi T, **Chiarelli LR**, Mori M, Gelain A, Costantino L, Villa S, Meneghetti F, Barlocco. New chromane-based derivatives as inhibitors of *Mycobacterium tuberculosis* salicylate synthase (MbtI): preliminary biological evaluation and molecular modeling studies. **Molecules.** (2018) 23:E1506
10. **Chiarelli LR**, Mori G, Orena BS, Esposito M, Lane T, de Jesus Lopes Ribeiro AL, Degiacomi G, Zemanová J, Szádocka S, Huszár S, Palčeková Z, Manfredi M, Gosetti F, Lelièvre J, Ballell L, Kazakova E, Makarov V, Marengo E, Mikusova K, Cole ST, Riccardi G, Ekins S, Pasca MR. A multitarget approach to drug discovery inhibiting *Mycobacterium tuberculosis* PyrG and PanK. **Sci. Rep.** (2018) 8:3187.
11. Viglio S, Cagnone M, **Chiarelli LR**, Salvini R, Iadarola P. The Role of One- and Two-Dimensional Electrophoretic Techniques in Proteomics of the Lung (2018) in **Electrophoresis - Life Sciences Practical Applications**. Boldura OM and Baltă C Eds (IntechOpen) pp. 22-44 <http://dx.doi.org/10.5772/intechopen.75042>
12. Hogan HM, Scoffone VC, Makarov V, Gislason A, Tesfu H, Stietz MS, Brassinga AK, Domaratzki M, Li X, Azzalin A, Biggiogera M, Riabova O, Monakhova N, **Chiarelli LR**, Riccardi G, Buroni S, Cardona ST. Competitive fitness of essential gene knockdowns reveals a broad-spectrum antibacterial inhibitor of the cell division protein FtsZ. **Antimicrob Agents Chemother.** (2018) 62:e01231-18.

13. Esposito M, Szadocka S, Degiacomi G, Orena BS, Mori G, Piano V, Boldrin F, Zemanova J, Huszár S, Barros D, Ekins S, Lelièvre J, Manganelli R, Mattevi A, Pasca MR, Riccardi G, Ballell L, Mikušová K, **Chiarelli LR[§]**. *A phenotypic based target screening approach delivers new antitubercular CTP synthetase inhibitors.* **ACS Infect Dis.** (2017) 3:428-437. ([§]**Corresponding author**)
14. Mori G, **Chiarelli LR**, Riccardi G, Pasca MR. *New prodrugs against tuberculosis.* **Drug Discov Today** (2017) 22:519-525.
15. Scoffone VC, **Chiarelli LR**, Trespidi G, Mentasti M, Riccardi G, Buroni S. *Burkholderia cenocepacia* infections in cystic fibrosis patients: drug resistance and therapeutic approaches. **Front. Microbiol.** (2017) 8:1592.
16. Oliveira PFM, Guidetti B, Chamayou A, André-Barrès C, Madacki J, Kordulakova J, Mori G, Orena BS, **Chiarelli LR**, Pasca MR, Lherbet C, Carayon C, Massou M, Baron M, Baltas M. Mechanochemical synthesis and biological evaluation of novel isoniazid derivatives with potent antitubercular activity. **Molecules.** (2017) 22:1457.
17. Israyilova A, Buroni S, Forneris F, Scoffone VC, Shixaliyev NQ., Riccardi G, **Chiarelli LR[§]**. Biochemical characterization of glutamate racemase, a new candidate drug target against *Burkholderia cenocepacia* infections. **Plos One** (2016) 11:e0167350. ([§]**Corresponding author**)
18. **Chiarelli LR**, Mori G, Esposito M, Orena BS, Pasca MR. *New and old hot drug targets in tuberculosis.* **Curr Med Chem.** (2016) 23:3813-3846.
19. Meneghetti F, Villa S, Gelain A, Barlocco D, **Chiarelli LR**, Pasca MR, Costantino L. *Iron acquisition pathways as targets for antitubercular drugs.* **Curr Med Chem.** (2016) 23:4009-4026.
20. Scoffone VC*, **Chiarelli LR***, Makarov V*, Brackman G, Israyilova A, Azzalin A, Forneris F, Riabova O, Savina S, Coenye T, Riccardi G, Buroni S. *Discovery of new diketopiperazines inhibiting Burkholderia cenocepacia quorum sensing in vitro and in vivo.* **Sci. Rep.** 2016. 6:32487 (***First co-authors**) (**F1000Prime Recommended article**).
21. Spadaro F, Scoffone VC, **Chiarelli LR[§]**, Fumagalli M, Buroni S, Riccardi G, and Forneris F[§]. *The crystal structure of Burkholderia cenocepacia DfsA provides insights into substrate recognition and quorum sensing fatty acid biosynthesis.* **Biochemistry** (2016) 55:3241-50. ([§]**Co-corresponding author**)
22. Tiwari R, Miller PA, **Chiarelli LR**, Mori G, Šarkan M, Centárová I, Cho S, Mikušová K, Franzblau SG, Oliver AG and Miller MJ. *Design, Syntheses, and Anti-TB Activity of 1,3-Benzothiazinone Azide and Click Chemistry Products Inspired by BTZ043* **ACS Med Chem Lett.** (2016) 7:266-270 .
23. Mori G*, **Chiarelli LR***, Esposito M*, Makarov V*, Bellinzoni M, Hartkoorn RC, Degiacomi G, Boldrin F, Ekins S, de Jesus Lopes Ribeiro AL, Marino LB, Centárová I, Svetlíková Z, Blaško J, Kazakova E, Lepioshkin A, Barilone N, Zanoni G, Porta A, Fondi M, Fani R, Baulard AR, Mikušová K, Alzari PM, Manganelli R, de Carvalho LPS, Riccardi G, Cole ST, and Pasca MR. *Thiophenecarboxamide derivatives activated by EthA kill Mycobacterium tuberculosis by inhibiting the CTP synthetase PyrG.* **Chem. Biol.** (2015) 22: 917-927. (***First co-authors**)
24. Maggi M*, **Chiarelli LR***, Valentini G, and Scotti C. *Tackling Critical Catalytic Residues in Helicobacter pylori L-Asparaginase.* **Biomolecules** (2015) 5: 306-317. (***First co-authors**)
25. Maggi M*, **Chiarelli LR***, Valentini G, and Scotti C. *Engineering of Helicobacter pylori L-Asparaginase: Characterization of Two Functionally Distinct Groups of Mutants.* **PLoS ONE** (2015) 10: e0117025. (***First co-authors**)
26. Albesa-Jové D, Comino N, Tersa M, Mohorko E, Urresti S, Dainese E, **Chiarelli LR**, Pasca MR, Manganelli R, Makarov V, Riccardi G, Svergun DI, Glockshuber R, and Guerin ME. *The redox state regulates the conformation of Rv2466c to activate the antitubercular prodrug TP053.* **J Biol Chem.** (2015) 290: 31077–31089 .
27. Neres J*, Hartkoorn RC*, **Chiarelli LR***, Gadupudi R*, Pasca MR, Mori G, Farina D, Savina S, Makarov V, Kolly GS, Molteni E, Binda C, Dhar N, Ferrari S, Brodin P, Delorme V, Landry V, Ribeiro AL, Venturelli A, Saxena P, Pojer F, Carta A, Luciani R, Porta A, Zanoni G, De Rossi E, Costi MP, Riccardi G, and Cole ST. *2-Carboxyquinoxalines kill Mycobacterium tuberculosis through non-covalent inhibition of DprE1.* **ACS Chem Biol.** (2015) 10: 705–714 (***First co-authors**) (**F1000Prime Recommended article**)