

## G. Maga Publications (last five years)

- 1: Famiglini V, La Regina G, Coluccia A, Masci D, Brancale A, Badia R, Riveira Muñoz E, Este JA, Crespan E, Brambilla A, Maga G, Catalano M, Limatola C, Formica FRR, Cirilli R, Novellino E, Silvestri R. Chiral Indolylarylsulfone Non-Nucleoside Reverse Transcriptase Inhibitors as New Potent and Broad Spectrum anti-HIV-1 Agents. *J Med Chem.* 2017 Jun 19. doi: 10.1021/acs.jmedchem.6b01906. [Epub ahead of print]
- 2: Garbelli A, Riva V, Crespan E, Maga G. How to win the HIV-1 drug resistance hurdle race: running faster or jumping higher? *Biochem J.* 2017 Apr 26;474(10):1559-1577. doi: 10.1042/BCJ20160772.
- 3: Tassini S, Sun L, Lanko K, Crespan E, Langron E, Falchi F, Kissova M, Armijos-Rivera JI, Delang L, Mirabelli C, Neyts J, Pieroni M, Cavalli A, Costantino G, Maga G, Vergani P, Leyssen P, Radi M. Discovery of Multitarget Agents Active as Broad-Spectrum Antivirals and Correctors of Cystic Fibrosis Transmembrane Conductance Regulator for Associated Pulmonary Diseases. *J Med Chem.* 2017 Feb 23;60(4):1400-1416. doi: 10.1021/acs.jmedchem.6b01521.
- 4: Musumeci F, Fallacara AL, Brullo C, Grossi G, Botta L, Calandro P, Chiariello M, Kissova M, Crespan E, Maga G, Schenone S. Identification of new pyrrolo[2,3-d]pyrimidines as Src tyrosine kinase inhibitors in vitro active against Glioblastoma. *Eur J Med Chem.* 2017 Feb 15;127:369-378. doi: 10.1016/j.ejmech.2016.12.036.
- 5: Mentegari E, Crespan E, Bavagnoli L, Kissova M, Bertoletti F, Sabbioneda S, Imhof R, Sturla SJ, Nilforoushan A, Hübscher U, van Loon B, Maga G. Ribonucleotide incorporation by human DNA polymerase  $\eta$  impacts translesion synthesis and RNase H2 activity. *Nucleic Acids Res.* 2017 Mar 17;45(5):2600-2614. doi: 10.1093/nar/gkw1275.
- 6: Mentegari E, Kissova M, Bavagnoli L, Maga G, Crespan E. DNA Polymerases  $\lambda$  and  $\beta$ : The Double-Edged Swords of DNA Repair. *Genes (Basel).* 2016 Aug 31;7(9). pii: E57. doi: 10.3390/genes7090057.
- 7: Kissova M, Maga G, Crespan E. The human tyrosine kinase Kit and its gatekeeper mutant T670I, show different kinetic properties: Implications for drug design. *Bioorg Med Chem.* 2016 Oct 1;24(19):4555-62. doi: 10.1016/j.bmc.2016.07.059.
- 8: El-Moghazy SM, George RF, Osman EE, Elbatrawy AA, Kissova M, Colombo A, Crespan E, Maga G. Novel pyrazolo[3,4-d]pyrimidines as dual Src-Abl inhibitors active against mutant form of Abl and the leukemia K-562 cell line. *Eur J Med Chem.* 2016 Nov 10;123:1-13. doi: 10.1016/j.ejmech.2016.07.034.
- 9: Radi M, Schneider R, Fallacara AL, Botta L, Crespan E, Tintori C, Maga G, Kissova M, Calgani A, Richters A, Musumeci F, Rauh D, Schenone S. A cascade

screening approach for the identification of Bcr-Abl myristate pocket binders active against wild type and T315I mutant. *Bioorg Med Chem Lett.* 2016 Aug 1;26(15):3436-40. doi: 10.1016/j.bmcl.2016.06.051.

10: Brai A, Fazi R, Tintori C, Zamperini C, Bugli F, Sanguinetti M, Stigliano E, Esté J, Badia R, Franco S, Martinez MA, Martinez JP, Meyerhans A, Saladini F, Zazzi M, Garbelli A, Maga G, Botta M. Human DDX3 protein is a valuable target to develop broad spectrum antiviral agents. *Proc Natl Acad Sci U S A.* 2016 May 10;113(19):5388-93. doi: 10.1073/pnas.1522987113.

11: Crespan E, Furrer A, Rösinger M, Bertoletti F, Mentegari E, Chiapparini G, Imhof R, Ziegler N, Sturla SJ, Hübscher U, van Loon B, Maga G. Impact of ribonucleotide incorporation by DNA polymerases  $\beta$  and  $\lambda$  on oxidative base excision repair. *Nat Commun.* 2016 Feb 26;7:10805. doi: 10.1038/ncomms10805.

12: Tintori C, Brai A, Dasso Lang MC, Deodato D, Greco AM, Bizzarri BM, Cascone L, Casian A, Zamperini C, Dreassi E, Crespan E, Maga G, Vanham G, Ceresola E, Canducci F, Ariën KK, Botta M. Development and in Vitro Evaluation of a Microbicide Gel Formulation for a Novel Non-Nucleoside Reverse Transcriptase Inhibitor Belonging to the N-Dihydroalkyloxybenzyloxypyrimidines (N-DABOs) Family. *J Med Chem.* 2016 Mar 24;59(6):2747-59. doi: 10.1021/acs.jmedchem.5b01979.

13: Llona-Minguez S, Höglund A, Jacques SA, Johansson L, Calderón-Montaña JM, Claesson M, Loseva O, Valerie NC, Lundbäck T, Piedrafita J, Maga G, Crespan E, Meijer L, Burgos Morón E, Baranczewski P, Hagbjörk AL, Svensson R, Wiita E, Almlöf I, Visnes T, Jeppsson F, Sigmundsson K, Jensen AJ, Artursson P, Jemth AS, Stenmark P, Warpman Berglund U, Scobie M, Helleday T. Discovery of the First Potent and Selective Inhibitors of Human dCTP Pyrophosphatase 1. *J Med Chem.* 2016 Feb 11;59(3):1140-8. doi: 10.1021/acs.jmedchem.5b01741.

14: Fazi R, Tintori C, Brai A, Botta L, Selvaraj M, Garbelli A, Maga G, Botta M. Homology Model-Based Virtual Screening for the Identification of Human Helicase DDX3 Inhibitors. *J Chem Inf Model.* 2015 Nov 23;55(11):2443-54. doi: 10.1021/acs.jcim.5b00419.

15: Bavagnoli L, Cucuzza S, Campanini G, Rovida F, Paolucci S, Baldanti F, Maga G. The novel influenza A virus protein PA-X and its naturally deleted variant show different enzymatic properties in comparison to the viral endonuclease PA. *Nucleic Acids Res.* 2015 Oct 30;43(19):9405-17. doi: 10.1093/nar/gkv926. Epub 2015

16: Spallarossa A, Caneva C, Caviglia M, Alfei S, Butini S, Campiani G, Gemma S, Brindisi M, Zisterer DM, Bright SA, Williams CD, Crespan E, Maga G, Sanna G, Delogu I, Collu G, Loddo R. Unconventional Knoevenagel-type indoles: Synthesis and cell-based studies for the identification of pro-apoptotic agents. *Eur J Med Chem.* 2015 Sep 18;102:648-60. doi: 10.1016/j.ejmech.2015.08.009.

- 17: Vincetti P, Caporuscio F, Kaptein S, Gioiello A, Mancino V, Suzuki Y, Yamamoto N, Crespan E, Lossani A, Maga G, Rastelli G, Castagnolo D, Neyts J, Leyssen P, Costantino G, Radi M. Discovery of Multitarget Antivirals Acting on Both the Dengue Virus NS5-NS3 Interaction and the Host Src/Fyn Kinases. *J Med Chem.* 2015 Jun 25;58(12):4964-75. doi: 10.1021/acs.jmedchem.5b00108.
- 18: Tintori C, La Sala G, Vignaroli G, Botta L, Fallacara AL, Falchi F, Radi M, Zamperini C, Dreassi E, Dello Iacono L, Orioli D, Biamonti G, Garbelli M, Lossani A, Gasparrini F, Tuccinardi T, Laurenzana I, Angelucci A, Maga G, Schenone S, Brullo C, Musumeci F, Desogus A, Crespan E, Botta M. Studies on the ATP Binding Site of Fyn Kinase for the Identification of New Inhibitors and Their Evaluation as Potential Agents against Tauopathies and Tumors. *J Med Chem.* 2015 Jun 11;58(11):4590-609. doi: 10.1021/acs.jmedchem.5b00140.
- 19: Crespan E, Hübscher U, Maga G. Expansion of CAG triplet repeats by human DNA polymerases  $\lambda$  and  $\beta$  in vitro, is regulated by flap endonuclease 1 and DNA ligase 1. *DNA Repair (Amst).* 2015 May;29:101-11. doi: 10.1016/j.dnarep.2015.01.005.
- 20: Tintori C, Fallacara AL, Radi M, Zamperini C, Dreassi E, Crespan E, Maga G, Schenone S, Musumeci F, Brullo C, Richters A, Gasparrini F, Angelucci A, Festuccia C, Delle Monache S, Rauh D, Botta M. Combining X-ray crystallography and molecular modeling toward the optimization of pyrazolo[3,4-d]pyrimidines as potent c-Src inhibitors active in vivo against neuroblastoma. *J Med Chem.* 2015 Jan 8;58(1):347-61. doi: 10.1021/jm5013159.
- 21: Famiglini V, La Regina G, Coluccia A, Pelliccia S, Brancale A, Maga G, Crespan E, Badia R, Riveira-Muñoz E, Esté JA, Ferretti R, Cirilli R, Zamperini C, Botta M, Schols D, Limongelli V, Agostino B, Novellino E, Silvestri R. Indolylarylsulfones carrying a heterocyclic tail as very potent and broad spectrum HIV-1 non-nucleoside reverse transcriptase inhibitors. *J Med Chem.* 2014 Dec 11;57(23):9945-57. doi: 10.1021/jm5011622.
- 22: Rotili D, Tarantino D, Nawrozki MB, Babushkin AS, Botta G, Marrocco B, Cirilli R, Menta S, Badia R, Crespan E, Ballante F, Ragno R, Esté JA, Maga G, Mai A. Exploring the role of 2-chloro-6-fluoro substitution in 2-alkylthio-6-benzyl-5-alkylpyrimidin-4(3H)-ones: effects in HIV-1-infected cells and in HIV-1 reverse transcriptase enzymes. *J Med Chem.* 2014 Jun 26;57(12):5212-25. doi: 10.1021/jm500284x.
- 23: Vignaroli G, Zamperini C, Dreassi E, Radi M, Angelucci A, Sanità P, Crespan E, Kissova M, Maga G, Schenone S, Musumeci F, Botta M. Pyrazolo[3,4-d]pyrimidine Prodrugs: Strategic Optimization of the Aqueous Solubility of Dual Src/Abl Inhibitors. *ACS Med Chem Lett.* 2013 May 20;4(7):622-6. doi: 10.1021/ml4000782.
- 24: Famiglini V, La Regina G, Coluccia A, Pelliccia S, Brancale A, Maga G, Crespan E, Badia R, Clotet B, Esté JA, Cirilli R, Novellino E, Silvestri R. New indolylarylsulfones as highly potent and broad spectrum HIV-1 non-nucleoside

reverse transcriptase inhibitors. *Eur J Med Chem.* 2014 Jun 10;80:101-11. doi: 10.1016/j.ejmech.2014.04.027.

25: Khan A, Garbelli A, Grossi S, Florentin A, Batelli G, Acuna T, Zolla G, Kaye Y, Paul LK, Zhu JK, Maga G, Grafi G, Barak S. The Arabidopsis STRESS RESPONSE SUPPRESSOR DEAD-box RNA helicases are nucleolar- and chromocenter-localized proteins that undergo stress-mediated relocalization and are involved in epigenetic gene silencing. *Plant J.* 2014 Jul;79(1):28-43. doi: 10.1111/tpj.12533.

26: Vignaroli G, Mencarelli M, Sementa D, Crespan E, Kissova M, Maga G, Schenone S, Radi M, Botta M. Exploring the chemical space around the privileged pyrazolo[3,4-d]pyrimidine scaffold: toward novel allosteric inhibitors of T315I-mutated Abl. *ACS Comb Sci.* 2014 Apr 14;16(4):168-75. doi:10.1021/co500004e.

27: Maga G, Crespan E, Markkanen E, Imhof R, Furrer A, Villani G, Hübscher U, van Loon B. DNA polymerase δ-interacting protein 2 is a processivity factor for DNA polymerase λ during 8-oxo-7,8-dihydroguanine bypass. *Proc Natl Acad Sci U S A.* 2013 Nov 19;110(47):18850-5. doi: 10.1073/pnas.1308760110.

28: Tomasso A, Casari G, Maga G. What makes y family pols potential candidates for molecular targeted therapies and novel biotechnological applications. *Curr Mol Med.* 2014 Jan;14(1):96-114. Review. PubMed PMID: 24160487.

29: Gemma S, Brogi S, Novellino E, Campiani G, Maga G, Brindisi M, Butini S. HCV-targeted antivirals: current status and future challenges. *Curr Pharm Des.* 2014;20(21):3445-64. Review. PubMed PMID: 24001232.

30: Costi R, Crucitti GC, Pescatori L, Messore A, Scipione L, Tortorella S, Amoroso A, Crespan E, Campiglia P, Maresca B, Porta A, Granata I, Novellino E, Gouge J, Delarue M, Maga G, Di Santo R. New nucleotide-competitive non-nucleoside inhibitors of terminal deoxynucleotidyl transferase: discovery, characterization, and crystal structure in complex with the target. *J Med Chem.* 2013 Sep 26;56(18):7431-41. doi: 10.1021/jm4010187.

31: Tintori C, Laurenzana I, La Rocca F, Falchi F, Carraro F, Ruiz A, Esté JA, Kissova M, Crespan E, Maga G, Biava M, Brullo C, Schenone S, Botta M. Identification of Hck inhibitors as hits for the development of antileukemia and anti-HIV agents. *ChemMedChem.* 2013 Aug;8(8):1353-60. doi: 10.1002/cmdc.201300204.

32: Radi M, Tintori C, Musumeci F, Brullo C, Zamperini C, Dreassi E, Fallacara AL, Vignaroli G, Crespan E, Zanolli S, Laurenzana I, Filippi I, Maga G, Schenone S, Angelucci A, Botta M. Design, synthesis, and biological evaluation of pyrazolo[3,4-d]pyrimidines active in vivo on the Bcr-Abl T315I mutant. *J Med Chem.* 2013 Jul 11;56(13):5382-94. doi: 10.1021/jm400233w.

- 33: Amoroso A, Maga G, Daghia M. Cytotoxicity of  $\alpha$ -dicarbonyl compounds submitted to in vitro simulated digestion process. *Food Chem.* 2013 Oct 15;140(4):654-9. doi: 10.1016/j.foodchem.2012.10.063.
- 34: Mori M, Tintori C, Christopher RS, Radi M, Schenone S, Musumeci F, Brullo C, Sanità P, Delle Monache S, Angelucci A, Kissova M, Crespan E, Maga G, Botta M. A combination strategy to inhibit Pim-1: synergism between noncompetitive and ATP-competitive inhibitors. *ChemMedChem.* 2013 Mar;8(3):484-96. doi: 10.1002/cmdc.201200480.
- 35: Bertoletti F, Crespan E, Maga G. Tyrosine kinases as essential cellular cofactors and potential therapeutic targets for human immunodeficiency virus infection. *Cell Mol Biol (Noisy-le-grand).* 2012 Dec 22;58(1):31-43.
- 36: Maga G, Veljkovic N, Crespan E, Spadari S, Prljic J, Perovic V, Glisic S, Veljkovic V. New in silico and conventional in vitro approaches to advance HIV drug discovery and design. *Expert Opin Drug Discov.* 2013 Jan;8(1):83-92. doi: 10.1517/17460441.2013.741118. Epub 2012 Nov 20.
- 37: Zucca E, Bertoletti F, Wimmer U, Ferrari E, Mazzini G, Khoronenkova S, Grosse N, van Loon B, Dianov G, Hübscher U, Maga G. Silencing of human DNA polymerase  $\lambda$  causes replication stress and is synthetically lethal with an impaired S phase checkpoint. *Nucleic Acids Res.* 2013 Jan 7;41(1):229-41. doi: 10.1093/nar/gks1016.
- 38: Crespan E, Pasi E, Imoto S, Hübscher U, Greenberg MM, Maga G. Human DNA polymerase  $\beta$ , but not  $\lambda$ , can bypass a 2-deoxyribonolactone lesion together with proliferating cell nuclear antigen. *ACS Chem Biol.* 2013 Feb 15;8(2):336-44. doi: 10.1021/cb300542k.
- 39: La Regina G, Coluccia A, Brancale A, Piscitelli F, Famiglini V, Cosconati S, Maga G, Samuele A, Gonzalez E, Clotet B, Schols D, Esté JA, Novellino E, Silvestri R. New nitrogen containing substituents at the indole-2-carboxamide yield high potent and broad spectrum indolylarylsulfone HIV-1 non-nucleoside reverse transcriptase inhibitors. *J Med Chem.* 2012 Jul 26;55(14):6634-8. doi: 10.1021/jm300477h.
- 40: Samuele A, Crespan E, Garbelli A, Bavagnoli L, Maga G. The power of enzyme kinetics in the drug development process. *Curr Pharm Biotechnol.* 2013;14(5):551-60. Review. PubMed PMID: 22429137.
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- 42: Crespan E, Czabany T, Maga G, Hübscher U. Microhomology-mediated DNA strand annealing and elongation by human DNA polymerases  $\lambda$  and  $\beta$  on normal and repetitive DNA sequences. *Nucleic Acids Res.* 2012 Jul;40(12):5577-90. doi: 10.1093/nar/gks186.

- 43: Radi M, Pagano M, Franchi L, Castagnolo D, Schenone S, Casaluce G, Zamperini C, Dreassi E, Maga G, Samuele A, Gonzalo E, Clotet B, Esté JA, Botta M. Synthesis, biological activity, and ADME properties of novel S-DABOs/N-DABOs as HIV reverse transcriptase inhibitors. *ChemMedChem*. 2012 May;7(5):883-96. doi: 10.1002/cmdc.201200056.
- 44: Crespan E, Czabany T, Maga G, Hübscher U. Microhomology-mediated DNA strand annealing and elongation by human DNA polymerases  $\lambda$  and  $\beta$  on normal and repetitive DNA sequences. *Nucleic Acids Res*. 2012 Jul;40(12):5577-90. doi:10.1093/nar/gks186.
- 45: Radi M, Falchi F, Garbelli A, Samuele A, Bernardo V, Paolucci S, Baldanti F, Schenone S, Manetti F, Maga G, Botta M. Discovery of the first small molecule inhibitor of human DDX3 specifically designed to target the RNA binding site: towards the next generation HIV-1 inhibitors. *Bioorg Med Chem Lett*. 2012 Mar 1;22(5):2094-8. doi: 10.1016/j.bmcl.2011.12.135.
- 46: Manfroni G, Meschini F, Barreca ML, Leyssen P, Samuele A, Iraci N, Sabatini S, Massari S, Maga G, Neyts J, Cecchetti V. Pyridobenzothiazole derivatives as new chemotype targeting the HCV NS5B polymerase. *Bioorg Med Chem*. 2012 Jan 15;20(2):866-76. doi: 10.1016/j.bmc.2011.11.061.