OMB No. 0925-0001 and 0925-0002 (Rev. 11/16 Approved Through 10/31/2018)

BIOGRAPHICAL SKETCH

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NAME: Stefano Alcaro

eRA COMMONS USER NAME (credential, e.g., agency login):

POSITION TITLE: Full Professor of Medicinal Chemistry

EDUCATION/TRAINING *(Begin with baccalaureate or other initial professional education, such as nursing, include postdoctoral training and residency training if applicable. Add/delete rows as necessary.)*

INSTITUTION AND LOCATION	DEGREE *(if applicable)*	Completion Date MM/YYYY	FIELD OF STUDY
University “La Sapienza”, Rome (Italy)	B.S.	07/1990	Medicinal Chemistry
University “La Sapienza”, Rome (Italy)	Ph.D	11/1993	Pharmacology, Pharmacognosy and Toxicology
Columbia University, NYC (USA)	Postdoctoral	10/1994	Computational Chemistry
University “La Sapienza”, Rome (Italy)	Second B.S.	07/1995	Pharmacy

A. Personal Statement

His scientific interests are related to the development of new molecular modeling tools useful in the drug discovery process and to the application of them and other methods, mainly in the design of anticancer and antiviral agents.

B. Positions and Honors

1996-2002 Assistant Professor of Medicinal Chemistry, Faculty of Pharmacy at University "Magna Græcia" of Catanzaro (Italy);
2002-2011 Associate Professor of Medicinal Chemistry, Faculty of Pharmacy at University "Magna Græcia" of Catanzaro (Italy);
2011- Full Professor of Medicinal Chemistry, Department of Health Sciences at University "Magna Græcia" of Catanzaro (Italy);
2013- Coordinator of Life Science PhD Program at University "Magna Græcia" of Catanzaro;
2015- “Coordinator-Elect” of the Paul Ehrlich Euro-PhD Network for the period 2019-2021;
2016- Chair of the H2020 COST Action MuTaLig CA15135 (www.mutalig.eu);
2013-2016 Outstanding reviewer certificate for Journal of Medicinal Chemistry by the American Chemical Society

C. Contributions to Science

He is co-author of more than 170 peer-reviewed manuscripts and numerous communications presented at national and international meetings.
Bibliometric indexes, May 2017:
WOS H-index = 32
Scopus H-Index = 33
Google Scholar H-index = 38
TIS in Chemistry Area at the www.topitalianscientists.org
Evaluation of research quality (Italian VQR 2004-2010) = AAA (out of 3 products)
Evaluation of research quality (Italian VQR 2011-2014) = AA (out of 2 products)

List of 2016-2017 published/accepted papers

1. Alteri, C.; Surdo, M.; Di Maio, V.C.; Di Santo, F.; Costa, G.; Parrotta, L.; Romeo, I.; Gori, C.; Santoro, M.M.; Fedele, V.; Carta, S.; Continenza, F.; Pinnetti, C.; Bellagamba, R.; Liuzzi, G.; Orchi, N.; Latini, A.; Bertoli, A.; Girardi, E.; **Alcaro, S**.; Giuliani, M.; Petrosillo, N.; Andreoni, M.; Antinori, A.; Monforte, A.D.; Ceccherini-Silberstein, F.; Artese, A.; Perno, C.F.; Svicher, V. The HIV-1 reverse transcriptase polymorphism A98S improves the response to tenofovir disoproxil fumarate + emtricitabine-containing HAART both in vivo and in vitro. *Journal of Global Antimicrobial Resistance*, **2016,** *7,* 1-7. DOI: 10.1016/j.jgar.2016.06.005
2. Carradori, S.; Gidaro, M.C.; Petzer, A.; Costa, G.; Guglielmi, P.; Chimenti, P.; **Alcaro, S**.; Petzer, J.P. Inhibition of Human Monoamine Oxidase: Biological and Molecular Modeling Studies on Selected Natural Flavonoids. *Journal of Agricultural and Food Chemistry*, **2016,** *64,* 9004-9011. DOI: 10.1021/acs.jafc.6b03529
3. Talarico, C.; Dattilo, V.; D'Antona, L.; Menniti, M.; Bianco, C.; Ortuso, F.; **Alcaro, S**.; Schenone, S.; Perrotti, N.; Amato, R. SGK1, the New Player in the Game of Resistance: Chemo-Radio Molecular Target and Strategy for Inhibition. *Cellular Physiology and Biochemistry*, **2016,** *39,* 1863-1876. DOI: 10.1159/000447885
4. Costa, G.; Rocca, R.; Moraca, F.; Talarico, C.; Romeo, I.; Ortuso, F.; **Alcaro, S**.; Artese, A. A Comparative Docking Strategy to Identify Polyphenolic Derivatives as Promising Antineoplastic Binders of G-quadruplex DNA c-myc and bcl-2 Sequences. *Molecular Informatics*, **2016,** 391-402. DOI: 10.1002/minf.201501040
5. Rocca, R.; Costa, G.; Artese, A.; Parrotta, L.; Ortuso, F.; Maccioni, E.; Pinato, O.; Greco, M.L.; Sissi, C.; **Alcaro, S**.; Distinto, S.; Moraca, F. Hit Identification of a Novel Dual Binder for h-telo/c-myc G-Quadruplex by a Combination of Pharmacophore Structure-Based Virtual Screening and Docking Refinement. *ChemMedChem*, **2016,** *11,* 1721-1733. DOI: 10.1002/cmdc.201600053
6. Rocca, R.; Costa, G.; Artese, A.; Parrotta, L.; Ortuso, F.; Maccioni, E.; Pinato, O.; Greco, M.L.; Sissi, C.; **Alcaro, S**.; Distinto, S.; Moraca, F. Back Cover: Hit Identification of a Novel Dual Binder for h-telo/c-myc G-Quadruplex by a Combination of Pharmacophore Structure-Based Virtual Screening and Docking Refinement. *ChemMedChem,* **2016,** *11,* 1875. DOI: 10.1002/cmdc.201600393
7. Desideri, N.; Proietti Monaco, L.; Fioravanti, R.; Biava, M.; Yáñez, M.; **Alcaro, S**.; Ortuso, F. (E)-3-Heteroarylidenechroman-4-ones as potent and selective monoamine oxidase-B inhibitors. *European Journal of Medicinal Chemistry*, **2016,** *117,* 292-300. DOI: 10.1016/j.ejmech.2016.03.081
8. Costa, G.; Gidaro, M.C.; Vullo, D.; Supuran, C.T.; **Alcaro, S**. Active components of essential oils as anti-obesity potential drugs investigated by in silico techniques *Journal of Agricultural and Food Chemistry*, **2016,** 64 (26), pp. 5295-5300. DOI: 10.1021/acs.jafc.6b02004
9. Reis, J.; Cagide, F.; Chavarria, D.; Silva, T.; Fernandes, C.; Gaspar, A.; Uriarte, E.; Remião, F.; **Alcaro, S**.; Ortuso, F.; Borges, F. Discovery of New Chemical Entities for Old Targets: Insights on the Lead Optimization of Chromone-Based Monoamine Oxidase B (MAO-B) Inhibitors. *Journal of Medicinal Chemistry*, **2016,** *59,* 5879-5893. DOI: 10.1021/acs.jmedchem.6b00527
10. Varela, C.L.; Amaral, C.; Correia-Da-Silva, G.; Costa, S.C.; Carvalho, R.A.; Costa, G.; **Alcaro, S**.; Teixeira, N.A.A.; Tavares-Da-Silva, E.J.; Roleira, F.M.F. Exploring new chemical functionalities to improve aromatase inhibition of steroids. *Bioorganic and Medicinal Chemistry*, **2016,** *24,* 2823-2831. DOI: 10.1016/j.bmc.2016.04.056
11. Aiello, F.; Badolato, M.; Pessina, F.; Sticozzi, C.; Maestrini, V.; Aldinucci, C.; Luongo, L.; Guida, F.; Ligresti, A.; Artese, A.; Allarà, M.; Costa, G.; Frosini, M.; Schiano Moriello, A.; De Petrocellis, L.; Valacchi, G.; **Alcaro, S**.; Maione, S.; Di Marzo, V.; Corelli, F.; Brizzi, A. Design and Synthesis of New Transient Receptor Potential Vanilloid Type-1 (TRPV1) Channel Modulators: Identification, Molecular Modeling Analysis, and Pharmacological Characterization of the N-(4-Hydroxy-3-methoxybenzyl)-4-(thiophen-2-yl)butanamide, a Small Molecule Endowed with Agonist TRPV1 Activity and Protective Effects against Oxidative Stress. *ACS Chemical Neuroscience*, **2016,** *7,* 737-748. DOI: 10.1021/acschemneuro.5b00333
12. Gaudio, E.; Paduano, F.; Ngankeu, A.; Ortuso, F.; Lovat, F.; Pinton, S.; D'Agostino, S.; Zanesi, N.; Aqeilan, R.I.; Campiglia, P.; Novellino, E.; **Alcaro, S**.; Croce, C.M.; Trapasso, F. A Fhit-mimetic peptide suppresses annexin A4-mediated chemoresistance to paclitaxel in lung cancer cells. *Oncotarget*, **2016,** *7,* 29927-29936. DOI: 10.18632/oncotarget.9179
13. Talarico, C.; Dattilo, V.; Lucia D'Antona, Barone, A.; Amodio, N.; Belviso, S.; Musumeci, F.; Abbruzzese, C.; Bianco, C.; Trapasso, F.; Schenone, S.; **Alcaro, S**.; Ortuso, F.; Florio, T.; Paggi, M.G.; Perrotti, N.; Amato, R. SI113, a SGK1 inhibitor, potentiates the effects of radiotherapy, modulates the

response to oxidative stress and induces cytotoxic autophagy in human glioblastoma multiforme cells. *Oncotarget*, **2016,** *7,* 15868-15884. DOI: 10.18632/oncotarget.7520

14. Kaserer, T.; Rigo, R.; Schuster, P.; **Alcaro, S**.; Sissi, C.; Schuster, D. Optimized Virtual Screening Workflow for the Identification of Novel G-Quadruplex Ligands. *Journal of Chemical Information and Modeling,* **2016,** *56,* 484-500. DOI: 10.1021/acs.jcim.5b00658
15. Gidaro, M.C.; **Alcaro, S**.; Secci, D.; Rivanera, D.; Mollica, A.; Agamennone, M.; Giampietro, L.; Carradori, S. Identification of new anti-Candida compounds by ligand-based pharmacophore virtual screening. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2016,** 1-4. DOI: 10.3109/14756366.2016.1156103
16. Gidaro, M.C.; Astorino, C.; Petzer, A.; Carradori, S.; Alcaro, F.; Costa, G.; Artese, A.; Rafele, G.; Russo, F.M.; Petzer, J.P.; **Alcaro, S**. Kaempferol as Selective Human MAO-A Inhibitor: Analytical Detection in Calabrian Red Wines, Biological and Molecular Modeling Studies. *Journal of Agricultural and Food Chemistry*, **2016,** *64,* 1394-1400. DOI: 10.1021/acs.jafc.5b06043
17. Distinto, S.; Meleddu, R.; Yanez, M.; Cirilli, R.; Bianco, G.; Sanna, M.L.; Arridu, A.; Cossu, P.; Cottiglia, F.; Faggi, C.; Ortuso, F.; **Alcaro, S**.; Maccioni, E. Drug design, synthesis, in vitro and in silico evaluation of selective monoaminoxidase B inhibitors based on 3-acetyl-2-dichlorophenyl-5-aryl-2,3-dihydro-1,3,4-oxadiazole chemical scaffold. *European Journal of Medicinal Chemistry*, **2016,** *108,* 542-552. DOI: 10.1016/j.ejmech.2015.12.026
18. Doria, F.; Nadai, M.; Costa, G.; Sattin, G.; Gallati, C.; Bergamaschi, G.; Moraca, F.; **Alcaro, S**.; Freccero, M.; Richter, S.N. Extended Naphthalene Diimides with Donor/Acceptor Hydrogen-Bonding Properties Targeting G-Quadruplex Nucleic Acids. *European Journal of Organic Chemistry*, **2016,** *28*, 4824-4833. DOI: 10.1002/ejoc.201600757
19. Corona, A.; Meleddu, R.; Esposito, F.; Distinto, S.; Bianco, G.; Masaoka, T.; Maccioni, E.; Menéndez-Arias, L.; **Alcaro, S**.; Le Grice, S.F.J.; Tramontano, E. Ribonuclease H/DNA polymerase HIV-1 reverse transcriptase dual inhibitor: Mechanistic studies on the allosteric mode of action of isatin-based compound RMNC6 *PLoS ONE*, **2016,** *11*, e0147225, DOI: 10.1371/journal.pone.0147225
20. Meleddu, R.; Distinto, S.; Cirilli, R.; **Alcaro, S.**; Yanez, M.; Sanna, M.L.; Corona, A.; Melis, C.; Bianco, G., Matyus, P.; Cottiglia, F.; Maccioni, E. Through scaffold modification to 3,5-diaryl-4,5-dihydroisoxazoles: new potent and selective inhibitors of monoamine oxidase B. *J Enzyme Inhib Med Chem.* **2017**, *32*, 264-270. doi: 10.1080/14756366.2016.1247061
21. Moraca, F.; Amato, J.; Ortuso, F.; Artese, A.; Pagano, B.; Novellino, E.; **Alcaro, S**.; Parrinello, M.; Limongelli, V. Energetics and structural characterization of ligand binding to DNA: when berberine meets telomeric G-quadruplex. *PNAS*, **2017,** *114*, E2136-E2145
22. Milelli, A.; Marchetti, C.; Greco, ML.; Moraca, F.; Costa, G.; Turrini, E.; Catanzaro, E.; Betari, N.; Calcabrini, C.; Sissi, C.; Alcaro, S.; Fimognari, C.; Tumiatti, V.; Minarini, A..; Naphthalene diimide-polyamine hybrids as antiproliferative agents: Focus on the architecture of the polyamine chains. *Eur J Med Chem.* **2017,** *128*, 107-122
23. Sonar, VP.; Corona, A.; Distinto, S.; Maccioni, E.; Meleddu, R.; Fois, B.; Floris, C.; Malpure, NV.; Alcaro, S.; Tramontano, E.; Cottiglia, F. Natural product-inspired esters and amides of ferulic and caffeic acid as dual inhibitors of HIV-1 reverse transcriptase. *Eur J Med Chem.* **2017**, *130*, 248-260
24. Rocca, R.; Talarico, C.; Moraca, F.; Costa, G.; Romeo, I.; Ortuso, F.; Alcaro, S.; Artese, A. Molecular recognition of a carboxy pyridostatin towards G-quadruplex structures: why does it prefer RNA? *Chem Biol Drug Des.* **2017**, accepted for publication

Additional info at www.researchgate.net/profile/Stefano_Alcaro

D. Additional Information: Research Support and/or Scholastic Performance

Grants and funding resources

1997 NATO grant in collaboration with Prof. R. S. Coleman Ohio-State University (Columbus, USA) on a research computational project in anticancer field. Role: Co-Investigator

2000 Young research project CNR Agenzia 2000: "Computational study of interaction between biological active compounds and nucleic acids". Role: PI

2001 ST fellowship FIRC in the Prof. R.S Coleman's lab Ohio-State University Columbus (OH). Role: PI

2001 industrial grant on the project "Computational study of taxane based antitumor agents" Role: PI

2002 industrial grant on the project "Computational study of colchicine derivatives" Role: PI

2007 Grant MIUR on the project "Drug design, synthesis and biological evaluation of novel cyclooxygenase inhibitors". Role: PI of local unit

2008 Grant FIRB on the project "New agents in the specific anticancer therapy". Role: PI of local unit
2009 Grant MIUR on the project "Rational drug design and synthesis of ligands able to recognize the G-quadruplex motif of nucleic acids" Role: PI of local unit
2013 PON industrial grant for an advanced training course of young researchers. Role: Coordinator
2015 PON industrial grant for research activities - project “In silico studies of bioactive compounds”. Role: PI
2016 COST Action CA15135 starting activities www.cost.eu/COST_Actions/ca/CA15135 (running project). Role: Chair

Catanzaro, May 17th 2017 Prof. Stefano Alcaro