

Personal Data



citizenship:

Italian

DoB.:

09/10/1986

cell phone:

+39 328 5674705

email:

aspinello@sissa.it

Professional Experience

CNR-IOM Democritos National Simulation Center and International School for Advanced Studies (SISSA).

PI - Awarded with a "Mario e Valeria Rindi" FIRC-AIRC fellowship for Italy

04/2019 – 03/2022

CNR-IOM Democritos National Simulation Center and International School for Advanced Studies (SISSA).

Post Doctoral Fellow (Advisor Dr. Alessandra Magistrato).

05/2016 – 03/2019

Research Fellowships at European Research Institutions

Université de Lorraine, Structure and Reactivity of Complex Molecular Systems (SRSMC). COST Short-Term Scientific Mission and Invited Researcher (tutor Dr. Antonio Monari).

06/2015 – 07/2015

02/2016 – 02/2016

University of Groningen, Research Institute of Pharmacy. COST Short-Term Scientific Mission (tutor Prof. Angela Casini).

03/2015 – 05/2015

TU Braunschweig, Institut für Organische Chemie. Visiting PhD student (tutor Prof. Jörg Grunenberg).

03/2013 – 12/2013

Education

University of Palermo, PhD in Chemistry (tutor Prof. Giampaolo Barone).
Title: Interaction of Metal Complexes with G-quadruplex DNA.
Awarded with the Doctor Europaeus title.

01/2013 – 12/2015

University of Palermo, Master degree in Chemistry, summa cum laude.

01/2010 – 03/2012

Honours and Awards

Funding as Principal Investigator

- 2020: IscraB-SPLSeq - Tackling the molecular basis of critical splice sites recognition by the SF3b splicing factor via all-atoms simulations, approved on MARCONI100 machine of CINECA, Bologna (1.8 million core/h).
- 2019: IscraB-SPLMod - Unravelling the mechanism of action of novel small-molecule splicing modulators: A step forward towards precision medicine of hematologic cancers, approved on GALILEO machine of CINECA, Bologna (1.8 million core/h).
- 2018: "Mario e Valeria Rindi" FIRC-AIRC Fellowship for Italy (75k €).
- 2017: IscraB-TyrSwitc - The role of tyrosine 361 phosphorylation on aromatase catalytic activity, approved on MARCONI machine of CINECA, Bologna (1.0 million core/h).
- 2016: IscraC-METEOR - Modulation of estrogen production targeting the human aromatase/cytochrome reductase adduct interface, approved on MARCONI machine of CINECA, Bologna (200k core/h).

Awards and Travel Grant

- 2019 - Italfarmaco and SCI (Italian Chemical Society, Chemistry of the Biological System Division) Award "Gastone De Santis" (2500 €).
- 2018 - SCI (Chemistry of the Biological System Division) Fellowship to attend to "National Congress of the Division of Chemistry of Biological Systems", Siena, Italy.
- 2017 - SIBPA (Italian Society of Pure and Applied Biophysics) Fellowship to attend to "11th European Biophysical Societies' Association (EBSA) Congress", Edinburgh, United Kingdom.

- 2015 - COST Short-Term Scientific Mission (Université de Lorraine, France) (1800 €).
- 2015 - COST Short-Term Scientific Mission (University of Groningen, Netherlands) (2300 €).
- 2015 - EBSA (European Biophysical Societies' Association) Fellowship to attend to "10th European Biophysics Congress", Dresden, Germany.
- 2013 - PRACE (Partnership for Advanced Computing in Europe) Fellowship to attend to "Conference on Scientific Computing - CSC 2013", Paphos, Cyprus.

Speaking Engagement

- 2019 - National Congress of the Division of Chemistry of Biological Systems, Siena, Italy.
- 2019 - 6th Computationally Driven Drug Discovery (CDDD) Meeting, Rome, Italy.
- 2018 - National Congress of the Division of Chemistry of Biological Systems, Caserta, Italy.
- 2017 - 5th Computationally Driven Drug Discovery (CDDD) Meeting, Milan, Italy.
- 2016 - 3rd International Symposium on Functional Metal Complexes that Bind to Biomolecules, Palma, Spain.
- 2014 - XXII meeting of the "Italian Biophysical Society", Palermo, Italy.

Teaching

- Lab Assistant in "Summer School on Atomistic Simulation Techniques for Material Science, Nanotechnology, and Biophysics", 2017, Trieste.
<http://www.democritos.it/school2017/index.php/Main/HomePage>

Member of the Topic Editorial Board of *Molecules* (ISSN 1420-3049).

I am the author of 40 peer-reviewed papers published in international journals, (plus 2 are submitted) with 753 citations and H-index 15 (Google Scholar).

Publications

Submitted

- J. Caciolla, S. Martini, A. Spinello, M. Pavlin, F. Simonelli, A. Bisi, N. Zaffaroni, S. Gobbi, A. Magistrato Dual acting compounds targeting aromatase and estrogen receptor offer unprecedented therapeutic opportunities to counteract estrogen responsive breast cancer
- J. Xu, F. Simonelli, X. Li, A. Spinello, S. Laporte, V. Torre, A. Magistrato Molecular mechanisms of the blockage of glioblastoma motility

2020

- A. Spinello, A. Saltalamacchia, A. Magistrato: Is the Rigidity of SARS-CoV-2 Spike Receptor-Binding Motif the Hallmark for Its Enhanced Infectivity? Insights from All-Atom Simulations *J. Phys. Chem. Lett.*, 11 (2020) 4785.
- A. Spinello, J. Caciolla, S. Martini, A. Bisi, N. Zaffaroni, S. Gobbi, A. Magistrato: Targeting Orthosteric and Allosteric Pockets of Aromatase via Dual-Mode Novel Azole Inhibitors. *ACS J. Med. Chem. Lett.*, 11 (2020) 732.
- I. Ritacco, A. Saltalamacchia, A. Spinello, E. Ippoliti, A. Magistrato: Impact of Cytochrome Reductase Binding on its partner CYP450s: Insights from all-atoms Simulations of the Aromatase Enzyme. *J. Phys. Chem. Lett.*, 11 (2020) 1189.
- P. Janos, A. Spinello, A. Magistrato: All-atom simulations to studying metallodrugs/target interactions *Curr. Opin. Chem. Biol.*, 61 (2020) 1.
- G. Palermo, A. Spinello, A. Saha, A. Magistrato: Frontiers of metal-coordinating drug design *Expert Opin. Drug Discov.*, accepted.
- C. Zhang, T. Schilirò, M. Gea, S. Bianchi, A. Spinello, A. Magistrato, G. Gilardi, G. Di Nardo: Molecular Basis for Endocrine Disruption by Pesticides Targeting Aromatase and Estrogen Receptor *Int. J. Environ. Res.*, 17 (2020) 5664.

2019

- A. Spinello, S. Martini, F. Berti, M. Pennati, M. Pavlin, J. Sgrignani, G. Grazioso, G. Colombo, N. Zaffaroni, A. Magistrato: Rational design of allosteric modulators of the aromatase enzyme: An unprecedented therapeutic strategy to fight breast cancer. *Eur. J. Med. Chem.*, 168 (2019) 253.
- A. Spinello, E. Vecile, A. Abbate, A. Dobrina, A. Magistrato: How Can Interleukin-1 Receptor Antagonist Modulate Distinct Cell Death Pathways? Insights from Combined Experimental and Molecular Simulation Study. *J. Chem. Inf. Model.*, 59 (2019) 351.
- A. Spinello, A. Magistrato: Recent Advances in the Computational Design of Potent Aromatase Inhibitors: Open-eye on Endocrine-resistant Breast Cancers. *Expert Opin. Drug Discov.*, 14 (2019) 1065.
- A. Spinello, I. Ritacco, A. Magistrato: The Catalytic Mechanism of Steroidogenic Cytochromes P450 from All-Atom Simulations: Entwinement with Membrane Environment, Redox Partners, and Post-Transcriptional Regulation. *Catalysts*, 9 (2019) 81.

- A. Spinello, M.G. Cusimano, G. Barone, D. Schillaci, S. Cascioferro, A. Magistrato, B. Parrino, V. Arizza, M. Vitale: A synthetic derivative of antimicrobial peptide Holothuroidin 2 from Mediterranean sea-cucumber (*Holothuria tubulosa*) in the control of *Listeria monocytogenes*. *Mar. Drugs*, 17 (2019) 159.
- I. Ritacco, A. Spinello, E. Ippoliti, A. Magistrato: Post-Translational Regulation of CYP450s Metabolism As Revealed by All-Atoms Simulations of the Aromatase Enzyme. *J. Chem. Inf. Model.*, 59 (2019) 2930.
- J. Borisek, A. Saltalamacchia, A. Spinello, A. Magistrato: Exploiting Cryo-EM Structural Information and All-atom Simulations to Decrypt the Molecular Mechanism of Splicing Modulators. *J. Chem. Inf. Model.*, 60 (2019) 2510.
- A. Terenzi, H. Gattuso, A. Spinello, B.K. Keppler, C. Chipot, F. Dehez, G. Barone, A. Monari: Targeting G-quadruplexes with Organic Dyes: Chelerythrine-DNA Binding Elucidated by Combining Molecular Modeling and Optical Spectroscopy. *Antioxidants*, 8 (2019) 472.
- M. Pavlin, L. Gelsomino, I. Barone, A. Spinello, S. Catalano, S. Andò, A. Magistrato: Structural, Thermodynamic and Kinetic Traits of Antiestrogen-compounds Selectively Targeting the Y537S Mutant Estrogen Receptor in Breast Cancer Cell Lines. *Front. Chem.*, 7 (2019) 602.
- J. Sgrignani, L. Casalino, F. Doro, A. Spinello, A. Magistrato: Can Multi-Scale Simulations Unravel the Function of Metallo-Enzymes to Improve Knowledge-based Drug Discovery? *Future Med. Chem.*, 11 (2019) 771.

2018

- A. Spinello, M. Pavlin, L. Casalino, A. Magistrato: A Dehydrogenase Dual Hydrogen Abstraction Mechanism promotes Estrogen Biosynthesis. Can we Expand the Functional Annotation of the Aromatase Enzyme?, *Chem. Eur. J.*, 24 (2018) 10840.
- A. Spinello, M.G. Cusimano, D. Schillaci, L. Inguglia, G. Barone, V. Arizza: Antimicrobial and Antibiofilm Activity of a Recombinant Fragment of beta-thymosin of Sea-urchin *Paracentrotus Lividus*, *Mar. Drugs*, 16 (2018) 366.
- L. Casalino, G. Palermo, A. Spinello, U. Rothlisberger, A. Magistrato: All-Atom Simulations Disentangle the Functional Dynamics Underlying Gene Maturation in the Intron Lariat Spliceosome, *Proc. Natl. Acad. Sci. USA*, 115 (2018) 6584.
- M. Pavlin, A. Spinello, M. Pennati, N. Zaffaroni, S. Gobbi, A. Bisi, G. Colombo, A. Magistrato: A Computational Assay of Estrogen Receptor alpha Antagonists Reveals the Key Common Structural Traits of Drugs Effectively Fighting Refractory Breast Cancers, *Sci. Rep.*, 9 (2018) 649.
- R. Bonsignore, F. Russo, A. Terenzi, A. Spinello, A. Lauria, G. Gennaro, A.M. Almerico, B.K. Keppler, G. Barone: The interaction of Schiff Base complexes of nickel(II) and zinc(II) with duplex and G-quadruplex DNA, *J. Inorg. Biochem.*, 178 (2018) 106.

2017

- A. Spinello, A. Magistrato: An Omics Perspective to the Molecular Mechanisms of Anticancer Metallo-drugs in the Computational Microscope Era, *Expert Opin. Drug Discov.*, 12 (2017) 813.

2016

- A. Spinello, G. Barone, J. Grunenberg: Molecular Recognition of Naphthalene Diimide Ligands by Telomeric Quadruplex-DNA: The Importance of the Protonation State and non-Mediated Hydrogen Bonds, *Phys. Chem. Chem. Phys.*, 18 (2016) 2871.
- A. Spinello, A. de Almeida, A. Casini, G. Barone: The inhibition of glycerol permeation through aquaglyceroporin-3 induced by mercury(II): A molecular dynamics study, *J. Inorg. Biochem.*, 160 (2016) 78.
- A. Spinello, R. Bonsignore, G. Barone, B.K. Keppler, A. Terenzi: Metal Ions and Metal Complexes in Alzheimer's Disease, *Curr. Pharm. Des.*, 22 (2016) 3996.
- A. Spinello, G. Barone, F. Cappello, A. Pace, S. Buscemi, A.P. Piccionello: The binding mechanism of epolactaene to Hsp60 unveiled by in silico modelling, *Chem. Select*, 4 (2016) 1.
- H. Gattuso, A. Spinello, A. Terenzi, X. Assfeld, G. Barone, A. Monari: Circular Dichroism of DNA G-Quadruplexes: Combining Modeling and Spectroscopy To Unravel Complex Structures, *J. Phys. Chem. B*, 120 (2016) 3113.
- R. Bonsignore, A. Notaro, A.M. Pia Salvo, A. Spinello, G. Fiasconaro, A. Terenzi, F. Giacalone, B.K. Keppler, M. Giuliano, M. Gruttadauria, G. Barone: DNA-Binding and Anticancer Activity of Pyrene-Imidazolium Derivatives, *Chem. Select*, 1 (2016) 6755.
- R. Bonsignore, A. Terenzi, A. Spinello, A. Martorana, A. Lauria, A.M. Almerico, B.K. Keppler, G. Barone: G-quadruplex vs. duplex-DNA binding of nickel(II) and zinc(II) Schiff base complexes, *J. Inorg. Biochem.*, 161 (2016) 115.
- D. Schillaci, G. Barone, M.G. Cusimano, S. Cascioferro, A. Spinello, M. Vitale, V. Arizza: A peptide from human beta-thymosin as a platform for the development of new anti-biofilm agents for *Staphylococcus* spp. and *Pseudomonas aeruginosa*, *World J. Microbiol. Biotechnol.*, 32 (2016) 124.

2015

- A. Spinello, M.G. Ortore, F. Spinozzi, C. Ricci, G. Barone, A. Marino Gammazza, A.P. Piccionello: Quaternary structure of GroEL and naive-Hsp60 chaperones: a combined SAXS-MD study, *RSC Adv.*, 5 (2015) 49871.
- I. Pibiri, L. Lentini, R. Melfi, G. Gallucci, A. Pace, A. Spinello, G. Barone, A. Di Leonardo: Enhancement of Premature Stop Codon Readthrough in the CFTR Gene by Ataluren (PTC124) Derivatives, *Eur. J. Med. Chem.*, 101 (2015) 236.

2014

- J. Grunenberg, G. Barone, A. Spinello: The right answer for the right electrostatics: Force field methods are able to describe relative energies of DNA guanine quadruplexes, *J. Chem. Theory Comp.*, 10 (2014) 2901.
- A. Biancardi, A. Burgalassi, A. Terenzi, A. Spinello, G. Barone, T. Biver, B. Mennucci: A combined theoretical-experimental investigation of the spectroscopic properties of a DNA-intercalator ZnII Salphen-type complex, *Chem. Eur. J.*, 20 (2014) 7439.
- L. Lentini, R. Melfi, A. Di Leonardo, A. Spinello, G. Barone, A. Pace, A.P. Piccionello, I. Pibiri: Towards a rationale for the PTC124 (Ataluren) promoted readthrough of premature stop codons: a computational approach and GFP-reporter cell-based assay, *Mol. Pharmaceutics*, 11 (2014) 653.

- A. Lauria, R. Bonsignore, A. Terenzi, A. Spinello, F. Giannici, A. Longo, A.M. Almerico, G. Barone: Nickel(II), copper(II) and zinc(II) metallo-intercalators: structural details of the DNA-binding by a combined experimental and computational investigation, *Dalton Trans.*, 43 (2014) 6108.
- A. Terenzi, R. Bonsignore, A. Spinello, C. Gentile, A. Martorana, C. Ducani, B. Högberg, A.M. Almerico, A. Lauria, G. Barone: Selective G-Quadruplex Stabilizers: Schiff-base Metal Complexes with Anticancer Activity, *RSC Adv.*, 4 (2014) 33245.
- D. Schillaci, M.G. Cusimano, A. Spinello, G. Barone, M. Vitale, D. Russo, D. Parrinello, V. Arizza: Paracentrin 1, a synthetic antimicrobial peptide from the sea-urchin *Paracentrotus lividus*, interferes with staphylococcal and *Pseudomonas aeruginosa* biofilm formation, *AMB express*, 4 (2014) 78.

2013

- A. Spinello, A. Terenzi, G. Barone: Metal Complex-DNA Binding: Insights from Molecular Dynamics and DFT/MM Calculations, *J. Inorg. Biochem.*, 124 (2013) 63.

2012

- A. Terenzi, L. Tomasello, A. Spinello, G. Bruno, C. Giordano, G. Barone: (Dipyrido[3,2-a:2',3'-c]phenazine) (glycinato) copper(II) perchlorate: A novel DNA-intercalator with anti-proliferative activity against thyroid cancer cell lines, *J. Inorg. Biochem.*, 117 (2012) 103.