ALL. B

Decreto Rettore Università di Roma "La Sapienza" n 2590/2017 del 12.10.2017

Daniela De Vita

Curriculum Vitae

"ai fini della pubblicazione"

Place Sao Carlos (SP-Brazil)

Date 04/12/2017

Part I – General Information

Full Name	Daniela De Vita
Spoken Languages	Italian, English, Brazilian Portuguese

Part II – Education

Type	Year	Institution	
University graduation	2004	Sapienza University of Rome, Faculty of Pharmacy	MSc. in Pharmaceutical Chemistry and Technologies; Level in National Classification :110/110 cum laude with the thesis "D-cycloserine derivatives as potential nootropic agents"
PhD	2008	Sapienza University of Rome, Faculty of Pharmacy	PhD in Pharmaceutical Sciences, with the thesis "4-Aminopyridine derivatives as ChE inhibitors"
Licensure	2005	Sapienza University of Rome, Faculty of Pharmacy	Qualification for practise pharmacist's profession

Part III – Appointments

IIIA – Academic Appointments

Start	End	Institution	Position
01/03/2016	present	IQSC-USP Sao Carlos (SP, Brazil)	Post-doc fellow
01/06/2014	31/05/2015	Sapienza, University of Rome	Assegnista di Ricerca, group of Prof. Di Santo
02/05/2013	01/05/2014	Sapienza, University of Rome	Assegnista di Ricerca, group of

			Prof. Silvestri
01/10/2012	31/10/2012	Sapienza, University of Rome	Incarico occasionale, group of Prof.Costi
01/11/2011	30/11/2011	Sapienza, University of Rome	Incarico di lavoro autonomo, group of Dr. Di Rienzo
01/03/2011	31/08/2011	Sapienza, University of Rome	Collaborazione coordinata e continuativa (co.co.co.) , group of Prof. Fornarini
01/09/2010	28/02/2011	Sapienza, University of Rome	Collaborazione coordinata e continuativa (co.co.co.) , group of Prof. Biava
02/04/2008	02/04/2009	Sapienza, University of Rome	Collaborazione coordinata e continuativa (co.co.co.) , group of Prof. Biava
01/11/2004	31/10/2007	Sapienza, University of Rome	PhD student, group of Dr. Scipione

Part IV – Teaching experience

Year	Institution	Lecture/Course
AA 2012-2013	Tuscia University, at DEB (Dipartimento di Scienze Ecologiche e Biologiche	Teaching of General and Inorganic Chemistry

Part V - Society memberberships

Year	Title
2014-2015	Member of the Italian Chemical Society (SCI).

Part VI - Funding Information [grants as PI-principal investigator or I-investigator]

Year	Title	Program	Grant value
2015	Targeting Trypanosomatids sterol biosynthesis and thiol redox metabolism enzymes for lead drug discovery-*Investigator*	**Sapienza Università di Roma- Grandi progetti di Ateneo- Grant number C26H15WYPW**	20000 Euro

Part VII – Research Activities

Keywords	Brief Description

Caffeic acid, cinnamic acid, anti-biofilm agents, antifungal agents	Caffeic and cinnamic acids are naturally present in many aromatic plants and spices and were initially extracted respectively from Thymus (*Thymus vulgaris*) and Cinnamon (in particular *Cinnamomum cassia*, commercially common) by extraction with hot Soxhlet apparatus and subsequent purifications by column chromatography. Since the obtained acids did not show any activity on biofilm of *Candida albicans*, new derivatives of caffeic and cinnamic acids have been designed and synthesized. These compounds have shown the ability to selectively inhibit the biofilm of *Candida albicans* both in formation and preformed with MIC values lower than fluconazole, with low cytotoxicity on human cell lines in culture. The search of new antifungal compounds involved synthetic azoles, as racemic mixtures or pure enantiomers. These compounds were more active than fluconazole against *Candida albicans* and non-*albicans* strains and not cytotoxic.
Physostigmine, 3,4-dihydroxybenzoic acid, acetylcholinesterase inhibitors	The structural modifications of the natural compounds physostigmine and 3,4-dihydroxybenzoic acid allowed to obtain acetylcholinesterase inhibitors, in particular: i) *N,N*-dialkylcarbamates which showed a percentage of inhibition of acetylcholinesterase up to 85%; ii) catechol derivatives that inhibit acetylcholinesterase at low micromolar range concentrations and possess metal chelating (Iron, Copper and Zinc) and radical scavenger properties. Additionally, in the field of cholinesterase inhibitors, new pyridine compounds able to inhibit the aggregation of β-amyloid, key peptide in the pathogenesis of Alzheimer's disease were found. Moreover, new multi-target compounds, able to inhibit simultaneously acetylcholinesterase and monoamino oxidase, have been identified.
Antitrypanosomal agents, azoles, antitubercular Agents, cysteine proteases, dipeptide	Azole-type compounds able to inhibit *Trypanosoma cruzi* 14-α-demethylase (TcCYP51), characterized by selective antiparasitic activity at nanomolar concentrations and low toxicity on cellular rat cell lines, have been designed and synthetized. The strongest inhibitors were co-crystallized with TcCYP51 and the co-crystal structures have been solved by X-ray crystallography. Some selected azole compounds have been studied as racemate or pure enantiomers as antitubercular agents, showing MIC values in the micromolar range against *Mycobacterium tuberculosis* H37Ra strain. Moreover, dipeptidyl nitrile derivatives have been synthesized and evaluated as cysteine-protease inhibitors (cruzain, cathepsin L) and for their antiparasitic activity. The current research activities are focused also on the potential anti-tripanosomal activity of naturally occurring compounds with special attention towards coumarin and flavonoids extracted by conventional methods from some plants of the *Rutaceae* family.

Part VIII – Summary of Scientific Achievements

Product type	Number	Data Base	Start	End
Papers [international]	25	Scopus	2006	2017

Total Impact factor	77.69
Total Citations	136

Average Citations per Product	5.44
Hirsch (H) index	7
Normalized H index*	0.58

*H index divided by the academic seniority, calculated since the first scientific publication (2006) up to date

Part IX– Selected Publications

1. **D. De Vita**, A. Angeli, F. Pandolfi, M. Bortolami, R. Costi, R. Di Santo, E. Suffredini, M. Ceruso, S. Del Prete, C. Capasso, L. Scipione, C. T. Supuran. Inhibition of the α-carbonic anhydrase from Vibrio cholerae with amides and sulfonamides incorporating imidazole moieties. *J. Enzyme Inhib. Med. Chem.* **2017**, 32(1),798-804. IF = 4.293*, citations =1 (ED. Taylor & Francis)
*The Impact Factor refers to 2016

2. **D. De Vita**, G. Simonetti, F. Pandolfi, R. Costi , R. Di Santo , F.D. D'Auria, L. Scipione. Exploring the anti-biofilm activity of cinnamic acid derivatives in Candida albicans. *Bioorg. Med. Chem. Lett.* **2016**, 26(24), 5931-5935. IF = 2.454, citations = 1 (ED. Elsevier)

3. **D. De Vita**, F. Pandolfi, R. Cirilli, L. Scipione, R. Di Santo, L. Friggeri, M. Mori, D. Fiorucci, G. Maccari, R.S. Arul Christopher, C. Zamperini, V. Pau, A. De Logu, S. Tortorella, M. Botta. Discovery of in vitro antitubercular agents through in silico ligand-based approaches. *Eur. J. Med. Chem.* **2016**, 121, 169-180. IF = 4.519, citations = 2 (ED. Elsevier)

4. **D. De Vita**, F. Pandolfi, L. Ornano, M. Feroci, I. Chiarotto, I. Sileno, F. Pepi, R. Costi, R. Di Santo, L. Scipione. New N,N-dimethylcarbamate inhibitors of acetylcholinesterase: design synthesis and biological evaluation. *J. Enzyme Inhib. Med. Chem.* **2016**, 31, 106-113. IF = 4.293, citations =1 (ED. Taylor & Francis)

5. **D. De Vita**, F. Moraca, C. Zamperini, F. Pandolfi, R. Di Santo, A. Matheeussen, L. Maes, S. Tortorella, L. Scipione. In vitro screening of 2-(1H-imidazol-1-yl)-1-phenylethanol derivatives as antiprotozoal agents and docking studies on Trypanosoma cruzi CYP51. *Eur. J. Med. Chem.* **2016**, 113, 28-33. IF = 4.519, citations =6 (ED. Elsevier)

6. **D. De Vita**, L. Friggeri, F. D. D'Auria, F. Pandolfi, F. Piccoli, S. Panella, A. T. Palamara, G. Simonetti, L. Scipione, R. Di Santo, R. Costi, S. Tortorella. Activity of caffeic acid derivatives against Candida albicans biofilm. *Bioorg. Med. Chem. Lett.* **2014**, 24, 1502–1505. IF = 2.420, citations = 16 (ED. Elsevier)

7. **D. De Vita**, L. Scipione, S. Tortorella, P. Mellini, B. Di Rienzo, G. Simonetti, F.D. D'Auria, S. Panella, R. Cirilli, R. Di Santo, A.Palamara. Synthesis and antifungal activity of a new series of 2-(1H-imidazol-1-yl)-1-phenylethanol derivatives. *Eur. J. Med. Chem.* **2012**, 49, 334-342. IF = 3.499, citations = 21 (ED. Elsevier)

8. F. Moraca, **D. De Vita**, F. Pandolfi, R. Di Santo, R. Costi, R. Cirilli, F. D. D'Auria, S. Panella, A. T. Palamara, G. Simonetti, M. Botta, L. Scipione. Synthesis, biological evaluation and structure-activity correlation study of a series of imidazol-based compounds as Candida albicans inhibitors. *Eur. J. Med. Chem.* **2014**, 83, 665-673. IF = 3.447, citations = 8 (ED. Elsevier)

9. L. Friggeri, **D. De Vita***, F. Pandolfi, S. Tortorella, R. Costi, R. Di Santo, L. Scipione. Design, synthesis and evaluation of 3,4-dihydroxybenzoic acid derivatives as antioxidants, bio-metal chelating agents and acetylcholinesterase inhibitors. *J. Enzyme Inhib. Med. Chem.* 2015, 30(1), 166–172. IF = 3.428, citations = 1 (ED. Taylor & Francis)

10. P. Mellini, **D. De Vita***, B. Di Rienzo, S. La Rosa, A. Padova, L. Scipione, S. Tortorella, L. Friggeri. Efficient Synthesis of 3,5-dicarbamoyl-1,4-dihydropyridines from pyridinium salts. Key Molecules in Understanding NAD(P)+/NAD(P)H Pathways. *J. Heterocyclic Chem*. **2015**, 52, 221-226. IF = 0.685, citations = 1 (Ed. Lyle W. Castle, Wiley Online Library)

11. L. Friggeri, L. Scipione, R. Costi, M. Kaiser, F. Moraca, C. Zamperini, B. Botta, R. Di Santo, **D. De Vita***, R. Brun, S. Tortorella. New Promising Compounds with in Vitro Nanomolar Activity against Trypanosoma cruzi. *ACS Med. Chem. Lett*. **2013**, 4, 538−541. IF = 3.073, citations = 10 (ED. ACS Publications)

12. S. Carradori, F. Ortuso, A. Petzerc, D. Bagetta, C. De Monte, D. Secci, **D. De Vita**, P. Guglielmi, G. Zengin, A. Aktumsek, S. Alcaro, J.P. Petzer. Design, synthesis and biochemical evaluation of novel multi-target inhibitors as potential anti-Parkinson agents. *Eur. J. Med. Chem.* **2017**, in press doi.org/10.1016/j.ejmech.2017.10.050 IF = 4.293*, citations = 0 (In press, ED. Elsevier) The article is not indexed on Scopus Database yet.
*The Impact Factor refers to 2016

13. D.G.Silva, J. F.R.Ribeiro, **D. De Vita**, L. Cianni, C. H. Franco, L. H. Freitas-Junior, C. Borsoi Moraes, J. R.Rocha, A. C.B. Burtoloso, P. W. Kenny, A. Leitão, C. A. Montanari. A comparative study of warheads for design of cysteine protease inhibitors. *Bioorg. Med. Chem. Lett.* **2017**, 27(22), 5031-5035. IF = 2.454*, citations = 0 (ED. Elsevier)
*The Impact Factor refers to 2016

14. F. Pandolfi, **D. De Vita**, M. Bortolami, A. Coluccia, R. Di Santo, R. Costi, V. Andrisano, F. Alabiso, C. Bergamini, R. Fato, M. Bartolini, L. Scipione. New pyridine derivatives as inhibitors of acetylcholinesterase and amyloid aggregation. *Eur. J. Med. Chem*. **2017**, 141, 197-210. IF = 4.519*, citations = 0 (ED. Elsevier)
*The Impact Factor refers to 2016

15. M. D'Ascenzio, P. Chimenti, M.C. Gidaro, C. De Monte, **D. De Vita**, A. Granese, L. Scipione,R. Di Santo, G. Costa, S. Alcaro, M. Yáñez, S. Carradori. (Thiazol-2-yl)hydrazone derivatives from acetylpyridines as dual inhibitors of MAO and AChE: synthesis, biological evaluation and molecular modeling studies. *J. Enzyme Inhib. Med. Chem*. **2015**, 30(6), 908-919. IF = 3.428, citations = 5 (ED. Taylor & Francis)

16. L. Friggeri, T. Y. Hargrove, G. Rachakonda, A. D. Williams, Z. Wawrzak, R. Di Santo, **D. De Vita**, M. R. Waterman, S. Tortorella, F. Villalta, G. I. Lepesheva. Structural Basis for Rational Design of Inhibitors Targeting Trypanosoma cruzi Sterol 14α-Demethylase: Two Regions of the Enzyme Molecule Potentiate Its Inhibition. *J. Med. Chem.* **2014**, 57 (15), 6704−6717. IF = 5.447, citations = 16 (ED. ACS Publications)

17. L. Friggeri, F. Ballante, R. Ragno, I. Musmuca, D. De Vita, F. Manetti, M. Biava, L. Scipione, R. Di Santo, R. Costi, M. Feroci, S. Tortorella. Pharmacophore Assessment Through 3-D QSAR: Evaluation of the Predictive Ability on New Derivatives by the Application on a Series of Antitubercular Agents. *J. Chem. Inf. Model.* **2013**, 53, 1463−1474. IF = 4.068, citations = 6 (ED. ACS Publications)

18. P. Mellini, V. Carafa, B. Di Rienzo, D. Rotili, **D. De Vita**, R. Cirilli, B. Gallinella, D.P. Provvisiero, S. Di Maro, E. Novellino, L. Altucci, A. Mai. Carprofen Analogues as Sirtuin Inhibitors: Enzyme and Cellular Studies. *Chem. Med. Chem*. **2012**, 7, 1905-1908. IF = 2.835, citations = 7 (ED. Wiley-VCH)

19. B. Di Rienzo, P. Mellini, S. Tortorella, **D. De Vita**, L.Scipione. Facile and Efficient Synthesis of 4-Alkyl Derivatives of 3-Carbamoyl- and 3,5 Dicarbamoylpyridines as Nicotinamide Mimetics. *Synthesis*. **2010**, 22, 3835-3838. IF = 2.260, citations = 1 (Ed.Thieme)

20. L. Scipione, **D. De Vita**, A. Musella, L. Flammini, S. Bertoni, E. Barocelli. 4-Aminopyridine derivatives with anticholinesterase and antiamnesic activity. *Bioorg. Med. Chem. Lett.* **2008**, 18, 309-312. IF = 2.531, citations = 8 (ED. Elsevier)

ADDIONAL INFORMATION

ORAL COMMUNICATION

1. NPCF8 New Prospective in Pharmaceutical Chemistry, Parma (Italy) June 9-11 2014

Imidazole derivatives with in vitro antichagas activity.

2. XXII NMMC. Rome, September 10-13 2013 (session infectious diseases and drug resistance)

Imidazole derivatives with in vitro antichagas activity: synthesis, biological evaluation and docking studies.

3. Drug's day "Antitumoral drugs, orphan drugs and rare diseases". Salerno (Italy) April 12 2013

New imidazole derivatives in vitro highly active vs T.cruzi

POSTERS

1. 4th EFMS-YMCS. Vienna (Austria) - August 31-September 1, 2017

DG Silva, JFR Ribeiro, D. De Vita, L. Cianni, JR Rocha, ACB Burtoloso, PW Kenny, CA Montanari. Synthesis of cruzain inhibitors for dipeptidyl nitriles warhead exchange.

2. IUPAC 2017 - 46th World Chemistry Congress

L. Cianni, G. Sartori, D. De Vita, F. Rosini, CA Montanari, A. Leitão. On the study of halogen bond interaction to increase cruzain affinity of covalently bound reversible inhibitors.

3. XXIII NMMC. Salerno (Italy) September 6-9 2015

L. Scipione, R. Di Santo, R. Costi, S. Tortorella, G. Simonetti, F. D. D'Auria, F. Pandolfi, and D. De Vita. Cinnamic and caffeic acid derivatives against Candida albicans biofilm.

F. Pandolfi, D. De Vita, R. Di Santo, R. Costi, S. Tortorella, M. Bartolini, V. Andrisano, and L. Scipione. New dual binding site acetylcholinesterase inhibitors.

4. XXII NMMC. Rome (Italy) September 10-13 2013

D. De Vita, S. Panella, G. Simonetti, F. D. D'Auria, L. Scipione, R. Di Santo, L. Friggeri, S. Tortorella. Synthesis and antifungal activity of a new series of 2-(1H-imidazol-1-yl)-1-phenylethanol derivatives.

L. Friggeri, D. De Vita, F. Pandolfi, S. Tortorella, R. Costi, R. Di Santo, L. Scipione. Synthesis and evaluation of 3,4-dihydroxybenzoic acid derivatives as antioxidants, bio-metal chelating agents and acetylcholinesterase inhibitors.

5. Drug's day "Antitumoral drugs, orphan drugs and rare diseases". Salerno (Italy) April 12 2013

D. De Vita, L. Friggeri, L. Scipione, R. Di Santo, R. Costi, F. Moraca, B. Botta, R. Brun, M. Kaiser, S. Tortorella. New imidazole derivatives in vitro highly active vs T.cruzi.

6. Cost-CM801 WG1/WG3 Meeting: "New Drugs for Neglected Disease", Siena (Italy) May 31-June 1 2012

D. De Vita, L. Friggeri, P. Mellini, S. Tortorella, L. Scipione, M. Kaiser, R. Brun, R. Di Santo. New 4-aminopyridine and imidazole compounds highly active against T. Cruzi.

7. XXIV National Congress of the Italian Chemical Society, Lecce (Italy) September 11-16 2011

P. Mellini, D. De Vita, V. Carafa, L. Scipione, B. Di Rienzo and L. Altucci. New carbazole scaffolds as SIRT inhibitors.

8. NPCF5 New Prospective in Pharmaceutical Chemistry, Trieste (Italy) March 28-30 2011

L. Pescatori, D. De Vita, G. Cuzzucoli Crucitti, P. Mellini, B. Saint Joanis, R.Brosh, S. Tortorella, L. Scipione, R. Costi, R. Di Santo. Design, synthesis and biological activities of new active agents against mycobacteriun tuberculosis.

L. Pescatori, D. De Vita, P. Mellini, L. Scipione, S. Tortorella, R. Di Santo, G. Cuzzucoli Crucitti, R. Costi, L. Fattorini, G. Piccaro. Activity of drugs against dormant mycobacterium tuberculosis.

9.Conference on scientific research, faculty of Pharmacy- Rome (Italy), December 9-10 2004

L.Scipione, S Tortorella, V. Fabbri, E.Fabbrini, D. De Vita. Choline derivatives with potential antialzheimer activity.

TECHNICAL SKILLS

The participation in the above mentioned research projects allowed to acquire good experience in the field of extraction and purification techniques, chemical synthesis and analytical methodologies necessary to check the purity of the compounds and to elucidate the chemical structures of natural and synthetic compounds.
In particular, the methodologies and skills acquired are:

- Extraction of active compounds from pharmaceutical forms or from natural sources. Solid/liquid extraction by Soxhlet.
- Continuous or discontinuous liquid/liquid extraction by extractors for heavy and light solvents.
- Simple and fractional distillation, distillation at reduced pressure and azeotropic distillation.
- Purification of compounds by PLC.
- Purification of compounds by silica gel or alumina column chromatography.
- Purification of compounds by manual and automated flash chromatography.
- Purification of compounds by HPLC in reverse or normal phase.
- Separation of racemic mixtures by HPLC using semi-preparative amylose and cellulose-based chiral columns in normal or inverse phase.
- Analysis of mixtures by HPLC-MS in isocratic or gradient elution, using C18, C8, biphenyl analytical columns and amylose and cellulose-based chiral columns having immobilized chiral selectors.
- Analysis of mixtures by TLC (silica gel, alumina, C18).
- Determination of the purity of the compounds by HPLC and qNMR.
- Characterization and determination of purity of compounds by measurement of optical activity.
- Elucidation of the chemical structure of the compounds by NMR (^{1}H, ^{13}C, ^{19}F, COSY) and IR.
- Determination of compounds stability to auto-hydrolysis or enzymatic hydrolysis, by ^{1}H-NMR and HPLC.
- Inhibition study of acetylcholinesterase and butyrylcholinesterase by Ellman's spectrophotometric method.
- Evaluation of antioxidant activity by DPPH tests.

• Determination of chelating metal activity by spectrophotometric titrations and evaluation of stoichiometry of complexes by Job method.

Instrumentation used
Biotage Isolera ™ Prime; UFLC Shimadzu; NMR Bruker ADVANCE-400 spectrometer and data processing by WN-NMR Bruker Daltonik GMbH, 6.1.0.0, Topspin 2.1, Mestre; FT-IR spectrophotometer Perkin-Elmer Spectrum One ATR; UV-Vis lambda spectrophotometer 40 Perkin Elmer; ESI-MS ThermoQuest Finnigan, ESI-MS Amazon-SL. Digital polarimeter (P2000, Jasco).

Common Software Applications and Databases

ACDLABS Chemsketch, Chem Draw Ultra, IsisDraw, Marvin Sketch, Microsoft Office, Sigmaplot; ScifindeScholar, Reaxys, Scopus, PubMed, PubChem.

OTHER SCIENTIFIC ACHIEVEMENTS

Peer reviewer for international journals:

Journal of Medicinal Chemistry
European Journal of Medicinal Chemistry
Molecules
Bioorganic and Medicinal Chemistry Letters

Guest editor:
Journal of Chemistry

Il presente curriculum vitae è conforme a quanto prescritto dall'art. 4 del Codice in materia di protezione dei dati personali e dall'art. 26 del D. Lgs. 14 marzo 2013, n. 33, al fine della pubblicazione.

Luogo e data

Sao Carlos, 04/12/2017

Firma Daniela De Vita