CURRICULUM VITAE

PERSONAL INFORMATION

Name:	Antonio
Surname:	de la Vega de León
Birth Date:	18 September 1986
ID Number:	53615149-X
Address:	Clemensstrasse 57, 53225 Bonn, NRW, Germany
Telephone Number:	+49-176-47951874
Email:	antoniovega86@gmail.com / vega@bit.uni-bonn.de

ACADEMIC FORMATION

2010 - 2012: M. Sc. Life Science Informatics from the Bonn-Aachen International Center for Information Technology, part of the Rheinische Friedrich-Wilhelms-Universität Bonn, Germany. Grade: 1.2 (≈ 9.5/10)

2004 - 2010: *Licenciado* in Biology from the *Universidad Complutense de Madrid*, Spain. Grade: 8.67/10

2002 - 2004: *Bachillerato* in Life Science from *Colegio Everest*, Madrid, Spain. Grade: *Matrícula de Honor* (9.1/10)

PROFESSIONAL EXPERIENCE

November 2016 – Present: Postdoctoral research assistant (Marie-Curie fellow) at the group of Prof. Gillet (University of Sheffield) for the European project Diagnostic and Drug Discovery Initiative for Alzheimer's Disease (FP7-PEOPLE-2013-IAPP)

November 2012 – October 2016: Research assistant on the workgroup from Prof. Bajorath (University of Bonn), doing my PhD Thesis on the topic of applications of MMPs and visualization techniques for computational compound optimization

May 2012 – November 2012: Student assistant (SHK) on the workgroup from Prof. Bajorath (University of Bonn), developing a new multi-target activity landscape as the Master Thesis for the Life Science Informatics Masters

October 2011 – February 2012: Student assistant (SHK) in the University of Bonn, tutoring the exercise part of the lecture Foundations of Information Management WS 11/12 for the Life Science Informatics Masters

October 2009 - May 2010: Assistant on a bioinformatics project assembling and annotating the genomes of *Rhodococcus ruber* and *Gordonia cholesterolivorans* under supervision of Prof. Julian Perera, Biochemistry and Molecular Biology department of the Universidad Complutense de Madrid

July - September 2009: Internship on the molecular genetics laboratory for diagnostic GENYCA INNOVA.

October 2008 - Februar 2009: Assistant of Professor Tomás Naranjo Pompa on the cytogenetic laboratory of the Universidad Complutense de Madrid

October 2006 - June 2007: Small experiment on the population genetics laboratory of the University

September 2006: Laboratory assistant in Barcelona on the company Ecofloat S.A.

July - August 2006: Costumer service of Iberia Equipajes S.A., working on phone service.

JOURNAL PUBLICATIONS

Anighoro A, **de la Vega de León A** & Bajorath J. Predicting bioactive conformations and binding modes of macrocycles. J Comput-Aided Mol Des, in press. dx.doi.org/10.1007/s10822-016-9973-5

de la Vega de León A & Bajorath J. Chemical space visualization: transforming multi-dimensional chemical spaces into similarity-based molecular networks. Future Med Chem 8, 1769-1778, 2016. dx.doi.org/10.4155/fmc-2016-0023

Horvath D, Marcou G, Varnek A, Kayastha S, **de la Vega de León A** & Bajorath J. Prediction of activity cliffs using condensed graphs of reaction representations, descriptor recombination, support vector machine classification, and support vector regression. J Chem Inf Model, in press. dx.doi.org/10.1021/acs.jcim.6b00359

Shanmugasundaram V, Zhang L, Kayastha S, **de la Vega de León A**, Dimova D & Bajorath J. Monitoring the progression of structure-activity relationship information during lead optimization. J Med Chem 59, 4235-4244, 2016. dx.doi.org/10.1021/acs.jmedchem.5b01428

de la Vega de León A, Kayastha S, Dimova D, Schultz T & Bajorath J. Visualization of multi-property landscapes for compound selection and optimization. J Comput-Aided Mol Des 29, 695-705, 2015. dx.doi.org/10.1007/s10822-015-9862-3

Hameed A, Khan K, Zehra S, Ahmed R, Shafiq Z, Bakht S, Yaqub M, Hussain M, **de la Vega de León A**, Furtmann N, Bajorath J, Ahmad H, Tahir M & Iqbal J. Synthesis, biological evaluation and molecular docking of N-phenyl thiosemicarbazones as urease inhibitors. Bioorg Chem 61, 51-57, 2015. dx.doi.org/10.1016/j.bioorg.2015.06.004

Kayastha S, **de la Vega de León A**, Dimova D & Bajorath J. Target-based analysis of ionization states of bioactive compounds. Med Chem Commun 6, 1030-1035, 2015. dx.doi.org/10.1039/C5MD00051C

de la Vega de León A & Bajorath J. Prediction of compound potency changes in matched molecular pairs using support vector regression. J Chem Inf Model 54, 2654-2663, 2014. dx.doi.org/10.1021/ci5003944

de la Vega de León A, Hu Y & Bajorath J. Systematic identification of matching molecular series and mapping of screening hits. Mol Inf 33, 257-263, 2014. dx.doi.org/10.1002/minf.201400017

Stumpfe D, **de la Vega de León A**, Dimova D & Bajorath J. Advancing the activity cliff concept, part II [v1; ref status: indexed, f1000r.es/34p] F1000Research 3:75, 2014. dx.doi.org/10.12688/f1000research.4057

de la Vega de León A & Bajorath J. Formation of activity cliffs is accompanied by systematic increases in ligand efficiency from lowly to highly potent compounds. AAPS J 16, 335-341, 2014. dx.doi.org/10.1208/s12248-014-9567-x

Hu Y, **de la Vega de León A**, Zhang & Bajorath J. Matched molecular pair-based data sets for computer-aided medicinal chemistry [v2; ref status: indexed, f1000r.es/2w9] F1000Research 3:36, 2014. dx.doi.org/10.12688/f1000research.3-36.v2

de la Vega de León A & Bajorath J. Matched molecular pairs derived by retrosynthetic fragmentation. Med Chem Commun 5, 64-67, 2014. dx.doi.org/10.1039/C3MD00259D

Fernandez de las Heras L, Alonso S, **de la Vega de León A**, Xavier D, Perera J & Navarro Llorens JM. Draft genome sequence of the steroid degrader Rhodococcus ruber Strain Chol-4. Genome Announc 1:e00215-13, 2013. dx.doi.org/10.1128/genomeA.00215-13

de la Vega de León A & Bajorath J. Compound optimization through data set-dependent chemical transformations. J Chem Inf Model 53, 1263-1271, 2013. dx.doi.org/10.1021/ci400165a

de la Vega de León A & Bajorath J. Design of a three-dimensional multi-target activity landscape. J Chem Inf Model 52, 2876-2883, 2012. dx.doi.org/10.1021/ci300444p

OTHER SCIENTIFIC WORK

Shanmugasundaram V, Liying Z, Kayastha S, **de la Vega de León A**, Dimova D & Bajorath J. Data sets for SAR progression analysis. Freely available data set. dx.doi.org/10.5281/zenodo.32794

de la Vega de León A, Kayastha S, Dimova D, Schultz T & Bajorath J. ChEMBL20 data sets for multi-property landscape analysis. Freely available data set. dx.doi.org/10.5281/zenodo.21782

Hu Y, **de la Vega de León A**, Zhang B & Bajorath J. Detailed data sets of MMP-cliffs, SAR transfer series, RECAP-MMPs and compound activities. Freely available data set. dx.doi.org/10.5281/zenodo.8418

Kayastha S, **de la Vega de León A**, Dimova D, Schultz T & Bajorath J. Visualization of multi-property landscapes for compound selection and optimization. Poster at Chemoinformatics Strasbourg Summer School 2016

Dimova D, Kayastha S, **de la Vega de León A** & Bajorath J. Monitoring the progression of structure-activity relationship information during lead optimization. Poster at 2016 Frontiers in Medicinal Chemistry

Zhang L, Starr J, Dimova D, Iyer P, Gupta-Ostermann D, **de la Vega de León A** & Bajorath J, Shanmugasundaram V. Novel applications of SAR matrices in pharmaceutical research. Poster at the Spring 2014 Dallas ACS National Meeting

Müller G, Benningshof J, van Meurs P, Stumpfe D, **de la Vega de León A**, Furtmann N, Dimova D & Bajorath J. Synthetic and cheminformatic exploration of macrocyclic and peptidomimetic medicinal chemistry space. Poster at XXIII International Symposium on Medicinal Chemistry (EFMC-ISMC 2014)

de la Vega de León A & Bajorath J. Compound optimization through data set-dependent chemical transformations. Poster at 9th German Conference on Chemoinformatics (GCC 2013)

de la Vega de León A, Lounkine E, Vogt M & Bajorath J. Design of diverse and focused compound libraries. In: Tutorials in Cheminformatics. Eds: Varnek A. (in preparation)

Vogt M, **de la Vega de León A** & Bajorath J. Algorithmic chemoinformatics. In: Tutorials in Cheminformatics. Eds: Varnek A. (in preparation)

TEACHING EXPERIENCE

SS2016: Assistant in the Python-based Programming Lab Course II

WS2015/16: Two theoretical lectures for Chemoinformatics; assistant in the exercises of Chemoinformatics and Structural Bioinformatics lectures

SS2015: Assistant in the Python-based Programming Lab Course II

WS2014/15: Two theoretical lectures for Bridging Course Chemistry; assistant in the Research Practical invitational lab course

SS2014: Three theoretical lectures for Bioinformatics II; assistant in the Python-based Lab Course II

WS2013/14: One theoretical lecture for Bridging Course Chemistry; assistant in the Java-based Chemoinformatics Lab Course

SS2013: Assistant in the MOE-based Molecular Modeling and Drug Design Lab Course

WS2012/13: Assistant in the Java-based Chemoinformatics Lab Course

WS2011/12: Assistant in the Foundations of Information Management Exercises

LANGUAGES

Spanish: Native level

English: High level
Certificate in Advanced English (CAE) from Cambridge University
Internet based TOEFL test (iBT) score: 107
12 years of studies in a bilingual school

German: Medium/high level
Zentrale Mittelstufenprüfung (ZMP) Certificate from *Goethe Institut*
Advanced level from the *Escuela Oficial de Idiomas*
More than six years living in Germany

SKILLS

Programming: Java, Python, R

Scientific Software: MOE, AutoDock, KNIME

Computer Software: Microsoft Office, Inkscape, Latex