Antonio de la Vega de León

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Professional Experience

11/2016 – Present **Postdoctoral research assistant, University of Sheffield**
Development of novel machine learning research on the context of Alzheimer's disease for the European project D3i4AD (FP7-PEOPLE-2013-IAPP)

11/2012 – 10/2016 **Research assistant, University of Bonn**
Development of chemoinformatics technique to analyse complex chemical data with a focus on data mining and visualization techniques

05/2012 – 11/2012 **Student assistant (SHK), University of Bonn**
Development of a multitarget chemical visualization during the Master thesis

10/2011 – 02/2012 **Student assistant (SHK), University of Bonn**
Teaching assistant for the lecture Foundations of Information Management

10/2009 – 05/2010 **Laboratory assistant, Universidad Complutense de Madrid**
Work on a bioinformatics project assembling and annotating the genomes of *Rhodococcus ruber* and *Gordonia cholesterolivorans*

07/2009 – 09/2009 **Laboratory assistant, GENYCA INNOVA**
Work on molecular genetics techniques such as DNA extraction and PCR

10/2008 – 02/2009 **Laboratory assistant, Universidad Complutense de Madrid**
Work on cytogenetics techniques such as fluorescence in-situ hybridization

10/2006 – 06/2007 **Laboratory assistant, Universidad Complutense de Madrid**
Work on population genetics for *Drosophila melanogaster*

09/2006 **Laboratory assistant, Ecofloat**

07/2006- 08/2006 **Call operator, Costumer service Iberia Equipajes**

Academic Formation

2012 – 2016 **PhD Computational Life Sciences, University of Bonn**
Grade: 0.7 (≈ 9.5/10)

2010 – 2012 **M. Sc. Life Science Informatics, University of Bonn**
Grade: 1.2 (≈ 9.5/10)

2004 – 2010 **Biology undergraduate, Universidad Complutense de Madrid**
Grade: 8.67/10

2002 – 2004 **Life Science secondary school, Colegio Everest**
Grade: *Matrícula de Honor* (9.1/10)

Journal Publications

de la Vega de León A, Chen B & Gillet VJ. Effect of missing data on multitask prediction methods. J Cheminf, *in press*. dx.doi.org/10.1186/s13321-018-0281-z

de la Vega de León A & Bajorath J. Design of chemical space networks incorporating compound distance relationships. F1000Research 5(Chem Inf Sci):2634, 2016. dx.doi.org/10.12688/f1000research.10021.2

Anighoro A, **de la Vega de León A** & Bajorath J. Predicting bioactive conformations and binding modes of macrocycles. J Comput-Aided Mol Des 30, 841, 2016. 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 56, 1631-1640, 2016. 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 B & 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

Funding and Awards

SRUK/UAM Summer Studentships 2018 Supervisor for Master student from UAM for short summer scientific project

Bayer promotionspreis 2017 The pharmaceutical company Bayer awards this price to outstanding doctoral theses related to the biomedical field

Other Scientific Work

de la Vega de León A. Visualizations for chemical data. Oral presentation at the DataViz Hub launch event at the University of Sheffield. April 2018

de la Vega de León A & Gillet V. Comparison of multitask prediction methods for chemical data. UK-QSAR and Molecular Graphics and Modelling Society (MGMS) Meeting. April 2018

de la Vega de León A & Gillet V. Deep learning application to aid phenotypic assay campaigns with public chemical data. Poster at 13th German Conference of Chemoinformatics. 2017

de la Vega de León A & Gillet V. Deep learning application to aid phenotypic assay campaigns with public chemical data. Oral presentation at the Fall 2017 ACS National Meeting

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. (ISBN: 978-1-119-13796-2)

Vogt M, **de la Vega de León A** & Bajorath J. Algorithmic chemoinformatics. In: Tutorials in Cheminformatics. Eds: Varnek A. (ISBN: 978-1-119-13796-2)

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 ACS National Meeting

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

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)

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

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

Teaching Experience

University of Sheffield: teaching assistant for Data mining and visualization (SS2018), Designing webpages (WS2017/18), and Chemoinformatics (SS2017). Gave one lecture for Data Mining and Visualization (SS2018) and one lecture for Designing webpages (WS2017/18).

University of Bonn: teaching assistant for Chemoinformatics (WS2015/16), Programming Lab Course II (SS2015, SS2014), Structural Bioinformatics (WS2015/16), Chemoinformatics Lab Course (WS2013/14, WS2012/13), Molecular Modeling and Drug Design (SS2013), and Foundations of Information Management (WS2011/12). Gave two lectures for Chemoinfomatics (WS2015/16), three lectures for the Chemistry Bridging Course (WS2014/15, WS2013/14) module, and three lectures for Bioinformatics II (SS2014).

Skills

Supervision: supporting supervision for Jessica Stacey

Leadership: science outreach event organization as a volunteer of the British Science Association and as secretary of the Yorkshire constituency of the Society of Spanish Researchers in the UK

Programming: Large amount of experience in Python (numpy, matplotlib, tensorflow, scikit-learn, RDKit) and Java (OpenEye, JUNG). Moderate experience with R

Software: Experience with MOE for chemical modeling, Autodock for docking, KNIME for data mining and analysis, Inkscape and Illustrator for media creation, and Latex and Office for document creation

Languages: Native Spanish; Fluent English and German; Basic level of Chinese