## Dr Stéphane VELLAY, PharmD — Computational scientist in drug research

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**Keywords:**
Pharmacy, drug discovery & development, life science, modeling & simulation, computational chemistry, QSAR, imaging, data visualization

## Summary of qualifications

– 5 years experience in pharmaceutical and software industries for drug discovery & development

– Expert in life science: chemistry, biology, drug absorption distribution metabolism and elimination (ADME), imaging, virtual screening

– Conversant with computational modelling & simulation, scientific programming

– Lead by example, excellent interpersonal communication skills, promote team work across different disciplines, build trust relationship

– Native French speaker, fluent in English, intermediate in German

## Work Experience

**since 2007**
**4 years**

**Senior Application Scientist**
**Accelrys, Platform & Informatics Technologies, Cambridge UK (E Vande Water)**
Grow usage of Pipeline Pilot (scientific workflow technology) in the scientific community by identifying users' needs and advising or developing appropriate solutions, via various ways:

– *Demonstration*: Explaining benefits to users, and developing tailored proof-of-concept, each week in a different scientific environment or company;

– *Training*: Leading by example, provided more than a hundred training, with excellent feedback from both new and expert users, about most of the component collections;

– *Support*: Became a trusted advisor (inside and outside company) in a variety of Pipeline Pilot component collections (esp. Imaging, Reporting, Text Analytics) and in data visualization;

– *Consulting Services*: Engaged in various projects for scientific expertise (e.g. imaging, PKPD, computational chemistry) or interface usability.

Initiated and developed projects recognized and reused by the community or my team:

– The creation of the Bibliography Platform led to a publication and the wide promotion of the Text Analytics collection;

– The integration of PKPD tools like NONMEM, PsN, and WinBUGS generated new business in advance on the long-term company strategy to go towards clinical drug development;

– Managed team effort to create a standard, and now essential, demonstration slide deck, summarizing on all component collections.

Received 2 Accelrys Excellence Awards in 2009 for exceptional performance, initiative and continuous improvement.

**2005-2006**
**13 months**

**Computational Chemist**
**Technologie Servier, Biopharmaceutical research department, Orléans (Dr Ph Vayer)**
Defined a global *in silico* strategy to predict human intestinal absorption, based on three quantitative structure-property relationship models predicting (1) passive absorption, (2) P-Glycoprotein involvement, and (3) its impact on drugs.
Created these multivariate data analysis models based on physicochemical (Volsurf approach) and pharmacophoric (Almond approach) 3D descriptors derived from GRID molecular interaction fields. Compiled literature data and advised to conduct assays to fill in missing data.
Conceived a Python-based Intranet application (1) predicting ADME properties including these models as well as other models, (2) operating dissimilarity-based compound selection.
Trained the department for using this tool to validate *in vitro* and *in vivo* assays.

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| 2005<br>2 months | **Bioinformatician**<br>**UMR CNRS 5558, School of Medicine, Lyon 1 University (Pr JP Flandrois)**<br>Created bioinformatics Python-based object-oriented webwares, adapted to routine practice: PhyID (bacterial and viral phylogenetic identification) and SequenceColourist* (nucleotide or peptide sequences colouring).<br>Trained the hospital users, evaluated the applications with their feedback and wrote manuals. |
| 2004<br>3 months | **Clinical and pharmaceutical fellowship training**<br>**Toliara's Province Reference Hospital Centre, Madagascar**<br>Introduced a sustainable hospital hygiene improvement program in cooperation with the hospital administration and the medical team.<br>Clinical fellowship training at psychiatry departement and maternity ward. |
| 2003-2004<br>9 months | **Clinical and pharmaceutical fellowship training**<br>**Poissy Saint-Germain-en-Laye Hospital Centre (Pr D Brossard)**<br>Clinical fellowship training in geriatrics: Investigated statistical analysis of prescriptions.<br>Pharmaceutical fellowship training: Dispensed drugs, and reconstituted antineoplastic agent. |
| 2002-2003<br>6 months | **C Developer**<br>**Biomathematics laboratory, School of Pharmacy, Paris 5 University (Pr S Bénazeth)**<br>Created a population sampling simulation software, based on Monte-Carlo simulation.<br>Participated in the development of a complex speciation software. |
| 2000-2001<br>3 months | **PHP MySQL Developer**<br>**ViralGames, Incubator of the Telecommunications National School of Paris**<br>Created a PHP/MySQL dynamic statistics graphics rendering engine. |
| 1998-2000<br>8 months | **Steward**<br>**Air France, Roissy Charles De Gaulle airport**<br>Steward on the North American, African, Asian and European networks. |

## Education

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| 2006 | **Doctor of Pharmacy, with Honours**<br>National competitive examination<br>Research Thesis: *An application of molecular modelling: the human intestinal absorption*<br>*School of Pharmacy, René Descartes Paris 5 University (Pr S Bénazeth)*<br>*Technologie Servier, Biopharmaceutical research department, Orléans (Dr Ph Vayer)* |
| 2006 | **2nd level MSc Degree equivalent "Bioinformatics", with Distinction**<br>*Denis Diderot Paris 7 University (Pr C Etchebest)* |
| 2005 | **1st level MSc Degree equivalent "Structural Bioinformatics", with Honours**<br>*School of Pharmacy, René Descartes Paris 5 University (Pr S Bénazeth)* |
| 2004 | **1st level MSc Degree equivalent "Biological and Medical Sciences"**<br>*School of Pharmacy, René Descartes Paris 5 University* |

## Publication

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| 2009 | *Interactive text mining with Pipeline Pilot: a bibliographic web-based tool for PubMed.*<br>Vellay SG, Latimer NE, Paillard G.<br>*Infect Disord Drug Targets.* 2009 Jun;9(3):366-74. |

## Computational Skills

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| Scientific applications | **Data Pipelining** <br> Pipeline Pilot (expert in most component collections) <br><br> **Molecular Modelling** <br> Tripos (SYBYL & SYBYL Programming Language), GROMACS, CHARMM <br><br> **Quantitative Structure-Activity Relationships (QSAR)** <br> Pipeline Pilot data modeling collections, VolSurf, Almond, GRID, Golpe, MetaSite, ComFa <br><br> **Bioinformatics** <br> Pipeline Pilot biology collections, Muscle, Clustalw, NJPlot, PhyID, Seaview, SequenceColourist* |
| Computer sciences | **Operating systems** <br> Mac, Linux, Windows <br><br> **Programming & Scripting** <br> Python, PHP, R, Linux Shell, C, OpenGL <br><br> **Databases & Web Design** <br> MySQL, PHPMyAdmin, Apache, JavaScript, HTML, CSS, LaTeX |

## Associative Activities & Interests

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| Musical training | **Advanced Musical Studies Diploma in clarinet and in chamber music (DFE)** <br> Bass clarinet, Sopranino, soprano, alto, tenor and bass recorders, Symphonic orchestra <br> *Francis Poulenc music conservatory, Paris 16 & Ménestrel music school, Chantilly 60* <br><br> **Sans dessus de Sons, association president (since 2007)** <br> Coaching the soundpainting ensemble Amalgammes <br><br> **Takalo-mozika, jazz association founder president (1999-2005)** <br> Planned, budgeted and organized a cultural exchange tour with artists throughout Madagascar. <br> Performed tours, regular concerts, and led a weekly jazz jam session with PavéJazz. |
| Volunteer work | **Huma Pharma, association member (1998-2004) and vice-president (1999-2001)** <br> Created an annual hospital hygiene improvement program in Madagascar (since 2002). <br> Started a weekly program aimed at working with homeless (since 2001). <br> Founded an annual cultural festival, making public aware of volunteer work (since 2000). |
| First aid | **Obtained the first aid training certificate.** |

## References

**References available upon request**