

PhD in Chemical Sciences  
Department of Chemistry "Ugo Schiff"  
University of Florence

PhD course ""  
**CURRICUL VITAE**

**Dr Michela Simone M.Sc. (1<sup>st</sup> Class Hons), D.Phil. (University of Oxford)**



## 1 Short CV

**Email:** [michela.simone@csiro.au](mailto:michela.simone@csiro.au)

**Webpages:**

- Google Scholar: <https://scholar.google.com.au/citations?user=TCvPqaAAAAAJ&hl=it>
- ORCID: <https://orcid.org/0000-0002-1339-8236>
- Researchgate: [https://www.researchgate.net/profile/Michela\\_Simone2](https://www.researchgate.net/profile/Michela_Simone2)

**Areas of Research:** Renewable Fuels from Biomass, Ionic Liquids, Spectroscopy, Mechanistic Studies, Medicinal Chemistry, Glycobiology/Carbohydrate Chemistry, Bioinorganic Chemistry, Organic Boron.

**Languages** English (fluent), Italian (native), Spanish (advanced), German (advanced).

### CURRENT POSITION

**May 2022- Current: Project Leader** in Renewable Fuels: Hydrogen from cool Water Splitting via a Multi-Pronged Catalytic Approach. Leading a team of 8 in this research program at the interface of physical chemistry, physics and engineering. *Commonwealth Scientific and Industrial Research Organisation (CSIRO), 10 Murray Dwyer CCT, Mayfield West NSW2304, Australia.* CSIRO is Australia's National Scientific Agency.

### PREVIOUS POSITIONS HELD

**Jan 2014-Oct 2021: Lecturer in Medicinal Chemistry and Chemical Biology (Level B, tenured, full time),** *School of Environmental and Life Sciences, Discipline of Chemistry, The University of Newcastle, Australia.*

**Dec 2010-Dec 2013: Lecturer in Chemistry (Medicinal and Biological, Level B, fixed-term, tenure-track, full time),** *School of Chemistry, University of Sydney, Australia.*

**Feb-Nov 2010: Post-Doctoral Fellow,** *Chemistry Research Laboratory, University of Oxford, U.K.,* Advisor: Vice-Chancellor Professor Andrew D. Hamilton. Research position in protein-protein interactions, initial development of my research in drug leads containing organic boron.

**2007-2010: Post-Doctoral Fellow,** *Wolfson Institute for Biomedical Research, University College London, U.K.,* Advisor: Professor David Selwood. Research position in medicinal chemistry, encompassing synthetic development of low Fsp<sup>3</sup> index drug leads, biological evaluations and *in silico* work.

### HIGHEST TERTIARY QUALIFICATION

Doctor of Philosophy (D.Phil.), Dyson Perrins Laboratory/Chemistry Research Laboratory, University of Oxford, U.K., Supervisor: Professor George W. J. Fleet. Thesis title: Studies on Branched Sugar Lactones.

#### TECHNICAL CONSULTING AND ADVISORY ACTIVITIES (SINCE 2012)

Consulting with clients in Academia, Industry and the Public Service in the following:

- **Teaching:** the Australian Federal Government as a Ramboll Pty subcontractor. Scope of work: online teaching modules in Chemistry for public servants.
- **Forensics:** analysis of illegal drug samples for the NSW Forensic Evidence and Technical Services Command. Evidence to be used in a court case.
- **Research:** Biomass for renewable energy production (for physical chemistry applications), NMR/IR/UV/Mass Spec/X-ray crystallography advanced analytical skills (inorganic chemistry), mechanistic skills (for novel biological fluorescent tags), carbohydrate/Maillard chemistry (for nutrition/industry project about manuka honey production).
- **Senior Editing** for Wiley, the medicinal chemistry journal Chemical Biology & Drug Design.

#### SELECTED HONOURS AND AWARDS

- **\*Awarded\* the Royal Australian Chemical Institute Nyholm Youth Lectureship 2015-2016**
- Selected to attend the annual conference of the Australian Academy of Sciences, *Science at the Shine Dome* – for Early- and Mid-career Researcher Program, Canberra (2014).
- **\*Finalist\*** of the Biohackathon science competition (aims at producing *novel approaches and solutions* to a selected life science problem of great importance to the community. This year: **Quick and inexpensive detection of biofilms in the clinic** - <http://atp-innovations.com.au/biohackathon/> (2013).
- **\*Awarded\*** four courses (for a total of £12,000) from the Centre for Scientific Enterprise Ltd (CSEL), London, U.K. to attend four MBA elective course (2007-2009).
- My D.Phil. Studies were financially supported by the European Union for 3.5 years *via* a European Research Training Network Award (for a total of £37,000) (2002-2006).
- **\*Socrates Awardee from the European Union\*** to spend the academic year 2000-2001 studying and getting involved in research at the Institut für Organische Chemie, Georg-August-Universität, Göttingen, Germany (for a total of €8,000) (2000).

#### PRINCIPAL INSTRUMENTATION AND SOFTWARE SKILLS

**Physical Chemical Analytical Methods:** Include Nuclear Magnetic Resonance, Circular Dichroism, Infrared, Ultraviolet, Mass Spectrometry, X-Ray Crystallography, HPLC, LCMS, GC, AAS, dissolution apparatus.

**Software and operating systems:** Molecular Operating Environment, PyMol, Chimera, VIDA.

**Experimental Biology:** Proficient in culturing cell, working in sterile environment, running ATPase assays. Proficient in the use of the Spectrophotometer ND-1000, the plate-reader Rosys-Anthos 2001, the liquid handler Hamilton MicrolabStar.

**Flow Chemistry Instruments:** H-Cube, Microwave, RevelR.

**Certificate in handling of unsealed radioactive materials.**

**Mechanical Engineering:** 3D printers, water jet cutter.

#### RESEARCH

**RESEARCH FUNDING:** AUD 1.33 M (since 2011, as sole applicant or as co-applicant, including for the Priority Research Centre for Drug Development at the University of Newcastle).

**SCIENTIFIC PUBLICATIONS: 61 (since 2004). Patents: 1**

<https://patentscope.wipo.int/search/en/detail.jsf?docId=WO2010097604>.

Scholar Metrics: 1181 Citations (on 29 March 2022). H-Index = 19.

Publications available from:

- Google Scholar: <https://scholar.google.com.au/citations?user=TCvPqaAAAAAJ&hl=it>
- ORCID: <https://orcid.org/0000-0002-1339-8236>

#### VERBAL SCIENTIFIC COMMUNICATIONS

Engagements at National and International Chemistry Conferences: 34 (since 2004). Research Seminars in Universities and other Institutions: 22 (since 2003, inclusive in German).

#### STUDENT RESEARCH SUPERVISIONS AT CSIRO

Undergraduate: 2 (Project).

#### **STUDENT RESEARCH SUPERVISIONS (since 2011)**

Graduate (Ph.D.): 7. Undergraduate: 9 (Honours), 24 (Project, inclusive of two international students), 9 (voluntary).

#### **EXAMINER (since 2011)**

Ph.D. Candidatures: Progress: 1; Confirmations: 5; Completions: 2.

Honours Thesis and Seminar Examiner (about 7 *pa*); Project student coursework (about 18 *pa*).

External (National and International) Ph.D. Completion Examinations: 4.

#### **SCIENTIFIC ASSESSOR OF DOMESTIC AND INTERNATIONAL FUNDING PROPOSALS**

for the National Science Centre, Poland (since 2021); for Australian Research Council (ARC) Discovery Project funding rounds (since 2021); for the Croatian Science Foundation (HRZZ) (since 2020); for the Priority Research Centre for Drug Development at the University of Newcastle (2017-2018).

### **COMMUNICATIONS AND TEACHING**

#### **HONOURS AND AWARDS IN COMMUNICATIONS AND TEACHING**

Royal Australian Chemical Institute Nyholm Youth Lectureship 2015-2016 (2014) for outstanding Science Communication.

Certificate in University Assessment, Centre for Teaching & Learning, University of Newcastle (2018).

#### **LECTURE COURSES, TEACHING LABORATORIES, AND CURRICULUM DEVELOPMENT (SINCE 2011)**

At the University of Newcastle (2014-2021):

- Lecturer in 1<sup>st</sup>, 2<sup>nd</sup> and 3<sup>rd</sup> Year undergraduate courses: 6 (2014); 7 (2015); 9 (2016); 10 (2017); 6 (2018); 3 (2019), 9 (2020).
- Supervisor in 1<sup>st</sup>, 2<sup>nd</sup> and 3<sup>rd</sup> Year undergraduate teaching laboratories: 6 (2014), 7 (2015), 6 (2016), 6 (2017), 1 (2019), 5 (2020).
- Curriculum developer for courses I taught, including the transfer to online technology during COVID-19: 3 (2014); 2 (2015, inclusive of teaching laboratory component); 3 (2016, inclusive of teaching laboratory component); 1 (2019, I spearheaded the Faculty of Science move to online modules); 5 (2020, inclusive of move to online modules due to COVID-19).
- Course Coordinator of 1<sup>st</sup>, 2<sup>nd</sup> and 3<sup>rd</sup> Year undergraduate courses: 2 (2015); 4 (2016); 2 (2017); 2 (2018); 4 (2020); 1 (2021).

At the University of Sydney (2011-2013): Taught in two 1<sup>st</sup> Year courses *pa* and supervised 1<sup>st</sup>, 2<sup>nd</sup> and 3<sup>rd</sup> Year undergraduate teaching laboratories. I developed curriculum for the two 1<sup>st</sup> Year courses I taught into.

**LARGEST OPERATIONS** I led: the One-on-One Tutoring Scheme for 1<sup>st</sup> Year Chemistry Cohorts, Course Coordination for 1<sup>st</sup> Year Chemistry Courses (2017-2020).

**GRANTS FOR COURSE DEVELOPMENT:** 2 (AUD 8150).

**TEACHING AT ENAP MIGLIANICO WHILE ON MATERNITY LEAVE (2019):** Physics and Chemistry to migrant teenagers from Africa and the Middle East studying to achieve middle school certificate (Licenza Media).

#### **PROFESSIONAL DEVELOPMENT**

1. Modules: Online Assessment, Principles of Assessment, Effective and Engaged Supervision, Preventing Violence in the Workplace, Assessment and Feedback, Creating Multiple-Choice Questions, Assessment of Teaching, Rubrics, Higher Degree by Research (PhD) Thesis Examination.
2. Leadership Skills Enhancement: I was tapped at Faculty of Science level for a Personal Development Plan facilitated by Organisational Psychologist, over one-on-one sessions with Opra Psychology Group (<https://www.opragroup.com>).

### **COMMUNICATIONS AND OUTREACH**

**OUTREACH SEMINARS TO SECONDARY SCHOOL STUDENTS AND CAREER EVENTS:** 25 (2012-2018), inclusive of:

- Science Panel Discussion. Topic: Women in STEM. University of Newcastle (2018);

- RACI Award Ceremonies at the University of Newcastle (2018).
- Student Career Engagements with TAFE (2016-2017).
- Interview for Television Journalism on perfluorooctanesulfonate (PFOS) and perfluorooctanoic acid (PFOA) used at the Williamtown Royal Australian Air Force base, University of Newcastle (2016).
- **RACI Nyholm Youth Lectureship Occasional Speaker** at RACI Presidents' Dinner, Sydney (2016).
- **\*RACI Nyholm Youth Lectureship Outreach Seminars to Secondary School Students\***: James Ruse Agricultural School, Gosford Secondary School, Western Sydney University, University of New South Wales, Orange Secondary School, Abbotsleigh Secondary School, Merewether Secondary School, Koorringal Secondary School, Bowral Secondary School, Kadina Secondary School, University of Sydney (approx. 1800 students, 2015-2016).

**At University of Newcastle:** Outreach to Secondary Schools through presence at Science Award Ceremonies (2014-2016); Discipline of Chemistry Open-Days & Outreach events (2014-2017), inclusive of career seminars.

**At University of Sydney:** School of Chemistry Open-Days & Outreach events (2012-2013), inclusive of career seminars.

### **GOVERNANCE AND SERVICE**

#### **PROFESSIONAL ACTIVITIES AT UNIVERSITY OF NEWCASTLE**

- **Research Management:**
  - Member of the Managing Committee of the Priority Research Centre for Drug Development (2018-2019).
- **Committee Member for:**
  - Equity, Diversity and Inclusion Committee (2019-2020).
  - Faculty of Science's Teaching & Learning Committee (2017).
  - Faculty Award Committee on: Research Innovation Excellence, Teaching Excellence and Contribution to Student Learning, Sessional Staff Award for Teaching Excellence and Contribution to Student Learning.
  - Discipline of Chemistry, School and Faculty of Science Meetings (2014-2021).
- **Presentations:** RACI Award ceremonies, Faculty of Science Teaching Showcase: 2017 One-on-One Tutoring Scheme for CHEM1010 presentation, Panel discussion for O-Week organised by the Faculty of Science, Faculty of Science Graduation Ceremonies.
- **Coordinatorship:**
  - Seminar Program of the Discipline of Chemistry, University of Newcastle, Australia (2015).
  - Work Health & Safety Coordinator for the Organic Chemistry research labs (2014-2021).

#### **PROFESSIONAL ACTIVITIES AT UNIVERSITY OF SYDNEY**

- **Coordinatorship:**
  - School of Chemistry Open-Days & Outreach events (2012-2013).
  - Seminar Program in the School of Chemistry (2013).
- **Committee Member for:**
  - Member of the Science and Mathematics Network of Australian University Educators Committee (2011-2013).

#### **PROFESSIONAL MEMBERSHIPS**

Royal Society of Chemistry (MRSC, 2010-Curr.); Inorganic Chemistry Foundation at the University of Sydney (2012-Curr.); Royal Australian Chemical Institute (MRACI, 2012-Curr.); Priority Research Centre for Drug Development at University of Newcastle (2013-2019).

#### **JOURNAL PEER-REVIEWING AND ASSOCIATE EDITING**

*Chemical Biology & Drug Design* (Associate Editor since 2011); *PLoS ONE* (since 2011); *Australian Journal of Chemistry* (since 2012); *European Journal of Organic Chemistry* (since 2013); *Tetrahedron: Asymmetry* (since 2014); *ACS Applied Materials and Interfaces* (since 2015); *Bioorganic Medicinal Chemistry* (since 2017).

#### **SCIENTIFIC CONFERENCE ORGANISATION AND INVOLVEMENT WITH THE RACI**

**2015-2020:** President of the RACI Newcastle/Hunter Section. Main engagements: Job Readiness Seminar organised in conjunction with Technical And Further Education (TAFE) College colleagues for students at the University of Newcastle and TAFE (2016). Selected research seminars of the Discipline of Chemistry were sponsored by the

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Newcastle/Hunter RACI Section (2015-2016). Mentor for the RACI Mentoring Program of New South Wales, Australia (2016-2020).

**2012-2013:** Member of the Organising Committee for the RACI Institute Biomolecular Division National Conference "Biomolecular in the Bush", Leura, Australia, 14-17/07/2013. Organisation of this big Conference took almost two years, featured mostly international plenary speakers and was highly attended.

**2012:** Member of the Organising Committee for the RACI Biomolecular Division New South Wales Student Meeting, University of Sydney, Australia, 01/06/2012.

#### **FURTHER PROFESSIONAL DEVELOPMENT ENGAGEMENTS**

Women & Leadership Australia Leadership in Action high impact course (2022). Turbo-Charge Your Writing, Developing a Research Track-Record on a Shoestring, Planning Your Research Career, Statistics Course (2017), IP, Commercialisation and Contract Research Workshop, Research Development Series (2014), University of Newcastle. Future Research Leaders Program (CareerPath) (2013) Leading and Building Positive Working Relationships (CareerPath) (2012), Vibrational Spectroscopy Course: Theory and Practical Aspects, New Synchrotron and Neutron Users Symposium UNSW (2011).

Recruitment and Selection, Equal Opportunity, Think-Write: Quality Papers, Intellectual Property, University College London, U.K. (2009).

MBA Elective courses: Value Creation, Energy: Markets, Models and Strategies, New Technology Development, New Technology Ventures, London Business School, U.K. (2007-2009).

Spanish Basic intensive OPAL course, Spanish Intermediate intensive OPAL course (2005-2007), Oxford University Language Centre, U.K.

## 2 Bibliometric data

**Scholar metrics: 1294 (on 30 November 2022). h-Index = 19. SJR = Scimago Journal Ranking. Researchgate Research Interest Score = 568.** Relative to opportunity I have been highly successful with publications with 62 to date (27 as corresponding author (CA)), h-index of 19 (Scholar) and an upwards trajectory: 8 publications in 2011-2013 (130 cit), 8 in 2014-2016 (189 cit) and 15 in 2017-2019 (303 cit), so far 10 in 2020-2022 (so far 390 cit).

- Google Scholar: <https://scholar.google.com.au/citations?user=TCvPqaAAAAAJ&hl=it>
- ORCID: <https://orcid.org/0000-0002-1339-8236>
- Researchgate: [https://www.researchgate.net/profile/Michela\\_Simone2](https://www.researchgate.net/profile/Michela_Simone2)



ORCID Code

### 3. Selection of the 10 most relevant publications and/or patents

- A62 (CA27)** D. M. Campkin, Y. Shimadate, B. Bartholomew, P. V. Bernhardt, R. J. Nash, J. A. Sakoff, A. Kato, **Michela Simone\***, Borylated 2,3,4,5-Tetrachlorophthalimide and Their 2,3,4,5-Tetrachlorobenzamide Analogues: Synthesis, Their Glycosidase Inhibition and Anticancer Properties in View to Boron Neutron Capture Therapy, *Molecules*, **2022**, *27*, 3447-3475. *Invited Research Article for the Women in Bioorganic Chemistry Special Issue*. doi: <https://doi.org/10.3390/molecules27113447>.
- A57 (CA23)** A. Glenister, C. K. J. Chen, A. K. Renfrew, **Michela Simone\***, T. W. Hambley, Warburg Effect Targeting Cobalt(III) Cytotoxin Chaperone Complexes, *Journal of Medicinal Chemistry*, **2021**, *64*, 2678-2690. doi: [org/10.1021/acs.jmedchem.0c01875](https://doi.org/10.1021/acs.jmedchem.0c01875)
- A53 (CA20)** M. Ghorbani, **Michela Simone\***, Developing New Room-Temperature Ionic Liquids with High Thermal Stability and a Greener Synthetic Profile, *ACS Omega*, **2020**, *5*, 12637-12648. doi: [10.1021/acsomega.9b04091](https://doi.org/10.1021/acsomega.9b04091)
- A52 (CA19)** A. Glenister, **Michela Simone\***, T. W. Hambley, Synthesis and Evaluation of a Warburg Effect Targeting Vector to Increase the Uptake of Compounds by Cancer Cells, *PlosOne*, **2019**, e0217712. doi: [10.1371/journal.pone.0217712](https://doi.org/10.1371/journal.pone.0217712)
- A40** K. Latham, **Michela Simone**, W. Dose, J. Allen, S. Donne, Synchrotron Based NEXAFS Study on Nitrogen Doped Hydrothermal Carbon: Insights into Surface Functionalities and Formation Mechanisms, *Carbon*, **2017**, *114*, 566-578. doi: [10.1016/j.carbon.2016.12.057](https://doi.org/10.1016/j.carbon.2016.12.057)
- A33** A. Moyes, R. Khambata, I. Villar, K. Bubb, R. Baliga, N. Lumsden, F. Xiao, P. Gane, A.-S. Rebstock, R. Worthington, **Michela Simone**, F. Mota, F. Rivilla, S. Vallejo, C. Peiró, C. S. Ferrer, S. Djordjevic, M. Caulfield, R. MacAllister, D. Selwood, A. Ahluwalia A. Hobbs, Endothelial C-type natriuretic peptide maintains vascular homeostasis, *Journal of Clinical Investigation*, **2014**, *124*, 4039-4051. doi: [10.1172/JCI74281](https://doi.org/10.1172/JCI74281)
- P29** **Inventors:** D. Selwood, A.-S. Rebstock, **Michela Simone**, M. Gooding, K. Stoeber, S. Tudzarova, C. Boshoff, G. Williams, S. Kingsbury, D. Lagos, M. Funes Quesada, Guanidino-substituted bi- and polyphenyls as small molecule carriers. **Pub. No.:** WO/2010/097604; **International Application No.:** PCT/GB2010/000359; **Publication Date:** 02/09/2010; **International Filing Date:** 01/03/2010. <https://patentscope.wipo.int/search/en/detail.jsf?docId=WO2010097604>
- A28 (CA9)** **Michela Simone\***, R. G. Soengas, S. F. Jenkinson, E. L. Evinson, R. J. Nash, G. W. J. Fleet, Synthesis of three branched iminosugars [(3*R*,4*R*,5*S*)-3-(hydroxymethyl)piperidine-3,4,5-triol, (3*R*,4*R*,5*R*)-3-(hydroxymethyl)piperidine-3,4,5-triol and (3*S*,4*R*,5*R*)-3-(hydroxymethyl)piperidine-3,4,5-triol] and a branched trihydroxynipectic acid [(3*R*,4*R*,5*R*)-3,4,5-trihydroxypiperidine-3-carboxylic acid] from sugar lactones with a carbon substituent at C-2, *Tetrahedron: Asymmetry*, **2012**, *23*, 401-408. doi: [10.1016/j.tetasy.2012.03.007](https://doi.org/10.1016/j.tetasy.2012.03.007)
- A23 (CA7)** **Michela Simone\***, A. A. Edwards, G. E. Tranter, G. W. J. Fleet, C-3 Branched  $\delta$ -3,5-*cis*- and *trans*-THF Sugar Amino Acids: synthesis of the first generation of branched homooligomers, *Amino Acids*, **2011**, *41*, 643-661. *Invited Research Article for the Special Issue on Foldamers*. doi: [10.1007/s00726-011-0849-7](https://doi.org/10.1007/s00726-011-0849-7)
- A13** R. A. Jockusch, F. O. Talbot, P. S. Rogers, **Michela Simone**, G. W. J. Fleet, J. P. Simons, Carbohydrate Amino Acids: The Intrinsic Conformational Preference for a  $\beta$ -Turn-Type Structure in a Carbopeptoid Building Block, *Journal of the American Chemical Society*, **2006**, *128*, 16771-16777. doi: [10.1021/ja0607133](https://doi.org/10.1021/ja0607133)