To the Dean of the Faculty of Chemical Technology of the University of Chemistry and Technology, Prague

Proposal for commencement of Professor Appointment Proceedings for the field of Organic Chemistry

Name: Andrea Brancale
Birth code: XXXX
Residence address: XXXX,Prague
Workplace: Department of Organic Chemistry

Proposal supported in writing by:

1. Professor Pete Williams
2. Professor Kathie Seley-Radtke
3. Professor Chris Meier

Please find attached to my proposal (under Section 74, paragraph 2 of the Act No. 111/1998 Coll., on Higher Education Institutions and on Changes and Amendments of Other Acts) the following documents in written and electronic forms:

1. **File in non-modifiable binding containing** (Note: everything in 3 printed copies + electronic copy to be sent to the e-mail address of the Dean´s Office)
   a) curriculum vitae,
   b) overview of pedagogical and professional activities,
   c) overview of scientific and professional works, invention and realization activities, professional and social activities, international cooperation, domestic and foreign internships, and the most important creative activities,
   d) brief pedagogical project.

2. **I further attach to my proposal:**
   - Habilitation Certificate
   - Ph.D. Certificate
   - Master Certificate

Date: 22nd October 2025 Signature:

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1. Curriculum Vitae

1.1 Personal data

Name: Andrea Brancale
Date of birth: XXXX 1971
Place of birth: XXXX, Italy
Marital status: XXXX
Residence: XXXX, Prague, Czech Republic

1.2 Education

- 2001 Ph.D., Design, synthesis and evaluation of novel antiviral nucleosides, Welsh School of Pharmacy, Cardiff University. Supervisor: Prof. Chris McGuigan.
- 1996 Laurea in Chimica e Tecnologia Farmaceutiche, Universita' "La Sapienza", Roma. Research Project: Design and synthesis of novel heterocyclic compounds as anti-HIV agents.

Other Qualifications

- 1997 Qualified Pharmacist – University of Rome "La Sapienza"
- 2024 Industrial Property Course Patents 2024 – Certification ISO 9001:2015 – Polytechnic University of Milan

1.3 Career

- 2022 - date Chair of Medicinal Chemistry, University of Chemistry and Technology, Prague.
- 2017-2022 Professor of Medicinal Chemistry, Cardiff University.
- 2015-2017 Reader in Medicinal Chemistry, Cardiff University.
- 2011-2015 Senior Lecturer in Medicinal Chemistry, Cardiff University.
- 2002-2011 Lecturer in Medicinal Chemistry, Cardiff University.
- 2001-2002 Research Associate, Cardiff University.

2. Pedagogical Activity

2.1 Overview

Subject (typ of study- master, bachelor, PhD)	Scope (hours / week)	Number of semesters	Type (P=lecture, C=exercise, L=laboratory)	Number of students examined
Master of Pharmacy (year 1)- Organic chemistry laboratory classes	9h/week	22	L	110
Master of Pharmacy (year 2)- Organic chemistry laboratory classes	4h/week	15	L	100
Master of Pharmacy (year 2)- NMR Lectures	2h/year	12	P	100
Master of Pharmacy (year 2)- NMR coursework	2h/year	12	C	100
Master of Pharmacy (year 3)- Module Leader for "Optimisation of Drug Design" - Lectures	10h/semester	44	P	100
Master of Pharmacy (year 3)- Module Leader for "Optimisation of Drug Design" - Coursework	10h/semester	44	C	100
Master of Pharmacy (year 4)- Molecular Modelling workshops	8h/semester	14	C	100
MSc Bioinformatics - Lecture on Computer-aided drug design	2h/semester	10	P	20
MSc Medicinal Chemistry - Lecture on Computer-aided drug design	4h/semester	8	P	15
Ph.D. Drugs and Biomaterials – Drug Design and Discovery course	28h/semester	1	P	10

In grey, classes previously taught at Cardiff University

2.2 Supervision over students

Defended bachelor theses: 5 (at UCT)

Defended master theses: 46 (at Cardiff University)

Defended doctoral dissertation theses: 29 (at Cardiff University) – list below. The star indicates main supervision, others specialised co-supervision.

1. *2002/05, Dimitrios Vlakakis (departmental funding). Topic: Antiviral Drug Design. Subsequent post: Academic position in Greece.
2. *2003/06, Maria Chiara Barbera (Departmental funding). Topic: Anticancer Drug Design. Subsequent post: Regulatory body, Italy.
3. 2004/07, Mohamed Gomaa (Funded by The Embassy of the Arab Republic of Egypt – Main supervisor C. Simons). Topic: Anticancer Drug Design. Subsequent post: Research assistant, Cardiff University (CRUK grant; C. Simons and A. Brancale)
4. *2005/08, Sahar Kandil (Funded by The Embassy of the Arab Republic of Egypt). Topic: Antiviral Drug Design. Subsequent post: Research Assistant, Cardiff University (Prof. C. McGuigan)

5. 2005/08, Rocco Valente (Funded by the Leukaemia Research Appeal for Wales – Main supervisor C. McGuigan). Topic: Antiviral Drug Design. Subsequent post: employed at the Chemical Abstracts Service.

6. *2006/09, Nicola Zonta (66% Departmental – 33% Inhibitex Inc. funding). Topic: Antiviral Drug Design. Subsequent post: Software developer for Schrödinger Inc.

7. *2006/09, Mohammed Khedr (Funded by The Embassy of the Arab Republic of Egypt). Topic: Antiviral Drug Design. Subsequent post: Academic position in Saudi Arabia.

8. 2009/12, Salvatore Ferla (Funded by CRUK– Main supervisor C. Simons). Subsequent post: Lecturer, Swansea University (Dr.Brancale)

9. *2010/13, Marcella Bassetto (100% Biovitas funding). Topic: Antiviral Drug Design. Subsequent post: Lecturer, Swansea University (Prof. C. McGuigan)

10. *2010/14, Athanasios Anthopoulos, (The President's Studentship program). Subsequent post: Research Assistant, UCL.

11. 2010/13 Jitka Soukupova (The President's studentship program; Main supervisor Dr. Richard Clarkson - BIOSI). Topic: Anticancer Drug Design.

12. *2011, Iuni Trist (Funded by EU-ITN Euvirna). Topic: Antiviral Drug Design.

13. *2011, Michela Cancellieri (Funded by EU-ITN Euvirna). Topic: Antiviral Drug Design.

14. 2012, Olivia Hyward (funded by Cancer Research Wales; Main supervisor Dr. Richard Clarkson - BIOSI). Topic: Anticancer Drug Design.

15. 2012, Daniele Avancini (funded by HPC Wales; Main Supervisor Paul Lewis, Swansea University). Topic: Anticancer Drug Design.

16. *2013, Cinzia Bordoni (Funded by Cancer Research Wales). Topic: Anticancer Drug Design.

17. 2013, Dan Turnham (Funded by LSRNW/Biovitas; Main supervisor Dr. Richard Clarkson - BIOSI). Topic: Anticancer Drug Design.

18. *2014, Cecilia Cima (Funded by LSRNW/Henson Foundation). Topic: Antiviral Drug Design.

19. 2014, Gaia Pasqualetto (Funded by LSRNW/BIOSI; Main supervisor Dr. Mark Young - BIOSI). Topic: P2X-Receptors binders.

20. 2014, Edward James (Funded by LSRNW/PHRMY; Main supervisor Prof. C. McGuigan).

21. 2014, Carmen Jimenez Antunez (Funded by LSRNW/Nucana; Main supervisor Prof. C. McGuigan). Topic: Anticancer Drug Design.

22. *2015, Gilda Giancotti (Funded by Tiziana Life Sciences). Topic: Anticancer Drug Design.

23. *2015, Birgit Zonsics (Funded by H2020 ETN-ANTIVIRALS). Topic: Antiviral Drug Design.

24. *2015, Roberto Manganaro (Funded by H2020 ETN-ANTIVIRALS). Topic: Antiviral Drug Design.

25. 2015, Elisa Pileggi, (Funded by LSRNW/PHRMY; Main supervisor Dr. F. Pertusati). Topic: Anticancer Drug Design.

26. 2015, Gilda Padalino (Funded by LSRNW/ABER; Main supervisor Prof. K. Hoffmann, Aberystwyth University). Topic: Anthelmintics Drug Design.

27. 2016, Carmine Varricchio (Funded by PHRMY/OPTOM; Main supervisor Dr. C. Heard). Topic: Mitochondria modulators.

28. 2019, Marika Zuanon (Main Supervisor Dr. M. Young). Topic: P2X-Receptors binders

29. *2019, Marialuce Avigliano (Funded by Cancer Research Wales). Topic: Anticancer Drug Design.

Current doctoral dissertation theses: 1 as specialist supervisor (at UCT)

1. Jakub Harvalik; Topic: Computer aided design and synthesis of novel transcription factors modulators. Principal Supervisor: Cuřínová Petra Ing. Ph.D.

2.3 Authorship of teaching texts and aids, other pedagogical activities

- Preparation of original course material (lecture, handouts, coursework exercises) for the teaching classes indicated in section 2.1
- Preparation of study materials, including presentations, for the Drug design and Discovery courses, to support accreditation of the novel study program "Drugs and Biomaterials".
- External examiner for Chemical Pharmacology course in Oxford University (2014 – 2019)
- Ph.D. external examiner at Nottingham University, School of Pharmacy; Manchester University, School of Pharmacy; Trinity College, School of Pharmacy, Dublin; Kingston University, School of Pharmacy and Chemistry; Swansea University, School of Chemistry.
- External Ph.D. examiner for the University of Eastern Piedmont, Italy; IEO-University of Milan; University of Messina, Italy.

2.4 Innovative contribution to pedagogical work

During my tenure at Cardiff University, I was actively involved in teaching across all levels of the MPharm degree, covering various aspects of medicinal chemistry, from fundamental organic synthesis to more advanced computer-aided drug design techniques. Each year, I supervised 3-4 project students in my laboratory as part of their final (Master's) year research project assignment.

My specific contributions to teaching and scholarship within the Cardiff Master of Pharmacy (MPharm) included:

MPharm 1. PH1125: I was involved in laboratory classes where students engaged with fundamental organic chemistry methods and techniques. These sessions enabled students to perform basic organic chemistry experiments designed to support lecture content and enhance their understanding of theoretical principles.

MPharm 2. PH2112: In this module, I delivered lectures on NMR spectroscopy and conducted a workshop on analytical techniques used to determine chemical structures.

MPharm 3. PH3101 (Module Leader): This module introduced students to advanced drug design concepts. My initial lectures covered the fundamentals of computer-aided drug design, lead optimisation, and advanced medicinal chemistry methodologies. These topics were reinforced through a CAL session focused on the visualisation and manipulation of three-dimensional protein structures. Later in the module, I delivered lectures on two specific drug classes (Sulphonamides and DHFR inhibitors), illustrating how drug design principles were applied in real-world scenarios. Towards the end of the module, I led exam preparation activities, including a revision workshop and an interactive lecture using clickers to facilitate student participation. Additionally, I was responsible for organising and assessing the "Group Presentation on Infectious Diseases" coursework associated with this module.

MPharm 4. PH4117: In this module, I provided an introductory lecture on computer-aided drug design methods and techniques relevant to the coursework. To support this, I also conducted a CAL session where students learned to use a professional molecular modelling software package for basic experimental applications.

Beyond the MPharm programme, I also lectured in the Master's in Bioinformatics at the Cardiff Medical School and the Master's in Medicinal Chemistry and Drug Design at the Cardiff School of

Chemistry. As students in these programmes came from diverse academic backgrounds, I tailored my lectures to provide a broad overview of drug design and discovery, with a particular emphasis on molecular modelling methodologies.

Evidence of Teaching Innovation, Course Development, and Administration

From 2005 to 2016, I served as the Module Leader for PH3101 ("Optimisation of Drug Design"), overseeing the management, delivery, and assessment of the module content. My responsibilities included collecting student feedback and implementing revisions to enhance course materials. Given the module's interdisciplinary nature, I consistently sought innovative ways to integrate different scientific disciplines to provide students with a unified learning experience.

I used social media tools, such as a module wiki and a Facebook page, to encourage discussion around course content and highlight connections between different topics. Additionally, I introduced two workshop series on antibacterial and anticancer therapies, designed around specific case studies. These workshops successfully integrated scientific concepts with pharmacy practice considerations, proving to be highly popular with students.

To further enhance assessment strategies, I restructured the module's exam format in 2014. Instead of traditional compartmentalised questions, I designed an integrated approach, where the exam consisted of four multidisciplinary questions centred on specific topics, such as anticancer therapy. These questions encompassed various aspects of the topic, from drug design approaches to the clinical implications of treatments. To support student preparation, I provided a pool of 12 potential exam questions, from which four would appear in the final exam. This approach fostered a deeper engagement with the material and received praise from the External Examiner.

I championed the use of technology to improve student learning experiences. In 2012, I secured funding for the acquisition of 25 iPads for use in MPharm classes, a project well-received by faculty members. Due to increasing demand, the number of tablets was doubled in subsequent years to support a wider range of academic applications.

As a member of the Board of Studies and the Board of Examiners, I contributed to the ongoing design and evolution of the MPharm course. Additionally, I actively participated in peer assessment exercises, which provided valuable insights into teaching methodologies across different scientific backgrounds. Collaborations with pharmacy teaching practitioners, for example, helped me refine strategies for integrating science and practice more effectively.

Finally, I have always valued student feedback as a crucial component in the development of my teaching material. In addition to standard module feedback, I engaged with students directly as a rotating member of the Staff/Student Panel, ensuring that their perspectives contributed to continuous course improvements.

Currently at UCT, in the last academic year, I have started to deliver a course on Drug Design and Discovery, for PhD students, and in particular to the ones enrolled in the Drugs and Biomaterial scheme. I will discuss this more in details in section 2.5.

2.5 Pedagogical project

I currently teach a PhD course on *Drug Design and Discovery* for students in the *Drugs and Biomaterials* program. The course will be also adapted for a master study program (see below). This course covers all key aspects of modern drug discovery, from target validation to clinical trials. I designed the course with an emphasis on case studies and real-world examples, drawing from recent literature and news to provide students with up-to-date insights. Assessment is conducted through student presentations rather than traditional exams. Each student is assigned a therapeutic area of

interest and must develop a comprehensive drug discovery strategy, from target identification to potential therapy. This approach encourages students to critically reflect on the material and apply their knowledge to relevant research scenarios.

Building on this foundation, I plan to further enhance the course by inviting external specialists—researchers and clinicians actively engaged in drug discovery—to share their first-hand experiences with the students. This will provide valuable professional perspectives and bridge the gap between theoretical knowledge and practical application.

Additionally, based on my experience with PhD students, I contributed to designing a new master's program, *Chemoinformatics in Medicinal Chemistry*, in collaboration with the University of Strasbourg. This double-degree program is structured so that students complete their first year at the University of Chemical Technology and their second year at the Université de Strasbourg (UNISTRA), ensuring a cohesive learning experience. The curriculum includes key courses such as Fundamentals of Programming, Applied Programming, Molecular Modelling, Statistical Data Analysis, Multivariate Data Analysis, and Computational Drug Design. The master's program will join the *Erasmus Mundus Joint Master (EMJM) - ChEMoinformatics+* as an associate partner in 2026. By 2028, the University of Chemical Technology will become a full consortium member, and this program will serve as a dedicated EMJM track in *Chemoinformatics in Medicinal Chemistry*.

This international collaboration will offer significant opportunities, attracting high-calibre students from diverse backgrounds and strengthening the university's international profile. By participating in a globally recognised Erasmus Mundus programme, UCT will gain increased visibility, fostering academic excellence and research-driven innovation. Furthermore, this initiative will help build a strong international network, opening new avenues for collaboration with leading institutions and industry partners in medicinal chemistry and chemoinformatics.

3. Scientific Activity

3.1. Overview of scientific and research as well as innovative activities

	Activity	Count	Of that, in world language	SC[1]	Sum of IF/SJR[2]
1.	Research works in impacted journals recorded in the Web of Science (WoS)	223	English	7178	1122,2
2.	Research works in journals recorded in the Scopus database that are not stated in the Web of Science database				
3.	Research works in other peer-reviewed journals	1	English	0	-
4.	Chapters in monographies, monographies[3]	1	English	1	-
5.	Articles in journals without peer review, articles in proceedings	37	English	37	-
	TOTAL 1 – 5	**262**		**7216**	**1122,2**

	Activity	Count
6.	Personally given lectures abroad and at international conferences	27
7.	Co-author of other lectures and posters at international conferences	31
8.	Personally given lectures at national conferences	
9.	Co-author of other lectures and posters at national conferences	
	TOTAL 6 – 9	**58**
10.	Principal investigator of foreign grants and projects	24
11.	Principal investigator of domestic grants and projects	
12.	Co-investigator[4] of foreign grants and projects	25
13.	Co-investigator of domestic grants and projects	1
	TOTAL 10 – 13	50

[1] Sum of citations excluding self-citations according to the respective database (for WoS with the setup All Databases)
[2] Latest known IF or SJR of the journal
[3] SC represents the sum of citations excluding self-citations according to WoS with the setup All Databases
[4] Co-investigator is a person responsible for the professional part of the project to the co-recipient of the grant.

	Activity	Count
14.	Awarded European or international patents (EPO, WIPO), patents of USA and Japan	13
15.	Awarded Czech or other national patents utilized based on a valid licence agreement	
16.	Awarded Czech or other national patents utilized only by the owner of the patent or not utilized	
17.	Authorship of realized complex technical work with specified social benefit	1
18.	Pilot production, proven technologies	
19.	Utility models and industrial designs, prototypes, function samples, software	
	TOTAL 14 – 19	14

3.2. Research works in impacted journals recorded in the Web of Science database

ResearcherID: N-9445-2014

1. Ferenczei, J.; Blahout, V.; Dvorakova, H.; Brancale, A.; Curinova, P.; Labikova, M.; Kohout, M.; Setnicka, V.; Perlikova, P., Stereoanalysis of the Antiparasitic Natural Product Callunene and Its Synthetic Intermediates. J Nat Prod 2025**,** *88* (3), 723-731; Citations: 0; IF: 3.6
2. Queiros-Reis, L.; Kaarbø, M.; Al-Baldawi, H.; Alvites, R.; Mauricio, A. C.; Brancale, A.; Bassetto, M.; Mesquita, J. R., In Silico Discovery of a Novel Antiviral Scaffold for SARS-CoV-2 Targeting the Spike Glycoprotein through the Fatty Acid Binding Pocket. ACS Omega 2025, 10 (23), 24117-24132; Citations: 0; IF: 3.7
3. Rawat, M.; Padalino, G.; Adika, E.; Okombo, J.; Yeo, T.; Brancale, A.; Fidock, D. A.; Hoffmann, K. F.; Lee, M. C. S., Quinoxaline-based anti-schistosomal compounds have potent anti-plasmodial activity. PLoS Pathog 2025, 21 (2), e1012216; Citations: 0; IF: 4.9
4. Romagnoli, R.; Romagnoli, E.; Brancale, A.; Supuran, C. T.; Nocentini, A.; Manfreda, L.; Zanolli, A.; Bortolozzi, R.; Viola, G., Design and Synthesis of 2-substituted [1,2,4]Triazolo[1,5-a]pyrimidines Tethered with Umbelliferone as Selective Carbonic Anhydrase IX and XII Inhibitors. Anticancer Agents Med Chem 2025, 25 (18), 1429-1446; Citations: 0; IF: 2.8
5. Zuanon, M.; Brancale, A.; Young, M. T., Identification of New Human P2X7 Antagonists Using Ligand- and Structure-Based Virtual Screening. J Chem Inf Model 2025, 65 (13), 7143-7155; Citations: 0; IF: 5.7
6. Queiros-Reis, L., Alvites, R., Mauricio, A.C., Brancale, A., Bassetto, M. and Mesquita, J.R. Disrupting SARS-CoV-2 Spike Protein Activity, Int J Mol Sci, 2025, 26; DOI: 10.3390/ijms26010151; Citations: 0; IF: 4.9
7. Svobodova, K., Eigner, V., Brancale, A., Curinova, P. and Himl, M. Substituent-Driven Anion-Binding Selectivity in Aliphatic Chain-Substituted 1,2-Phenylene Urea Macrocycles and Optimized Synthetic Methodology, ChemistryOpen, 2025, e202400469; DOI: 10.1002/open.202400469; Citations: 0; IF: 2.9

8. Mariotto, E., Canton, M., Marchioro, C., Brancale, A., Hamel, E., Varani, K., Vincenzi, F., De Ventura, T., Padroni, C., Viola, G. and Romagnoli, R. Synthesis and Biological Evaluation of Novel 2-Aroyl Benzofuran-Based Hydroxamic Acids as Antimicrotubule Agents, Int J Mol Sci, 2024, 25; DOI: 10.3390/ijms25147519; Citations: 3; IF: 4.9
9. Seaton, G., Smith, H., Brancale, A., Westwell, A.D. and Clarkson, R. Multifaceted roles for BCL3 in cancer, Mol Cancer, 2024, 23; DOI: 10.1186/s12943-023-01922-8; Citations: 14; IF: 27.7
10. Tribble, J.R., Joe, M., Varricchio, C., Otmani, A., Canovai, A., Habchi, B., Daskalakis, E., Chaleckis, R., Loreto, A., Gilley, J., Wheelock, C.E., Johannesson, G., Wong, R.C.B., Coleman, M.P., Brancale, A. and Williams, P.A. NMNAT2 is a druggable target to drive neuronal NAD production, Nat Commun, 2024, 15; DOI: 10.1038/s41467-024-50354-5; Citations: 12; IF: 14.7
11. Mathez, G., Brancale, A. and Cagno, V. Novel Inhibitors of SARS-CoV-2 RNA Identified through Virtual Screening, J Chem Inf Model, 2024, 64; DOI: 10.1021/acs.jcim.4c00758; Citations: 3; IF: 5.7
12. Jia, X., Kullik, G.A., Bufano, M., Brancale, A., Schols, D. and Meier, C. Membrane-permeable tenofovir-di- and monophosphate analogues, Eur J Med Chem, 2024, 264; DOI: 10.1016/j.ejmech.2023.116020; Citations: 4; IF: 6.0
13. Padalino, G., Duggan, K., Mur, L.A.J., Maillard, J.Y., Brancale, A. and Hoffmann, K.F. Compounds Containing 2,3-Bis(phenylamino) Quinoxaline Exhibit Activity Against Methicillin-Resistant Staphylococcus aureus, Enterococcus faecalis, and Their Biofilms, Microbiologyopen, 2024, 13; DOI: 10.1002/mbo3.70011; Citations: 1; IF: 4.0
14. Lucero, B., Francisco, K.R., Varricchio, C., Liu, L.J., Yao, Y., Brancale, A., Brunden, K.R., Caffrey, C.R. and Ballatore, C. Design, Synthesis, and Evaluation of An Anti-trypanosomal [1,2,4]Triazolo[1,5-a]pyrimidine Probe for Photoaffinity Labeling Studies, ChemMedChem, 2024, 19; DOI: 10.1002/cmdc.202300656; Citations: 1; IF: 3.6
15. Pitasi, G., Brancale, A., Floris, S., Fais, A., Gitto, R. and De Luca, L. Computational Approach to Identifying New Chemical Entities as Elastase Inhibitors with Potential Antiaging Effects, Int J Mol Sci, 2024, 25; DOI: 10.3390/ijms252011174; Citations: 0; IF: 4.9
16. Miglioli, F., Joel, S., Tegoni, M., Neira-Pelen, P., Gunther, S., Carcelli, M., Fisicaro, E., Brancale, A., Fernandez-Garcia, Y. and Rogolino, D. Inhibitory interactions of the 2,3-dihydro-6,7-dihydroxy-1H-isoindol-1-one scaffold with Bunyavirales cap-snatching endonucleases expose relevant drug design features, Eur J Med Chem, 2024, 272; DOI: 10.1016/j.ejmech.2024.116467; Citations: 0; IF: 6.0
17. Giancotti, G., Nannetti, G., Padalino, G., Landini, M., Santos-Ferreira, N., Van Dycke, J., Naccarato, V., Patel, U., Silvestri, R., Neyts, J., Gozalbo-Rovira, R., Rodriguez-Diaz, J., Rocha-Pereira, J., Brancale, A., Ferla, S. and Bassetto, M. Structural Investigations on Novel Non-Nucleoside Inhibitors of Human Norovirus Polymerase, Viruses-Basel, 2023, 15; DOI: 10.3390/v15010074; Citations: 2; IF: 3.8
18. Pasqualetto, G., Zuanon, M., Brancale, A. and Young, M.T. Identification of the molecular determinants of antagonist potency in the allosteric binding pocket of human P2X4, Front Pharmacol, 2023, 14; DOI: 10.3389/fphar.2023.1101023; Citations: 8; IF: 4.4
19. Pasqualetto, G., Zuanon, M., Brancale, A. and Young, M.T. Identification of a novel P2X7 antagonist using structure-based virtual screening, Frontiers in Pharmacology, 2023, 13; DOI: 10.3389/fphar.2022.1094607; Citations: 4; IF: 4.4

20. Romagnoli, R., De Ventura, T., Manfredini, S., Baldini, E., Supuran, C.T., Nocentini, A., Brancale, A., Bortolozzi, R., Manfreda, L. and Viola, G. Design, synthesis, and biological investigation of selective human carbonic anhydrase II, IX, and XII inhibitors using 7-aryl/heteroaryl triazolopyrimidines bearing a sulfanilamide scaffold, J Enzyme Inhib Med Chem, 2023, 38; DOI: 10.1080/14756366.2023.2270180; Citations: 10; IF: 5.6
21. Francisco, K.R., Bruystens, J., Varricchio, C., McCurdy, S., Wu, J., Lopez-Ramirez, M.A., Ginsberg, M., Caffrey, C.R., Brancale, A., Gingras, A.R., Hixon, M.S. and Ballatore, C. Targeted Reversible Covalent Modification of a Noncatalytic Lysine of the Krev Interaction Trapped 1 Protein Enables Site-Directed Screening for Protein-Protein Interaction Inhibitors, ACS Pharmacol Transl Sci, 2023, 6; DOI: 10.1021/acsptsci.3c00156; Citations: 6; IF: 5.1
22. Salvadori, K., Onali, A., Mathez, G., Eigner, V., Dendisova, M., Matejka, P., Mullerova, M., Brancale, A. and Curinova, P. An Insight into Anion Extraction by Amphiphiles, ACS Omega, 2023, 8; DOI: 10.1021/acsomega.3c06767; Citations: 3; IF: 3.7
23. Xiang, H., Ferla, S., Varricchio, C., Brancale, A., Brown, N.L., Black, G.W., Turner, N.J. and Castagnolo, D. Biocatalytic and Chemo-Enzymatic Synthesis of Quinolines and 2-Quinolones by Monoamine Oxidase (MAO-N) and Horseradish Peroxidase (HRP) Biocatalysts, ACS Catal, 2023, ; DOI: 10.1021/acscatal.2c05902; Citations: 17; IF: 11.7
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3.3. Research works in journals recorded in the Scopus database that are not stated in the Web of Science database

Not stated

3.4. Research works in other peer-reviewed journals

1. Giancotti, G.; French, R.; Hayward, O.; Lee, K. Y.; Robinson, T.; Ribeiro da Silva, A. M.; Athina Varnava, A.; MacFarlane, M.; Richard W. E. Clarkson, R. W. E.; Westwell, A.; Brancale, A., The discovery of small-molecule inhibitors of cFLIP that sensitise tumour cells to TNF-related apoptosis-inducing ligand. Academia Oncology 2025, 2(2). doi:10.20935/AcadOnco7680.

3.5. Chapters in monographs, monographs

1. Bassetto, M.; Brancale, A.: The search for antivirals to treat alphavirus infections. In the book: CORONAVIRUSES AND OTHER NOVEL ANTIVIRAL TARGETS, Annual Reports in Medicinal Chemistry, Elsevier, pp. 133-151. Citation: 1

3.6. Articles in journal without peer review, articles in proceedings

1. Padalino, G; Duggan, K; Mur, LAJ; Maillard, JY; Brancale, A; Hoffmann, KF, Compounds Containing 2, 3-Bis(phenylamino) Quinoxaline Exhibit Activity Against Methicillin-Resistant Staphylococcus aureus, Enterococcus faecalis, and Their Biofilms, MICROBIOLOGYOPEN, 2024, 13, e011
2. Jöe, M; Tribble, JR; Varricchio, C; Brancale, A; Johannesson, G; Wheelock, C; Williams, P, Development of neuroprotective small molecular drugs targeting NMNAT2, INVESTIGATIVE OPHTHALMOLOGY & VISUAL SCIENCE, Annual Meeting of the Association-for-Research-in-Vision-and-Ophthalmology (ARVO), APR 23-27, 2023, New Orleans, LA, 2023, 64,
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6. Pasqualetto, G; Pileggi, E; Schepelmann, M; Heard, C; Young, MT; Rozanowska, MB; Brancale, A; Bassetto, M, Novel small-molecule chaperones to overcome opsin misfolding, mistrafficking and aggregation in retinal blinding diseases, INVESTIGATIVE OPHTHALMOLOGY & VISUAL SCIENCE, Annual Meeting of the Association-for-Research-in-Vision-and-Ophthalmology (ARVO), APR 28-MAY 02, 2019, Vancouver, CANADA, 2019, 60,
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8. Pileggi, E; Pasqualetto, G; Rozanowska, M; Brancale, A; Bassetto, M, Development of novel treatments against inherited blinding diseases Retinitis pigmentosa and Leber's congenital amaurosis, ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, 257th National Meeting of the American-Chemical-Society (ACS), MAR 31-APR 04, 2019, Orlando, FL, 2019, 257,
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10. Yarova, P; Schepelmann, M; Ferla, S; Huang, P; Telezhkin, V; Kidd, E; Ford, W; Broadley, K; Ward, J; Corrigan, C; Kemp, P; Brancale, A; Riccardi, D, Development of a new calcilytic for the treatment of inflammatory lung disease, EUROPEAN RESPIRATORY JOURNAL, 28th International Congress of the European-Respiratory-Society (ERS), SEP 15-19, 2018, Paris, FRANCE, 2018, 52,
11. Baker, A; Davies, J; Uusi-Kerttula, H; Ferla, S; Brancale, A; Wilkinson, G; Chester, J; Parker, A, Development of chimeric Ad5/Ad49 adenovirus vectors that exhibit enhanced tropism for tumour cell lines, HUMAN GENE THERAPY, Annual Conference of the British-Society-for-Gene-and-Cell-Therapy / Joint UK-Regenerative-Medicine-Platform Meeting, APR 19-21, 2017, Royal Welsh Coll Mus & Drama, Cardiff, WALES, 2017, 28, A14
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23. Bassetto, M; De Burghgrave, T; Leyssen, P; Neyts, J; Brancale, A, Design, synthesis, and evaluation of novel anti-CHIKV compounds, ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, Symposium on Physicochemical Characterization of Organic Matter - Past, Present, Future, and Role of Environment / 245th National Spring Meeting of the American-Chemical-Society (ACS), APR 07-11, 2013, New Orleans, LA, 2013, 245,
24. Ferla, S; Brancale, A; DeLuca, HF; Zhu, GJ; Simons, C, Small molecule inhibitors of CYP24A1 for treatment of various cancers, ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY, Symposium on Physicochemical Characterization of Organic Matter - Past, Present, Future, and Role of Environment / 245th National Spring Meeting of the American-Chemical-Society (ACS), APR 07-11, 2013, New Orleans, LA, 2013, 245,
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34. Brancale, A; Vlachakiis, D; Kandil, S; Biondaro, S; Berry, C; Neyts, J, Discovery of a novel HCV helicase inhibitor by a de novo drug design approach, ANTIVIRAL RESEARCH, 21st International Conference on Antiviral Research, APR 13-17, 2008, Montreal, CANADA, 2008, 78, A22
35. Derudas, M; McGuigan, C; Brancale, A; Bugert, J; Andrei, G; Snoeck, R; Balzarini, J, Design, synthesis and biological evaluation of novel acyclovir ProTides, ANTIVIRAL RESEARCH, 21st International Conference on Antiviral Research, APR 13-17, 2008, Montreal, CANADA, 2008, 78, A56
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37. Congiatu, C; McGuigan, C; Brancale, A, HINT as putative phosphoramidase responsible of pro-tides activation: Molecular modelling studies, ANTIVIRAL RESEARCH, 20th International Conference on Antiviral Research, APR 29-MAY 03, 2007, Palm Spring, CA, 2007, 74, A71

3.7. Personally given lectures abroad and at international conferences

1. 1st PANVIRIDE Drug Discovery Conference - Sep 29 - 30, 2025 – "The Promise and Challenges of Computer-Aided Drug Design in Antiviral Research"
2. Gordon Research Conference - Nucleosides, Nucleotides, and Oligonucleotides - Jun 25 - 30, 2023 - Salve Regina University "Nucleoside analogous beyond antivirals and anticancer: exploring their potential against schistosoma"
3. 18th Hellenic Symposium on Medicinal Chemistry – 25th February 2021: "The discovery of Bcl3 inhibitors as novel antimetastatic agents"
4. 32nd International Conference on Antiviral Research – Baltimore, USA, 14th May 2019: "Structure-based antiviral drug design"
5. 7th European Congress of Virology – Rotterdam, The Netherlands, 29th April 2018: "Computer-aided antiviral drug design (State of the art)"
6. 16th Medical Biodefence Congress – Munich, Germany, 29th October 2018: "Antivirals & antibiotics development"
7. The BMCS Mastering MedChem III: 3rd RCS-BMCS symposium on mastering medicinal chemistry – Cardiff, UK 22nd March 2017
8. 1st Medicinal Chemistry Ireland Conference – Dublin, Ireland 1st July 2016

9. China – United Kingdom Cancer (CUKC) Conference 2015 – Cardiff, UK 17th-18th July 2015: "Molecular modelling in anticancer drug design: The discovery of the BCL3 inhibitors"
10. "Tenth European Workshop in Drug Design" (X EWDD) – Siena, Italy, 17th – 22nd of May, 2015: "Computer-aided discovery Bcl3 inhibitors as potential anti-metastatic agents"
11. 3rd Antiviral Congress – Amsterdam, The Netherlands, 13th October 2014: "Antiviral Drug Design: recent developments and future challenges".
12. 2nd European Seminar in Virology (EuSeV) – Bertinoro, Italy, 13th June 2014: "Rational drug design: a state of the art look for next generation antivirals".
13. 27th International Conference on Antiviral Research – Raleigh, USA, 12th May 2014: "The Role of Molecular Modelling in Drug Discovery".
14. 26th International Conference on Antiviral Research – San Francisco, USA, 13th May 2013: "From irrational to rational antiviral drug design".
15. Welsh Cancer Conference 2010 – Cardiff, 14-15th April 2010: "Molecular graphics and computer visualisation in (cancer) drug discovery".
16. "Giornate scientifice dell'Istituto Pasteur" - Rome (IT), 23-24th October 2008: "Molecular modelling methods in anticancer drug discovery.
17. 1st International meeting "Nuove Prospettive in Chimica Farmaceutica" – Salerno (IT), 22-23rd February 2007: "Computer-aided design of a novel HCV helicase inhibitor"

Invited talks to Industries and Universities:

18. Karolinska Institute, Stockholm, Sweden, 14th of November 2023: "Drug design and discovery in academia: challenges and opportunities"
19. University of Padua, Padua, Italy, 17th April 2023: "The discovery of Bcl3 inhibitors by computer-based drug design"
20. University of California, San Diego, USA, 31st August 2018: "BCL3 inhibitors as novel anti-metastatic agents"
21. IFOM-IEO, Milan (IT), 23rd March, 2015: "Discovery of Bcl-3 inhibitors"
22. University of Hamburg, Faculty of Sciences, Department of Chemistry – Hamburg (D), 10th January, 2012: "Molecular Modelling and antiviral drug design"
23. Pennsylvania Biotechnology Center – Doylestown, PA (USA), 21st June 2010: "Computer modeling and its application in drug discovery"
24. University of Eastern Piedmont, Faculty of Pharmacy – Novara (IT), 15th November 2009: "Antiviral drug design: an irrational approach"
25. University of Rome "La Sapienza", Faculty of Pharmacy – Rome (IT) 22nd October 2008: "Design and Synthesis of novel antiviral compounds"
26. Morvus Technology ltd. – Carmarthen 29th August 2007: "Molecular modelling in drug discovery"
27. University of Padua, Faculty of Pharmacy – Padova (IT) 3rd May 2005: "Antiviral drug design"

3.8. Personally given lectures at national conferences

Not Stated

3.9. Principal investigator of foreign grants and projects (amounts allocated to the lab)

UCT Prague:

1. € 400,000 HORIZON-HLTH-2023-DISEASE-03-04, (UCT PI; Coordinator: Leiden University Medical Center) 2024-27; PANVIPREP - Developing broad-spectrum antiviral drugs for pandemic preparedness

Cardiff University:

2. £307,275 Wellcome Trust, 2021-24 (Cardiff PI): Refining the drug discovery paradigm for schistosomiasis
3. £53,887 Welsh Government - Ser Cymru III, 2020-21 (PI): Welsh Coronavirus Research (W-CoRe): A platform for the discovery of anti-betacoronaviruses agents.
4. £182,936 Welsh Government, 2020-23 (PI): Life Sciences Research Network Wales
5. £235,396 ImmuTep SAS, 2019-21 (PI): ImmuScreen - development of novel LAG3 inhibitors as anticancer compounds.
6. £130,854 NIH, 2019-21 (Cardiff PI) Optimization of microtubule-stabilizing triazolopyrimidines as therapeutics for Alzheimer's disease and related tauopathies
7. £100,000 Cancer Research Wales, PhD Studentship 2019-22 (PI): Design, synthesis and evaluation of novel CD200, PD-1 and CTLA-4 small-molecule inhibitors as potential cancer treatment
8. £20,000 The Bridging Fund, Wales, 2016 (PI): Development of a self-sustained Computer-aided drug discovery enterprise.
9. £100,000 Life Science Research Network of Wales Platform 2014/16 (PI): In silico platform to support drug discovery and development
10. £100,000 Life Science Research Network of Wales PDRA 2015/17 (PI): Discovery and development of a novel therapeutic for the treatment of inflammatory lung disorders.
11. £100,000 Tiziana Life Sciences PhD studentship 2015/18 (co-PI): Design, Synthesis and Evaluation of cFlip Inhibitors as Novel Anticancer Agents.
12. £180,000 Tiziana Life Sciences PDRA 2015/17 (PI) The Identification and Selection of Candidate Lead Compounds Against Bcl3.
13. £394,912 H2020-MSCA-ITN-2014 “ANTIVIRALS- European Training Network on Antiviral Drug Development” Coordinator: F. van Kuppeveld (The Radboud University Nijmegen Medical Centre, The Netherlands), A. Brancale (Cardiff PI; Leader of Research Sub-program).
14. £89,000 *Cancer Research Wales* studentship: 2013-16 (PI):*Discovery of Bcl-3 inhibitors for the potential treatment of metastatic breast cancer*
15. £45,000 LSRNW / PHRMY Ph.D. Studentship: 2013-16 (co-applicant):Fingolimod pro-drugs as a new therapeutic opportunity (PI: prof. Chris McGuigan)
16. £60,000 HPC Wales studentship: 2012-15 (co-applicant): A platform to determine mutation events in the cancer genome and chemical toxicity (PI: Dr. Paul Lewis, Swansea University)
17. £215,000 Biovitas project grant: 2013-14 (co-PI); Development of Bcl3 inhibitors for the treatment of metastastic breast cancer (PI)
18. £90,000 LSRNW / Biovitas Ph.D. Studentship: 2013-16 (co-PI): Development of Bcl3 inhibitors for the treatment of metastastic breast cancer (co-PIs: Dr. Andrew Westwell and Dr. Richard Clarkson)
19. £90,000 LSRNW / Henson Foundation Ph.D. Studentship: 2013-16; Design and synthesis of novel anti-DENV compounds (PI)

20. £105,000 Cancer Research Wales studentship: 2012-15 (co-applicant);Design and synthesis of molecular inhibitors of c-FLIP activity as a therapeutic strategy to target breast cancer stem cells (PI: Dr. Richard Clarkson)
21. £444,138 EU - FP7-PEOPLE-2010-ITN**,** 2011/2015, "EUVIRNA- European Training Network on (+)RNA Virus Replication and Antiviral"– Coordinator: F. van Kuppeveld (The Radboud University Nijmegen Medical Centre, The Netherlands), A. Brancale (Cardiff PI; Leader of Research Sub-program); €4,976,094 (€525,745 - allocated to CU/PHRMY).
22. £101,000 *Synergy Pharmaceuticals inc.*, 2010/11, "Molecular Modelling studies on bioactive peptides", A. Brancale.
23. £67,000 *Biovitas inc***.** 2010/12, "Computer-aided design of novel HCV helicase inhibitors", A. Brancale.
24. £31,304 *The President's research studentship*, 2010/2013, "Interactive drug design".

3.10. Principal investigator of domestic grants and projects

Not Stated

3.11. Co-investigator of foreign grants and projects (amounts allocated to the lab)

Cardiff University

1. £146,635 European Commission (Horizon 2020) MSC Fellowship 2018-20 (Coordinator; Fellow Dr. G. Nannetti)
2. £184,737 Ser Cymru II 2018/21: Individual Fellowship (Academic Sponsor; Fellow Dr. S. Ferla)
3. £721,566 Nucana Biomed Ltd., 2017-19 (co-applicant): Anticancer nucleosides.
4. £130,509 Demeter Therapeutics LLC, 2017 (co-applicant): Phosphoramidates for metabolic diseases.
5. £197,929 Ser Cymru II 2016/19: Individual Fellowship (Academic Sponsor; Fellow Dr. M. Bassetto)
6. £50,000 Life Science Research Network of Wales PDRA 2015/16 (co-applicant): Development of new prothrombotic lipids for haemostatic applications. (PI: Prof. V. O'Donnell)
7. £49,201 MRC 2015/16 (co-applicant): Development of new prothrombotic lipids for haemostatic applications. (PI: Prof. V. O'Donnell)
8. £50,000 Wellcome Trust 2015/16 (co-applicant): Role photosensitizing components of Burch's membrane in age-related macular degeneration (AMD) and therapeutic strategy to counteract their deleterious effects. (PI: Dr. Rozanowska)
9. £50,000 Life Science Research Network of Wales Platform 2015/16 (co-applicant): All Wales antivirals discovery and development platform. (PI: dr. J. Bugert)
10. £50,000 Life Science Research Network of Wales PDRA 2015/16 (co-applicant): Novel modulators of the visual cycle for treatment of retinal degenerations. (PI: Dr. Rozanowska)
11. £45,000 Life Science Research Network of Wales / MEDIC / PHRMY PhD Studentship 2015/18 (co-applicant): Developing Carbon Monoxide (CO) as a Synergistic Agent to Improve anti-VEGF Strategy for Triple-Negative Breast Cancer. (PI: Dr. J. Cai)
12. £49,360 Life Science Research Network of Wales PDRA 2015/16 (co-applicant): Discovery of Novel Site-Specific FAK Inhibitors for Potential Treatment of Metastatic Breast Cancer. (PI: Dr. Andrew Westwell)

13. £49,517 Life Science Research Network of Wales PDRA 2015/16 (co-applicant): Advancing Analogues of a Novel cFlip Inhibitor which Sensitizes Breast Cancer Cells and Stem Cells to TRAIL. (PI: Dr. Andrew Westwell)
14. £46,189 Life Science Research Network of Wales PDRA 2015/16 (co-applicant): Sensitizing to Radiotherapy: Pre-clinical Evaluation of a Novel Indication for Adjuvant Bcl3i. (PI: Dr. Clarkson)
15. £50,000 Life Science Research Network of Wales PDRA 2015/16 (co-applicant): Development of Novel CD200:CD200R Blockade Cancer Immunotherapy. (PI: Dr. Patel)
16. £115,380 Cancer Research Wales 2014/17 (co-applicant): Inhibitors of alphaB-Crystallin (CRYAB) for the Treatment of Triple-Negative Breast Cancer. (PI: Dr. Andrew Westwell)
17. £50,000 LSRNW Project Grant: 2014 (co-applicant): Targeting αB-crystallin (CRYAB): A possible novel strategy to impede triple-negative breast cancer growth (PI: Dr. J Cai)
18. £45,000 LSRNW / BIOSI Ph.D. studentship: 2014/17 (co-applicant):Structure-based design of human P2X4-selective small-molecule modulators (PI: Dr. Mark Young)
19. £45,000 LSRNW / PHRMY Ph.D. studentship: 2014/17 (co-applicant): Diastereoselective Synthesis of Phosphoroamidate Prodrugs (PI: Dr. Fabrizio Pertusati)
20. £115,000 Cancer Research Wales Project grant: 2014-16 (co-applicant): lnhibitors of oB-crystallin (CRYAB) for the treatment of triple negative breast cancer (PI: Dr. Andrew Westwell).
21. £505,140 *MRC/SARTRE*, 2009/11, "Development of new agents for colorectal cancer (CRC) using genetically defined autochthonous models", C. McGuigan, A. Brancale, A. Clarke, T. Maugham, P. Shaw; (£206,290 allocated to PHRMY).
22. £221,697 *CRUK*, 2008/10"Development of CYP26 Inhibitors as Cancer Therapeutics", C. Simons, A Brancale.
23. £130,370 *CRUK***,** 2009/12, "Small Molecule Inhibitors of CYP24A1– Prostate Cancer Therapeutics"; C. Simons, A. Brancale.
24. £23,500 *Inhibitex inc.,* 2008, "Molecular modelling studies on a novel anti-HCV nucleoside analogues", A. Brancale; (As part of the still ongoing Inhibitex deal of C. McGuigan; overall value to date >£700,000).
25. £60,000 *Leukaemia Research Appeal for Wales,* 2005/08, "New anti-leukaemia drug discovery", C. McGuigan, A. Brancale.

3.12. Co-investigator of domestic grants and projects

- ~80M CZK OP JAK, 2024-28 (Co-Applicant; Coordinator Charles University): NETPHARM - Nové technologie pro translační výzkum ve farmaceutických vědách

4. Technical and realization activities

4.1. Awarded European or international patents (EPO, WIPO), patents of USA and Japan

1. Small Molecule inhibitors of LAG-3, WO2024246563(A1), 05/12/2014, Godkin, A.; Brancale, A.; Mason, G.; Varricchio, C.; Michue-Seijas, S.
2. Epigallocatechin-3-gallate (egcg) analogs for use in the treatment of diseases in which an increase of nad+ is beneficial such as glaucoma WO2024170772(A1), 22/08/2024, WILLIAMS, P.; Brancale, A.; VARRICCHIO, C.; JÖE, M,I.
3. Antibacterial and antiparasitic quinoxaline 2,3 diamine derivatives. WO2021001661 (A1). 07/01/2021, Brancale A.; Padalino, G.; Hoffmann, K.
4. Monosaccharide phosphoarmidate prodrugs. WO2019118486(A1), 20/6/2019, Thomas, S.; Crutcher, P.; Perusati, F.; Sedlakova, J.; Brancale, A.
5. Androgen receptor modulators and their use as anti-cancer agents. WO2016079522(A1), 26/5/2016, Westwell, A.D.; Pertusati, F.; McGuigan, C.; Brancale, A.; Bassetto, M.; Ferla, S.; Kandil, S.
6. Androgen receptor modulators and their use as anti-cancer agents. WO2016079521(A1), 25/5/2016, Westwell, A.D.; Pertusati, F.; McGuigan, C.; Brancale, A.; Bassetto, M.; Ferla, S.; KAndil, S.
7. Bcl-3 Inhibitors, PCT/US2015/043333 31/07/2015, Westwell A. D.; Brancale A.; Clarkson R. W. E.
8. Novel anticancer 2-benzoylaminobenzamide derivatives., PCT/EP2014/066564, 31/07/2014, Westwell A. D.; Brancale A.; Clarkson R. W. E.; Soukupova J.
9. Substituted purine nucleosides, phosphoramidate and phosphordiamidate derivatives for treatment of viral infections, WO 2013070887 (A1) 16/05/2013, Chamberlain S.; Vernachio J.; Battina S.K.; Ramamurty C.V.S.; Rao C.S.; Mcguigan C.; Brancale A.
10. Indole derivatives, WO2011121629 (A1) 06/10/2011, Silvestri R.; La Regina G.; Hamel E.; Brancale A.; Lavia P.; Novellino E.
11. CYP26 inhibitors, WO2009153566 (A1), 23/12/2009, Simons C.; Brancale A.; Gomaa M. S. M.; Aboraia A. S. M.
12. Benzene derivatives, WO2009125191 (A1), 15/10/2009, Brancale A.; Valchakis D.; Berry C.; Neyts J.
13. Arythioindoles tubulin polymerisation inhibitors and methods of treating or preventing cancer using same, WO2006041961 (A1), 20/04/2006, Hamel E.; Silvestri R.; Brancale A.

4.2. Awarded Czech or other national patents utilized based on a valid licence agreement

Not Stated

4.3. Awarded Czech or other national patents utilized only by the owner of the patent or not utilized

Not Stated

4.4. Authorship of realized complex technical work with specified social benefit

Co-founder and Chairman of Awen Oncology Ltd., a spin-off company that was created around one of the research project developed in my lab. (http://awenoncology.com)

4.5. Pilot operation, proven technologies

Not stated

4.6. Utility models and industrial designs, prototypes, function samples, software

Not Stated

4.7. Expertise activity

Acted as Expert Witness in legal patent disputes, related to drug discovery, at the European Patent Office, at the UK Court, at the Canada court, and as an expert for the Department of Justice of the United States.

5. Organizational, professional and social activities related to the field

5.1. Membership and positions in international and national learned societies

- 2013-219 and 2022 – 2025; Elected to Board of Directors of the International Society for Antiviral Research
- Member of the International Society for Antiviral Research
- Member of the Royal Society of Chemistry

5.2. Membership in professional boards and advisory bodies

2022 – date Co-Founder and Chairman of the Board – Awen Oncology Ltd.
2021 – 2024 Member of the Scientific Advisory Board of TNA therapeutics
2016 – 2022 Scientific Director of the Life Sciences Research Network Wales (http://www.lsrnw.ac.uk)
2014 – 2017 Scientific Founder, member of the Scientific Advisory Board and Scientific Consultant of Tiziana Life Sciences
2012 – 2019 Member of the Scientific Advisory Board and Scientific Consultant of Synergy Pharmaceuticals Inc.

5.3. Membership and positions in editorial boards of professional journals

2017-date Editorial Board Member of Antiviral Research
2016 – 2023 Editor-in-Chief of Antiviral Chemistry and Chemotherapy
2004 – 2016 Chemistry Editor for Antiviral Chemistry and Chemotherapy

5.4. Membership and positions in organizational committees of conferences

- Current member of the Program Committee of the International Conference on Antiviral Research
- Organiser of the LSRNW annual congress - Cardiff, UK, 2016; Cardiff, UK, 2017; Cardiff, UK, 2018.
- Local organiser of the 28th International Conference on Antiviral Research - Rome, Italy, 2015.
- Local organiser for the SCI Fine Chemicals Group Graduate Symposium - Cardiff, 2005

5.5. Membership and positions in panels of grant agencies

- LS7 Panel member of the Italian Ministry of Education: Progetti di Rilevante Interesse Nazionale (PRIN)

5.6. Awards for research and development works

2026 Antonin Holy Memorial Award
2023 BIOVARIA Emerging Startup Award to Ceridwen Oncology (now Awen Oncology)
2016 Innovation in Healthcare Award for the "Development of a novel anti-metastatic agent"– Cardiff University
2013 William Prusoff Young Investigator Lecture Award – Presented by the International Society for Antiviral Research.

6. Foreign cooperation and stays abroad

6.1 Established productive collaborations

- Dr. Pete Williams, Karolinska Institute, Stockholm, Sweden
- Prof. Katherine Seley-Radtke, University of Maryland, USA
- Prof. Chris Meier, Hamburg Univeristy, Germany
- Prof. Romano Silvestri, University of Rome “La Sapienza”, Italy
- Prof. Sirio Dupont, Padua University, Italy
- Prof. Richard Clarkson, Cardiff Unviersity, UK
- Dr. Siang Boon Koh, Bristol University, UK
- Prof. Arianna Loragian, Padua University, Italy
- Prof. Enzo Tramontano, Cagliari Unvisrsity, Italy
- Prof. Frank van Kuppeveld, Utrecht University, The Netherlands
- Prof. Bruno canard, AFMB Marseille, France
- Prof. Johan Neyts, KU Leuven, Belgium
- Prof Graciela Andrei, KU Leuven, Belgium
- Dr. Dominik Rejman, IOCB Prague, Czech Republic
- Dr. Valeria Cagno, CHUV Lousanne, Switzerland

6.2 Stays abroad

- 2023 Visiting Professor at University of Rome “la Sapienza”, 2 months.
- 1999 Visiting Prof. Dominique Cahard, University of Rouen, France.

7. Most important creative activities

Below only some examples of my most innovating and creative activities.

7.1 Innovative Research Activities

Throughout my career, I have been deeply engaged in research activities that are both innovative and impactful, often extending beyond fundamental scientific inquiry to drive real-world applications in drug discovery. My work has consistently bridged the gap between academia and industry, fostering knowledge transfer and contributing to commercially relevant drug development projects.

Sustained Contribution to Knowledge Transfer

Since my PhD, I have actively participated in numerous drug discovery projects with high translational potential. My research has led to thirteen patents, highlighting my sustained contributions to intellectual property generation in medicinal chemistry.

For example, One of the most significant projects I have been involved in is the development of a Bcl-3 inhibitor as a selective anti-metastatic agent. This collaborative effort with Dr. Westwell and Dr. Clarkson began as a molecular modelling simulation in my lab, which successfully identified a potent Bcl-3 inhibitor (see reference 37). Over time, the project evolved into a commercially viable endeavour:

- The intellectual property (IP) was protected and subsequently licensed to a biotech incubator (*Biovitas*) (see patents 7 and 8).
- This led to the creation of a spin-off company, *Tiziana Life Sciences*, which was thenpublicly listed on the London Stock Exchange (AIM).
- The project has progressed towards clinical development, with a lead molecule selected and manufacturing of the Active Pharmaceutical Ingredient (API) initiated.
- The innovative nature of these projects was further recognised through the 2016 Innovation in Healthcare Award for the development of a novel anti-metastatic agent (section 5.6).

Another highly relevant project, based on unpublished research initiated in my lab, focuses on discovering a novel anticancer agent specifically targeting chordoma, a rare form of cancer. This project was selected for the Alderley Park Oncology Programme, leading to the establishment of a spin-off company, *Awen Oncology Ltd*, where I currently serve as Director. In recognition of this work, I was awarded the BIOVARIA Emerging Start-up Award in 2023 (see section 5.6).

Although these activities were primarily conducted during my tenure at Cardiff University, it is worth noting that we are currently in negotiations with an investor for the licensing of a research project that I initiated and am now carrying forward at UCT.

Future Directions in Innovative Research

Building on these successes, my future research will continue to focus on pioneering approaches in medicinal chemistry, particularly in:

- Rational drug design using AI-driven molecular modelling, accelerating the discovery of novel therapeutic agents.
- Expanding collaborations with biotech companies and pharmaceutical partners to facilitate knowledge transfer and clinical translation, as mentioned above.
- Exploring new chemical strategies to modulate neurodegenerative disease pathways (see, as an example, reference 5).

By integrating computational and experimental methodologies, I aim to further push the boundaries of drug discovery, ensuring that fundamental research translates into meaningful therapeutic advancements.

7.2 Innovation through leadership

In July 2016, I was appointed Scientific Director of the Life Sciences Research Network Wales (LSRNW), a Welsh Government-funded initiative under the *Ser Cymru* program. The network supported high-quality research projects at Welsh universities aimed at developing new treatments for unmet medical and veterinary needs. Under my leadership, LSRNW has provided funding for 56 PhD studentships, 42 research projects, and 10 platform grants, significantly contributing to capacity building and translational research in life sciences.

At the international level, I am an elected board member of the International Society for Antiviral Research (ISAR), the leading global professional association for scientists in the antiviral field. ISAR brings together experts from academia, industry, and government agencies, encompassing disciplines from medicinal chemistry to clinical research. Within ISAR, I also serve on various committees, including the Program Committee, which plays a key role in shaping the focus of the International Conference on Antiviral Research (ICAR), one of the most prestigious events in the field.

Through these leadership roles, I have contributed to shaping research priorities, fostering interdisciplinary collaboration, and supporting the next generation of scientists, further amplifying the impact of my work on global drug discovery efforts.