**Curriculum Vitae** 

Correct as of June 2024

Personal information

First name(s) / Surname(s)

Mark Timothy David CRONIN

Address

School of Pharmacy and Biomolecular Sciences

Liverpool John Moores University

Byrom Street Liverpool L3 3AF

United Kingdom

ORCID ID

0000-0002-6207-4158

Work experience

Dates | 2005 onwards

Occupation or position held Professor of Predictive Toxicology

Main activities and responsibilities

University professor with responsibilities for management of the QSAR and Modelling Research

Group, writing grants, managing research projects and consultancies, publication and dissemination of science. Teaching and academic administrative duties on the Master of Pharmacy and B.Sc. Applied

Chemical and Pharmaceutical Sciences degree programmes.

Name and address of employer | School of Pharmacy and Biomolecular Sciences, Liverpool John Moores University, Byrom Street,

Liverpool, L3 3AF, United Kingdom

Type of business or sector | University – Higher Education and Research

Dates 2001 – 2005

Occupation or position held Reader of Computational Chemistry

Main activities and responsibilities University reader with responsibilities for the writing of grants, managing research projects and

consultancies, publication and dissemination of science. Teaching and academic administrative duties on the Master of Pharmacy and B.Sc. Pharmaceutical and Chemical Sciences degree programmes.

Name and address of employer | School of Pharmacy and Chemistry, Liverpool John Moores University, Byrom Street, Liverpool, L3

3AF, United Kingdom

Type of business or sector | University – Higher Education and Research

Dates | 1994 – 2001

Occupation or position held | Lecturer / Senior Lecturer in Pharmaceutical Chemistry

Main activities and responsibilities | University lecturer with responsibilities for the writing of grants, publication and dissemination of

science. Teaching and academic administrative duties on the B.Sc. and Master of Pharmacy and

B.Sc. Pharmaceutical and Chemical Sciences degree programmes.

Name and address of employer | School of Pharmacy, Liverpool John Moores University, Byrom Street, Liverpool, L3 3AF, United

Kingdom

Type of business or sector | University – Higher Education and Research

Dates | 1991 - 1994

Occupation or position held Post – Doctoral Research Fellow

Main activities and responsibilities | Research into the prediction of human health effects e.g. skin sensitisation, skin permeability, skin

irritation through the application of quantitative structure-activity relationships (QSARs). The research

was funded by the Environmental Safety Laboratory of Unilever Research.

Name and address of employer | School of Pharmacy, Liverpool John Moores University, Byrom Street, Liverpool, L3 3AF, United

Kingdom

Type of business or sector | University – Higher Education and Research

### **Education and training**

Title of qualification awarded

PhD entitled "Quantitative Structure-Activity Relationships of Comparative Toxicity to Aquatic Organisms"

Name of organisation

Name of organisation

Liverpool Polytechnic, UK

Title of qualification awarded

B.Sc. (Hons) Applied Biology Liverpool Polytechnic, UK

# Personal skills and competences

I am an experienced academic (Full Professor at Liverpool John Moores University, England) and as such have a strong background in obtaining funding and managing research at both the international and national level. In addition I have considerable experience in teaching on under-graduate programmes (such as the Master of Pharmacy course).

I have over 35 years expertise in the development of *in silico* alternatives for toxicity testing. These alternatives include the use of *in silico* techniques such as quantitative structure-activity relationships (QSARs), category formation and read-across as well as threshold of toxicological concern (TTC). This includes a strong emphasis in toxicological data collection and curation. In particular this has included identifying appropriate data from the literature and organising them into usable datasets.

Underpinning my expertise in *in silico* techniques is a very strong technical background including toxicology, mechanisms of toxic action, computational chemistry, molecular modelling, expert systems for toxicity prediction and the multivariate statistical background in chemoinformatics.

I co-ordinated the COSMOS EU / Cosmetics Europe Project (part of the Suerat-1 Cluster) and have previously co-ordinated the InSilicoTox Marie Curie Project and projects for UK Defra. I am, and have been, a partner in numerous other projects including the OECD QSAR Toolbox, RISKHUNT3R, eTRANSAFE, eTox, NanoBridges, NanoPuzzles, CAESAR, EasyRing, IMAGETOX Projects etc.

Mother tongue(s)

#### **English**

Other language(s) Self-assessment European level (\*)

# French German

Г	rei	icn,	Gern	nan

Understanding			Speaking				Writing	
	Listening	Reading	S	Spoken interaction		Spoken production		
	A2	A2		A1		A1		A1
	A1	A1		A1		A1		A1

<sup>(\*)</sup> Common European Framework of Reference for Languages

# Organisational skills and competences

Strong organisation skills including the following:

- Management of research including European Union framework programme and national (UK)
  projects (as a partner and co-ordinator) in the area of quantitative structure-activity relationships to
  replace animal testing for toxicological assessment.
- Expertise in working in collaborative projects in the area of toxicological QSAR both within the UK, Europe and North America.
- Organisation of international and national conferences and workshops.
- Academic duties including organisation, administration and assessment of modules on the Master of Pharmacy programme.

#### Technical skills and competences

- Internationally recognised expertise in the area of "in silico toxicology". Specifically this relates to
  the development of quantitative structure-activity relationships for the prediction of the
  environmental and human health effects of chemicals. In particular the development of (Q)SARs for
  endpoints such as acute aquatic toxicity, skin sensitisation, chronic toxicity etc.
- Expertise reporting writing and publication, specifically with regard to scientific and technical workshops.
- Expertise in the development of approaches for the grouping of chemicals according to reactivity, mechanism of action, chemical similarity, analogues etc.
- Expertise in presenting scientific information through peer-reviewed publication and oral presentation.
- Expertise in training non-experts and experts alike in the development and application of *in silico* techniques for toxicity prediction.

#### Computer skills and competences

Wide ranging computer skills and expertise in the following areas:

- Use of specialist computational chemistry software including that required for the development of quantitative structure-activity relationships.
- Application of statistical software to develop multivariate QSARs.
- Expertise in the use and application of expert systems for toxicity and metabolism prediction.
- Microsoft Office: Word, Excel, Powerpoint.
- Trivial programming web-page design.

## Other skills and competences

- Four books and over 300 peer-reviewed journal articles published in the area of quantitative structure-activity relationships (QSARs) for the prediction of environmental and human health effects of chemicals.
- Over 150 conference and presentations as an invited or plenary speaker in the area of toxicological QSARs.
- Membership of various international and national expert working groups and committees including the OECD Expert Group on (Q)SAR, various ECVAM / ECB working groups and workshops, BioActive Sciences Group committee of the Society of Chemical Industry (including as past chairman), SETAC-UK Council.
- Holder of numerous grants include EU Framework Programmes (IMAGETOX (FP5), Easyring (FP5), ReProTect (FP6), CAESAR (FP6), OSIRIS (FP6), InSilicoTox Marie Curie Action (FP6), NanoPuzzles (FP7), NanoBridges (FP7), eTox (IMI), COSMOS (FP7), iPiE (IMI) eTRANSAFE (IMI), in3 (H2020); RISK-HUNT3R (H2020), OECD (Q)SAR Application Toolbox; UK grants from Defra, BBSRC etc.
- Consultancies and funded research in the area of toxicological QSAR with numerous companies including Unilever, L'Oreal, Lhasa Ltd, Health Canada, Defra (UK), Building Research Establishment and many others.
- Co-Editor-in-Chief of Computational Toxicology. Member of the editorial boards (past and on-going) of the following journals: Bulletin of Environmental Contamination and Toxicology; Current Medicinal Chemistry; Environmental Toxicology and Chemistry; Pest Management Science; SAR and QSAR in Environmental Research, ATLA, Molecular Informatics.

#### **Annexes**

### Selected Relevant Publications

A full list of Mark Cronin's publications can be viewed at: <a href="https://www.ljmu.ac.uk/about-us/staff-profiles/faculty-of-science/pharmacy-and-biomolecular-sciences/mark-cronin">https://orcid.org/0000-0002-6207-4158</a>

Annex: Selected Publications. In total I have edited 4 books and have over 300 publications (h-index>60; i10-index>250).

#### Selected Recent Relevant Refereed Journal Articles

- 1. DA Barnes, JW Firman, SJ Belfield, **MTD Cronin**, M Vinken, MJ Janssen, R Masereeuw (2024) Development of an adverse outcome pathway network for nephrotoxicity. *Archives of Toxicology* 98: 929-941.
- 2. **MTD Cronin**, SJ Belfield, KA Briggs, SJ Enoch, JW Firman, M Frericks, C Garrard, PH Maccallum, JC Madden, M Pastor, F Sanz, I Soininen, D Sousoni (2023) Making in silico predictive models for toxicology FAIR. *Regulatory Toxicology and Pharmacology* 140: 105385.
- 3. SJ Belfield, **MTD Cronin**, SJ Enoch, JW Firman (2023) Guidance for good practice in the application of machine learning in development of toxicological quantitative structure-activity relationships (QSARs). *PLoS ONE* 18: e0282924.
- 4. SE Escher, SP Felter, H Hollnagel, AP Boobis, C Yang, J Rathman, **MTD Cronin**, M Batke (2023) Workshop report on the evaluation of the updated and expanded carcinogen database to support derivation of threshold of toxicological concern values for DNA reactive carcinogens. *ALTEX Alternatives to animal experimentation* 40: 341-349
- 5. **MTD Cronin**, FJ Bauer, M Bonnell, B Campos, DJ Ebbrell, JW Firman, S Gutsell, G Hodges, G Patlewicz, M Sapounidou, N Spînu, PC Thomas, AP Worth (2022) A scheme to evaluate structural alerts to predict toxicity Assessing confidence by characterising uncertainties. *Regulatory Toxicology and Pharmacology* 135: 105249.
- C Westmoreland, HJ Bender, JE Doe, MN Jacobs, GEN Kass, F Madia, C Mahony, I Manou, G Maxwell, P Prieto, R Roggeband, T Sobanski, K Schütte, AP Worth, Z Zvonar, MTD Cronin (2022) Use of New Approach Methodologies (NAMs) in regulatory decisions for chemical safety: Report from an EPAA Deep Dive Workshop. Regulatory Toxicology and Pharmacology 135: 105261.
- 7. N Ball, R Bars, PA Botham, A Cuciureanu, **MTD Cronin**, JE Doe, T Dudzina, TW Gant, M Leist, B van Ravenzwaay (2022) A framework for chemical safety assessment incorporating new approach methodologies within REACH. *Archives of Toxicology* 76: 743-766.
- 8. C Alexander-White, D Bury, **M Cronin**, M Dent, E Hack, NJ Hewitt, G Kenna, J Naciff, G Ouedraogo, A Schepky, C Mahony, C Europe (2022) A 10-step framework for use of Read-Across (RAX) in Next Generation Risk Assessment (NGRA) for cosmetics safety assessment. *Regulatory Toxicology and Pharmacology* 129: 105094.
- N Spînu, MTD Cronin, J Lao, A Bal-Price, I Campia, SJ Enoch, JC Madden, L Mora Lagares, M Novič, D Pamies, S Scholz, DL Villeneuve, AP Worth, (2022) Probabilistic modelling of developmental neurotoxicity based on a simplified Adverse Outcome Pathway network. Computational Toxicology 21: 100206.
- 10. CB Pestana, JW Firman, **MTD Cronin** (2021) Incorporating lines of evidence from New Approach Methodologies (NAMs) to reduce uncertainties in a category based read-across: A case study for repeated dose toxicity. *Regulatory Toxicology and Pharmacology* 120: e104855.
- 11. C Mahony, RS Ashton, B Birk, AR Boobis, T Cull, GP Daston, L Ewart, TB Knudsen, I Manou, S Maurer-Stroh, L Margiotta-Casaluci, BP Müller, P Nordlund, RA Roberts, T Steger-Hartmann, E Vandenbossche, MR Viant, M Vinken, M Whelan, Z Zvonimir, MTD Cronin (2020) New ideas for non-animal approaches to predict repeated-dose systemic toxicity: Report from an EPAA Blue Sky Workshop. Regulatory Toxicology and Pharmacology 114: 104668
- 12. E Drakvik, R Altenburger, Y Aoki, T Backhaus, T Bahadori, R Barouki, W Brack, **MTD Cronin**, B Demeneix, S Hougaard Bennekou, J van Klaveren, C Kneuer, M Kolossa-Gehring, E Lebret, L Posthuma, L Reiber, C Rider, J Rüegg, G Testa, B van der Burg, H van der Voet, AM Warhurst, B van de Water, K Yamazaki, M Öberg, A Bergman (2020) Statement on advancing the assessment of chemical mixtures and their risks for human health and the environment. *Environment International* 134: 105267.
- 13. N Spinu, A Bal-Price, **MTD Cronin**, SJ Enoch, JC Madden, AP Worth (2019) Development and analysis of an Adverse Outcome Pathway network for human neurotoxicity. *Archives of Toxicology* 93:2759-2772.
- 14. B Desprez, B Birk, B Blaauboer, A Boobis, P Carmichael, MTD Cronin, R Curie, G Daston, B Hubesch, P Jennings, M Klaric, D Kroese, C Mahony, G Ouédraogo, A Piersma, A-N Richarz, M Schwarz, J van Benthem, B van de Water, M Vinken (2019) A mode-of-action ontology model for safety evaluation of chemicals: outcome of a series of workshops on repeated dose toxicity. *Toxicology in Vitro* 59: 44-50.
- 15. **MTD Cronin**, JC Madden, C Yang, AP Worth (2019) Unlocking the potential of *in silico* chemical safety assessment A report on a cross-sector symposium on current opportunities and future challenges. *Computational Toxicology* 10: 38-43.
- 16. C Laroche, E Annys, H Bender, D Botelho, P Botham, S Brendler-Schwaab, R Clayton, M Corvaro, G Dal Negro, F Delannois, M Dent, C Desaintes, B Desprez, S Dhalluin, A Hartmann, S Hoffmann-Doerr, B Hubesch, A Irizar, I Manou, BP Müller, S Nadzialek, P Prieto, M Rasenberg, Roggeband, TG Rowan, K Schutte, B van de Water, C Westmoreland, M Whelan, A Wilschut, Z Zvonimir, MTD Cronin (2019) Finding synergies for the 3Rs-Repeated Dose Toxicity testing: Report from an EPAA Partners' Forum. Regulatory Toxicology and Pharmacology 108: 104470.