

Table of Contents

EDITORIAL

Nicholas Sammut

ARTICLES

- 4 WanderRep A reporting Tool for Caregivers of Wandering Persons with Dementia **Research Article**
Colin Cachia, Conrad Attard and Matthew Montebello
- 10 Dynamics of Private Social Networks **Research Article**
Jonathan Mifsud and Matthew Montebello
- 16 Uniqueness Typing For A Higher-Order Language **Research Article**
Adrian Francalanza and Melanie Zammit
- 22 Formal Proofs for Broadcast Algorithms **Research Article**
Mandy Zammit and Adrian Francalanza
- 29 Monitoring Distributed Systems with Distributed PolyLarva **Research Article**
Ian Cassar, Adrian Francalanza, Christian Colombo
- 37 Warpage issues in large area mould embedding technologies **Research Article**
Russell Farrugia, Ivan Grech, Owen Casha, Joseph Micallef, Edward Gatt, Roseanne Duca and Conrad Cachia
- 45 Neuropathology and Neuropharmacology of Monoaminergic systems **Meeting Report**
Rona R. Ramsay and Philippe De Deurwaerdère
- 50 Annual Meeting of the COST ACTION CM1103 **Conference Proceedings**
- 101 Representational Momentum and the Human Face: an empirical note **Research Article**
Ian M. Thornton
- 111 2014 Science in the House with Members of Parliament **News**
David C. Magri
- 113 In memory of Prof. Giuseppe Amato (1944-2004) **News**
Giuseppe Crescimanno
- e1 Influence of antimony on structure and physical properties of tin **Research Article**
Andriy Yakymovych, Stepan Mudry, Yuriy Plevachuk, Vasyl Sklyarchuk, Valeri Sidorov
- e5 A Fruitful Fly Forward: The Role of the Fly in Drug Discovery for Neurodegeneration **Review Article**
Michelle Briffa, Neville Vassallo & Ruben J. Cauchi
- e17 Select polyphenols protect mitochondria against amyloid aggregates in Alzheimer and Parkinson diseases **Review Article**
Mario Caruana and Neville Vassallo
- e26 A 10 year review of the number of bovine dairy holdings and the dairy bovine population on the Maltese Islands **Research Article**
Mauro Buttigieg, Matteo Ganesella and Andrew James
- e34 Measuring b-cell function in vivo to understand the pathophysiology of type 2 diabetes **Review Article**
Luca P. Farrugia and Adrian Vella



COST Action no. CM1103

Structure-based drug design for diagnosis and treatment of neurological diseases: dissecting and modulating complex function in the monoaminergic systems of the brain

2011 | 2015

Objectives

- To forge interdisciplinary collaborations for structure-based drug design for multiple targets in the monoamine system
- To design chemical tools to diagnose and treat the pathology underlying neuropsychological disorders
- To quantify computationally and experimentally the efficacy of new multi-target lead compounds to a range of receptors, enzymes and transporters and take the best forward into behavioural studies
- To stimulate an interdisciplinary approach and the use of chemical tools to understand the molecular basis of behaviour in development and degeneration

Main Achievements

- Now 30 group leaders (40% female; 17% ESR).
- Predictive computational methods have identified novel drug-to-target interactions by data mining – (UK, RS; experimental tests in IT, DE).
- The crystal structure of a prototype compound with one target (MAO B) has been solved (ES,IT) – see figure.
- GPCR homology models published: <http://pubs.acs.org/doi/suppl/10.1021/ci900444q>.
- A novel compound (from DE) has been tested for antipsychotic efficacy in animal models of schizophrenia (IT) and autism (USA).
- 2 patents (ES). Joint publications: 18 published, 6 more submitted.
- Of four joint grant proposals submitted, one including IT and TR with external participants was successful (FP7-PEOPLE-2013-ITN).
- Vianello (HR) awarded a FP7 Marie Curie Career Integration Grant
- STSM: Last year, 9 were completed; Year 2 has 2 approved so far.

www.cost.eu/cmst



Chemistry and Molecular Sciences and Technologies (CMST)

Participating countries

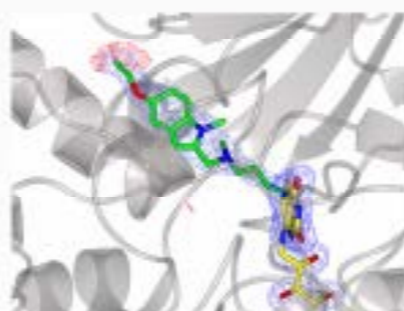
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Structure of the adduct of monoamine oxidase B and ASS234, a multipotent compound ([dx.doi.org/10.1021/jm200853t](https://doi.org/10.1021/jm200853t)) that inhibits monoamine oxidase A and acetyl- and butyryl-cholinesterase targets in Alzheimer's disease (ES and IT).

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WICT 2014

6th Workshop in Information and Communication Technology
2nd, 3rd April 2014 at Valletta Campus

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WICT 2014 is the 6th Workshop in Information and Communication Technology organized by the Faculty of ICT within the University of Malta.

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