PhD in Chemical Sciences
Department of Chemistry "Ugo Schiff"
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PhD Seminar

"Sugars, Drugs and Rock & Roll"

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Abstract

Michela's research interests span the areas of Medicinal Chemistry, Glycobiology/Carbohydrate Chemistry, Bioinorganic Chemistry, Organic Boron as Pharmacophore, Spectroscopy, and more recently Renewable Fuels and Ionic Liquids. These research programs reflect her varied career in research and the interdisciplinary nature of her research, spanning discoveries at the fundamental level with a clear pathway to applications. The main undercurrent to most of her research programs is carbohydrate chemistry.[1]

Synthetic development and spectroscopic analysis constitute the core of her and her research group's expertise. Cutting-edge skills in synthetic optimisation and development, and in spectroscopic analysis allow production of diastereoisomerically pure, high Fsp^3 index drug leads and the detailed analysis of complex systems, such as lactol mixtures, oligopeptides, equilibria of organic boron derivatives as they change from their boronate esters, to their boronic acid forms, to other intramolecularly bonded species, as the pH changes and as reactions proceed.

Organic boron as a pharmacophore. This is an area of paramount importance in medicinal chemistry, albeit still underdeveloped. The chemistry of organic boron is notoriously complex because it is so kaleidoscopic, however much is to be gained from its use as a pharmacophore due to its capacity to establish reversible covalent bonds with nucleophilic residues in active sites or around active sites of target enzymes. We have cutting-edge expertise in this area and developed protocols to functionalise low Fsp^3 and - most importantly - high Fsp^3 index molecules with organic boron groups, where we see potent and selective inhibition of the target enzymes. This opens up the way to new generations of boron neutron capture therapy (BNCT) agents.[2]

Glycosidase inhibition/modulation. Several novel drug lead libraries display selective and potent modulations against several glycosidases. These open up new strategies to inhibition of viral infections via a broad-spectrum antiviral strategy, diabetes management and management of selected lysosomal storage disorders.[3]

Ionic liquids, renewables and green chemistry. More recently, work in physical chemistry/engineering and green chemistry have yielded novel generations of ionic liquids with excellent thermal stabilities, green chemistry protocols for syntheses and purifications, and renewable fuels via biomass conversion and through water splitting processes.[4]

[1] *Journal of Medicinal Chemistry*, **2021**, 64, 2678; *PlosOne*, 2019, e0217712.
[2] *Molecules*, 2022, 27, 3447; *Beilstein Archives*, 2021, 20214; *Heterocyclic Communications*, **2017**, *23*, 167.
[3] *Chemical Biology Drug Design*, **2018**, *92*, 1171; *Tetrahedron: Asymmetry*, **2012**, *23*, 401.
[4] *Journal of Molecular Liquids*, 2020, 312, 114091; *ACS Omega*, 2020, 5, 12637; *Carbon*, **2017**, *114*, 566.