UNIVERSITÉ DE TOULON

LABORATOIRE MAPIEM

PERSONAL PROJECT OF RESEARCH

MOLECULARLY IMPRINTED POLYMERS FOR TOXIN DETECTION

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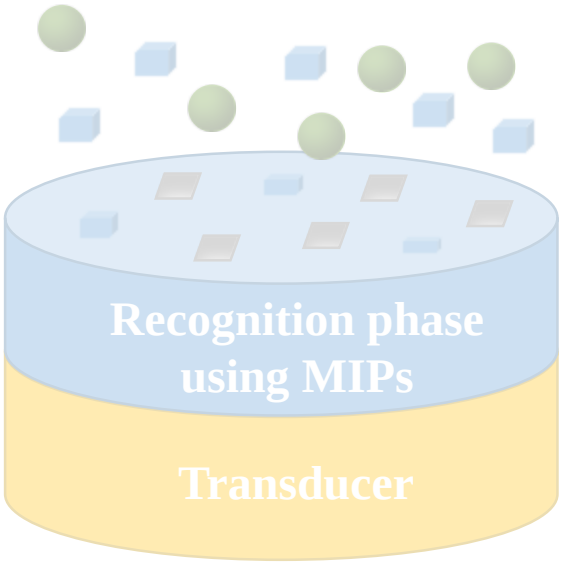
Made by SCOTE Tom L1 PC R

Outline of my Project

Molecularly Imprinted Polymer (MIP)



Sensor

Toxin Detection

What is a MIP ?

> **Inspired by antibodies**

LEGEND

: template (= target)

: functional monomers

MOLECULAR IMPRINTING TECHNIQUE:

1st STEP:

Copolymerization with a crosslinker

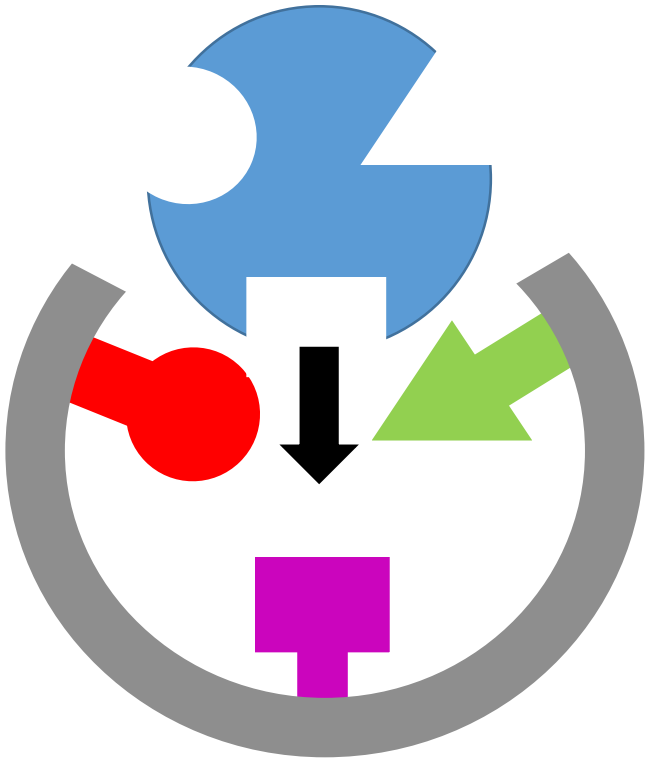
2nd STEP:

Solvent

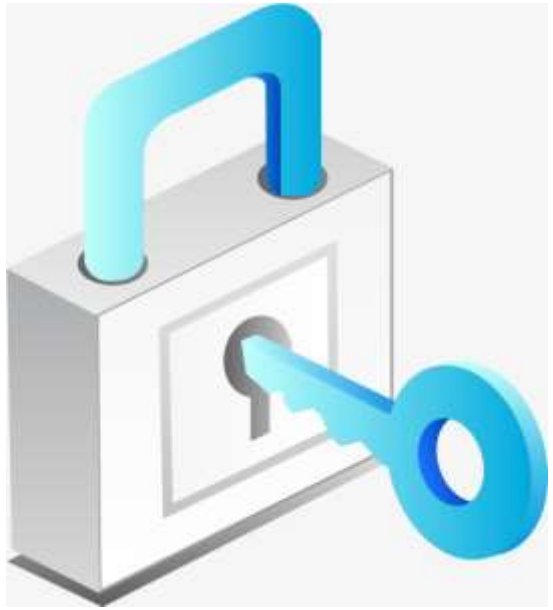
3rd STEP:

MIP

What is a MIP ?



SUM UP

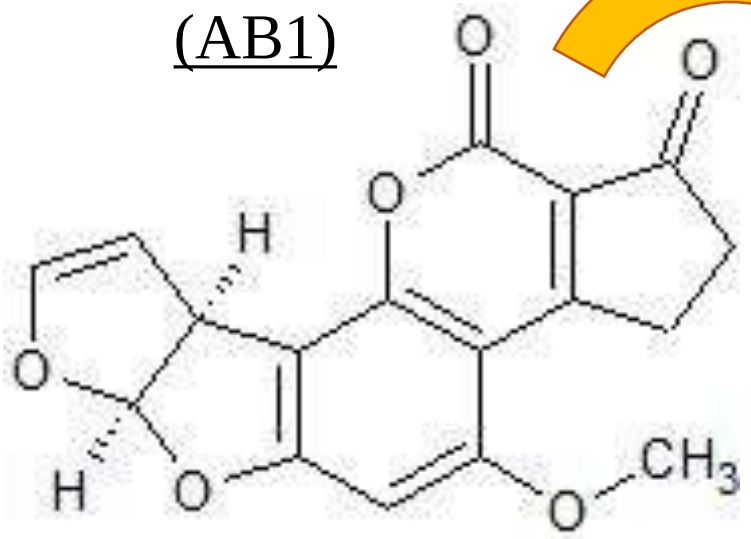


Source: *https://fr.pngtree.com/freepng/lock-and-key_2704040.html [Access: 29/05/19]*

A MIP and its template are like a lock and its key

Target toxin: Aflatoxin B1

Aflatoxin B1 (AB1)



2D structure

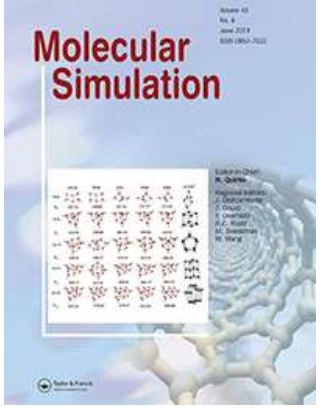
Source: *https://food20.fr/lait-anciens-nouveaux-usages/?lang=en [Access: 29/05/19]*

Acute toxic

Serious health hazard

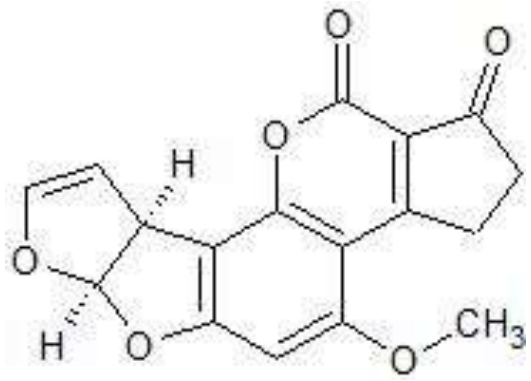
VERY DANGEROUS BECAUSE WE CAN FIND IT IN MILK, FOOD…

Source: *www.hse.gov.uk/chemical-classification/labelling-packaging/hazard-symbols-hazard-pictograms.htm [Access: 29/05/19]*

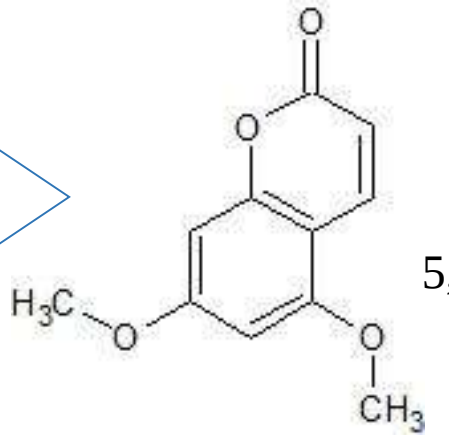


"Molecular modelling of a template substitute and monomers used in molecular imprinting for aflatoxin B1 micro-HPLC analysis". Miroslaw Wyszomirski and Wojciech Prus. *Molecular Simulation*, **38:11, 892-895**, 2012

Aflatoxin B1 (AB1)



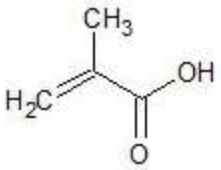
Replaced by a "dummy" template - less toxic



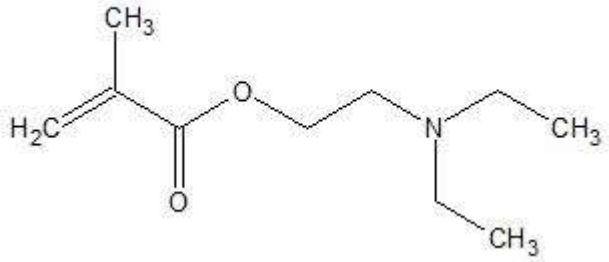
5,7-dimethoxycoumarin (DMC)

Functional monomers shortlisted for MIP design:

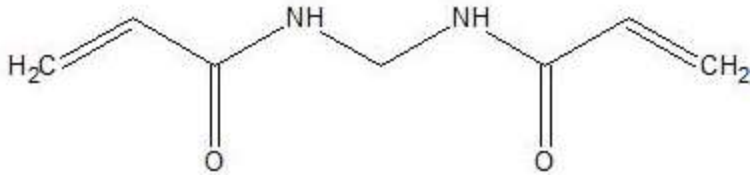
allylamine



methacrylic acid (MAA)



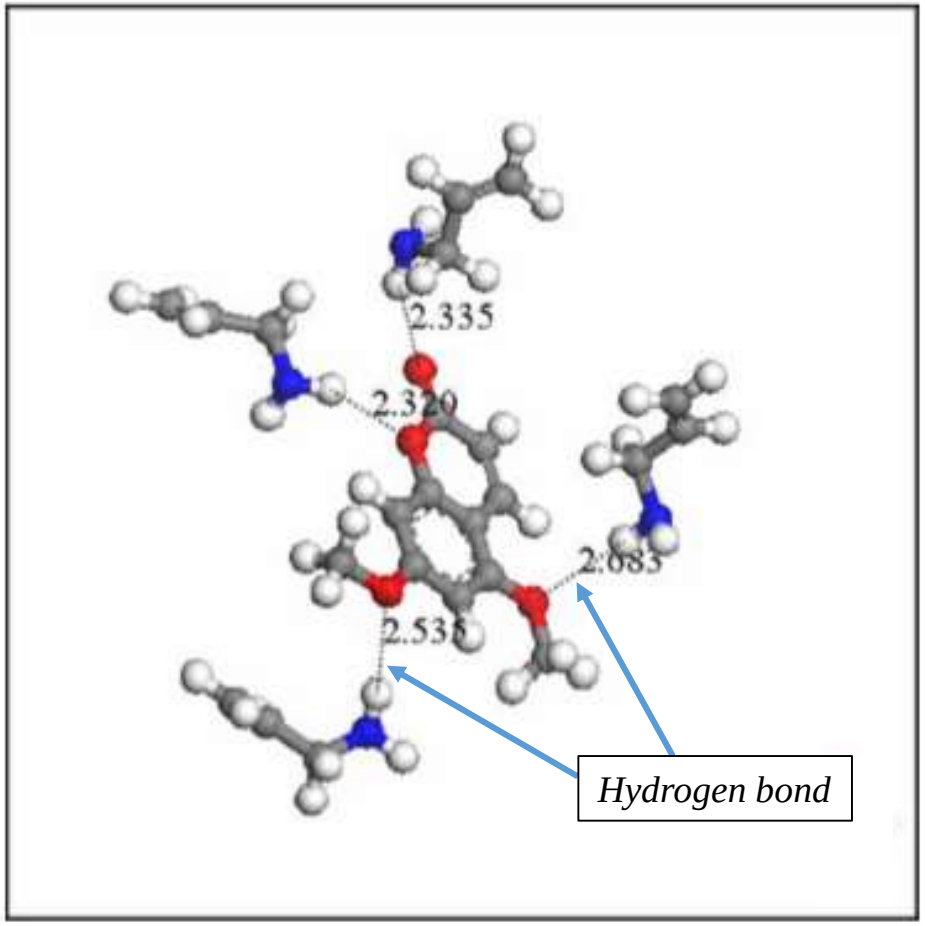
2-(diethyloamino)ethylmethacrylate (DEAEM)



N,N'-methylene bisacrylamide (MBA)

Which one is the best ?

Modelling results

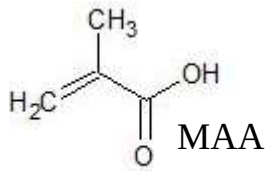


An example of a simulated system with the DMC molecule and MMA monomer molecules

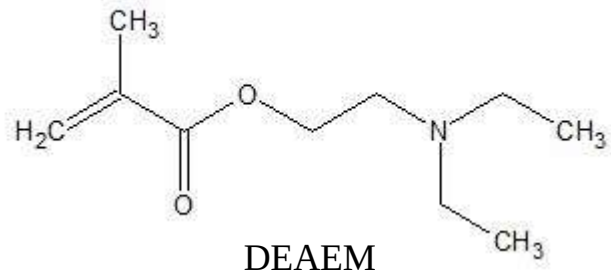
Result table. The energies of the interaction of the selected monomers with DMC and with AB1

Monomer	Interaction energy between the template molecule and the monomer (kcal/mol)	
	DMC	AB1
allylamine	-46,4 (± 1,2)	-43,1 (± 0,8)
MAA	-33,6 (± 1,0)	-32,0 (± 0,6)
DEAEM	-32,3 (± 1,1)	-23,5 (± 1,4)
MBA	-75,4 (± 0,9)	-86,8 (± 0,5)

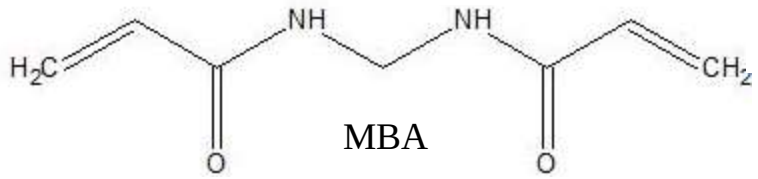
allylamine



MAA



DEAEM



MBA

Allylamine and MAA = Best monomers
MBA = Good choice for crosslinker

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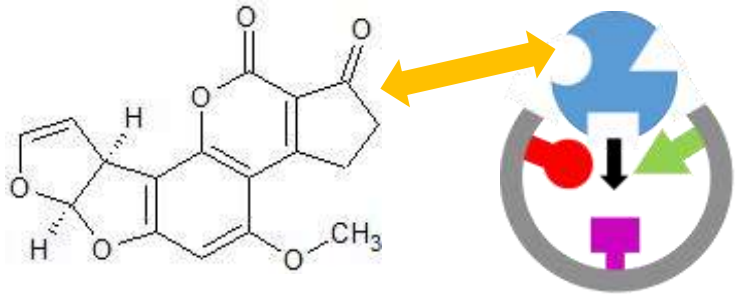
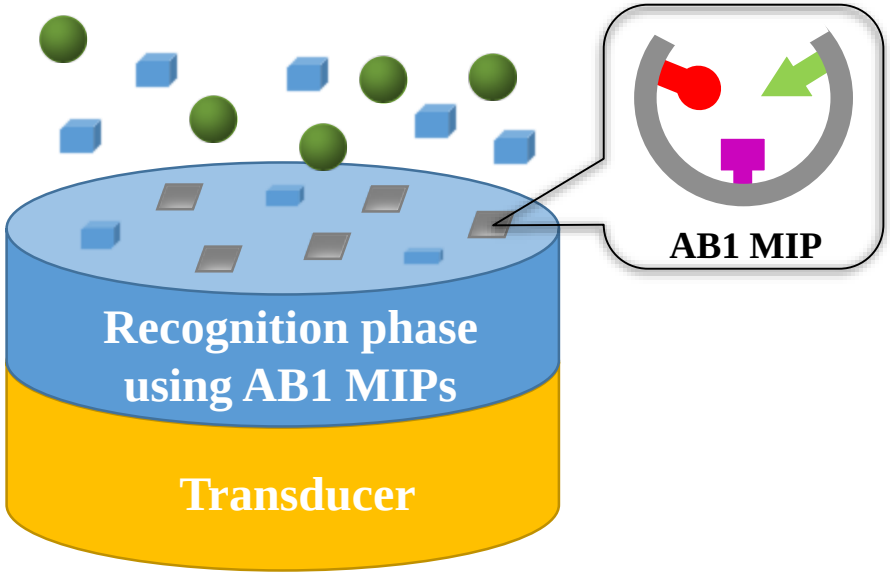
Conclusion and perspectives

- Synthesis conditions for a Aflatoxin B1 MIP



- Integration in a sensor



Sources: -*https://pixabay.com/fr/illustrations/bien-validé-dédié-okejka-2282499/*
-*https://ankiweb.net/shared/info/1577497098*
[Access: 29/05/19]