

# BeeToxAI: An Artificial Intelligence-Based Web Portal to Assess Acute Toxicity of Chemicals in Honey Bees



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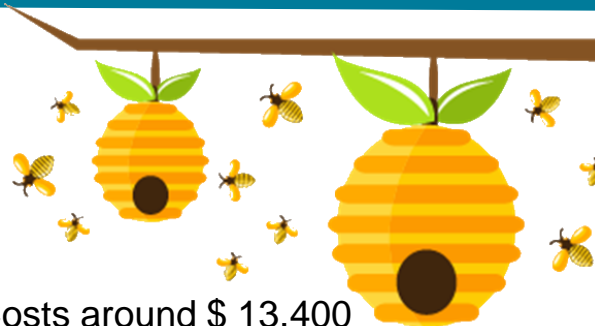
# The Honey Bees



$\frac{1}{3}$  of food is pollination dependent



Pollinate \$ 15 billion in crops annually

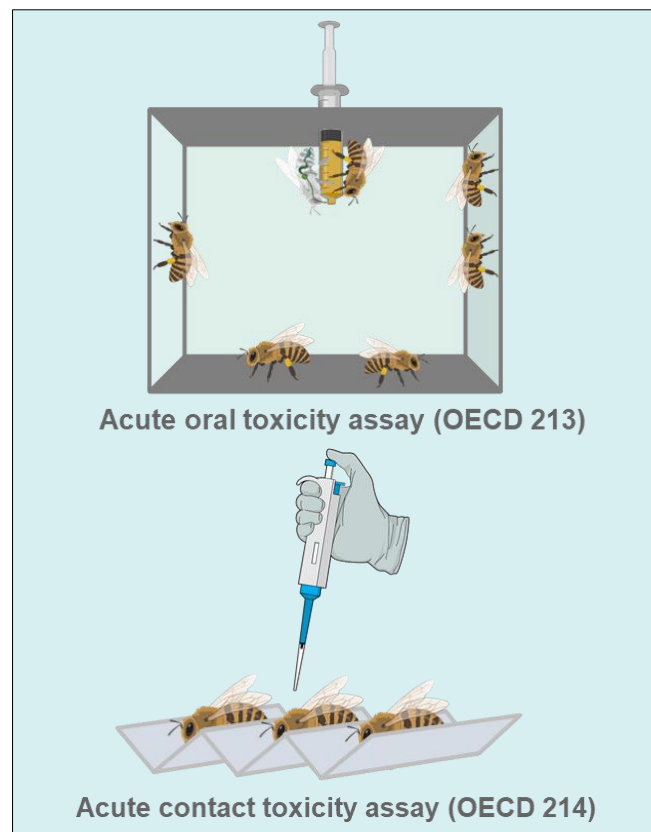
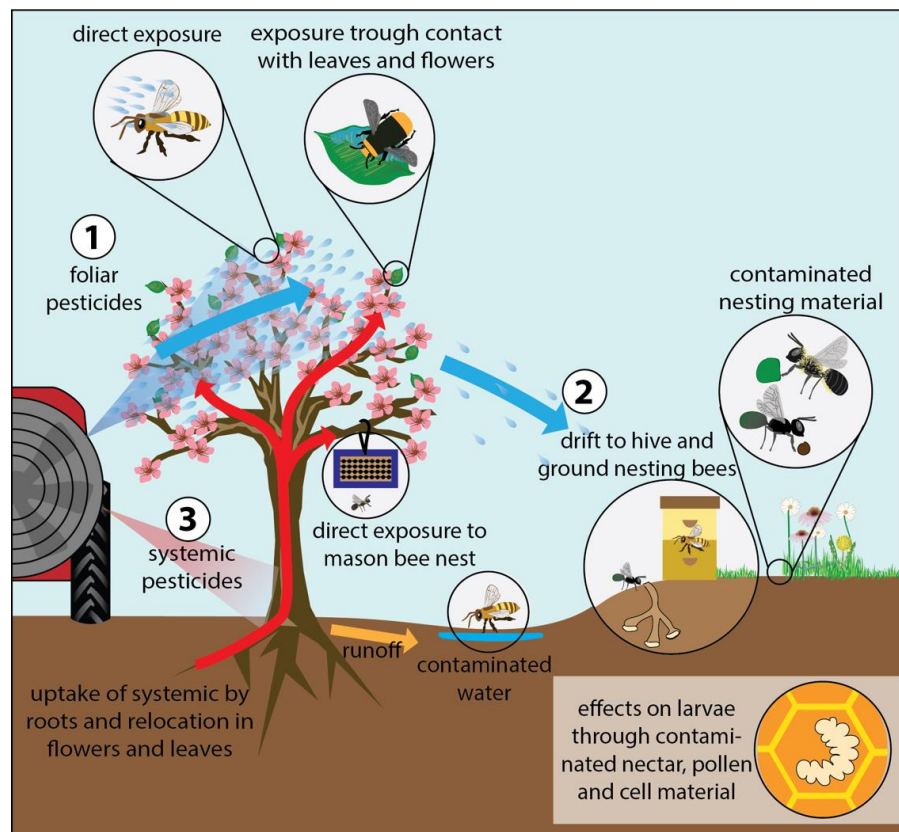


Costs around \$ 13,400 per compound

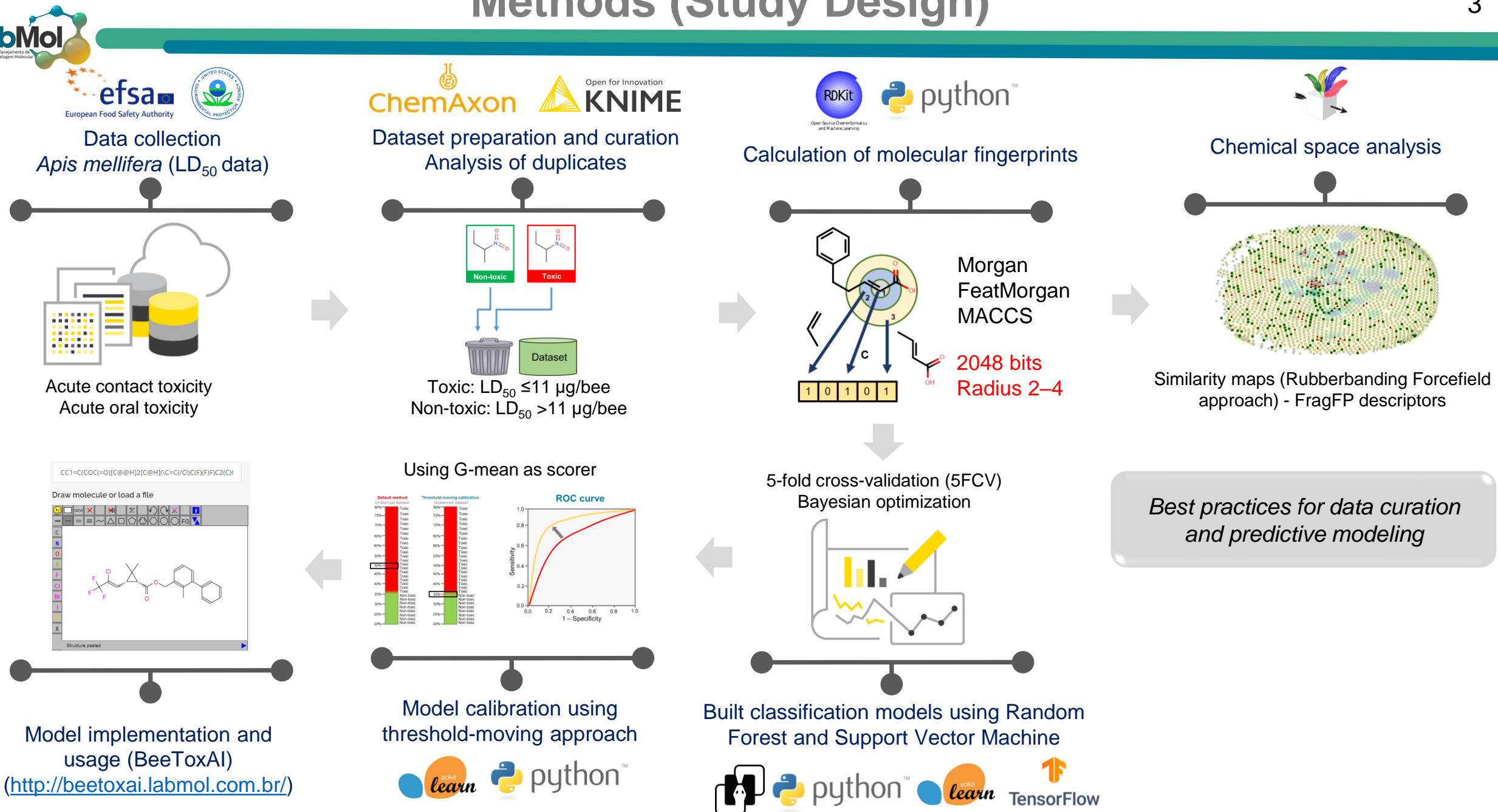
## Main goal of study

Development of predictive QSAR models to assess acute contact toxicity and acute oral toxicity of untested chemicals towards honey bee (*Apis mellifera*)

*In silico* methods are faster and cheaper alternatives to assess toxicity



# Methods (Study Design)

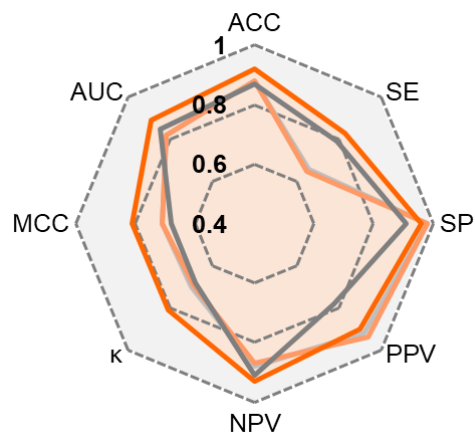


# Statistical Characteristics of Models

## Acute contact toxicity

### Morgan\_2 + RF

External validation

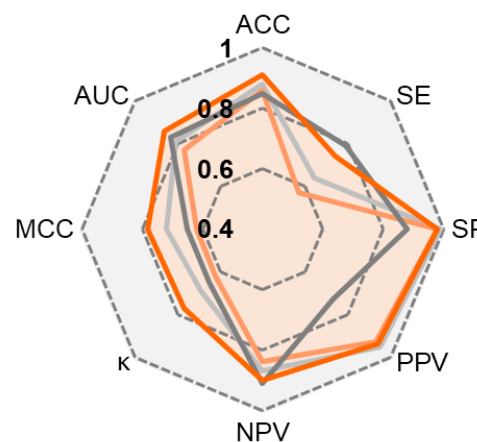


ACC = 0.92  
SE = 0.83  
SP = 0.96  
PPV = 0.90  
NPV = 0.93  
 $\kappa$  = 0.81  
MCC = 0.81  
AUC = 0.89

PT = 0.29

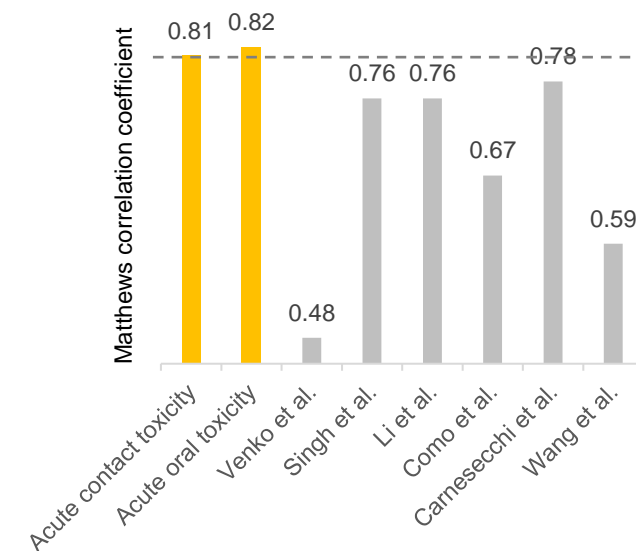
### Morgan\_4 + RF

External validation



ACC = 0.91  
SE = 0.74  
SP = 0.98  
PPV = 0.94  
NPV = 0.90  
 $\kappa$  = 0.77  
MCC = 0.78  
AUC = 0.87

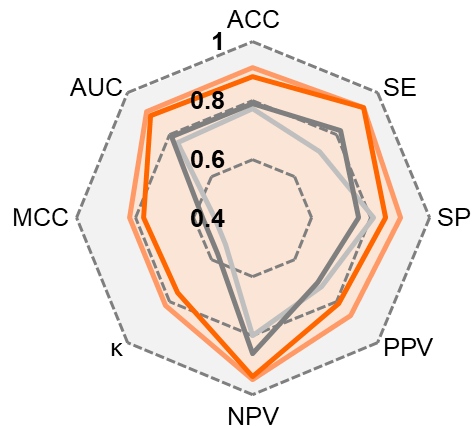
PT = 0.33



## Acute oral toxicity

### MACCS + SVM

External validation

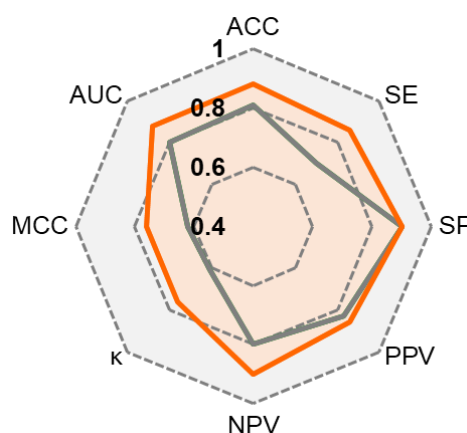


ACC = 0.91  
SE = 0.93  
SP = 0.90  
PPV = 0.87  
NPV = 0.95  
 $\kappa$  = 0.82  
MCC = 0.82  
AUC = 0.91

PT = 0.50

### MACCS + RF

External validation



ACC = 0.88  
SE = 0.86  
SP = 0.90  
PPV = 0.86  
NPV = 0.90  
 $\kappa$  = 0.76  
MCC = 0.76  
AUC = 0.88

PT = 0.50

The benchmarking with existing computational tools demonstrated predictive superiority of our models

Freely available at <http://beetoxai.labmol.com.br/>

# BeeTox



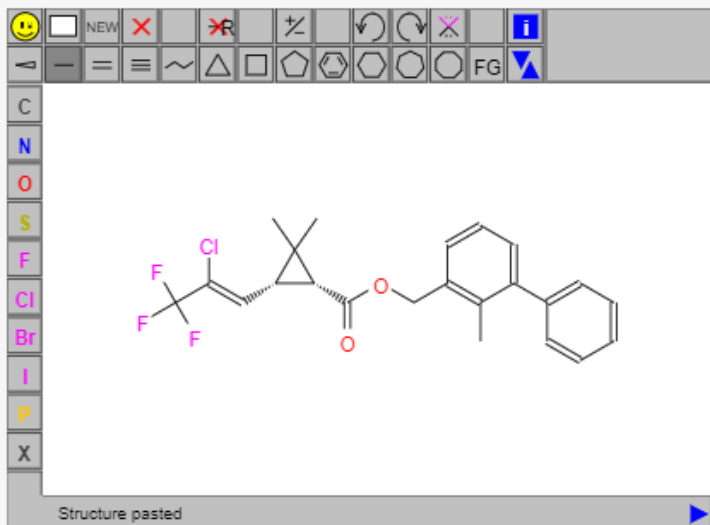
An artificial intelligence web app to assess acute toxicity of chemicals in honey bees



## Enter SMILES

CC1=C(COC(=O)[C@@H]2[C@H](\C=C(/Cl)C(F)(F)F)C2(C)(

Draw molecule or load a file



 SUBMIT ANALYSIS

## Endpoint

Acute oral Toxicity

Assay type: Acute Oral Toxicity Test (OECD 213)

Animal: Honey bee (*Apis mellifera*)

ML Algorithm: SVM

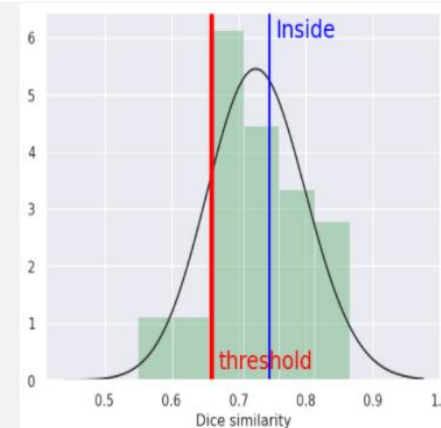
Descriptors: MACCS

## Prediction

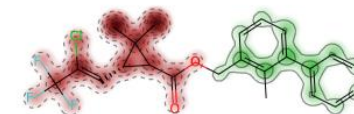
**Toxic (+)**

75.0%

## Applicability domain



## Contribution map



Acute Contact Toxicity

Assay type: Acute Contact Toxicity Test (OECD 214)

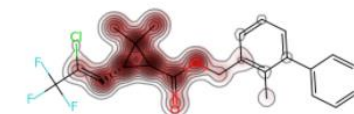
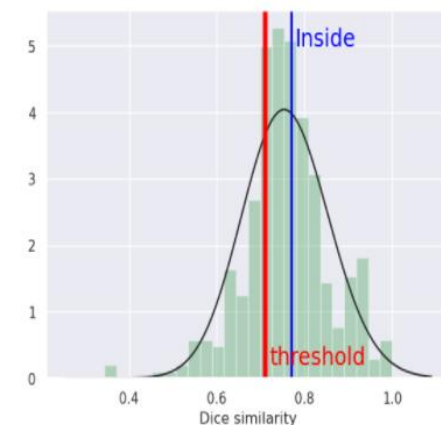
Animal: Honey bee (*Apis mellifera*)

ML Algorithm: Random Forest

Descriptors: Morgan EFCP2 with bit-vector size of 2048 bits

**Toxic (+)**

(100%)

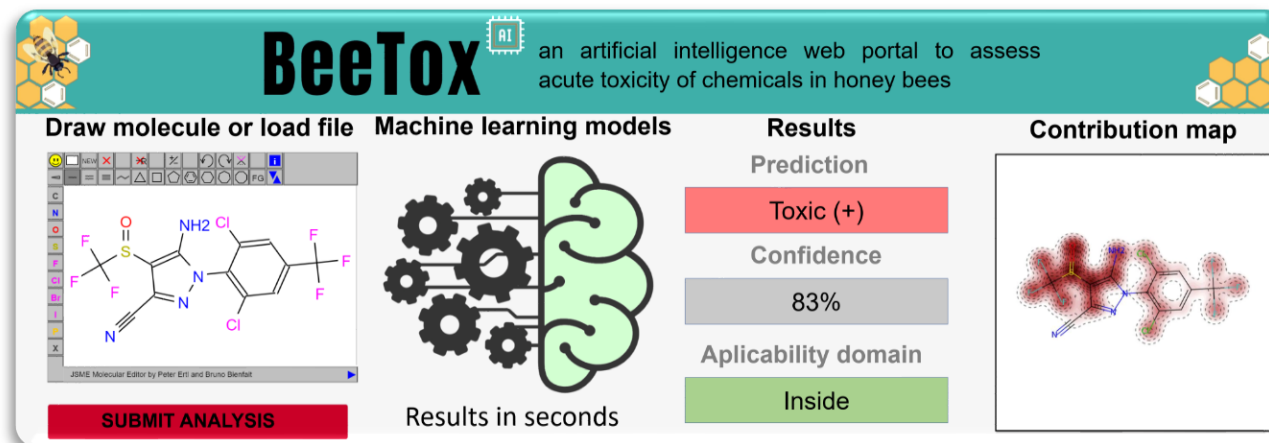




# Final Remarks

## Conclusion

BeeToxAI web app is fast, reliable, and user-friendly tool for the assessment of acute chemical toxicity to honey bees



**BeeTox<sup>AI</sup>** an artificial intelligence web portal to assess acute toxicity of chemicals in honey bees

**Draw molecule or load file** Machine learning models **Results** **Contribution map**

**Prediction**  
Toxic (+)

**Confidence**  
83%

**Aplicability domain**  
Inside

**Results in seconds**

**Contribution map**

**SUBMIT ANALYSIS**

## Acknowledgments



**UFG**  
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FEDERAL DE GOIÁS

