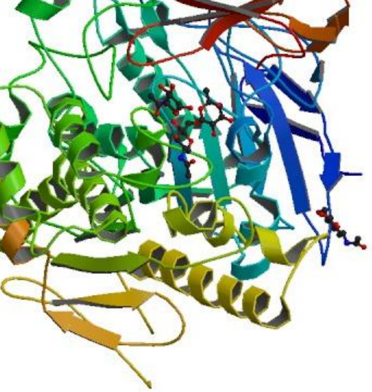

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# Leveraging Molecular Docking Techniques to Support Virtual Screening of Cross-species Susceptibility to Chemical Effects

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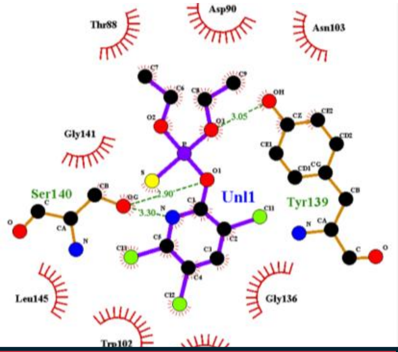
*[3]Safety and Environmental Assurance Centre (SEAC), Colworth Science Park, Sharnbrook MK44 1LQ.*



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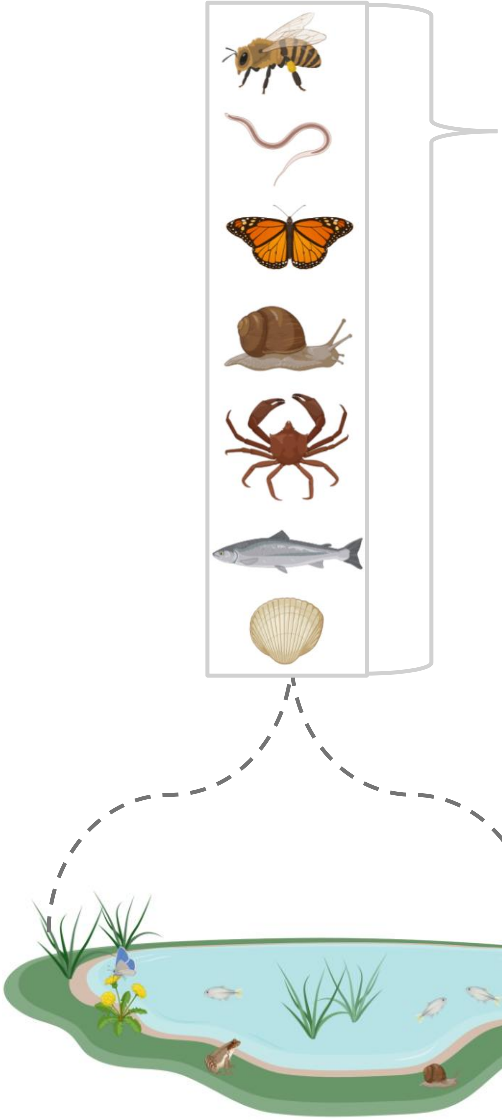
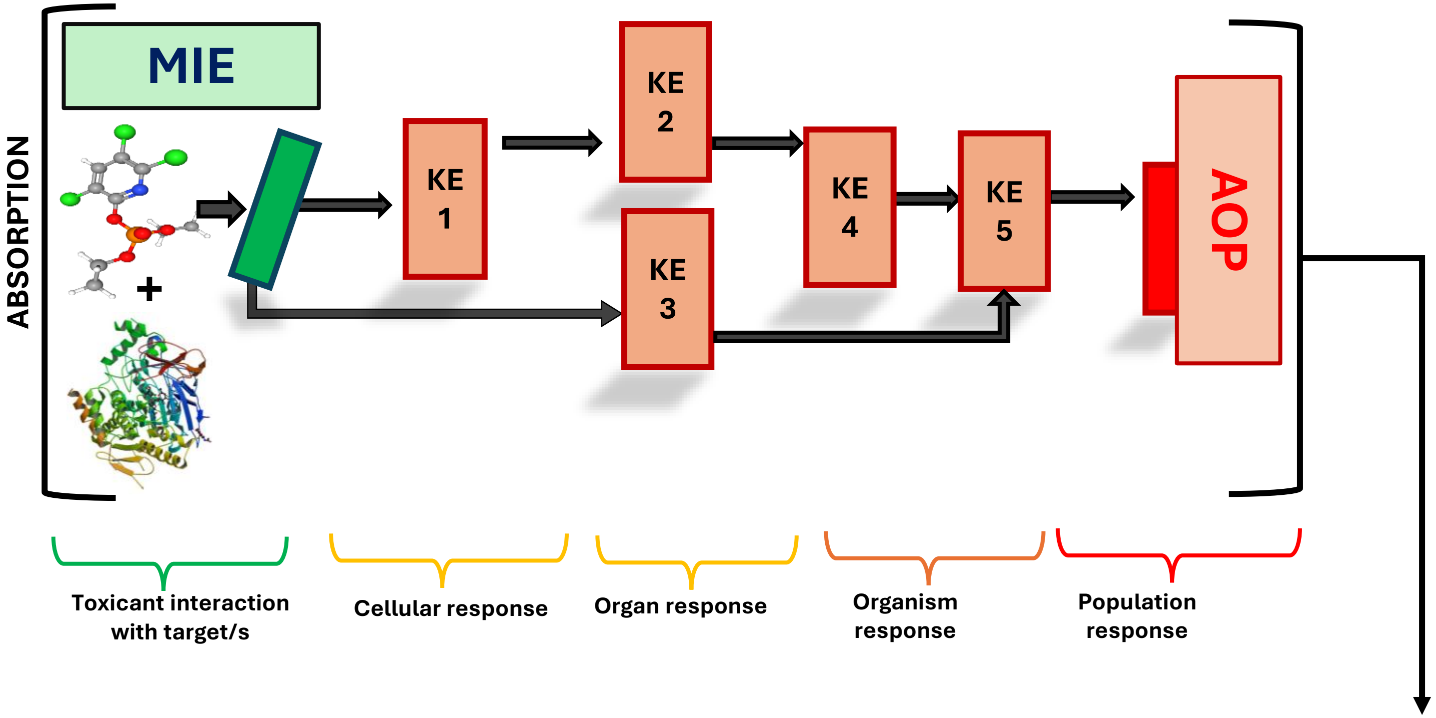
## ➢ Species are not equally sensitive to toxicants: making risk assessment difficult

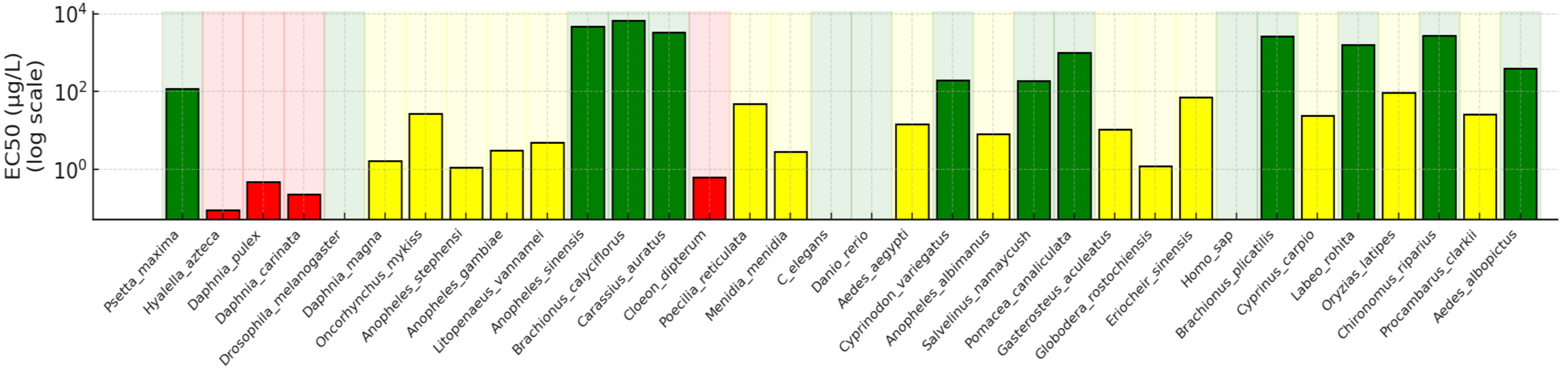


**Species sensitivities** = f

Statistical approach



**Species sensitivity distribution (SSD) for chlorpyrifos**



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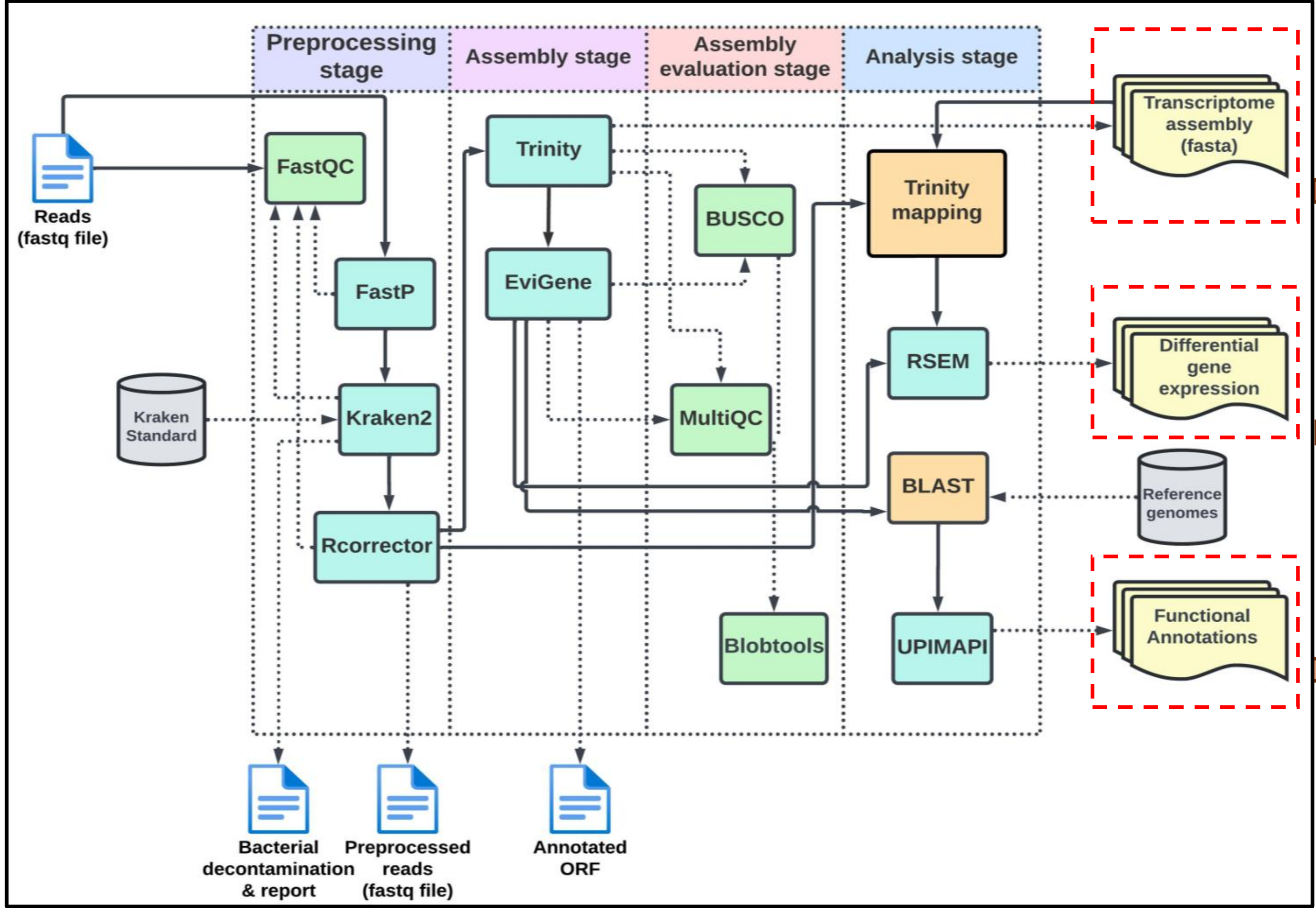
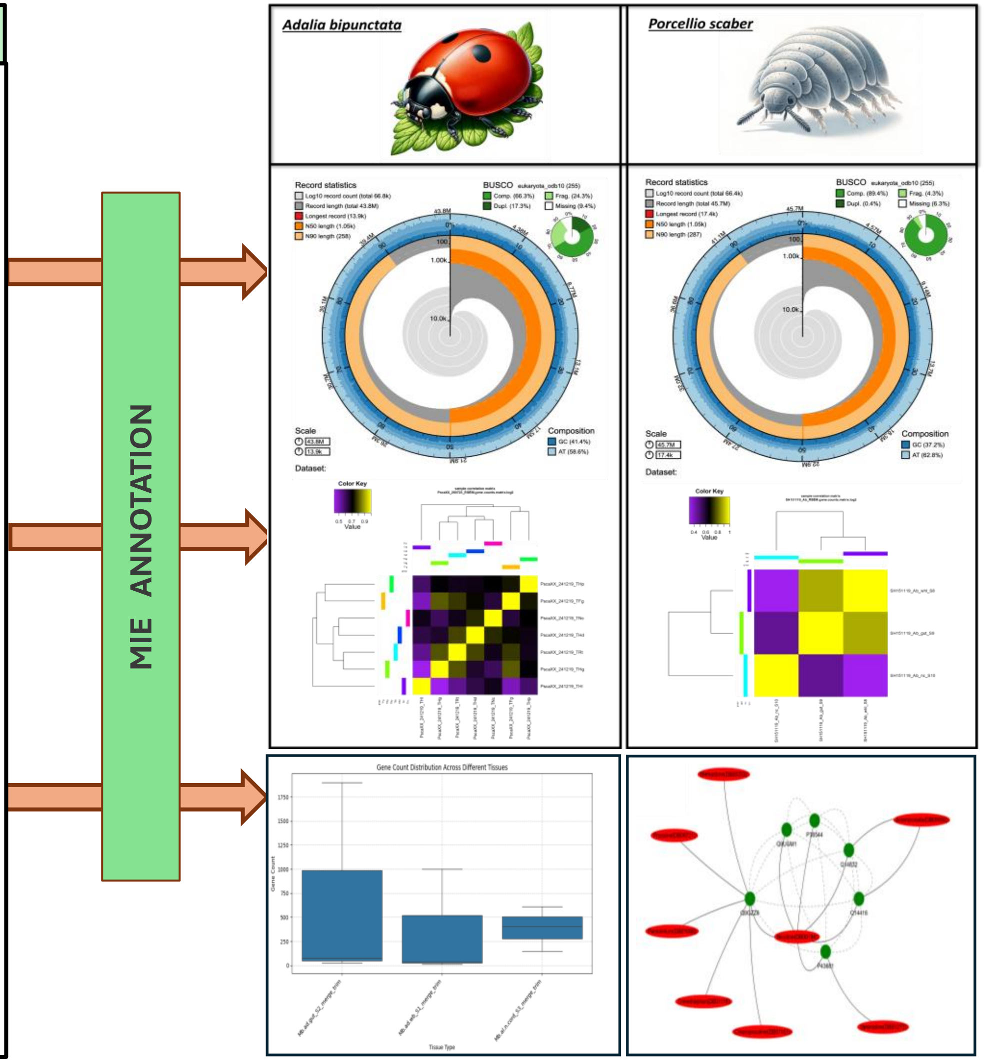
# Why is this important now? Helping the “too many” species scalability challenge

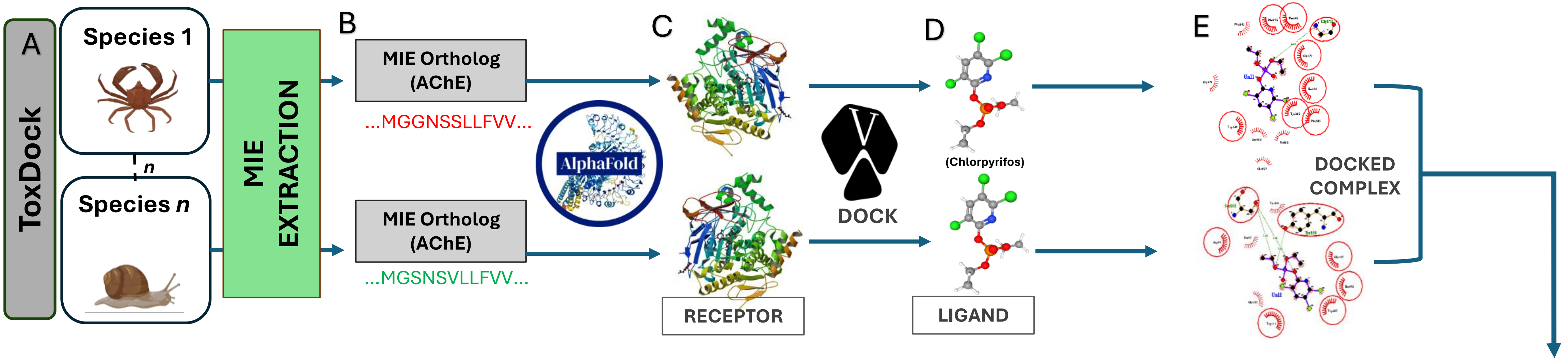
Darwin TREE of LIFE

- Over 1000 genomes and counting – goal of 70,000.
- Combining high-throughput exposure systems with RNA-seq can address chemical challenges and compensate for unavailable genome
- transFlow for fast and efficient transcriptome assembly, designed for: DGE analysis and MIE identification

**https://github.com/krishnan-Rama/transFlow (Nextflow/SLURM)**







A

**ToxDock**

Species 1

*n*

Species *n*

**MIE EXTRACTION**

B

MIE Ortholog (AChE)

...MGGNSSLLFVV...

MIE Ortholog (AChE)

...MGSNSVLLFVV...

AlphaFold

C

RECEPTOR

DOCK

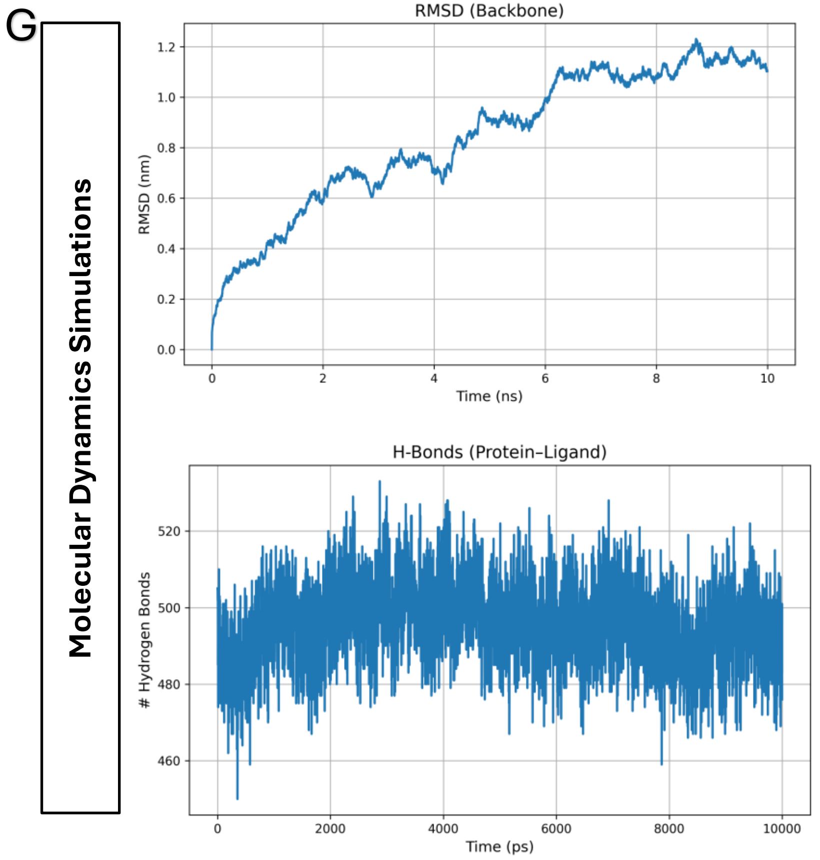
D

(Chlorpyrifos)

LIGAND

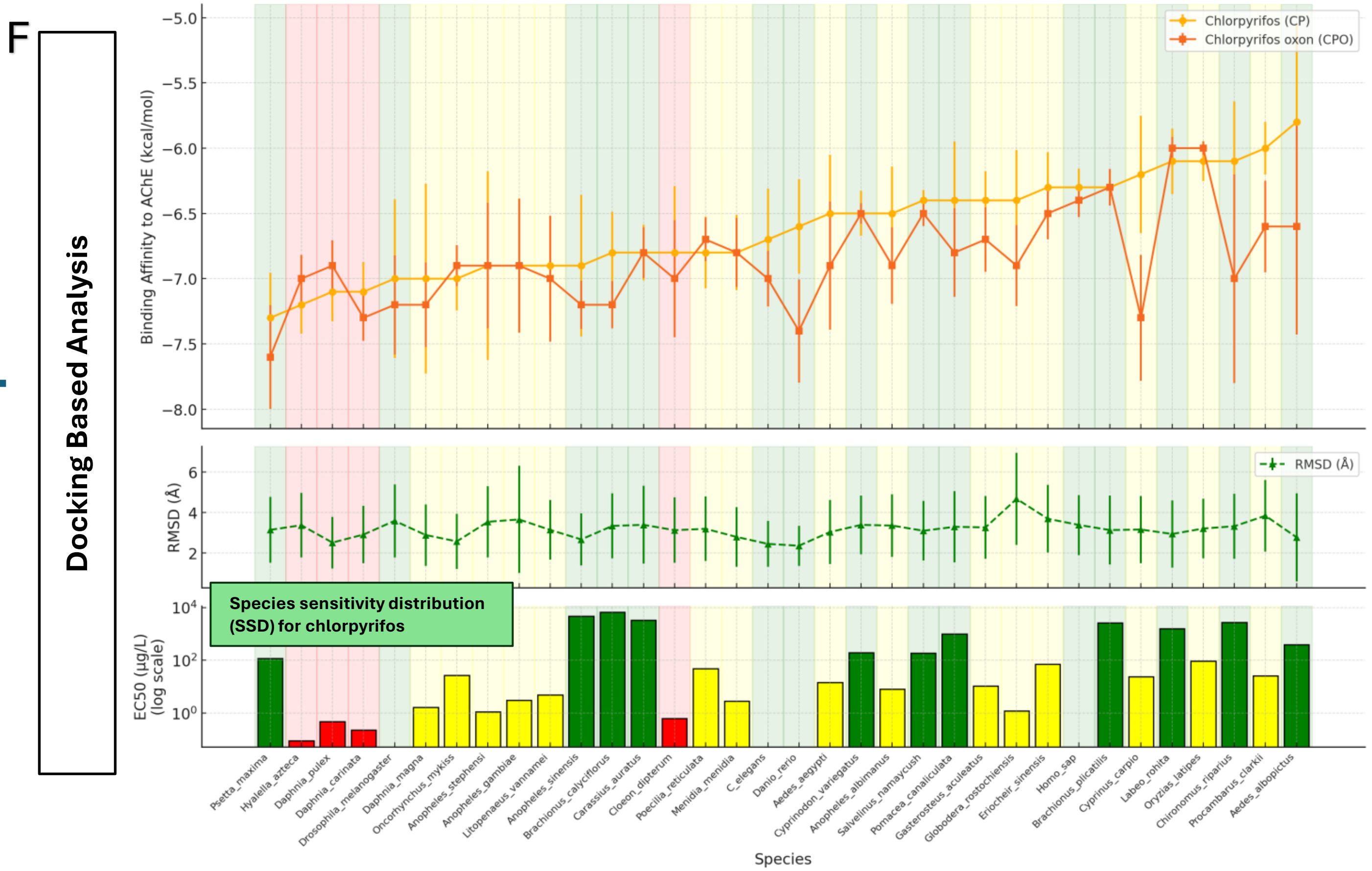
E

DOCKED COMPLEX



G

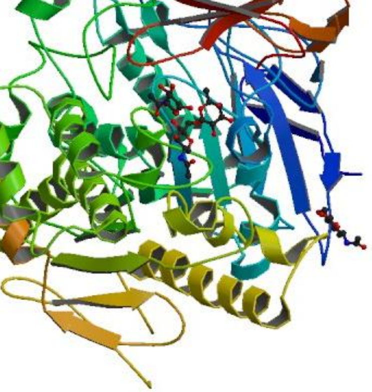
**Molecular Dynamics Simulations**



F

**Docking Based Analysis**

Species sensitivity distribution (SSD) for chlorpyrifos



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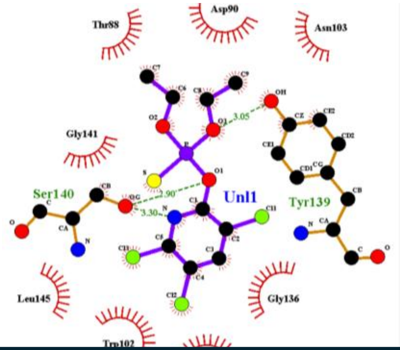
# Thank you, now let's get the theory into action…



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