

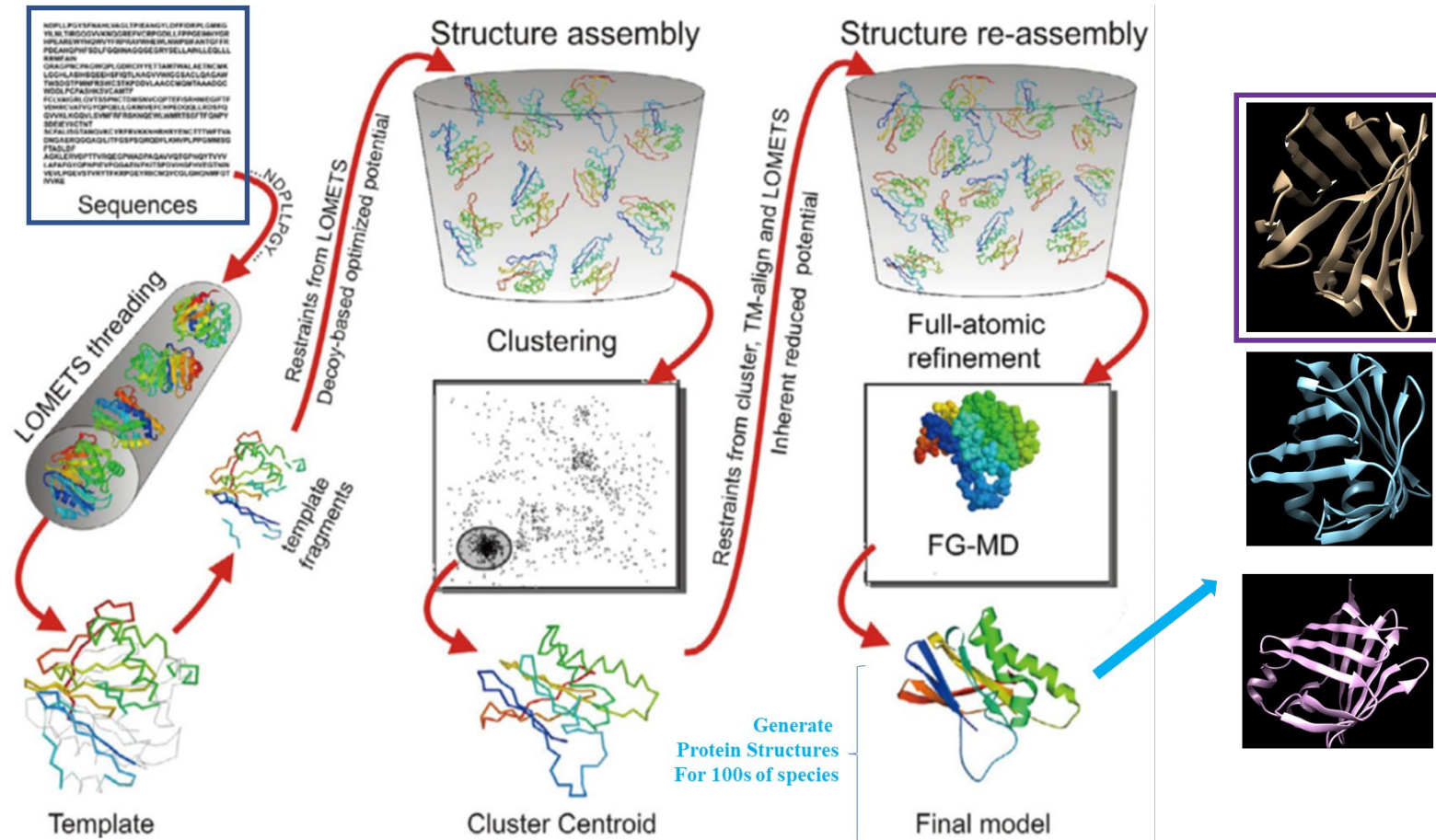
# Homology modeling and molecular docking recap

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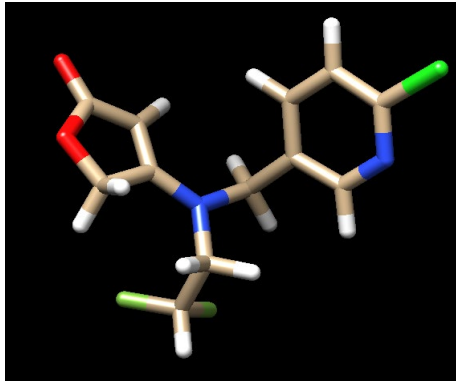


# Creating homology models with the Iterative Threading ASSEmbly Refinement (ITASSER) tool

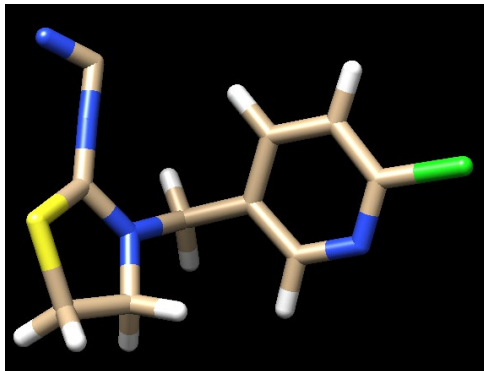




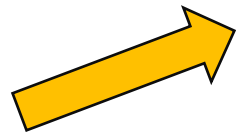
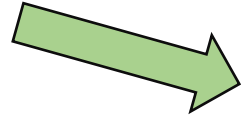
# Docking process



Flupyradifurone



Thiacloprid



## Docking box areas

EPA:

-17.098,-22.338,-11.492

20,15,15

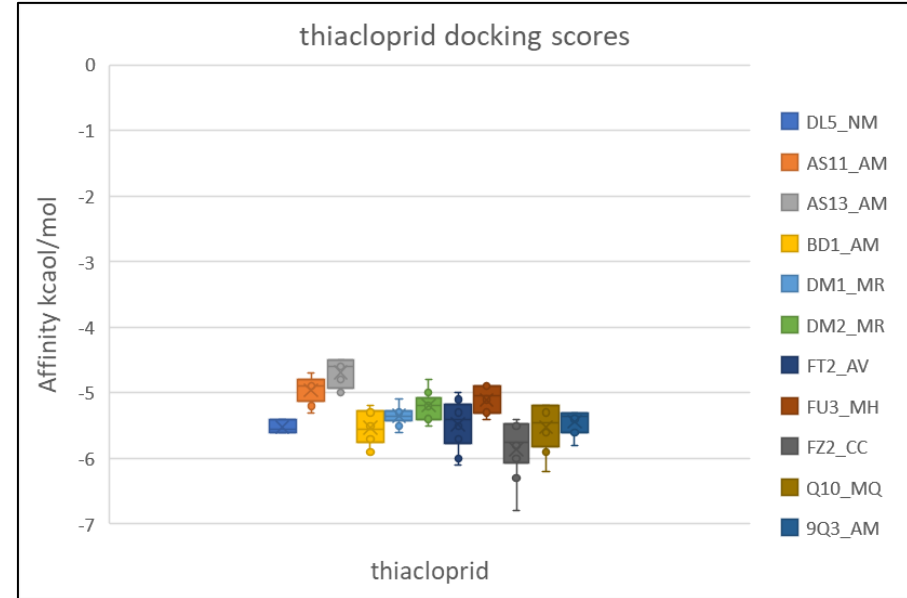
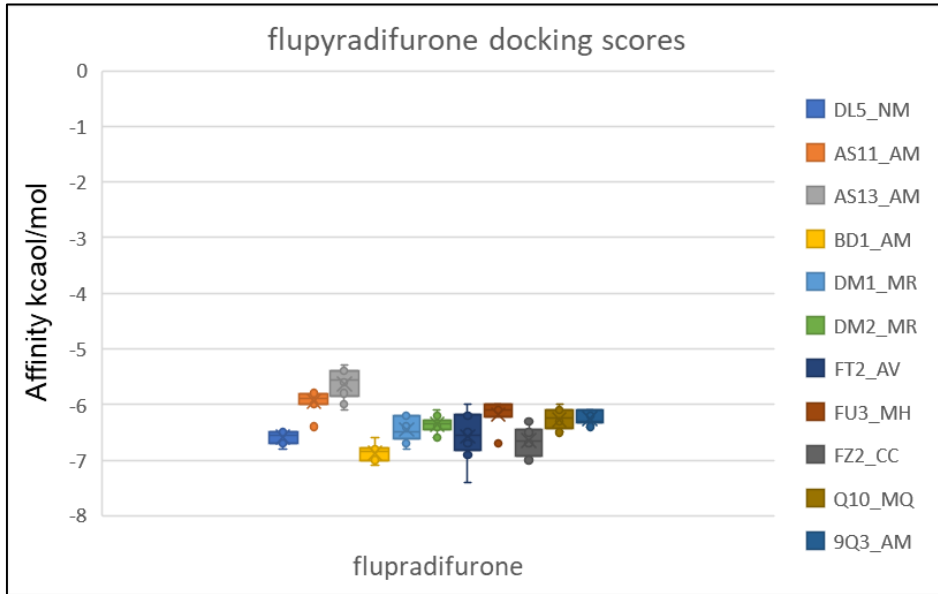
Bayer:

19.7332,25.7236,-4.67613

16.0055,17.7187,23.9048

(Used negative x,y,z coordinates due to location of ITASSER models)

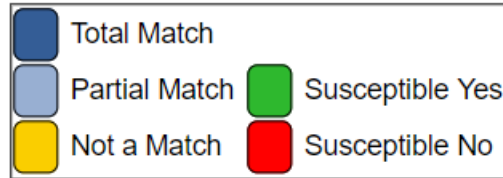
# Docking scores between models and boxes



		Average docking scores					
		AS11_AM	AS13_AM	BD1_AM	DM1_MR	DM2_MR	
flupyradifurone	EPA Box	-5.94	-5.63	-6.87	-6.45	-6.36	
	Bayer Box	-6	-5.68	-6.52	-6.54	-6.24	
thiacloprid	EPA Box	-4.96	-4.69	-5.53	-4.29	-5.19	
	Bayer Box	-5.3	-4.97	-5.4	-5.32	-4.91	
	flupy	thia					
Reference	-6.25	-5.44	EPA Box				
CYP9Q3_AM	-6.61	-5.64	Bayer Box				

“It includes 5 of the CYP9Q-orthologs we tested and have thiacloprid and flupyradifurone as their confirmed substrate and 5 enzymes (3 from the honey bee and two from Megachile rotundata), where metabolism of those insecticides is not present *in-vitro*.”

# Previously made SeqAPASS heat map



NCBI Accession	Scientific Name	Protein Name	Common Name	Similar Susceptibility	Amino Acid 1	Amino Acid 2	Amino Acid 3	Amino Acid 4	Amino Acid 5
XP_006562363.1	<i>Apis mellifera</i>	cytochrome P450 9e2	Honey bee	Y	111G	214N	310S	371V	372L
XP_016922294.2	<i>Apis cerana</i>	LOW QUALITY PROTEIN: cytochrome P450 9e2-like	Asiatic honeybee	Y	111G	214N	310S	371I	372L
XP_017758640.1	<i>Eufriesea mexicana</i>	PREDICTED: cytochrome P450 9e2-like	Orchid bees	N	110K	214M	307T	368I	369A
XP_031775226.1	<i>Apis florea</i>	cytochrome P450 9e2-like	Little honeybee	N	112K	216T	309T	370V	371V
XP_017794730.1	<i>Habropoda laboriosa</i>	PREDICTED: cytochrome P450 9e2-like	Digger bees	N	108K	212L	305T	366I	367V
XP_031837097.1	<i>Nomia melanderi</i>	cytochrome P450 9e2-like	Alkali bee	N	110K	214D	307S	368S	369P

