

Supplementary Materials

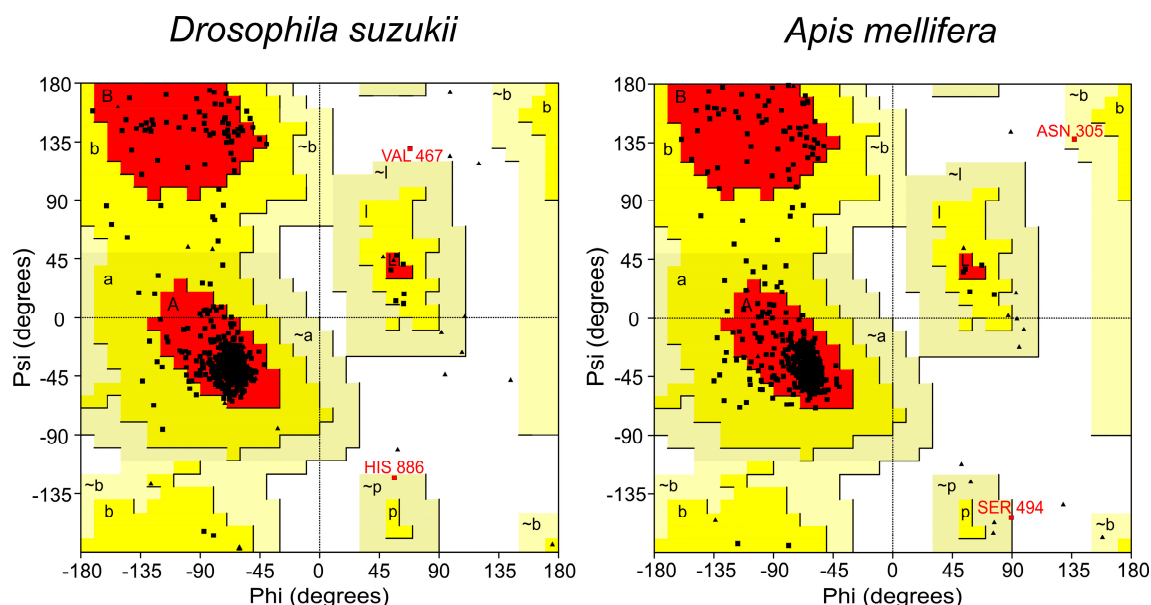


Figure S1. The Ramachandran plot of the GABA protein models. Based on an analysis of 118 structures of resolution of at least 2.0 Angstroms and R-factor no greater than 20%, a good quality model would be expected to have over 90% in the most favoured regions. Residues in most favoured regions [A,B,L]: *Drosophila suzukii* (425 – 92.2%), *Apis mellifera* (420 – 89.9 %); Residues in additional allowed regions [a,b,l,p]: *D. suzukii* (34 – 7.4 %), *A. mellifera* (45 – 9.6 %); Residues in generously allowed regions [\sim a, \sim b, \sim l, \sim p]: *D. suzukii* (1 – 0.2 %), *A. mellifera* (2 – 0.4 %); Residues in disallowed regions: *D. suzukii* (1 – 0.2 %), *A. mellifera* (0 – 0.0 %); Number of non-glycine and non-proline residues: *D. suzukii* (461 – 100.0 %), *A. mellifera* (467 – 100.0 %); Number of end-residues (excl. Gly and Pro): *D. suzukii* (5), *A. mellifera* (4); Number of glycine residues (shown as triangles): *D. suzukii* (40), *A. mellifera* (35); Number of proline residues: *D. suzukii* (24), *A. mellifera* (24); Total number of residues: *D. suzukii* (530), *A. mellifera* (530)

Binding of fipronil into GABA receptor proteins of *Drosophila suzukii* and *Apis mellifera*

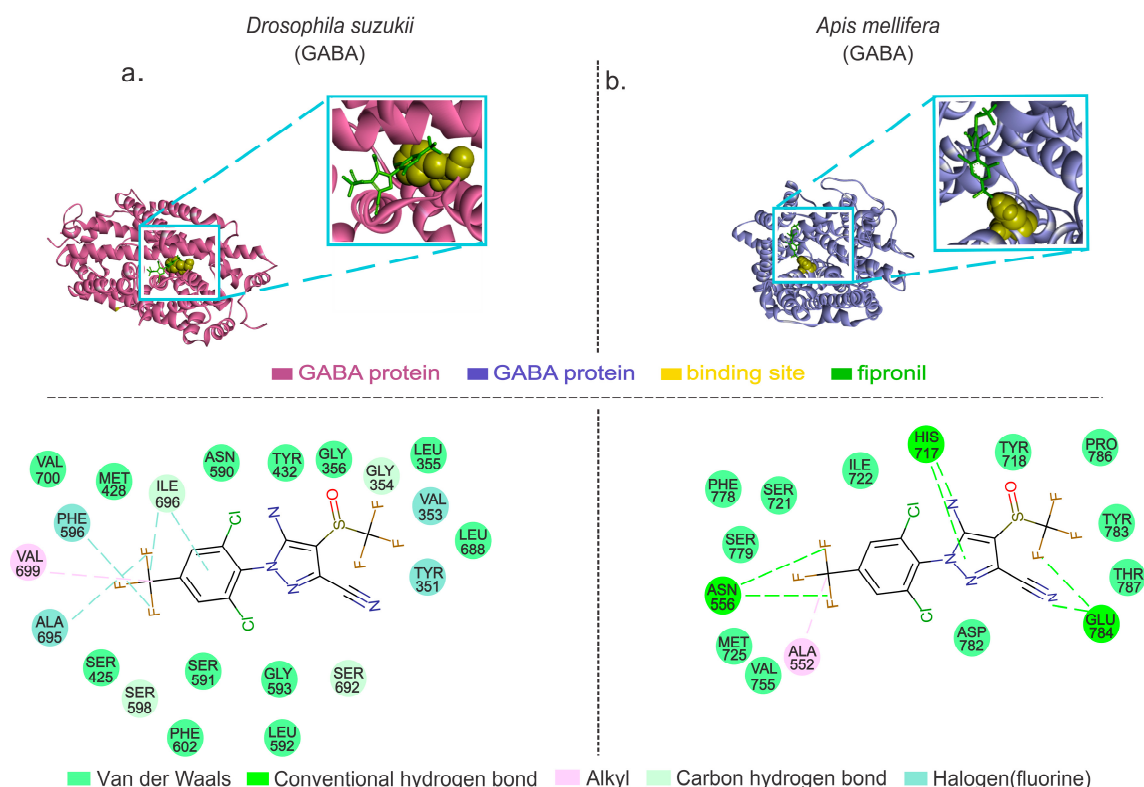


Figure S2. Fipronil interacting with GABA receptors of *Drosophila suzukii* and *Apis mellifera*. (a) Protein 3D structure of the *D. suzukii* GABA receptors with fipronil. (b) Protein 3D structure of the *A. mellifera* GABA receptors with fipronil. (c) 2D interaction maps showing the molecular interactions between amino acids from the binding site environments of *D. suzukii* GABA receptors with fipronil. (d) 2D interaction maps showing the molecular interactions between amino acids from the binding site environments of *A. mellifera* GABA receptors with fipronil.

Binding of citral isomers into acetylcholinesterase of *Drosophila suzukii* and *Apis mellifera*

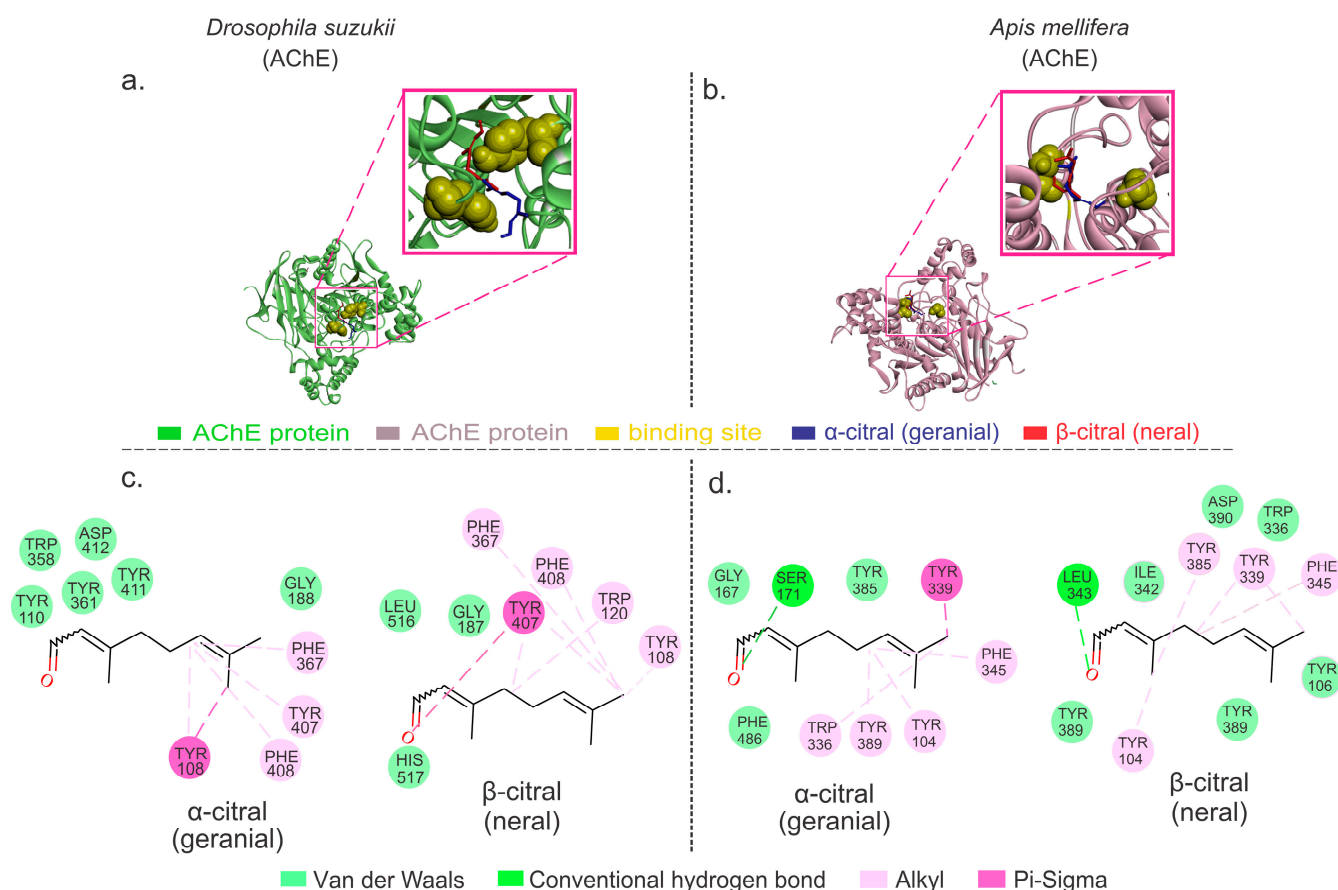


Figure S3. Citral isomers interacting with AChE protein from *Drosophila suzukii* and *Apis mellifera*. (a) Protein 3D structure of the *D. suzukii* AChE protein with the citral isomers. (b) Protein 3D structure of the *A. mellifera* AChE protein with the citral isomers. (c) 2D interaction maps showing the molecular interactions between amino acids from the binding site environments of *D. suzukii* AChE protein with the citral isomers. (d) 2D interaction maps showing the molecular interactions between amino acids from the binding site environments of *A. mellifera* AChE protein with the citral isomers

Binding of citral isomers into glutathioneS-transferase of *Drosophila suzukii* and *Apis mellifera*

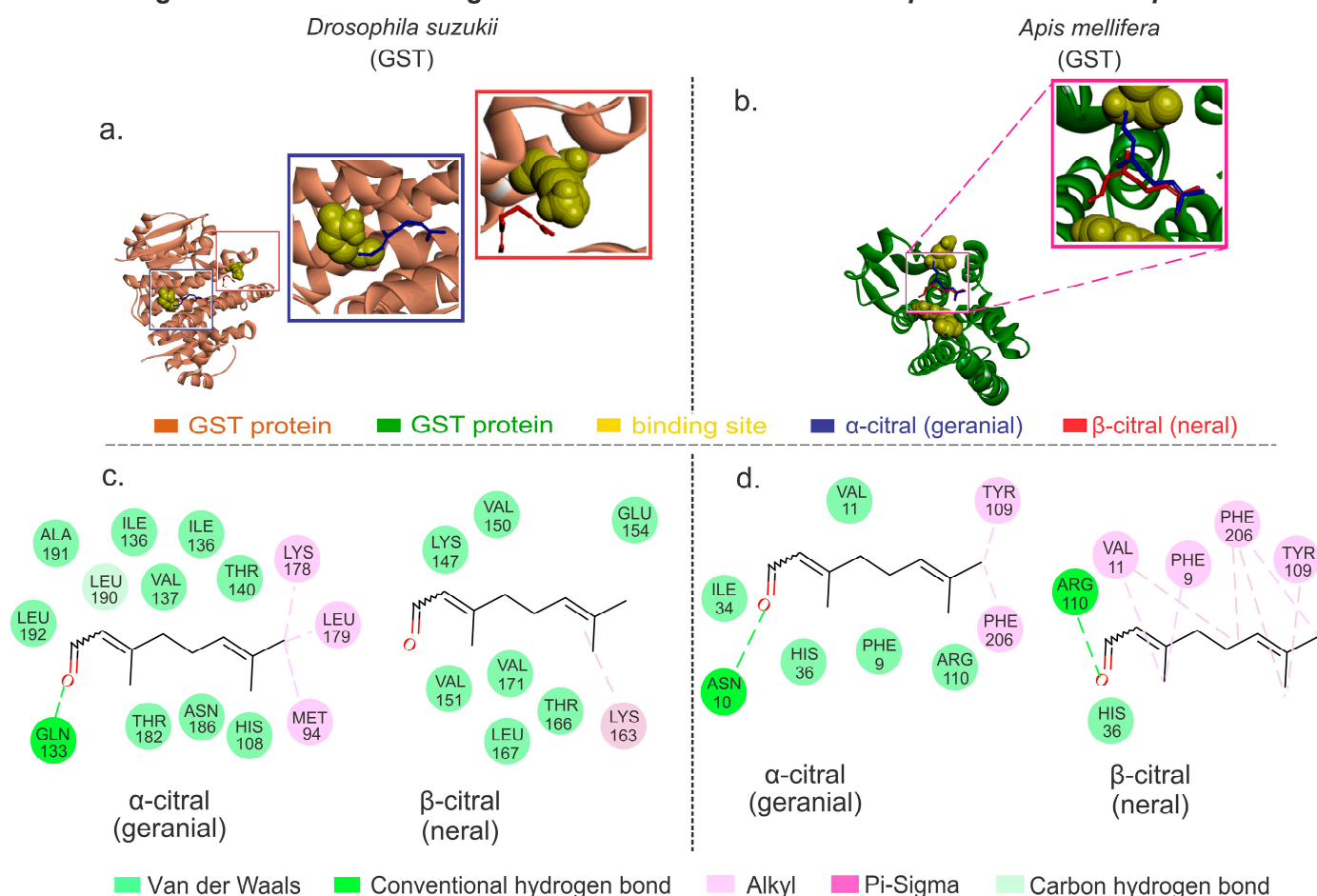


Figure S4. Citral isomers interacting with GST protein from *Drosophila suzukii* and *Apis mellifera*. (a) Protein 3D structure of the *D. suzukii* GST protein with the citral isomers. (b) Protein 3D structure of the *A. mellifera* GST protein with the citral isomers. (c) 2D interaction maps showing the molecular interactions between amino acids from the binding site environments of *D. suzukii* GST protein with the citral isomers. (d) 2D interaction maps showing the molecular interactions between amino acids from the binding site environments of *A. mellifera* GST protein with the citral isomers

Table S1 The coordinates of the receptor grids on the targets

γ -aminobutyric acid (GABA) receptor																	
<i>Drosophila suzukii</i>									<i>Apis mellifera</i>								
α -citral			β -citral			Fipronil			α -citral			β -citral			Fipronil		
124.039	6.693	42.925	124.039	6.693	42.925	124.039	6.693	42.925	-42.346	-0.589	54.926	-42.346	-0.589	54.926	-42.346	-0.589	54.926
Acetylcholinesterase (AChE)																	
<i>Drosophila suzukii</i>									<i>Apis mellifera</i>								
α -citral			β -citral			Fipronil			α -citral			β -citral			Fipronil		
24.426	63.184	9.919	24.426	63.184	9.919	<i>n.a</i>			24.326	63.259	10.076	24.326	63.259	10.076	<i>n.a</i>		
Glutathione-S-transferase (GST)																	
<i>Drosophila suzukii</i>									<i>Apis mellifera</i>								
α -citral			β -citral			Fipronil			α -citral			β -citral			Fipronil		
56.191	20.534	6.667	56.191	20.534	6.667	<i>n.a</i>			-0.300	0.923	-0.368	-0.300	0.923	-0.368	<i>n.a</i>		

*spacing 0.375; npts 40 40 40; *nt*- not applicable