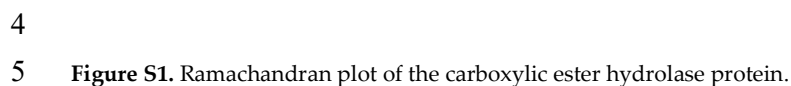


**Neurotoxic Effects of Linalool and  $\beta$ -Pinene on *Tribolium castaneum* Herbst**  
Nerlis Pajaro-Castro <sup>1,2</sup>, Karina Caballero-Gallardo <sup>1</sup> and Jesus Olivero-Verbel <sup>1,\*</sup>

3 Nerlis Pajaro-Castro <sup>1,2</sup>, Karina Caballero-Gallardo <sup>1</sup> and Jesus Olivero-Verbel <sup>1,\*</sup>



**Figure S1.** Ramachandran plot of the carboxylic ester hydrolase protein.

6



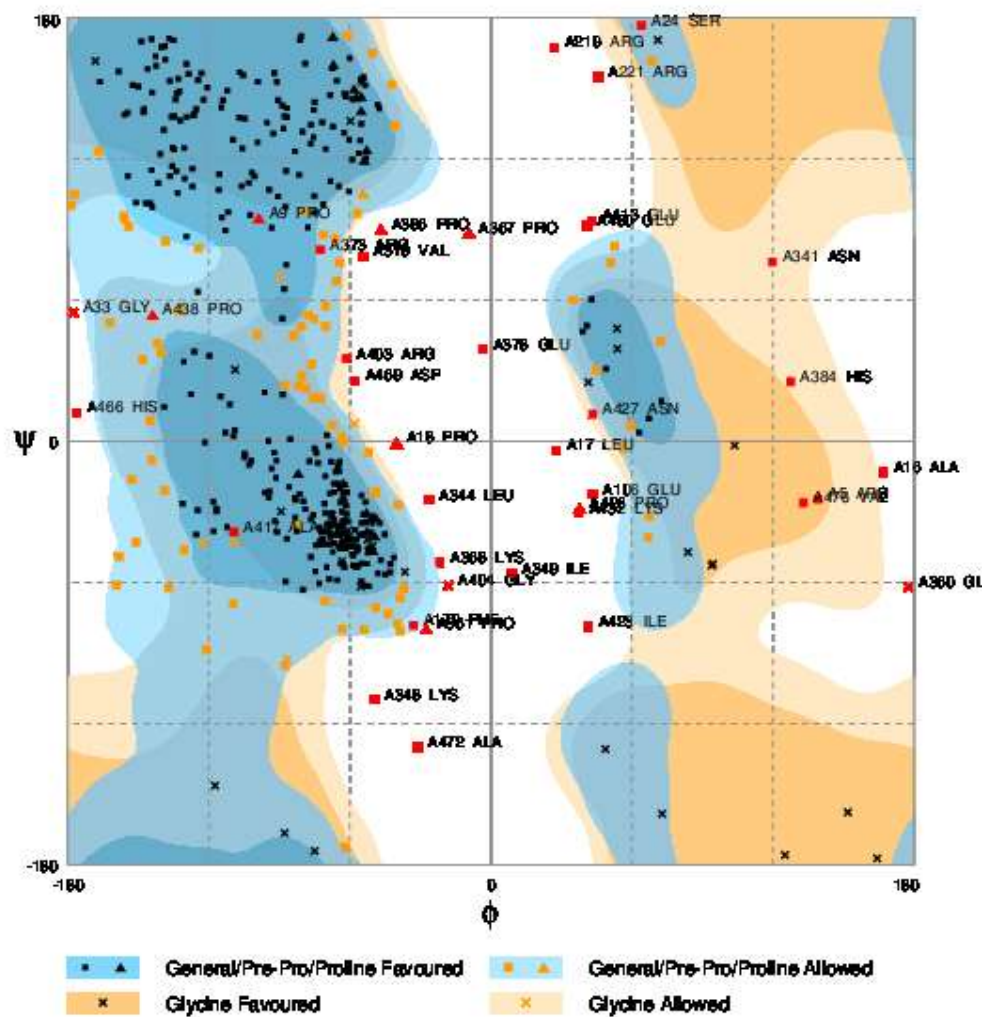


Figure S3. Ramachandran plot of the gamma-aminobutyric acid-gated anion channel splice variant 3a6a (GABA-RDL) protein.

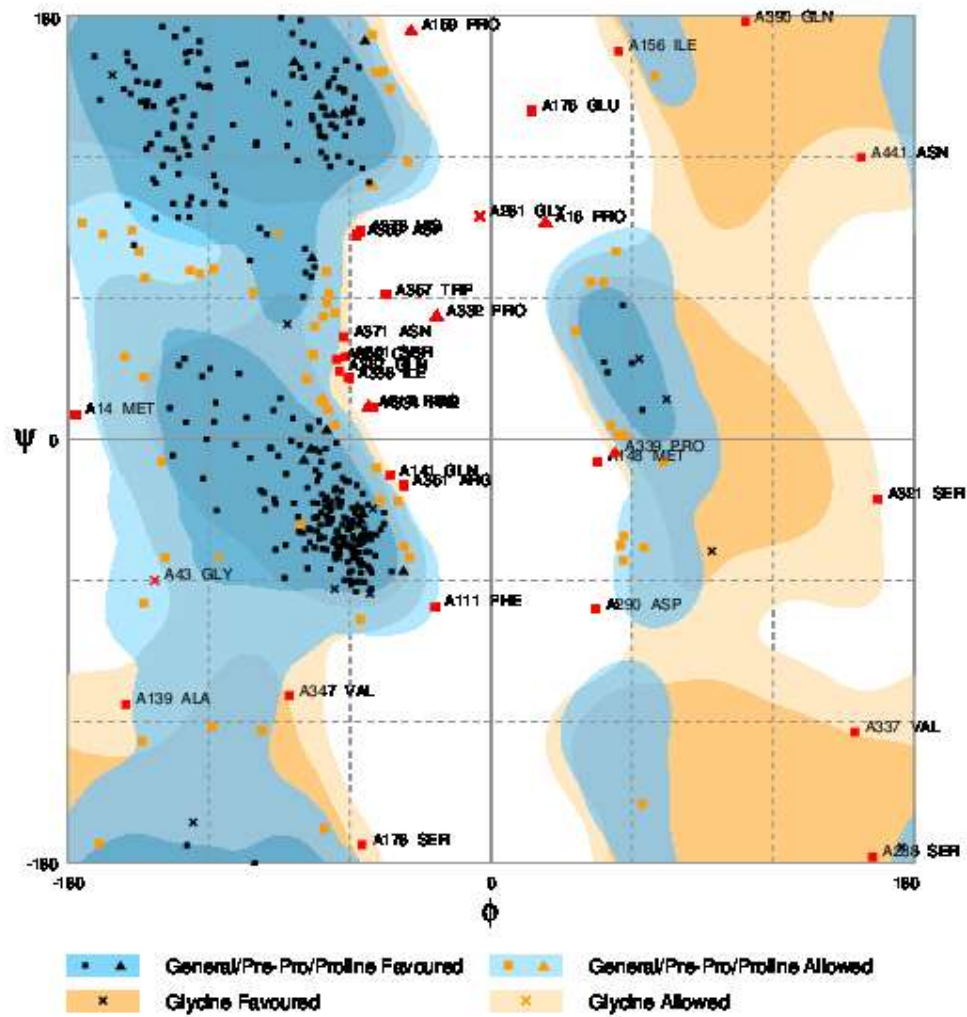


Figure S4. Ramachandran plot of the gamma-aminobutyric acid-gated ion channel (GABA-GRD) protein.

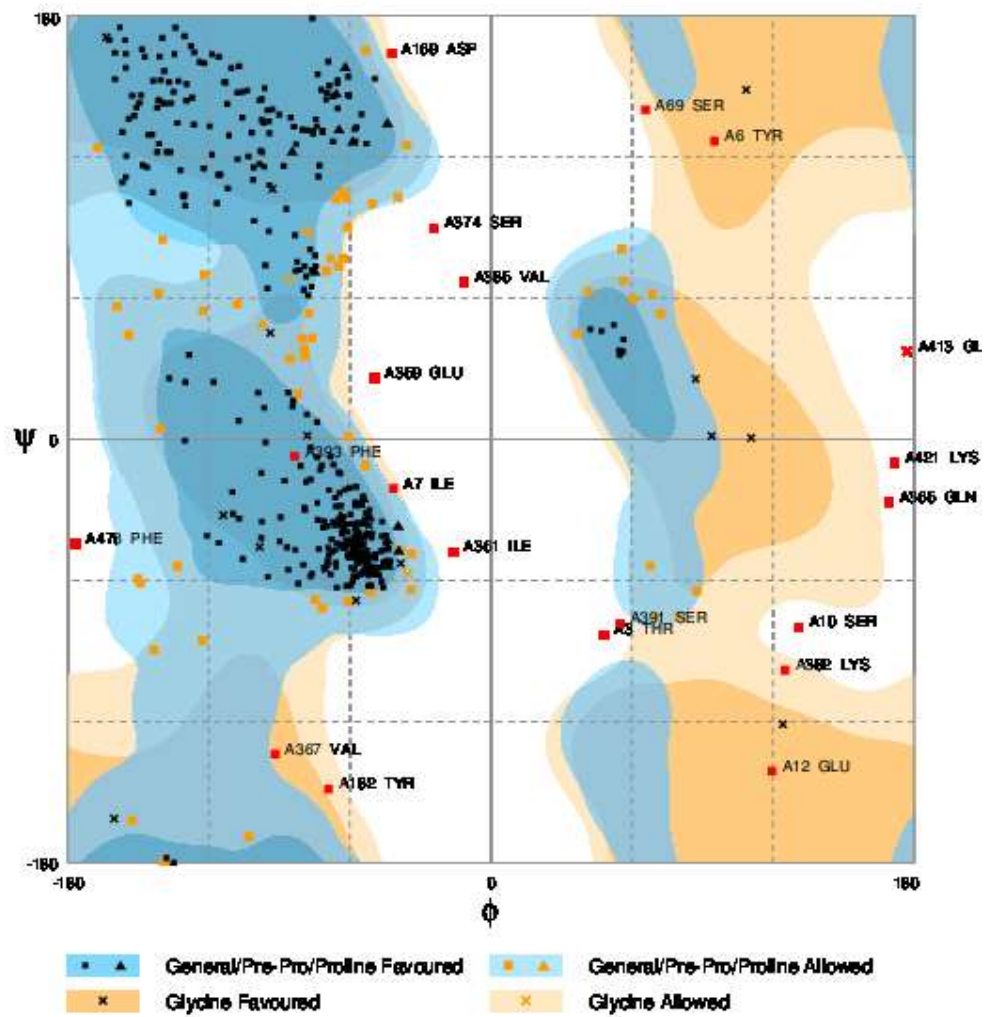


Figure S5. Ramachandran plot of the GABA-gated ion channel LCCH3 protein.



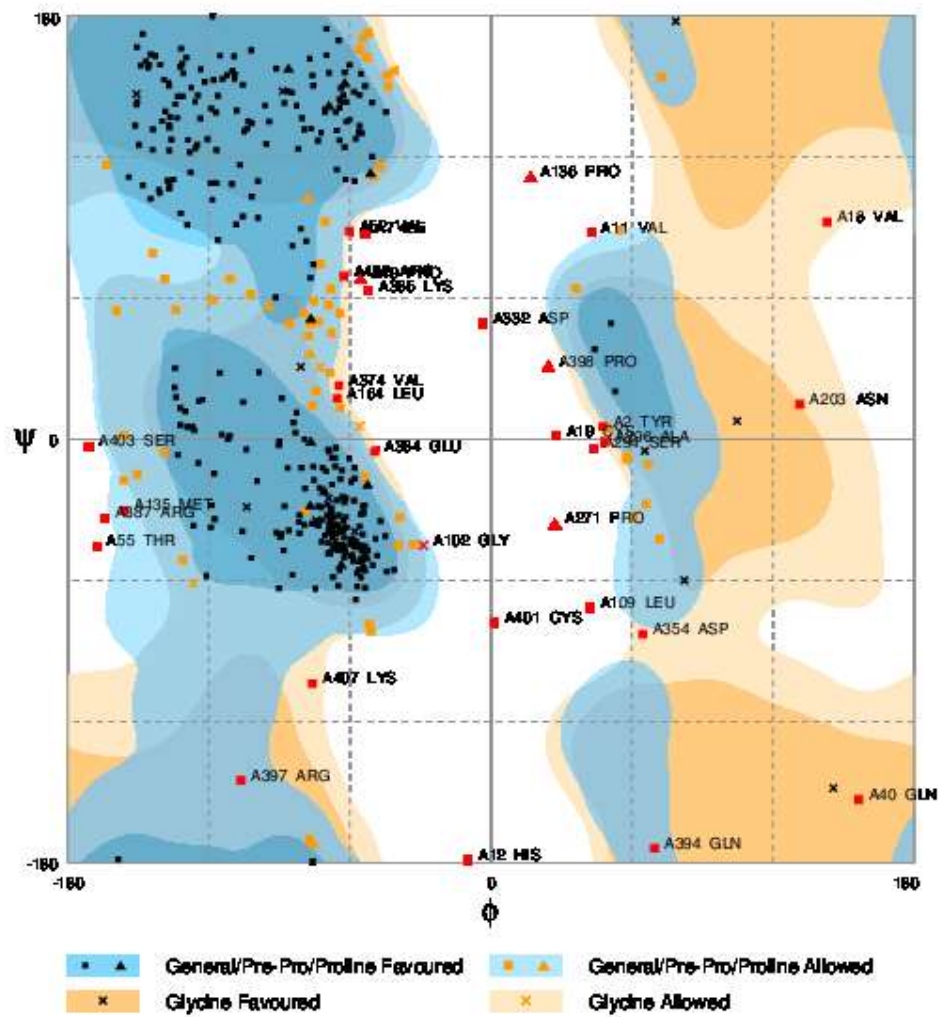


Figure S6. Ramachandran plot of the glutamate-gated chloride channel protein.

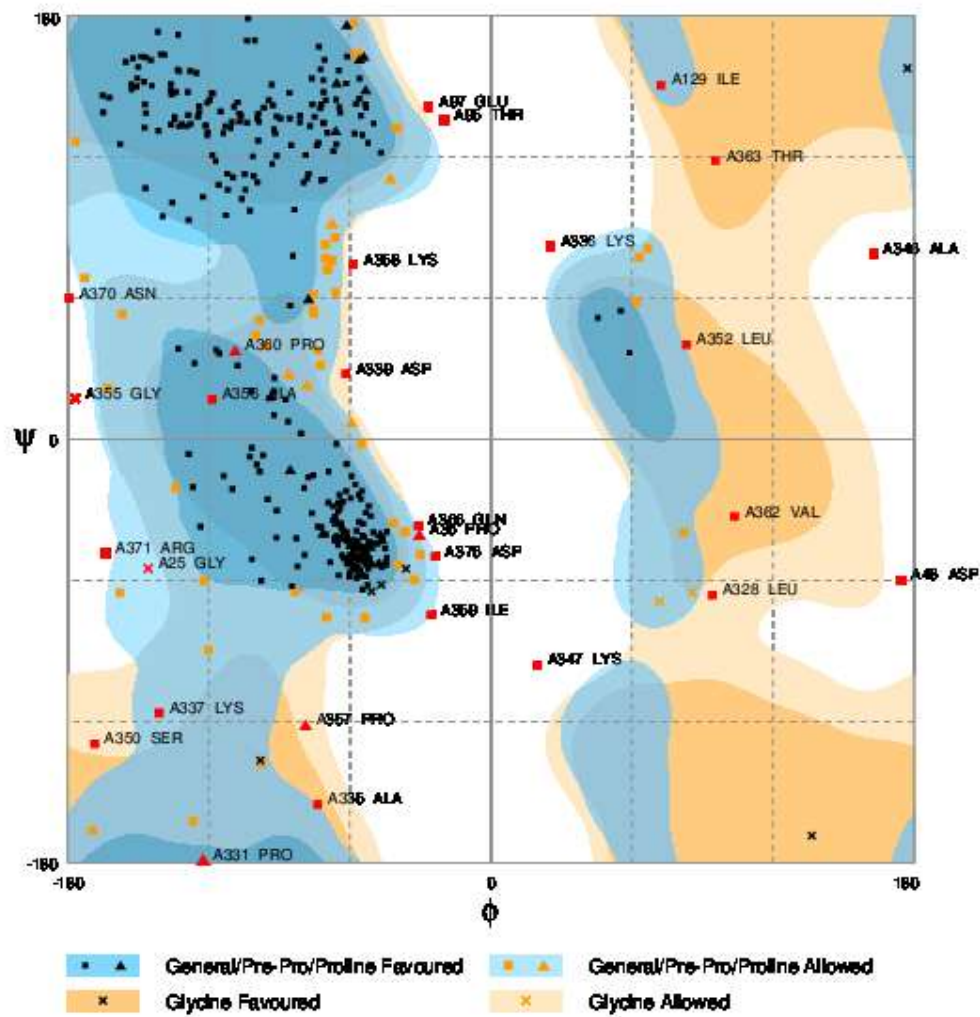


Figure S7. Ramachandran plot of the histamine-gated chloride channel 1 protein.





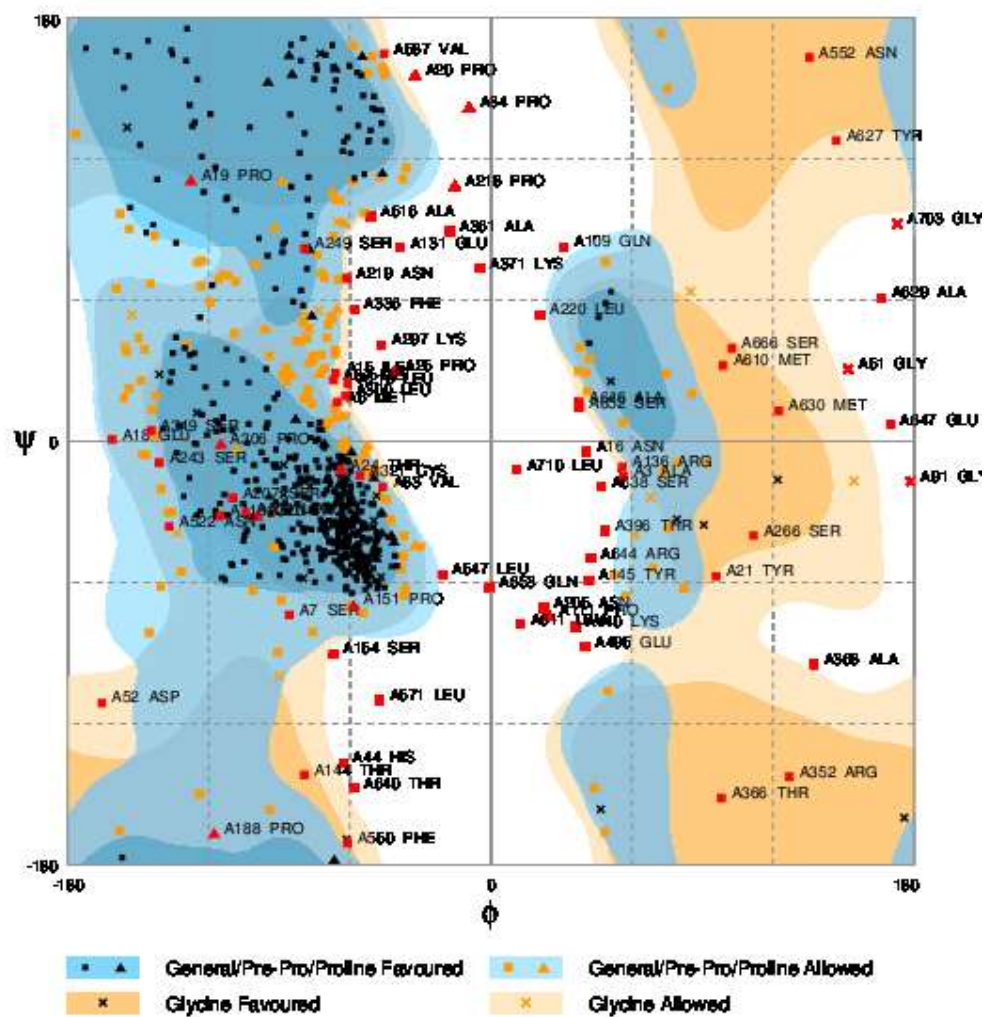


Figure S9. Ramachandran plot of the hormone receptor in the 39-like protein.



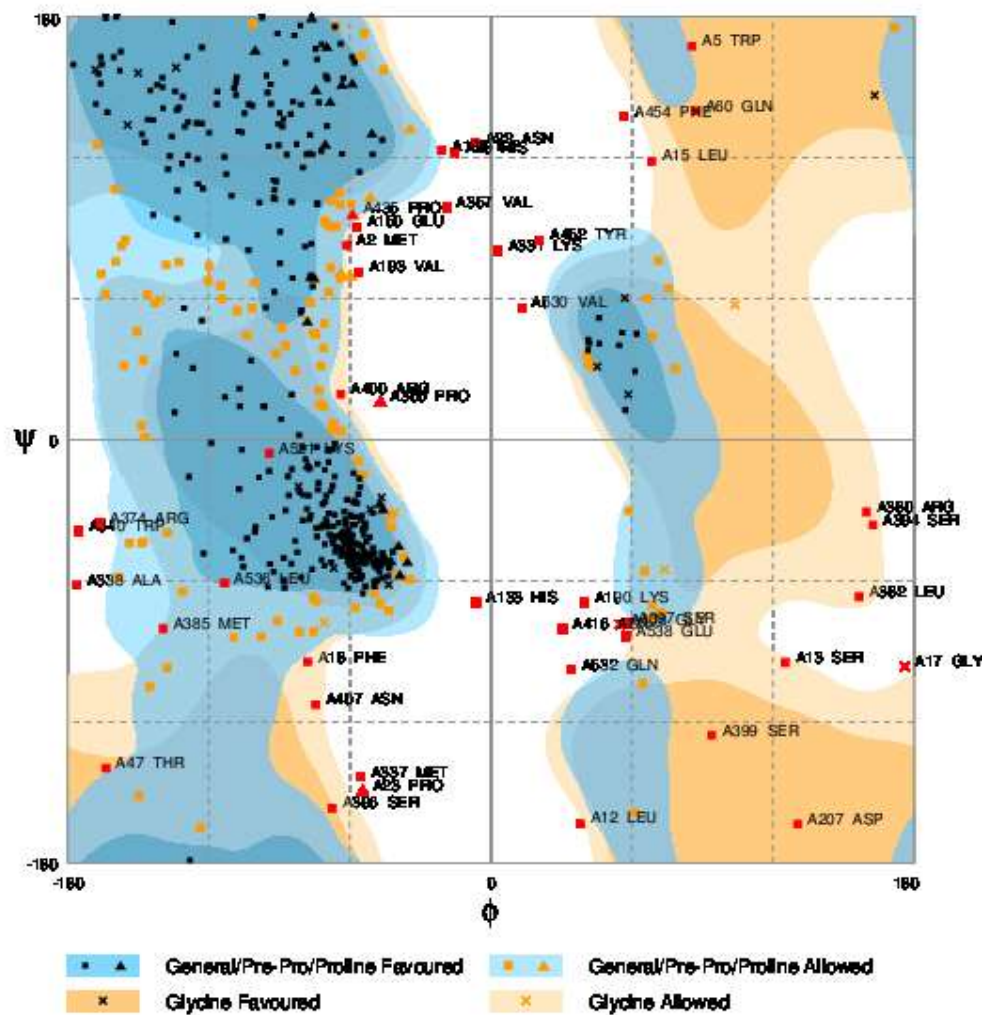


Figure S11. Ramachandran plot of the nicotinic acetylcholine receptor subunit alpha2 protein.

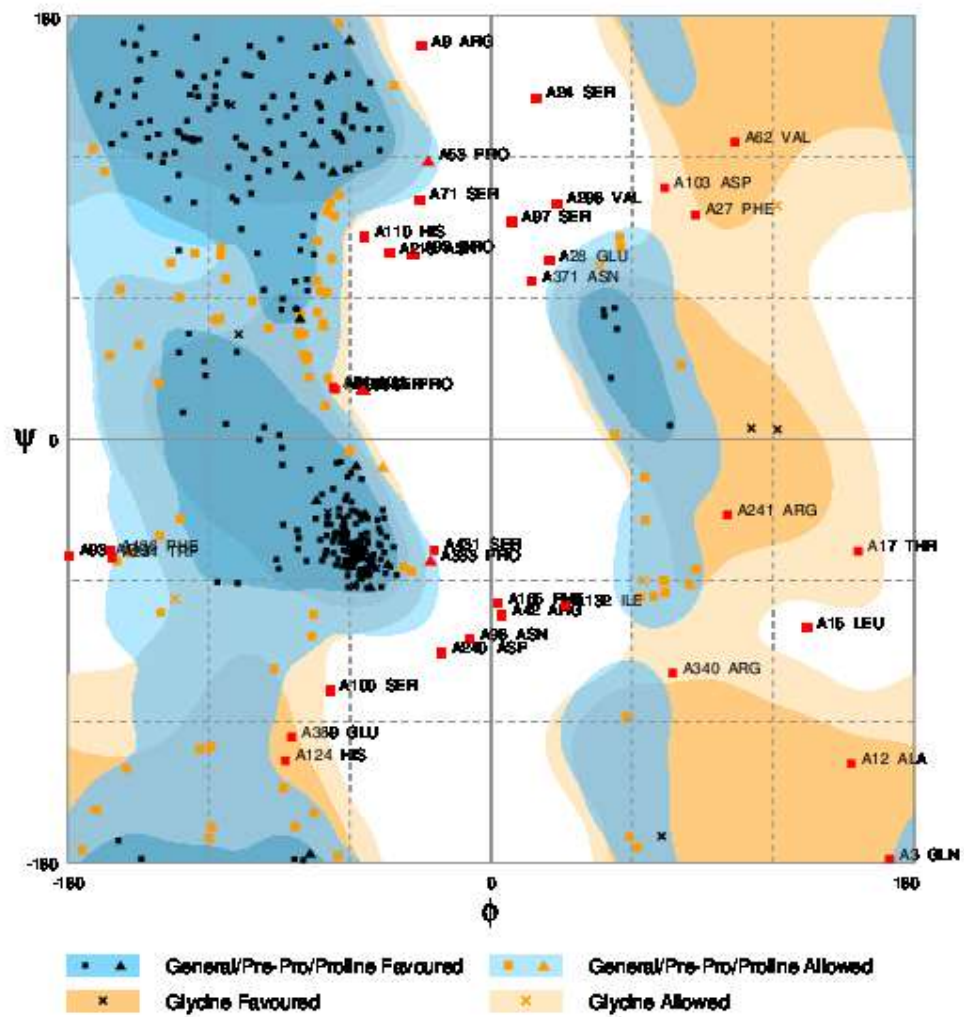


Figure S12. Ramachandran plot of the pH sensitive chloride channel protein.

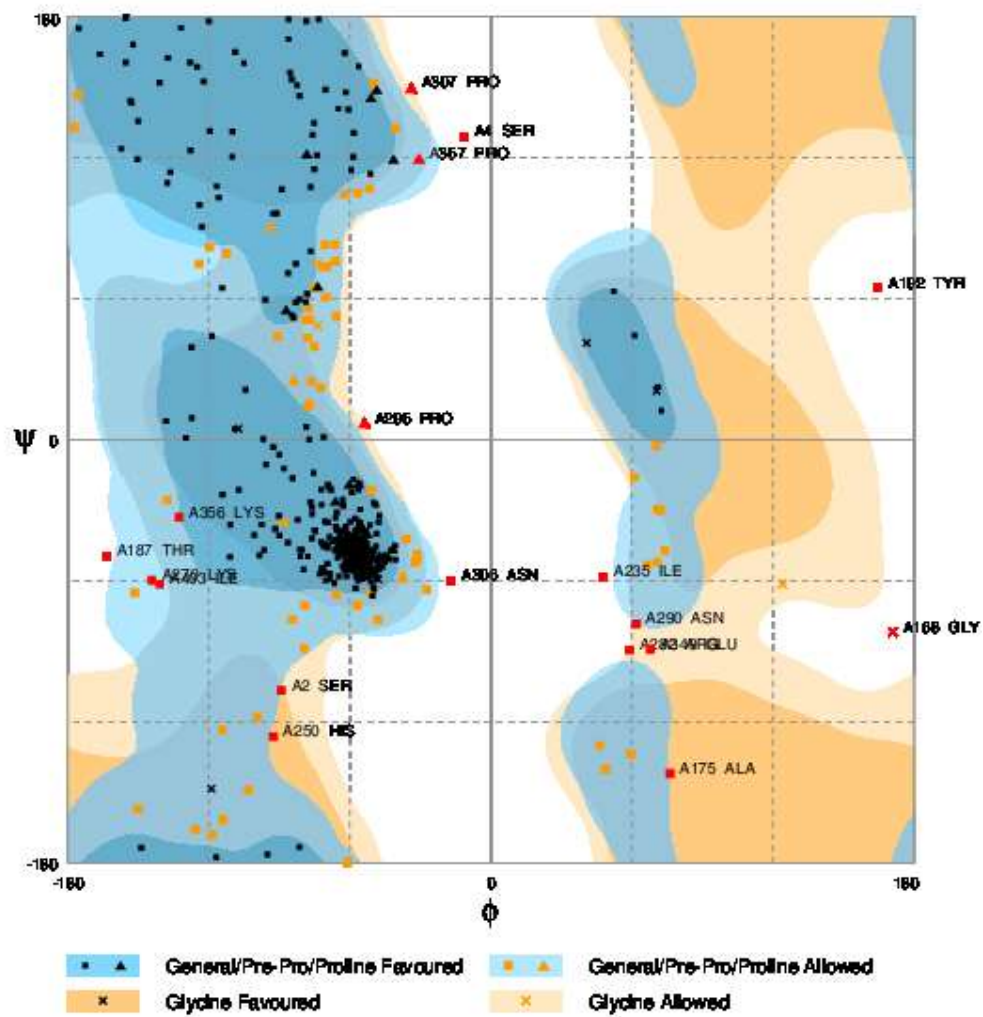
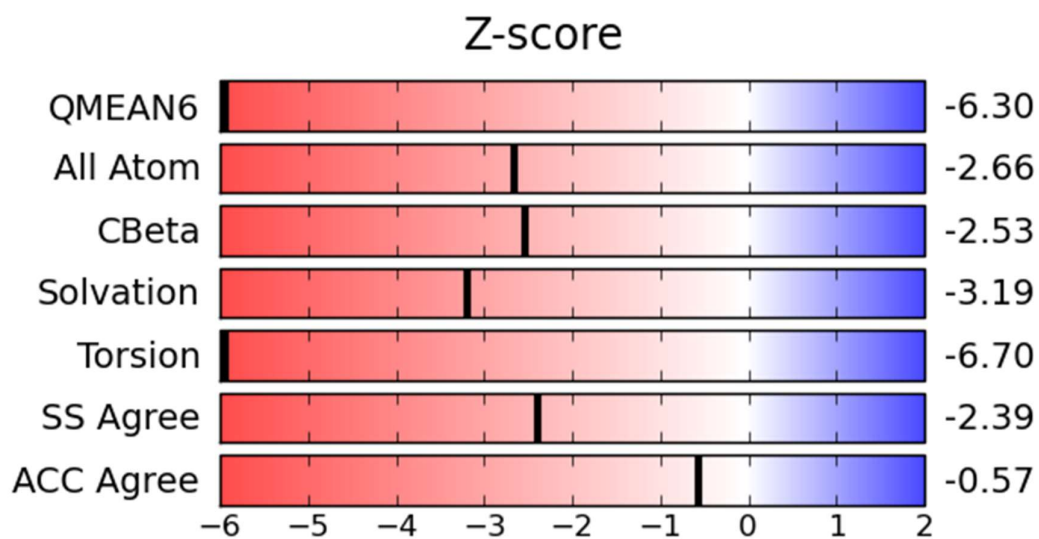
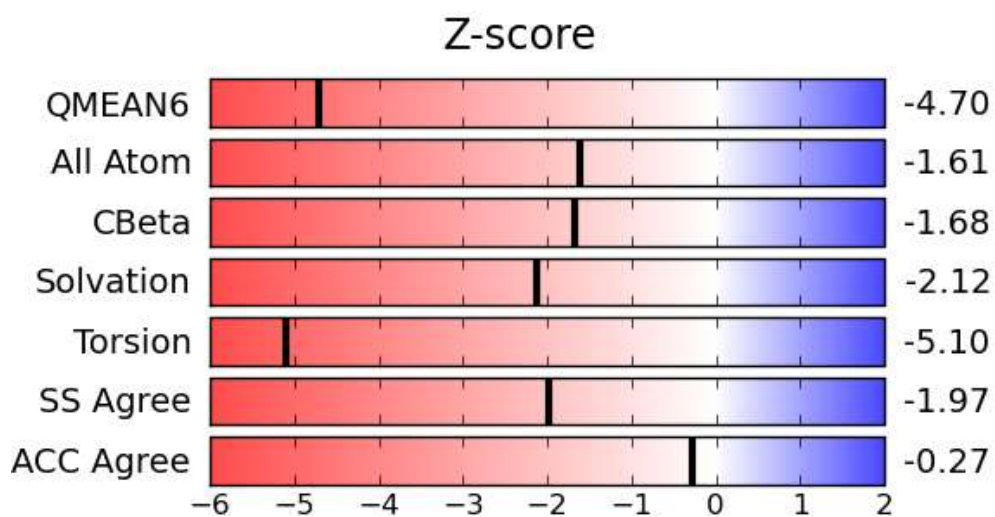


Figure S13. Ramachandran plot of the putative octopamine/tyramine receptor.

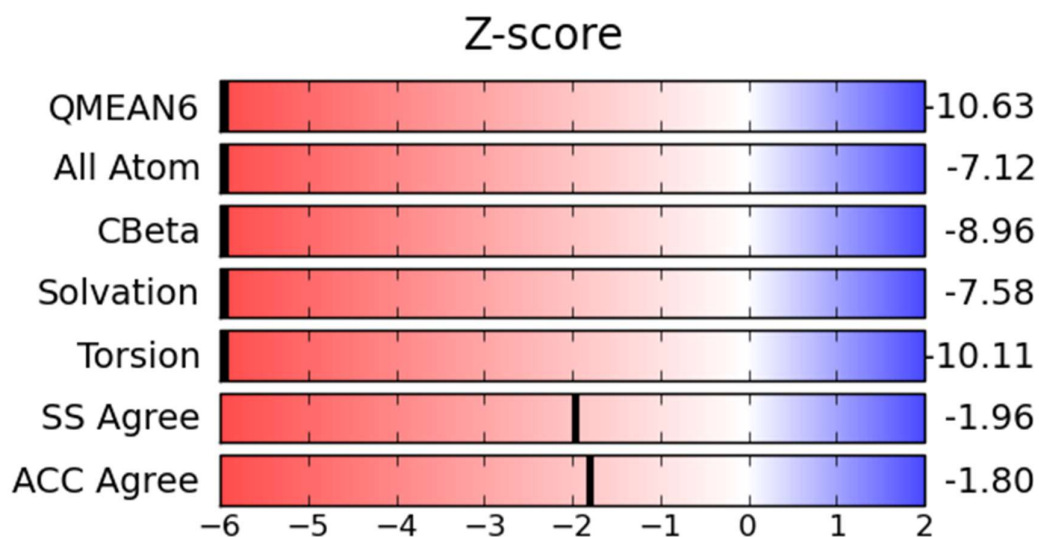




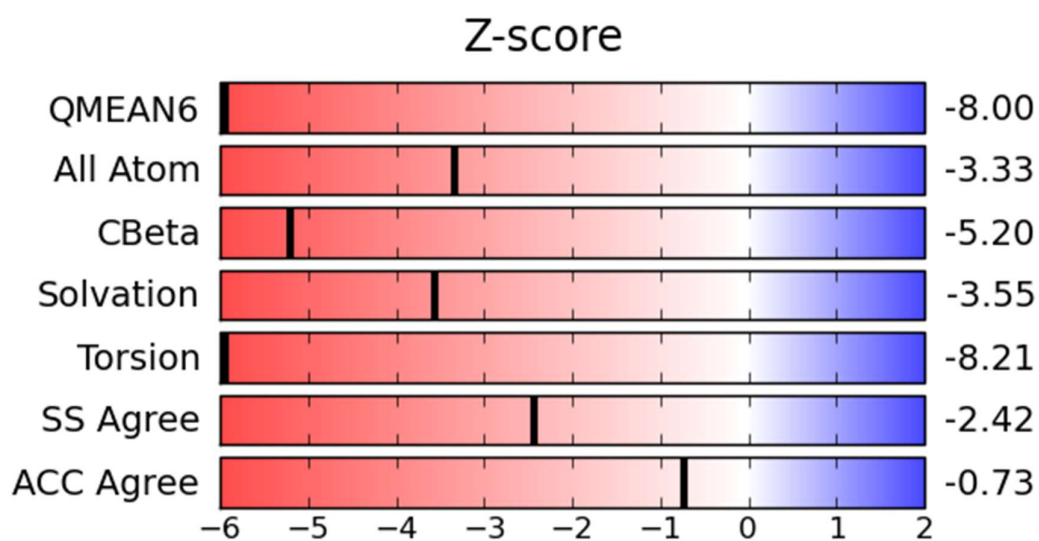
**Figure S14.** Z-score obtained by QMean for the carboxylic ester hydrolase protein.



**Figure S15.** Z-score obtained by QMean for the carboxylic ester hydrolase 2 protein.



**Figure S16.** Z-score obtained by QMean for the gamma-aminobutyric acid-gated anion channel splice variant 3a6a (GABA-RDL) protein.



**Figure S17.** Z-score obtained by QMean for the gamma-aminobutyric acid-gated ion channel (GABA-GRD) protein.

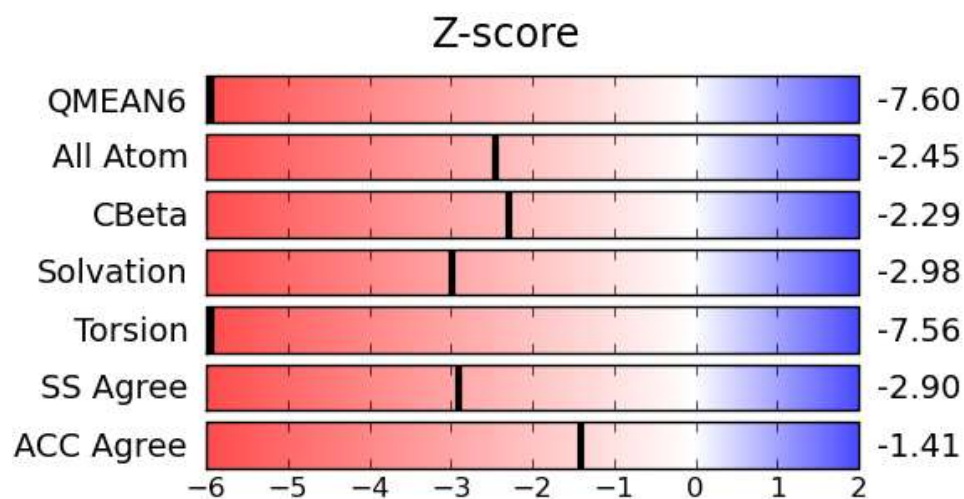


Figure S18. Z-score obtained by QMean for the GABA-gated ion channel LCCH3 protein.

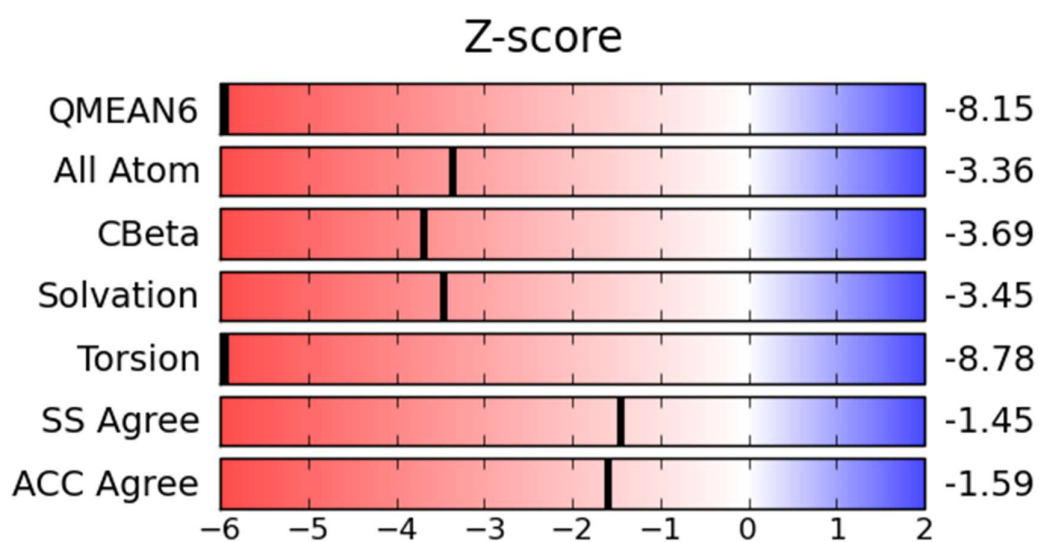


Figure S19. Z-score obtained by QMean for the glutamate-gated chloride channel protein.

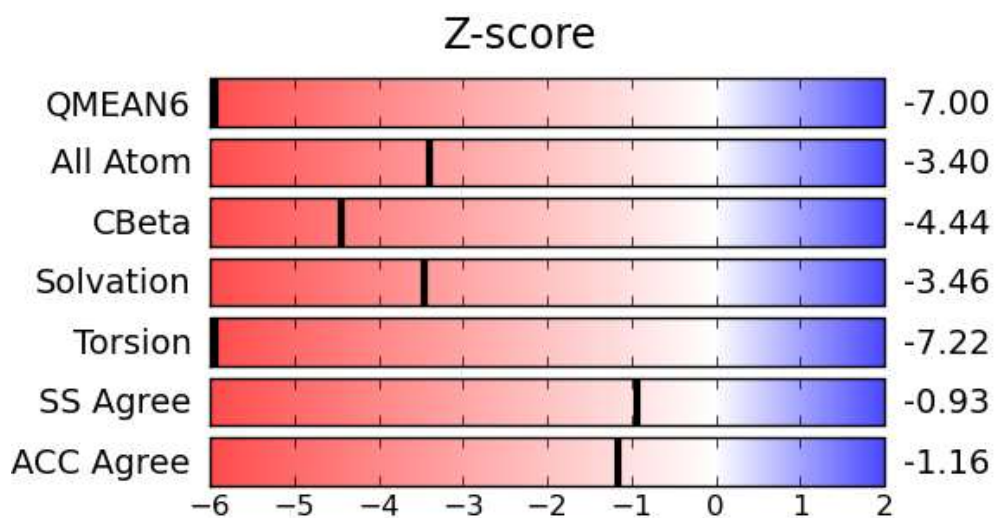


Figure S20. Z-score obtained by QMean for the histamine-gated chloride channel 1 protein.

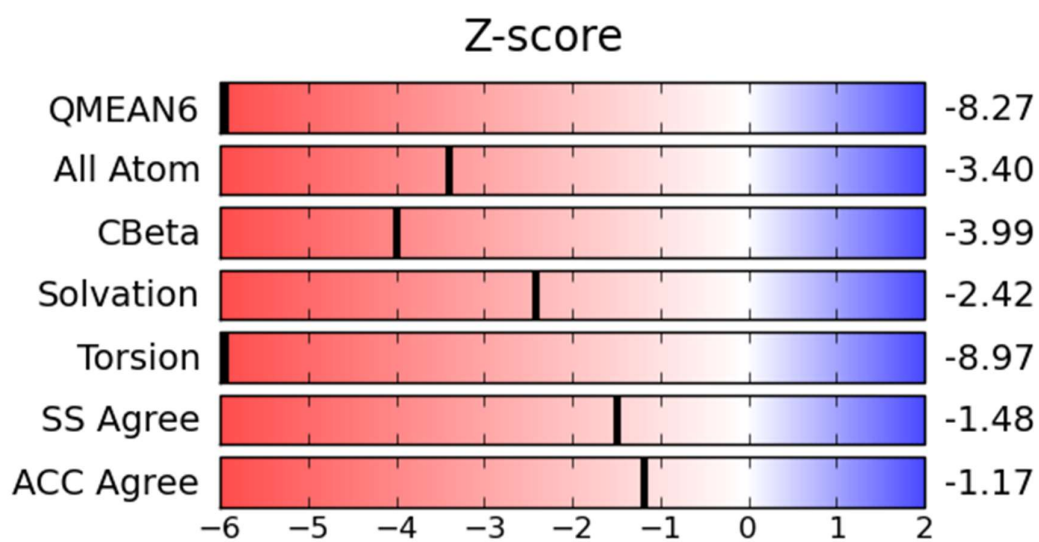
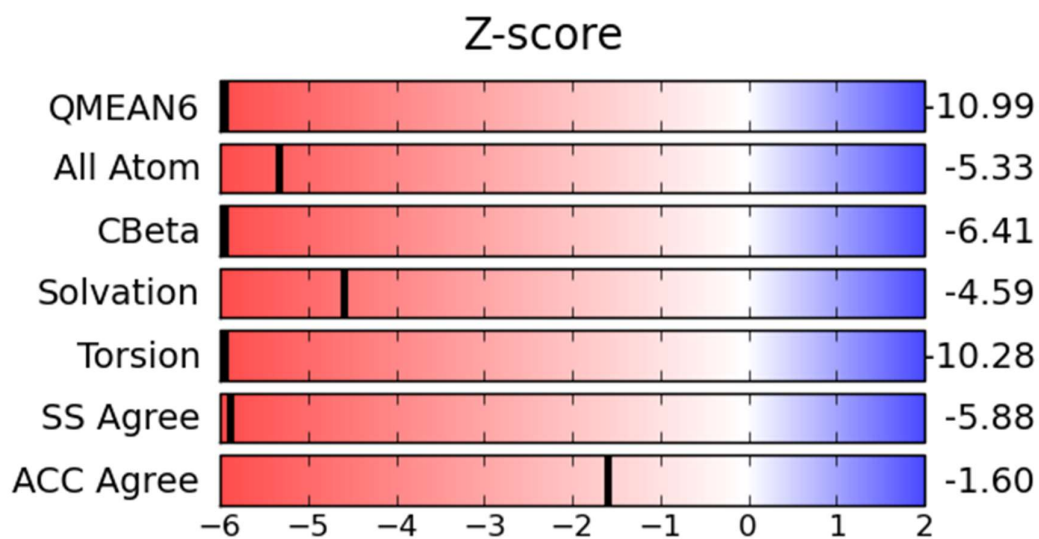
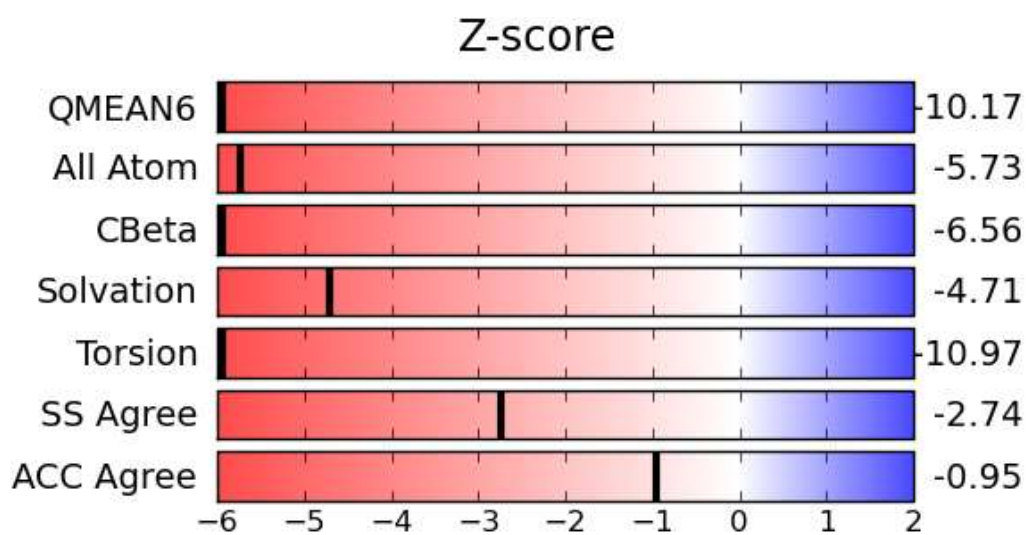


Figure S21. Z-score obtained by QMean for the histamine-gated chloride channel 2 protein.

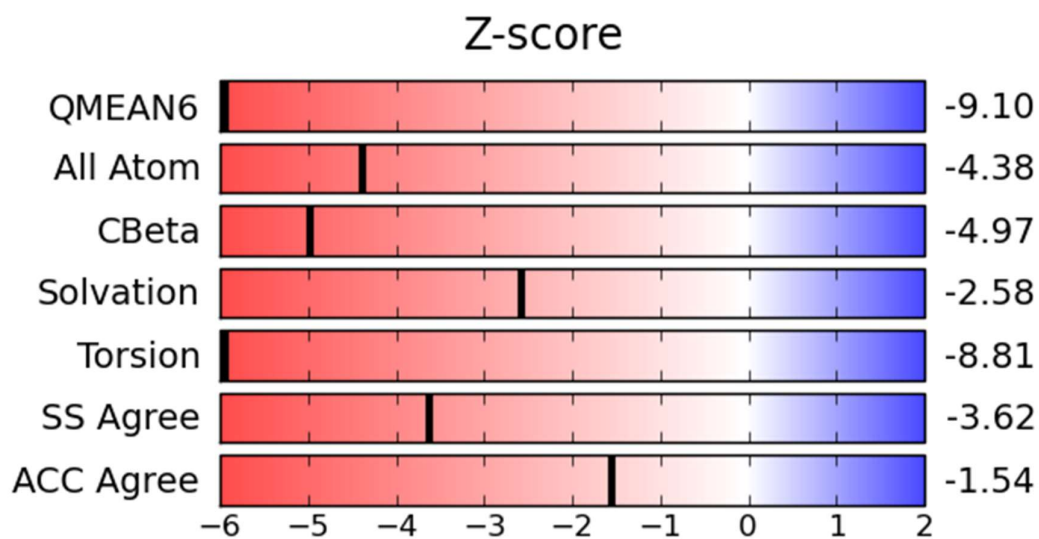


**Figure S22.** Z-score obtained by QMean for the hormone receptor in the 39-like protein.

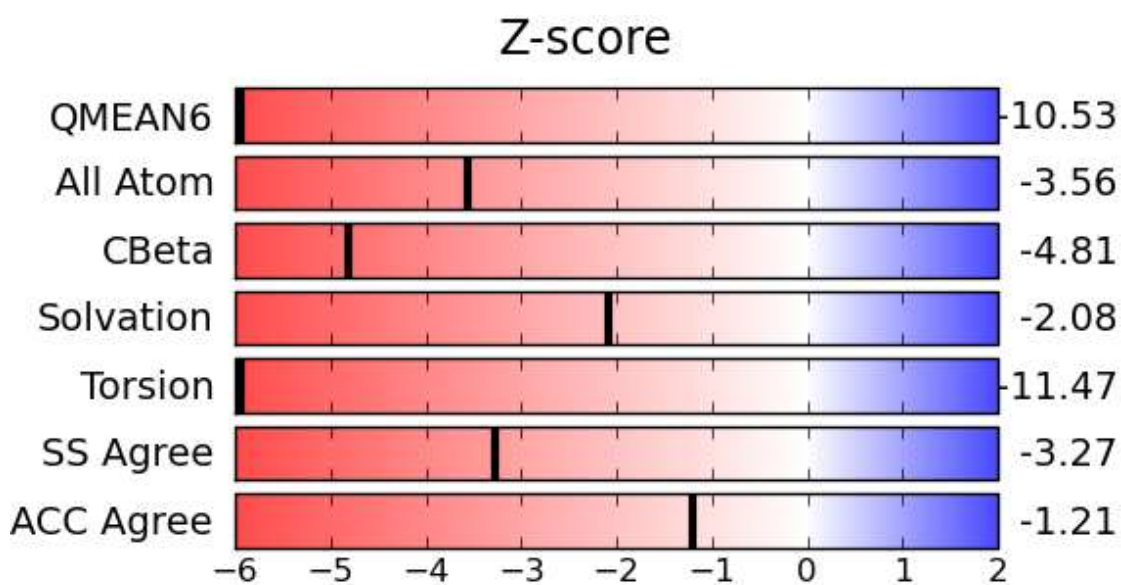


**Figure S23.** Z-score obtained by QMean for the nicotinic acetylcholine receptor subunit alpha1 protein.

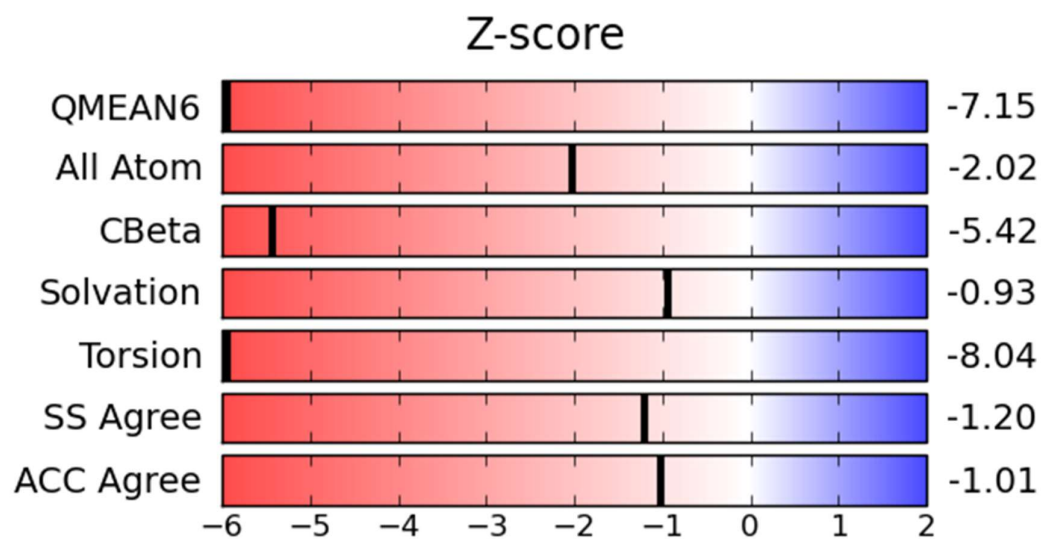




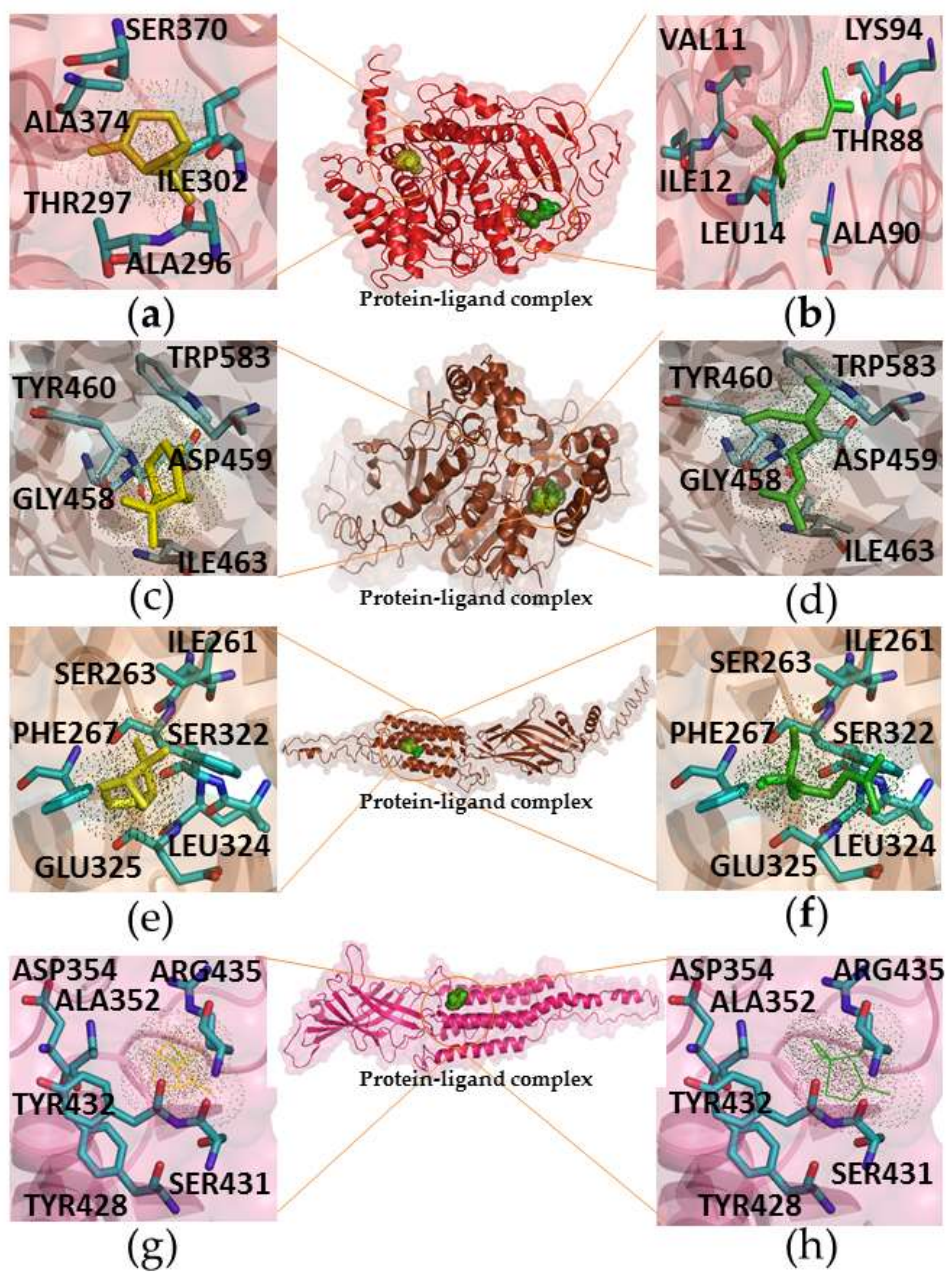
**Figure S24.** Z-score obtained by QMean for the nicotinic acetylcholine receptor subunit alpha2 protein.

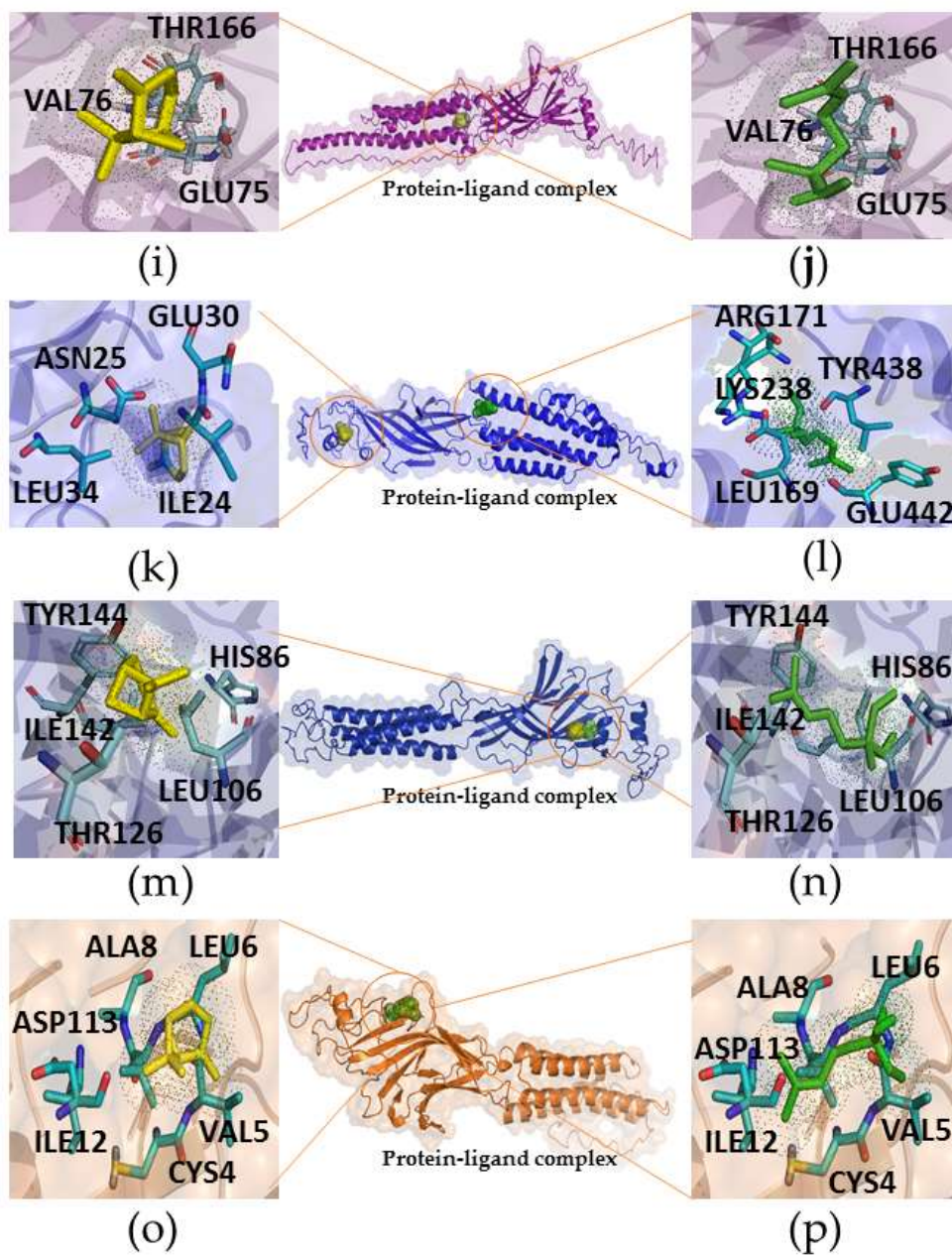


**Figure S25.** Z-score obtained by QMean for the pH sensitive chloride channel protein.



**Figure S26.** Z-score obtained by QMean for the putative octopamine/tyramine receptor.







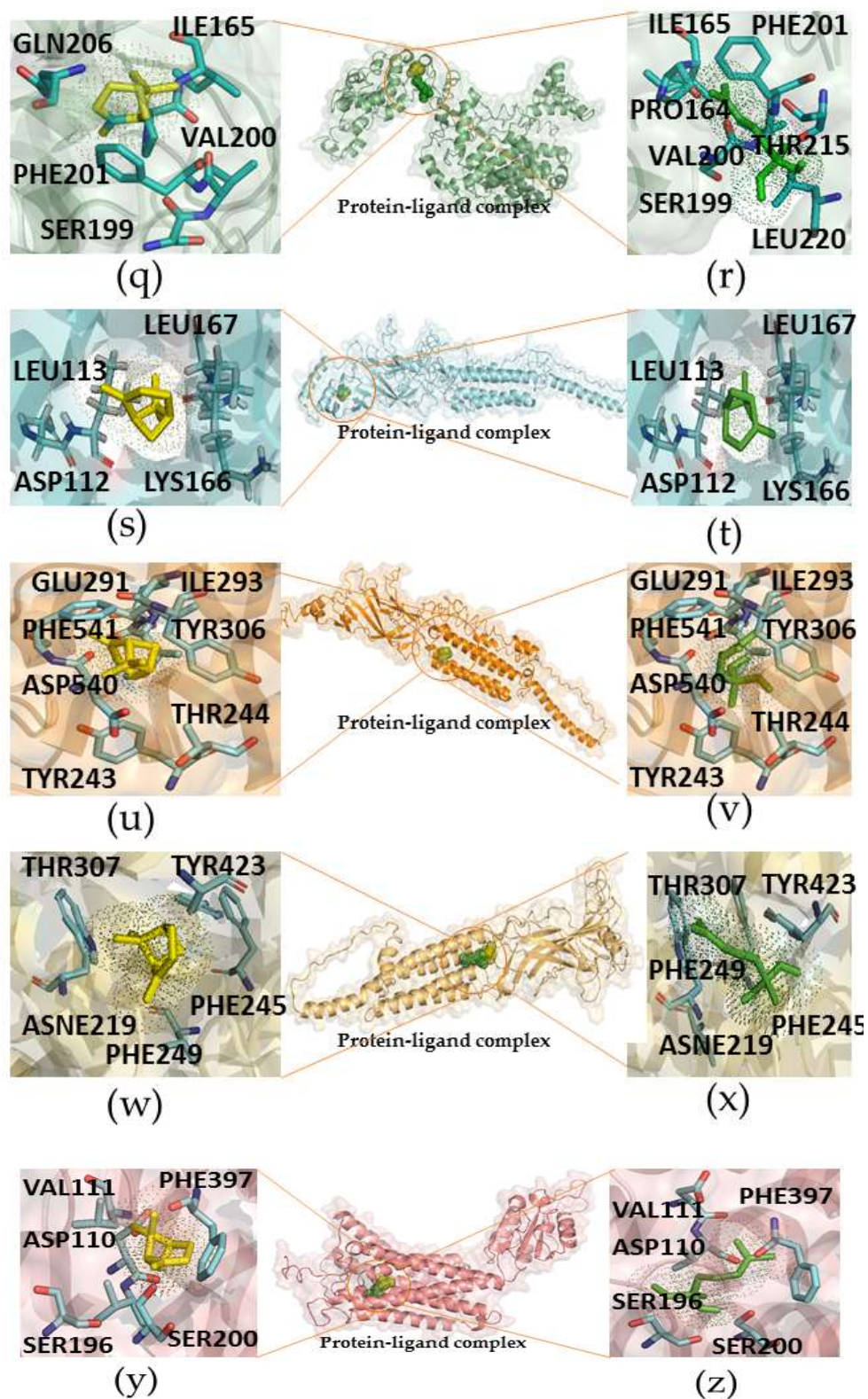


Figure S27. Predicted binding and interacting residues present in proteins from *T. castaneum*.



98 (a) carboxylic ester hydrolase- $\beta$ -pinene (yellow) complex; (b) carboxylic ester hydrolase-linalool  
99 (Green) complex; (c) carboxylic ester hydrolase2- $\beta$ -pinene complex; (d) carboxylic ester hydrolase2-  
100 linalool complex; (e) GABA-RDL- $\beta$ -pinene complex; (f) GABA-RDL-linalool complex; (g) GABA-  
101 GRD- $\beta$ -pinene complex; (h) GABA-GRD- linalool complex; (i) GABA-gated ion channel LCCH3- $\beta$ -  
102 pinene complex; (j) GABA-gated ion channel LCCH3- linalool complex; (k) glutamate-gated  
103 chloride channel- $\beta$ -pinene complex; (l) glutamate-gated chloride channel-linalool complex; (m)  
104 histamine-gated chloride channel 1- $\beta$ -pinene complex; (n) histamine-gated chloride channel 1-  
105 linalool complex; (o) histamine-gated chloride channel 2- $\beta$ -pinene complex; (p) histamine-gated  
106 chloride channel 2-linalool complex; (q) hormone receptor in the 39-like protein- $\beta$ -pinene complex;  
107 (r) hormone receptor in the 39-like protein-linalool complex; (s) nicotinic acetylcholine receptor  
108 subunit  $\alpha$ 1- $\beta$ -pinene complex; (t) nicotinic acetylcholine receptor subunit  $\alpha$ 1-linalool  
109 complex; (u) nicotinic acetylcholine receptor subunit  $\alpha$ 2- $\beta$ -pinene complex; (v) nicotinic  
110 acetylcholine receptor subunit  $\alpha$ 2-linalool complex; (w) pH sensitive chloride channel- $\beta$ -pinene  
111 complex; (x) pH sensitive chloride channel-linalool complex; (y) putative octopamine/tyramine  
112 receptor- $\beta$ -pinene complex; and (z) putative octopamine/tyramine receptor-linalool complex.

113