Supplementary Material

In silico investigation of selected pesticides and their determination in agricultural products using QuEChERS methodology and HPLC-DAD

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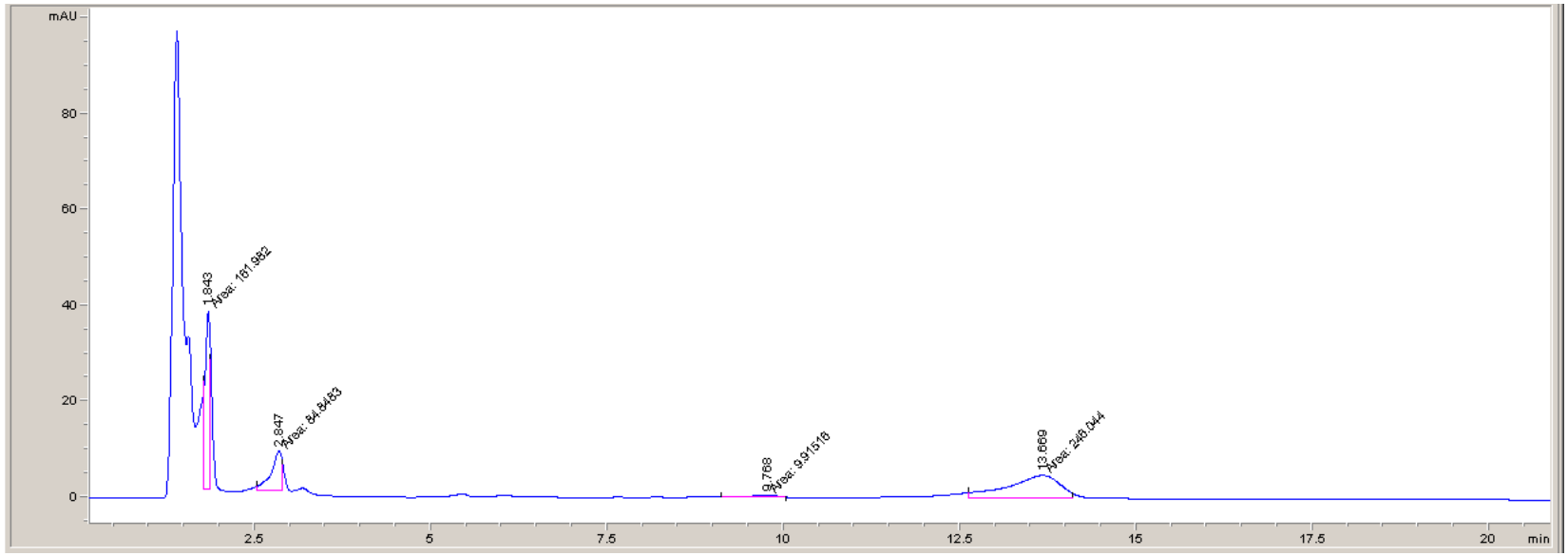
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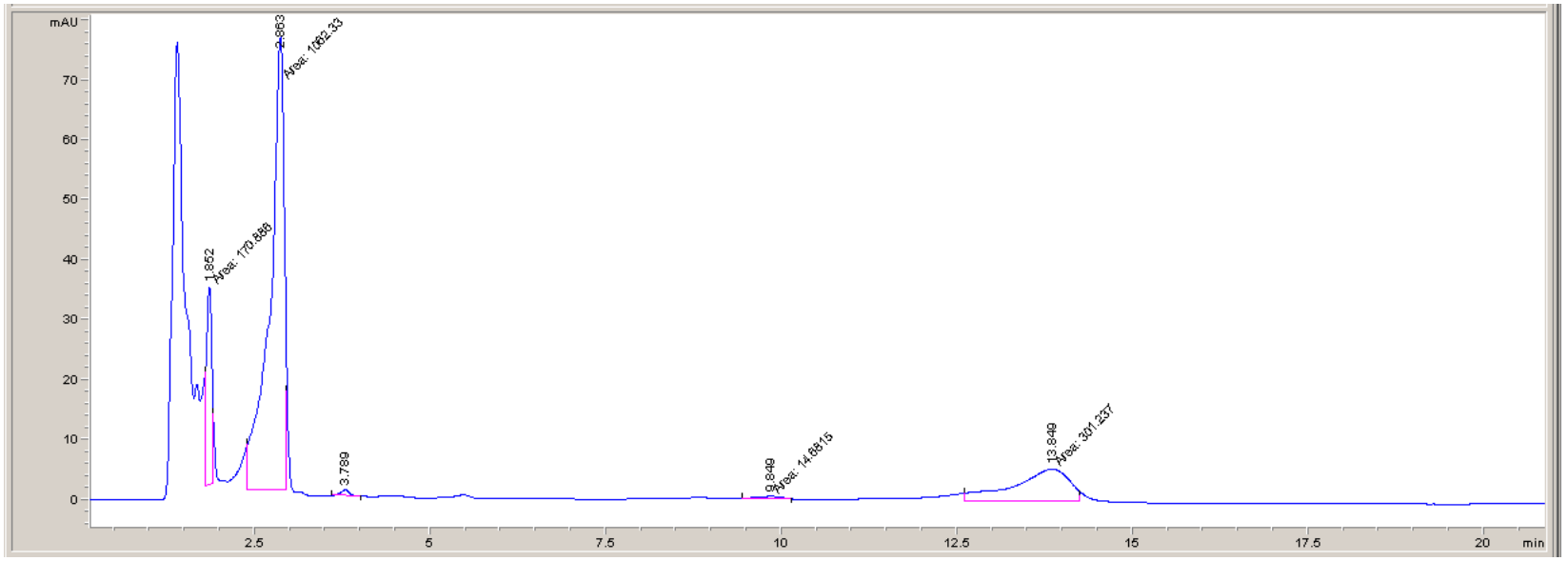
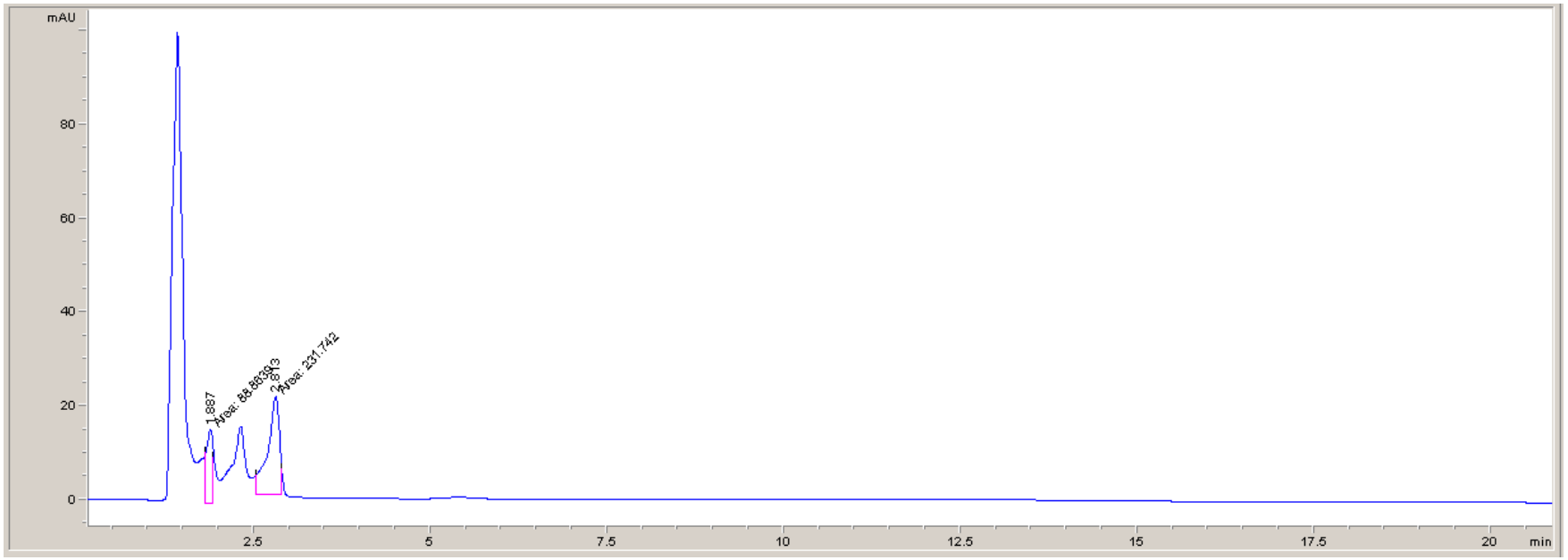
80
60
40
20
0
1.843
Area: 161.982
2.847
Area: 84.8483
9.768
Area: 9.91518
13.669
Area: 246.044
2.5
5
7.5
10
12.5
15
17.5
20
min

a)



b)

Figure S1. Representative chromatograms of a real sample of tomatoes spiked with standard solutions of selected pesticides (chlorantraniliprole, methomyl, metalaxyl and thiacloprid) and prepared using a) Method 1, and b) Method 2.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40
20
0
1.887
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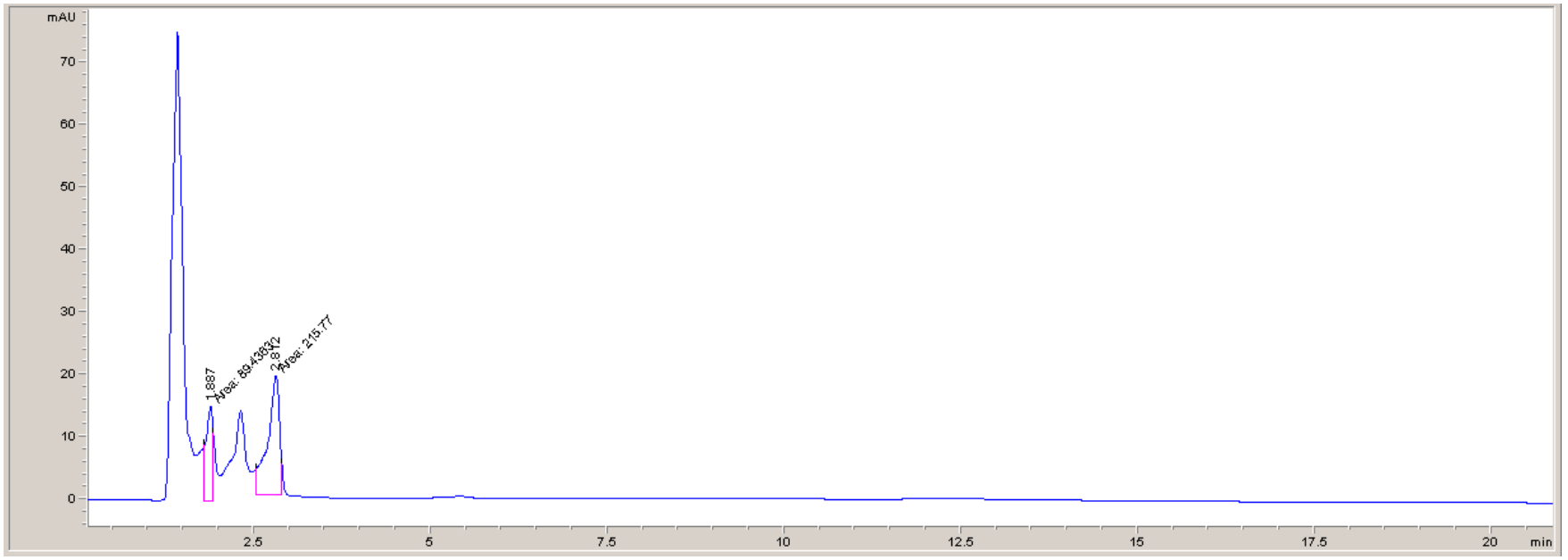
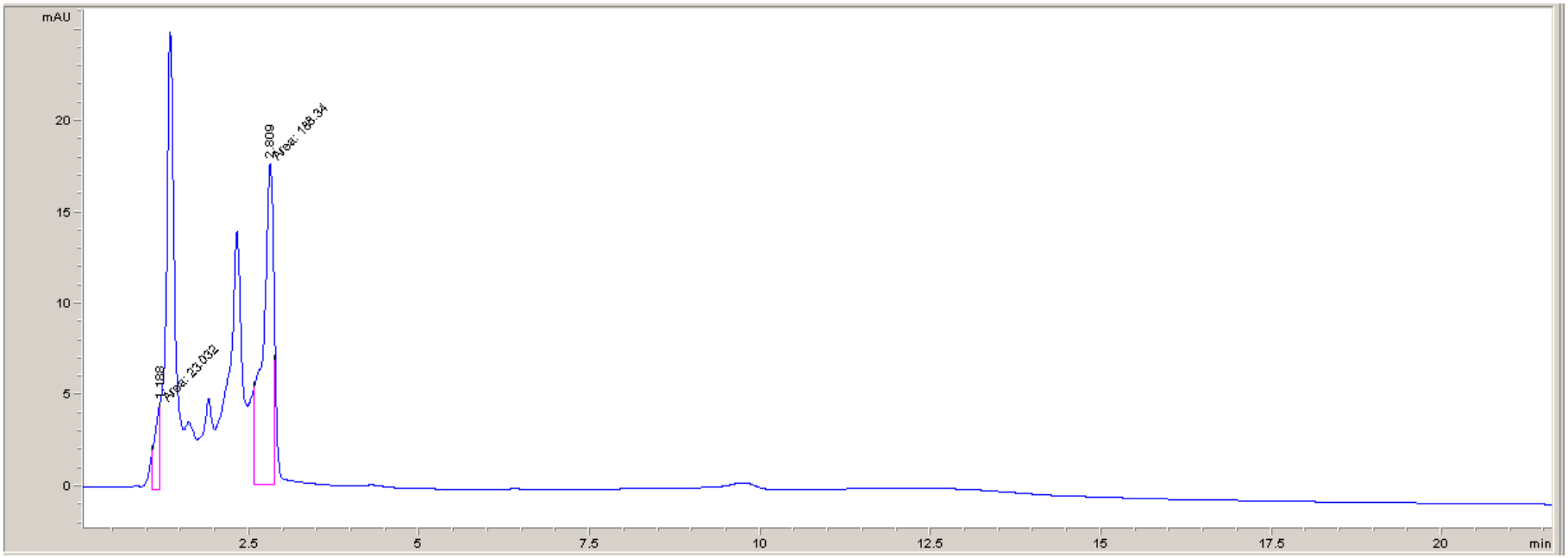
Area: 231.742
2.5
5
7.5
10
12.5
15
17.5
20
min

a)



b)

Figure S2. Representative chromatograms of real sample of cucumber spiked with standard solutions of selected pesticides (cymoxanil, famoxadone, and thiamethoxam) and prepared using a) Method 1, and b) Method 2.


mAU
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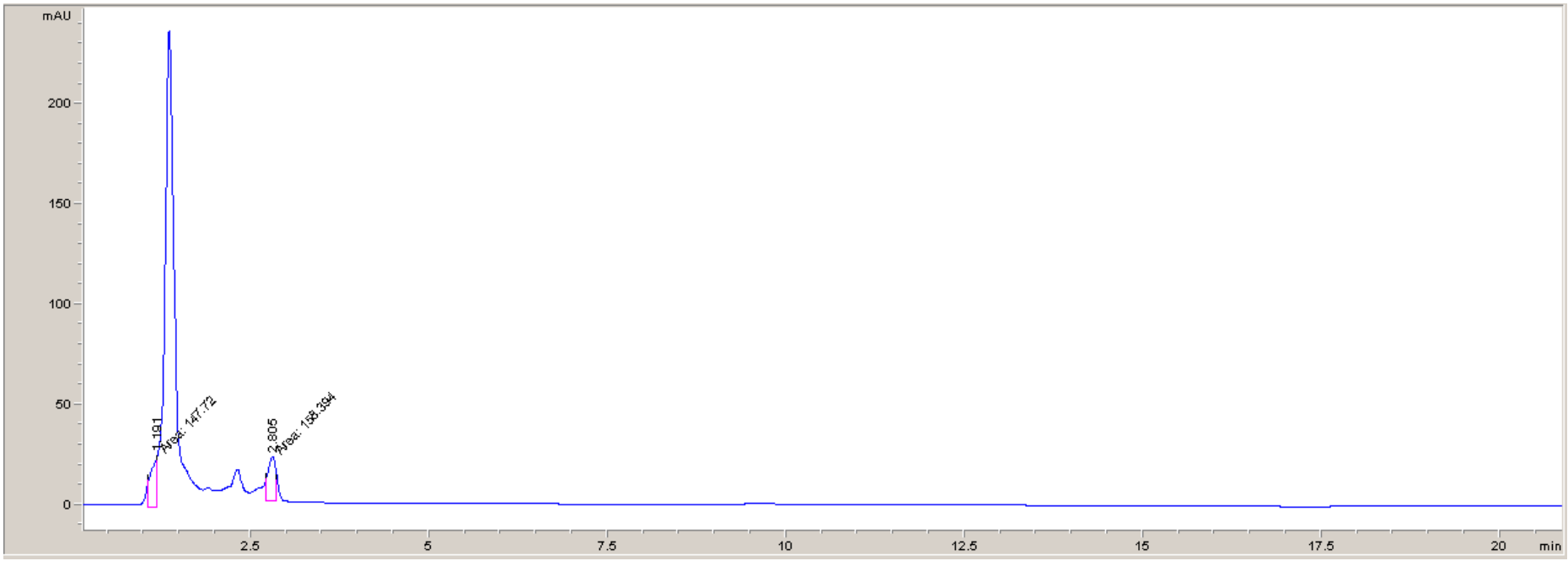
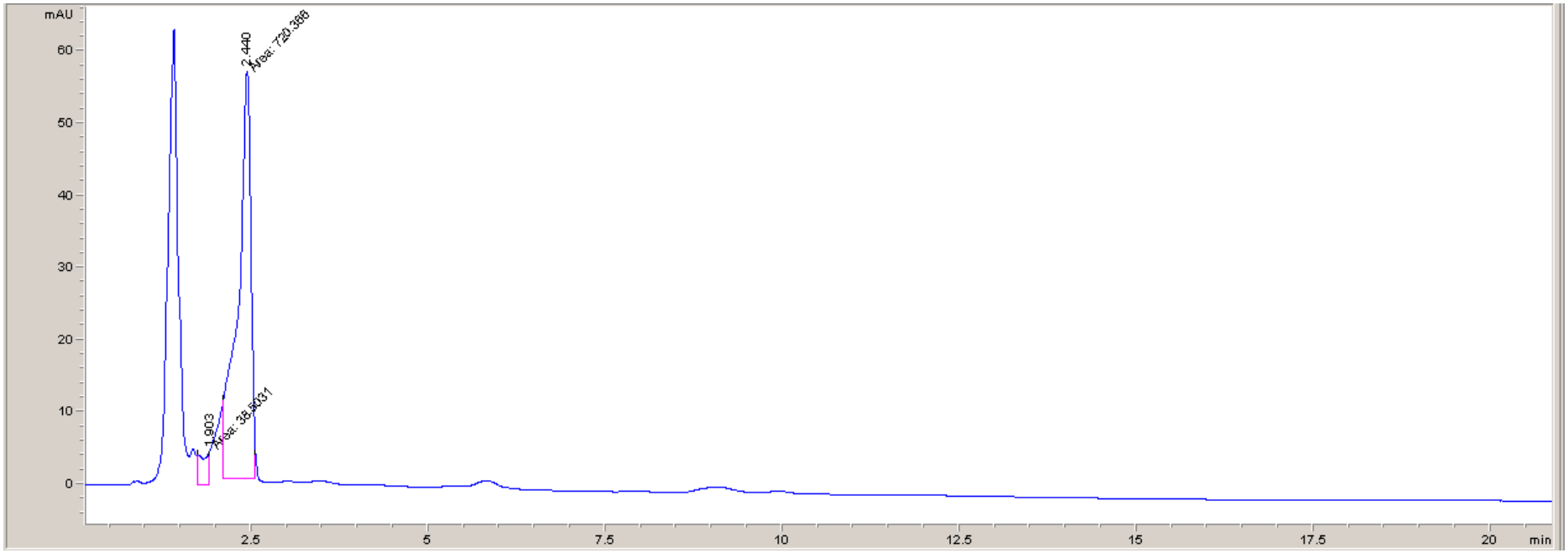
15
10
5
0
1.188
Area: 23.032
2.809
Area: 188.34
2.5
5
7.5
10
12.5
15
17.5
20
min

a)



b)

Figure S3. Representative chromatograms of real sample of grapes spiked with standard solutions of selected pesticides (abamectin, cymoxanil, metalaxyl-M, pyraclostrobin, propiconazole, and tebuconazole) and prepared using a) Method 1, and b) Method 2.


mAU
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40
30
20
10
0
2.440
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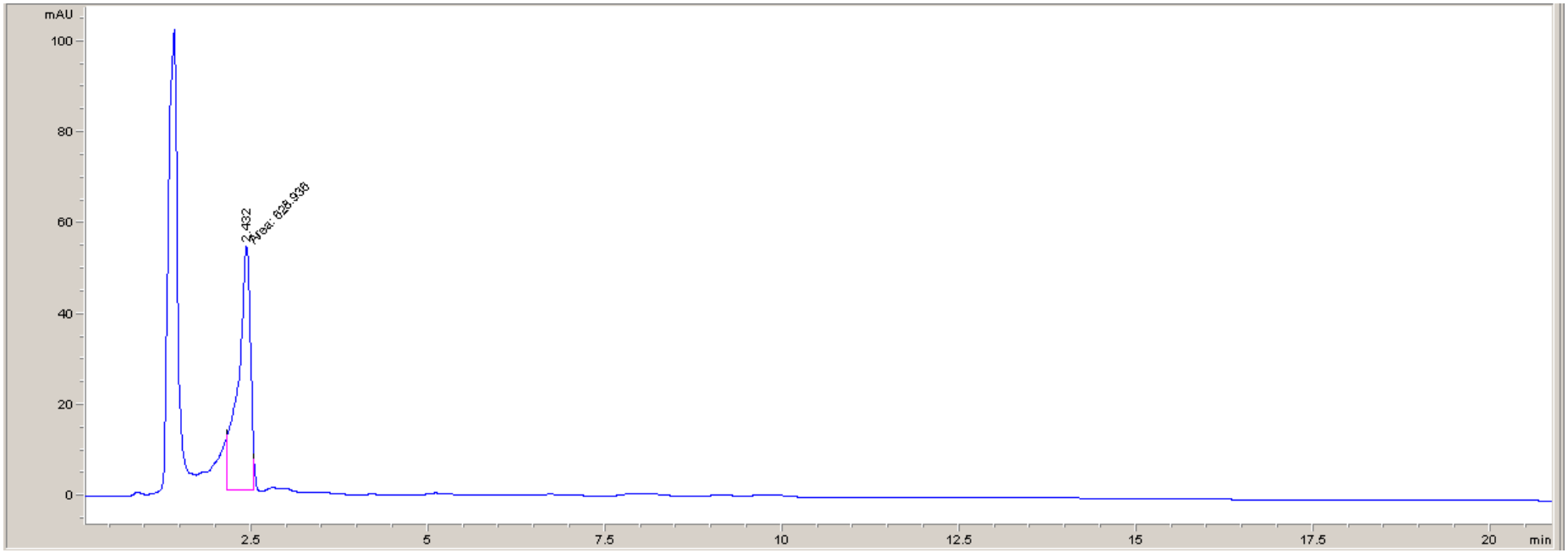
1.903
Area: 38.5431
2.5
5
7.5
10
12.5
15
17.5
20
min

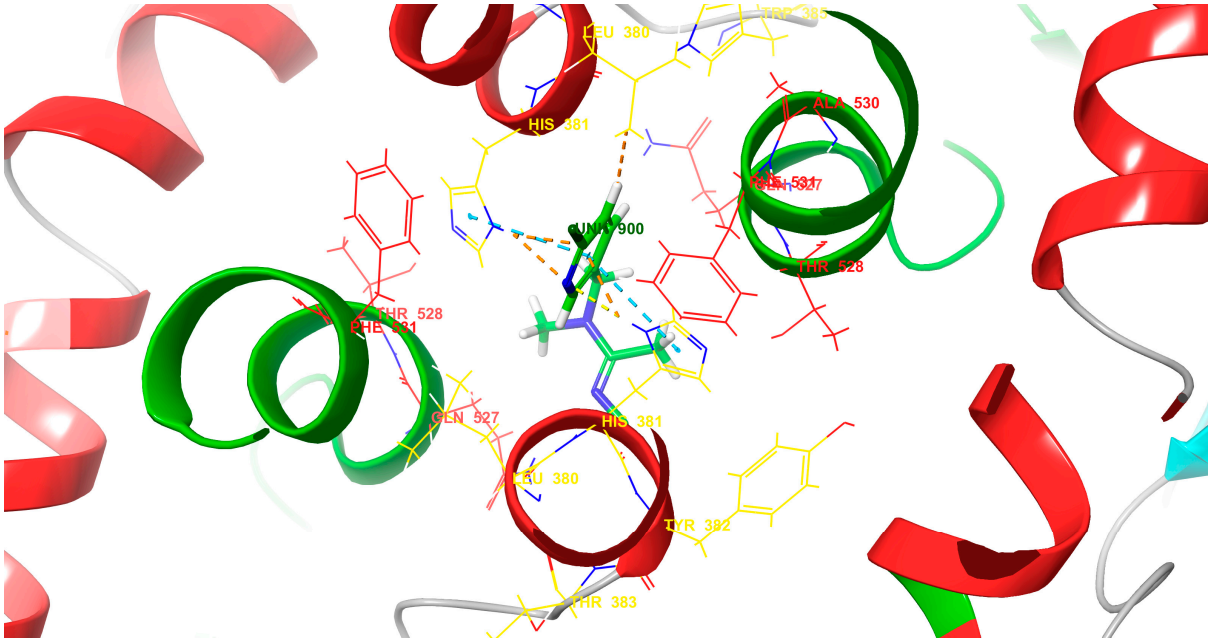
a)



b)

Figure S4. Representative chromatograms of real sample of pepper spiked with standard solutions of selected pesticides (acetamiprid, boscalid, emamectin benzoate, metalaxyl, pendimethalin, and pyraclostrobin) and prepared using a) Method 1, and b) Method 2.

a)



b)

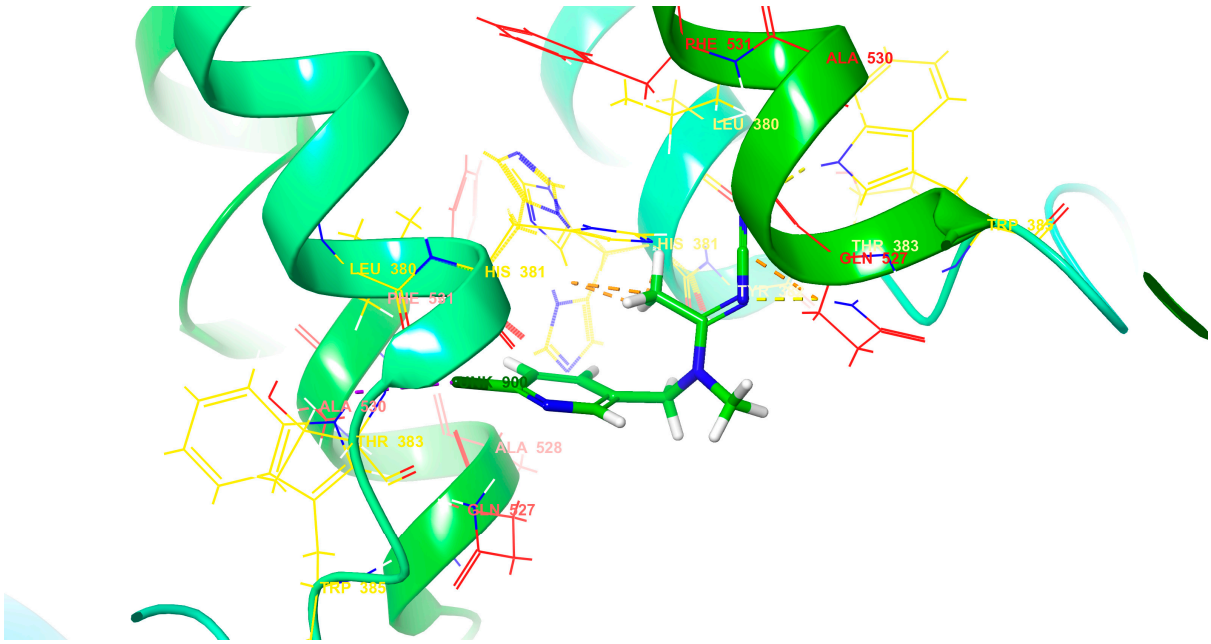
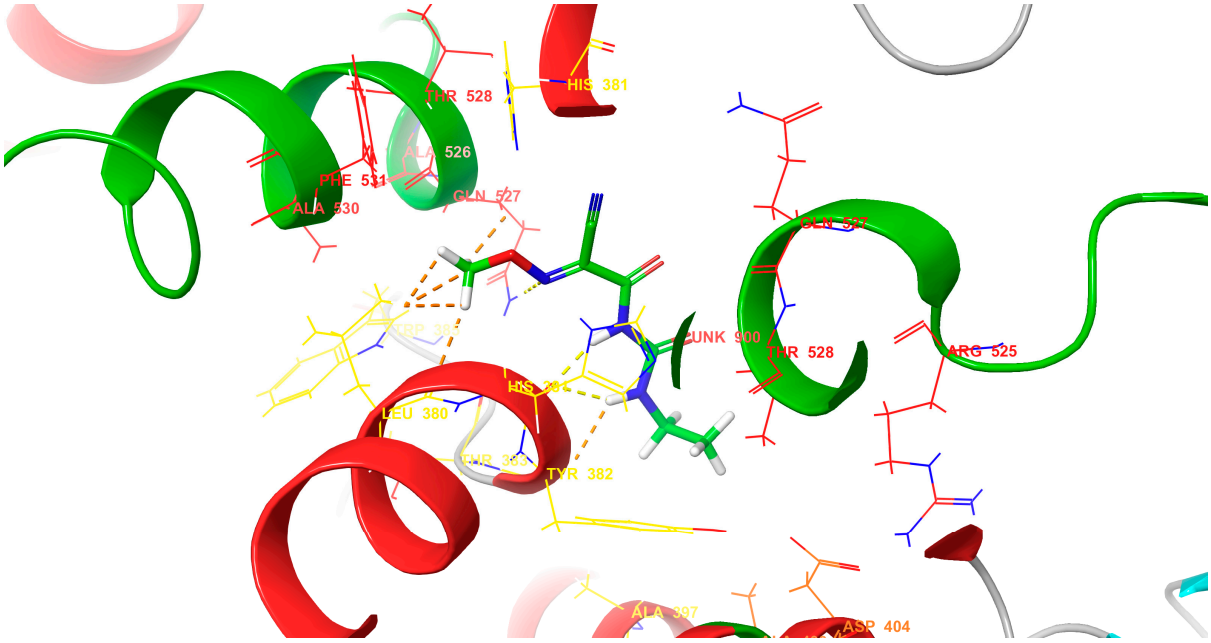


Figure S5. Graphic representations of docking acetamiprid into the structure of acetylcholine esterase from a) *Mus musculus*; b) *Homo sapiens*.

a)



b)

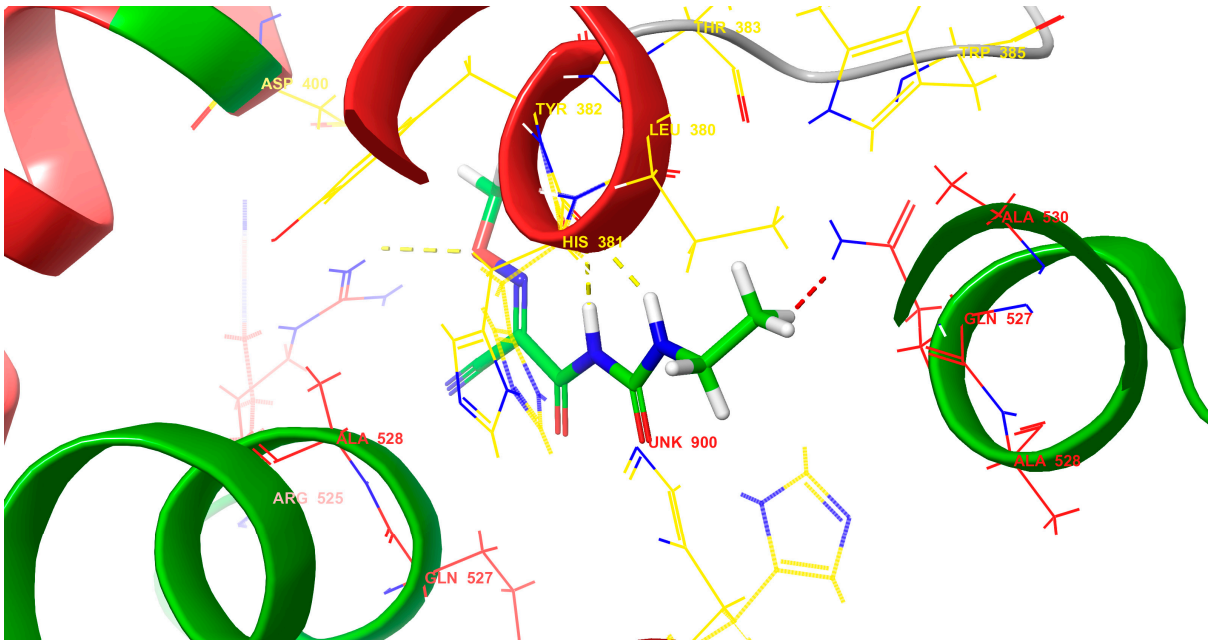
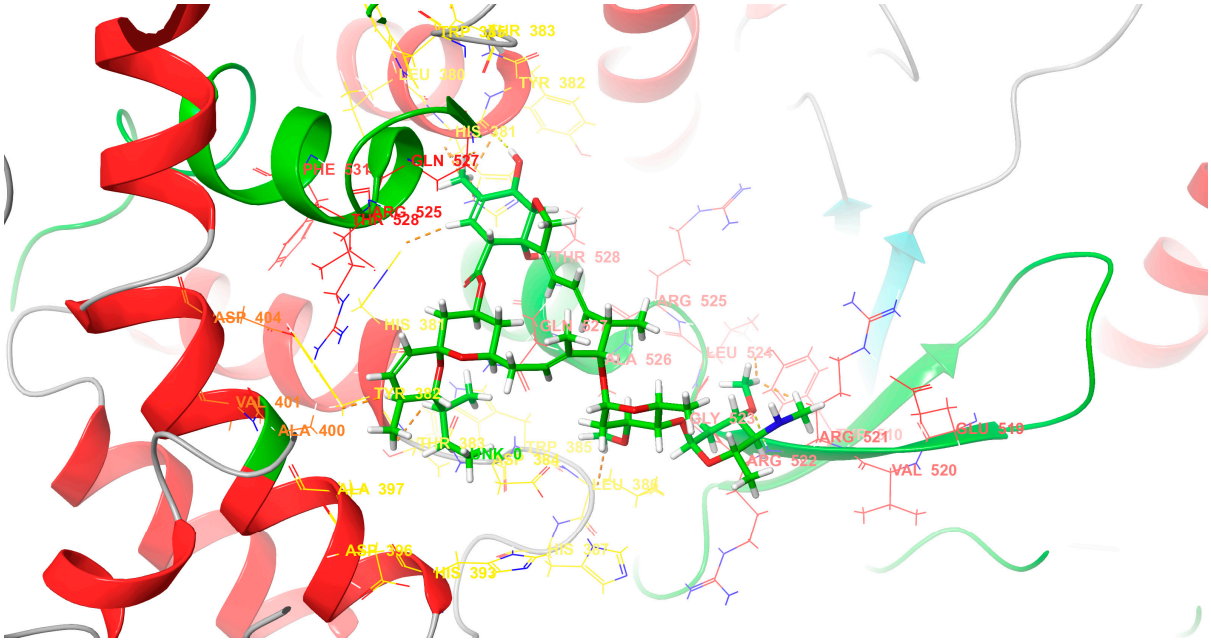


Figure S6. Graphic representations of docking cymoxanil into the structure of acetylcholine esterase from a) *Mus musculus*; b) *Homo sapiens*.

a)



b)

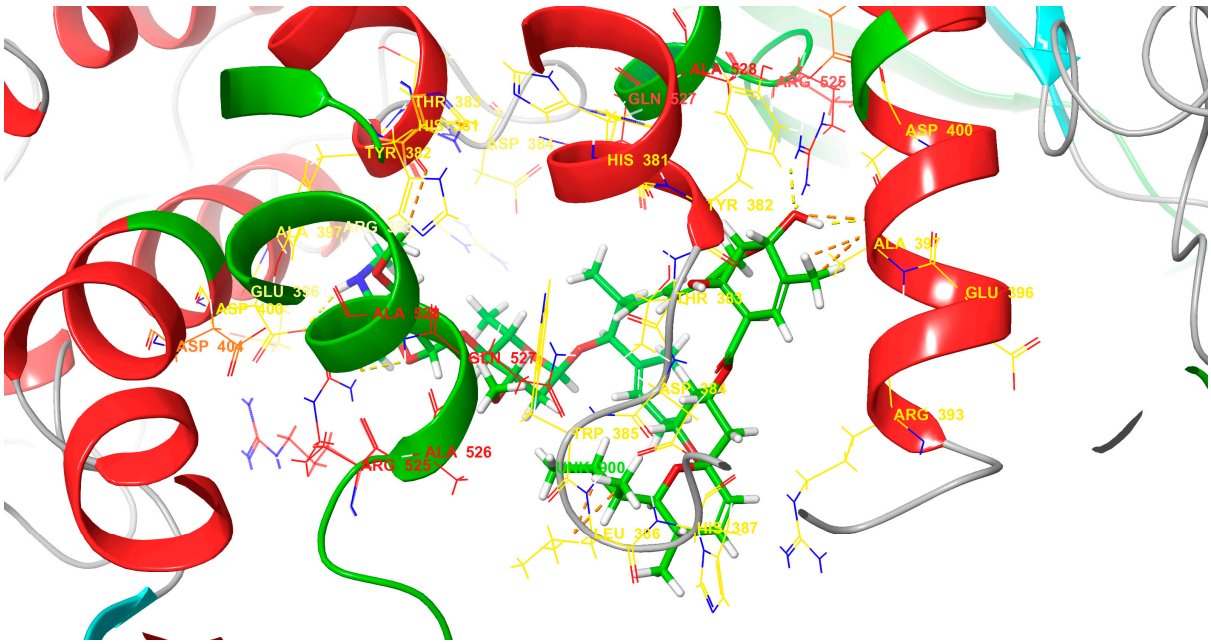
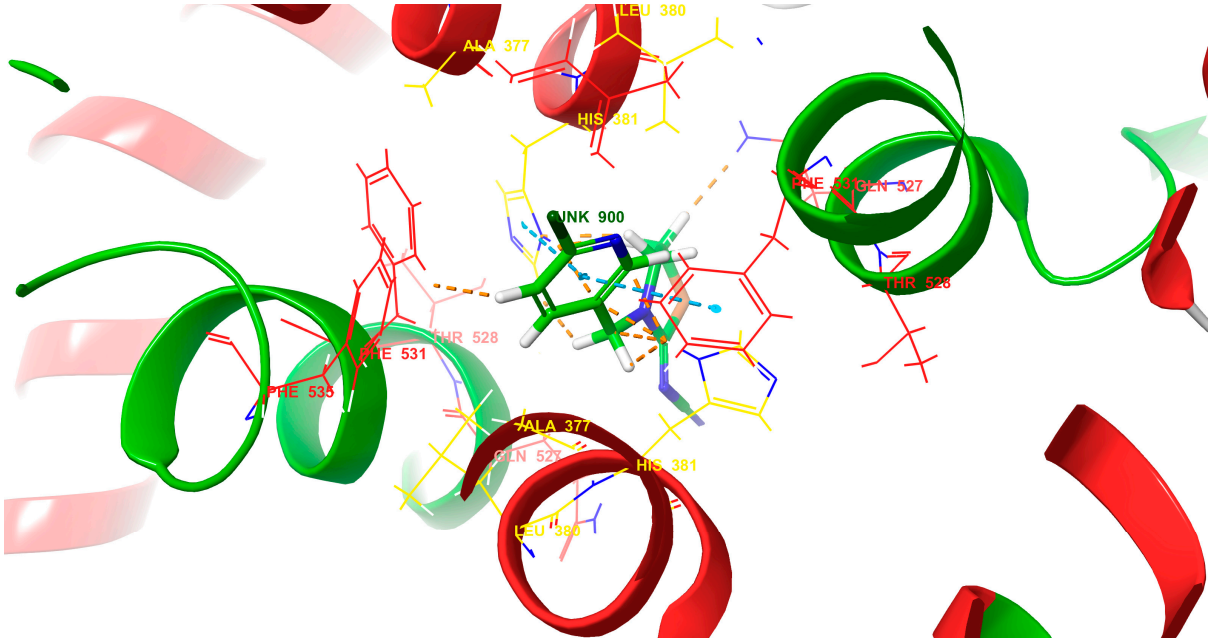


Figure S7. Graphic representations of docking emamectin into the structure of acetylcholine esterase from a) *Mus musculus*; b) *Homo sapiens*.

a)



b)

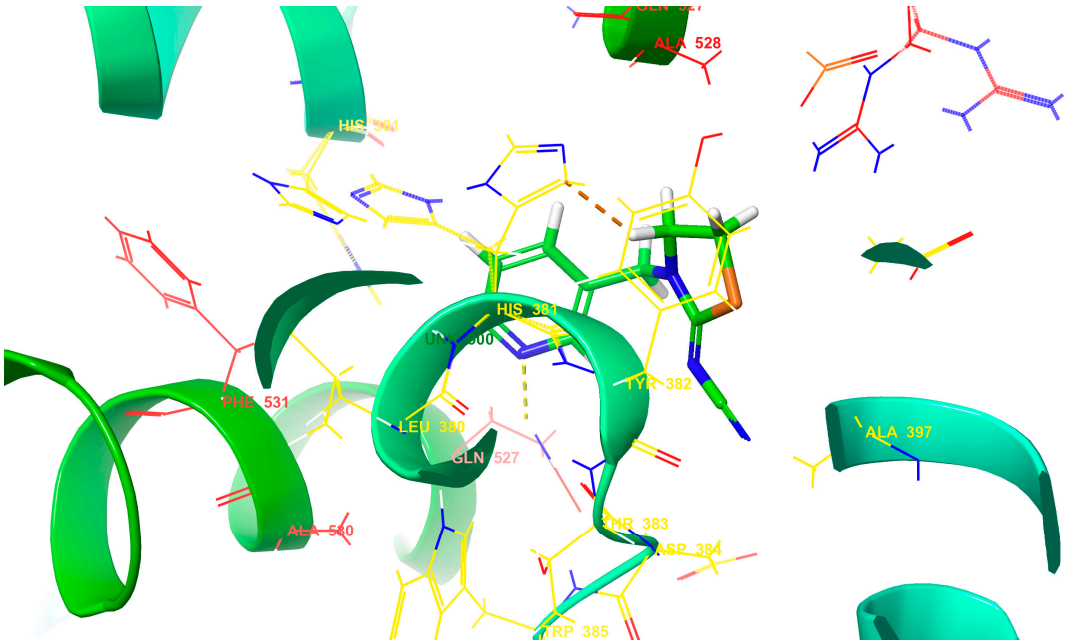
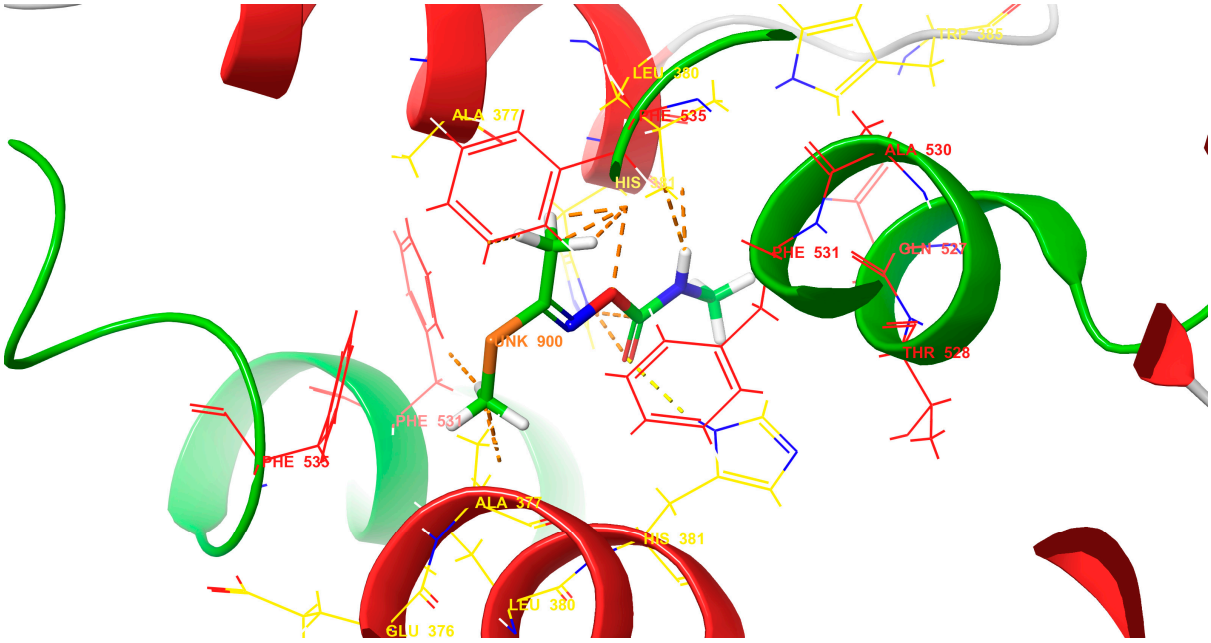


Figure S8. Graphic representations of docking thiacloprid into the structure of acetylcholine esterase from a) *Mus musculus*; b) *Homo sapiens*.

a)



b)

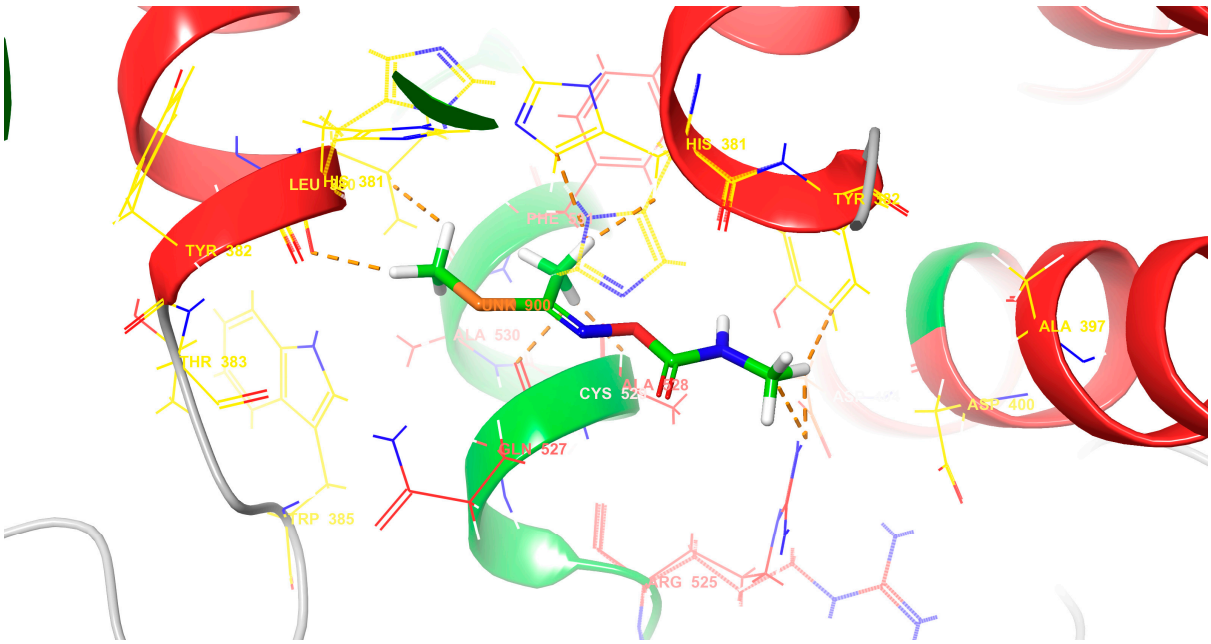
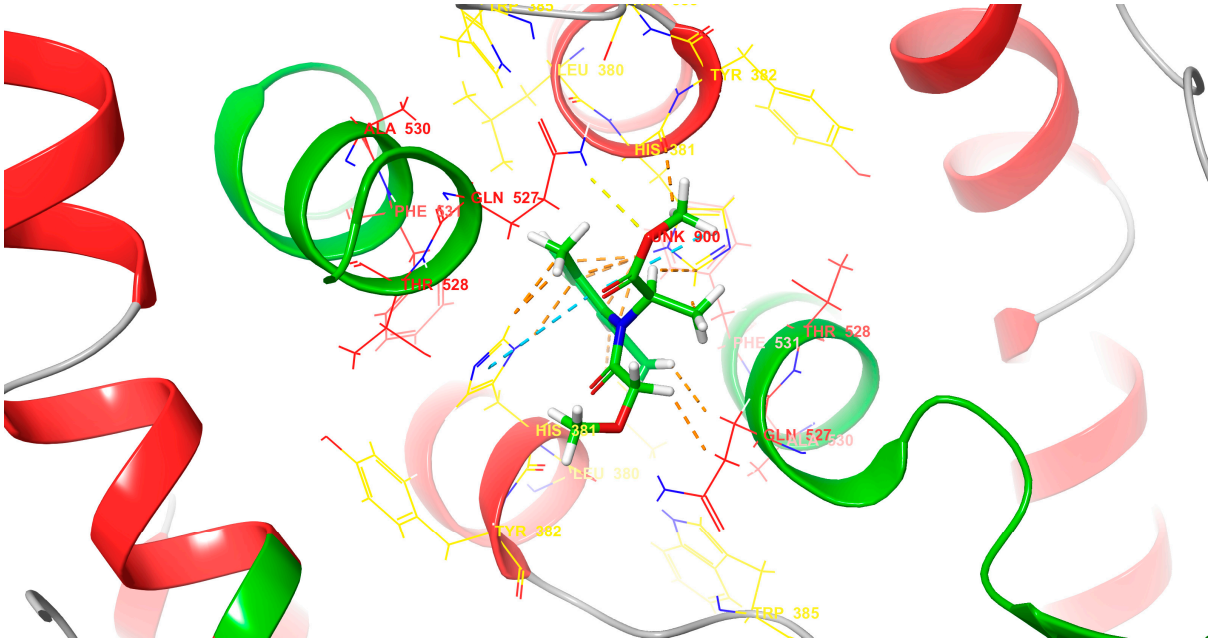


Figure S9. Graphic representations of docking methomyl into the structure of acetylcholine esterase from a) *Mus musculus*; b) *Homo sapiens*.

a)



b)

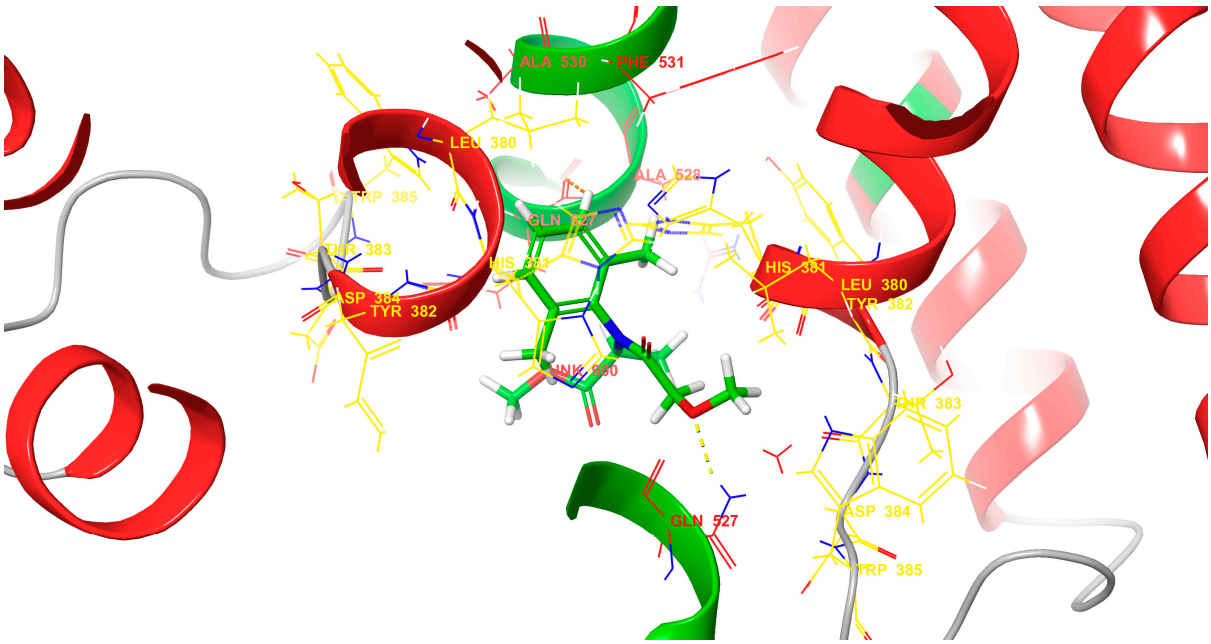
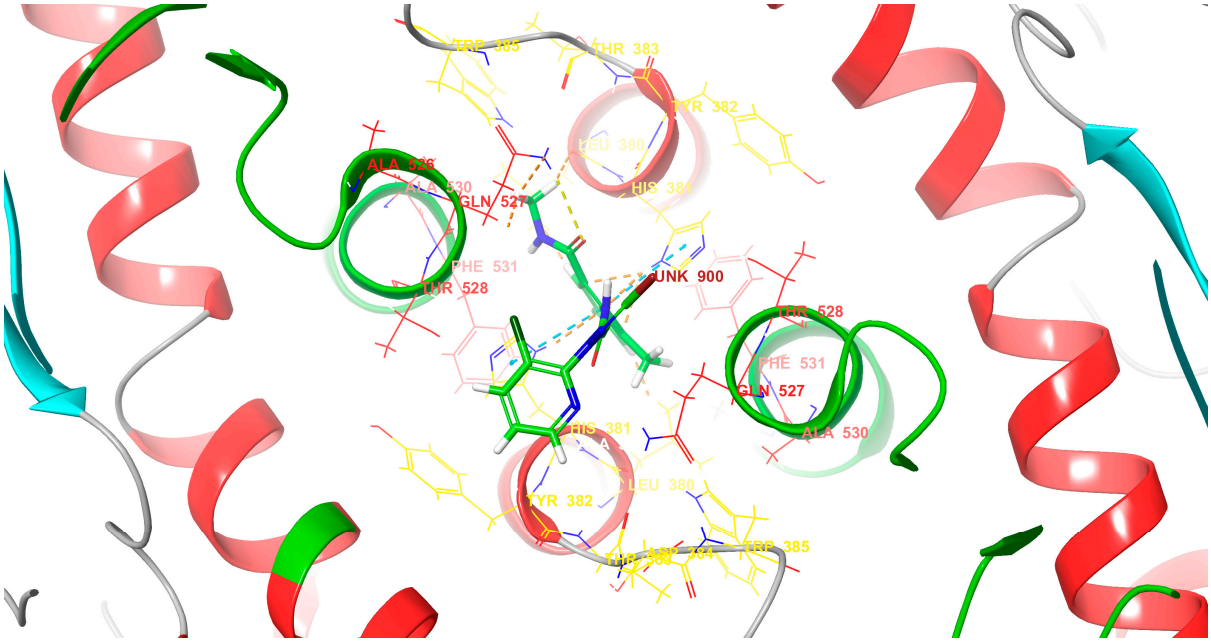


Figure S10. Graphic representations of docking metalaxyl into the structure of acetylcholine esterase from a) *Mus musculus*; b) *Homo sapiens*.

a)



b)

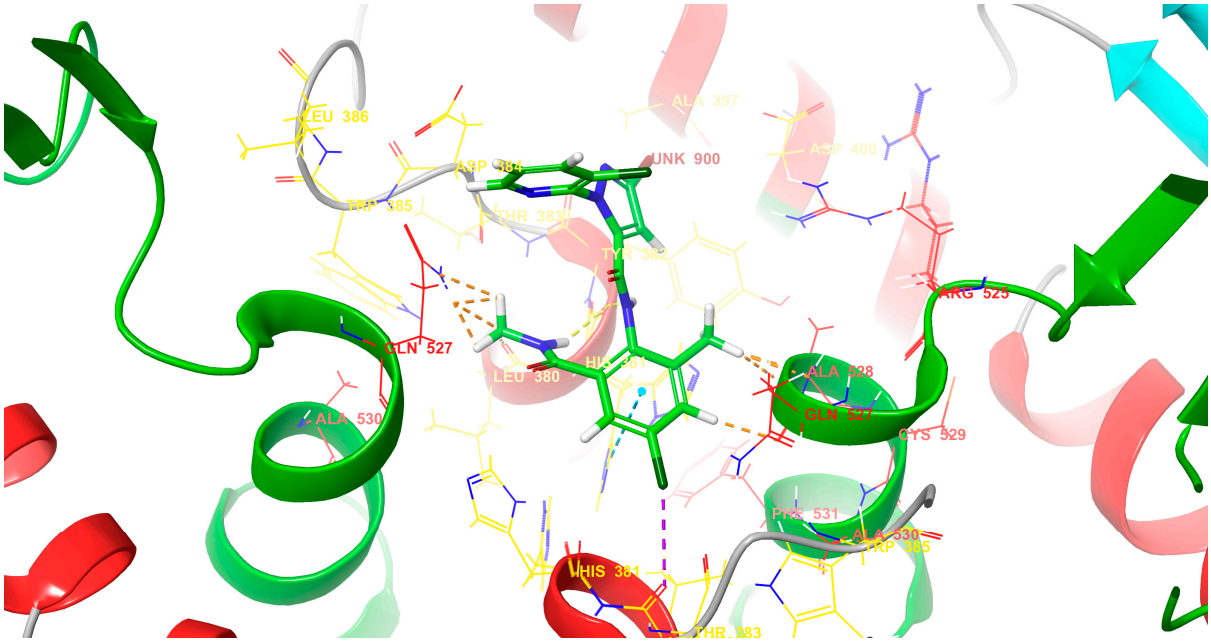


Figure S11. Graphic representations of docking chlorantraniliprole into the structure of acetylcholine esterase from a) *Mus musculus*; b) *Homo sapiens*.