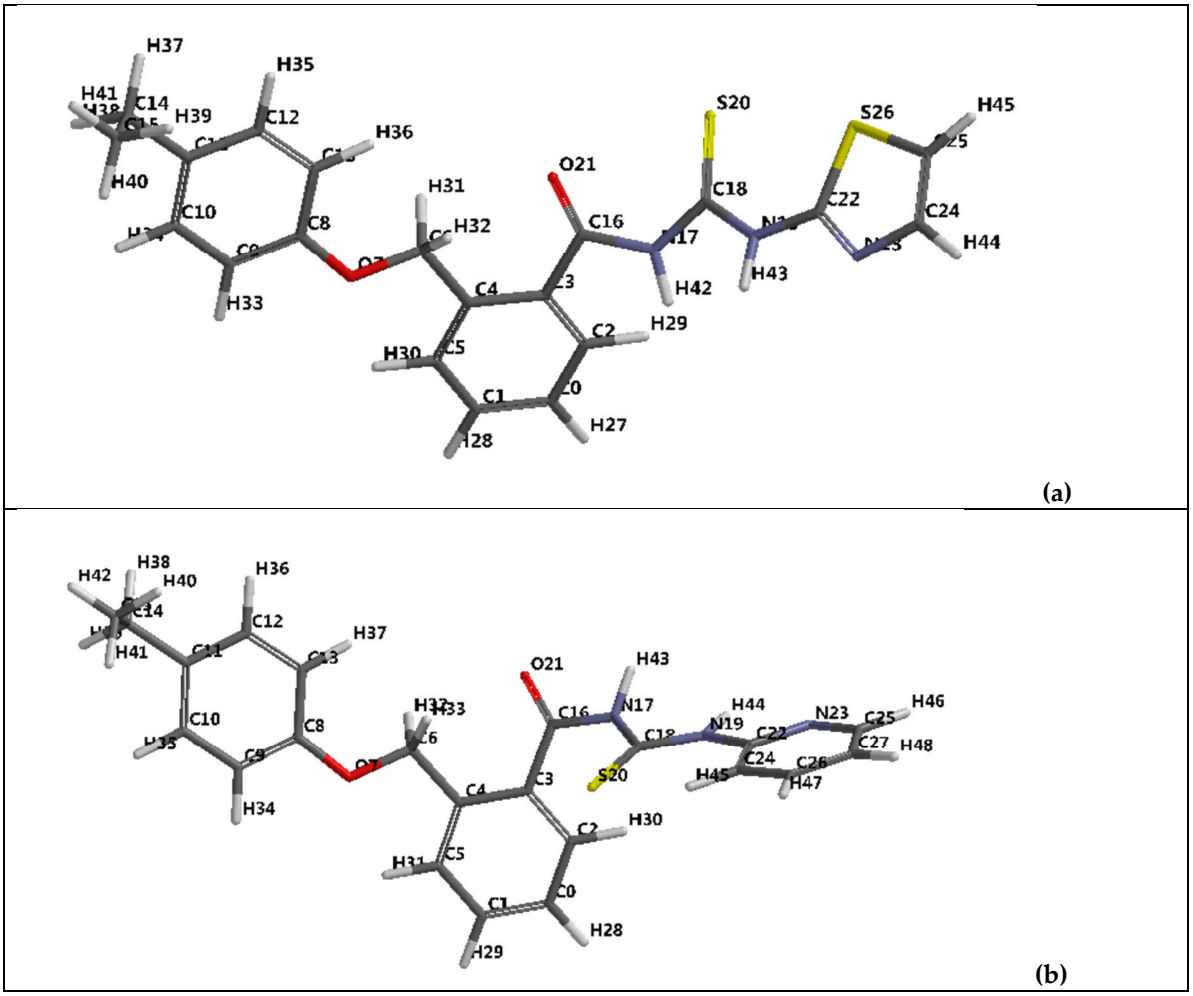
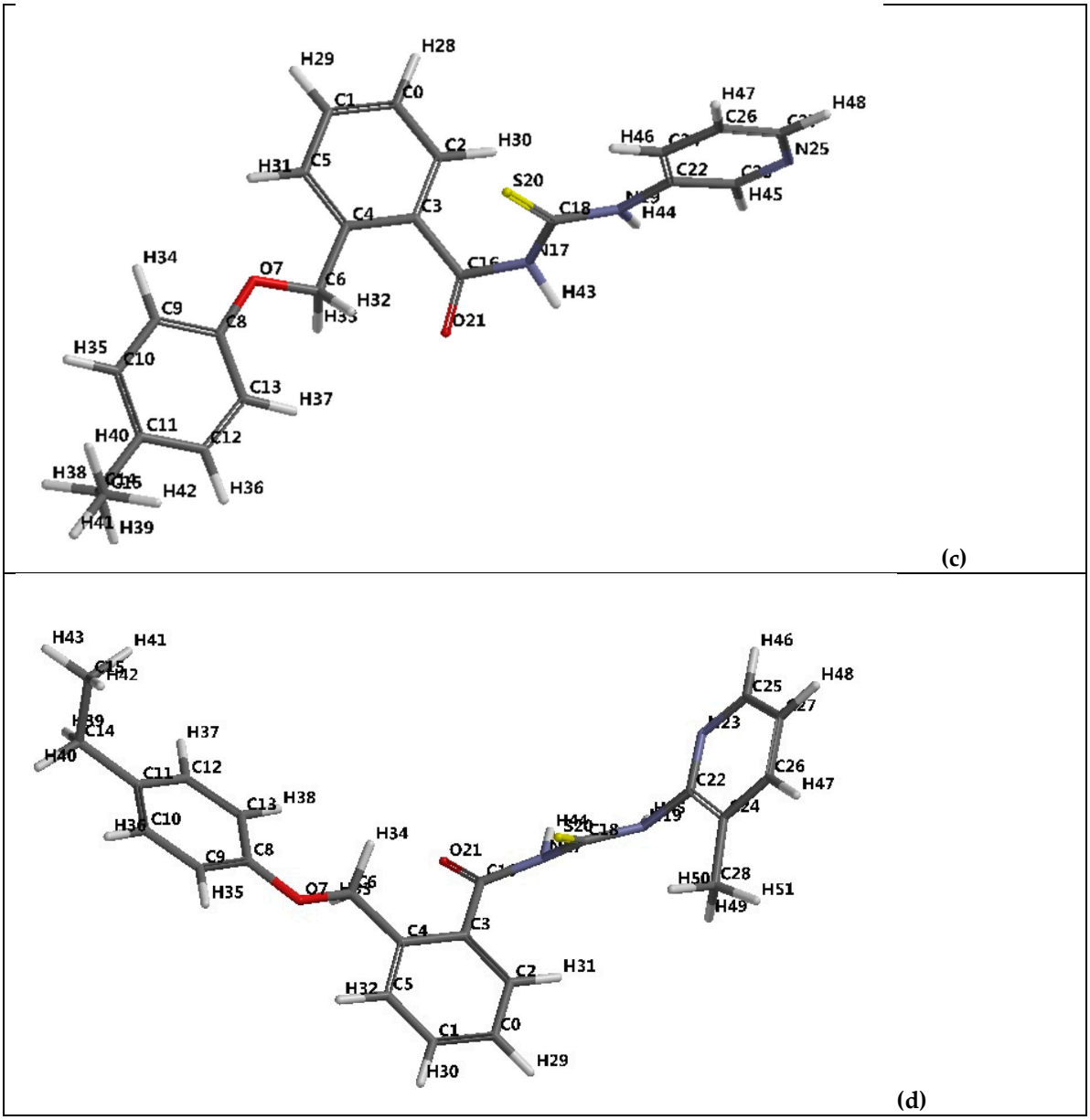
The present document consists of supplementary materials related to the ***In silico prediction, characterization and molecular docking studies on new benzamide derivatives*** research article.

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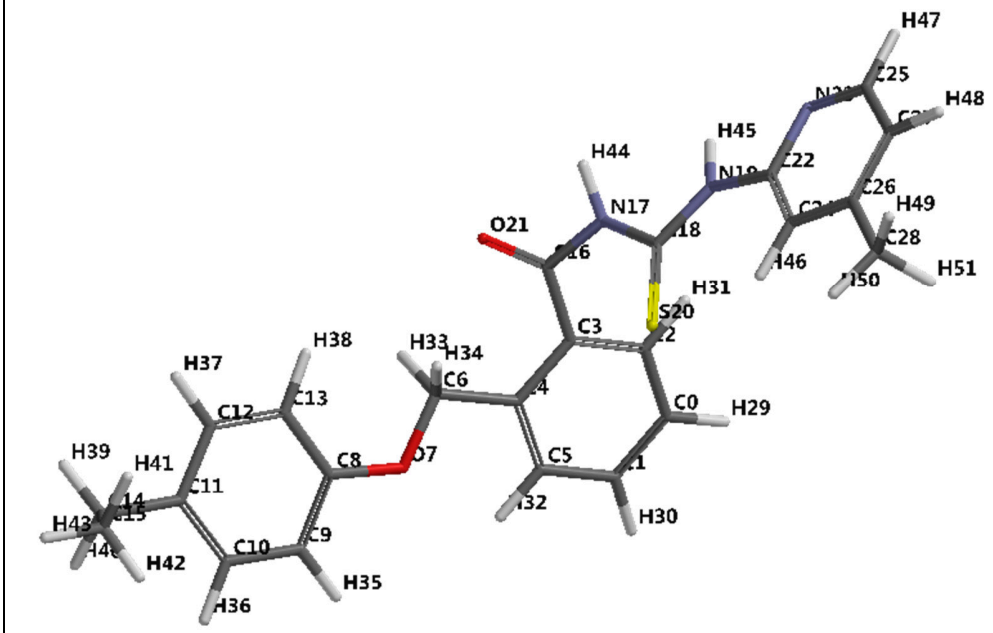
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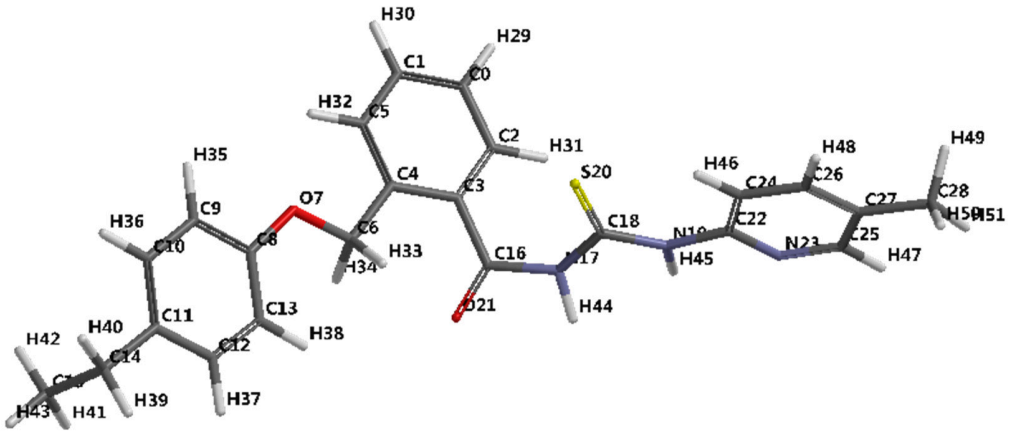
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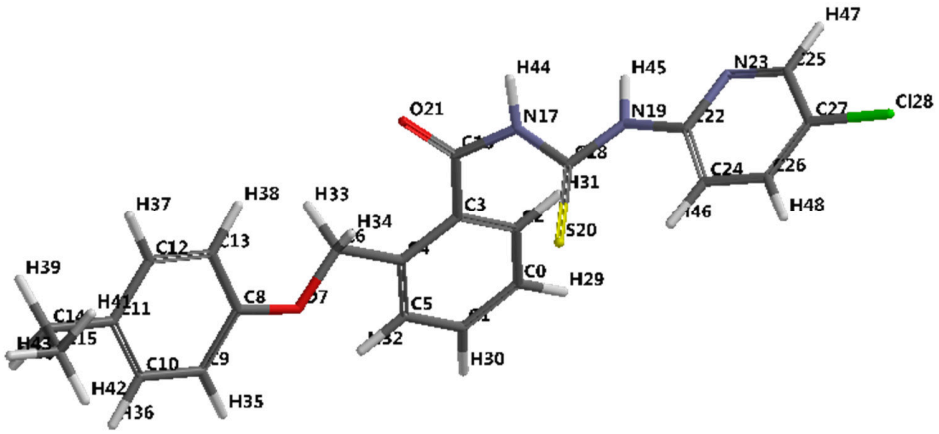
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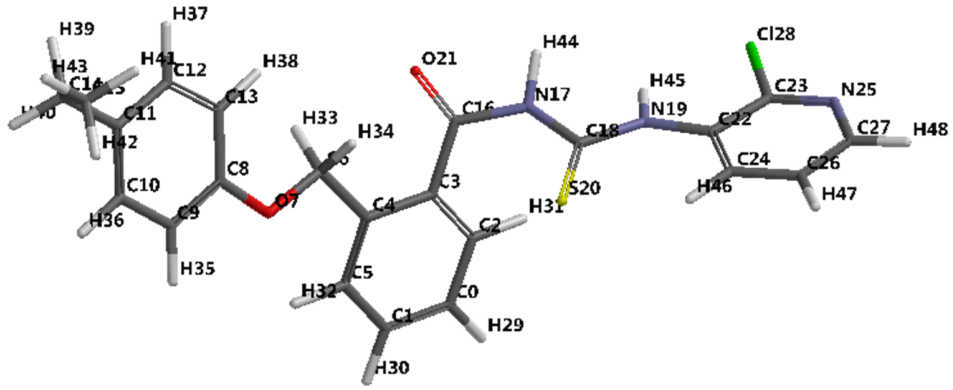
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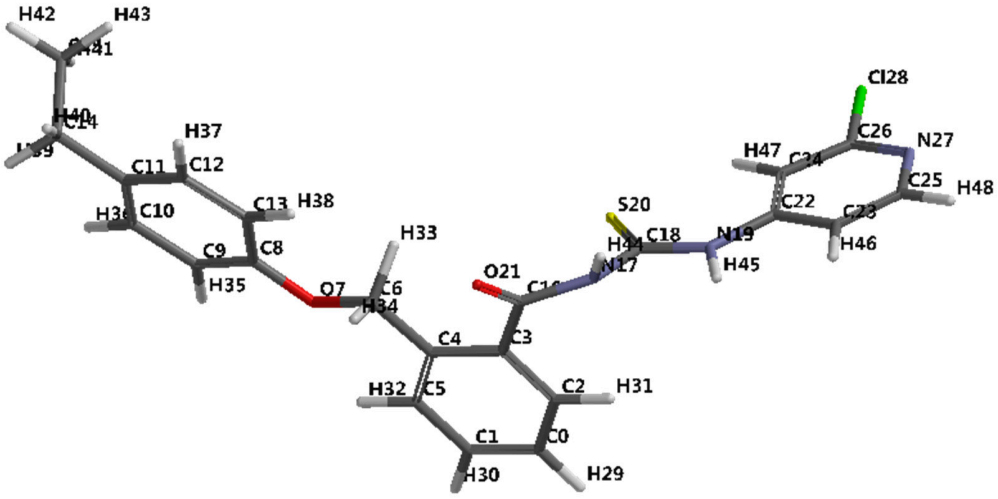
(h)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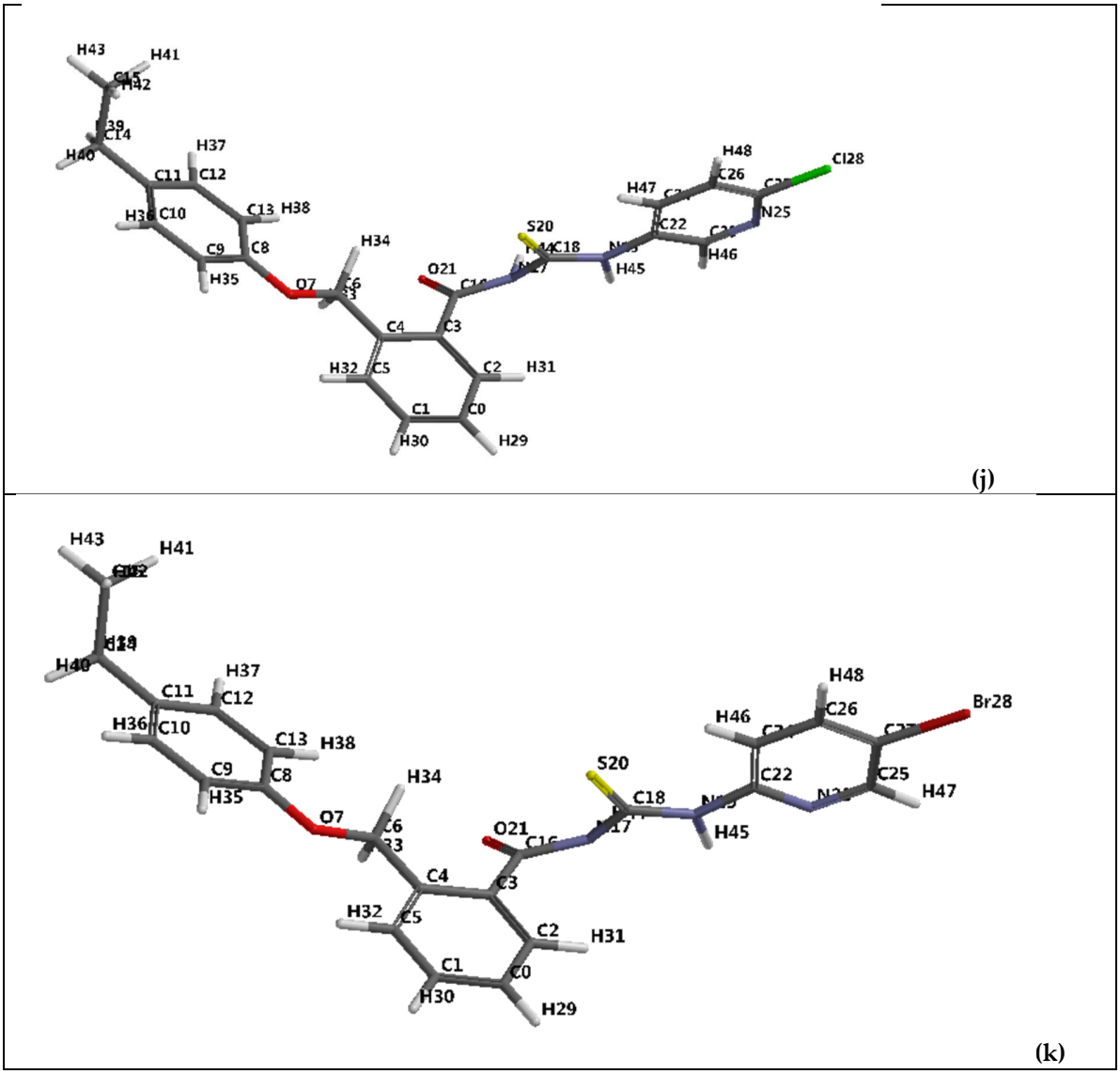
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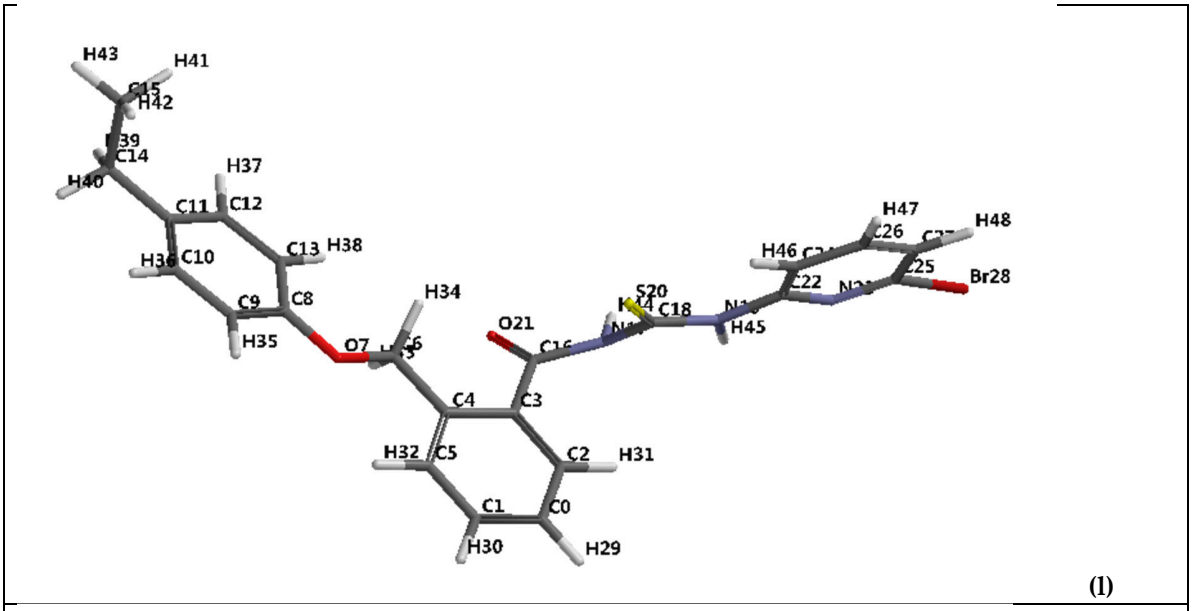
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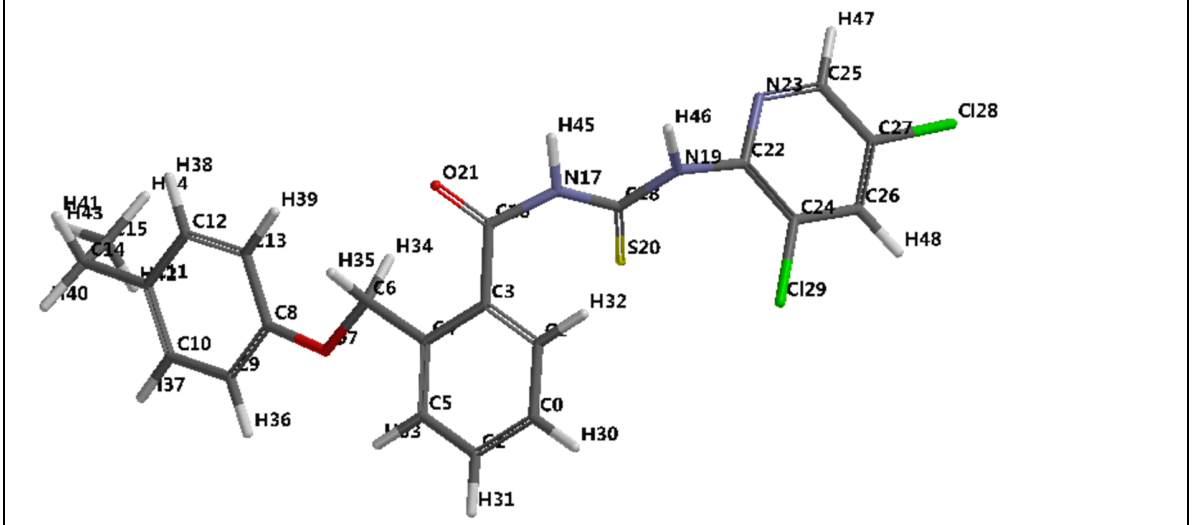
(l)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(m)

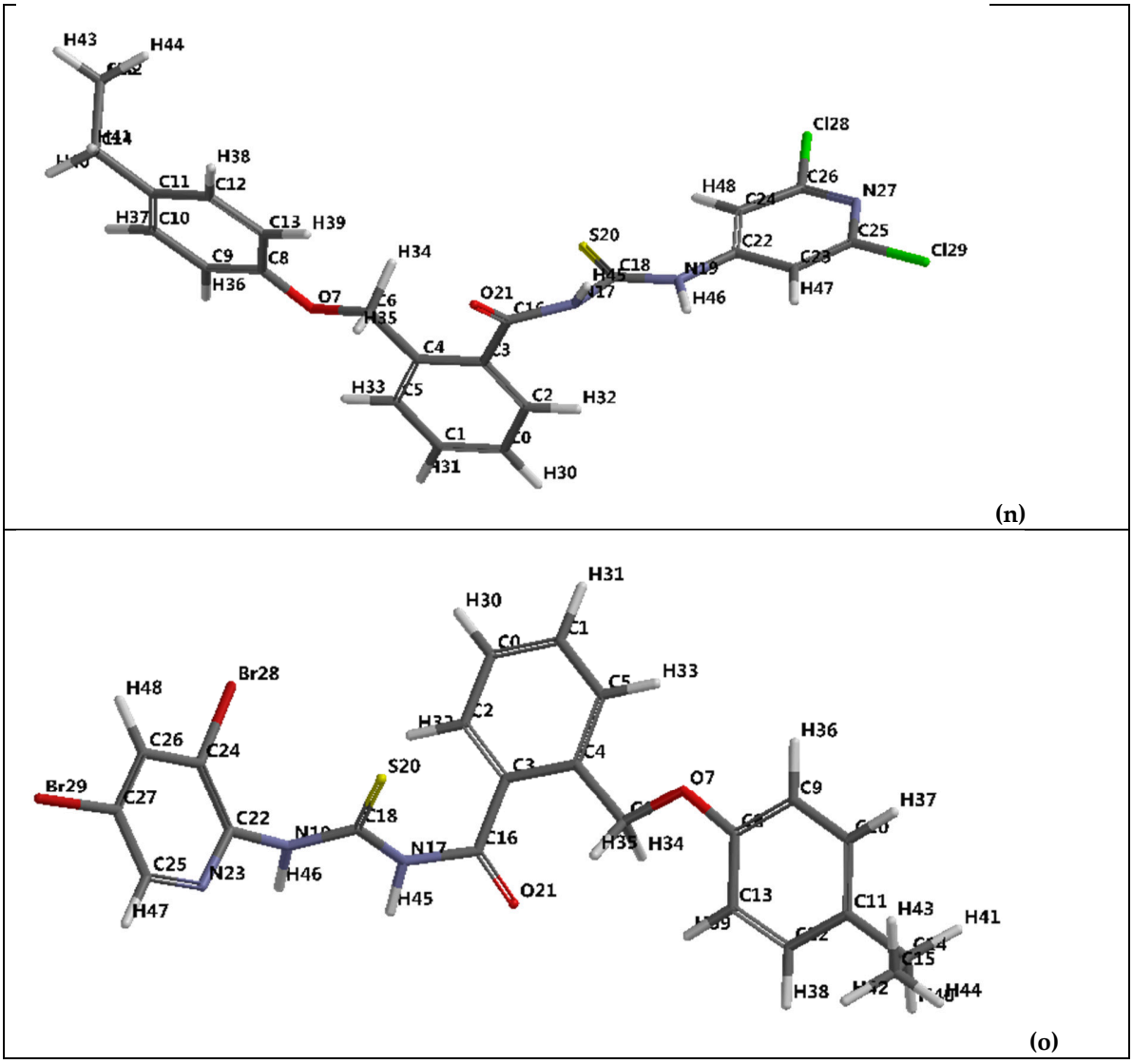
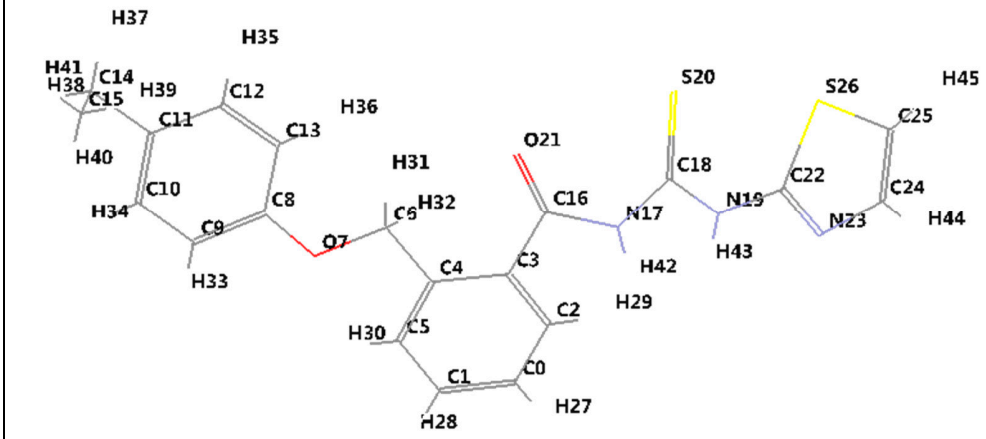


Figure S1. The tube label representation of the optimized molecular structure for the designed chemical compounds (a) **1a**; (b) **1b**; (c) **1c**; (d) **1d**; (e) **1e**; (f) **1f**; (g) **1g**; (h) **1h**; (i) **1i**; (j) **1j**; (k) **1k**; (l) **1l**; (m) **1m**; (n) **1n**; (o) **1o**.

By convention, the numbering of the atoms has been done in accordance with Spartan 14 software.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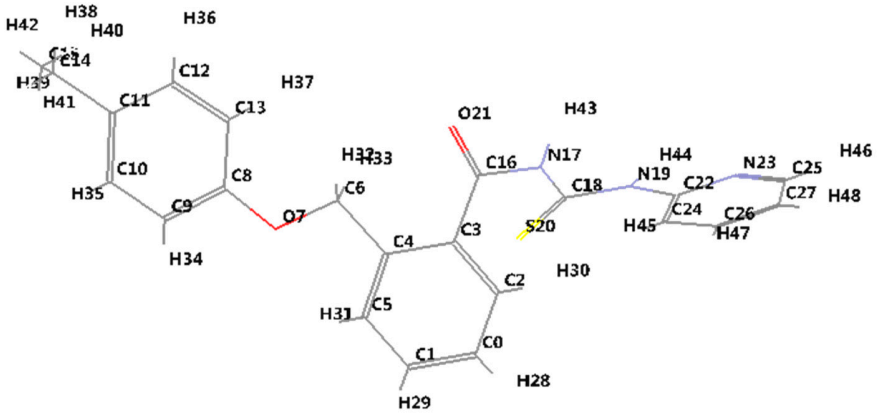
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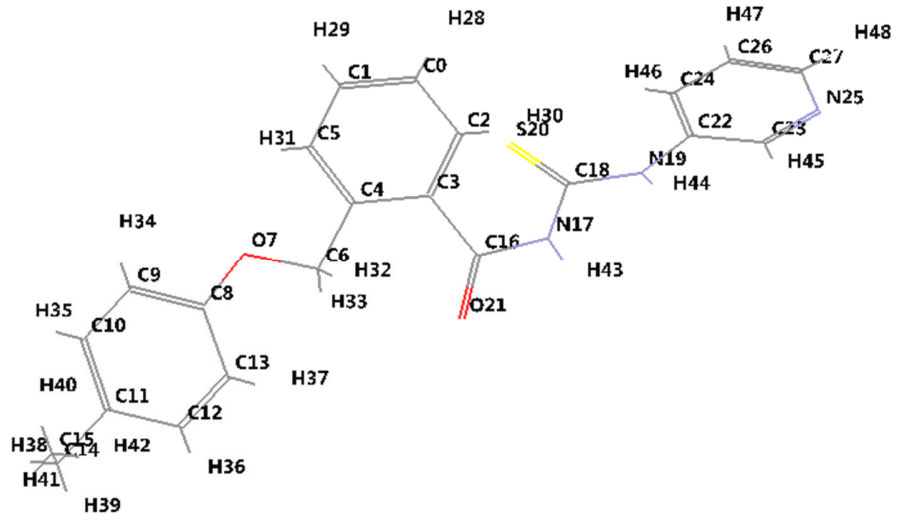
(b)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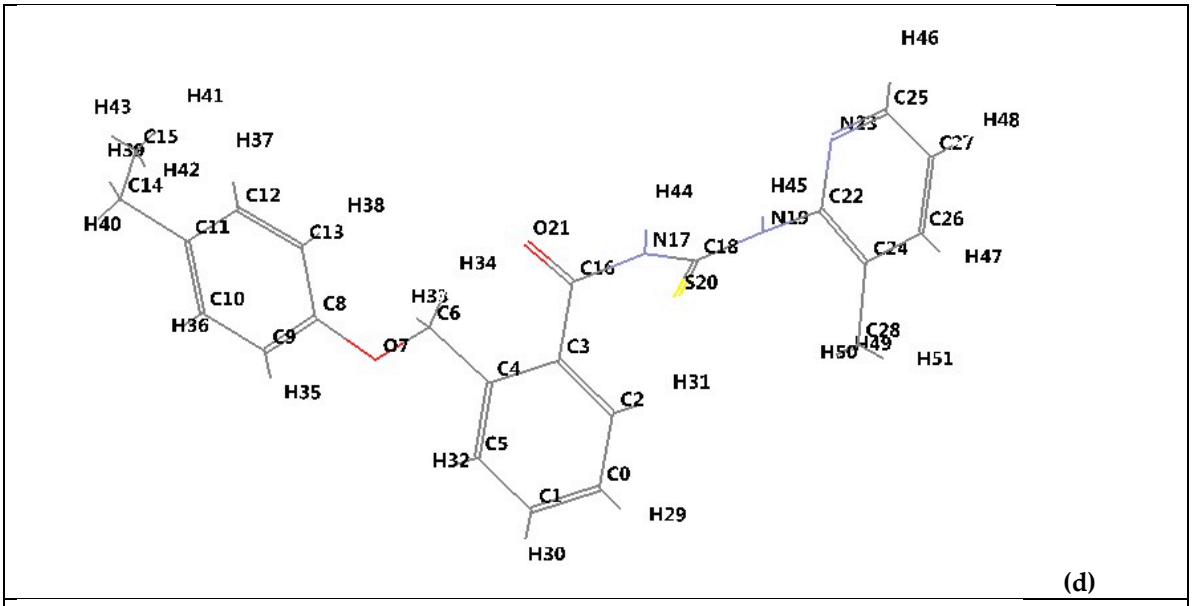
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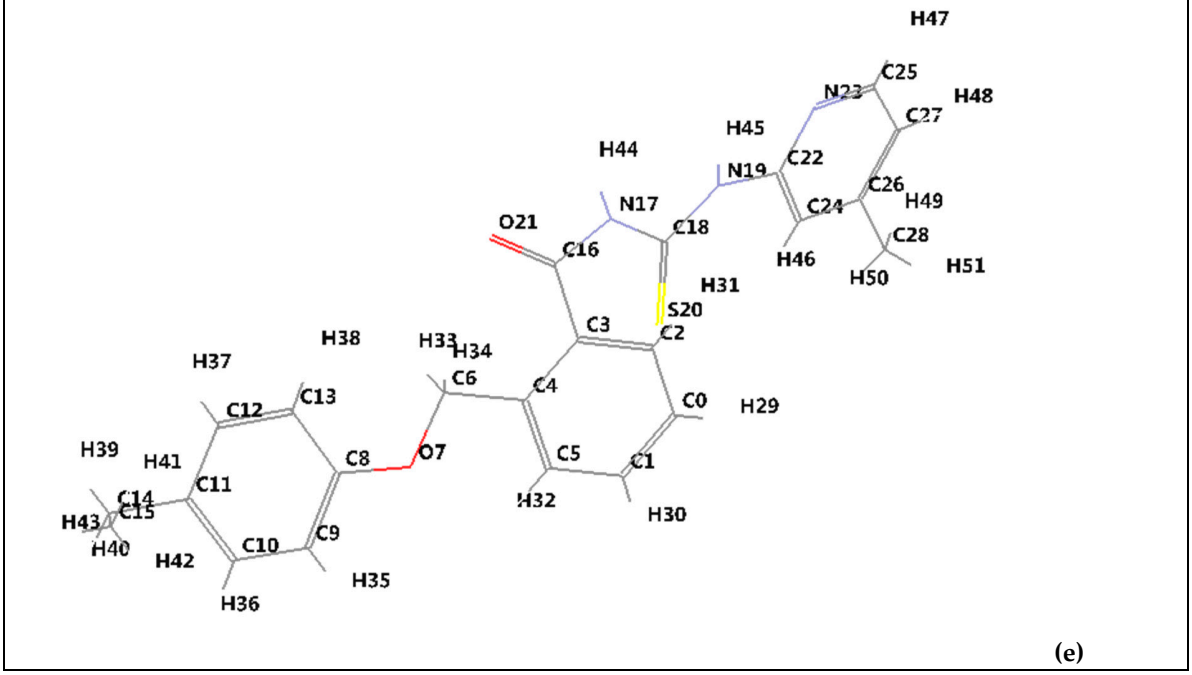
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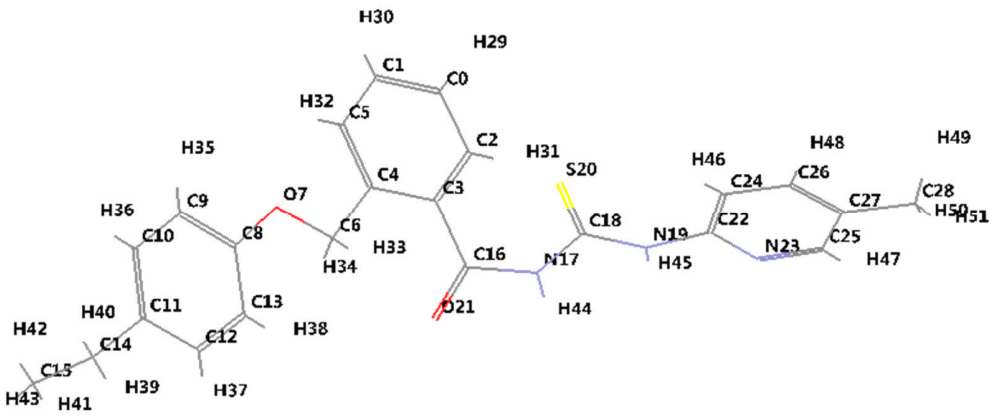
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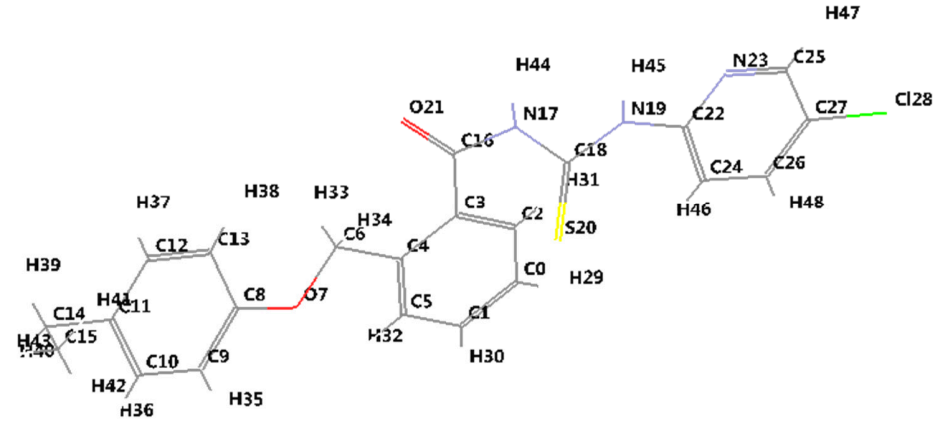
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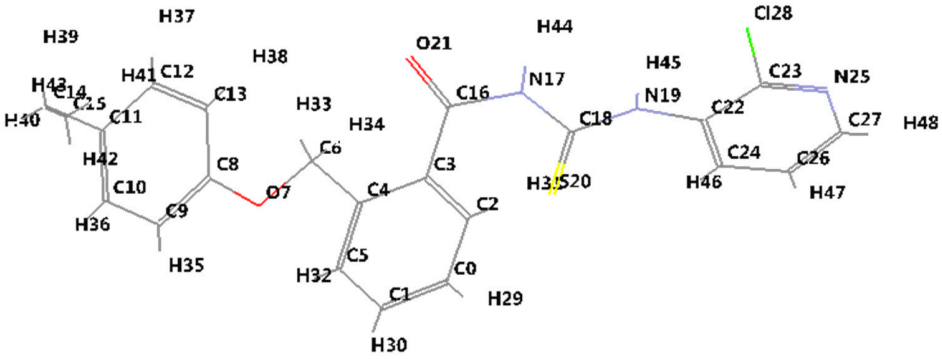
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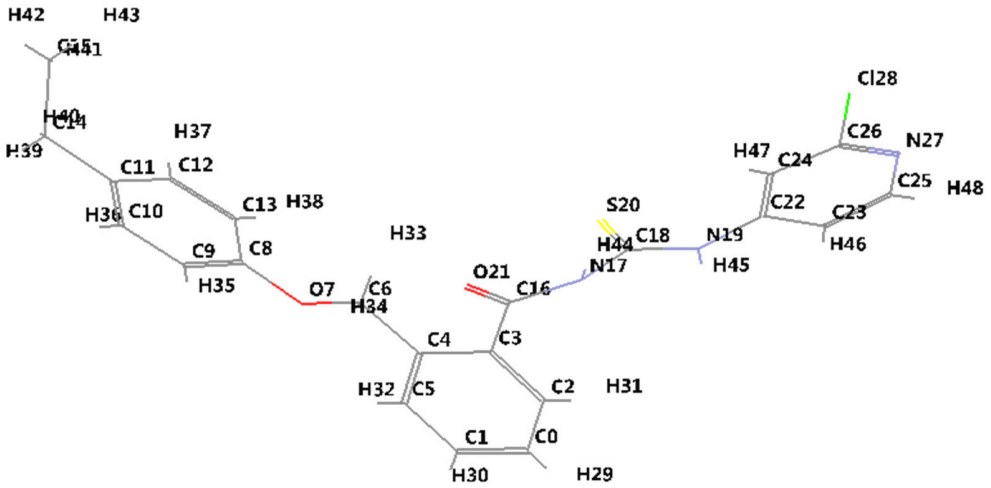
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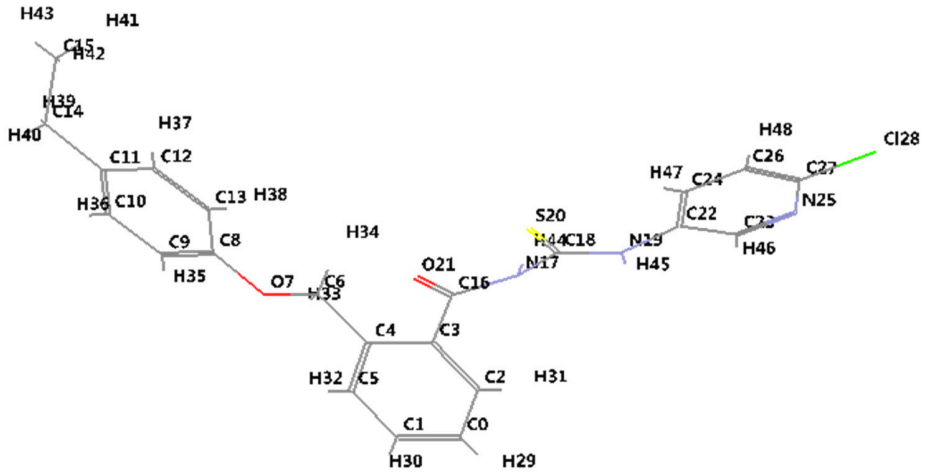
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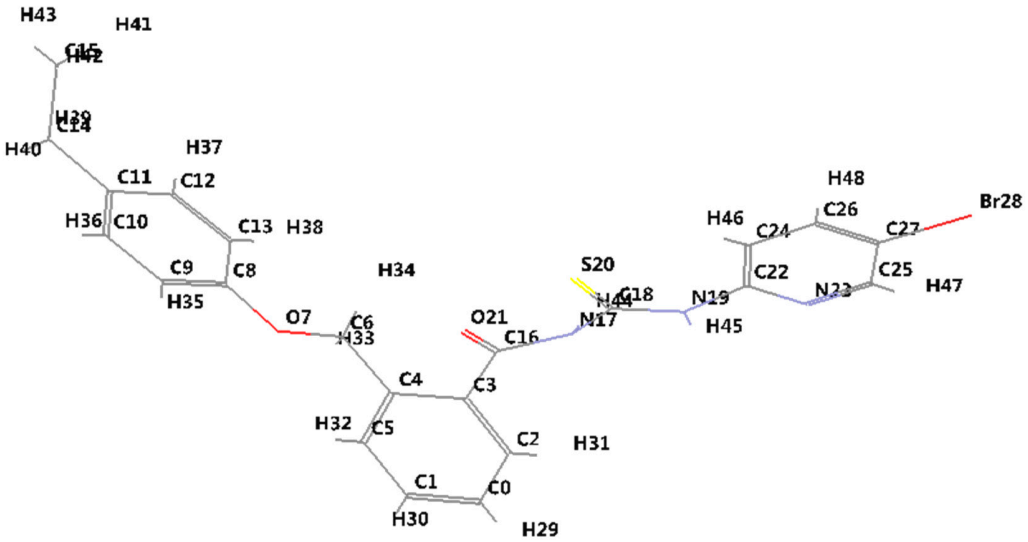
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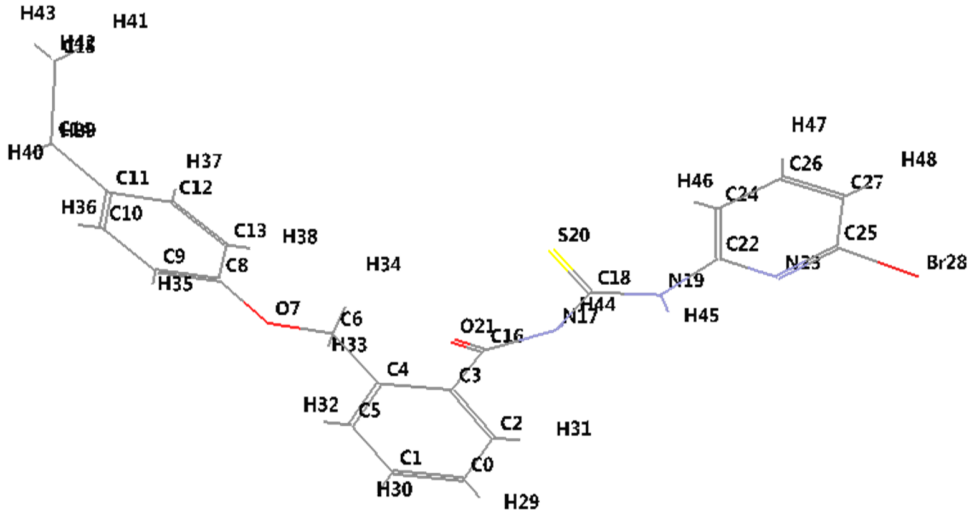
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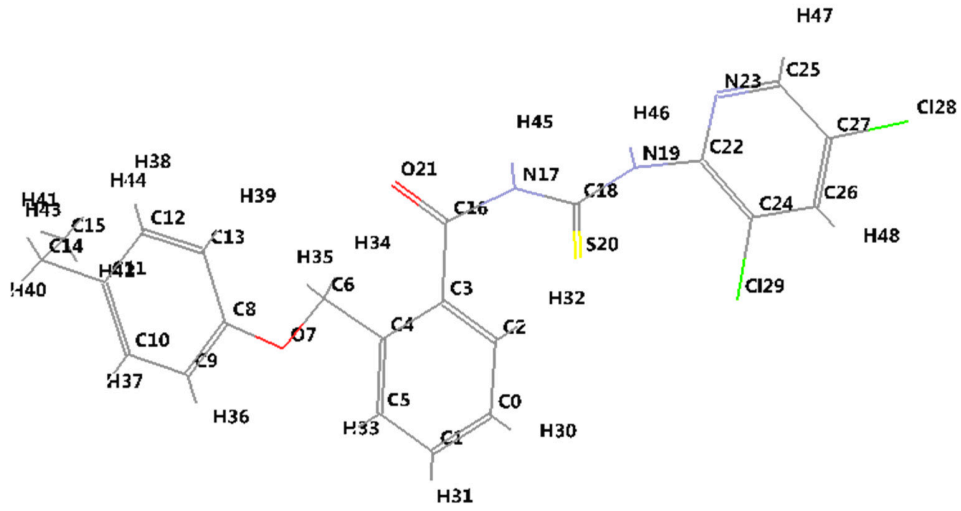
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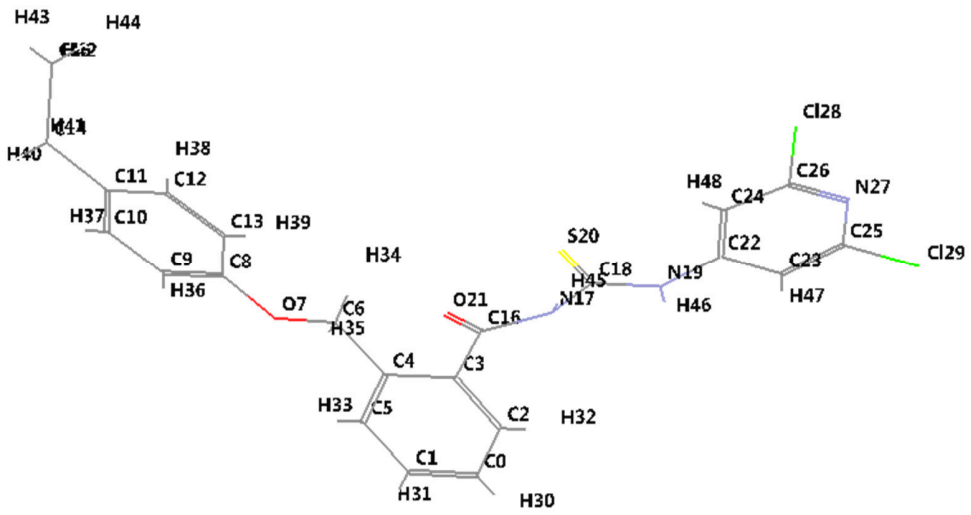
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(n)

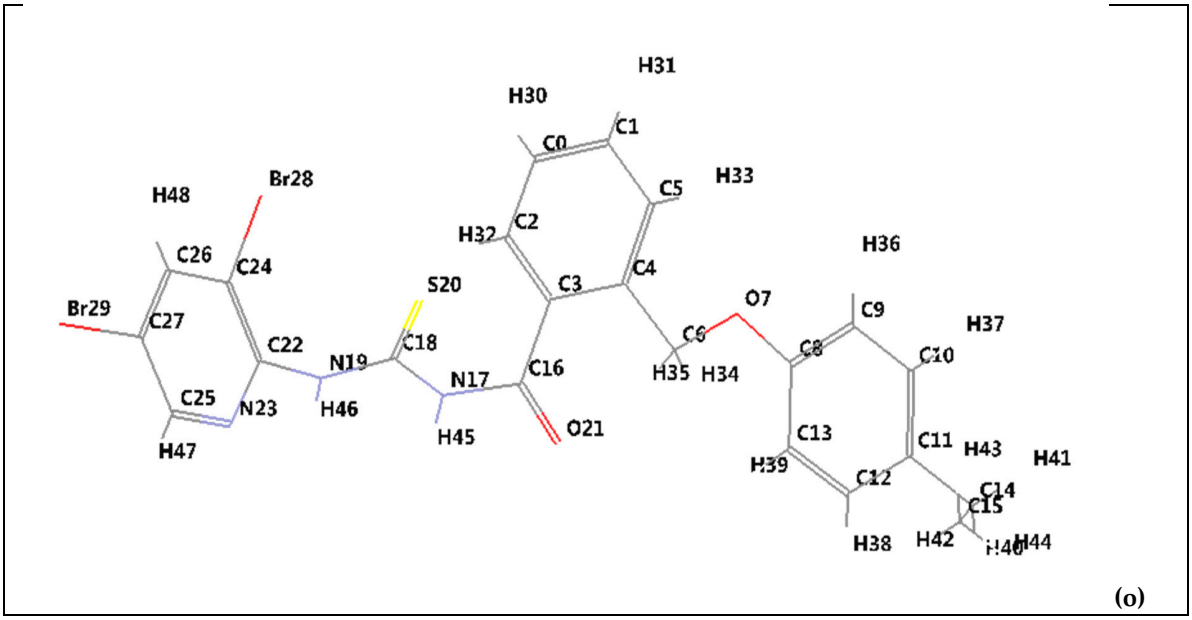
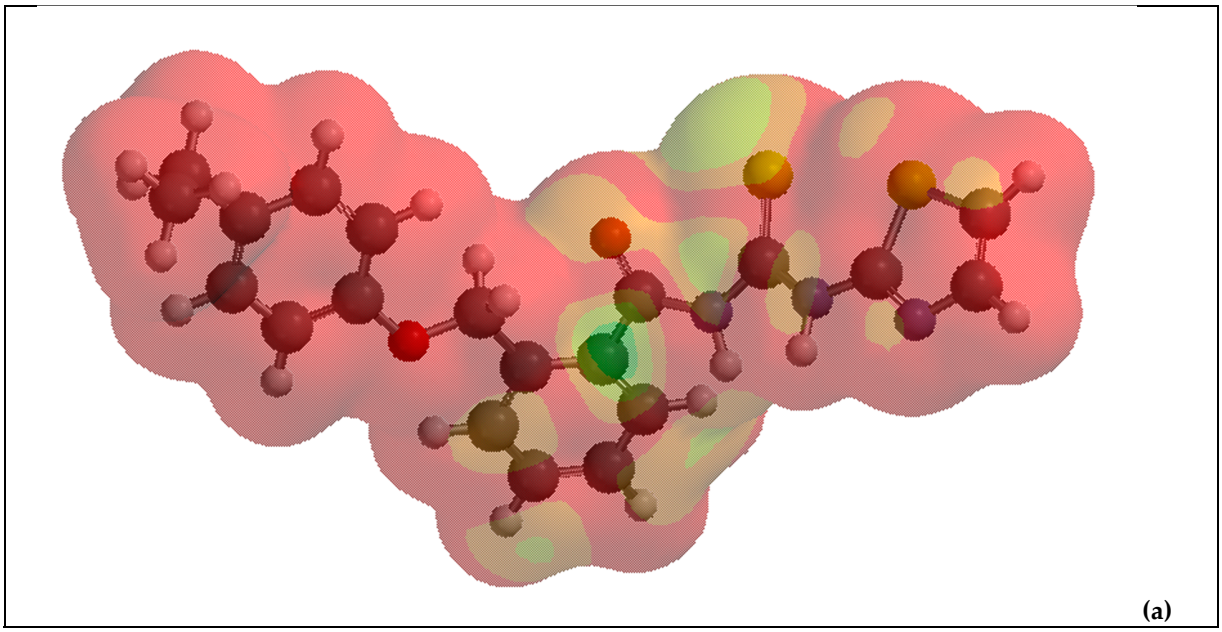
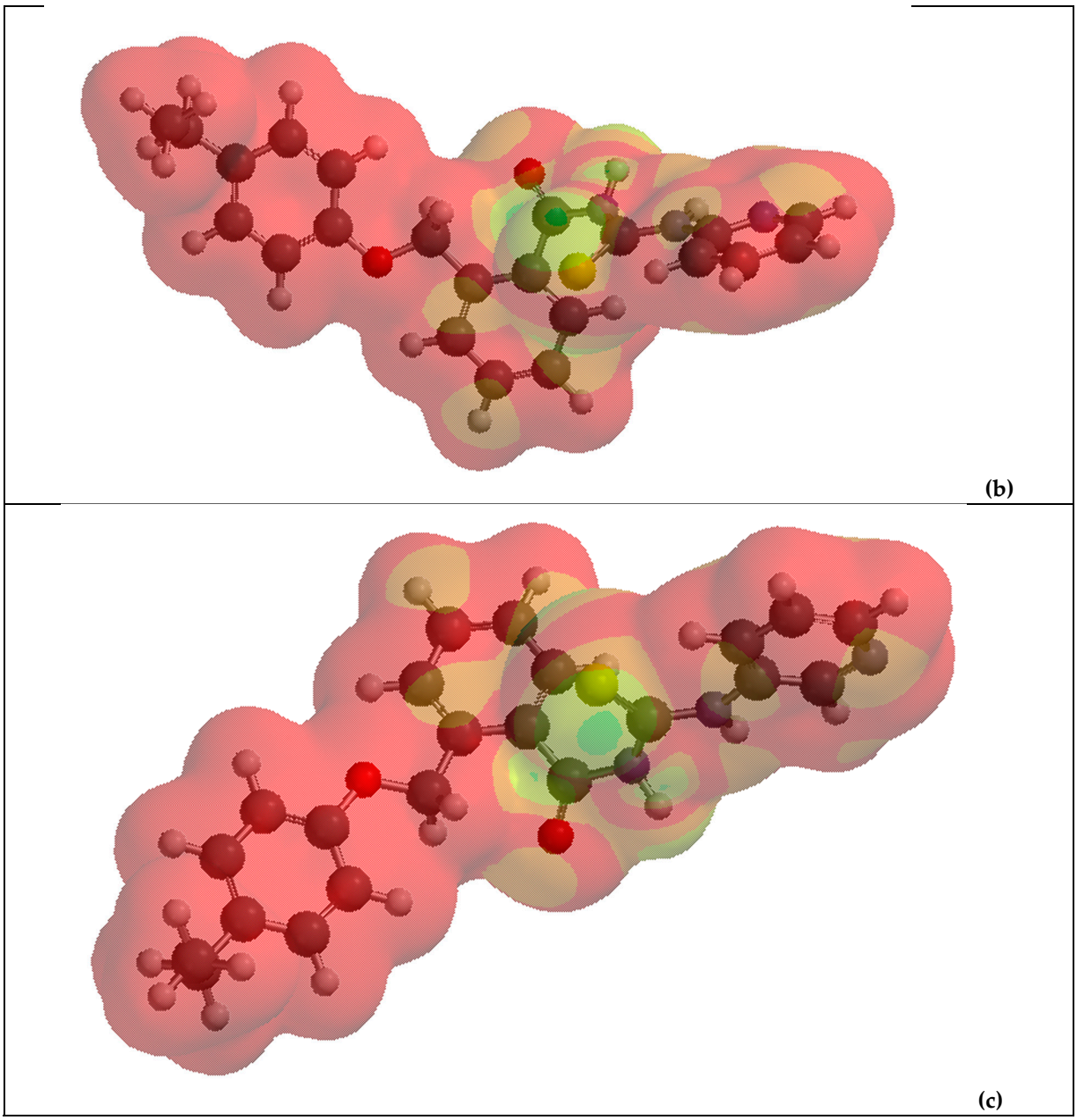
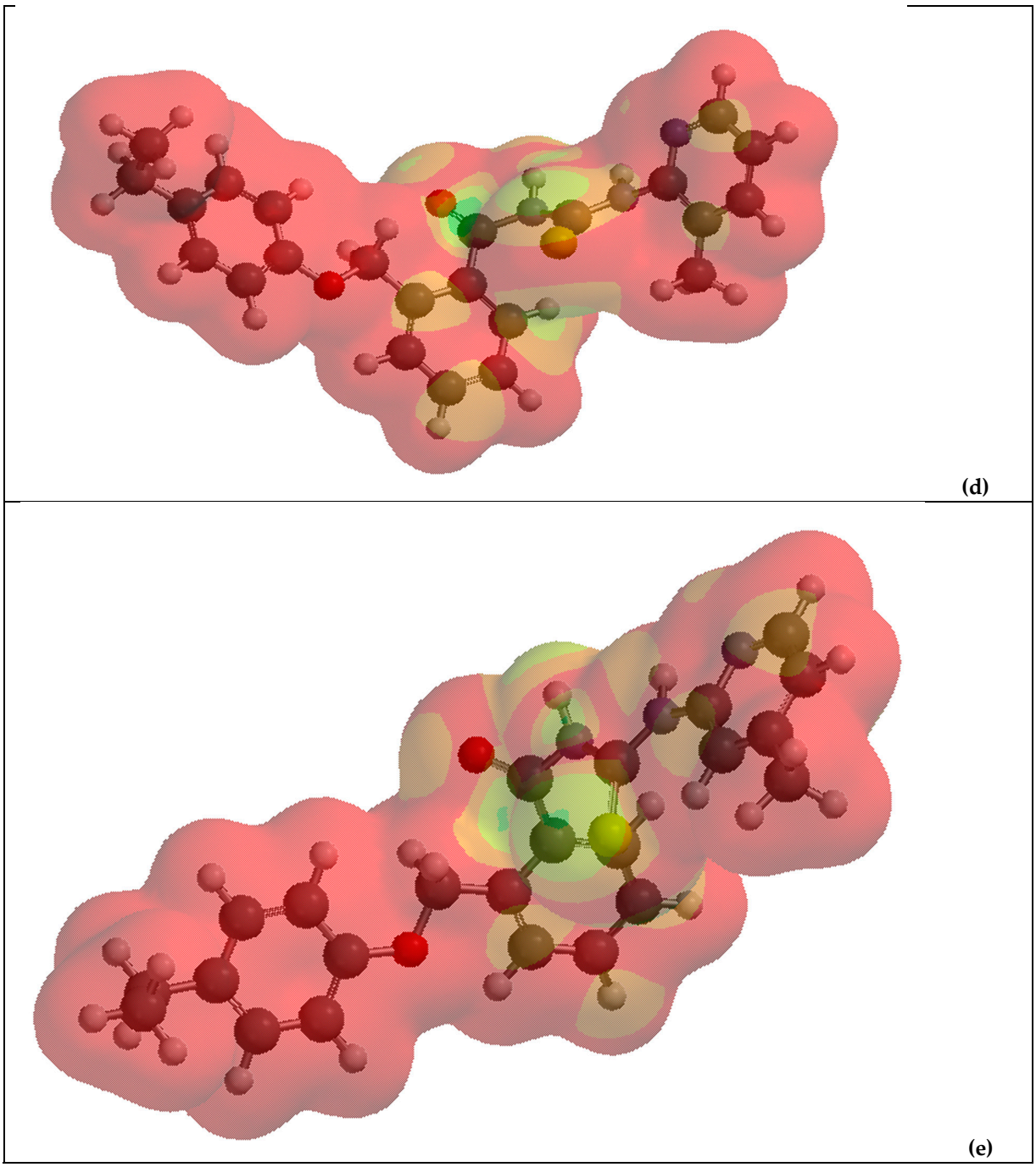


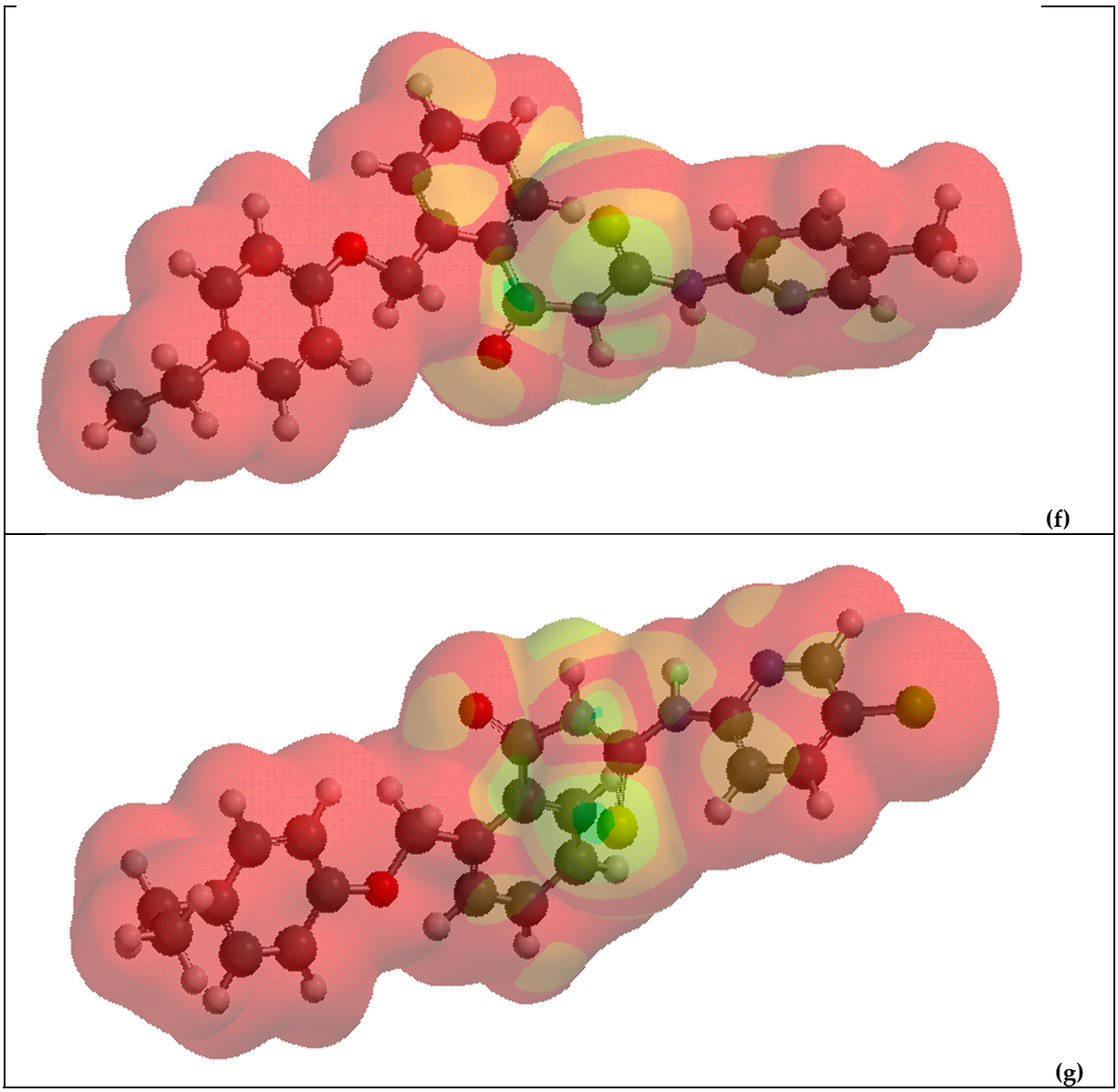
Figure S2. The wire label representation of the optimized molecular structure for the designed chemical compounds (a) **1a**; (b) **1b**; (c) **1c**; (d) **1d**; (e) **1e**; (f) **1f**; (g) **1g**; (h) **1h**; (i) **1i**; (j) **1j**; (k) **1k**; (l) **1l**; (m) **1m**; (n) **1n**; (o) **1o**.

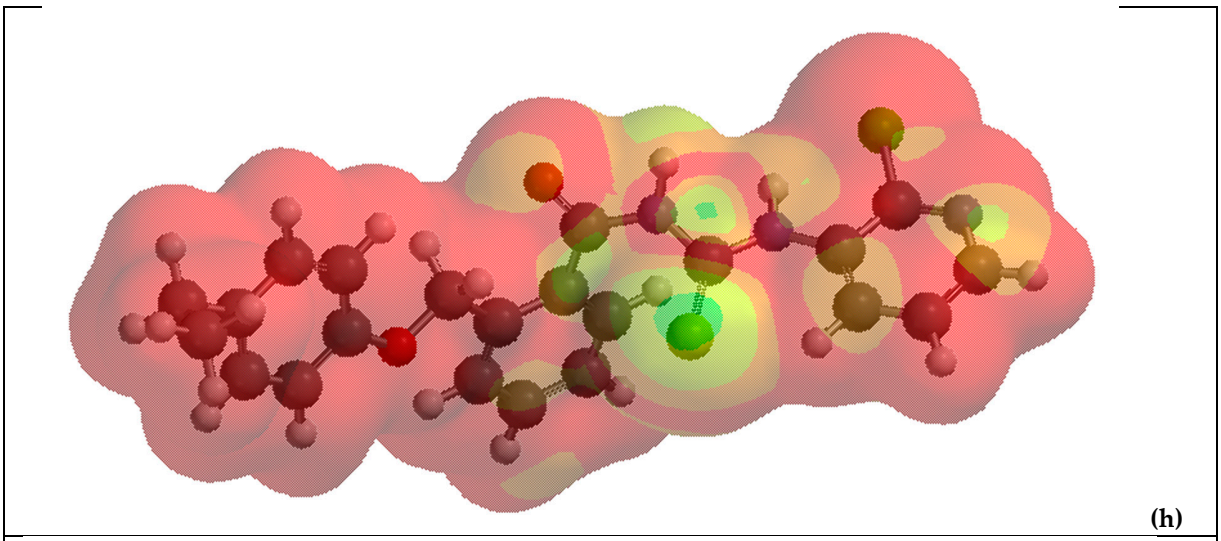
By convention, the numbering of the atoms has been done in accordance with Spartan 14 software.



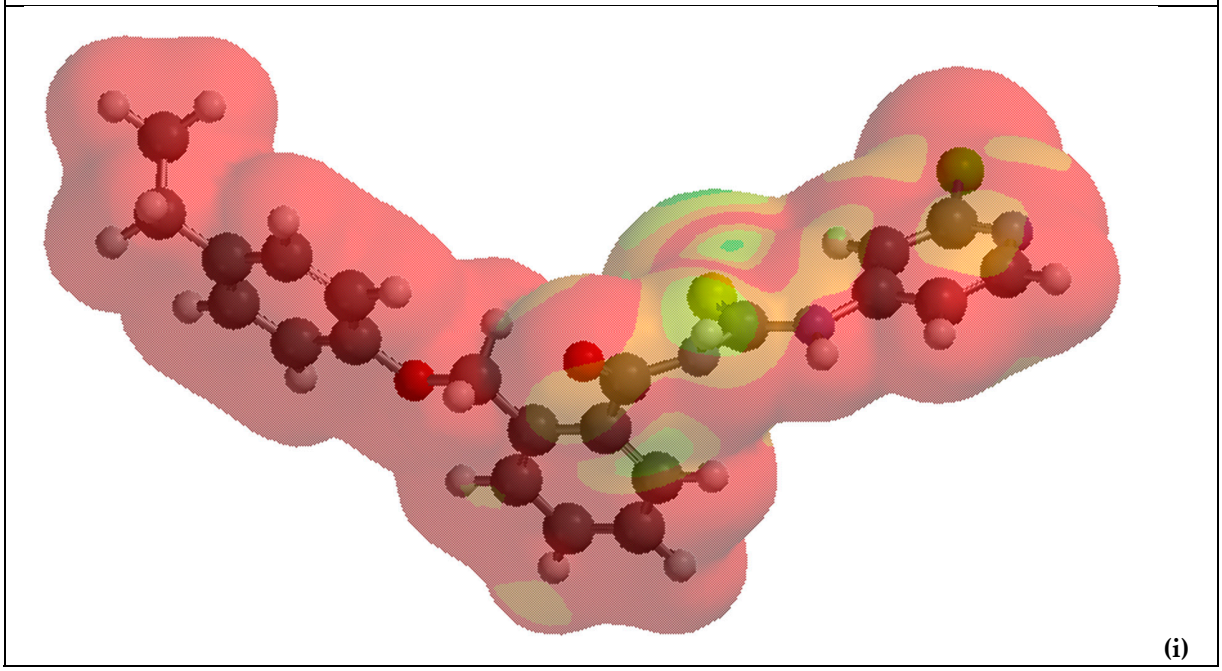

(b)
(c)


(d)
(e)

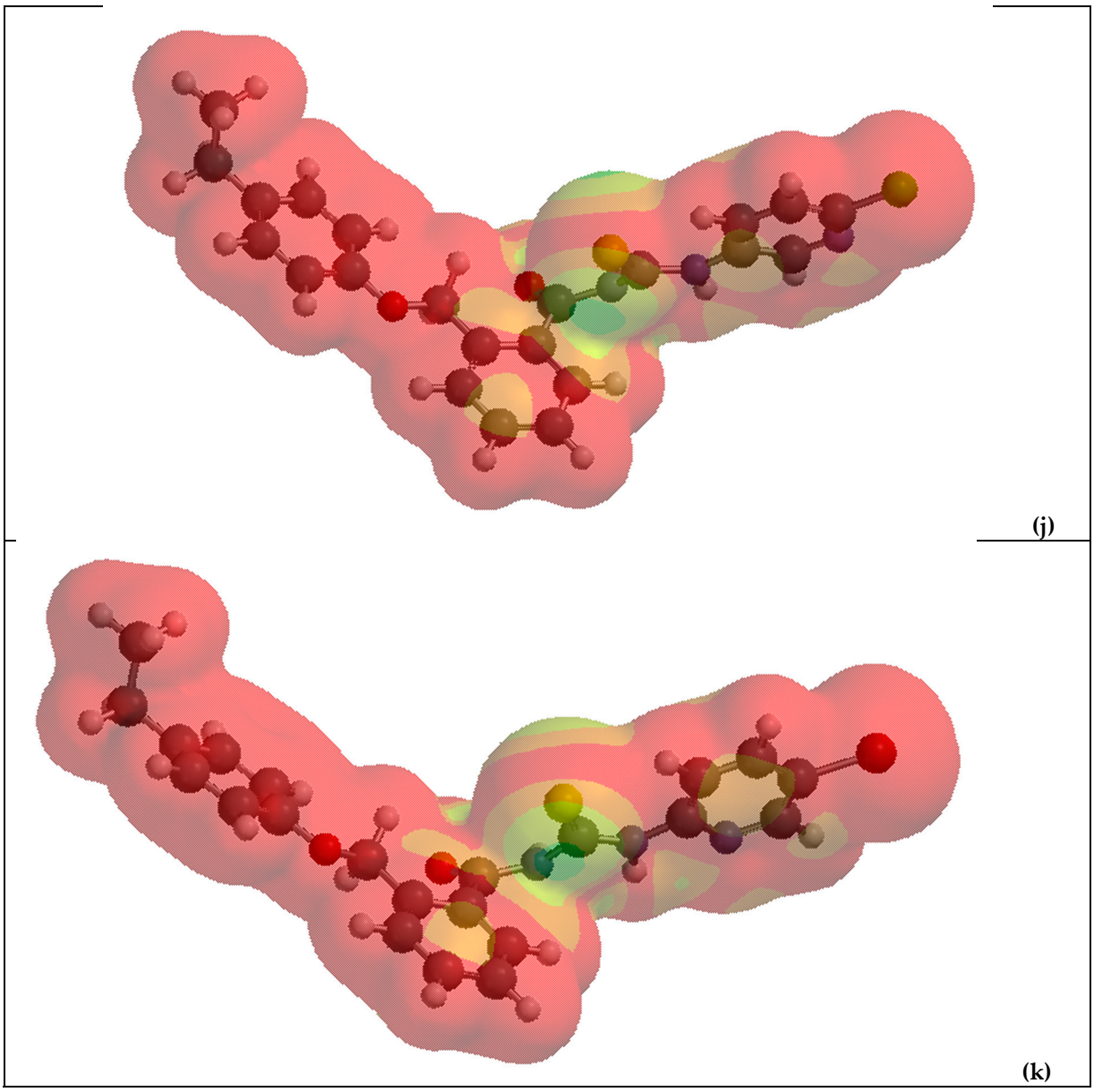

(f)
(g)



(h)

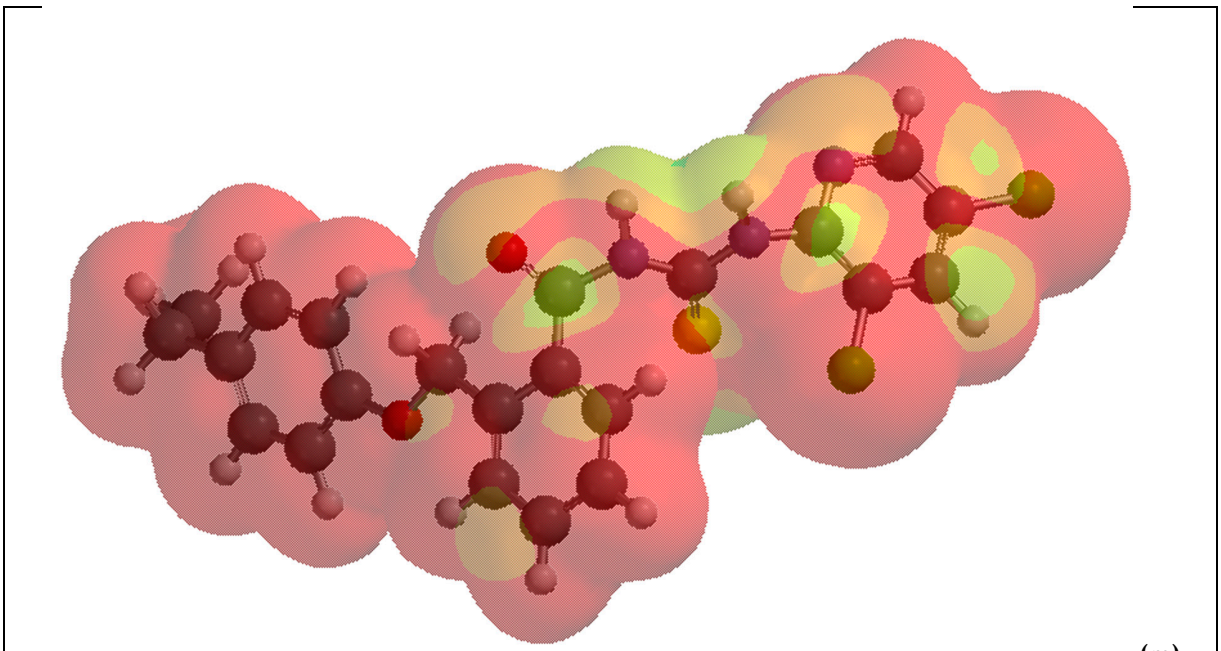


(i)

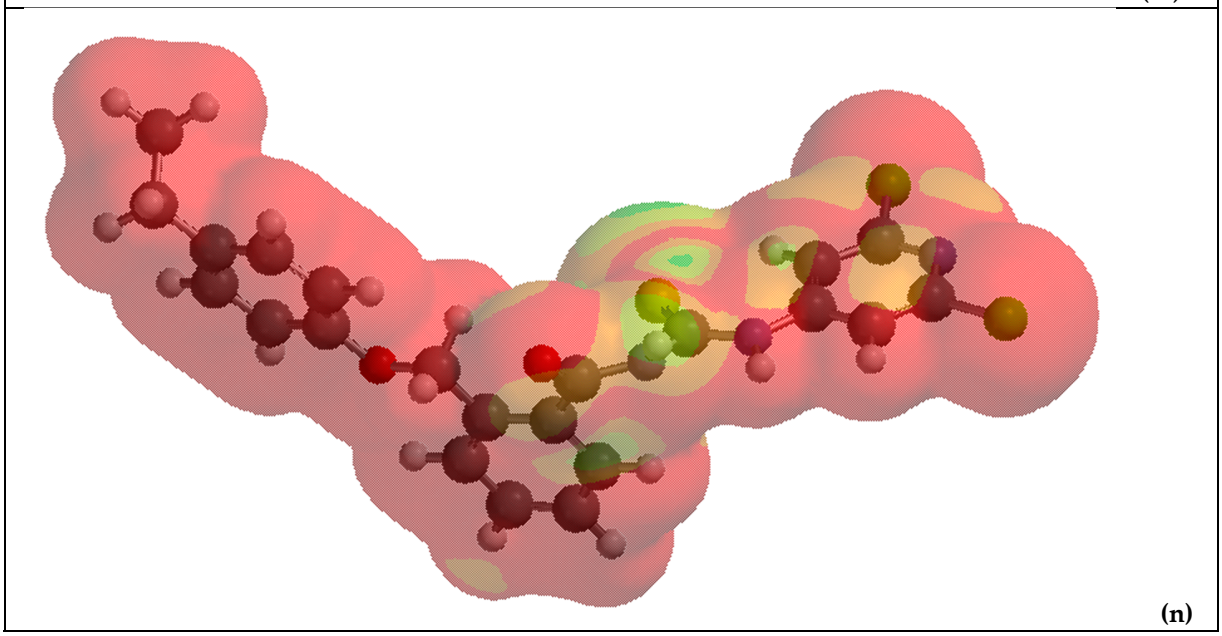


(j)

(k)



(m)



(n)

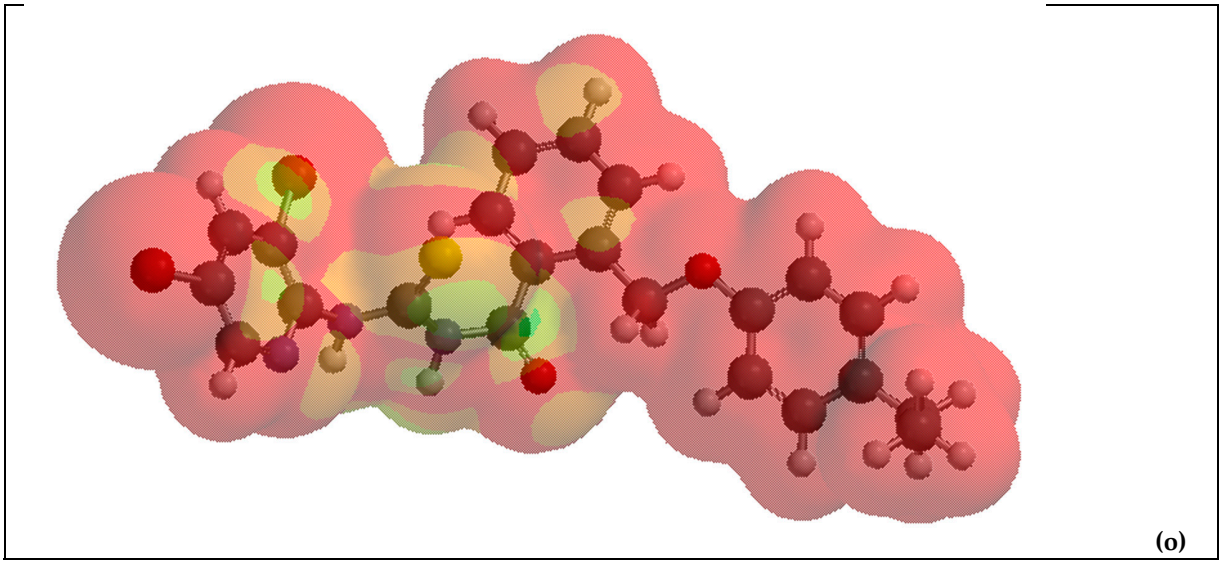
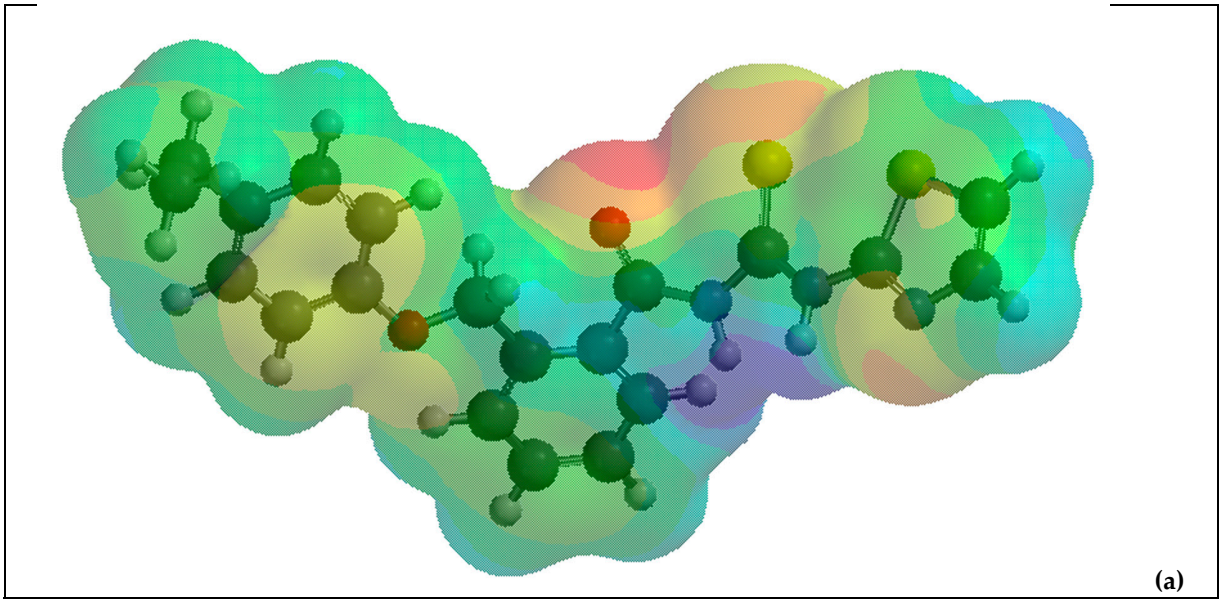
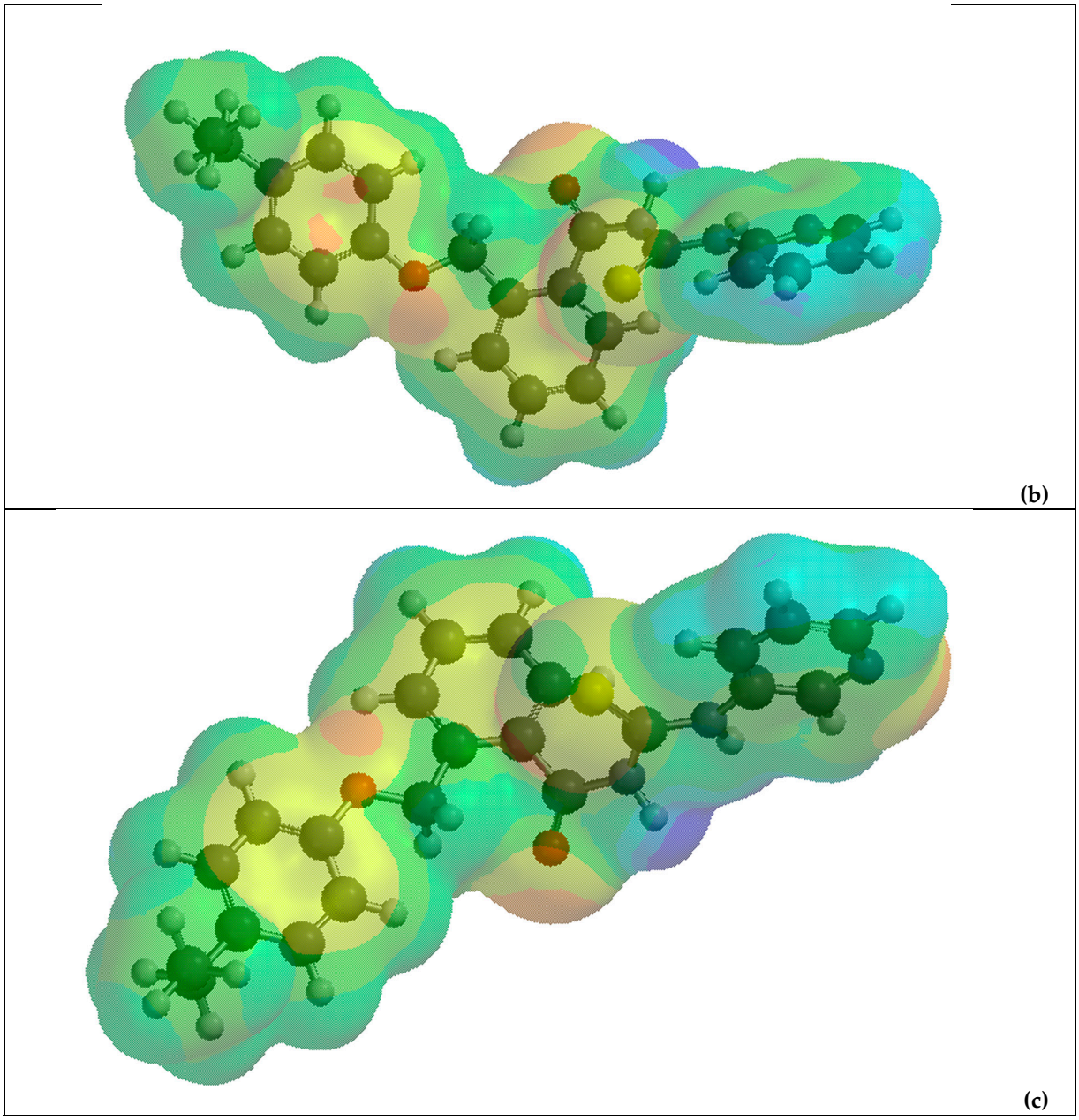
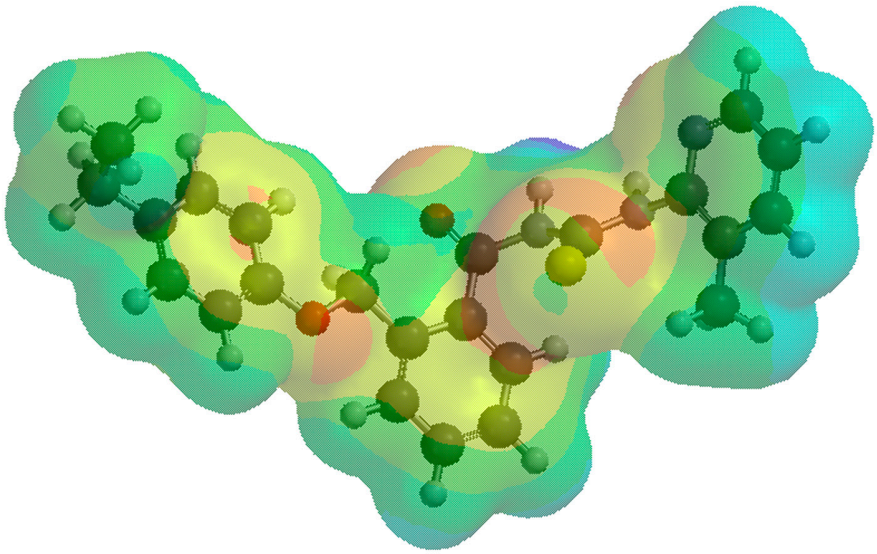


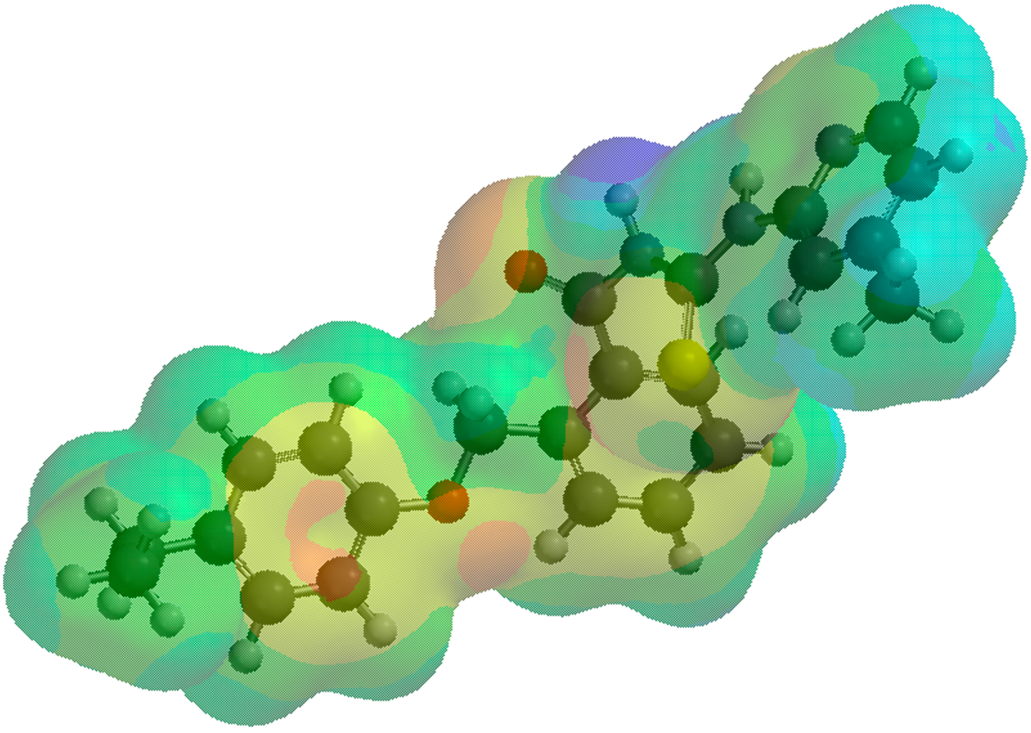
Figure S3. |LUMO| map for the compounds (a) **1a**; (b) **1b**; (c) **1c**; (d) **1d**; (e) **1e**; (f) **1f**; (g) **1g**; (h) **1h**; (i) **1i**; (j) **1j**; (k) **1k**; (l) **1l**; (m) **1m**; (n) **1n;** (o) **1o**. The red colour or colours toward red represents the minimum value of the LUMO (absolute values near zero), and the blue colour is used for indicating the maximum absolute values.



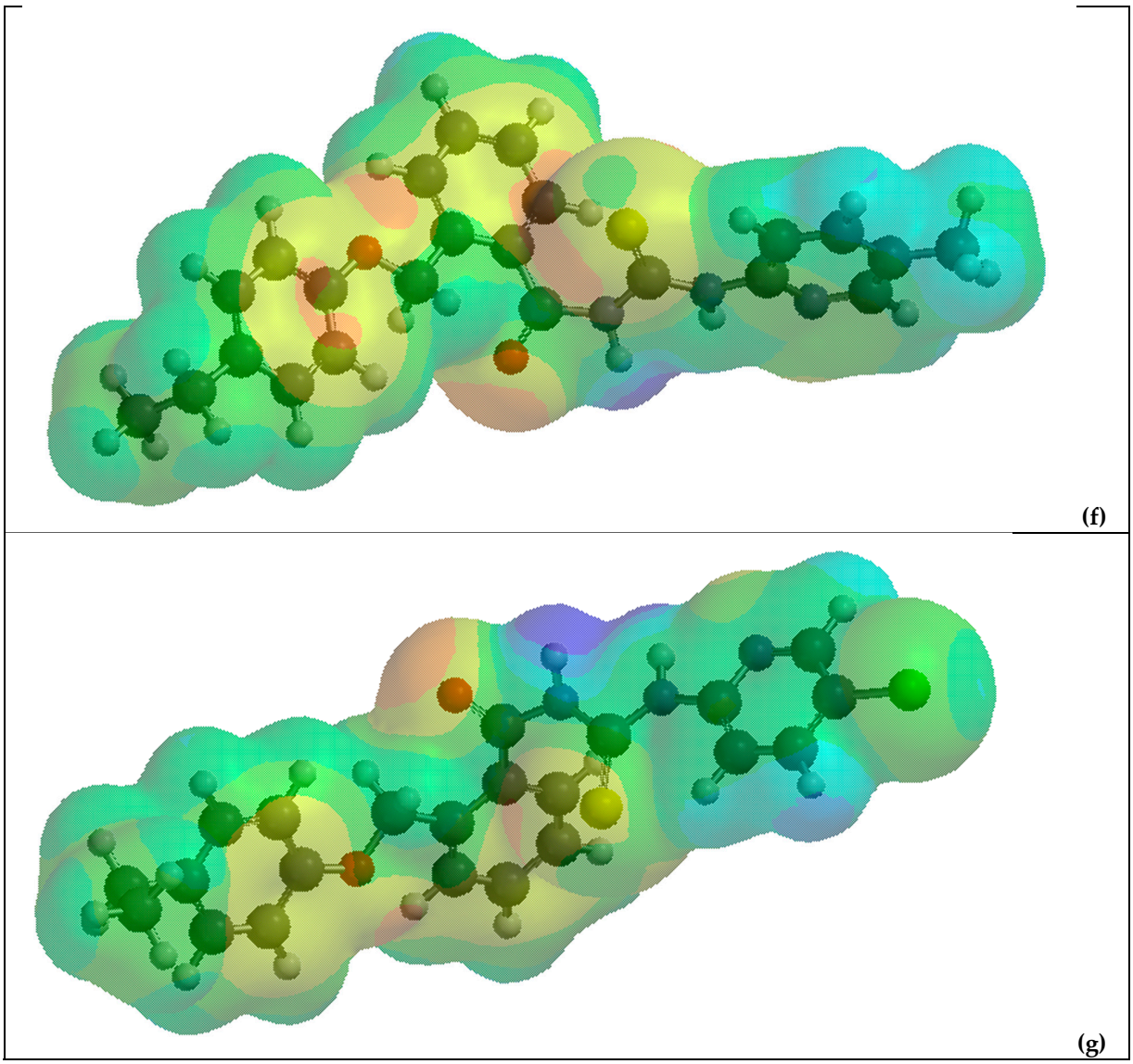

(b)
(c)

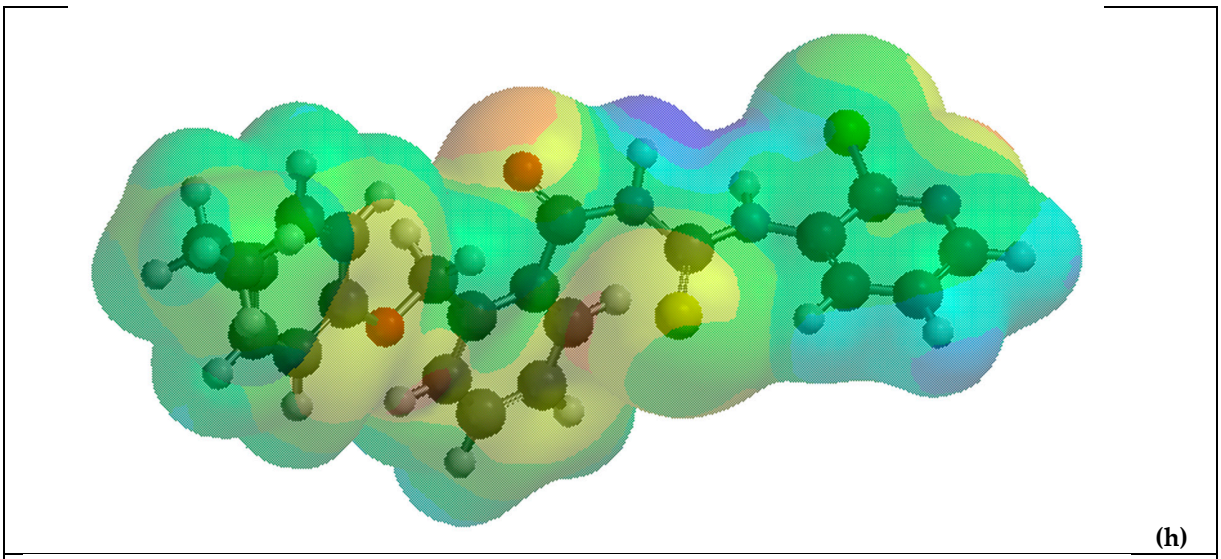


(d)

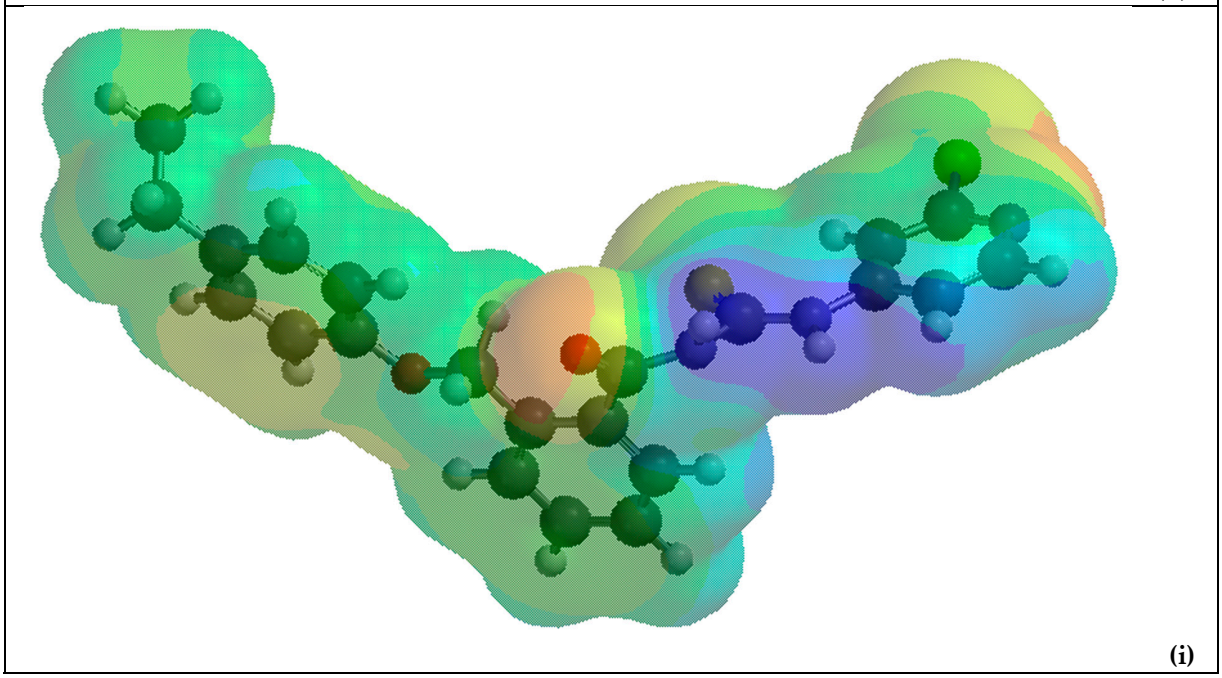


(e)

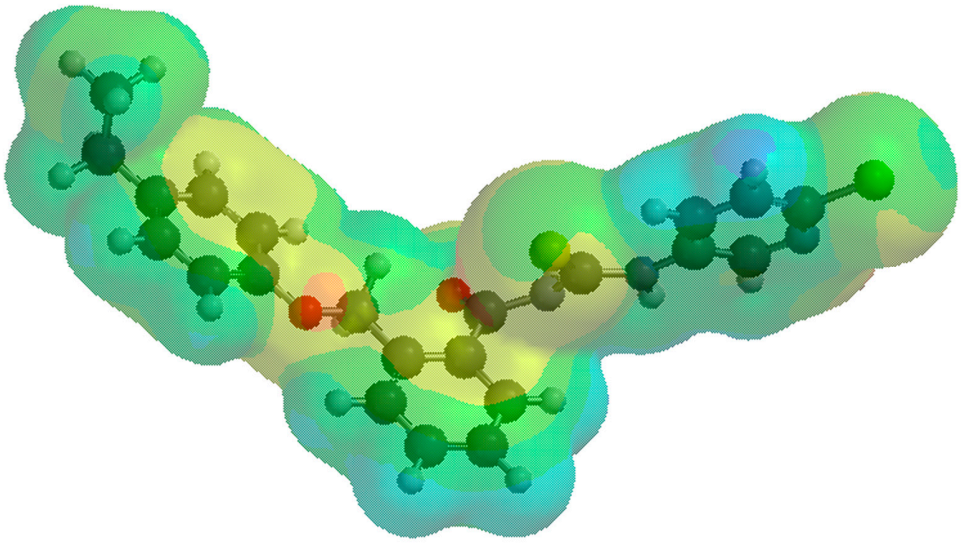

(f)
(g)



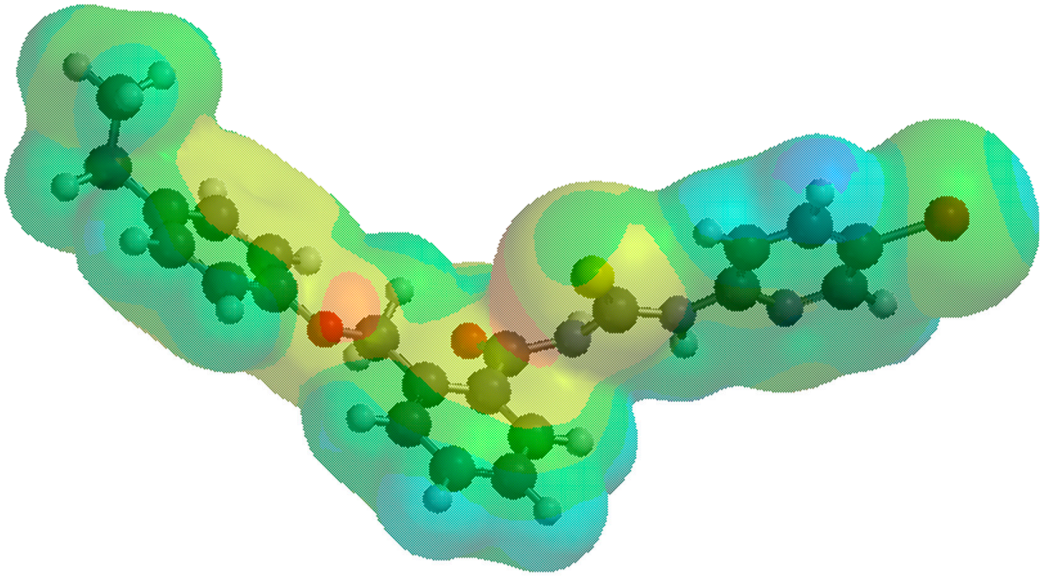
(h)



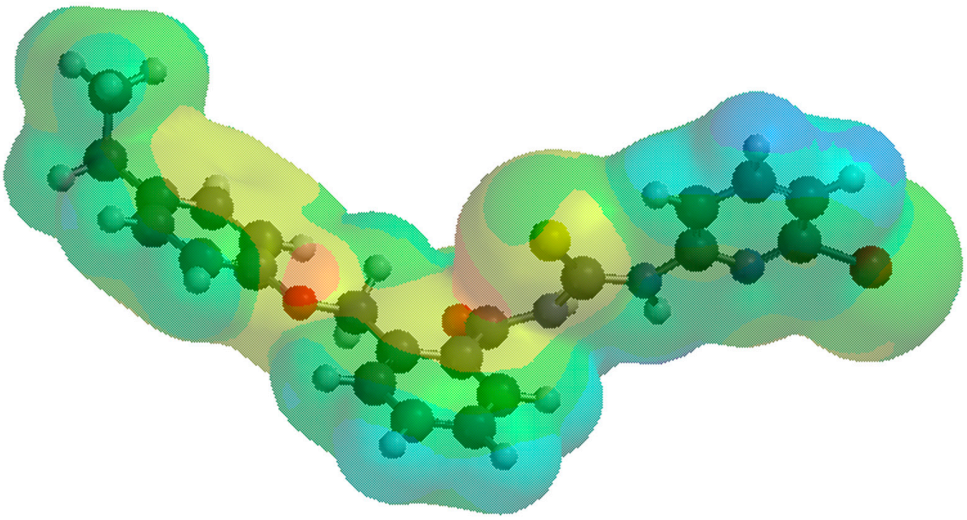
(i)



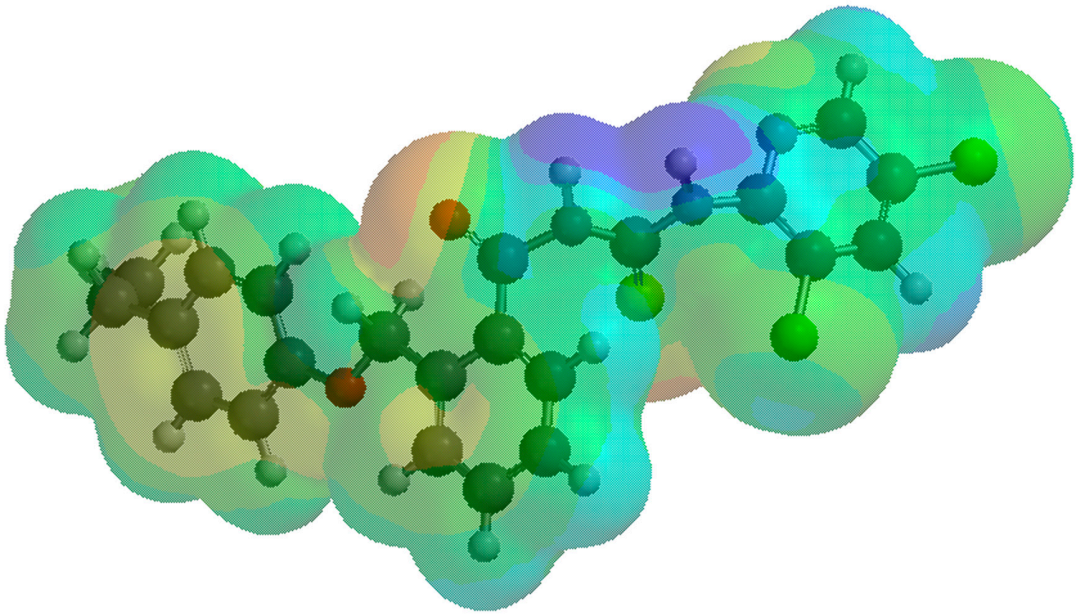
(j)



(k)



(l)



(m)

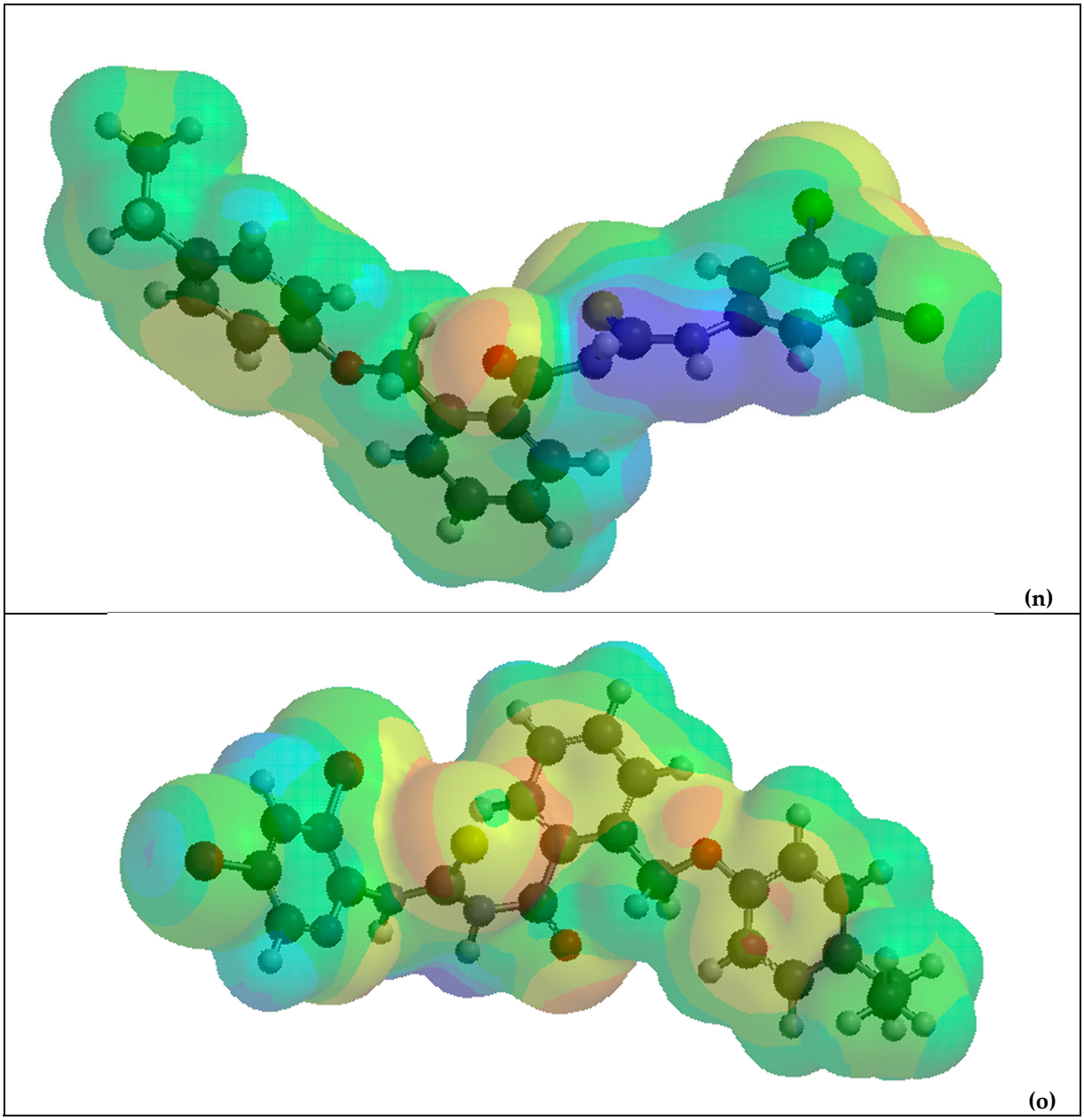
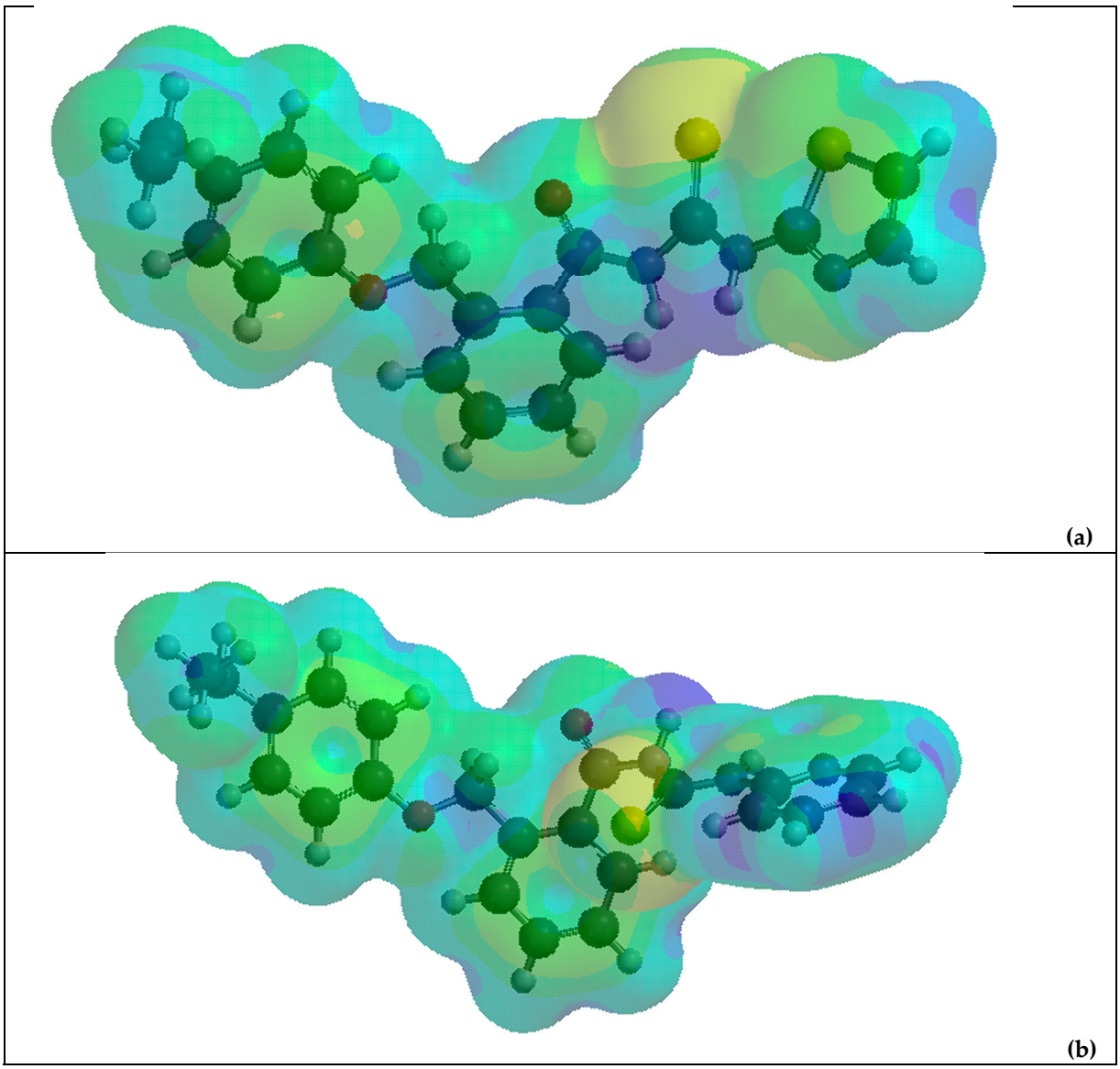
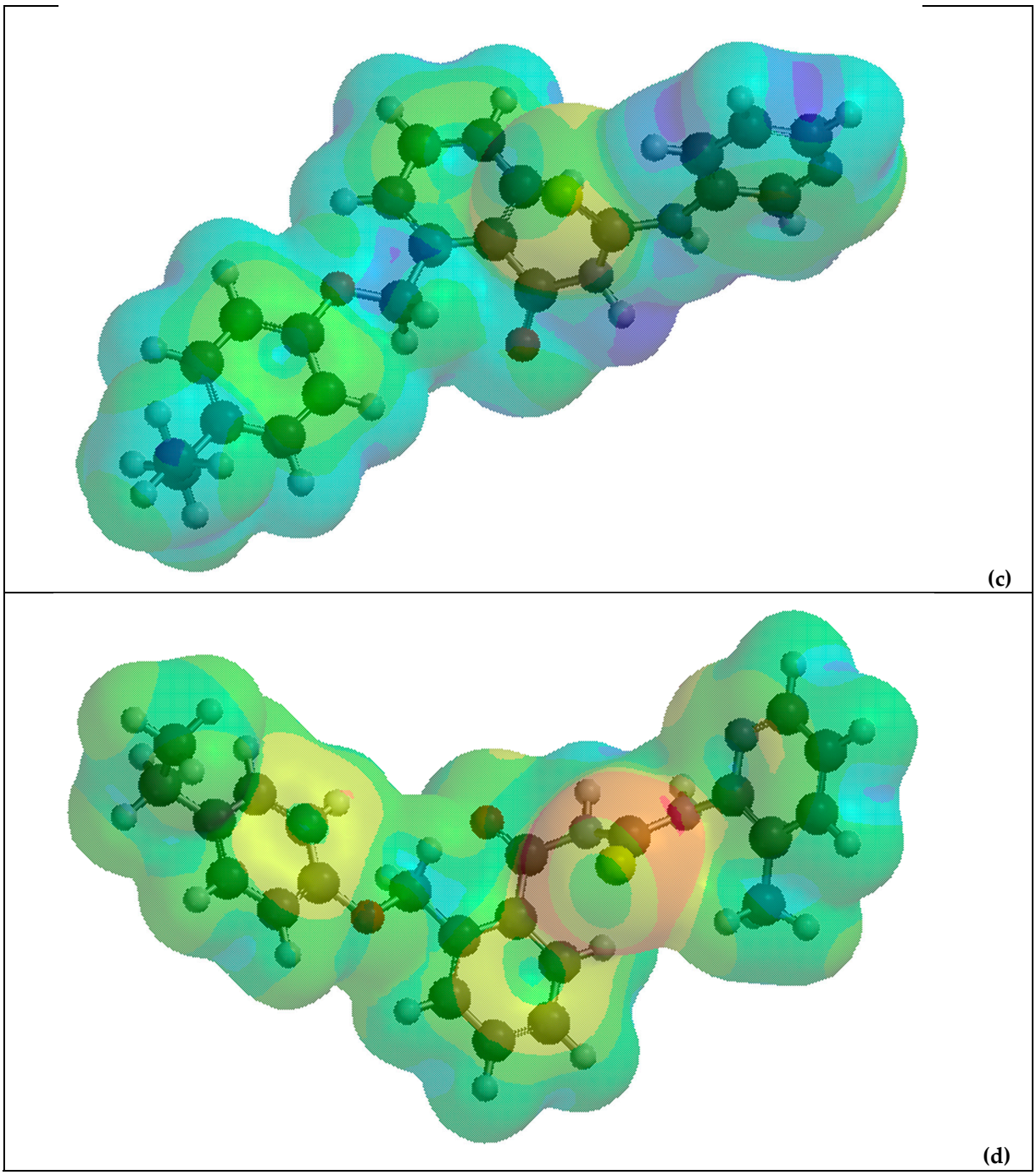
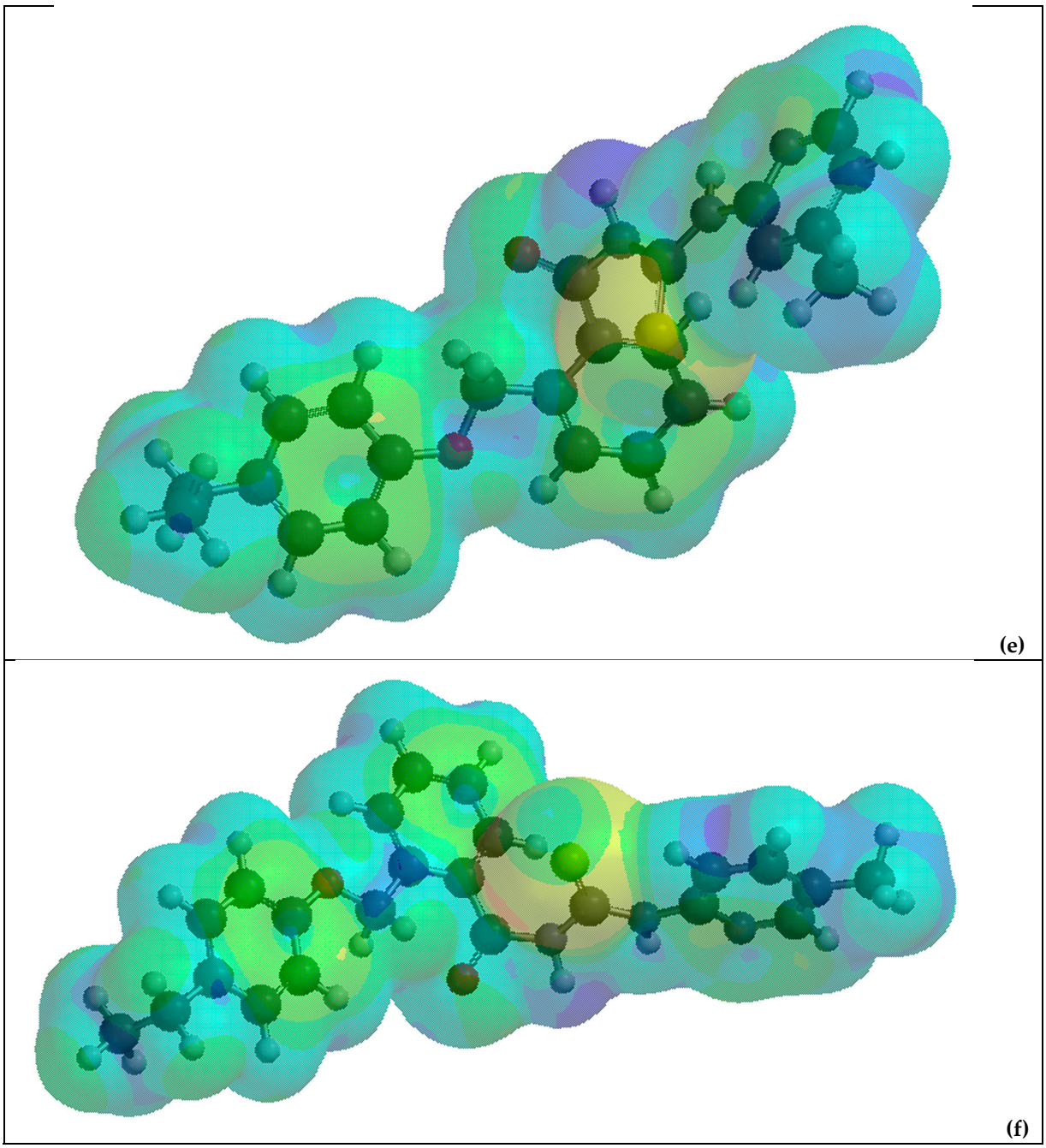
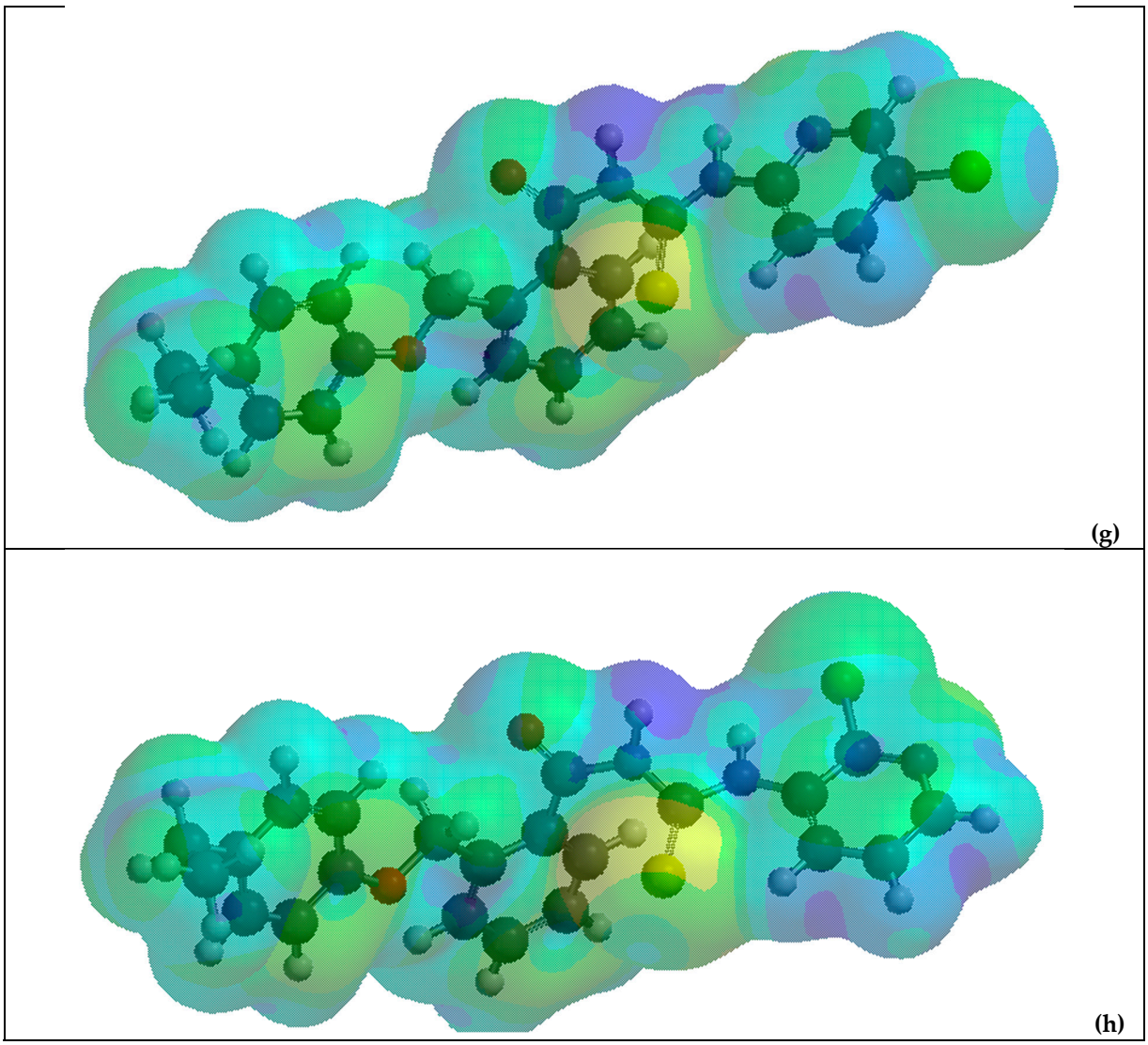


Figure S4. Molecular electrostatic potential map (on the electronic density) for the compounds (a) **1a**; (b) **1b**; (c) **1c**; (d) **1d**; (e) **1e**; (f) **1f**; (g) **1g**; (h) **1h**; (i) **1i**; (j) **1j**; (k) **1k**; (l) **1l**; (m) **1m**; (n) **1n**; (o) **1o**. Red colour or colours toward red mark the negative potential. On the other hand, colours toward blue indicate the positive potential.


(a)
(b)

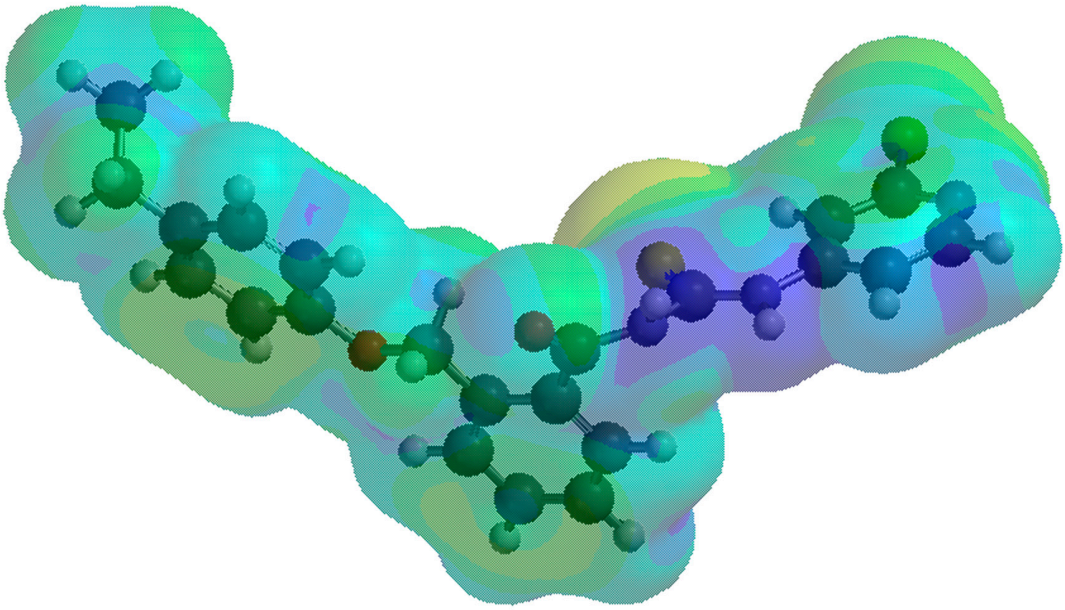

(c)
(d)


(e)
(f)

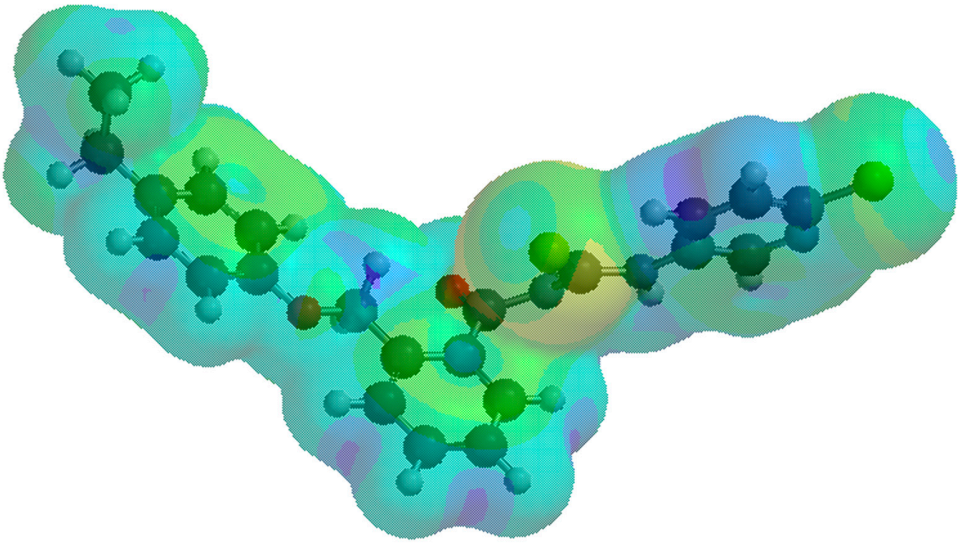


(g)

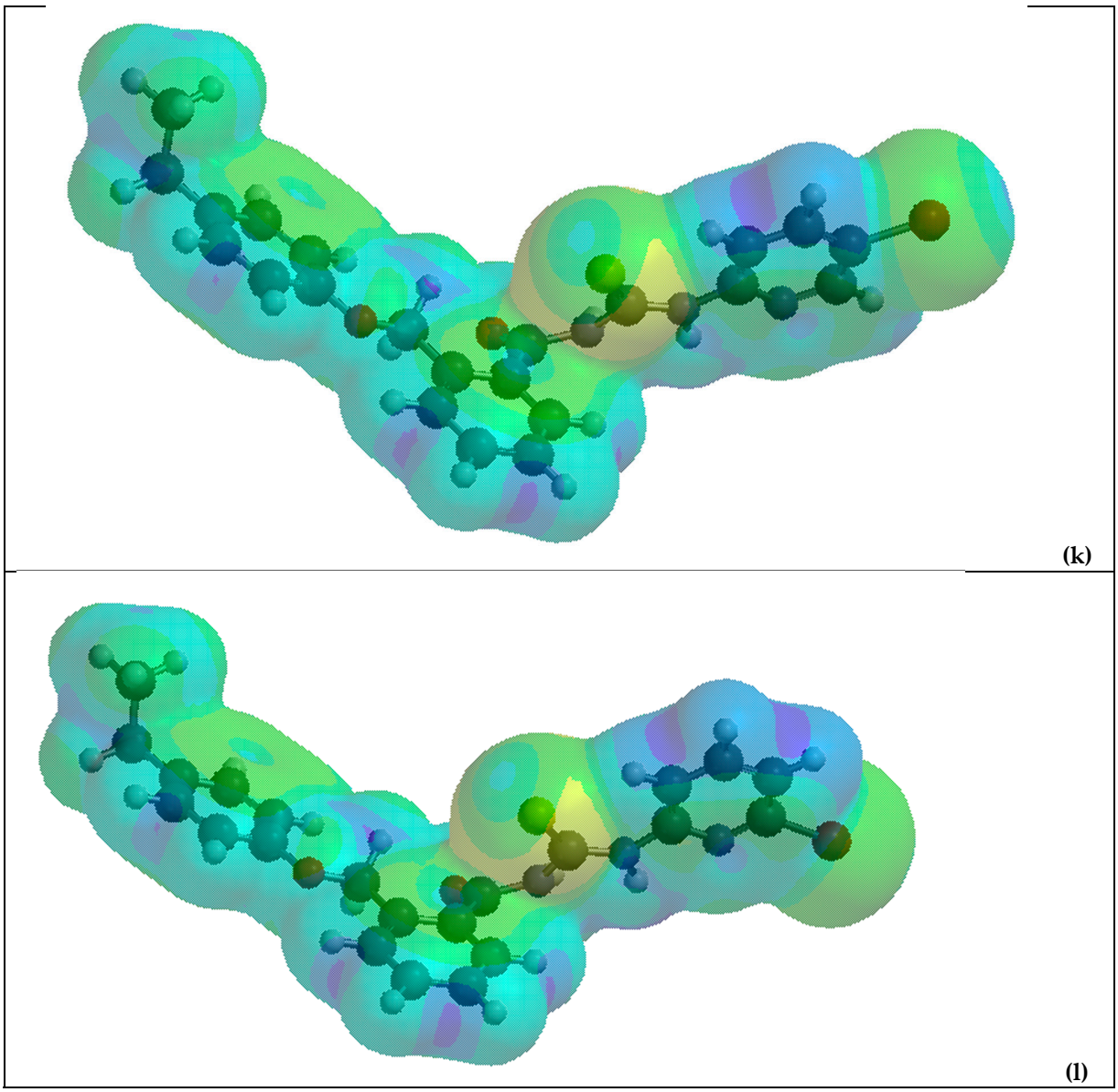
(h)

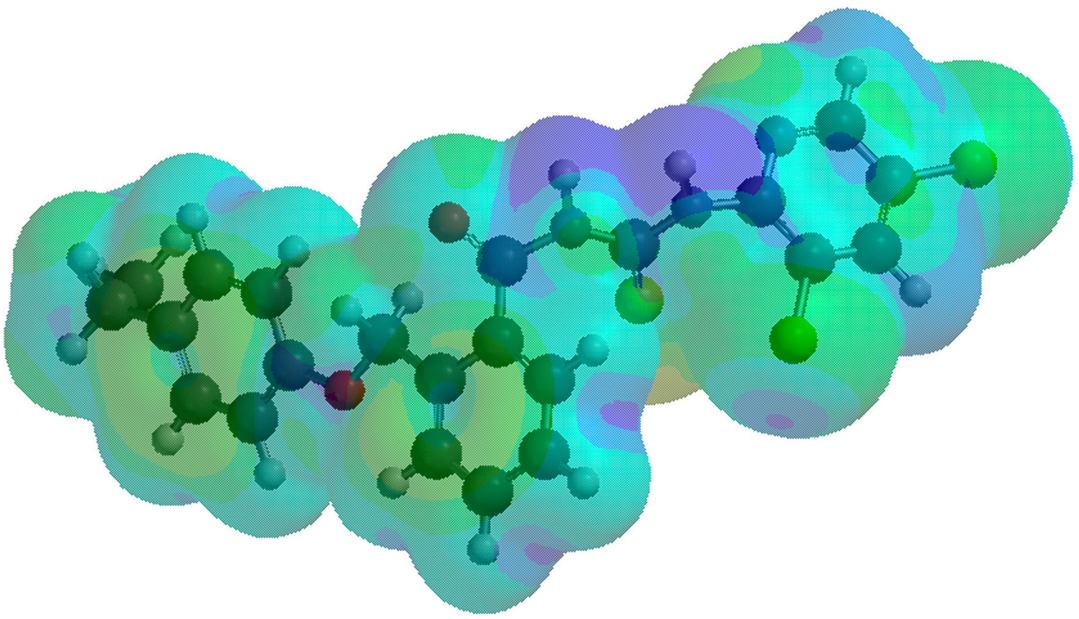


(i)

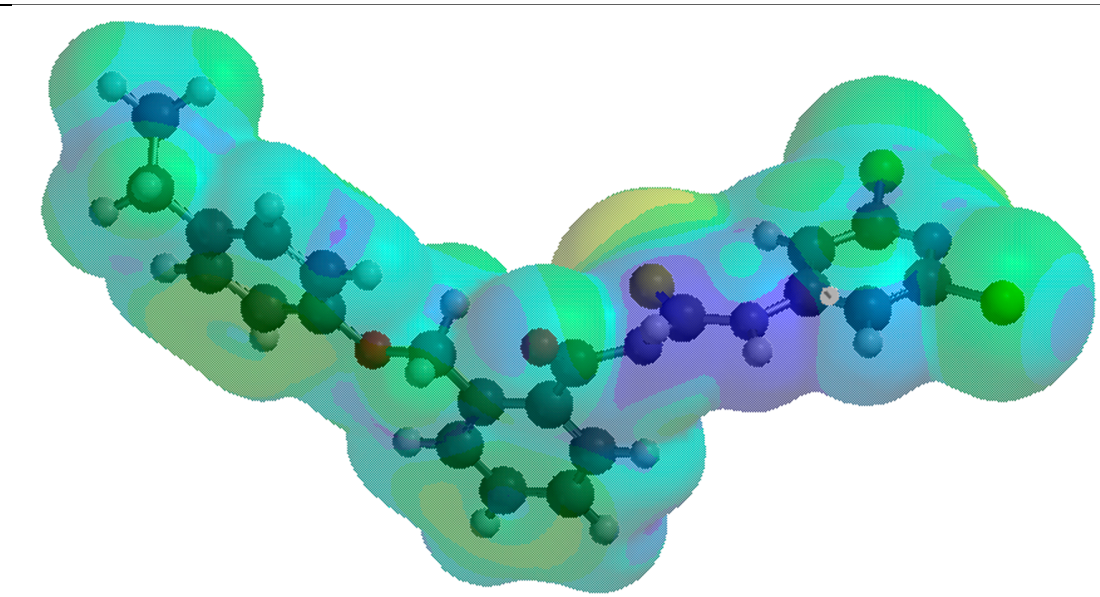


(j)


(k)
(l)



(m)



(n)

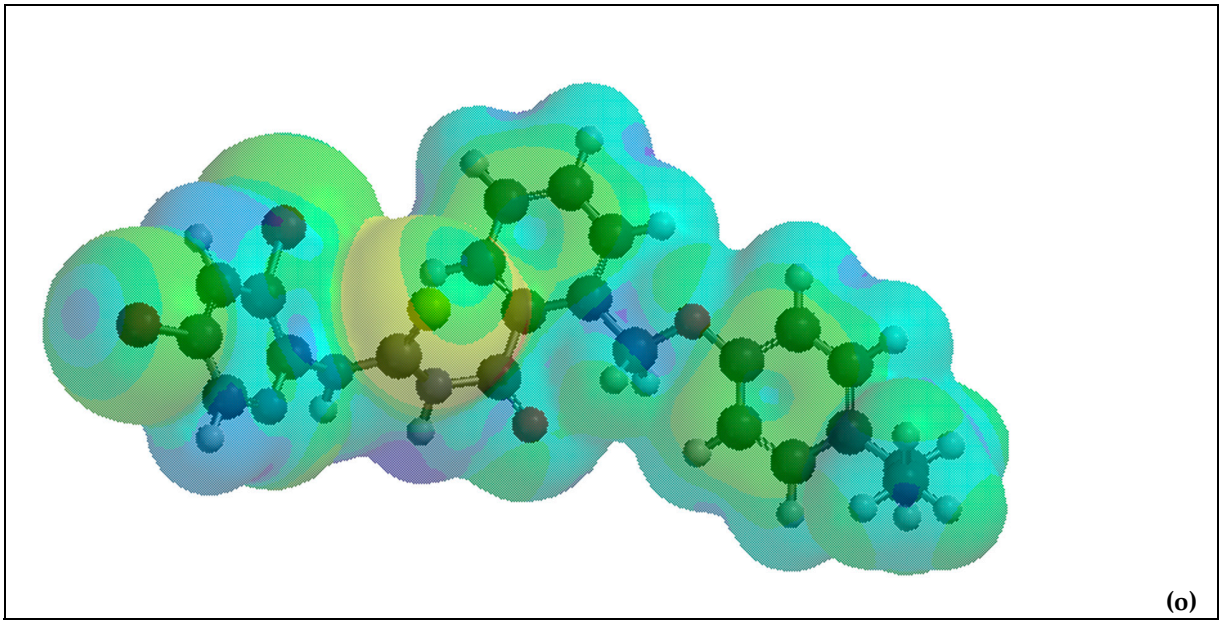


Figure S5. Local ionization potential map for the compounds (a) **1a**; (b) **1b**; (c) **1c**; (d) **1d**; (e) **1e**; (f) **1f**; (g) **1g**; (h) **1h**; (i) **1i**; (j) **1j**; (k) **1k**; (l) **1l**; (m) **1m**; (n) **1n**; (o) **1o**. The regions in blue indicate the areas where the ionization is tough. In other words, red regions indicate low ionization potential, while blue regions mark high ionization potential.

Docking outcome correlated with co-crystallized compounds

Figures S6 – S35 are graphic representations of intermolecular interactions between the ligand molecules docked with 2XCS (*S. aureus* DNA gyrase B, chain F) using CLC Drug Discovery Workbench Software

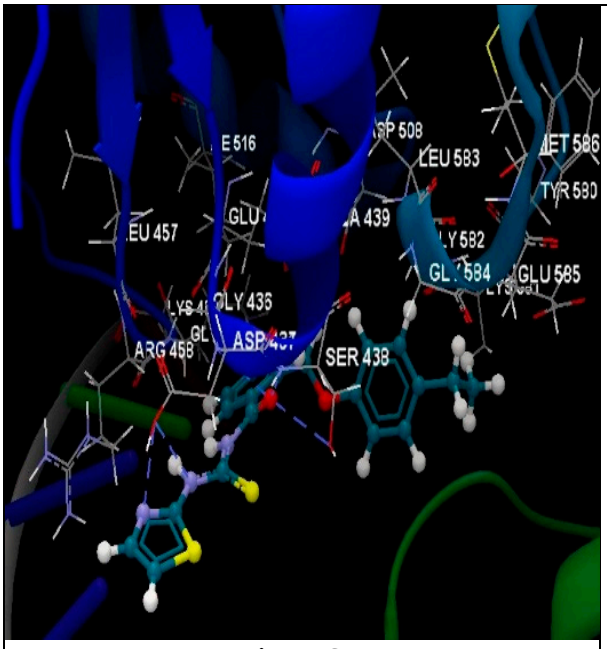


Figure S6.
The interaction group for the ligand **1a.**

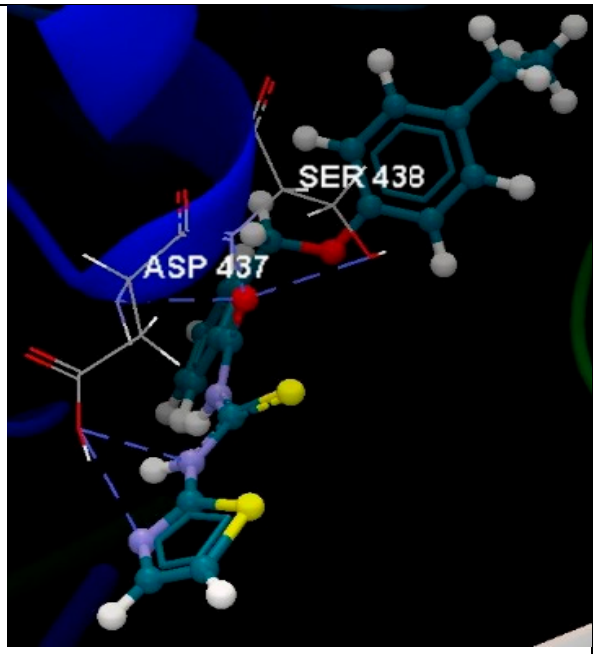


Figure S7. Hydrogen bounds created between the ligand **1a** and amino acids: ASP 437, SER 438.

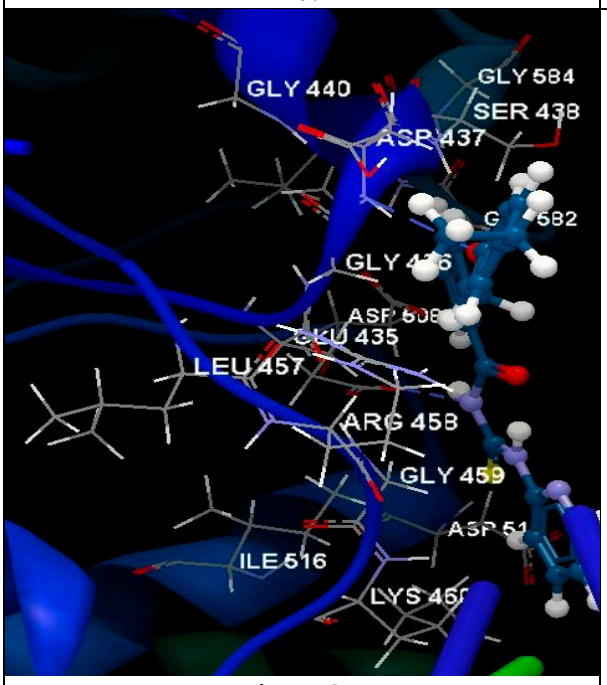


Figure S8.
The interaction group for the ligand **1b.**

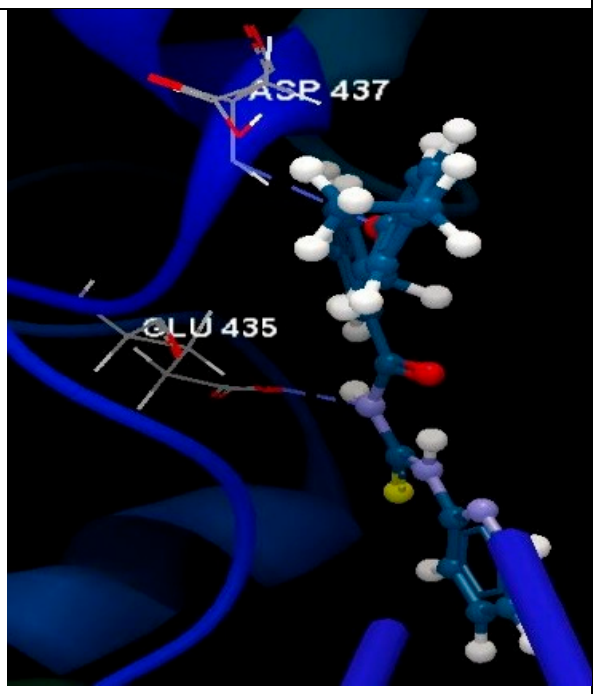


Figure S9. Hydrogen bounds created between the ligand **1b** and amino acids: ASP 437, GLU 435.

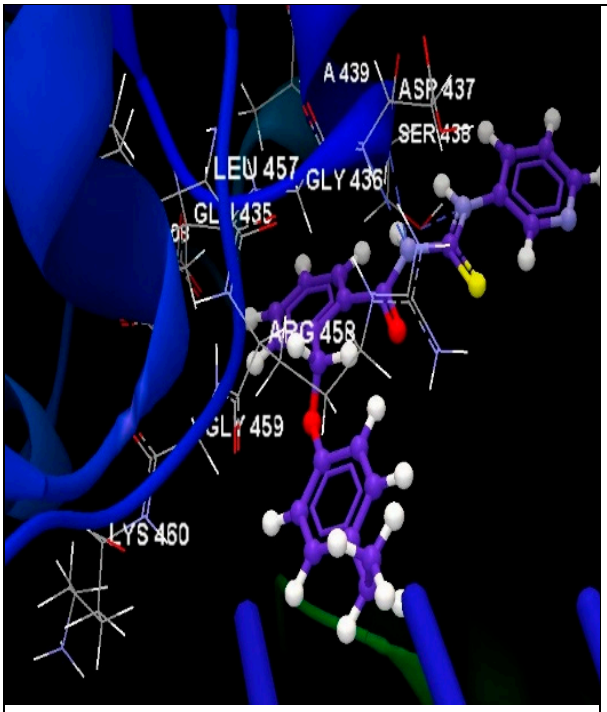


Figure S10.
The interaction group for the ligand **1c.**

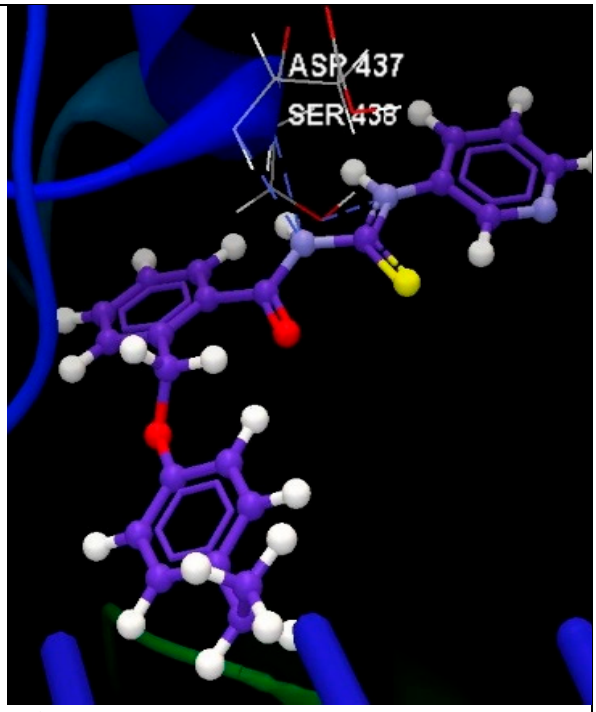


Figure S11. Hydrogen bounds created between the ligand **1c** and amino acids: ASP 437, SER 438.

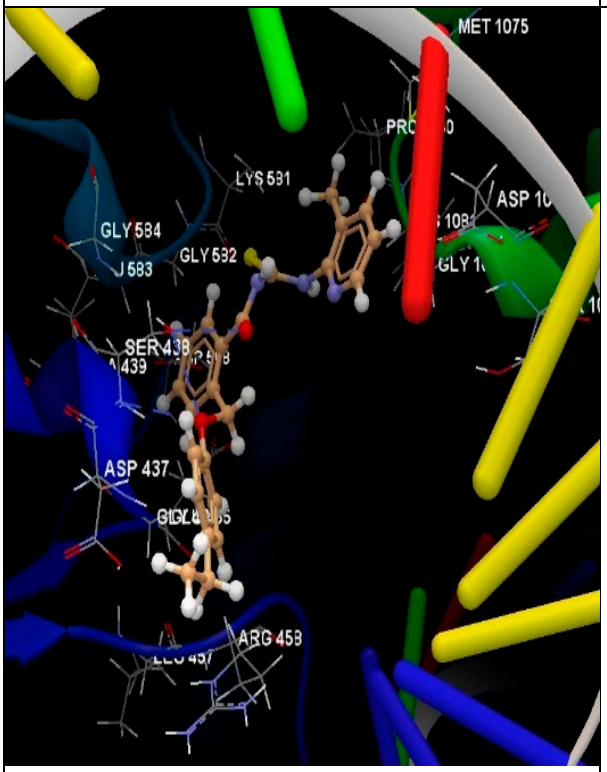


Figure S12.
The interaction group for the ligand **1d.**

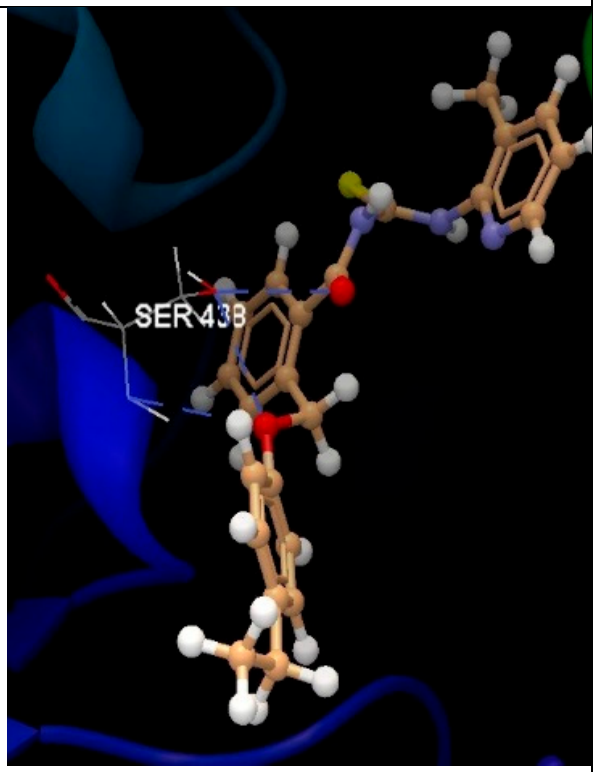


Figure S13. Hydrogen bounds created between the ligand **1d** and amino acid: SER 438.

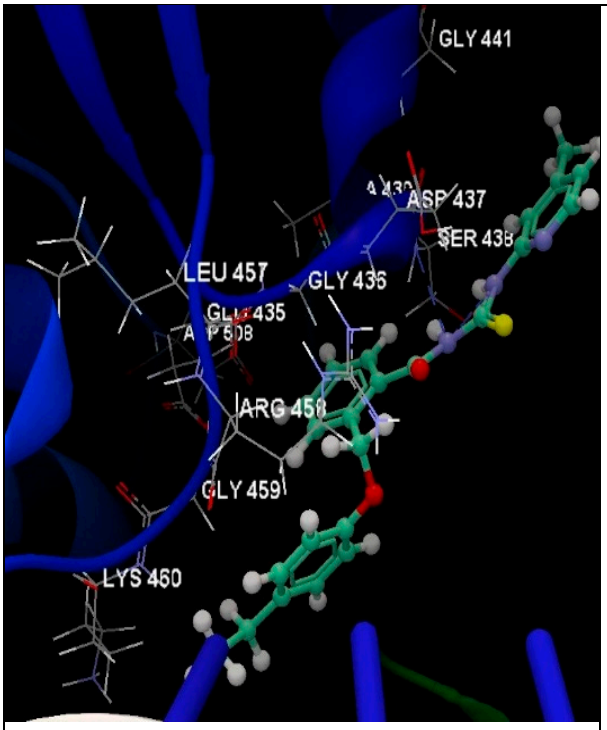


Figure S14.
The interaction group for the ligand **1e.**

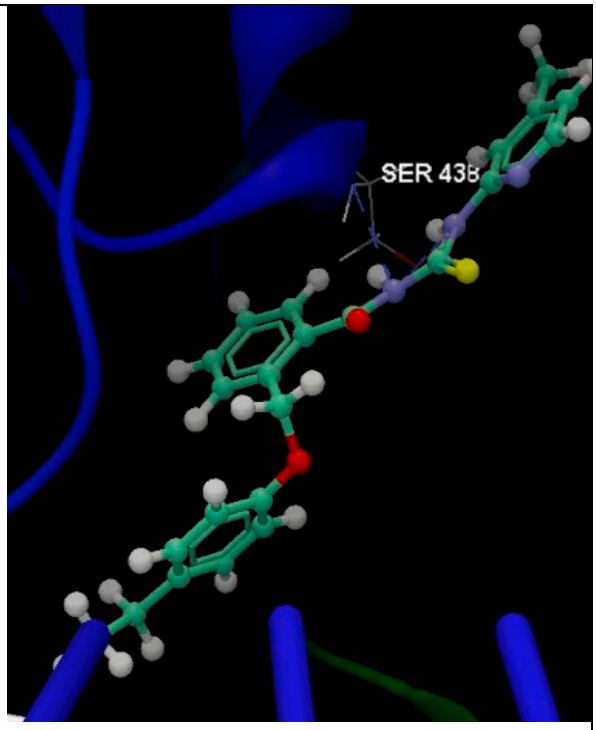


Figure S15. Hydrogen bounds created between the ligand **1e** and amino acid:
SER 438.

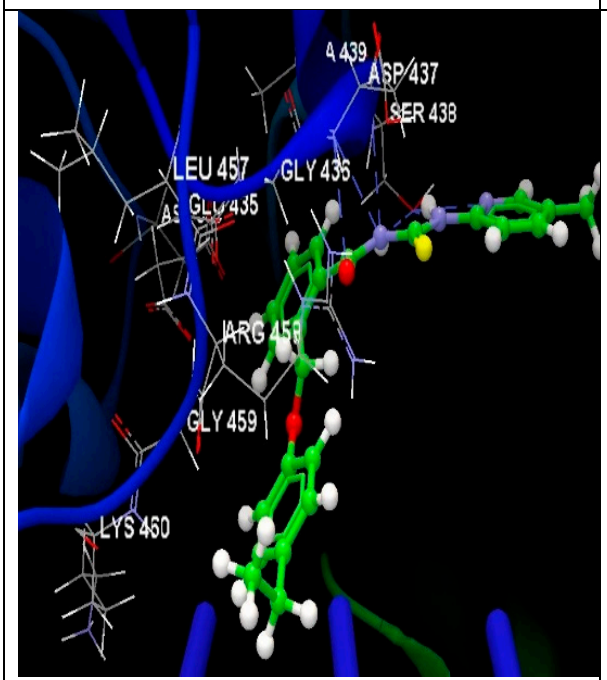


Figure S16.
The interaction group for the ligand **1f.**

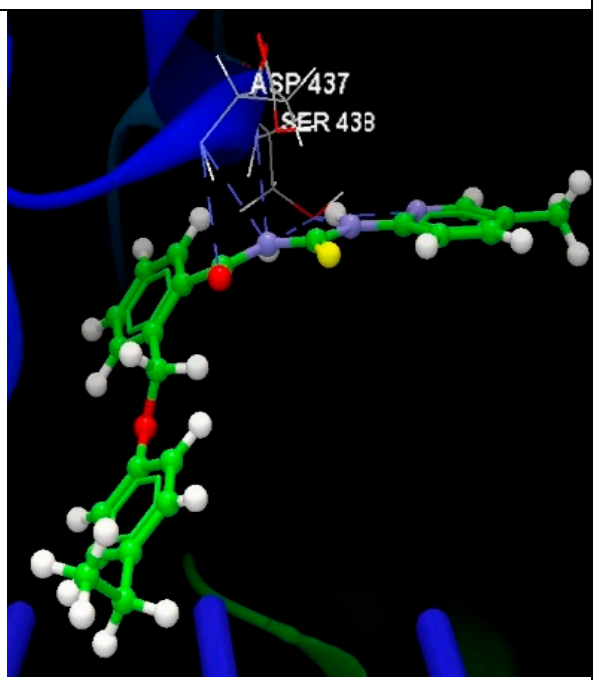


Figure S17. Hydrogen bounds created between the ligand **1f** and amino acids:
ASP 437, SER 438.

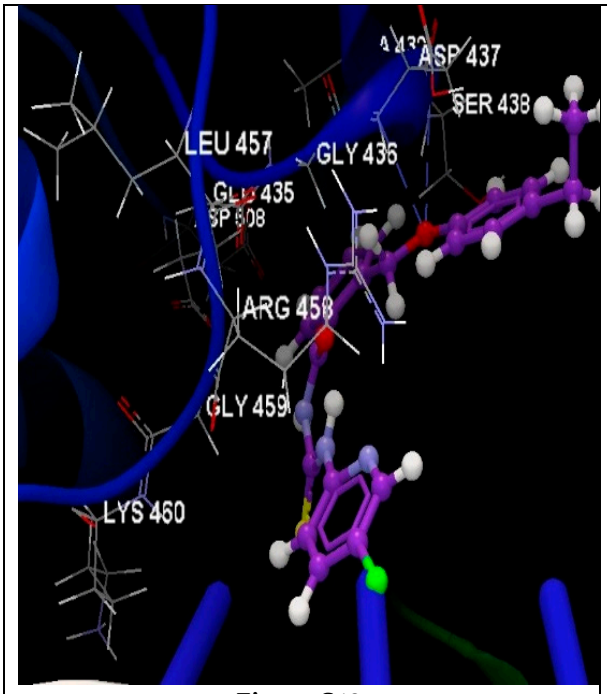


Figure S18.
The interaction group for the ligand **1g.**

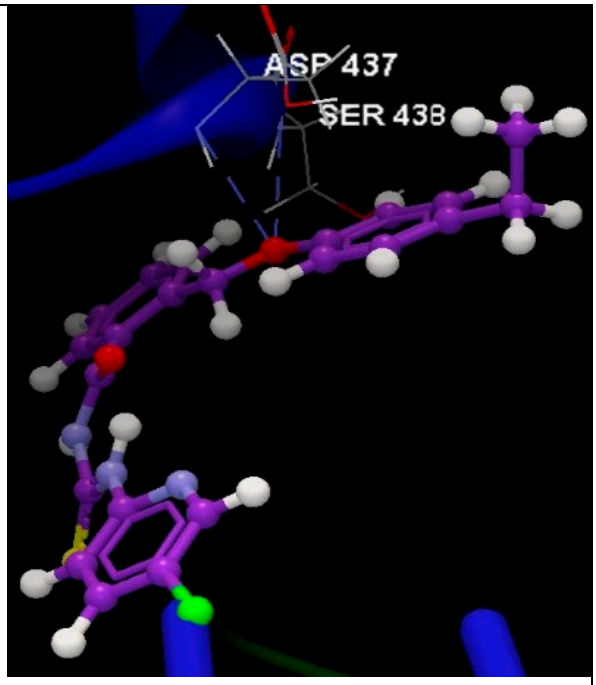


Figure S19. Hydrogen bounds created between the ligand **1g** and amino acids: ASP 437, SER 438.

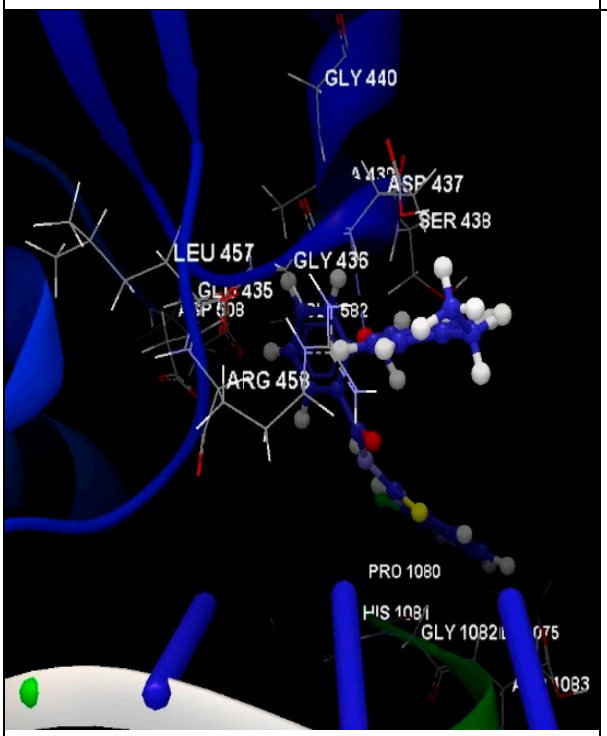


Figure S20.
The interaction group for the ligand **1h.**

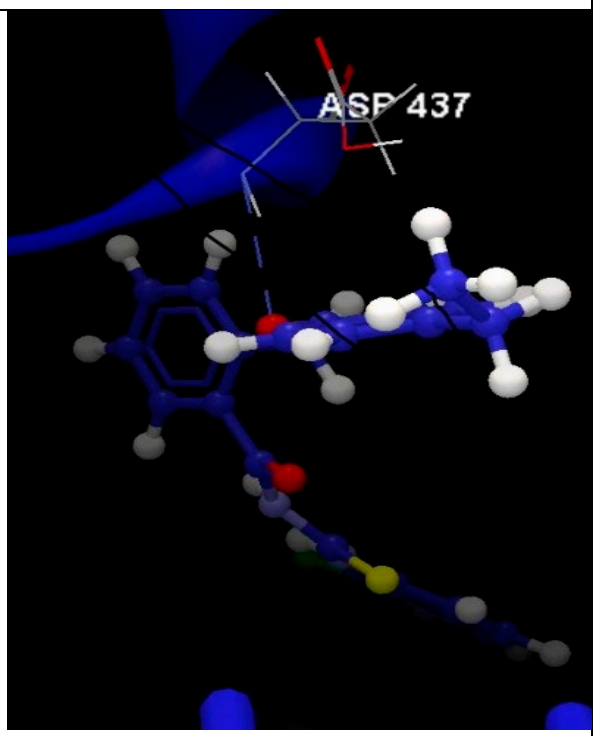


Figure S21. Hydrogen bounds created between the ligand **1h** and amino acid: ASP 437.

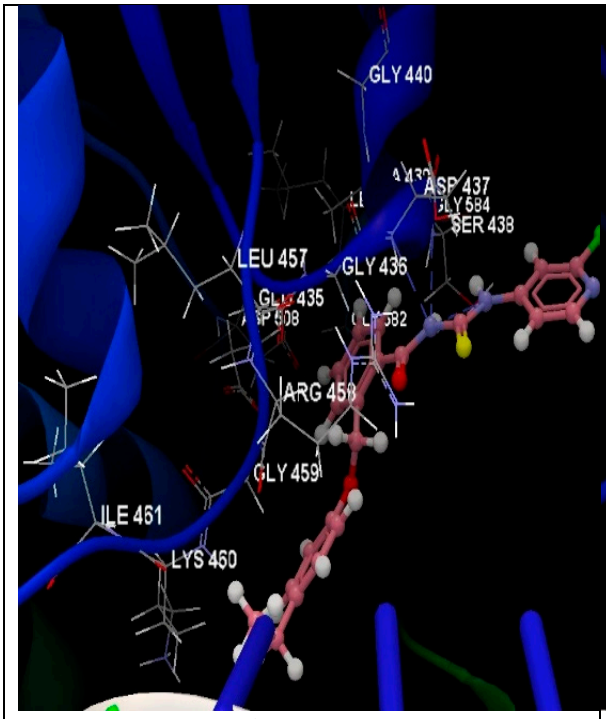


Figure S22.
The interaction group for the ligand **1i.**

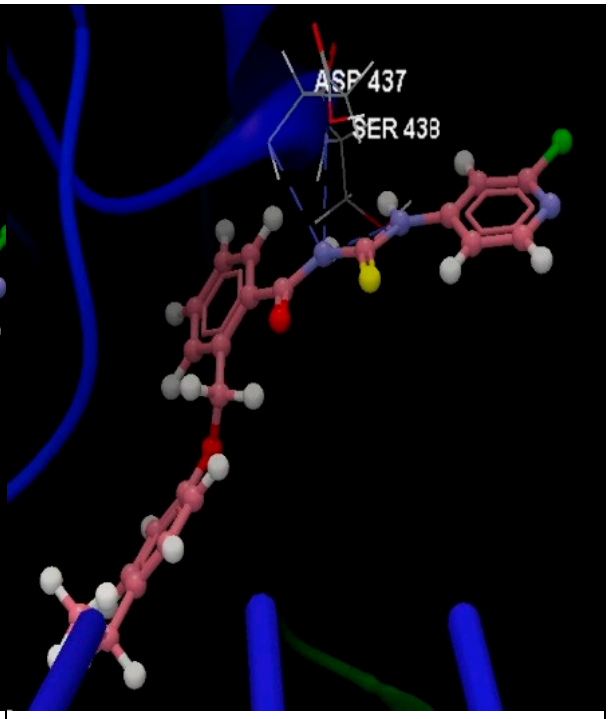


Figure S23. Hydrogen bounds created between the ligand **1i** and amino acids: ASP 437, SER 438.

Figure S24.
The interaction group for the ligand **1j.**

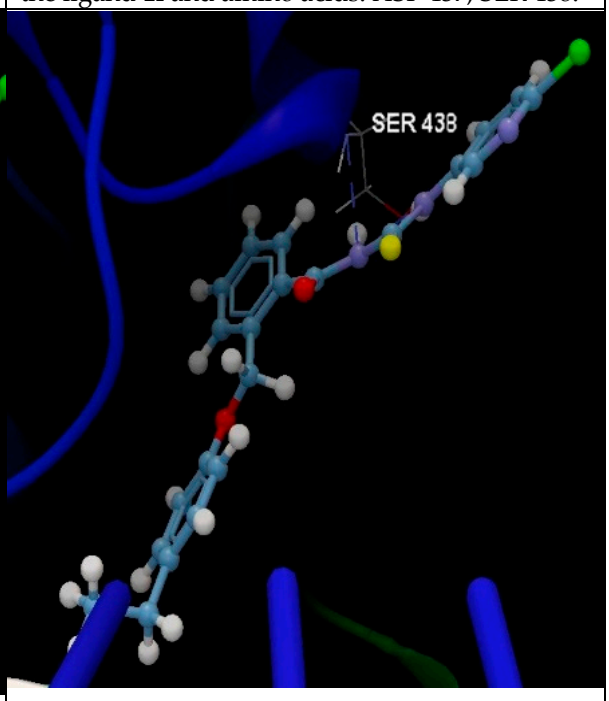


Figure S25. Hydrogen bounds created between the ligand **1j** and amino acid: SER 438.

Figure S26.
The interaction group for the ligand **1k.**

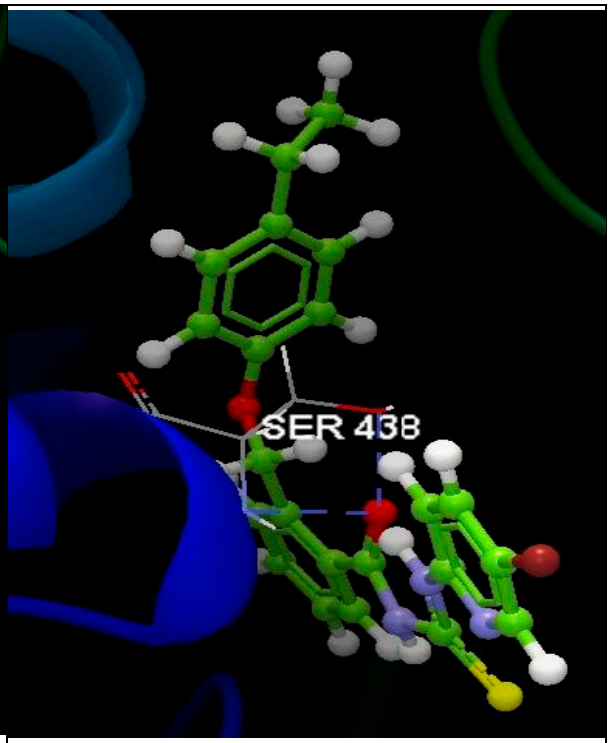


Figure S27. Hydrogen bounds created between the ligand **1k** and amino acid: SER 438.

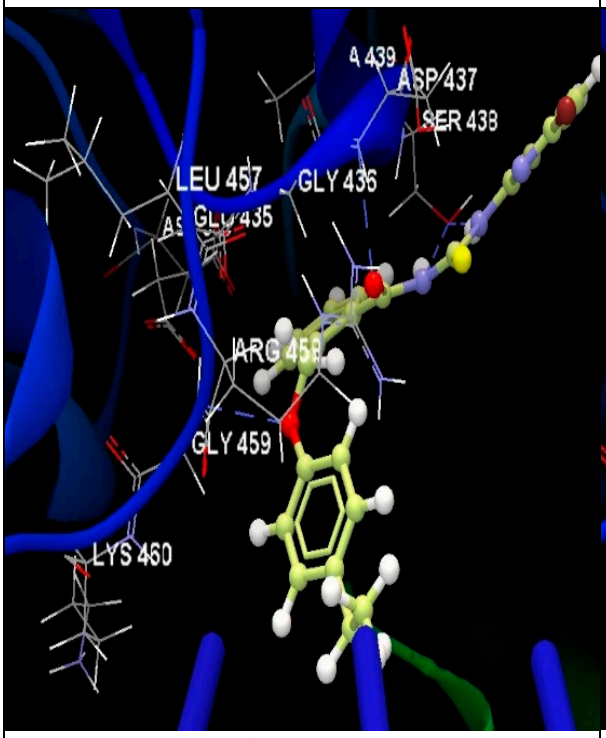


Figure S28.
The interaction group for the ligand **1l.**

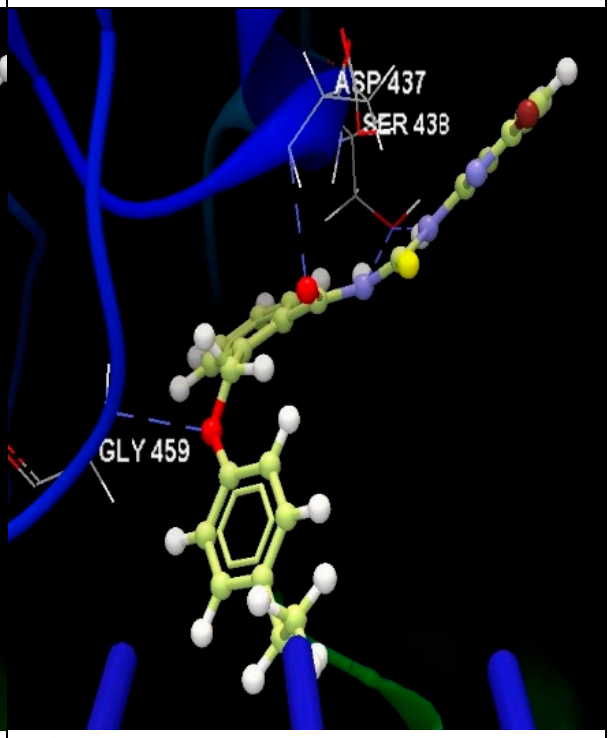


Figure S29. Hydrogen bounds created between the ligand **1l** and amino acids: ASP 437, SER 438, GLY 459.

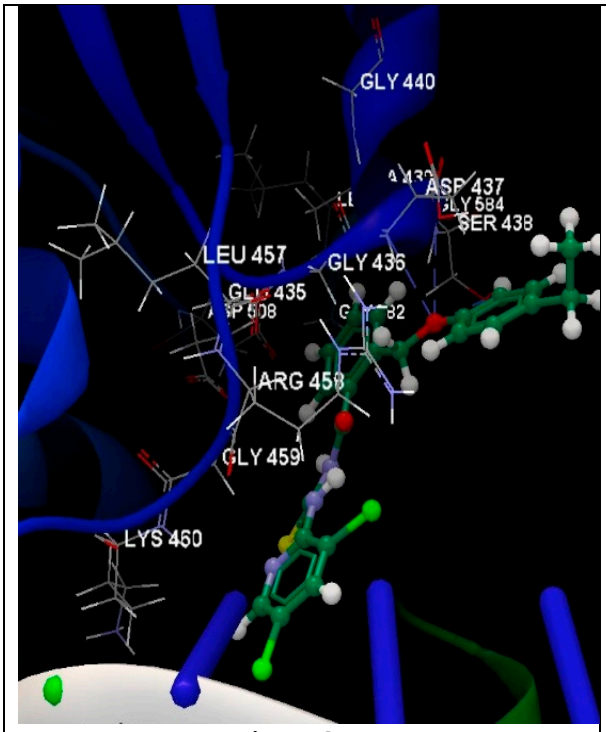


Figure S30.
The interaction group for the ligand **1m.**

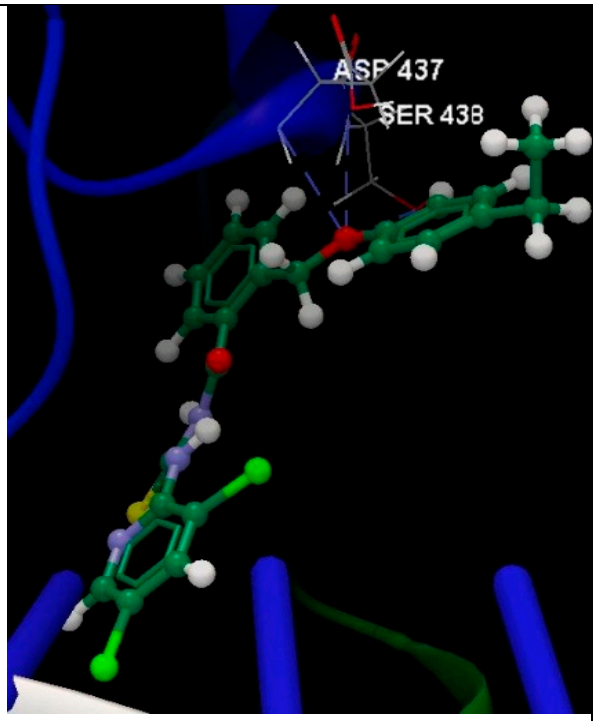


Figure S31. Hydrogen bounds created between the ligand **1m** and amino acids: ASP 437, SER 438.

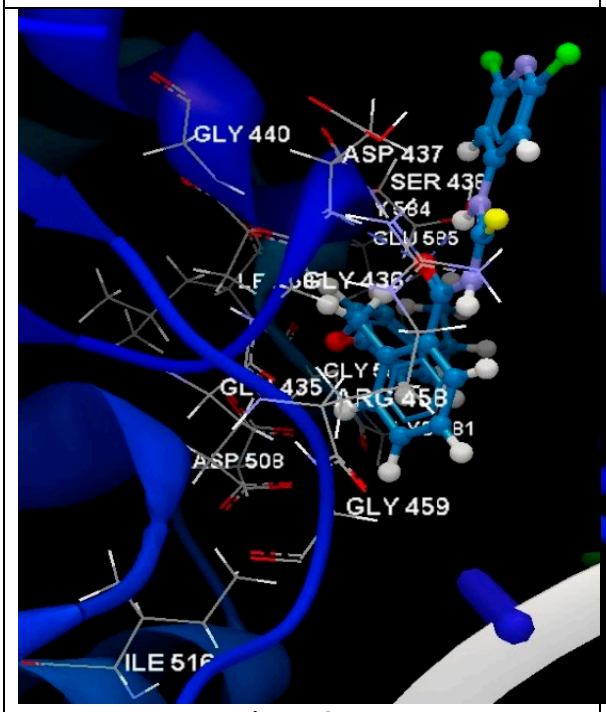


Figure S32.
The interaction group for the ligand **1n.**

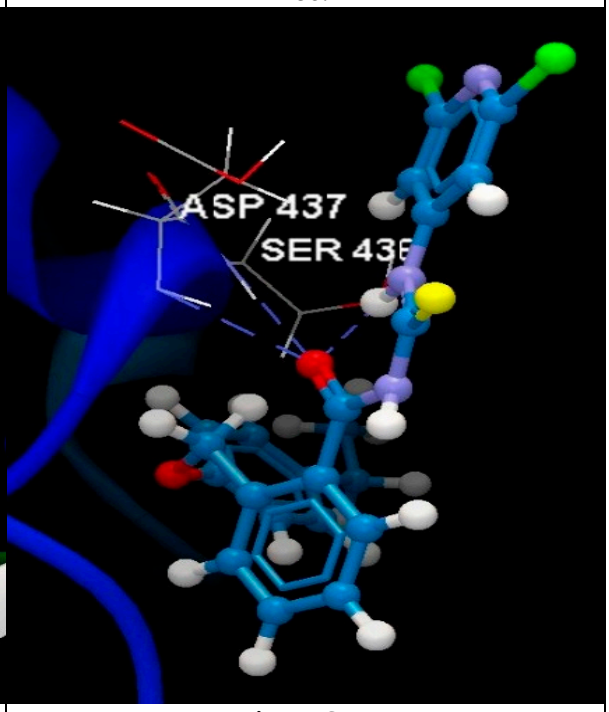


Figure S33.
Hydrogen bounds created between the ligand **1n** and amino acids: ASP 437, SER 438.

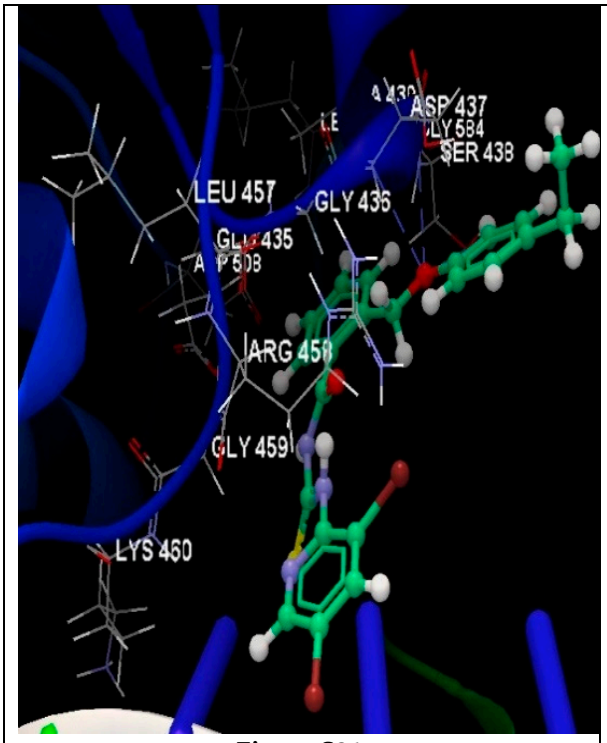


Figure S34.
The interaction group for the ligand **1o.**

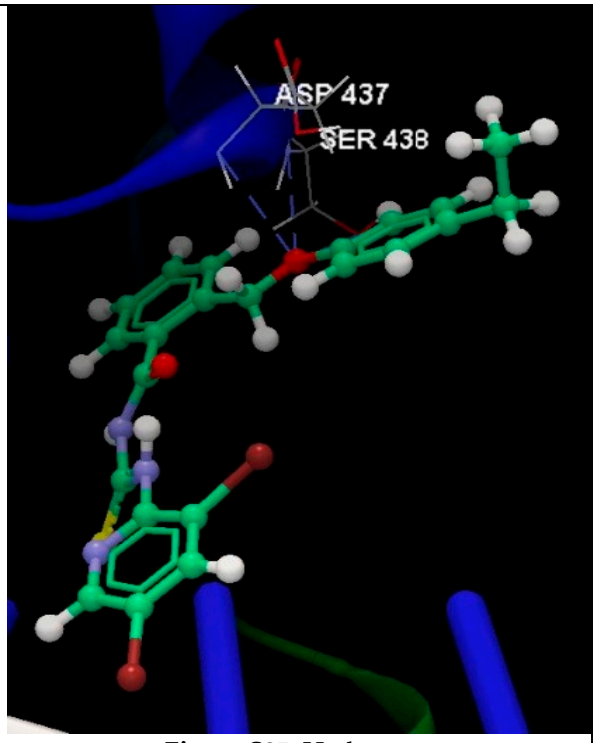


Figure S35. Hydrogen bounds created between the ligand **1o** and amino acids: ASP 437, SER 438.

Figures S36– S65 illustrate intermolecular interactions between the ligand molecules docked with 4DUH (*E. coli* DNA gyrase B, chain A) using CLC Drug Discovery Workbench Software.
For a comprehensive visualization of the interactions between each the designed compound and selected microbial agents, the **figures S36 – S65** reveal the interaction group generated by the docking software. The present hydrogen bonds are also exemplified in the figures attached to the present search.

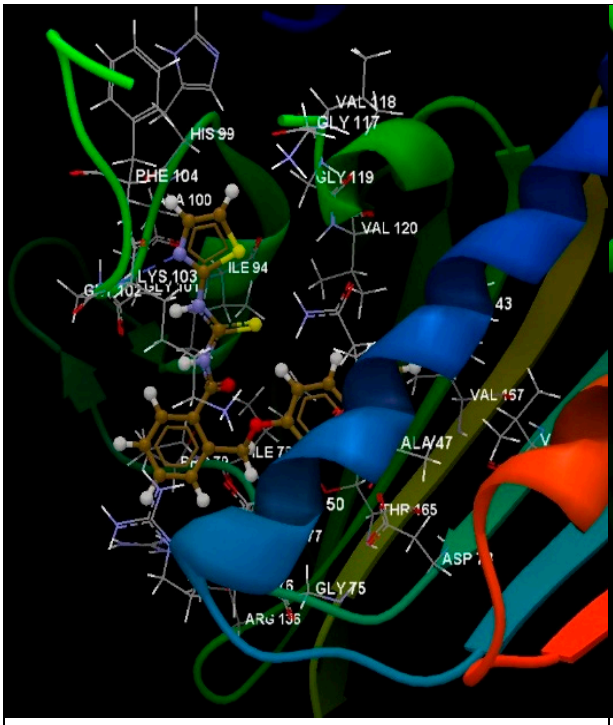


Figure S36.
The interaction group for the ligand **1a.**

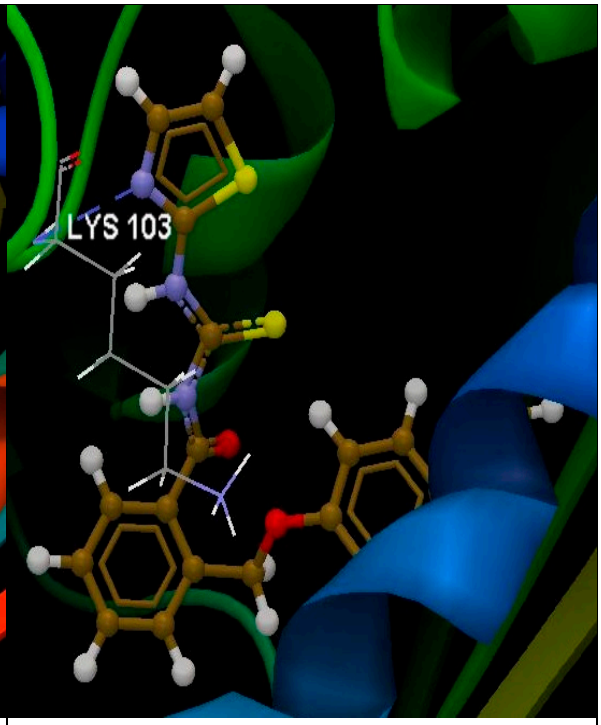


Figure S37.
Hydrogen bounds created between the ligand **1a** and amino acid: LYS 103

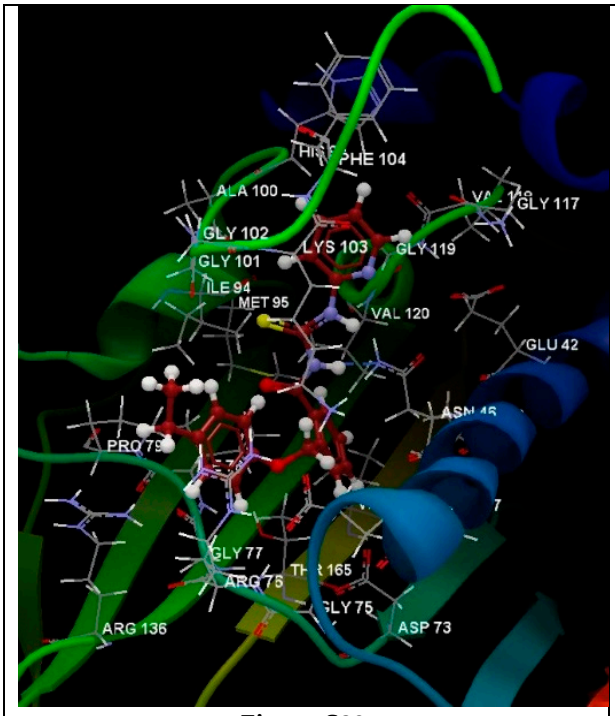


Figure S38.
The interaction group for the ligand **1b.**

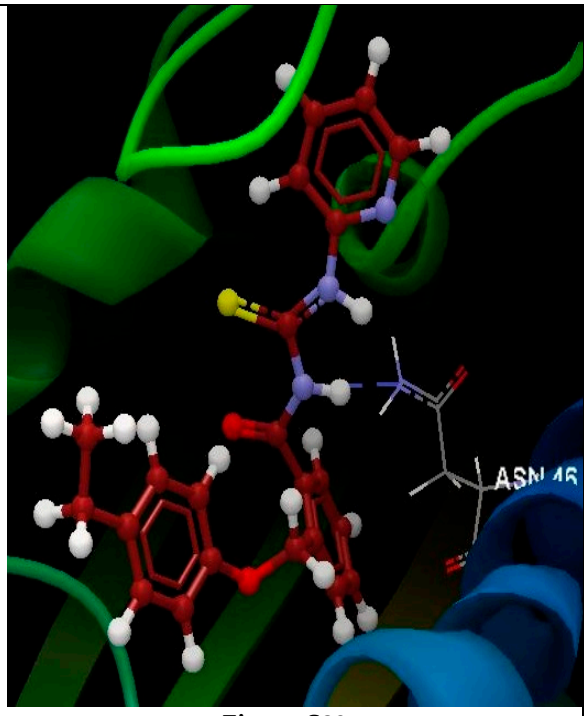


Figure S39.
Hydrogen bounds created between the ligand **1b** and amino acid: ASN 46.

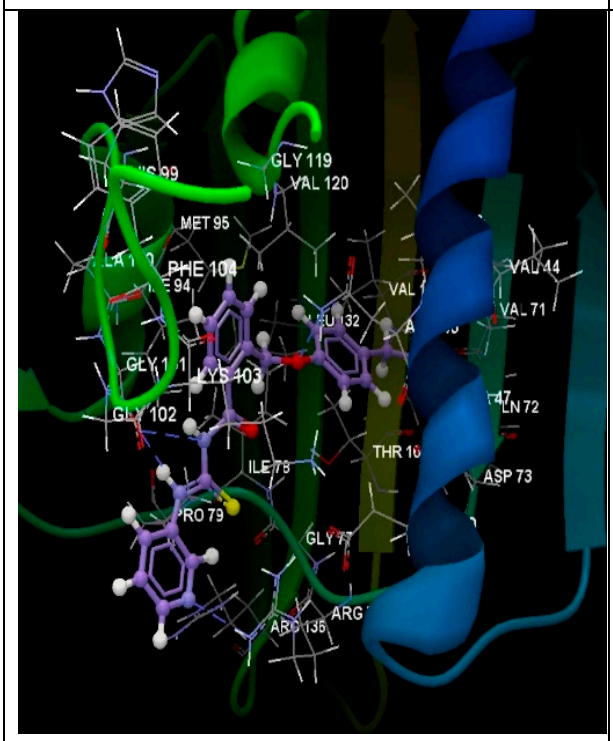


Figure S40.
The interaction group for the ligand **1c.**

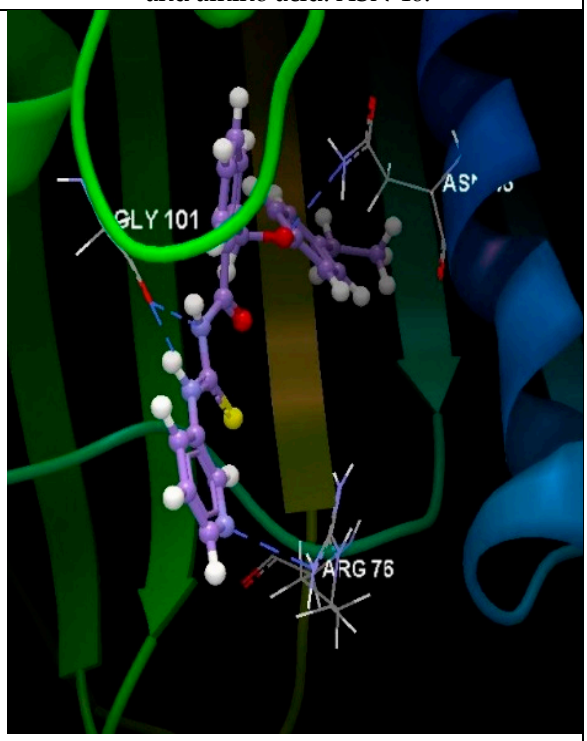


Figure S41.
Hydrogen bounds created between the ligand **1c** and amino acids: ASN 46, GLY 101, ARG 76.

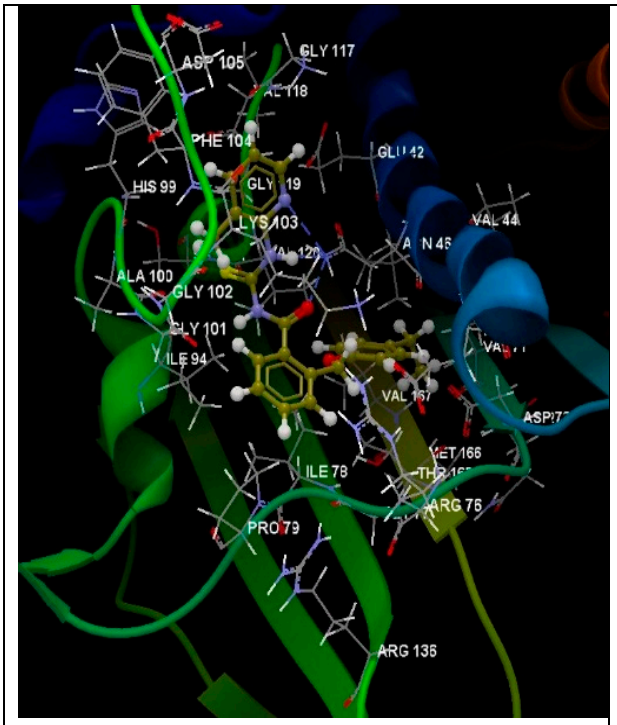


Figure S42.
The interaction group for the ligand **1d.**

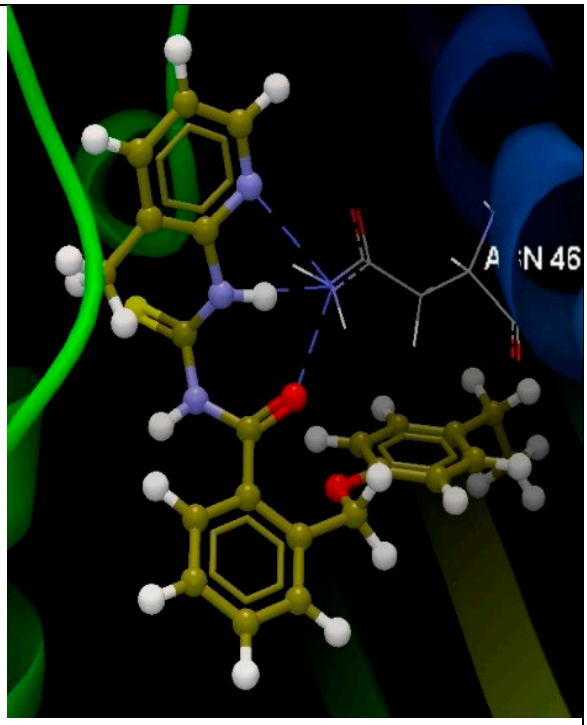


Figure S43.
Hydrogen bounds created between the ligand **1d** and amino acid: ASN 46.

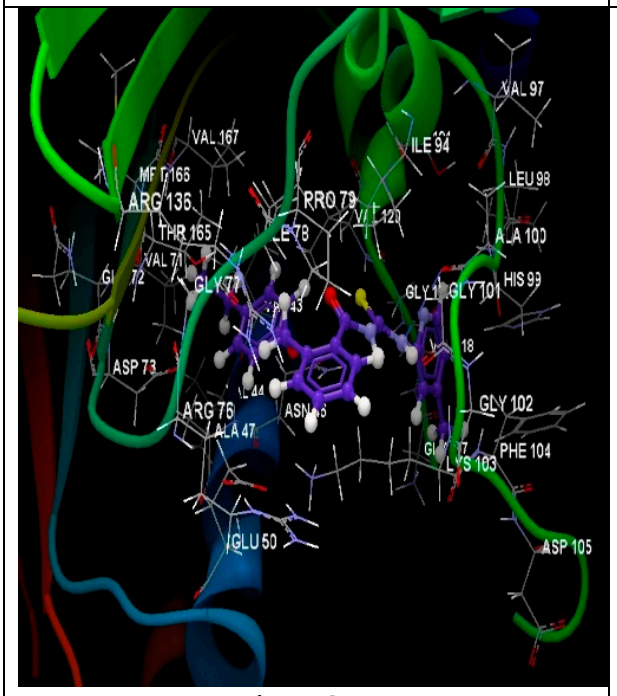


Figure S44.
The interaction group for the ligand **1e.**

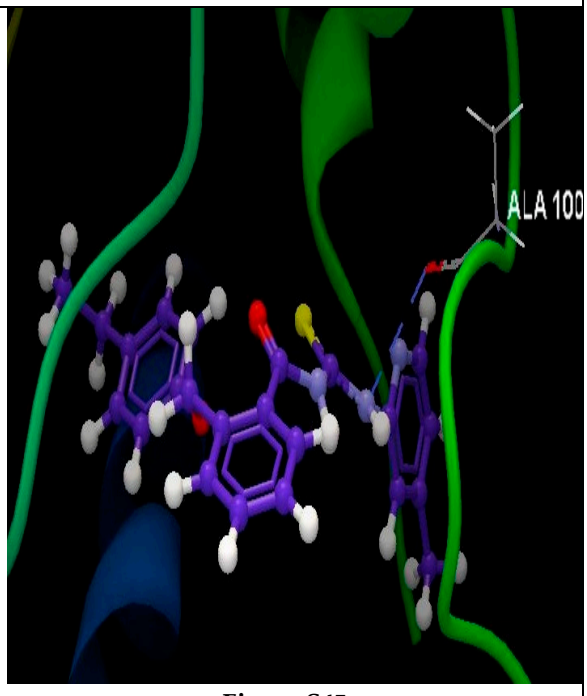


Figure S45.
Hydrogen bounds created between the ligand **1e** and amino acid: ALA 100.

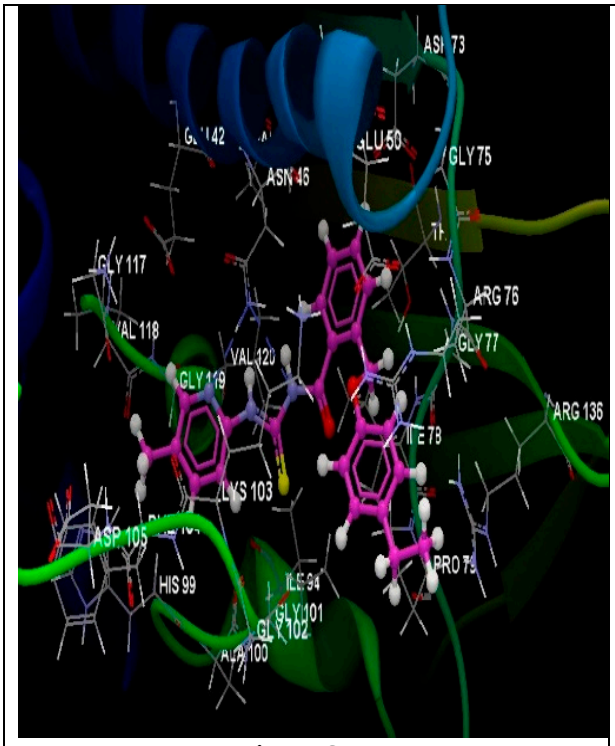


Figure S46.
The interaction group for the ligand **1f.**

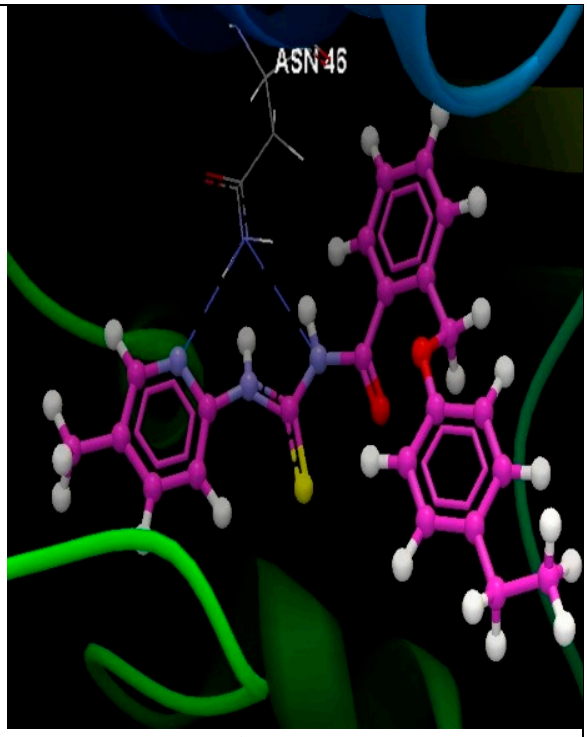


Figure S47.
Hydrogen bounds created between the ligand **1f** and amino acid: ASN 46.

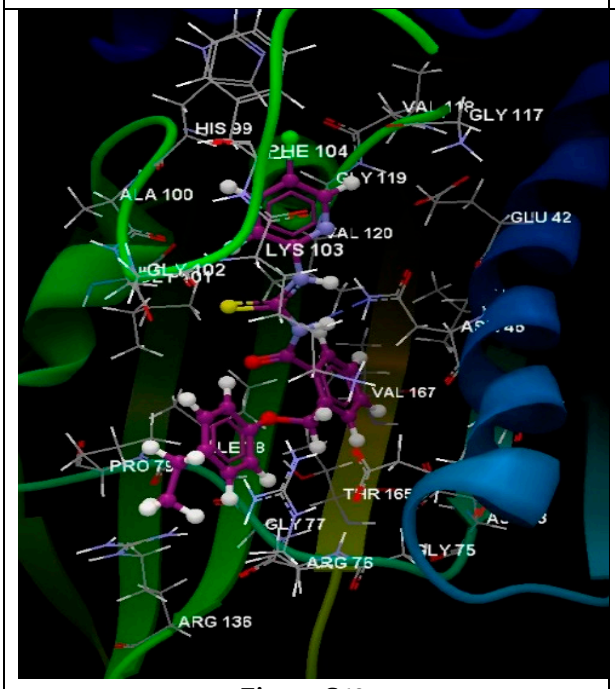


Figure S48.
The interaction group for the ligand **1g.**

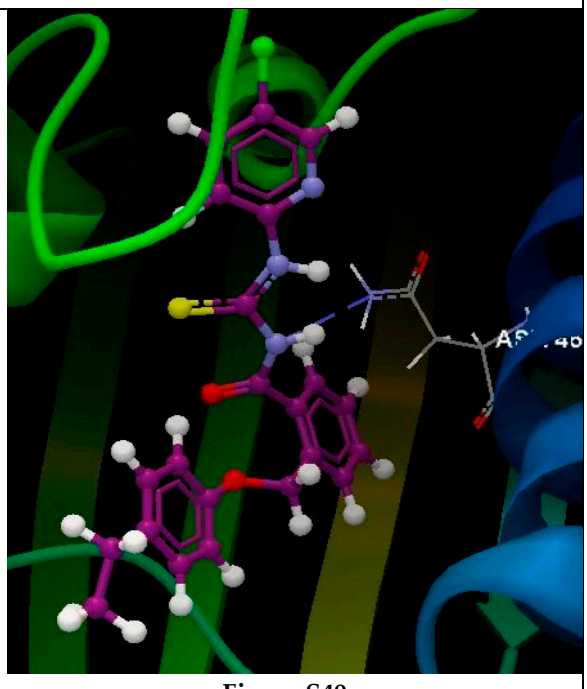


Figure S49.
Hydrogen bounds created between the ligand **1g** and amino acid: ASN 46.

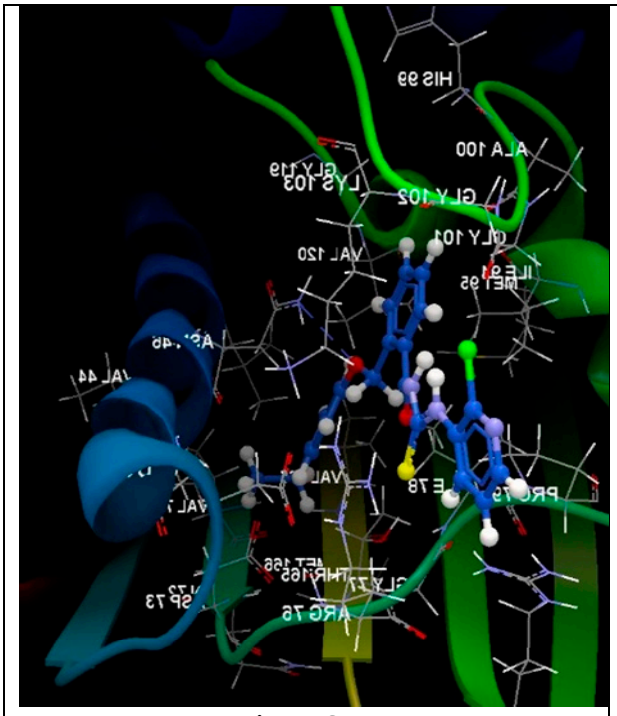


Figure S50.
The interaction group for the ligand **1h.**

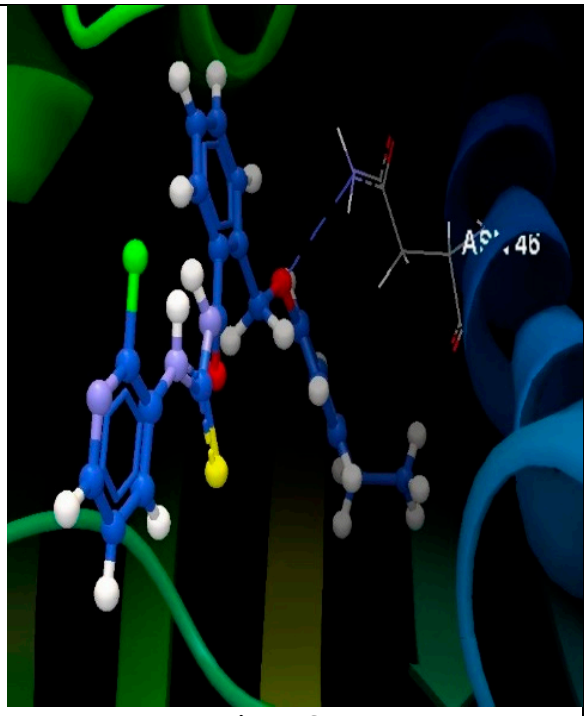


Figure S51.
Hydrogen bounds created between the ligand **1h** and amino acid: ASN 46.

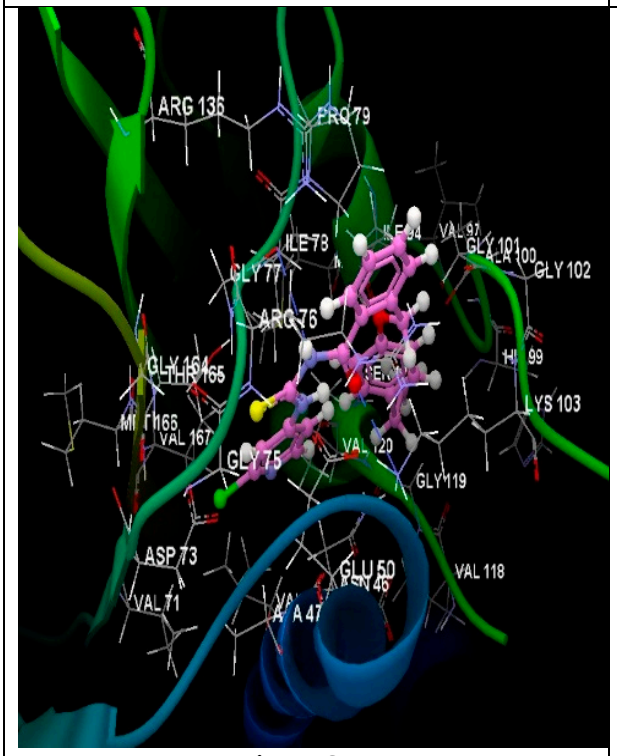


Figure S52.
The interaction group for the ligand **1i.**

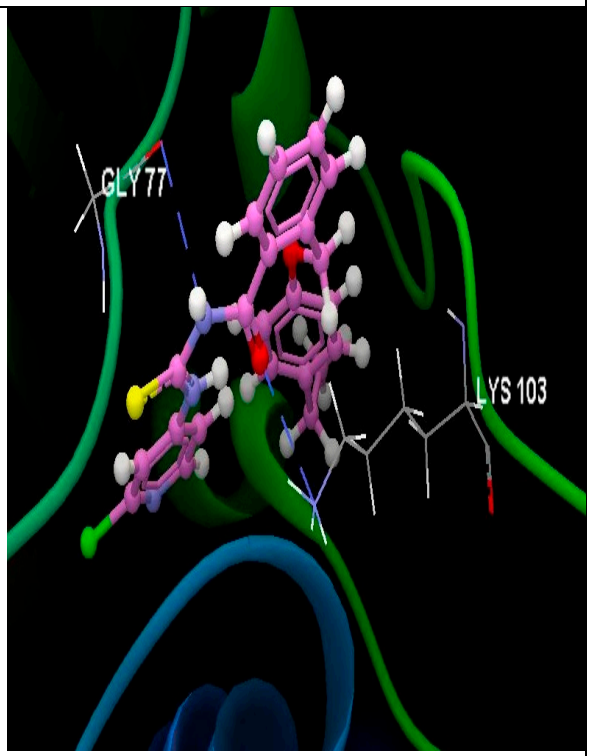


Figure S53.
Hydrogen bounds created between the ligand **1i** and amino acids: GLY 77, LYS 103.

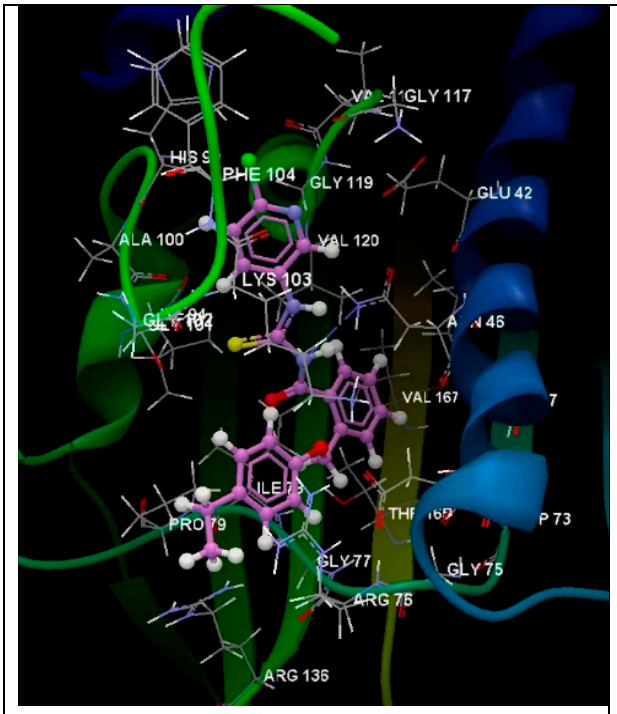


Figure S54.
The interaction group for the ligand **1j.**

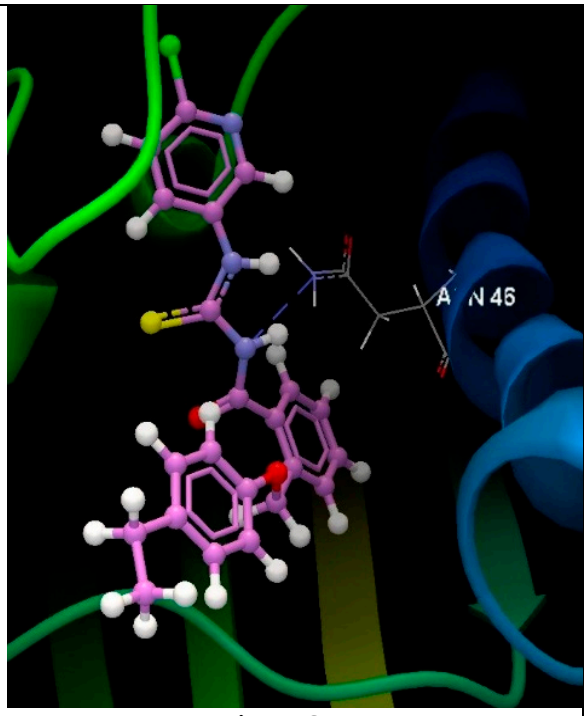


Figure S55.
Hydrogen bounds created between the ligand **1j** and amino acid: ASN 46.

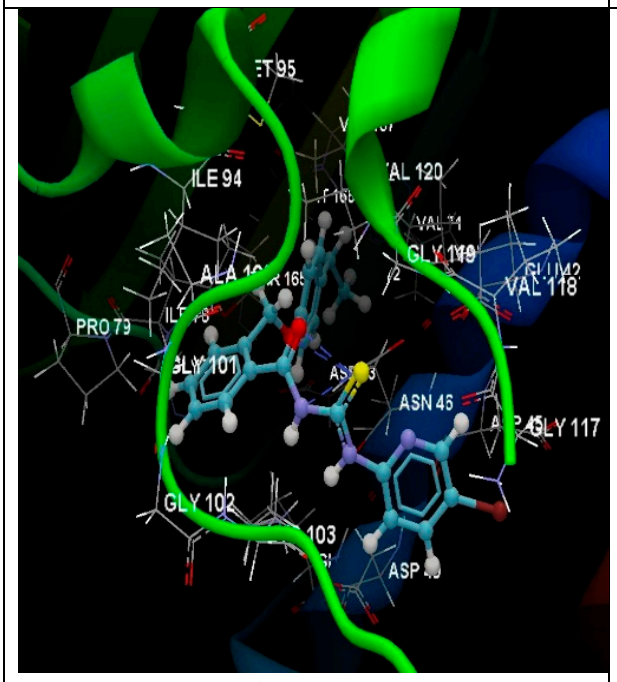


Figure S56.
The interaction group for the ligand **1k.**

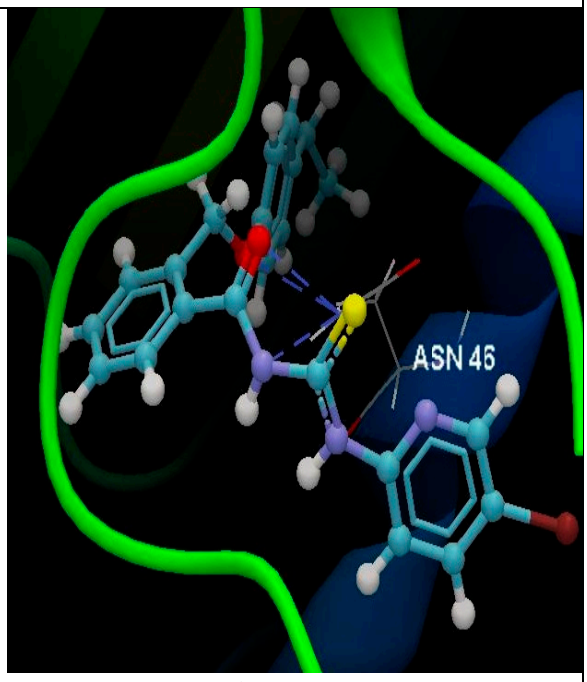


Figure S57.
Hydrogen bounds created between the ligand **1k** and amino acid: ASN 46.

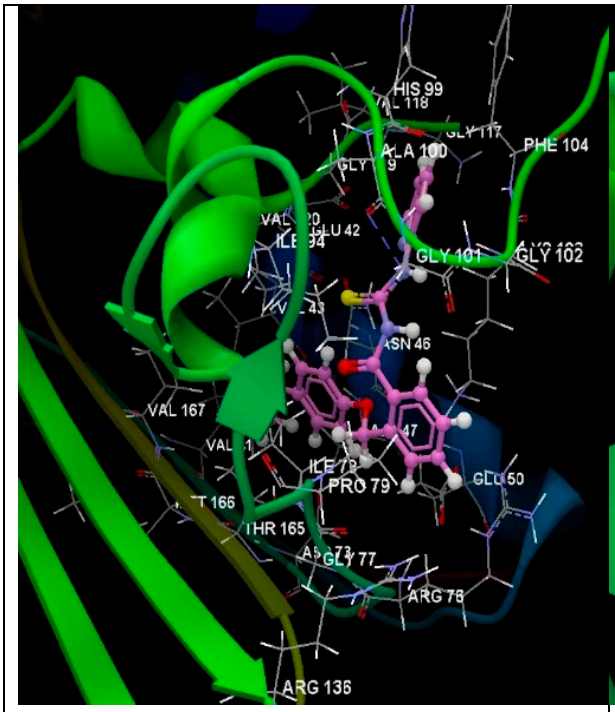


Figure S58.
The interaction group for the ligand **1l.**

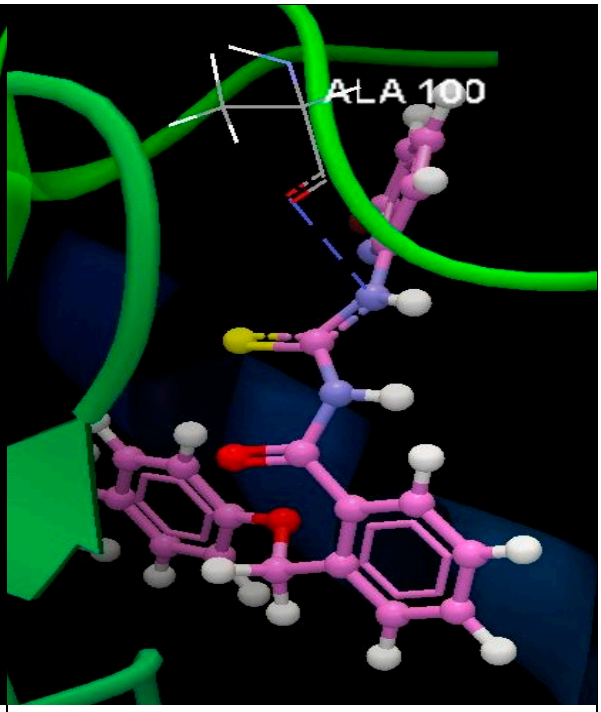


Figure S59.
Hydrogen bounds created between the ligand **1l** and amino acid: ALA 100.

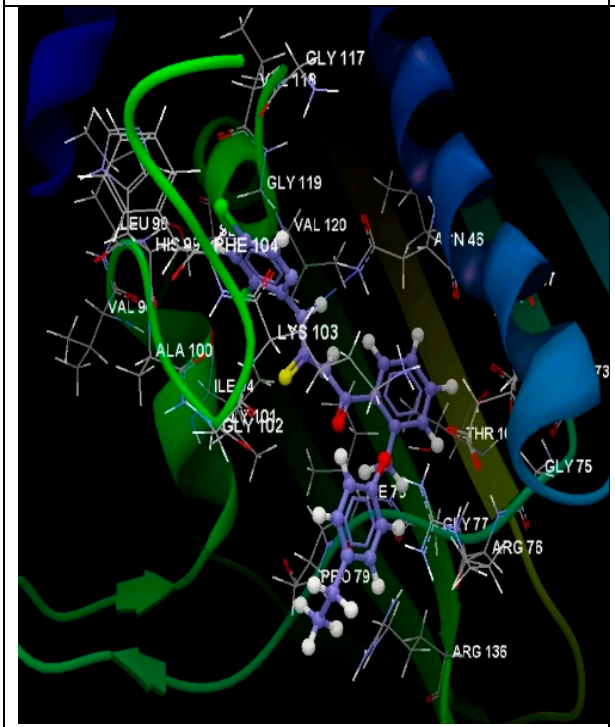


Figure S60.
The interaction group for the ligand **1m.**

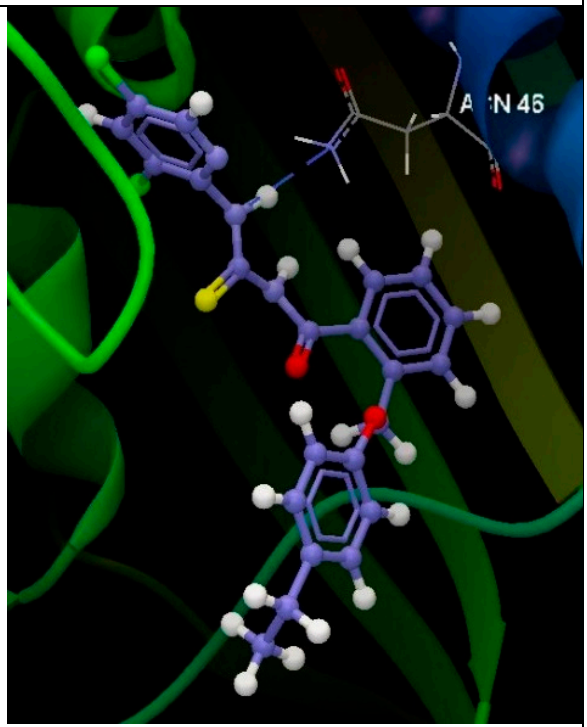


Figure S61.
Hydrogen bounds created between the ligand **1m** and amino acid: ASN 46.

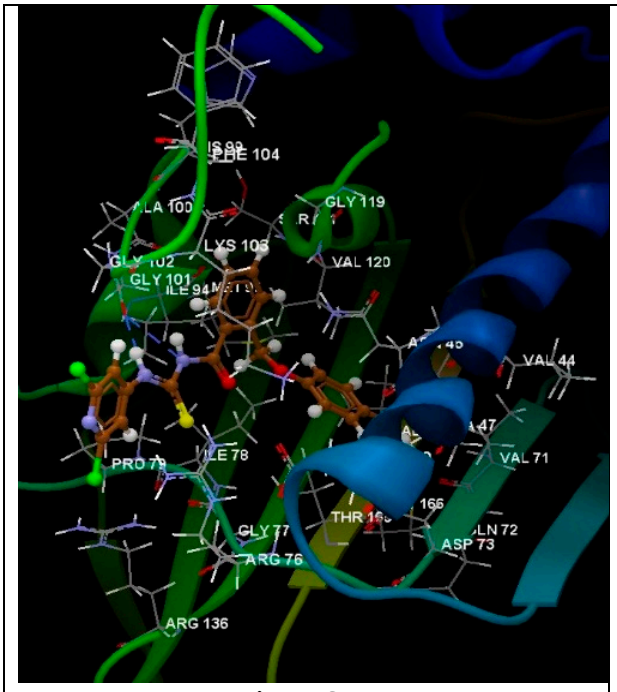


Figure S62.
The interaction group for the ligand **1n.**

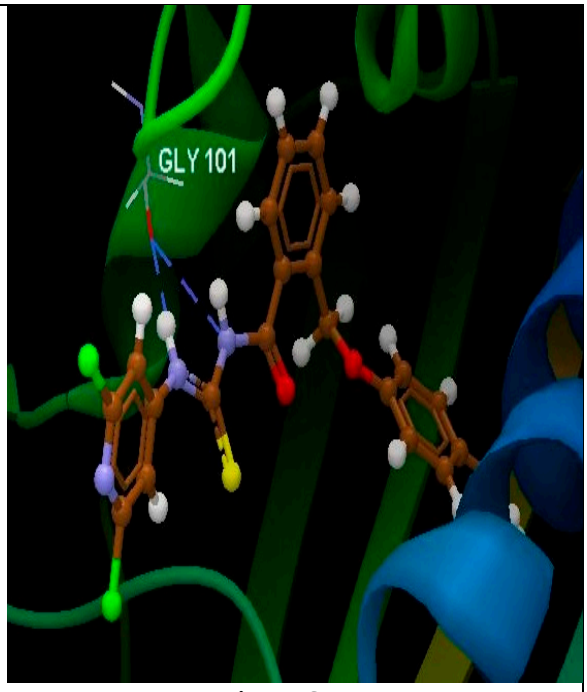


Figure S63.
Hydrogen bounds created between the ligand **1n** and amino acid: GLY 101.

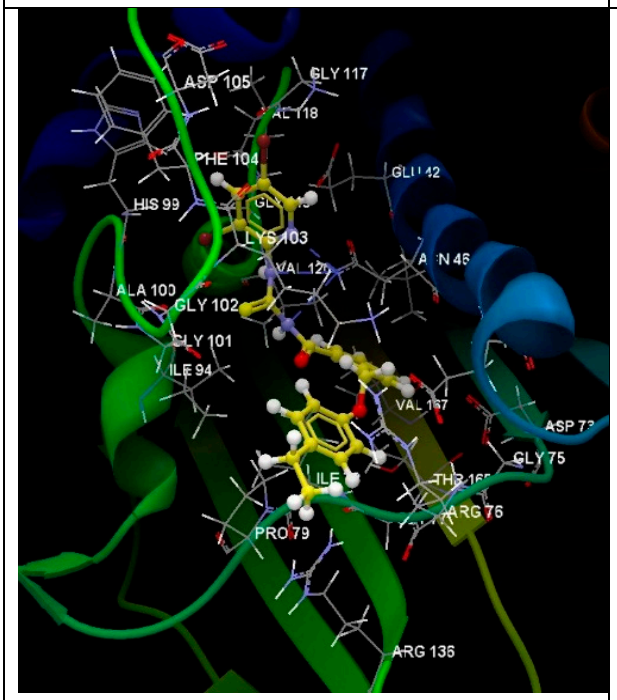


Figure S64.
The interaction group for the ligand **1o.**

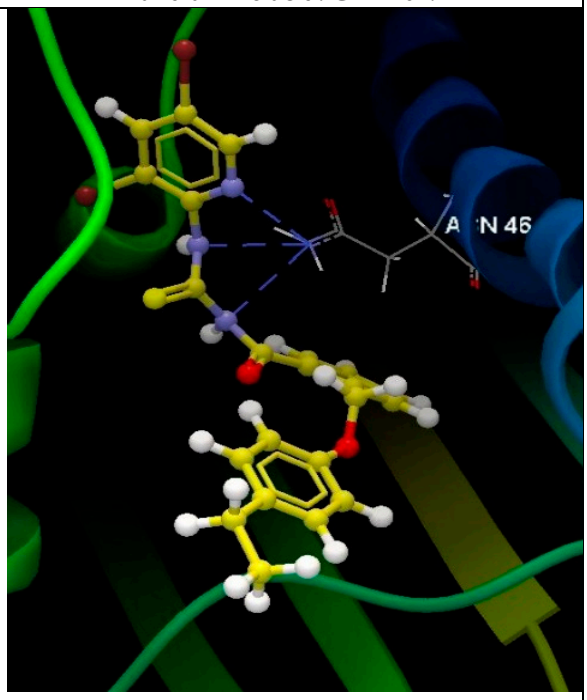


Figure S65.
Hydrogen bounds created between the ligand **1o** and amino acid: ASN 46.