Supplementary Materials

Figure S1(a)

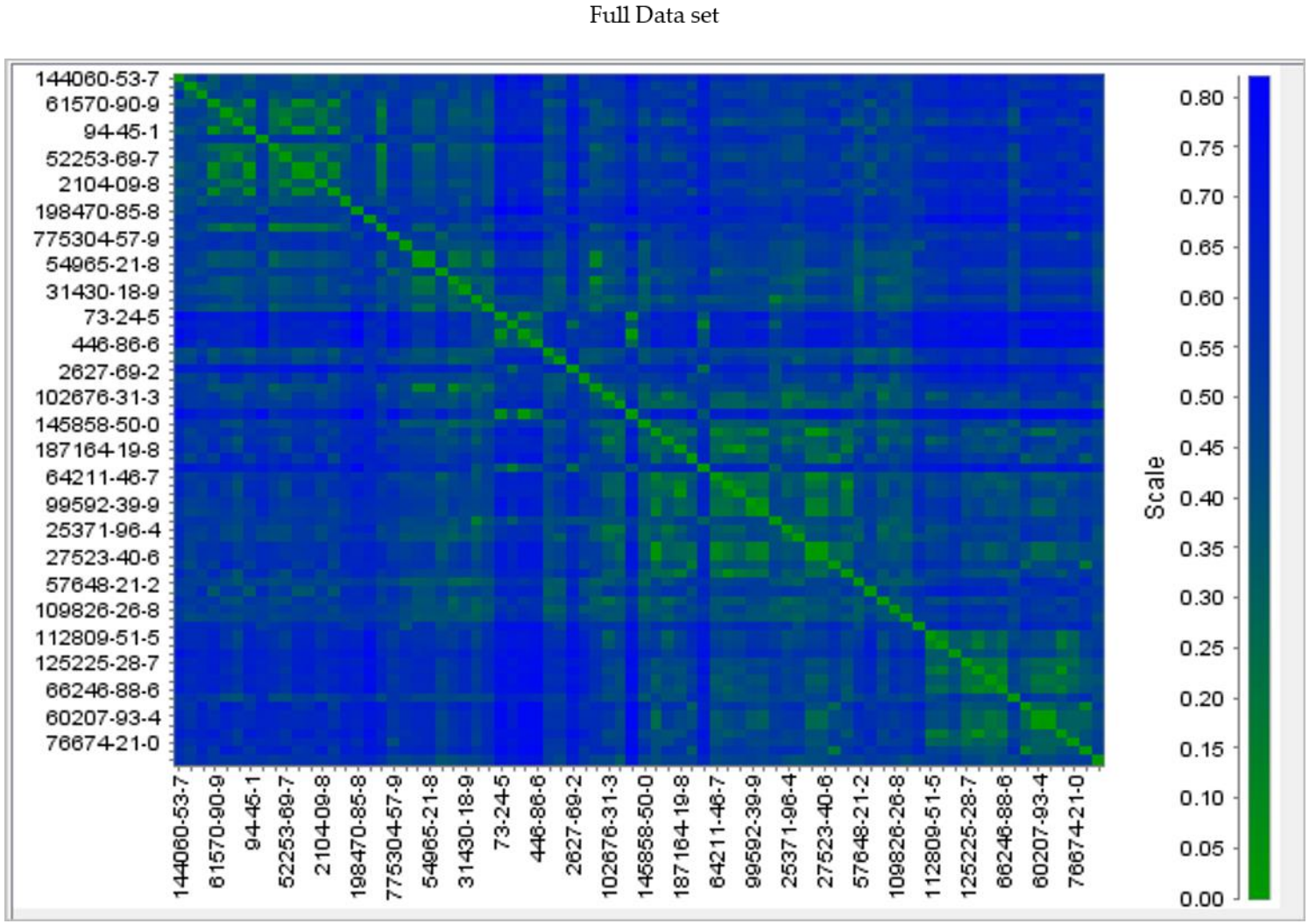
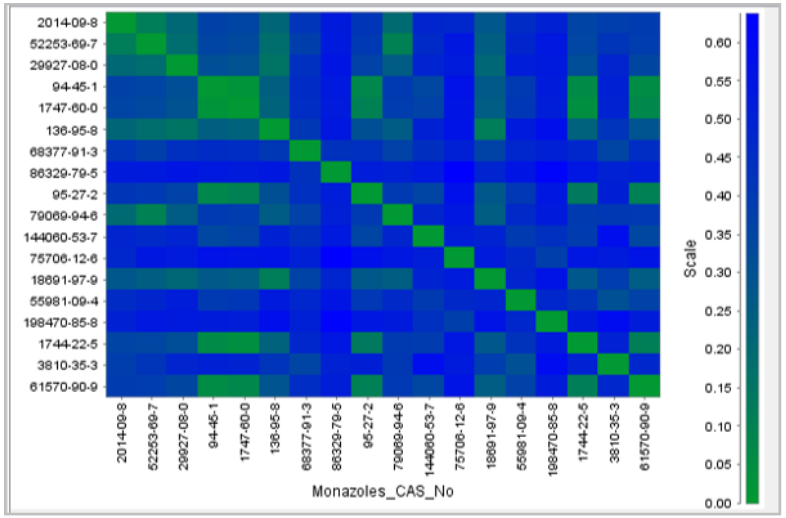
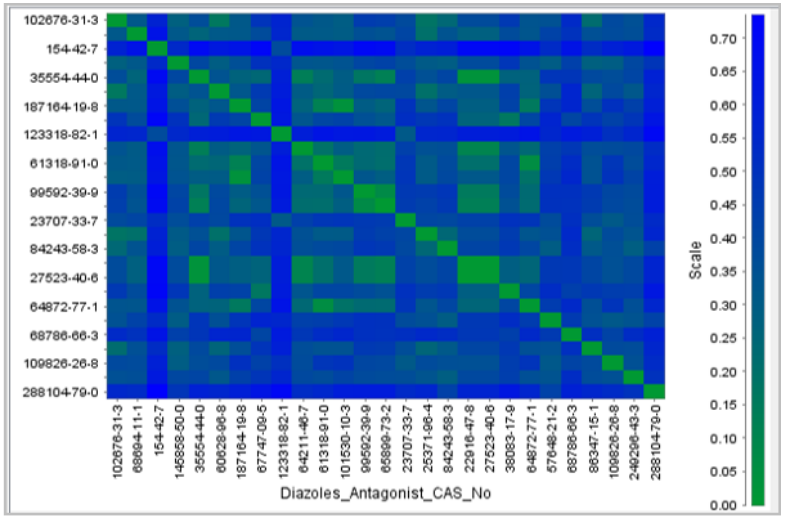


Figure S1(b)



(**c**)



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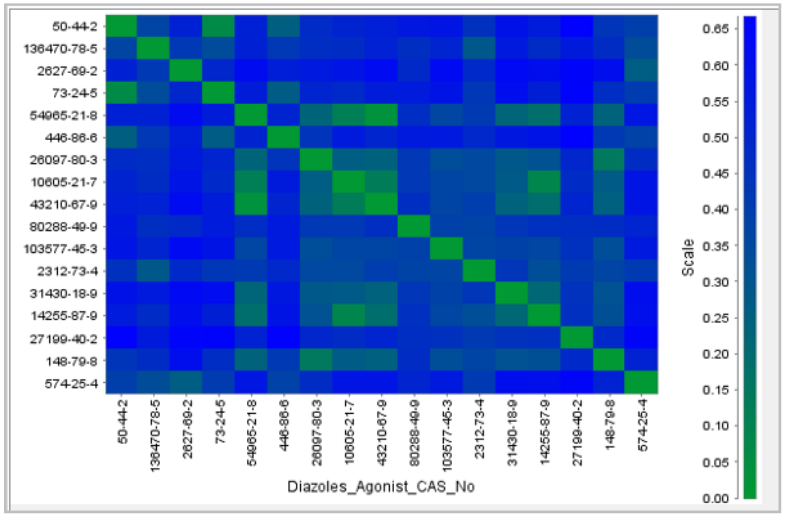

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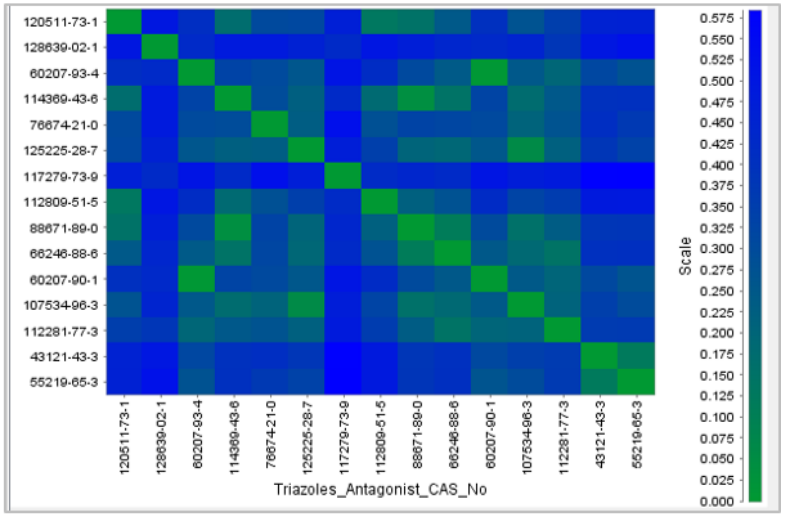
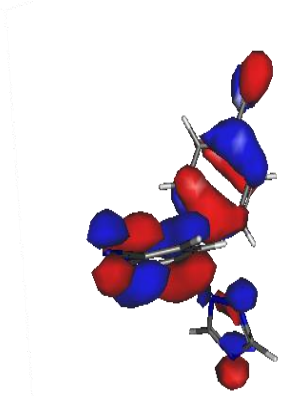
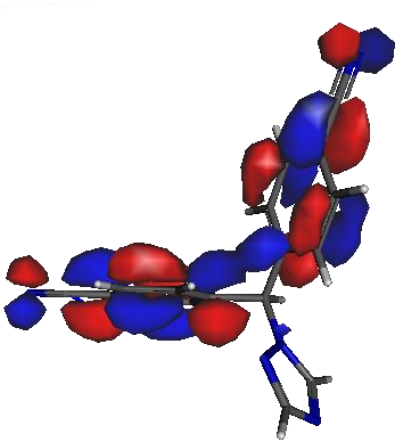
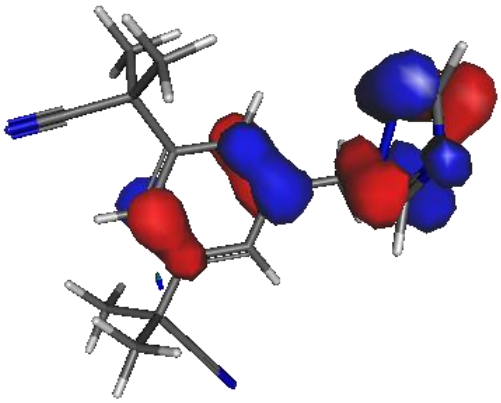
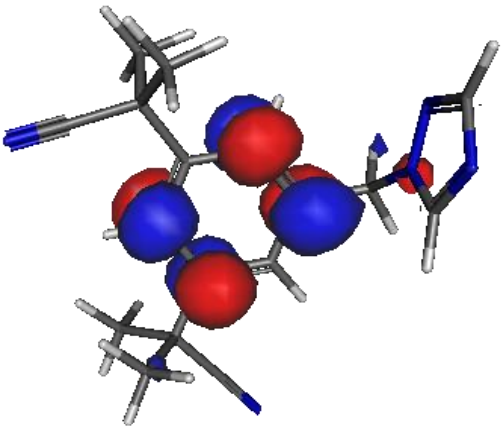
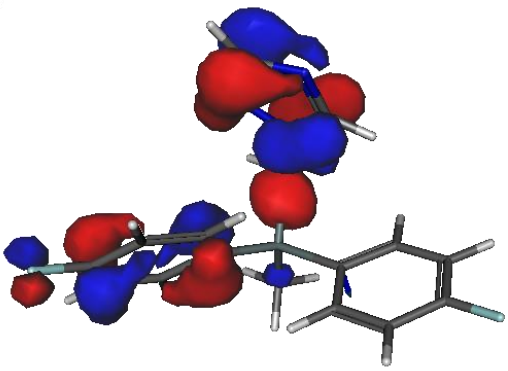
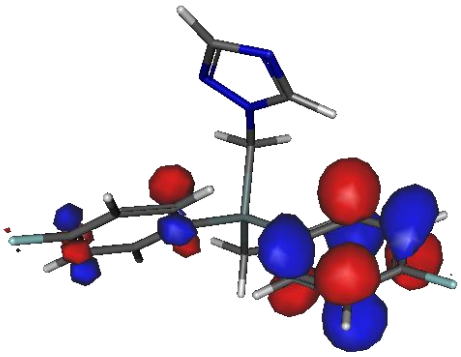
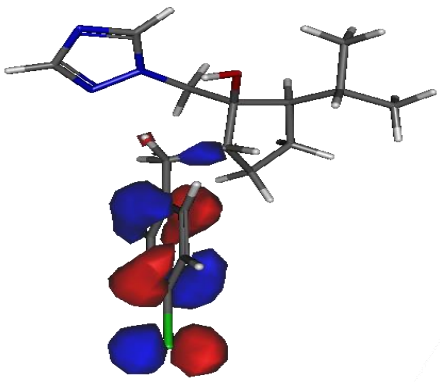
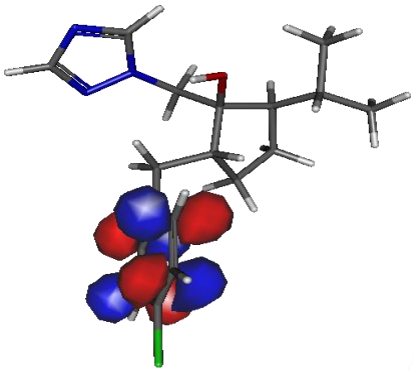
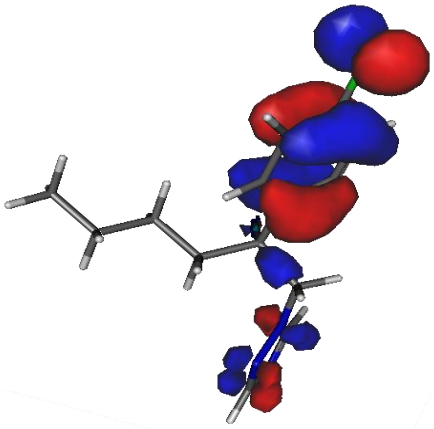


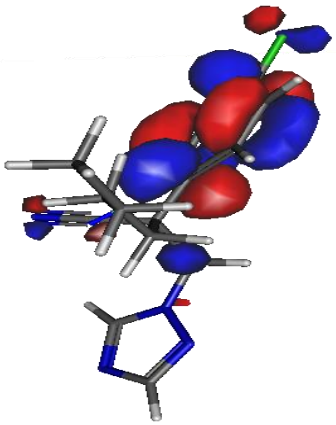
(**f**)

Figure S1: The heat maps showing the diversity of the data set. a.) Heat map for full data set. b) Heat map for the classified data set based on activity and class of the azole. On left side agonist monazoles (Thiazole/oxazole) (c) and agonist diazoles (imidazoles and benzimidazole) (e). On right side antagonist diazoles (imidazoles and benzimidazole) (d) and antagonist triazoles (f).

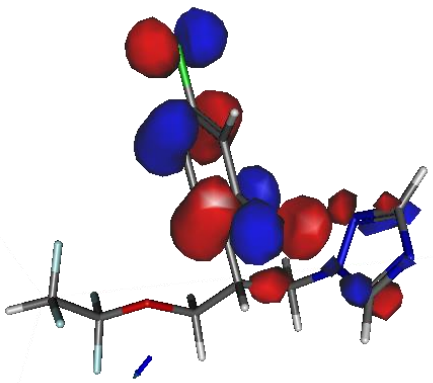
Molecule	HOMO	LUMO
Litrazole		
Anastrazole		
Flusilazole		
Ipiconazole		

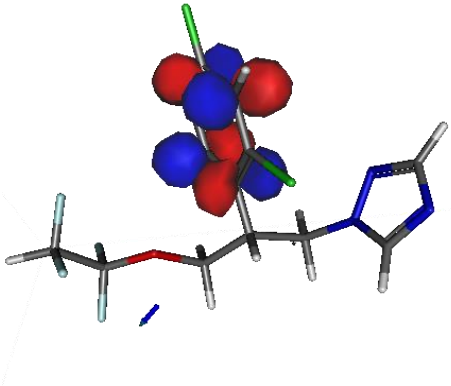
Myclobutanil



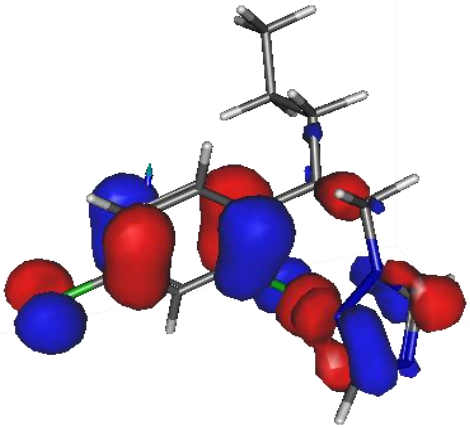


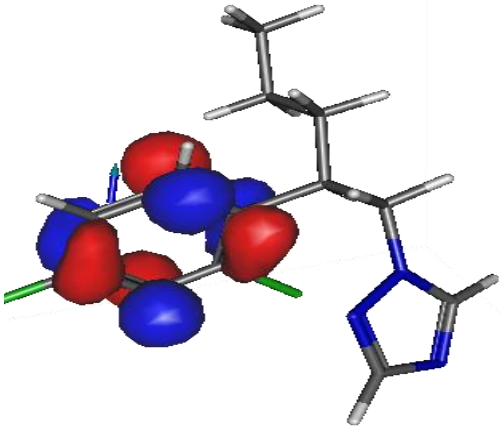
Tetraconazole



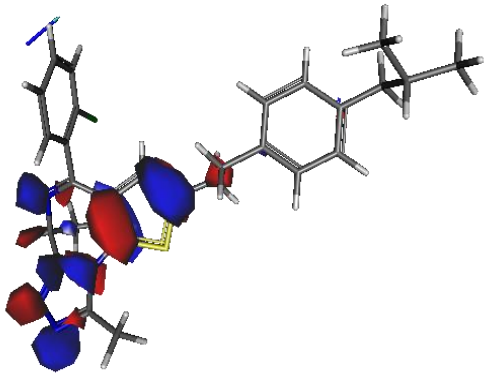


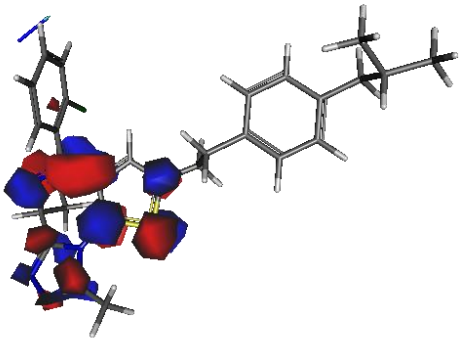
Penconazole



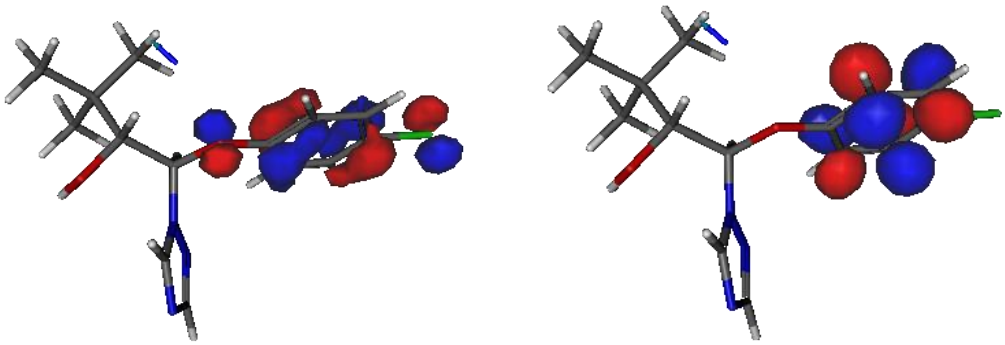


Israpafant

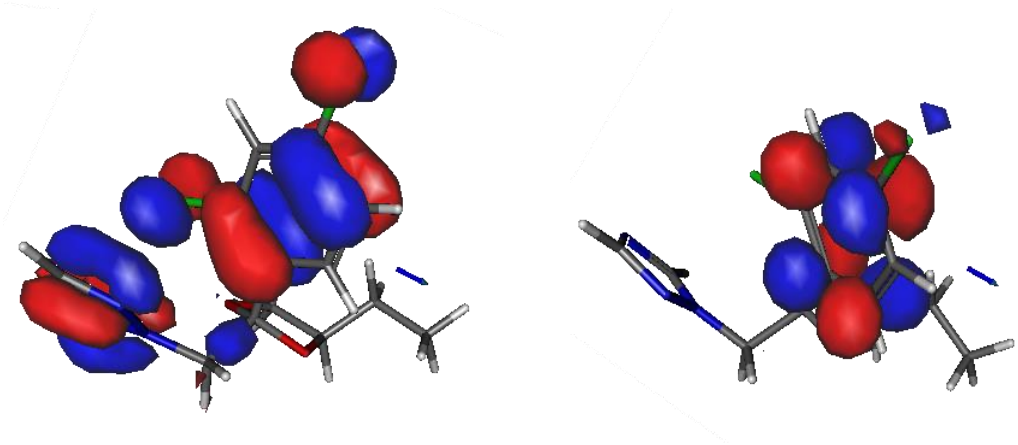




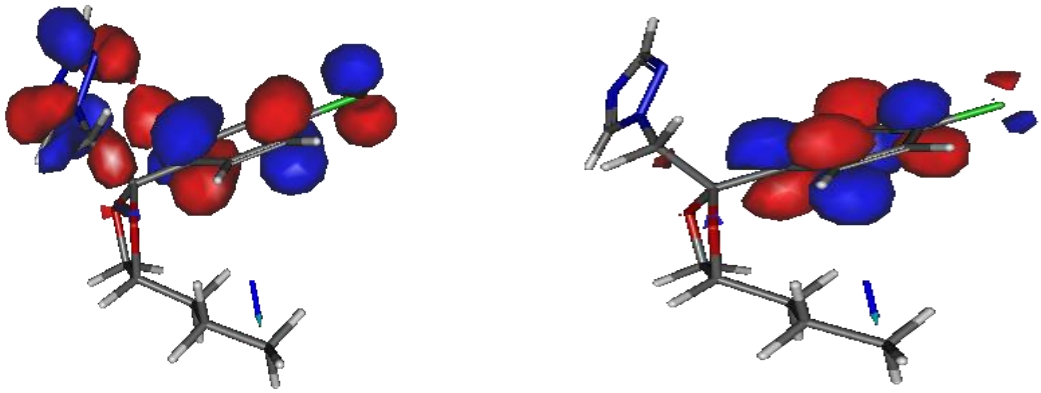
Triadimenol



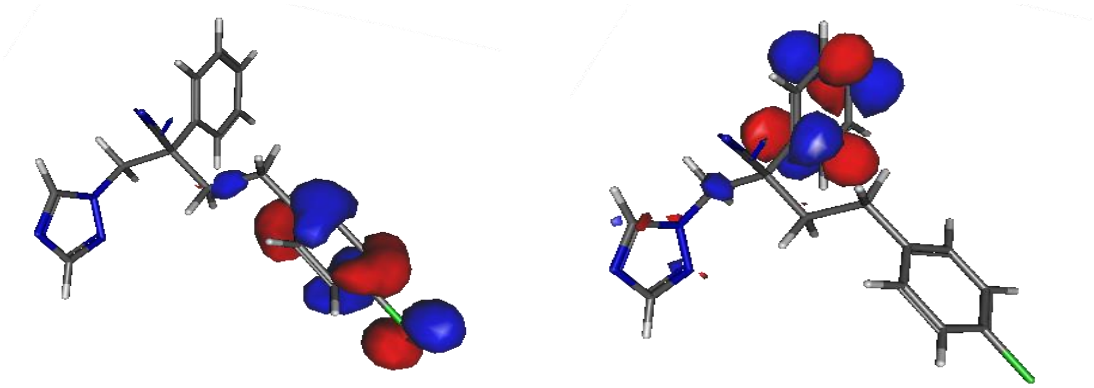
Etaconazole



Propiconazole



Fenbuconazole



Flutriafol

Triadimefon

Carfentrazone-ethyl

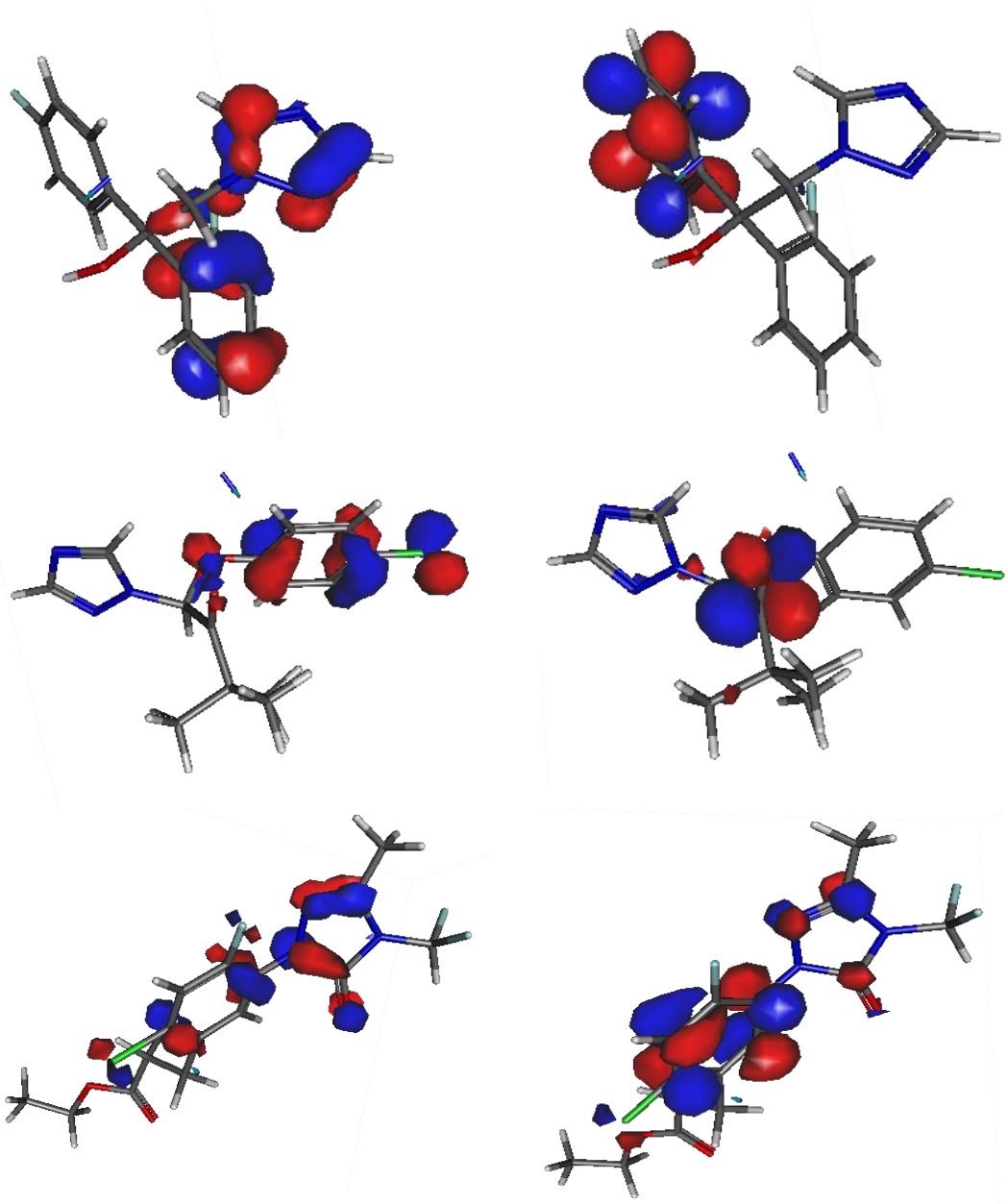


Figure S2: Representations of HOMO and LUMO isosurfaces for the antagonist triazoles computed using the single point at B3LYP/def2-SV(P) method on the structure obtained following complete optimisation with PM7.

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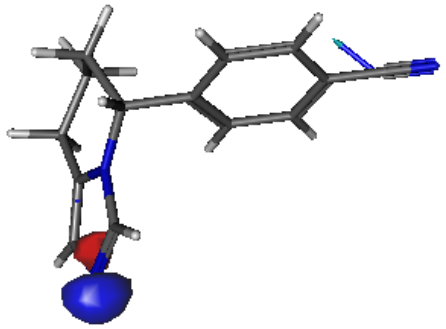
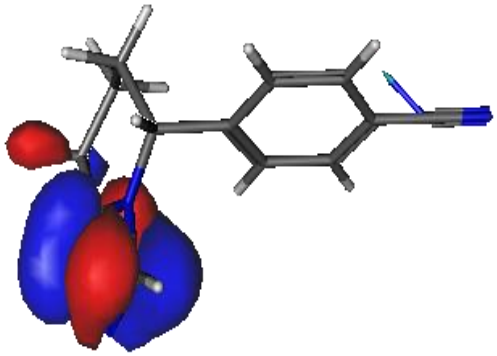
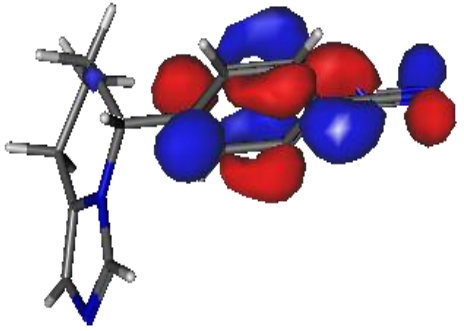
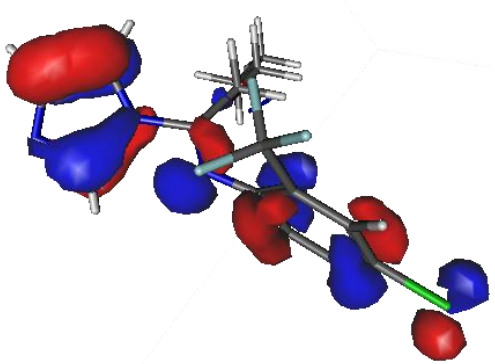
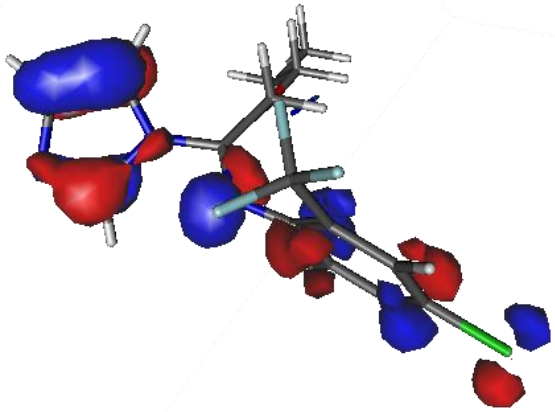
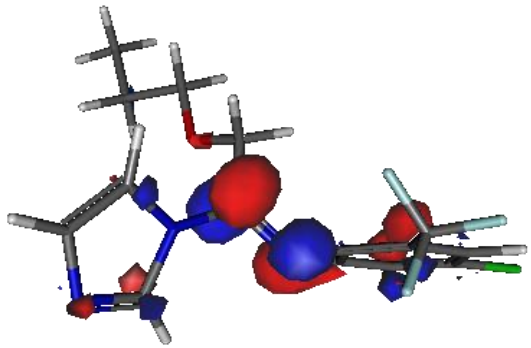
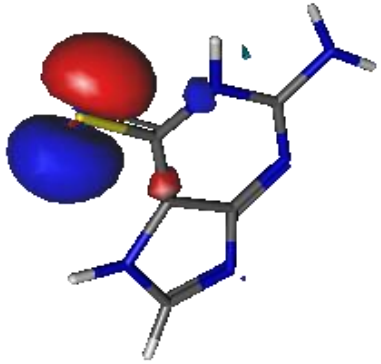
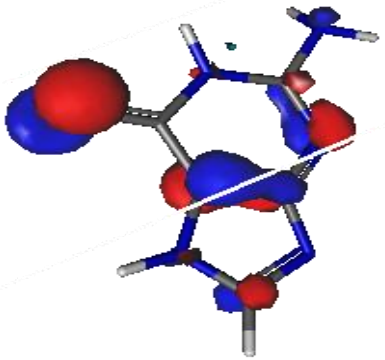
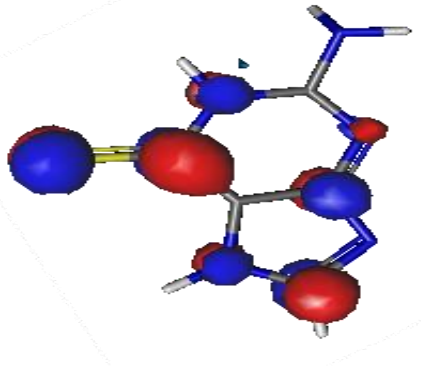
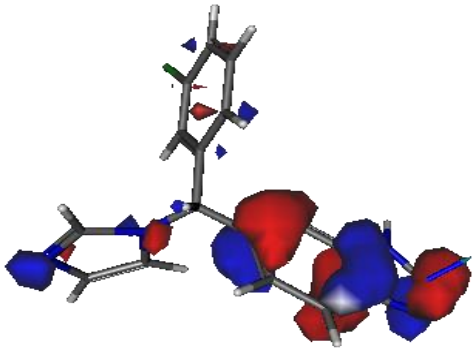
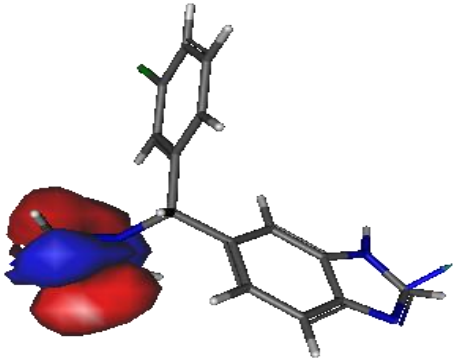
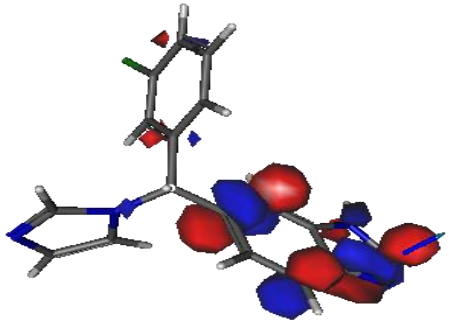
	HOMONL	HOMO	LUMO
Fadrozole			
Triflumizole			
6-Thioguanine			

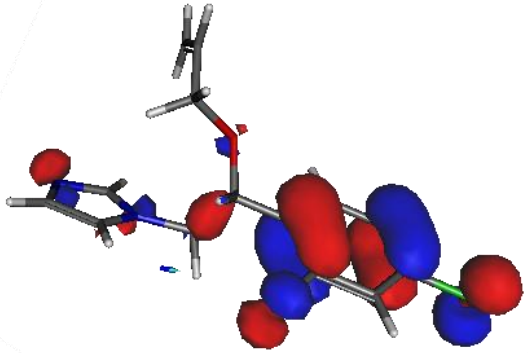
Liarozole

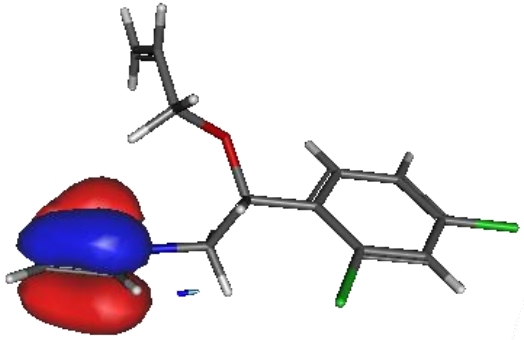


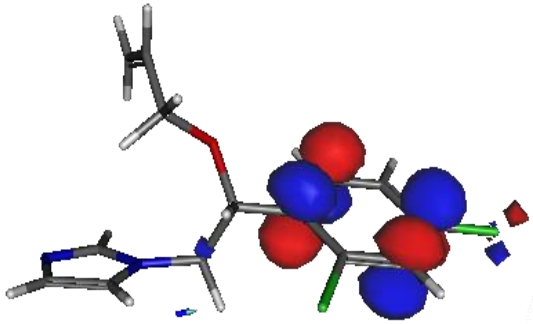




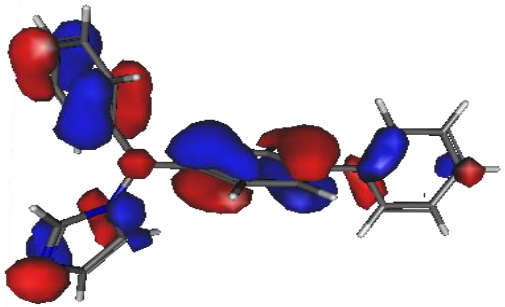
Imazalil

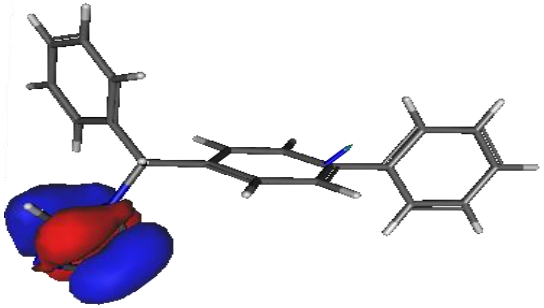


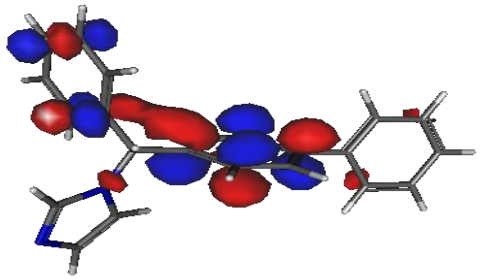




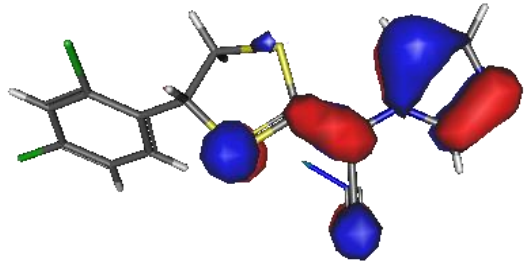
Bifonazole

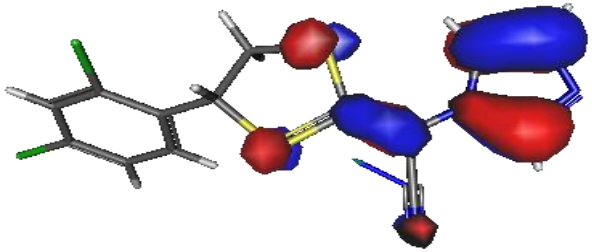


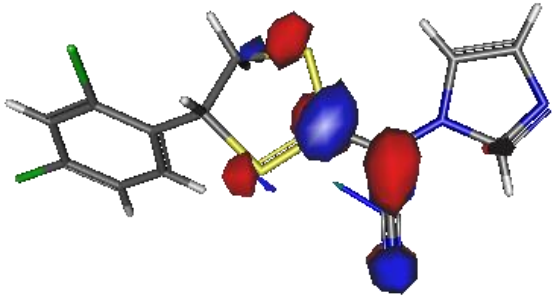




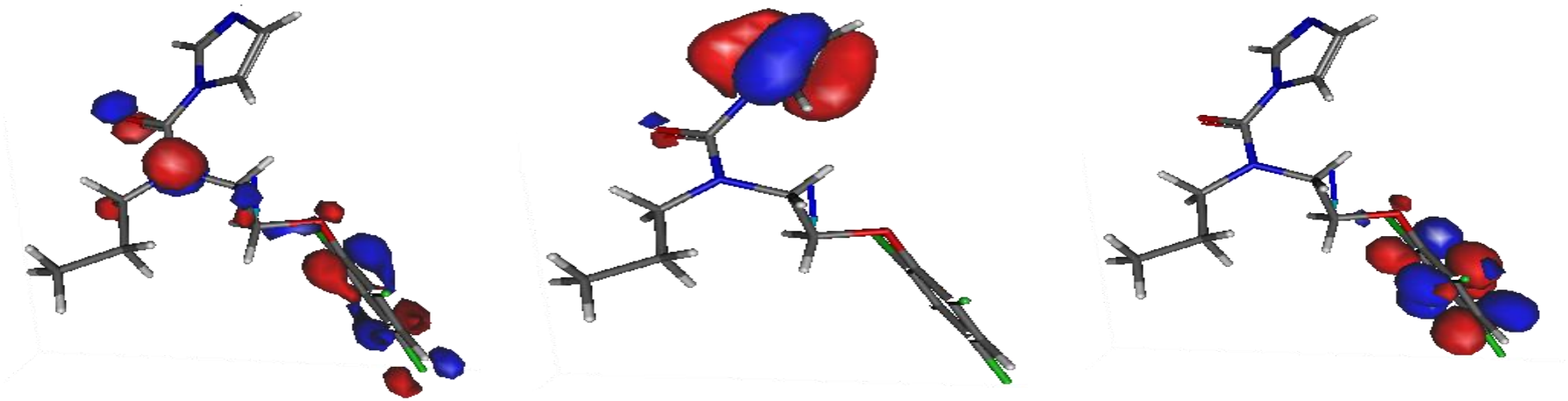
Luliconazole



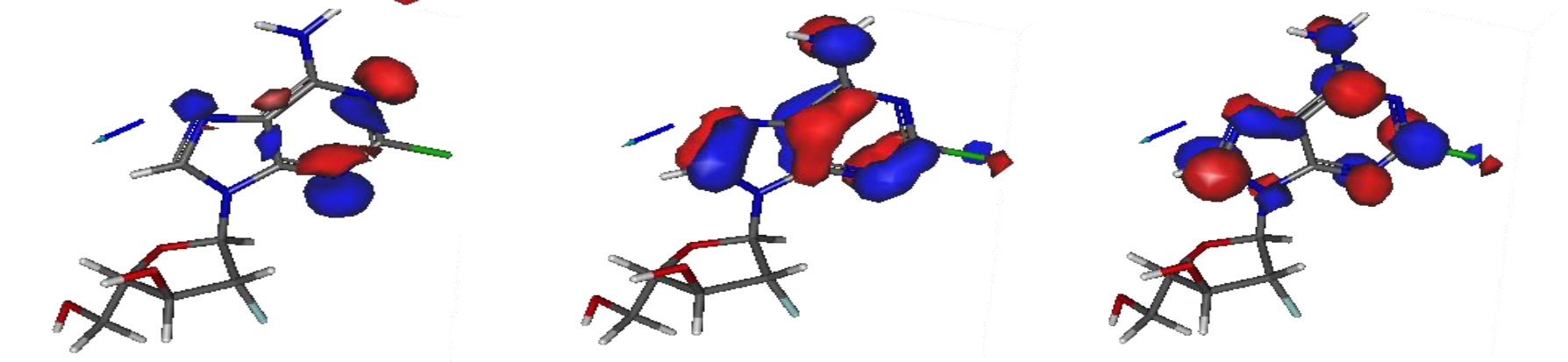




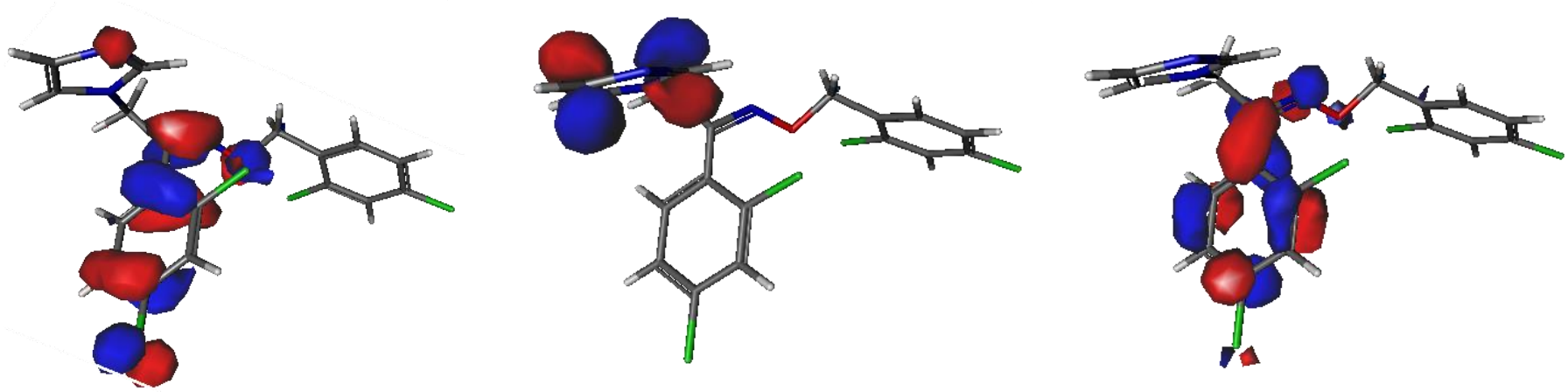
Prochloraz



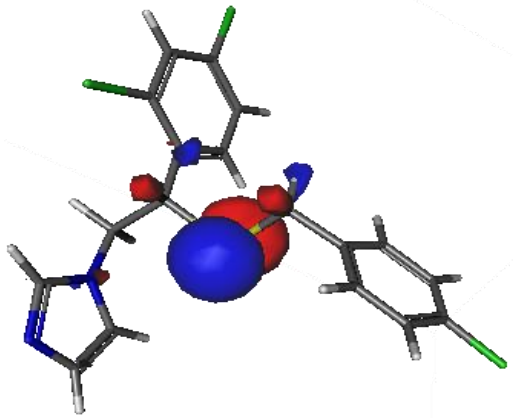
Clofarabine

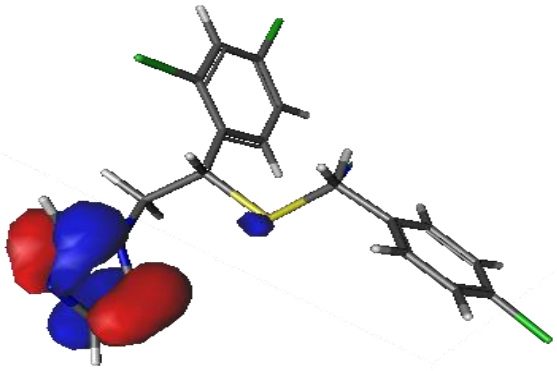


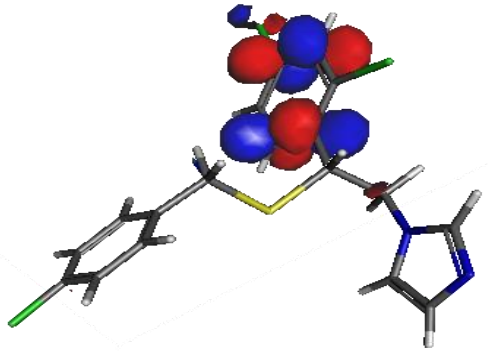
Oxiconazole



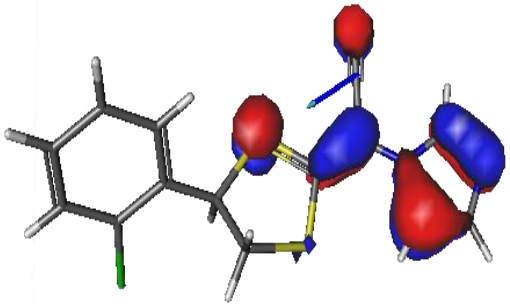
Sulconazole

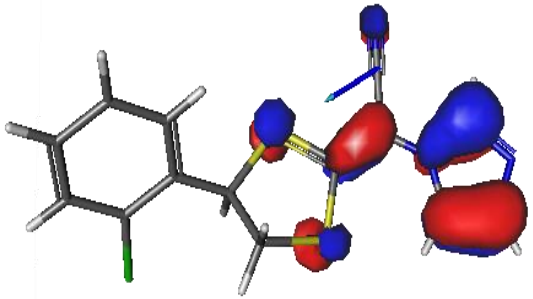


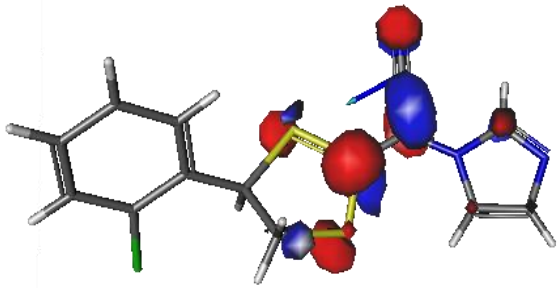




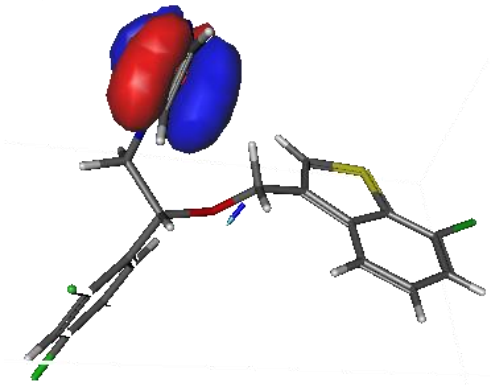
Lanoconazole

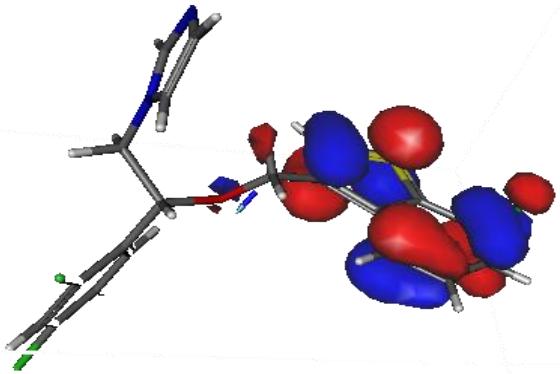


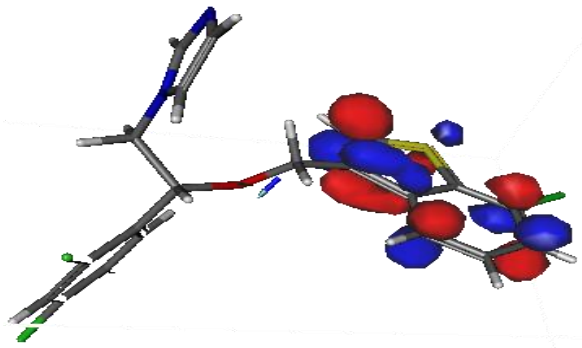




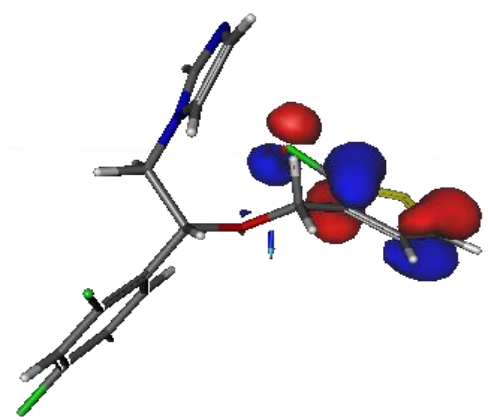
Sertaconazol

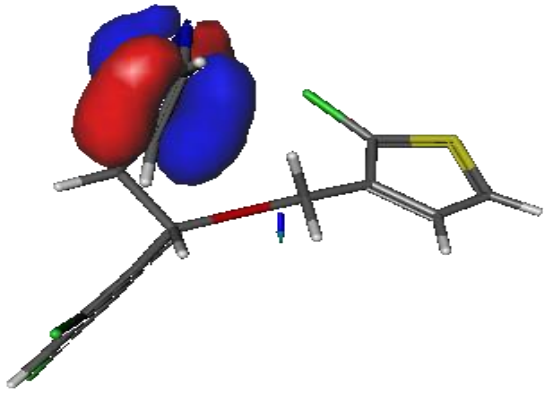


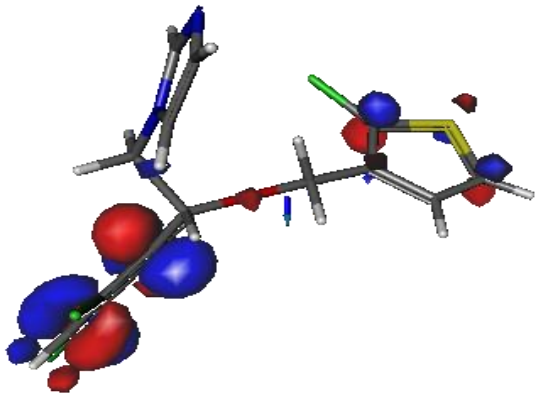




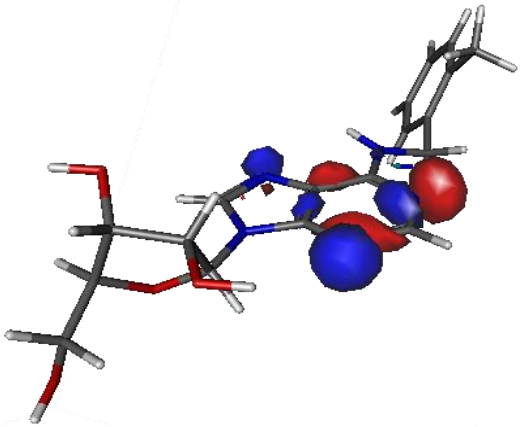
Tioconazole

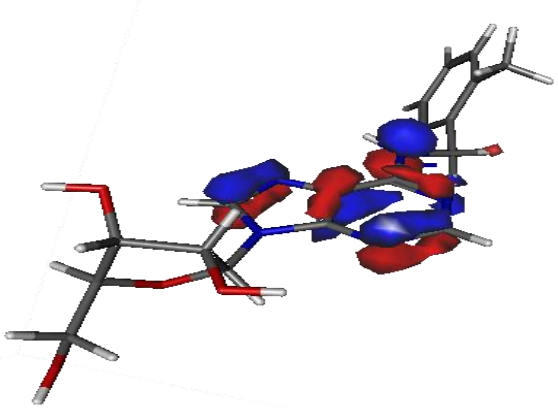


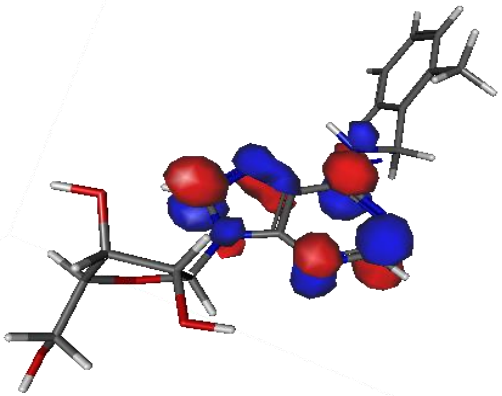




Metrifudil







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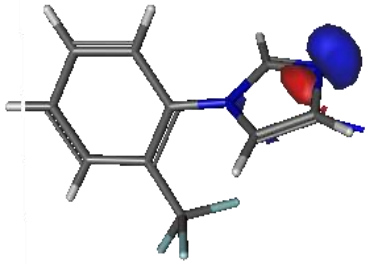
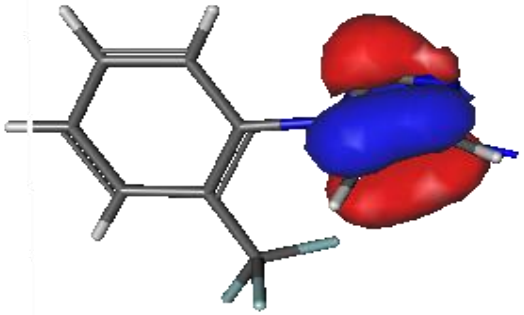
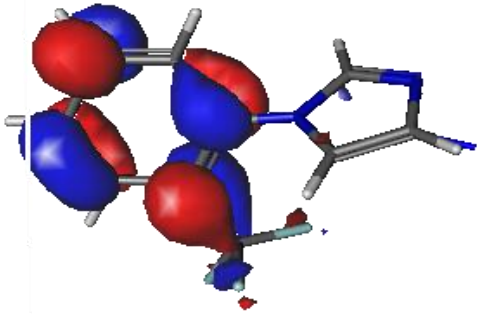
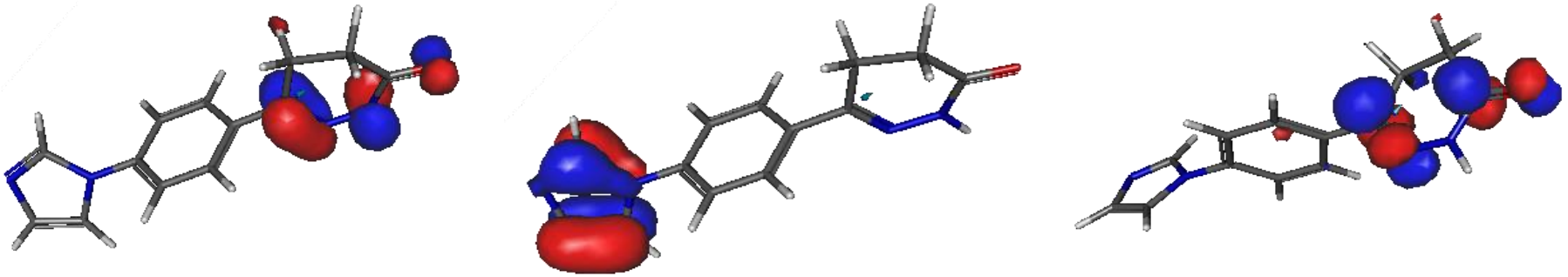






Imazodan



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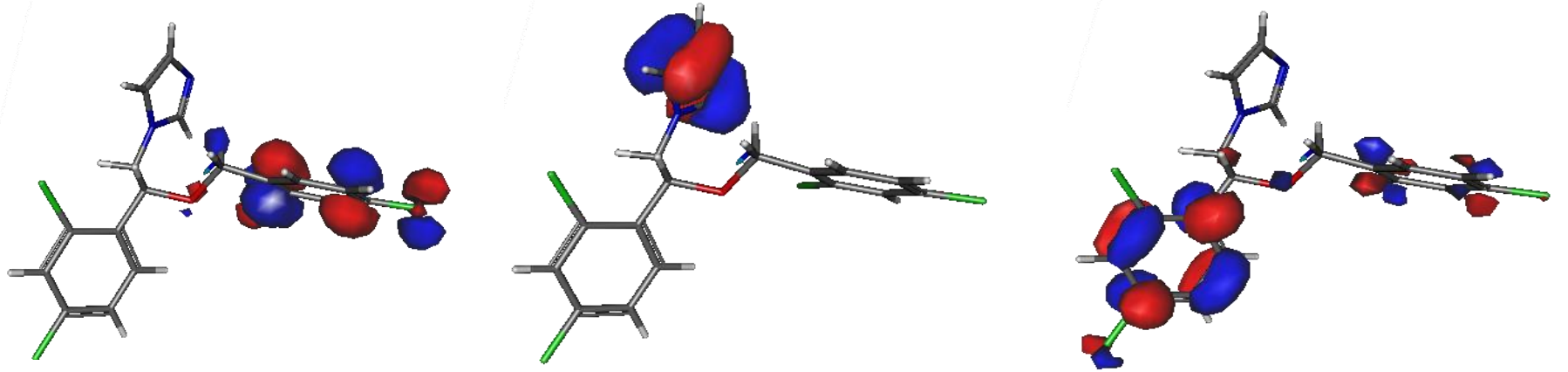

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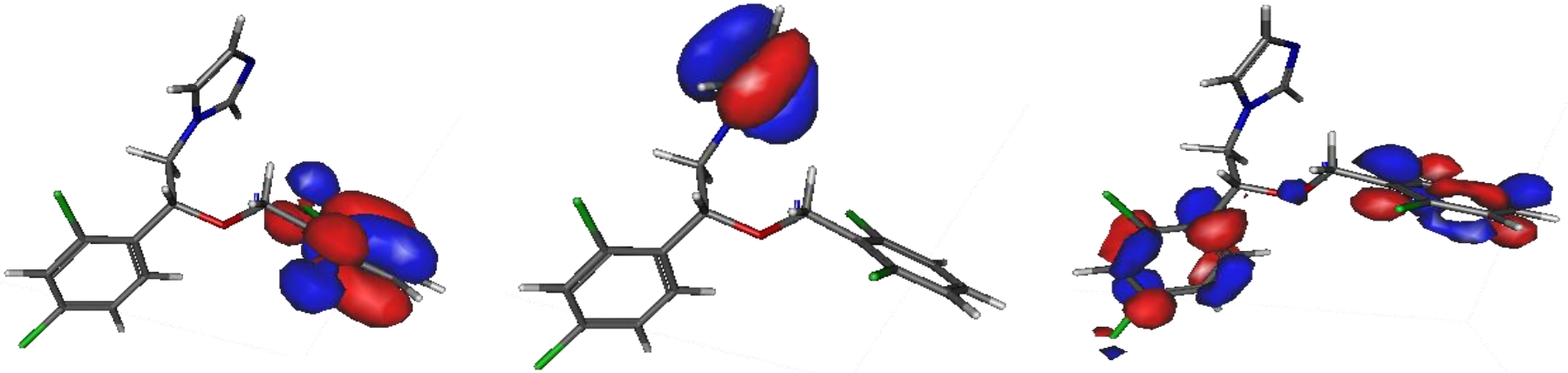
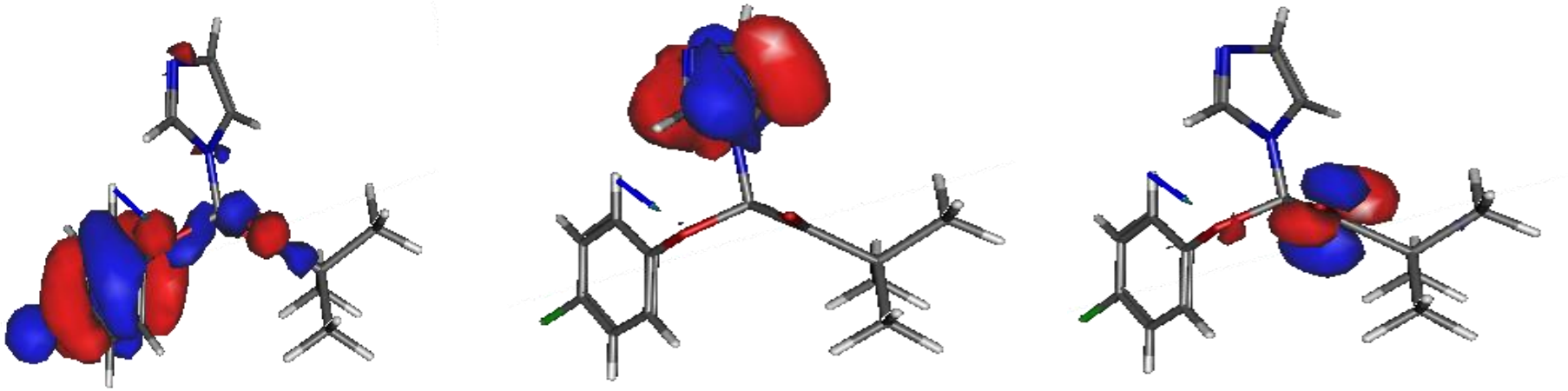


Climbazole



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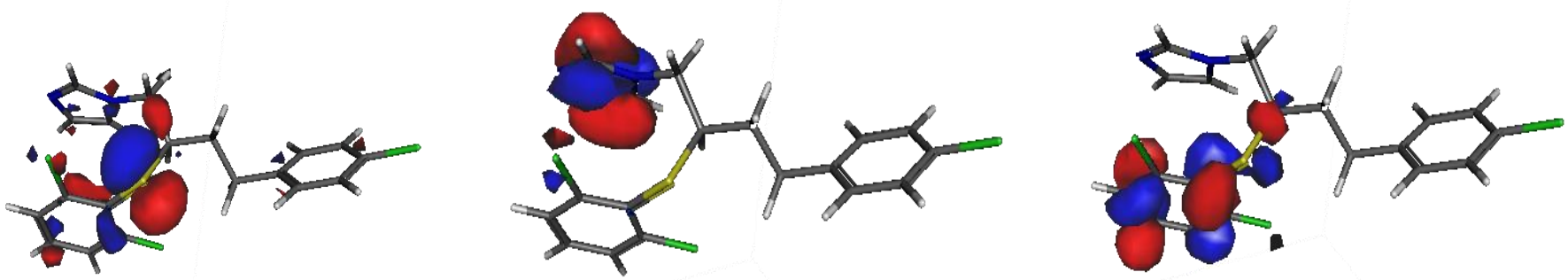

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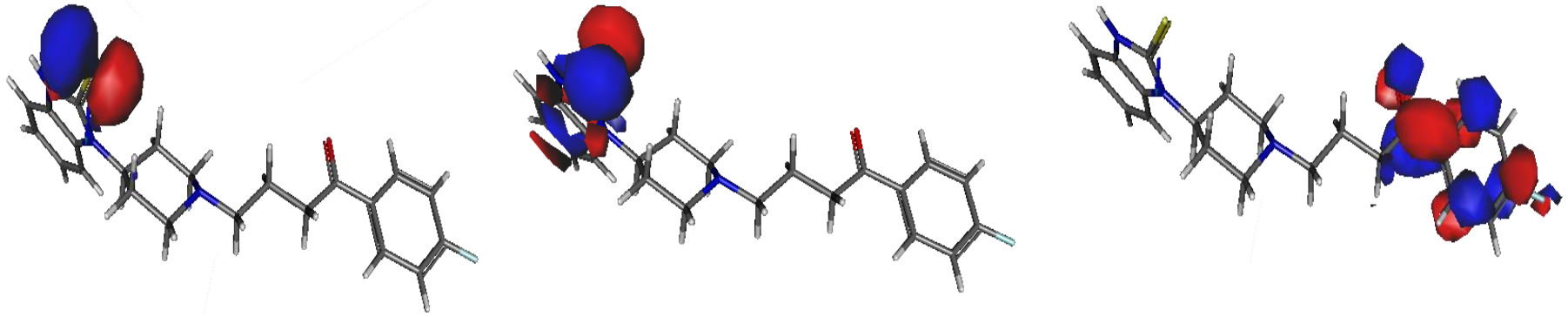

Triclabendazol
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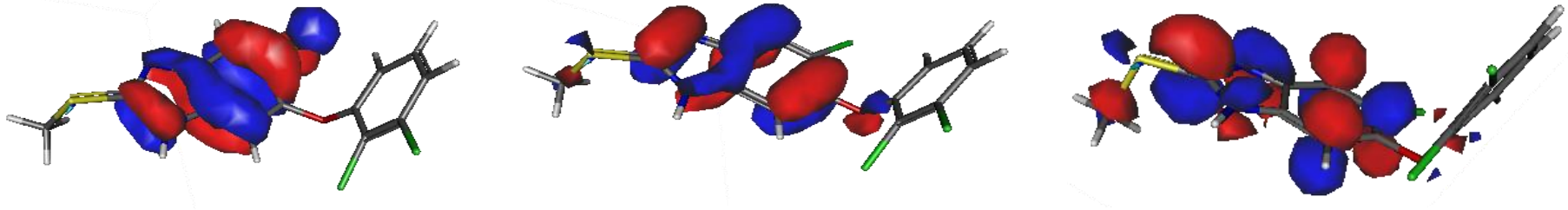
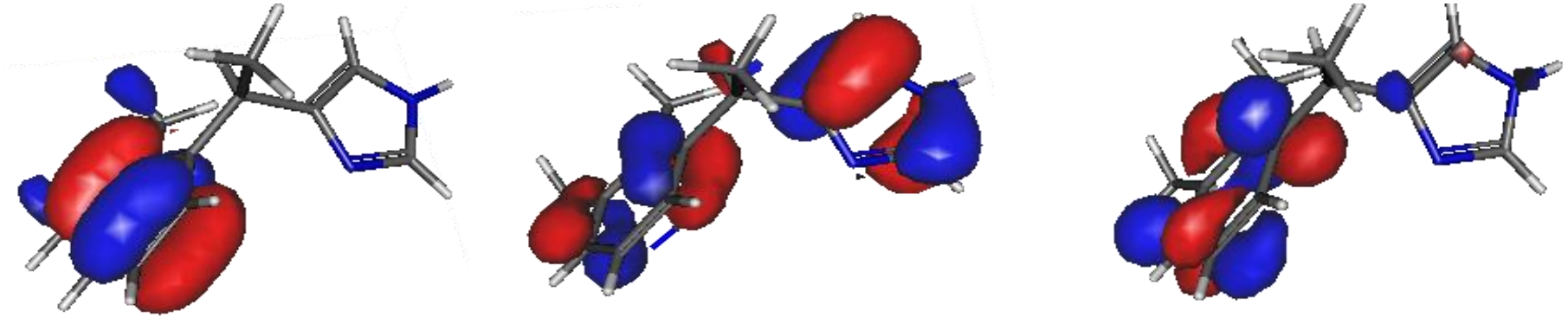
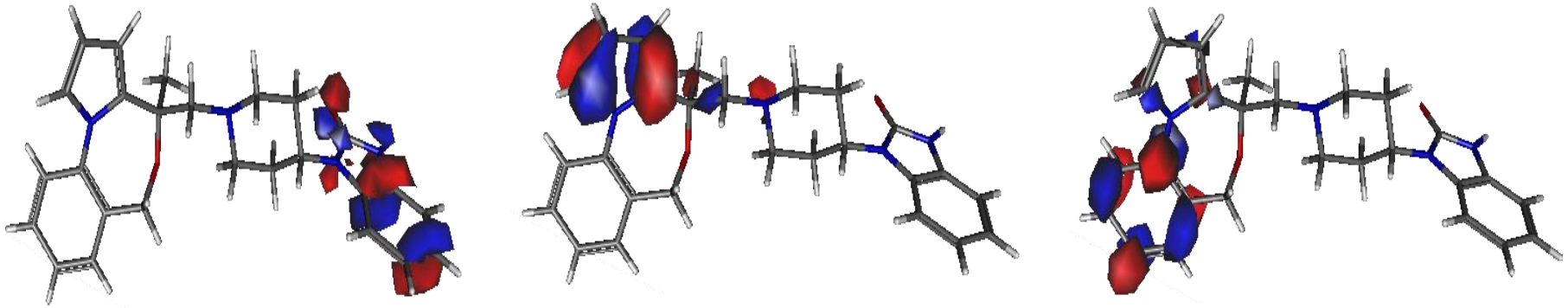


Medetomidine



Zaldaride



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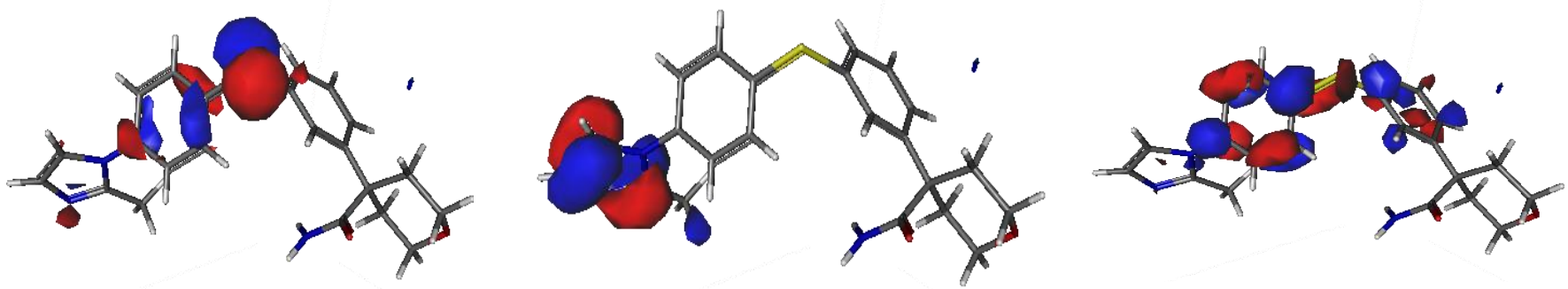

Surinabant

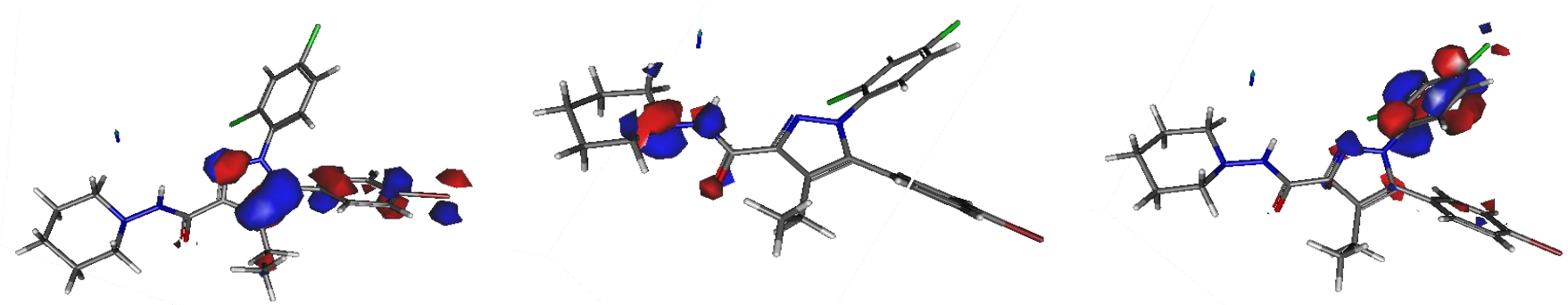

Figure S3: Representation of HOMO-1 (HOMONL), HOMO and LUMO isosurfaces of antagonist diazoles computed using the single point at B3LYP/def2-TZVP method on the structure obtained following complete optimisation with PM7

Figure S4

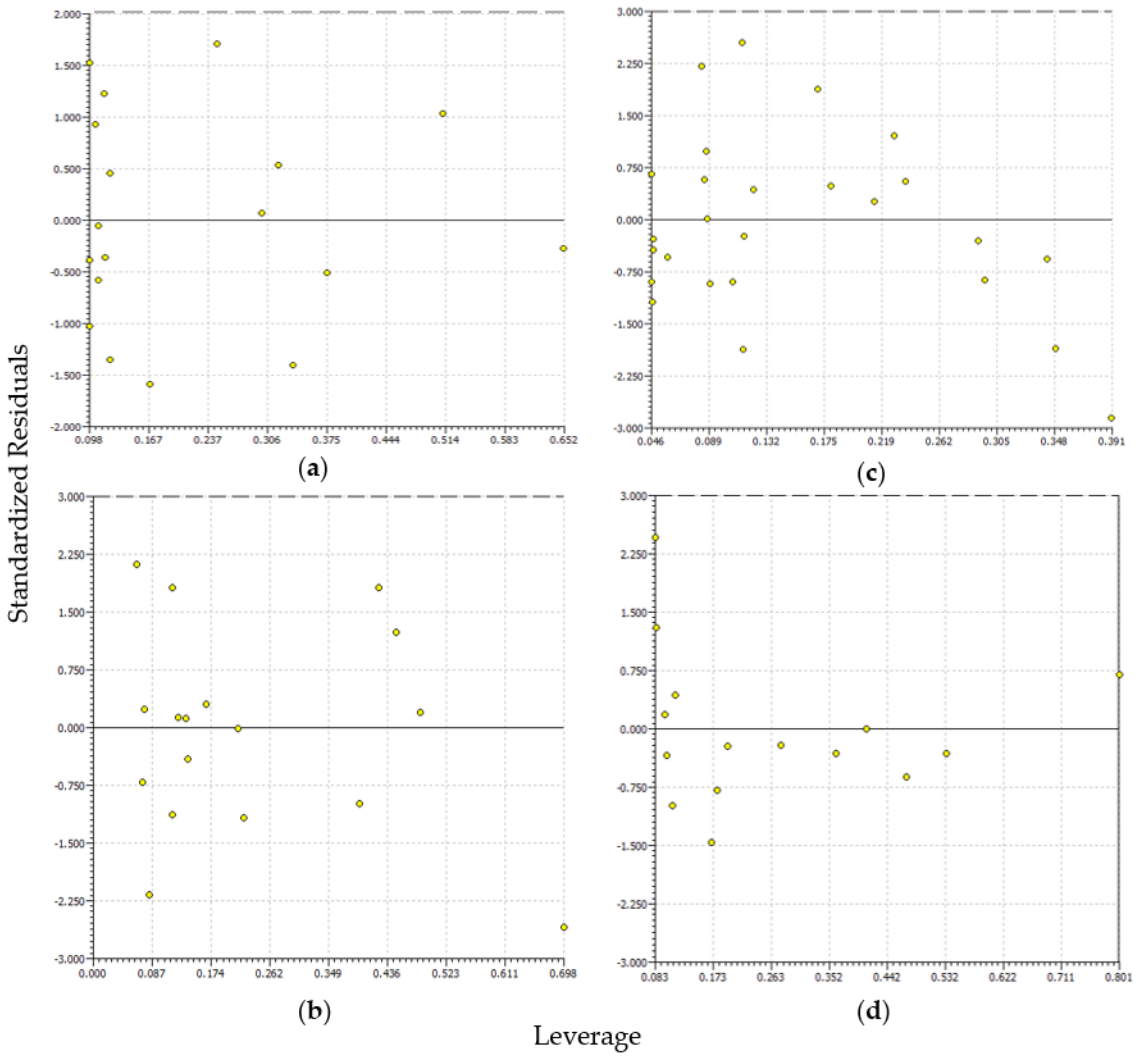

Figure S4. Williams plots of leverage vs standardised residuals for equations (1, 2, 4, 5) for: (**a**) agonist monazoles *(Thiazole/oxazole)*; (**b**) agonist Diazoles *(imidazoles and benzimidazole);* (**c**) antagonist Diazoles (*imidazoles and benzimidazole);* (**d**) antagonist Triazoles.