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Supporting information for article:

The different modes of chiral [1,2,3]triazolo[5,1-*b*][1,3,4]thiadiazines: crystal packing, conformation investigations and cellular activity

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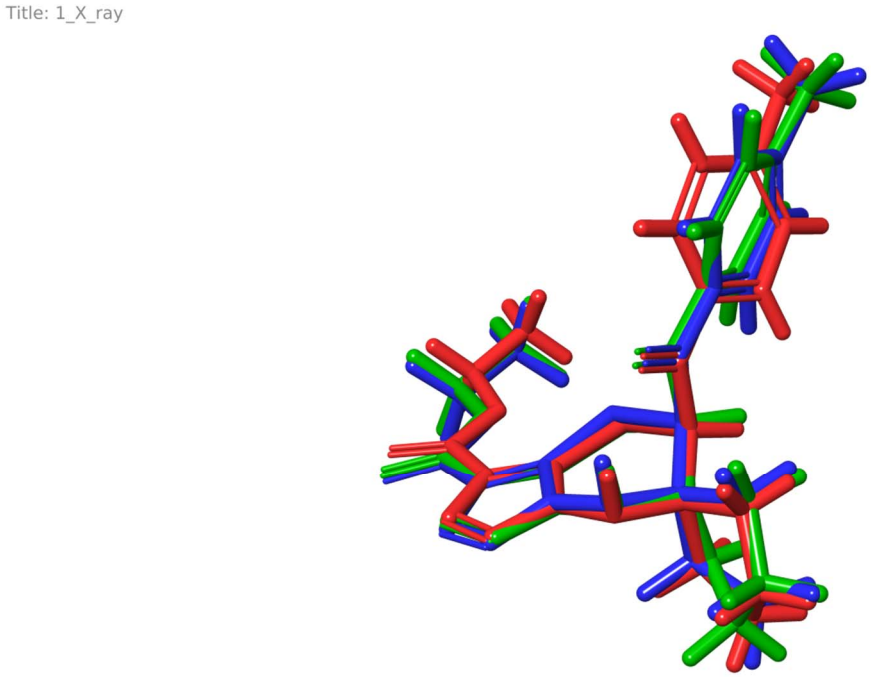


Figure S1 The superimposition showing the conformational differences between x-ray geometry (red), MM–optimized geomertry (green) and DFT–optimized geometry (blue) of the molecule (I).

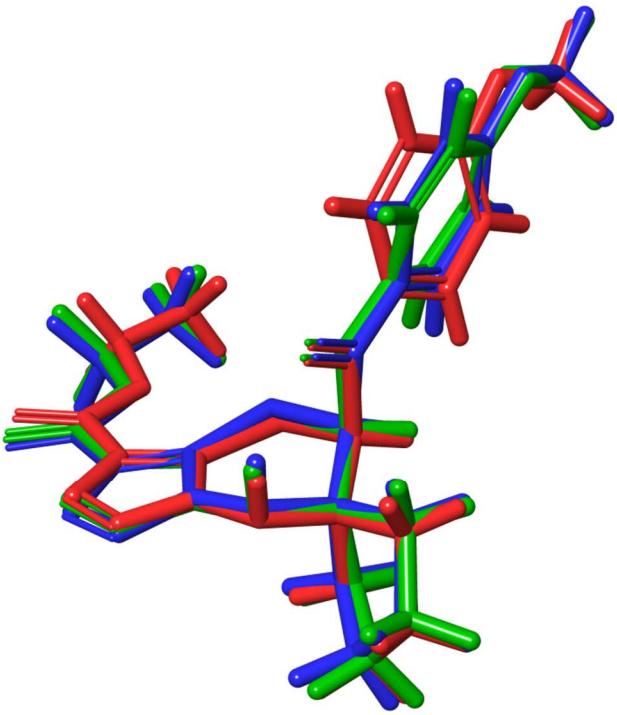


Figure S2 The superimposition showing the conformational differences between x-ray geometry (red), MM–optimized geomertry (green) and DFT–optimized geometry (blue) of the molecule (II).

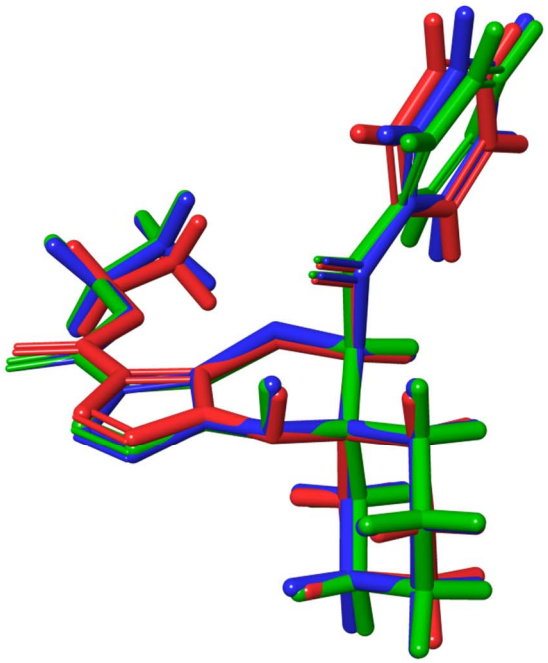


Figure S3 The superimposition showing the conformational differences between x-ray geometry (red), MM–optimized geomertry (green) and DFT–optimized geometry (blue) of the molecule (III).

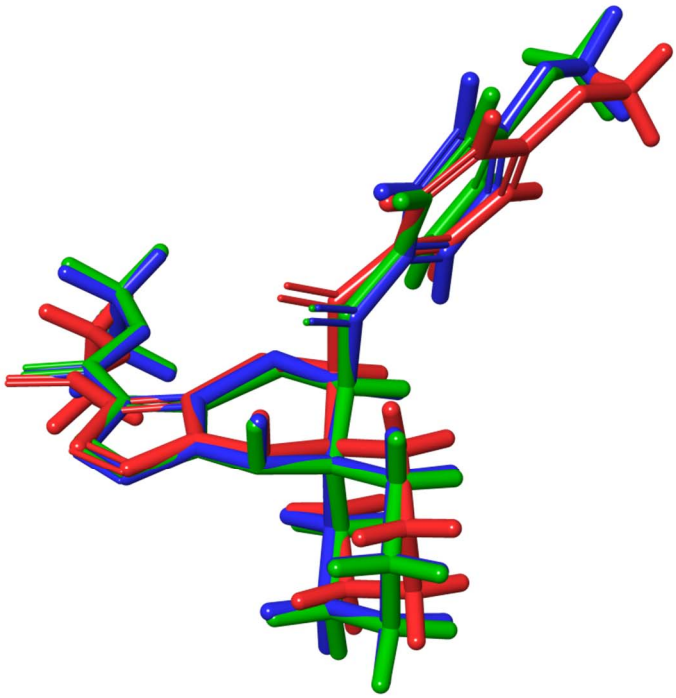


Figure S4 The superimposition showing the conformational differences between x-ray geometry (red), MM–optimized geomertry (green) and DFT–optimized geometry (blue) of the molecule (IV).

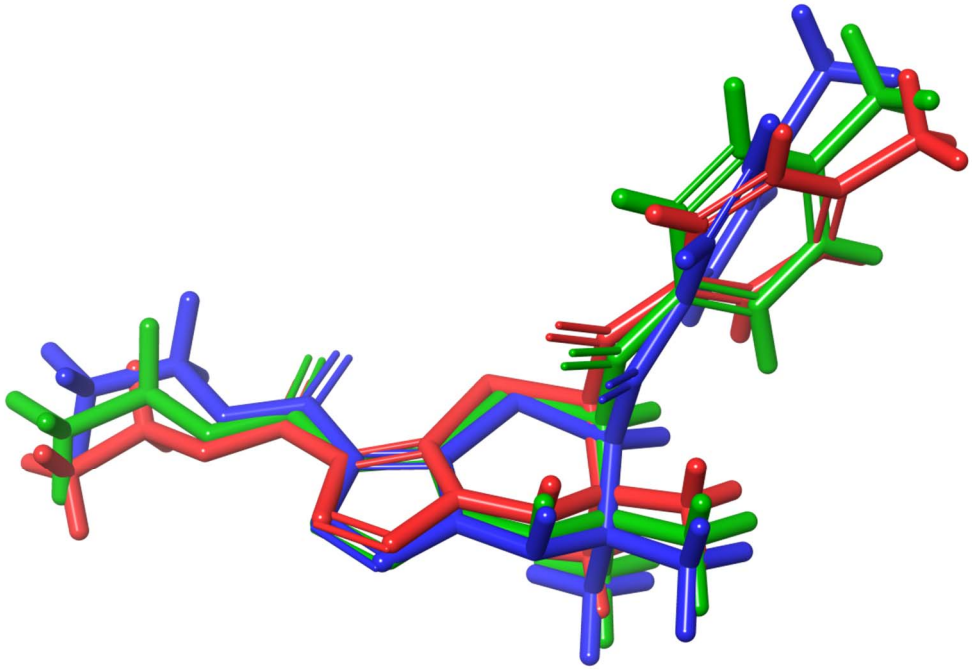


Figure S5 The superimposition showing the conformational differences between x-ray geometry (red), MM–optimized geomertry (green) and DFT–optimized geometry (blue) of the molecule (V).

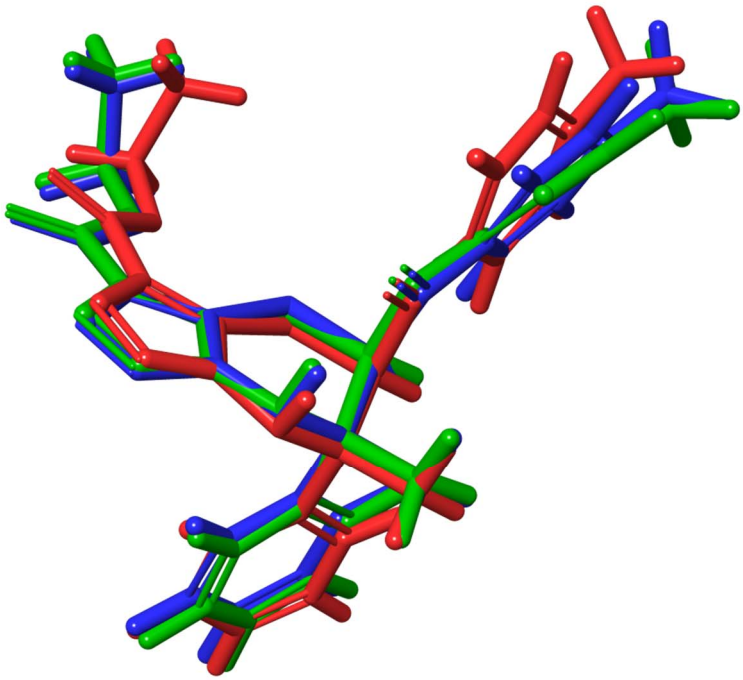


Figure S6 The superimposition showing the conformational differences between x-ray geometry (red), MM–optimized geomertry (green) and DFT–optimized geometry (blue) of the molecule (VI).

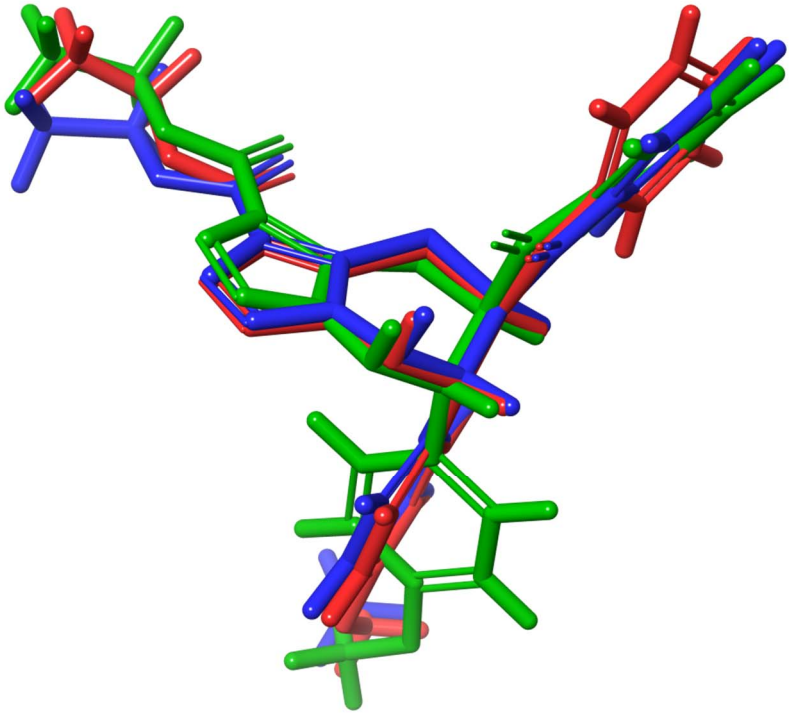


Figure S7 The superimposition showing the conformational differences between x-ray geometry (red), MM–optimized geomertry (green) and DFT–optimized geometry (blue) of the molecule (VII).

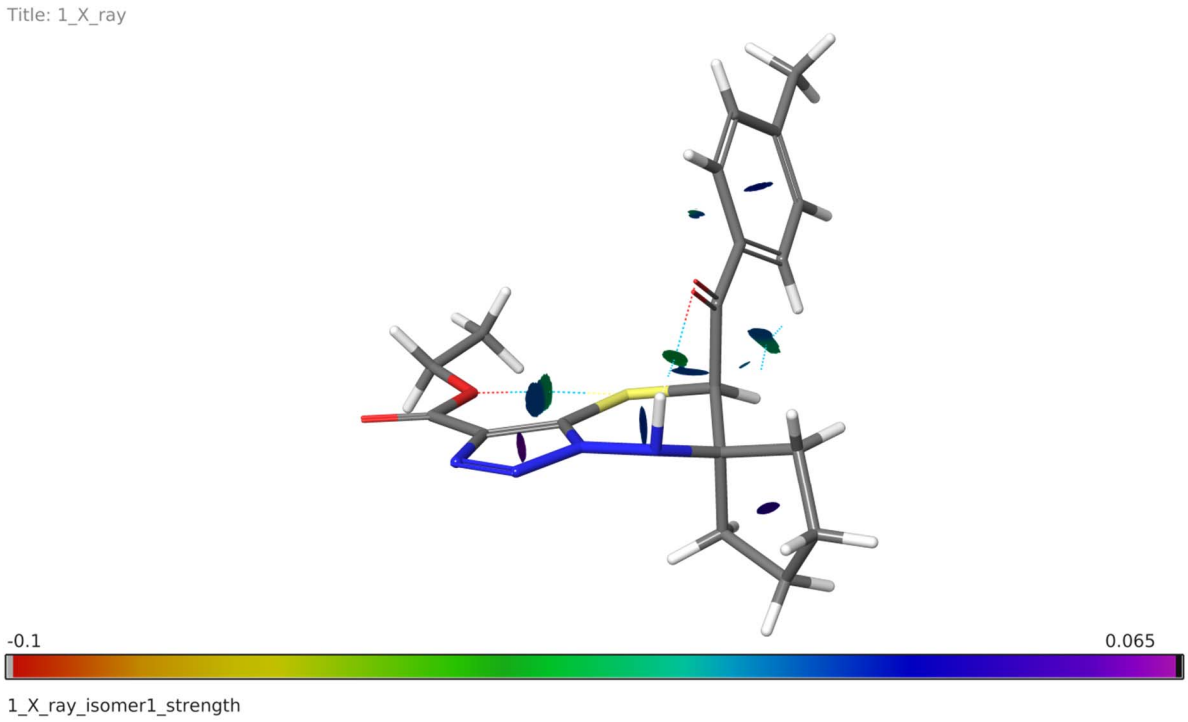


Figure S8 3D isosurface representation of the NCI plot for x-ray geometry of the molecule (I). The surfaces are colored on a rainbow scale according to values of sign(λ_2)ρ, ranging from –0.01 to +0.065 au and gradient cut-off is s = 0.30 au.

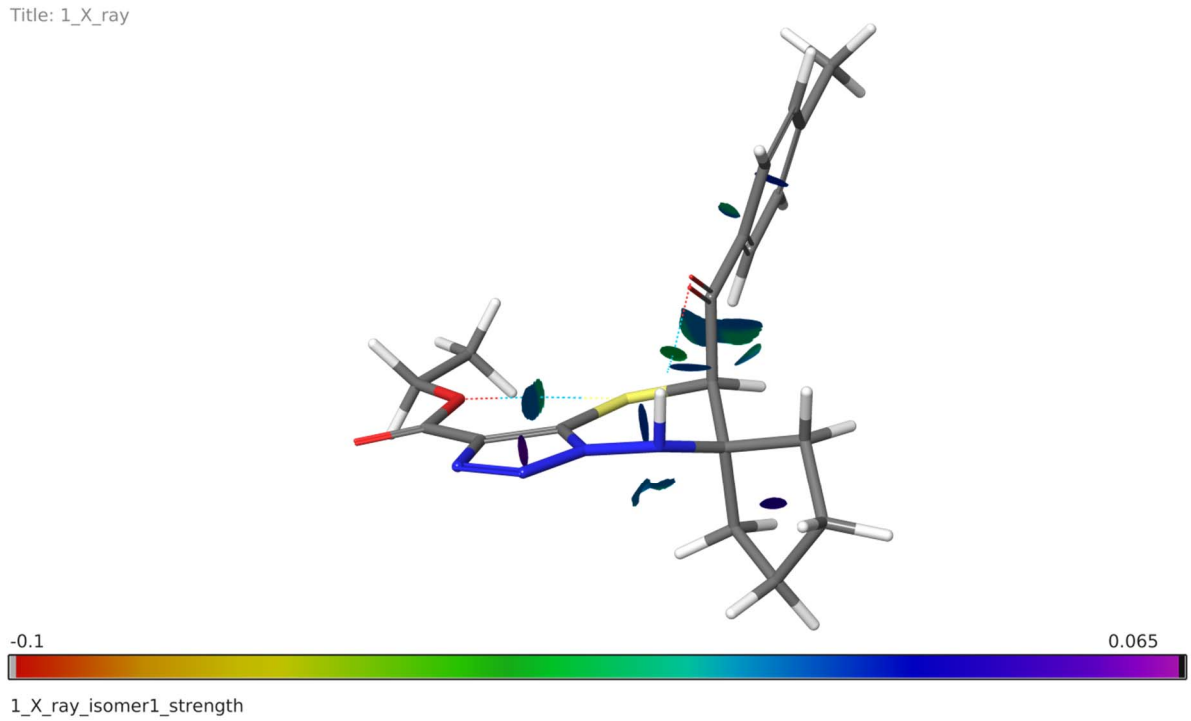


Figure S9 3D isosurface representation of the NCI plot for MM-optimized of the molecule (I). The surfaces are colored on a rainbow scale according to values of sign(λ_2)ρ, ranging from –0.01 to +0.065 au and gradient cut-off is s = 0.30 au.

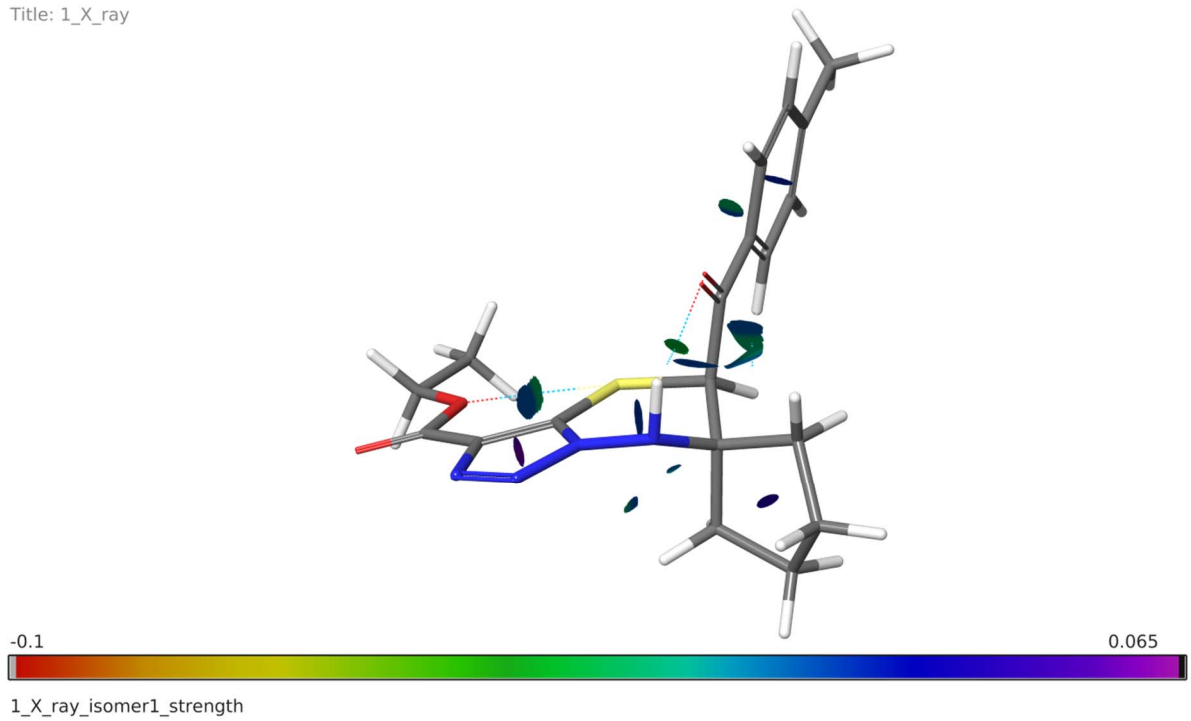


Figure S10 3D isosurface representation of the NCI plot for DFT-optimized of the molecule (I). The surfaces are colored on a rainbow scale according to values of sign(λ_2)ρ, ranging from –0.01 to +0.065 au and gradient cut-off is s = 0.30 au.

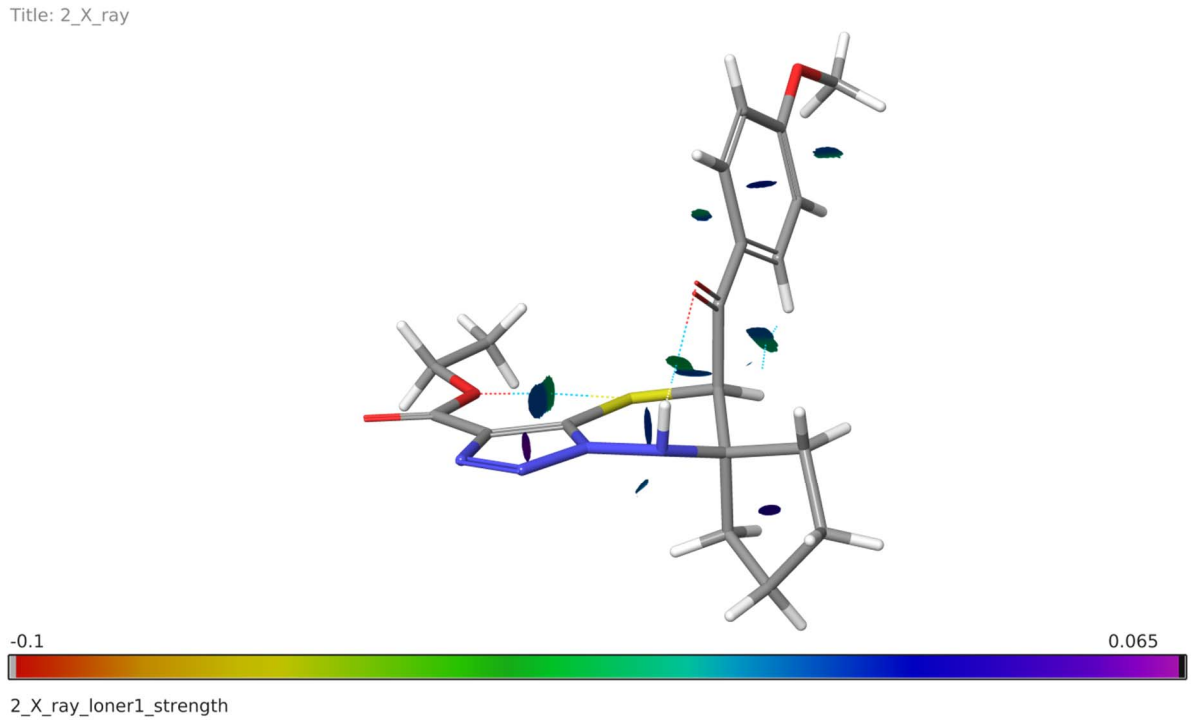


Figure S11 3D isosurface representation of the NCI plot for x-ray geometry of the molecule (II). The surfaces are colored on a rainbow scale according to values of sign(λ_2)ρ, ranging from –0.01 to +0.065 au and gradient cut-off is s = 0.30 au.

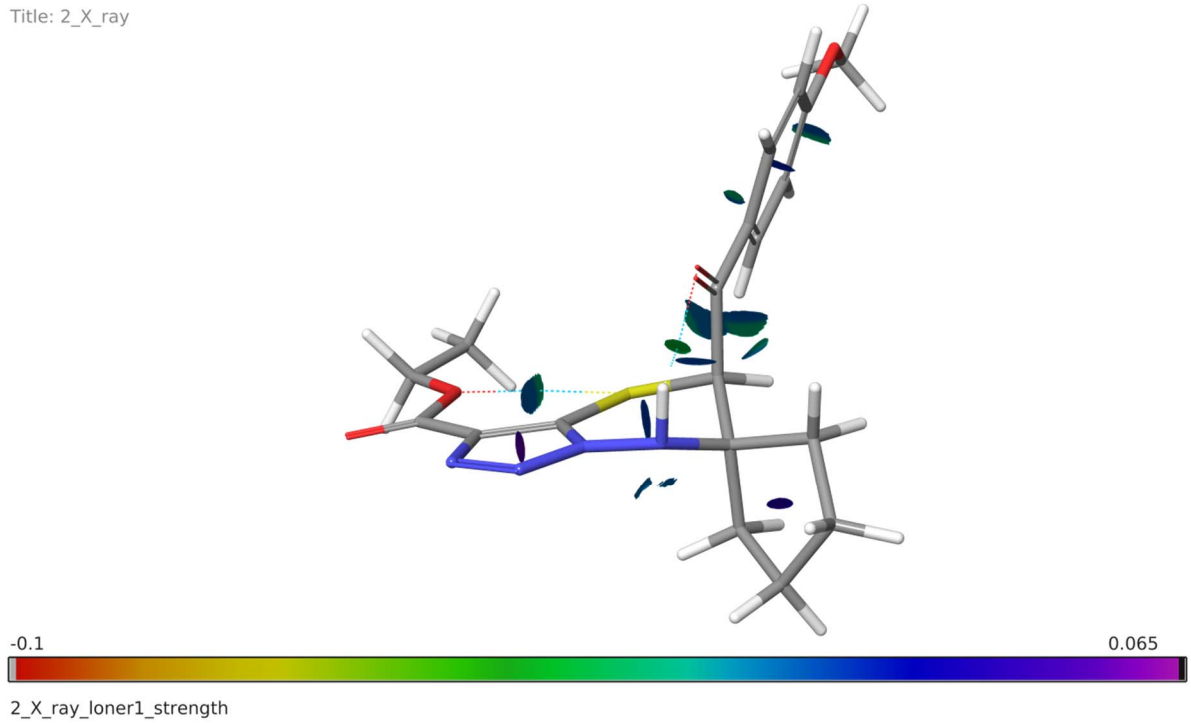


Figure S12 3D isosurface representation of the NCI plot for MM-optimized of the molecule (II). The surfaces are colored on a rainbow scale according to values of sign(λ_2)ρ, ranging from –0.01 to +0.065 au and gradient cut-off is s = 0.30 au.

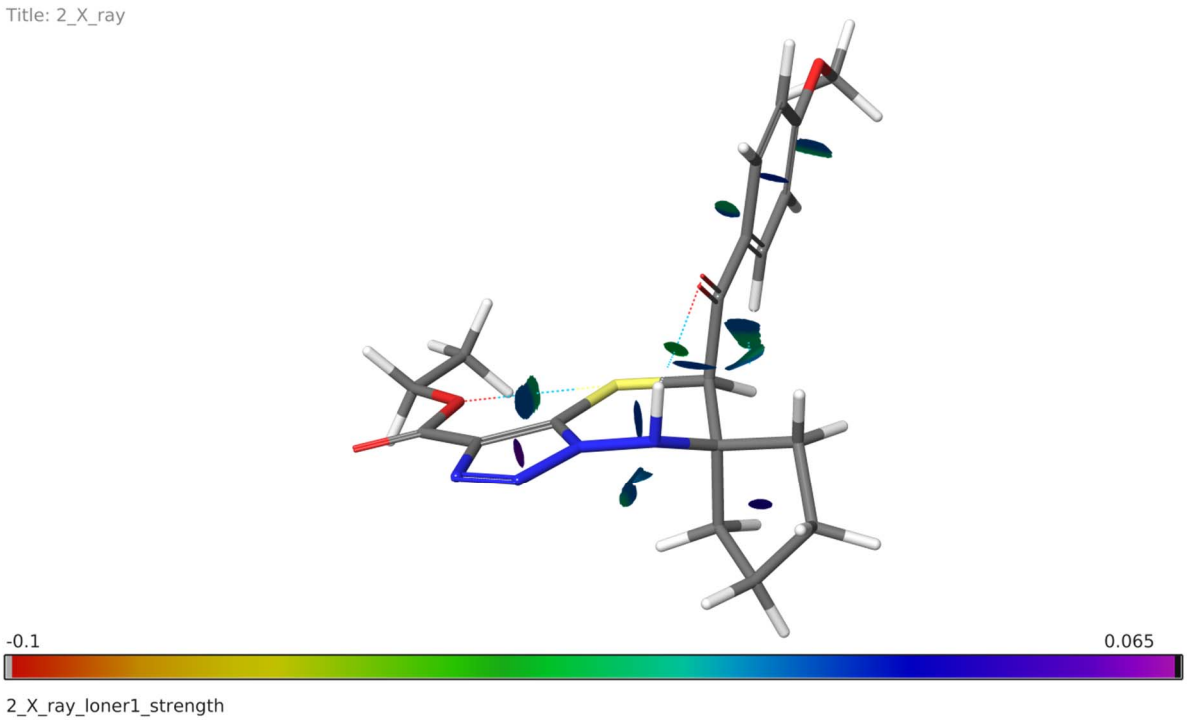


Figure S13 3D isosurface representation of the NCI plot for DFT-optimized of the molecule (II). The surfaces are colored on a rainbow scale according to values of sign(λ_2)ρ, ranging from –0.01 to +0.065 au and gradient cut-off is s = 0.30 au.

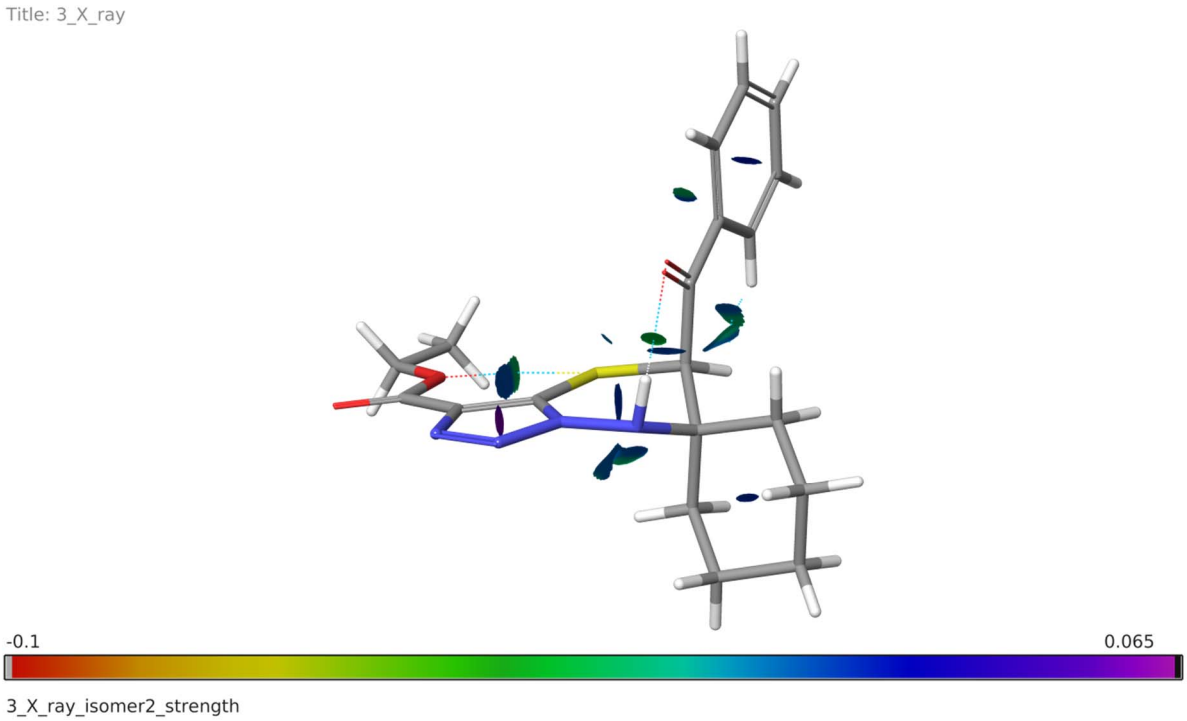


Figure S14 3D isosurface representation of the NCI plot for x-ray geometry of the molecule (III). The surfaces are colored on a rainbow scale according to values of sign(λ_2)ρ, ranging from –0.01 to +0.065 au and gradient cut-off is s = 0.30 au.

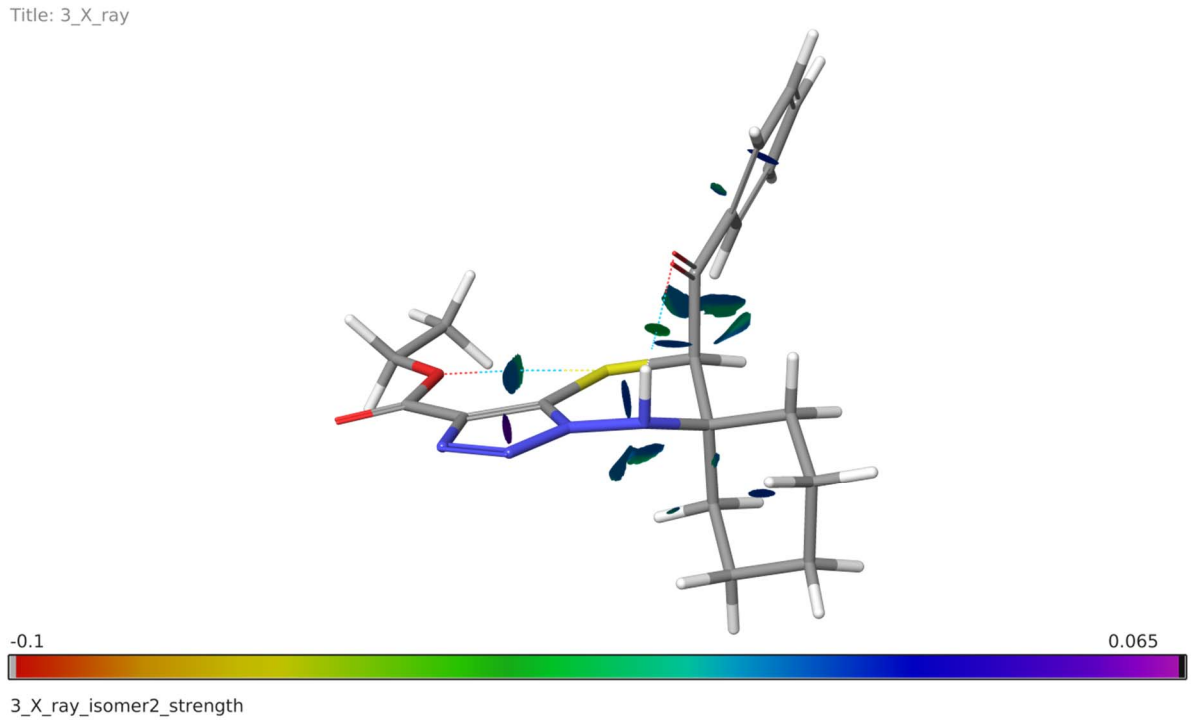


Figure S15 3D isosurface representation of the NCI plot for MM-optimized of the molecule (III). The surfaces are colored on a rainbow scale according to values of sign(λ_2)ρ, ranging from –0.01 to +0.065 au and gradient cut-off is s = 0.30 au.

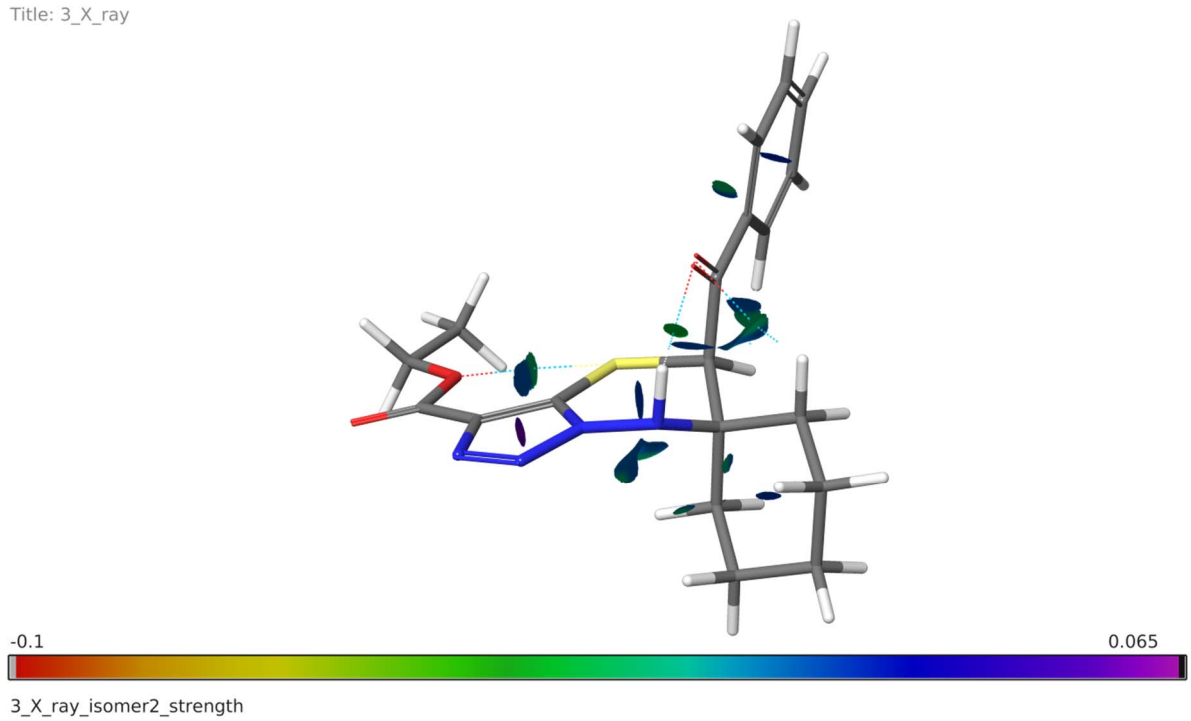


Figure S16 3D isosurface representation of the NCI plot for DFT-optimized of the molecule (III). The surfaces are colored on a rainbow scale according to values of sign(λ_2)ρ, ranging from –0.01 to +0.065 au and gradient cut-off is s = 0.30 au.

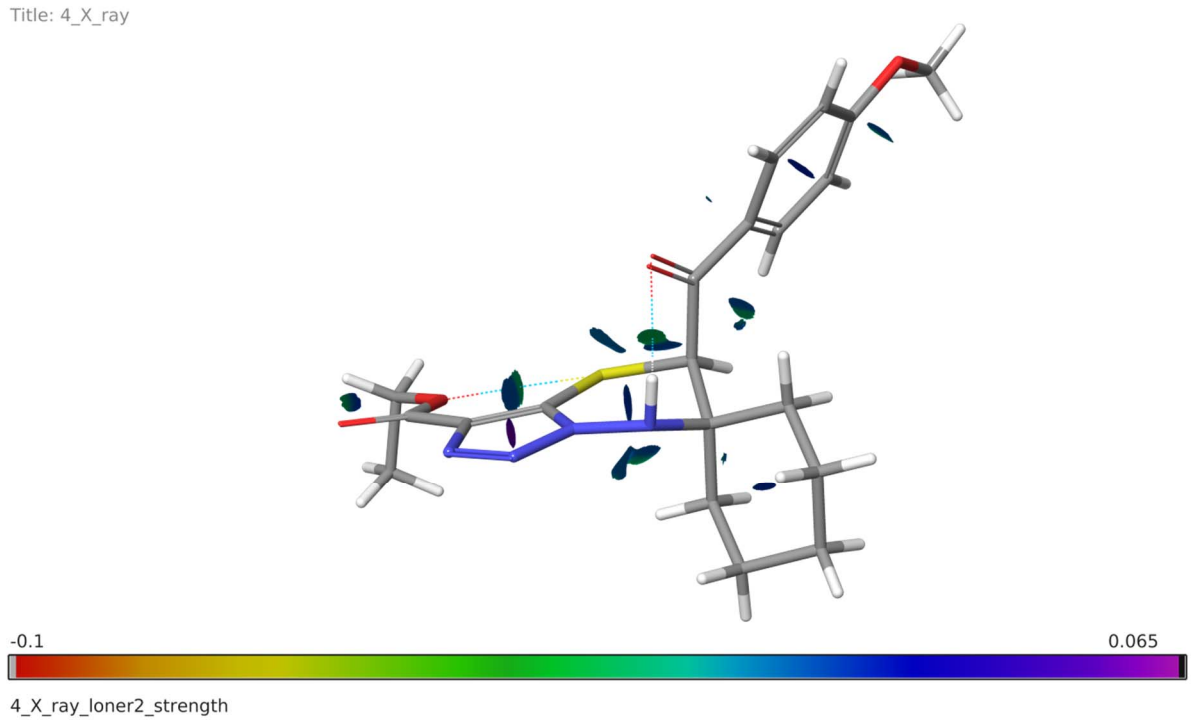


Figure S17 3D isosurface representation of the NCI plot for x-ray geometry of the molecule (IV). The surfaces are colored on a rainbow scale according to values of sign(λ_2)ρ, ranging from –0.01 to +0.065 au and gradient cut-off is s = 0.30 au.

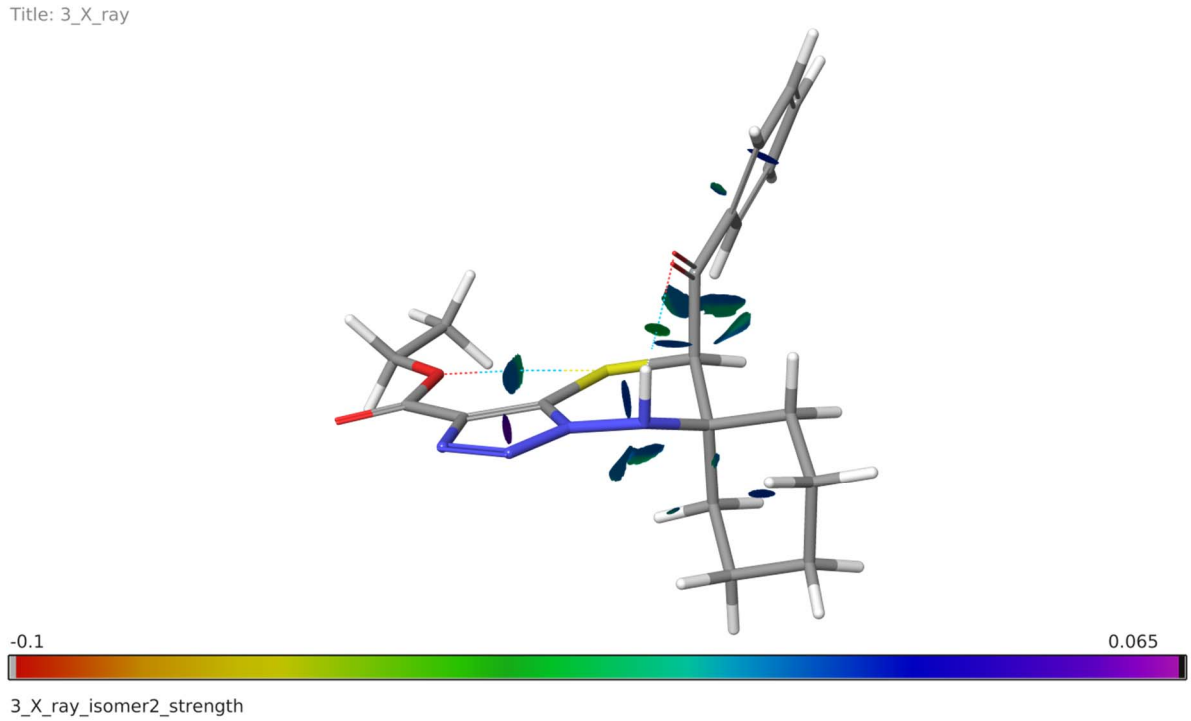


Figure S18 3D isosurface representation of the NCI plot for MM-optimized of the molecule (IV). The surfaces are colored on a rainbow scale according to values of sign(λ_2)ρ, ranging from –0.01 to +0.065 au and gradient cut-off is s = 0.30 au.

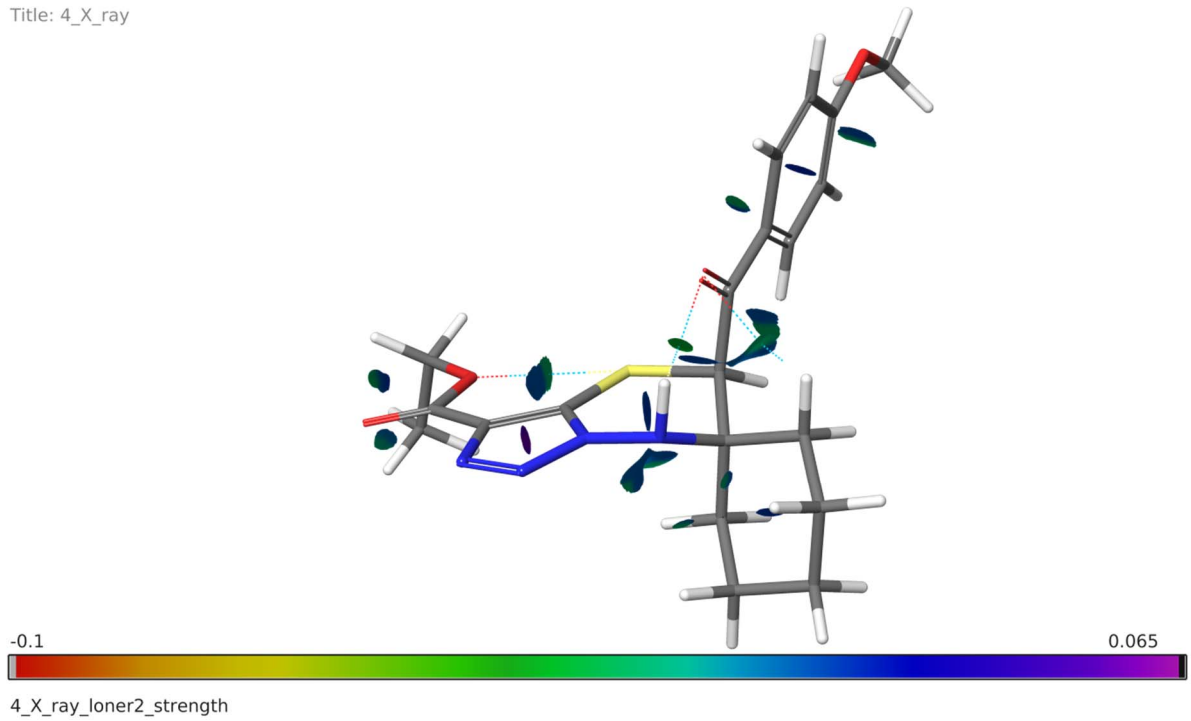


Figure S19 3D isosurface representation of the NCI plot for DFT-optimized of the molecule (IV). The surfaces are colored on a rainbow scale according to values of sign(λ_2)ρ, ranging from –0.01 to +0.065 au and gradient cut-off is s = 0.30 au.

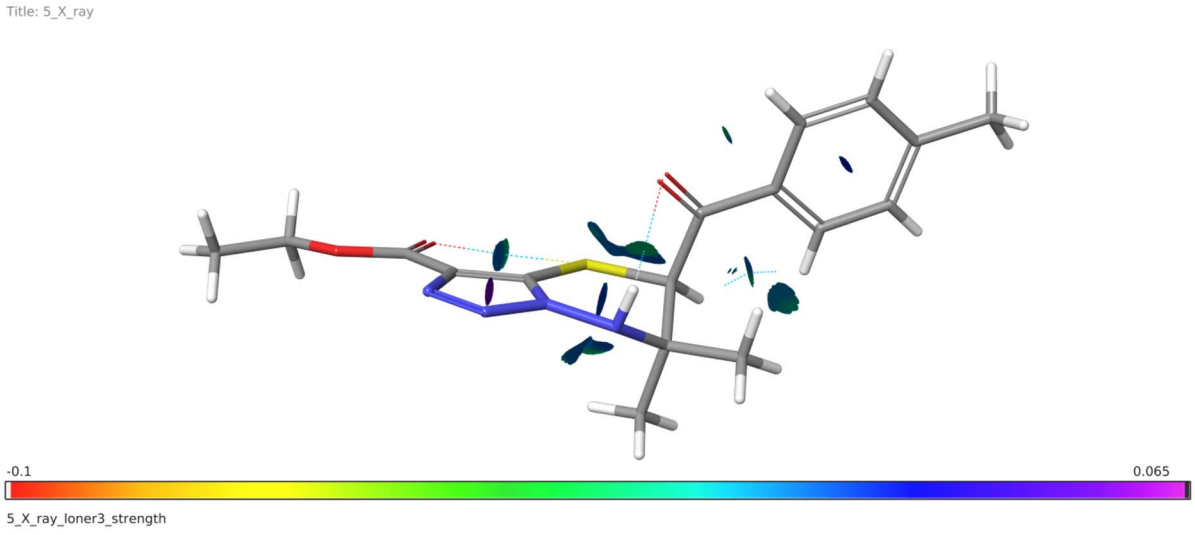


Figure S20 3D isosurface representation of the NCI plot for x-ray geometry of the molecule (V). The surfaces are colored on a rainbow scale according to values of sign(λ_2)ρ, ranging from –0.01 to +0.065 au and gradient cut-off is s = 0.30 au.

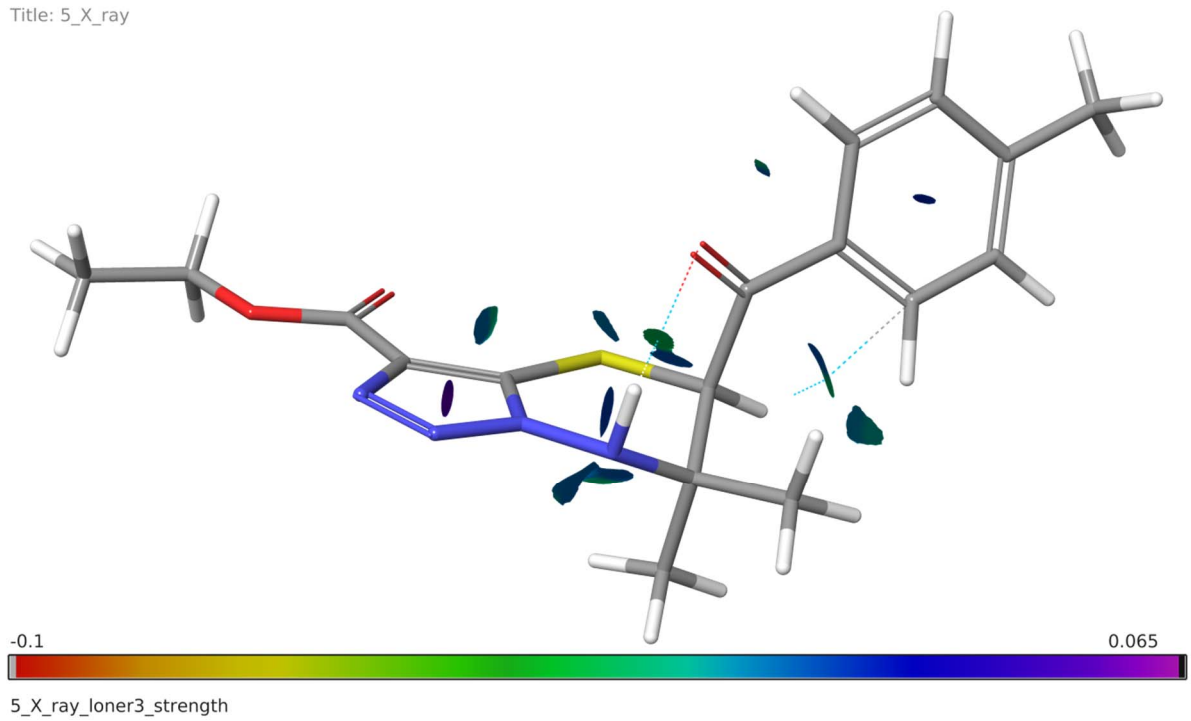


Figure S21 3D isosurface representation of the NCI plot for MM-optimized of the molecule (V). The surfaces are colored on a rainbow scale according to values of sign(λ_2)ρ, ranging from –0.01 to +0.065 au and gradient cut-off is s = 0.30 au.

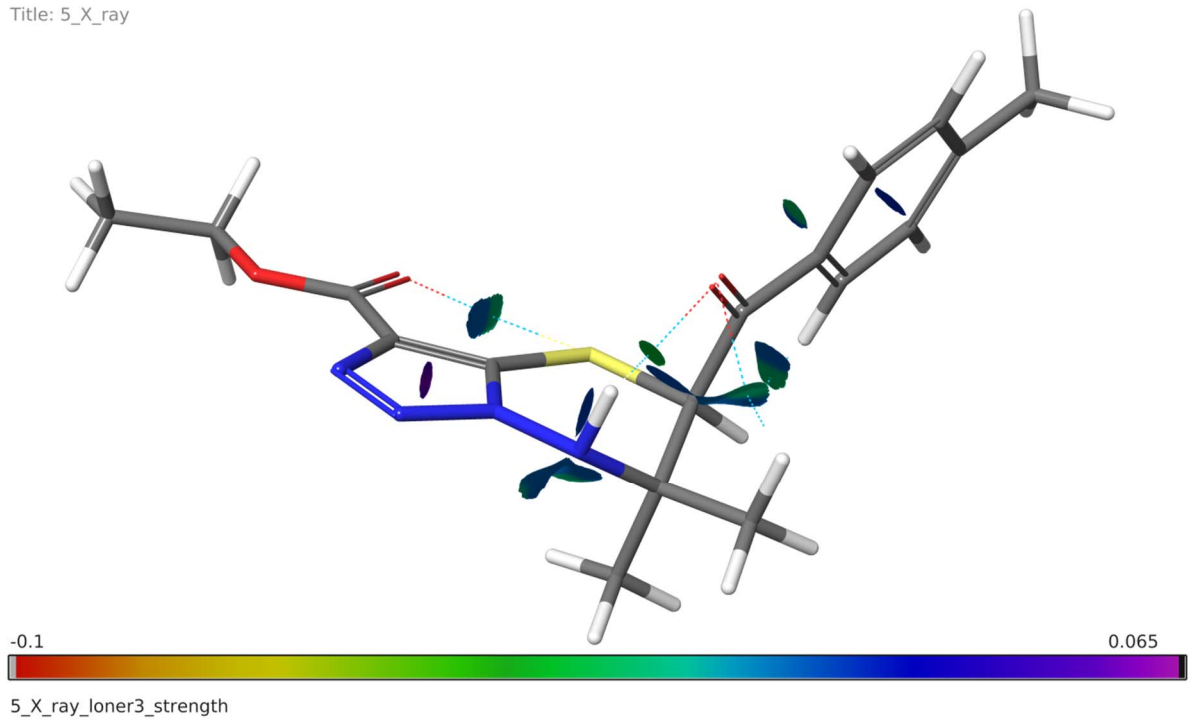


Figure S22 3D isosurface representation of the NCI plot for DFT-optimized of the molecule (V). The surfaces are colored on a rainbow scale according to values of sign(λ_2)ρ, ranging from –0.01 to +0.065 au and gradient cut-off is s = 0.30 au.

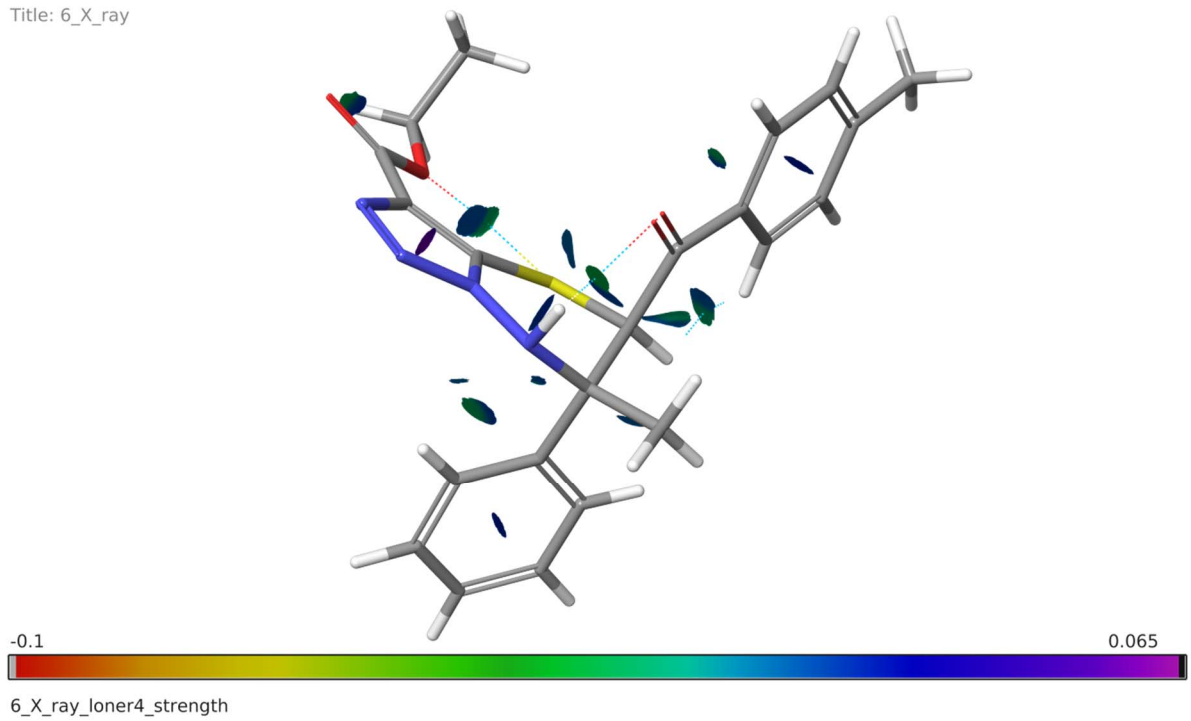


Figure S23 3D isosurface representation of the NCI plot for x-ray geometry of the molecule (VI). The surfaces are colored on a rainbow scale according to values of sign(λ_2)ρ, ranging from –0.01 to +0.065 au and gradient cut-off is s = 0.30 au.

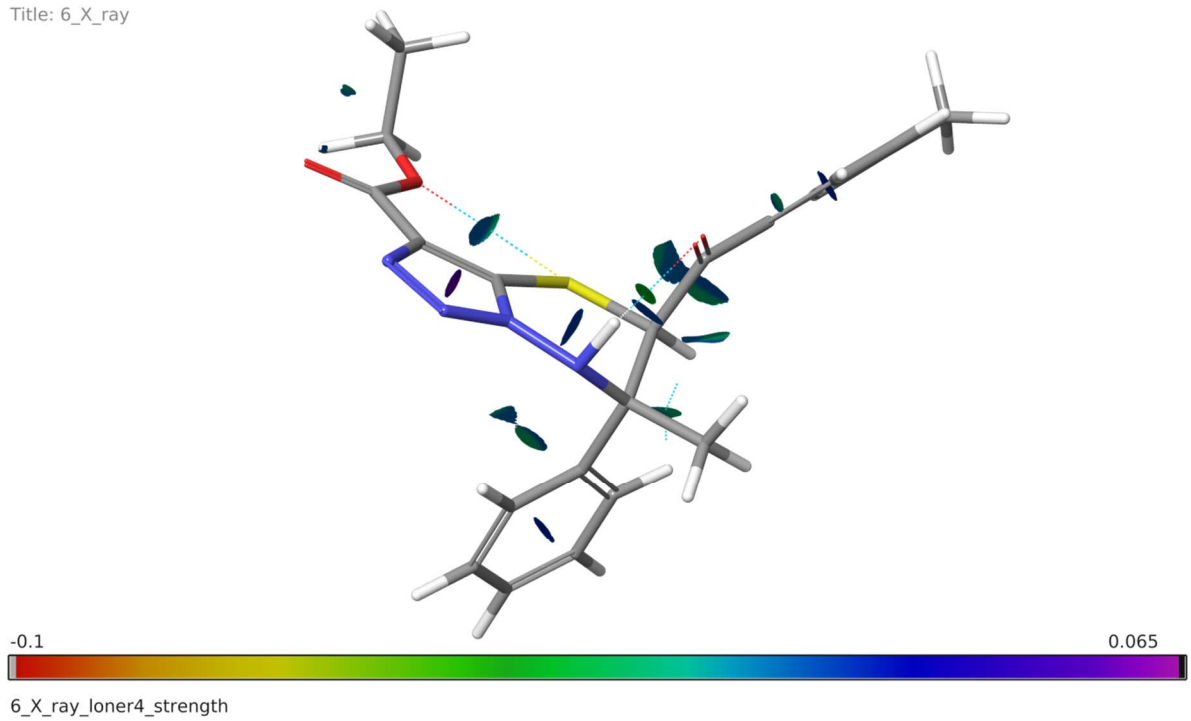


Figure S24 3D isosurface representation of the NCI plot for MM-optimized of the molecule (VI). The surfaces are colored on a rainbow scale according to values of sign(λ_2)ρ, ranging from –0.01 to +0.065 au and gradient cut-off is s = 0.30 au.

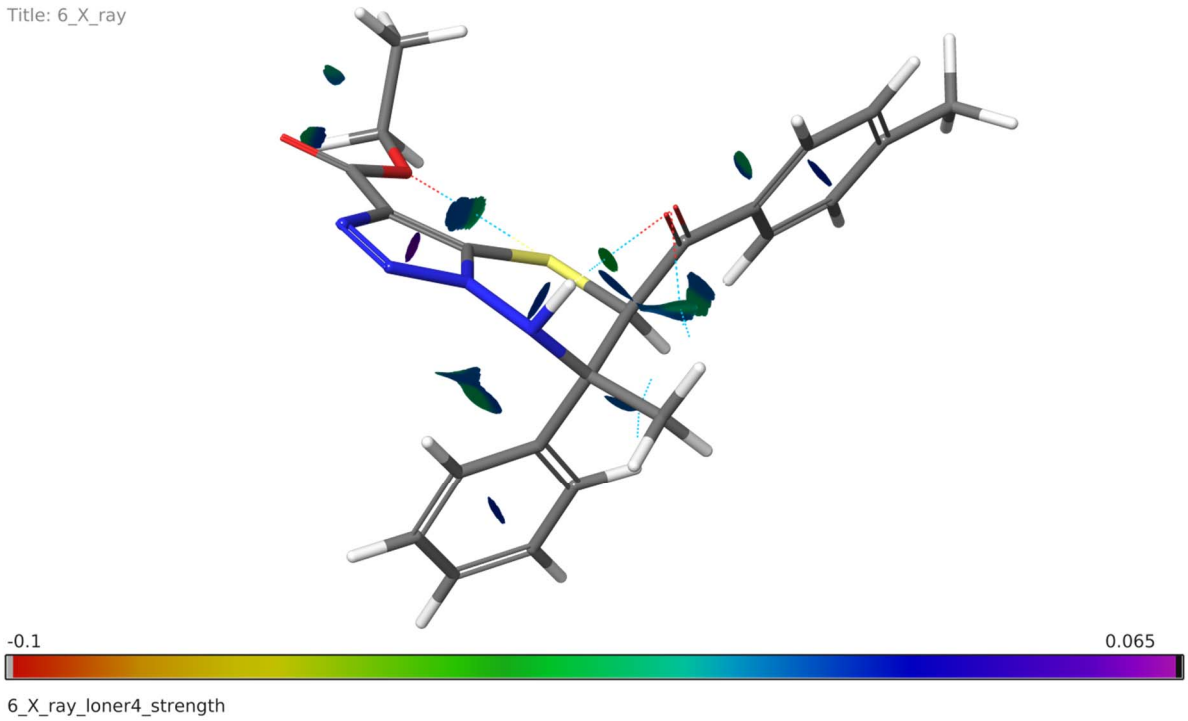


Figure S25 3D isosurface representation of the NCI plot for DFT-optimized of the molecule (VI). The surfaces are colored on a rainbow scale according to values of sign(λ_2)ρ, ranging from –0.01 to +0.065 au and gradient cut-off is s = 0.30 au.

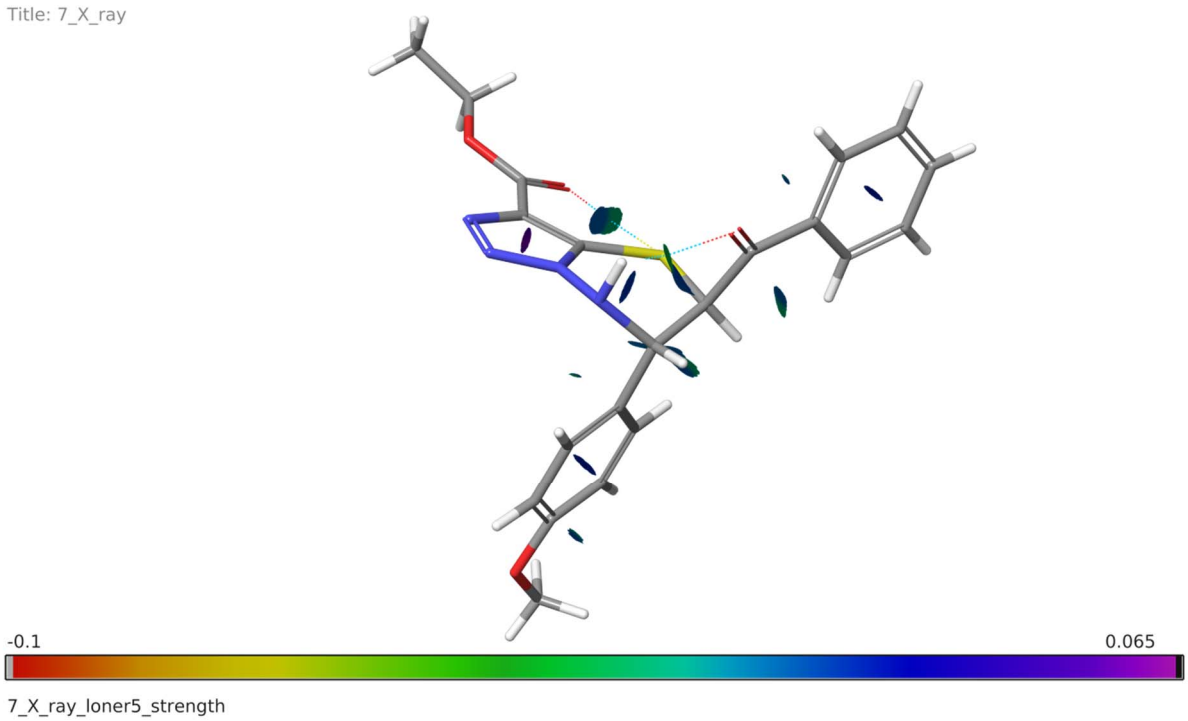


Figure S26 3D isosurface representation of the NCI plot for x-ray geometry of the molecule (VII). The surfaces are colored on a rainbow scale according to values of sign(λ_2)ρ, ranging from –0.01 to +0.065 au and gradient cut-off is s = 0.30 au.

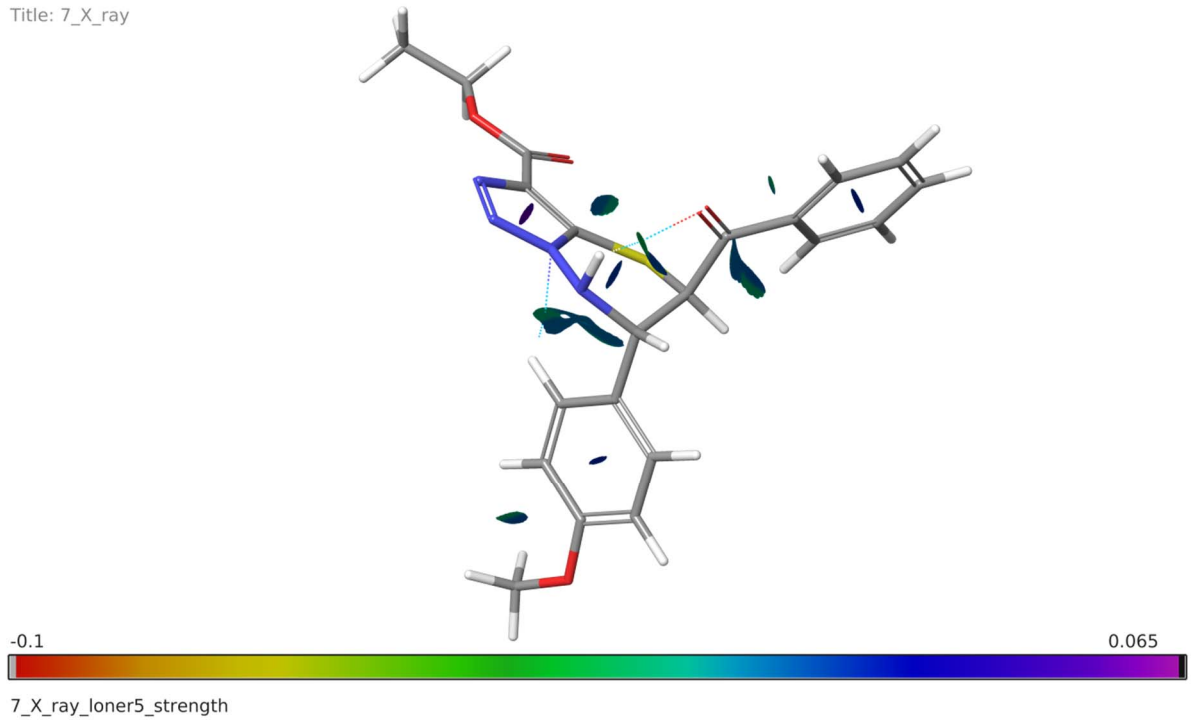


Figure S27 3D isosurface representation of the NCI plot for MM-optimized of the molecule (VII). The surfaces are colored on a rainbow scale according to values of sign(λ_2)ρ, ranging from –0.01 to +0.065 au and gradient cut-off is s = 0.30 au.

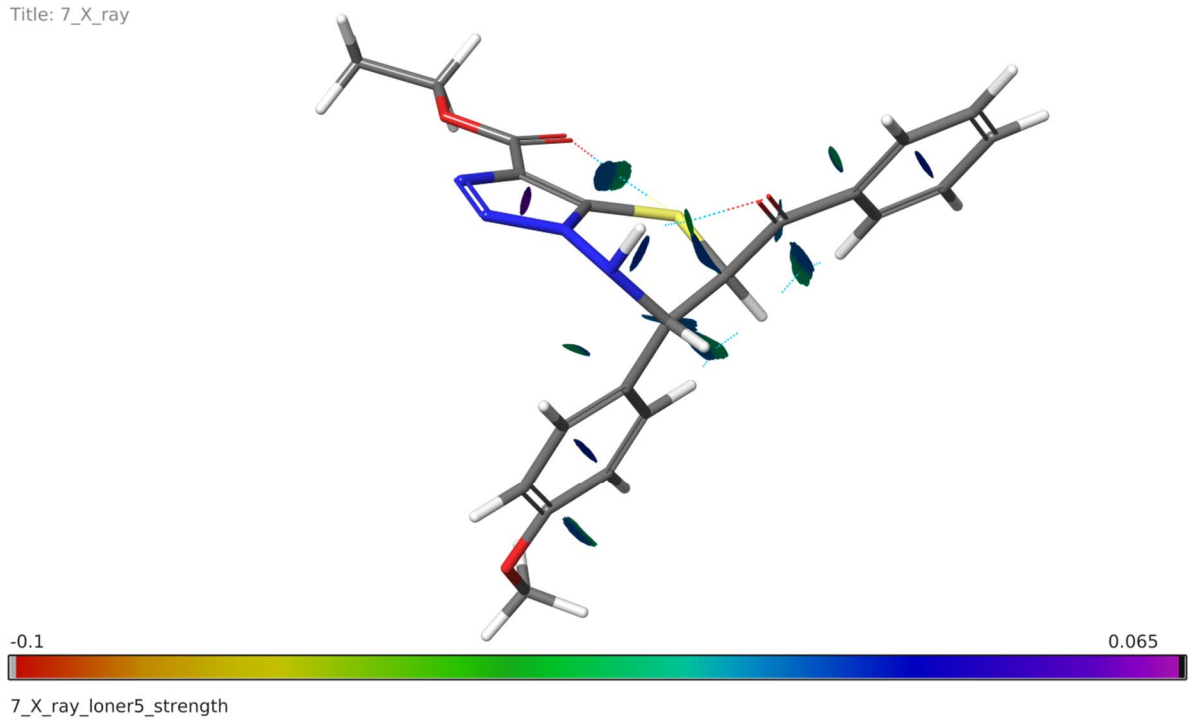


Figure S28 3D isosurface representation of the NCI plot for DFT-optimized of the molecule (VII). The surfaces are colored on a rainbow scale according to values of sign(λ_2)ρ, ranging from –0.01 to +0.065 au and gradient cut-off is s = 0.30 au.

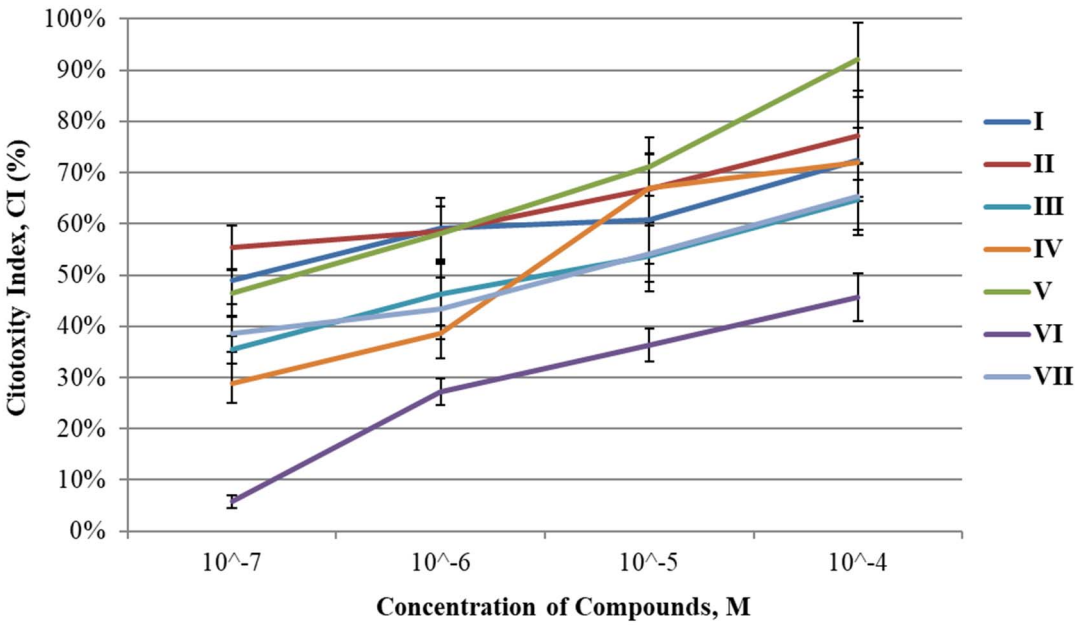


Figure S29 Toxic effects of compounds **I–VII** with increasing concentrations (10^{-7}–10^{-4} mol/L) on proliferation of Hela cells for 72 h, the proliferative response was assessed by MTT assay.

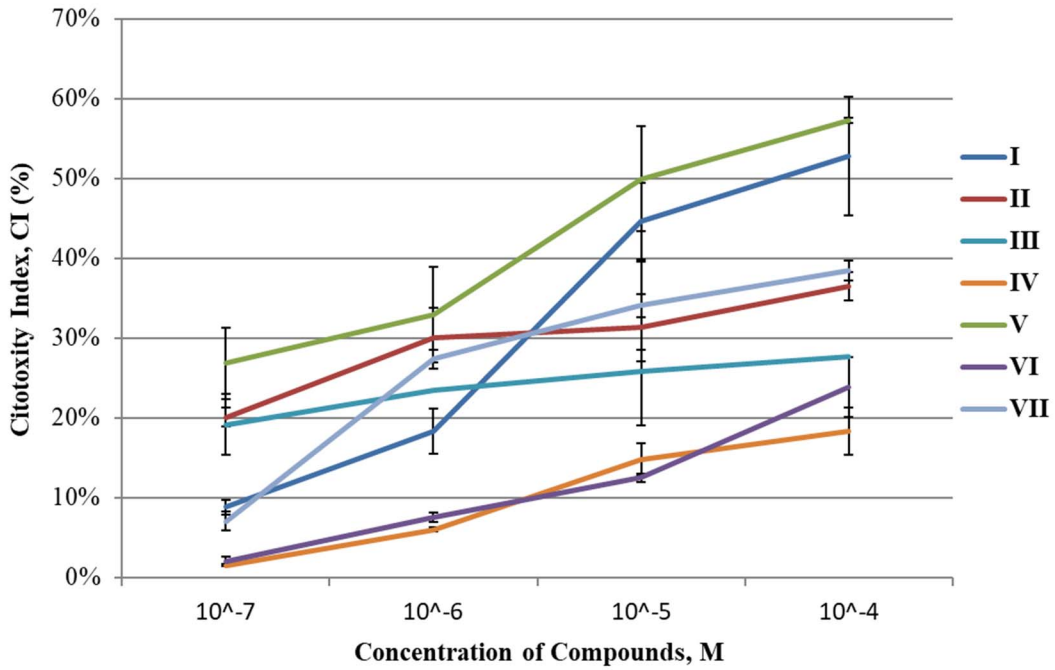


Figure S30 Toxic effects of Compounds **I–VII** with increasing concentrations (10^{-7}–10^{-4} mol/L) on proliferation of RD cells for 72 h, the proliferative response was assessed by MTT assay.

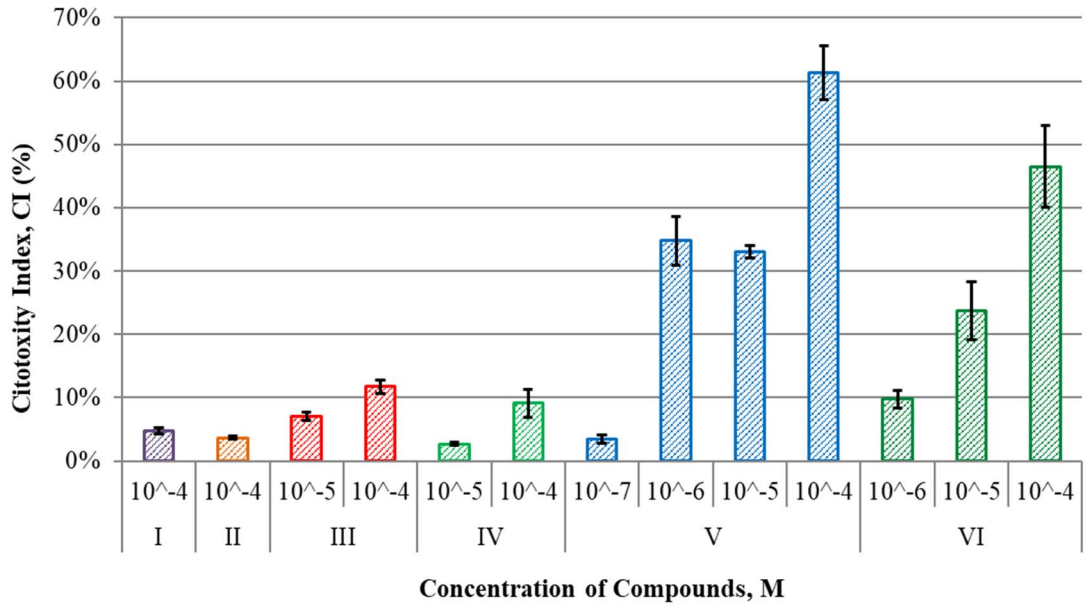


Figure S31 Toxic effects of some concentrations of compounds **I–VII** on proliferation of HEK293 cells for 72 h, the proliferative response was assessed by MTT assay.

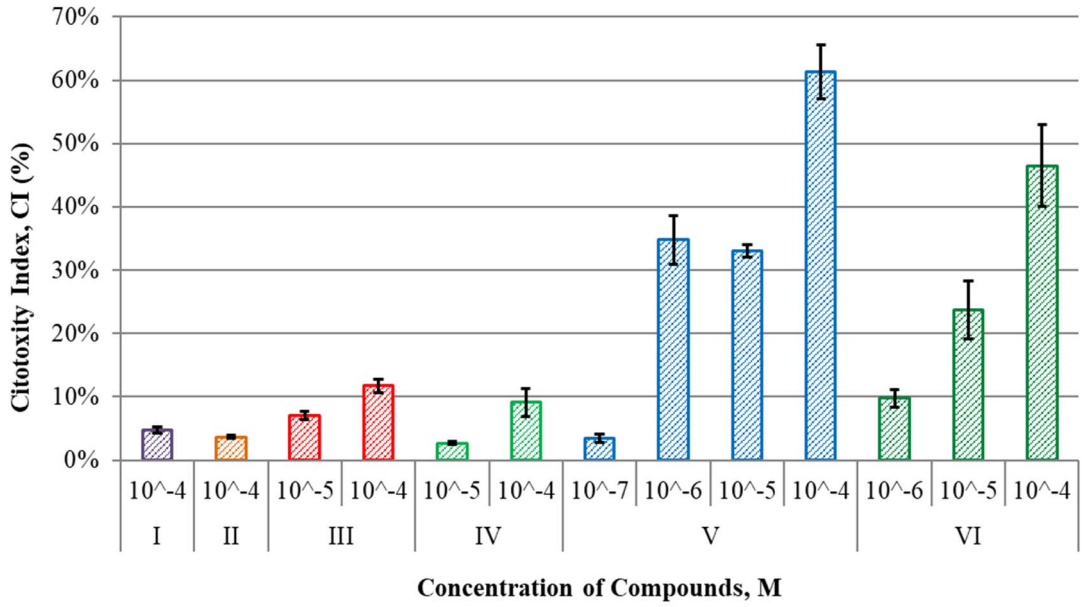


Figure S32 Toxic effects of some concentrations of compounds **I–VII** on proliferation of HF cells for 72 h, the proliferative response was assessed by MTT assay.

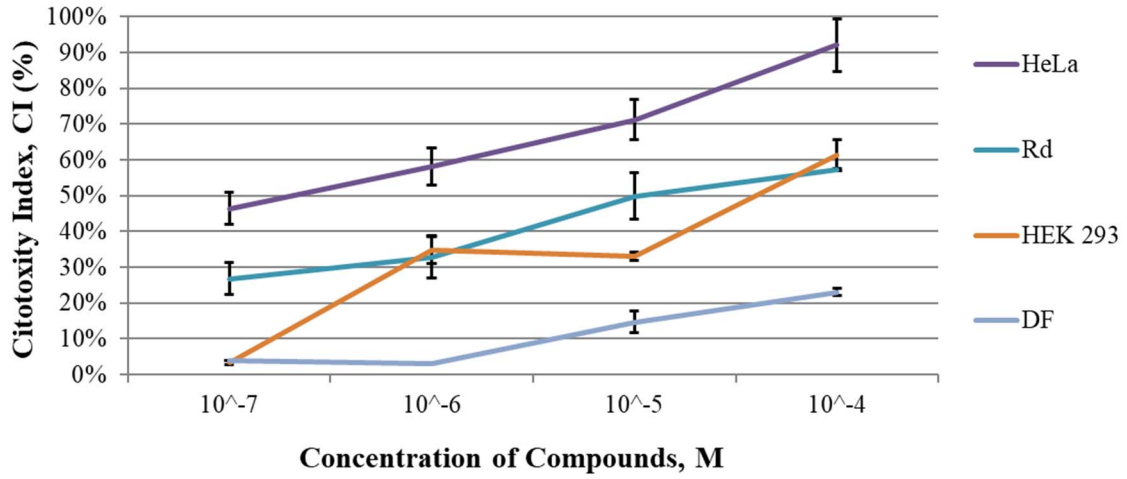


Figure S33 Effects of the most toxic compound **V** with increasing concentrations (10^{-7}–10^{-4} mol/L) on proliferation of cell lines for 72 h, the proliferative response was assessed by MTT assay.

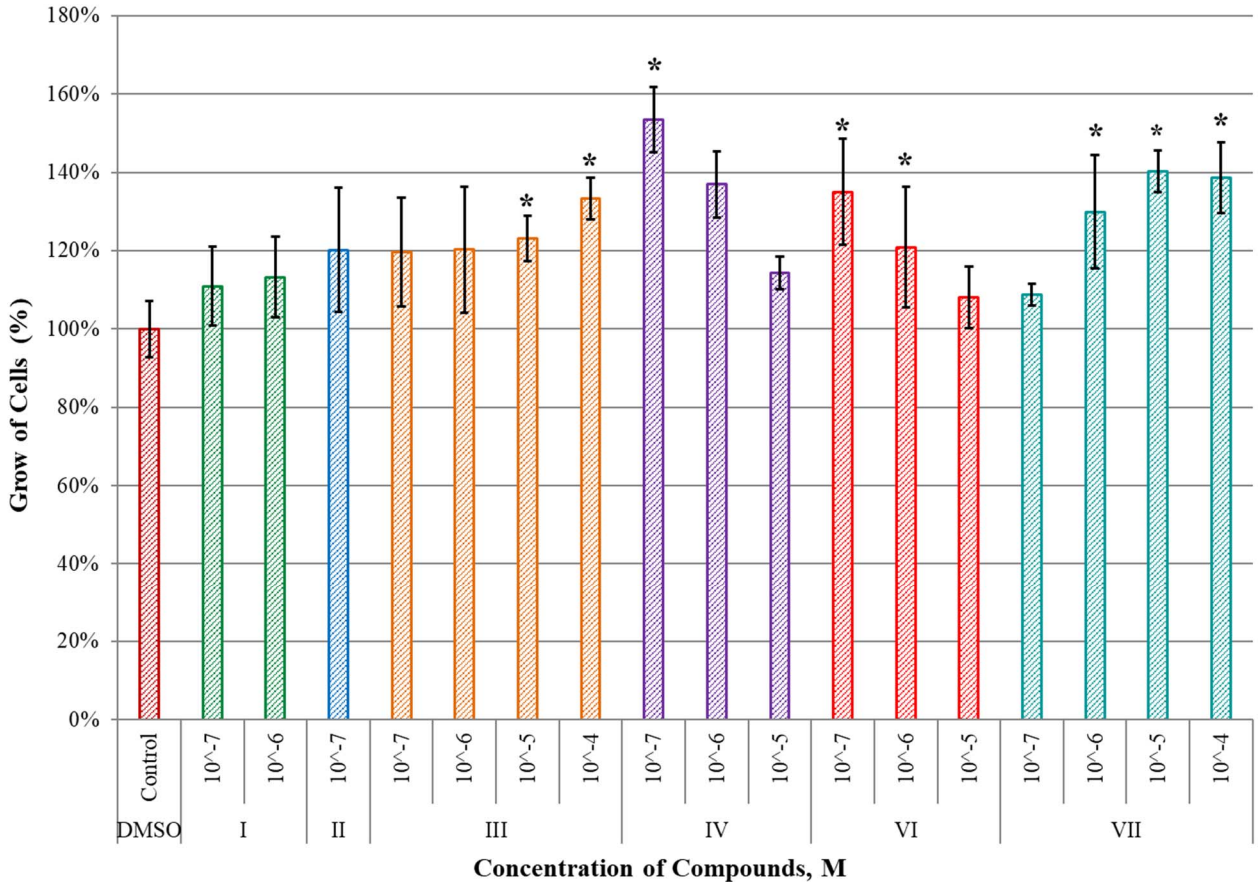
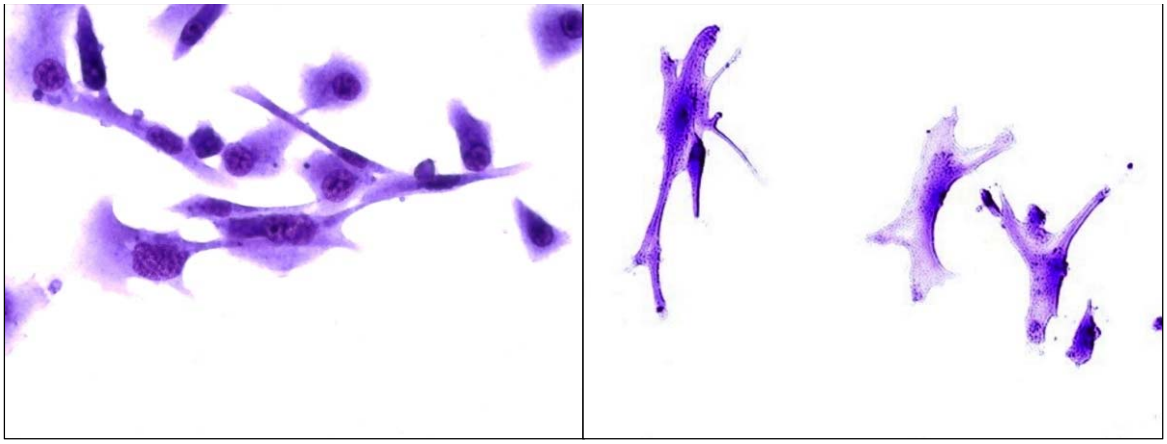


Figure S34 Stimulating effect of some concentrations of compounds I–IV,VI,VII on proliferation of cells for 72 h, the proliferative response was assessed by MTT assay. * – $p < 0.05$ in comparison with the positive control (Mann–Whitney U test).



a b

Figure S35 Morphology of FD cells (***a***) treated with compound **I** (10^{-7} M) and (***b***) untreated × 400. Giemsa staining assay.