

Supplementary Material (ESI) for Chemical Communications
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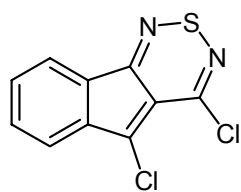
Cyclopentathiadiazines, new heterocyclic materials from cyclic enaminonitriles.

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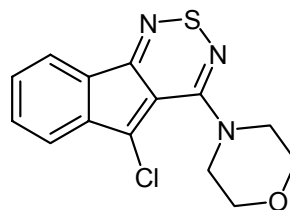
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A comparison between UV spectra of compounds **4-5** and **7-8** and some rotational studies to show steric hindrance that prevents conjugation of morpholine nitrogen and thiadiazine ring in **5** and **8**.

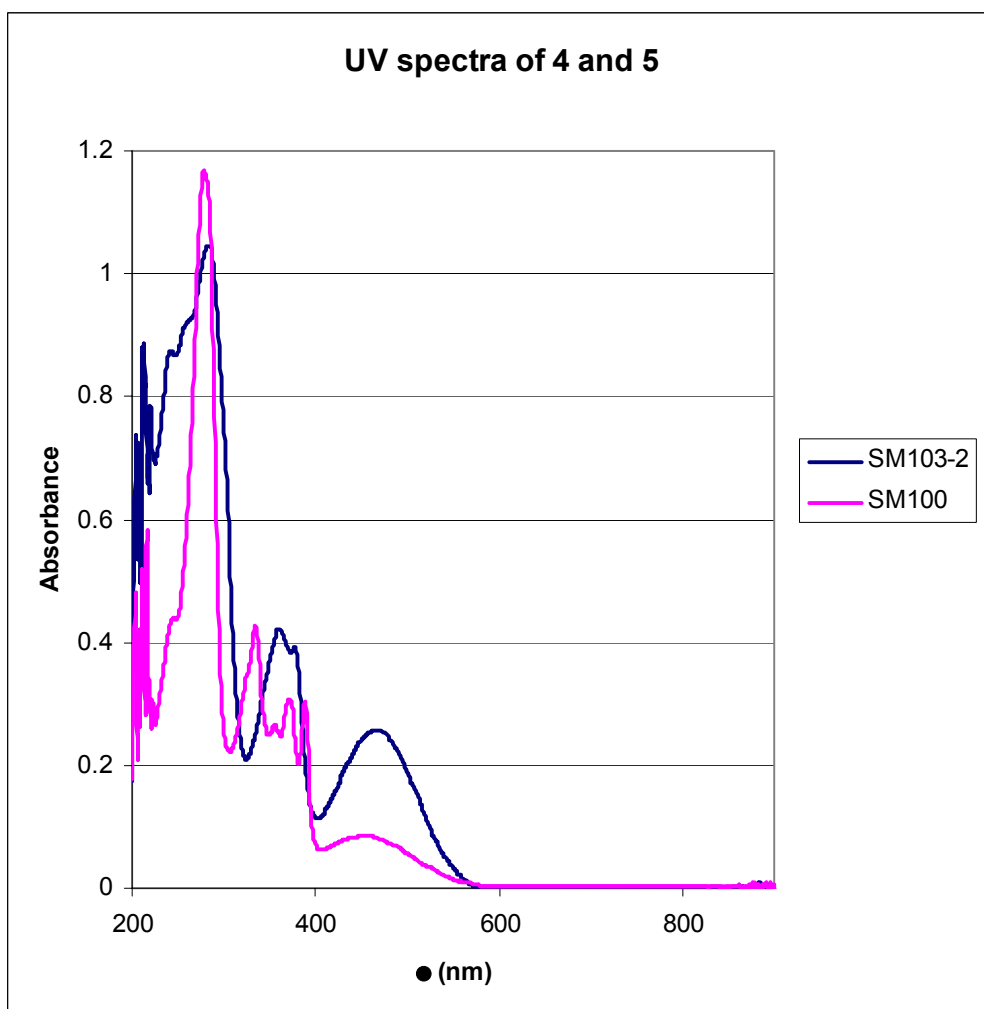


4 (SM100)



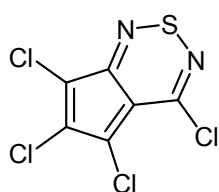
5 (SM103-2)

$6,54 \times 10^{-5}$ M in CH_2Cl_2

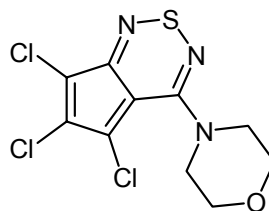


4: ($\lambda_{\text{max}} = 453$ nm, $\epsilon = 1809$ in CH_2Cl_2)

5: ($\lambda_{\text{max}} = 469$ nm, $\epsilon = 3917$ in CH_2Cl_2)

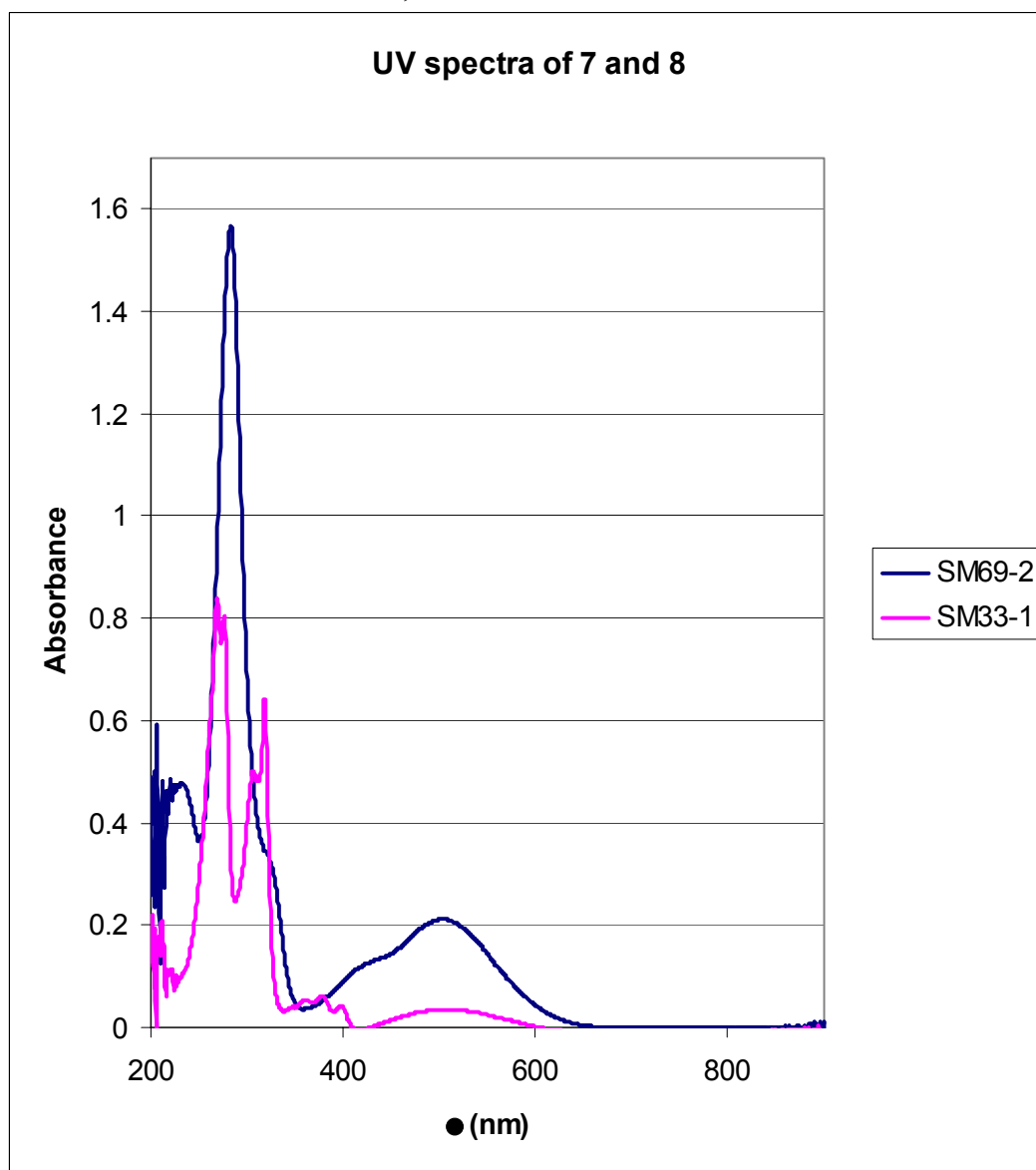


7 (SM33-1)



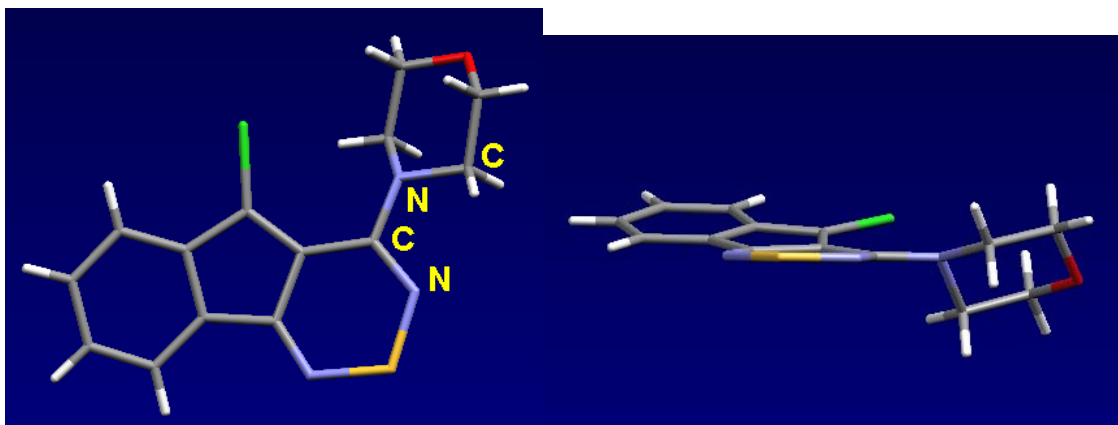
8 (SM69-2)

$6,16 \times 10^{-5}$ M in CH_2Cl_2

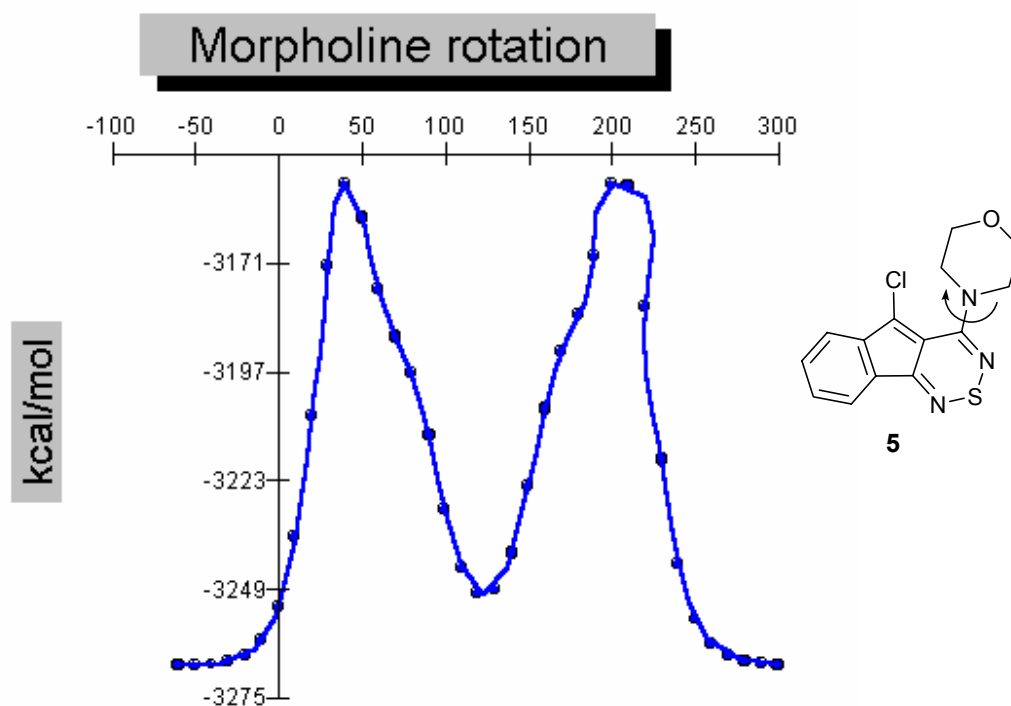


7: ($\lambda_{\text{max}} = 504$ nm, $\epsilon = 573$ in CH_2Cl_2)

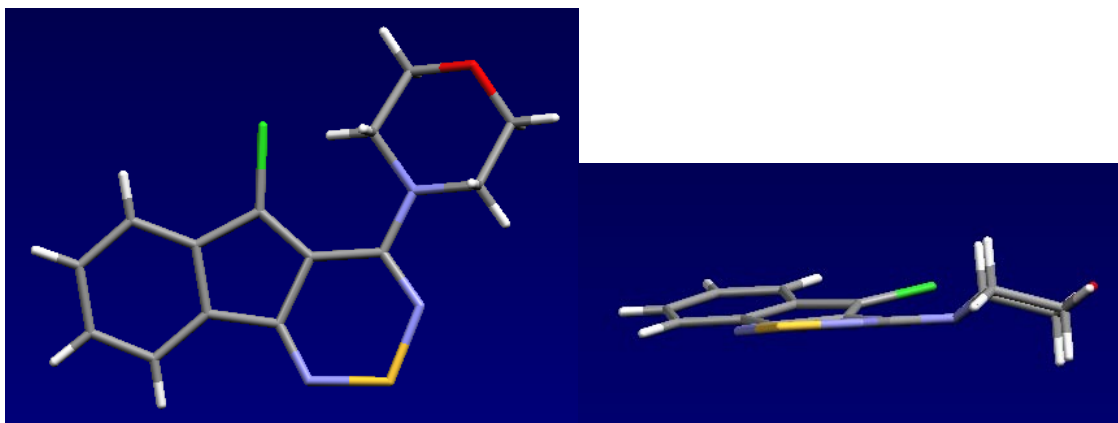
8: ($\lambda_{\text{max}} = 501$ nm, $\epsilon = 3443$ in CH_2Cl_2)



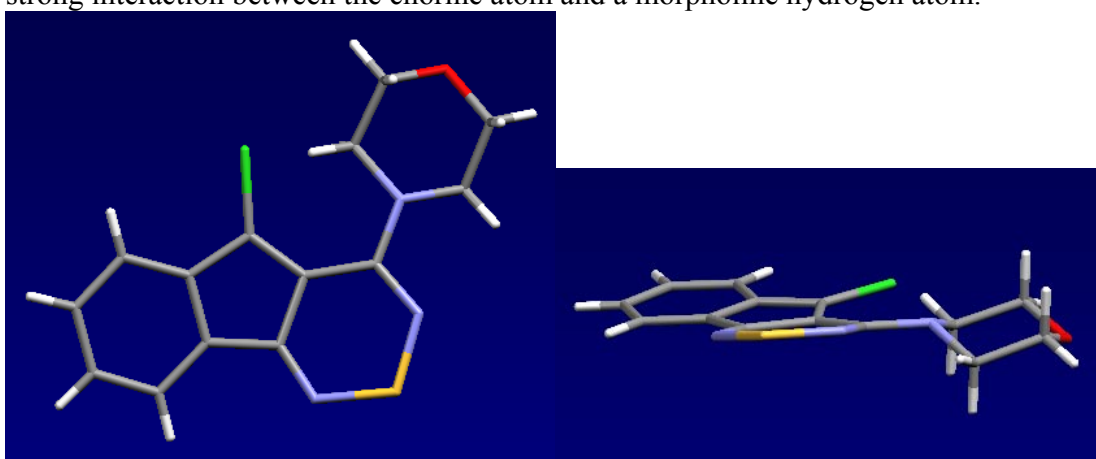
Two different views of the X-ray diffraction structure of compound **5** showing the relative position of the morpholine ring with respect to the thiadiazine ring. Dihedral angle N(thiadiazine)-C-N(morpholine)-C = -14.25° .



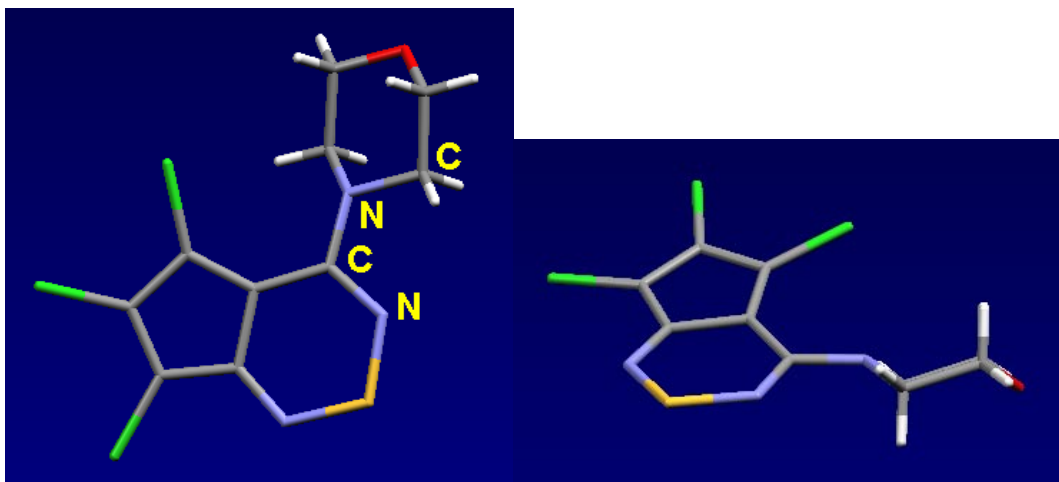
Plot of relative energies corresponding to rotation of the morpholine ring with respect to the thiadiazine ring. The two maxima correspond to dihedral angles of roughly 200 and 37.5° of the N(thiadiazine)-C-N(morpholine)-C dihedral angle as indicated in the first figure.



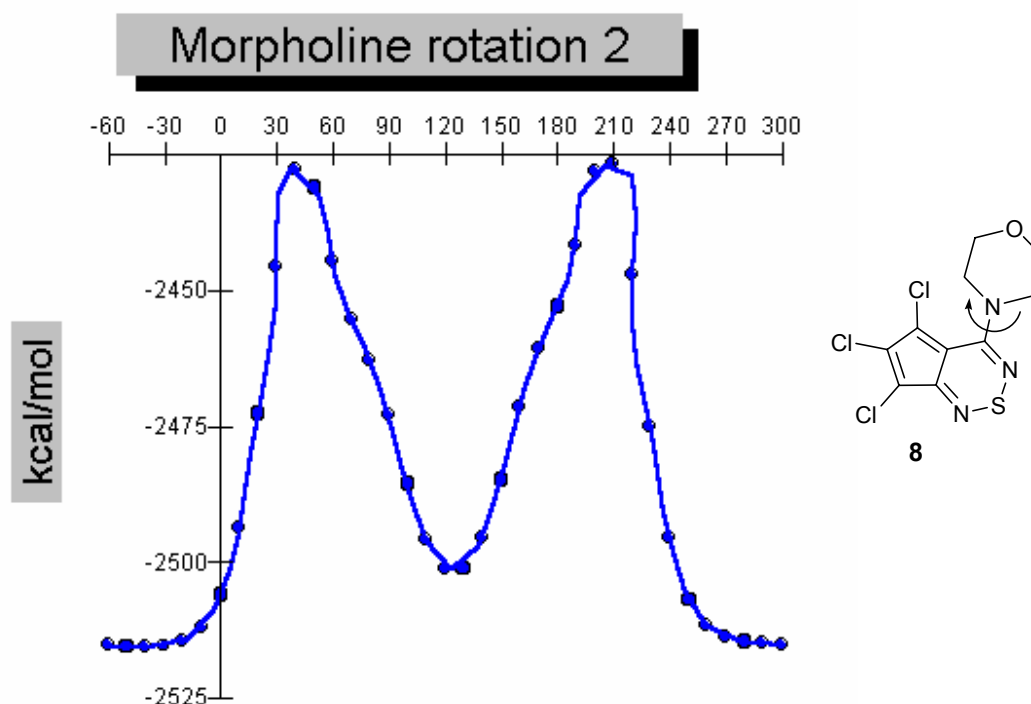
Two different views of the first maximum (dihedral angle 200 °) showing that the conjugation of the morpholine nitrogen lone pair and the thiadiazine ring is hindered by a strong interaction between the chlorine atom and a morpholine hydrogen atom.



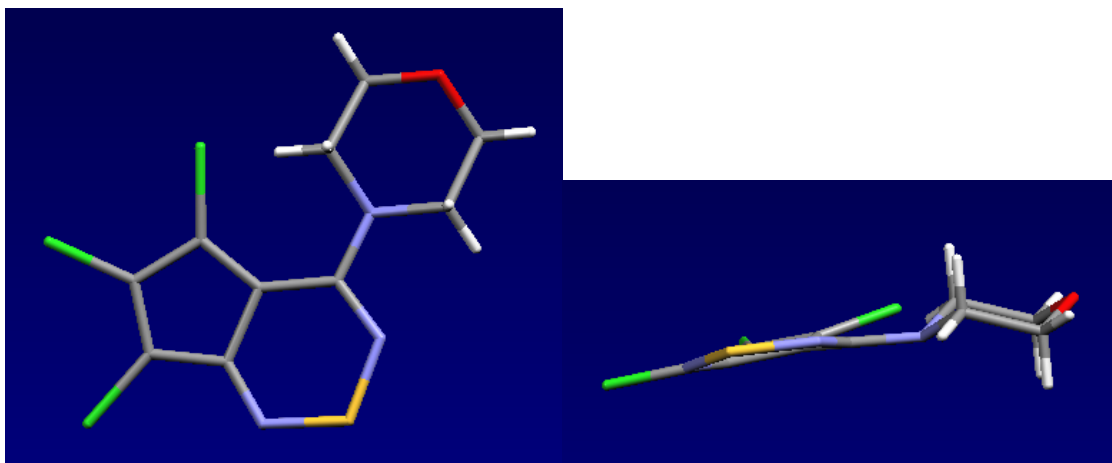
Two different views of the second maximum (dihedral angle 37.5 °) showing that the conjugation of the morpholine nitrogen lone pair and the thiadiazine ring is hindered by a strong interaction between the chlorine atom and a morpholine hydrogen atom.



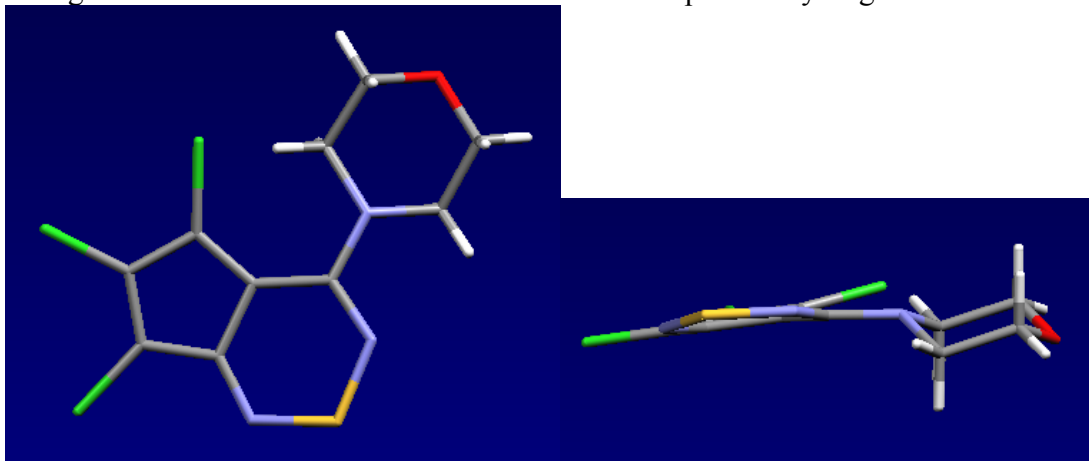
Two different views of the X-ray diffraction structure of compound **8** showing the relative position of the morpholine ring with respect to the thiadiazine ring.



Plot of relative energies corresponding to rotation of the morpholine ring with respect to the thiadiazine ring. The two maxima correspond to dihedral angles of roughly 210 and 37.5 ° of the N(thiadiazine)-C-N(morpholine)-C dihedral angle as indicated in the first figure.



Two different views of the first maximum (dihedral angle 210 °) showing that the conjugation of the morpholine nitrogen lone pair and the thiadiazine ring is hindered by a strong interaction between the chlorine atom and a morpholine hydrogen atom.



Two different views of the second maximum (dihedral angle 37.5 °) showing that the conjugation of the morpholine nitrogen lone pair and the thiadiazine ring is hindered by a strong interaction between the chlorine atom and a morpholine hydrogen atom.