Supplementary Information

A facile synthesis, characterization and biological evaluation of novel spiro-thiazolidinone and quinazolinone-thiazolidine derivatives

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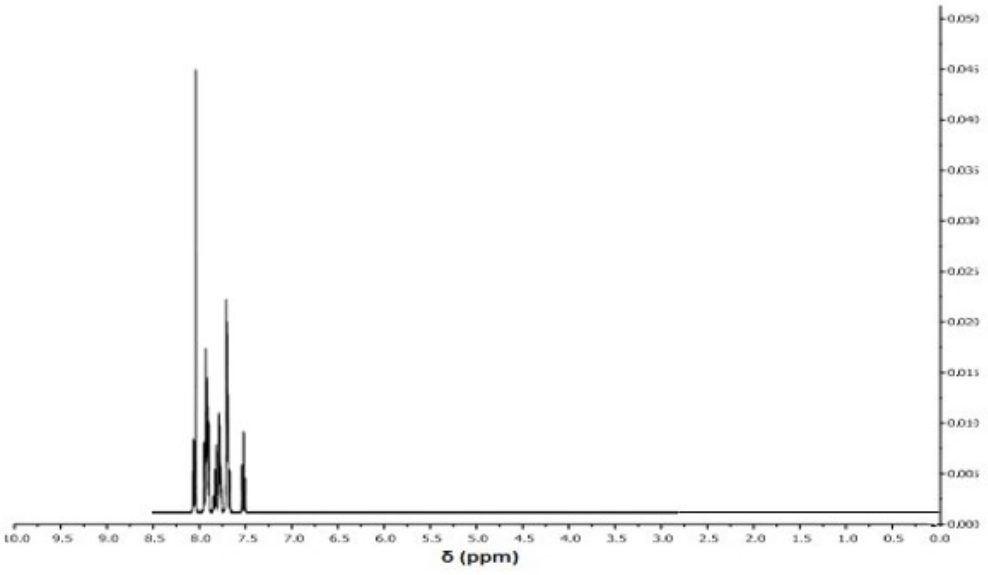
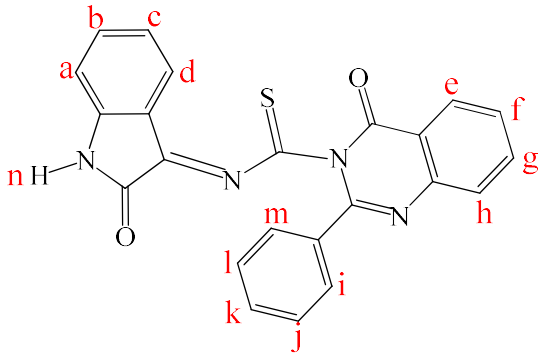


Figure S1. [1]HNMR spectra of compound **4a**



Compound **4a**

Multiplet for 13H (Aromatic $H^{a\ to\ m}$) at δ 7.53-8.05 ppm.

Singlet of 1 NH^{n} proton at δ 8.02 ppm.

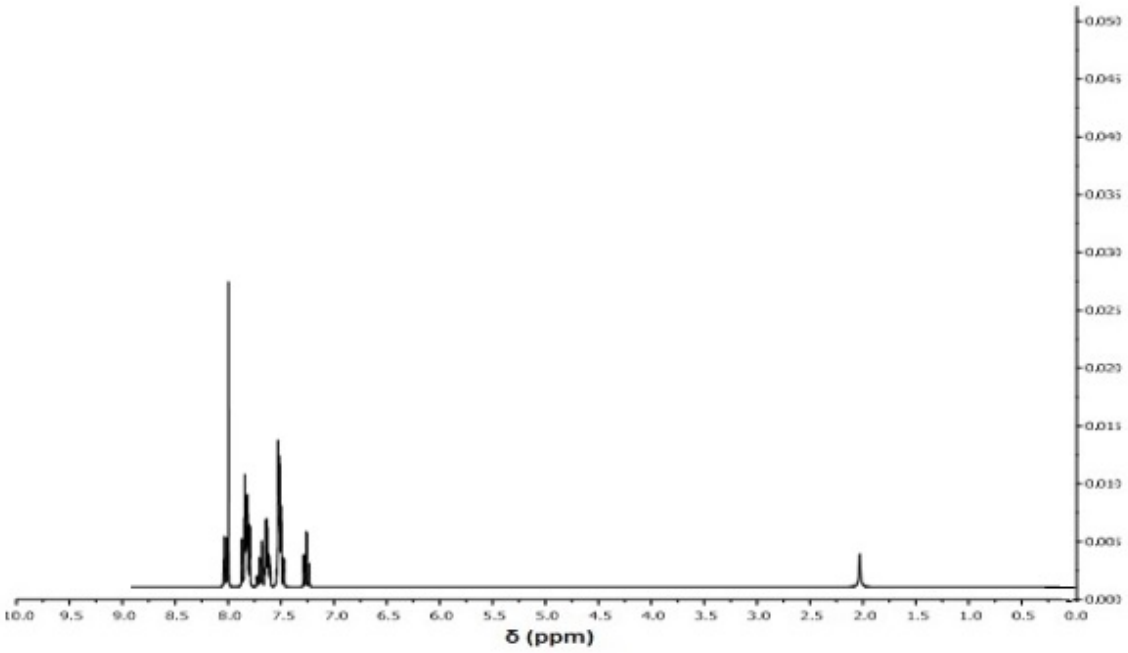
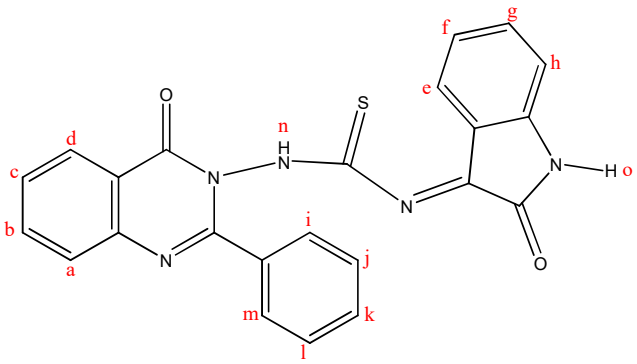


Figure S2. ^{1}HNMR spectra of compound **6a**



Compound **6a**

Multiplet for 13H (Aromatic $H^{a\ to\ m}$) at δ 7.53-8.05 ppm.

Singlet of 1 NH^{n} proton at δ 8.02 ppm.

Singlet of 1 NH^{o} proton at δ 2.02 ppm.

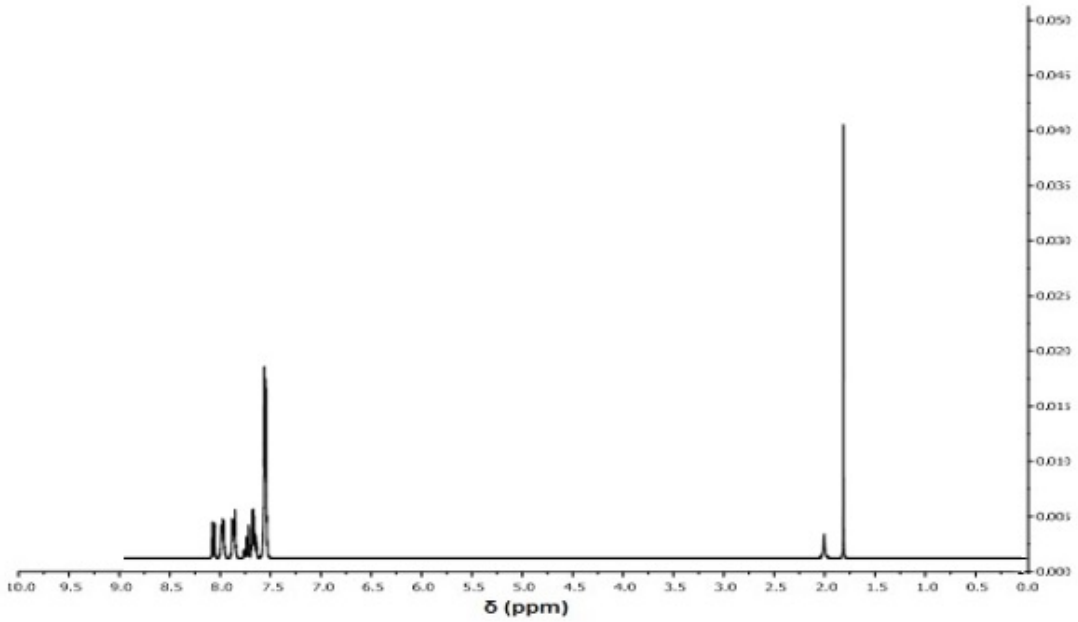
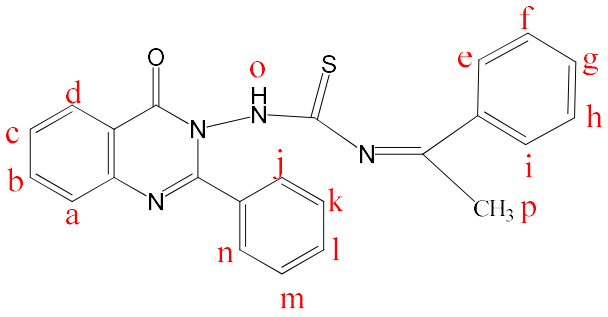


Figure S3. ^{1}HNMR spectra of compound **7a**



Compound **7a**

Multiplet for 14H (Aromatic $H^{a\ to\ n}$) at δ 7.53-8.05 ppm.

Singlet of 1 NH^{o} proton at δ 2.02 ppm.

Singlet of 3 CH^{p} proton at δ 1.83 ppm.

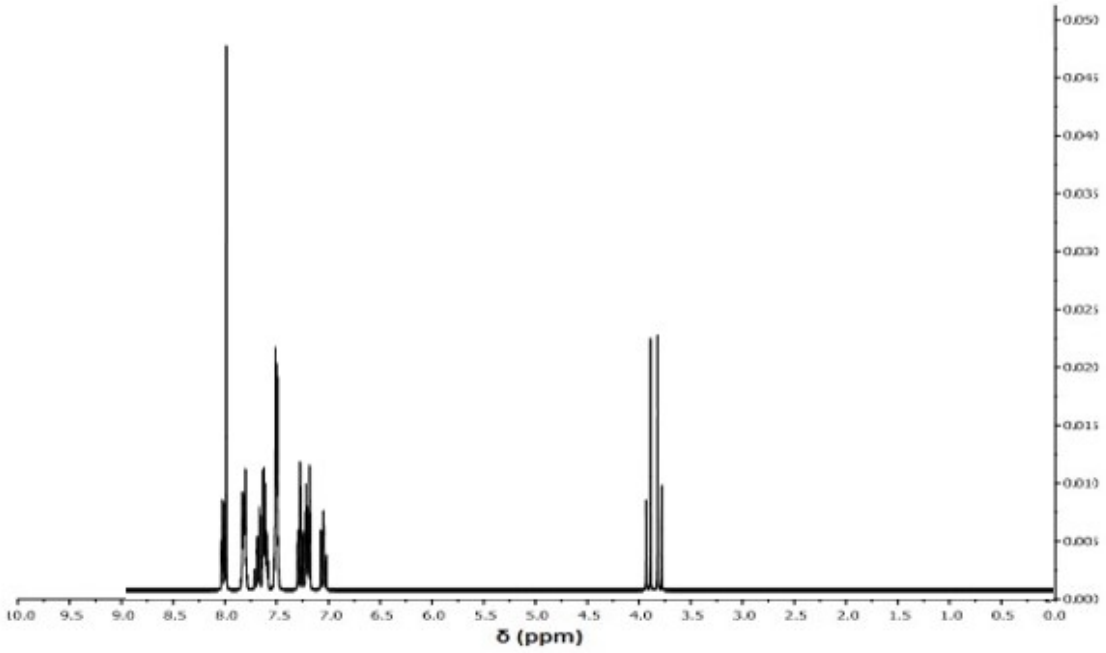
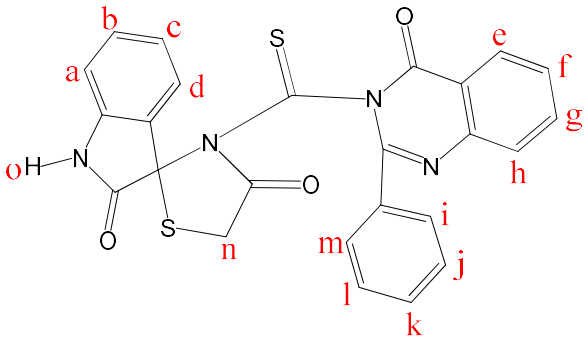


Figure S4. ^{1}HNMR spectra of compound **8a**



Compound 8**a**

Multiplet for 13H (Aromatic $H^{a\ to\ m}$) at δ 7.08-8.05 ppm.

Singlet of 1 NH^{o} proton at δ 8.02 ppm.

Doublet of doublets for 2H (CH_2^{n}) at 3.84 & 3.96 (J = 12.3 Hz). The two proton of CH_2^{n} are diastereotopic in nature, couples together and appears as doublet of doublets.

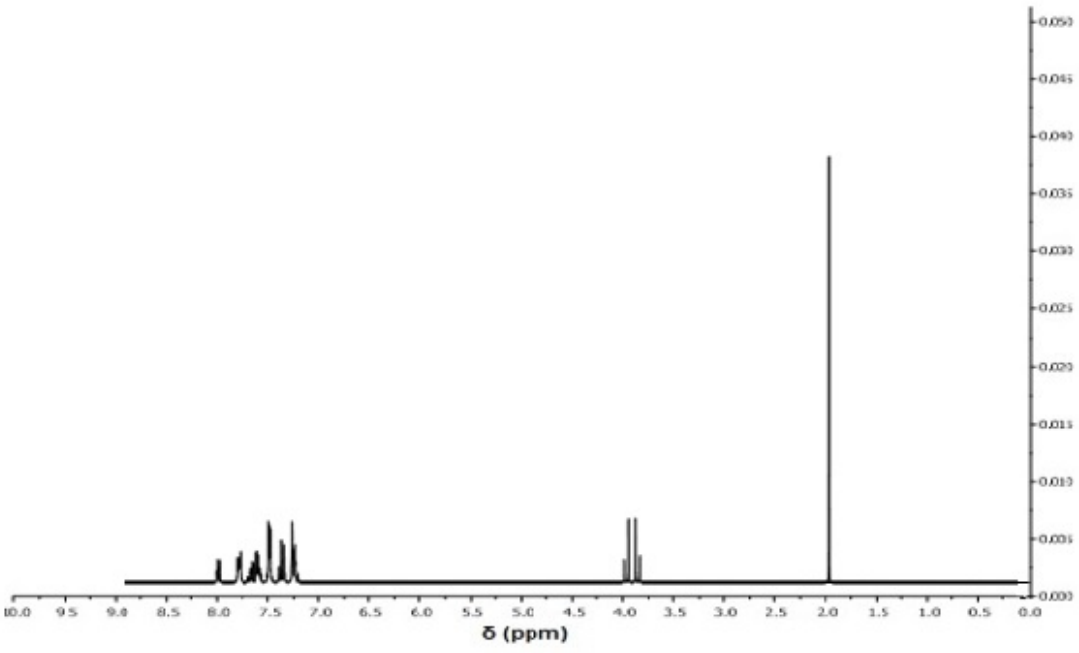
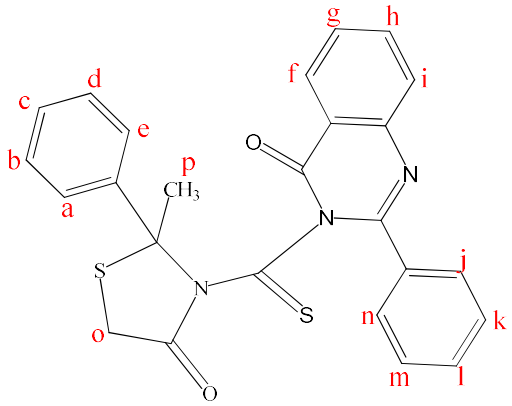


Figure S5. ^{1}HNMR spectra of compound **9a**



Compound 9**a**

Multiplet for 14H (Aromatic $H^{a\ to\ n}$) at δ 7.28-8.05 ppm.

Singlet of 3 CH^{p} proton at δ 1.91 ppm.

Double doublet of 2 CH^{o} at δ 3.84 & 3.96 ppm (J = 12.3 Hz).

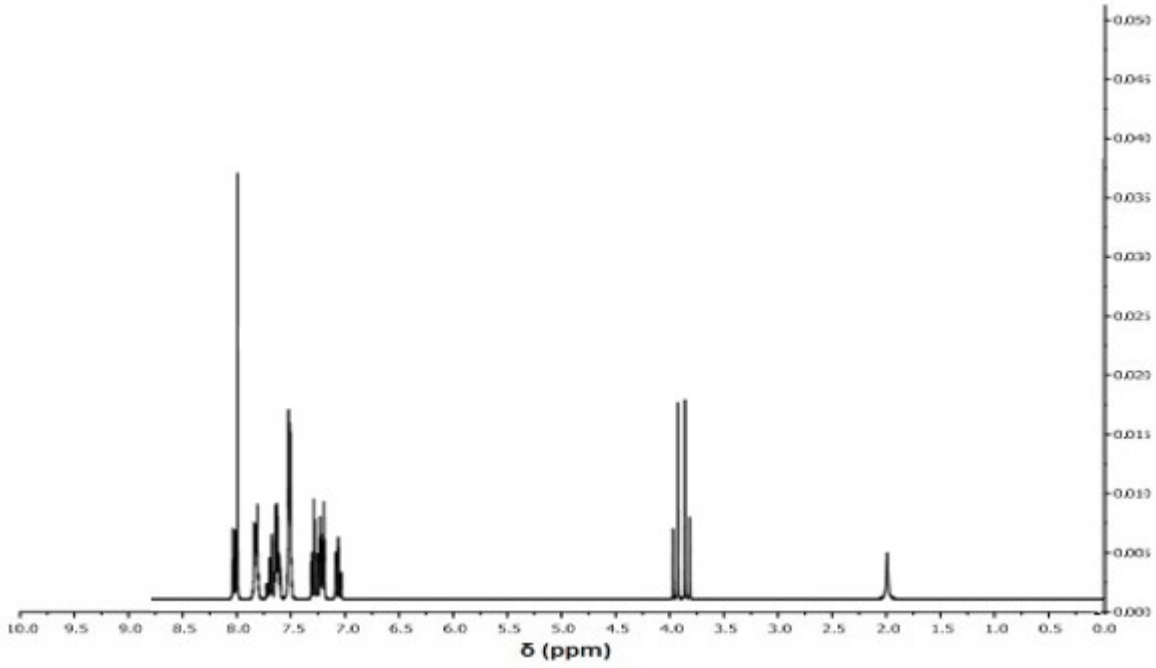
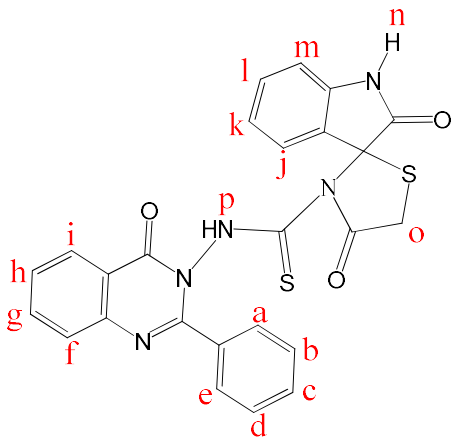


Figure S6. ^{1}HNMR spectra of compound **10a**



Compound **10a**

Multiplet for 13H (Aromatic $H^{a\ to\ m}$) at δ 7.08-8.05 ppm.

Singlet of 1 NH^{n} proton at δ 8.02 ppm.

Singlet of 1 NH^{p} proton at δ 2.02 ppm.

Double doublet of 2 CH^{o} at δ 3.84 & 3.96 ppm (J = 12.3 Hz).

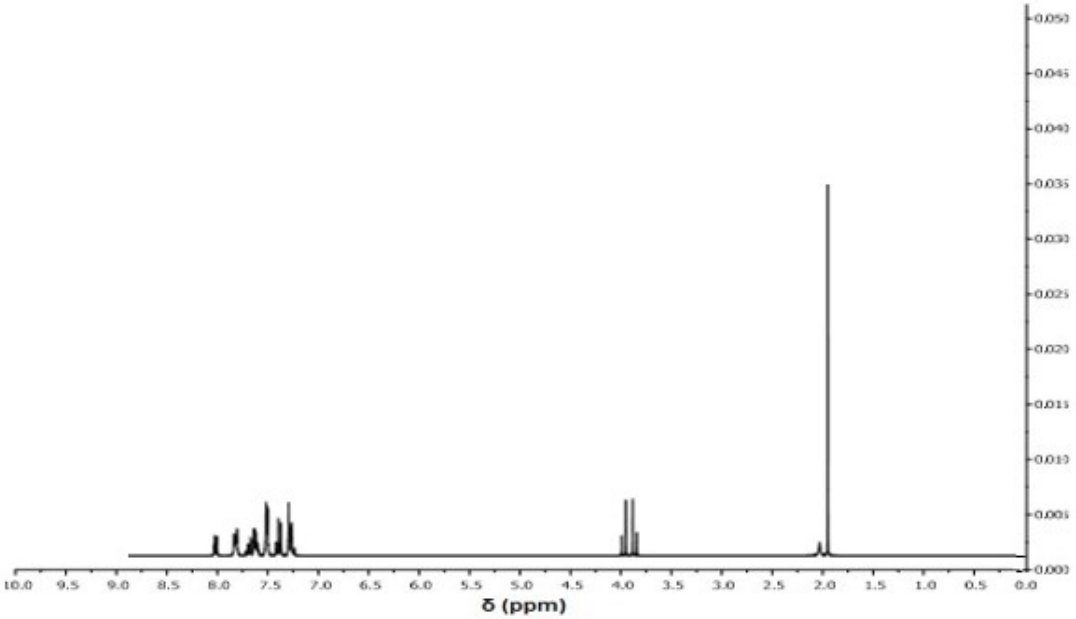
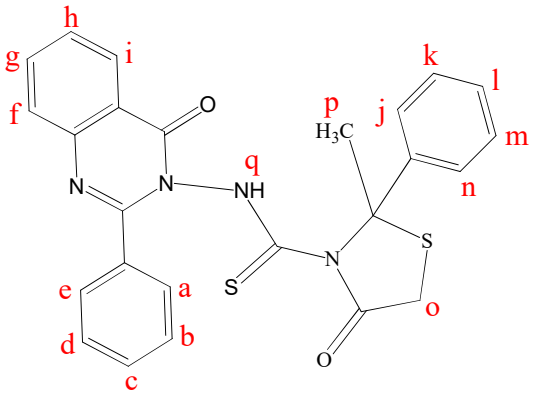


Figure S7. ^{1}HNMR spectra of compound **11a**



Compound **11a**

Multiplet for 14H (Aromatic $H^{a\ to\ n}$) at δ 7.30-8.05 ppm.

Singlet of 3 CH^{p} proton at δ 1.91 ppm.

Singlet of 1 NH^{q} proton at δ 2.02 ppm.

Double doublet of 2 CH^{o} at δ 3.84 & 3.96 ppm (J = 12.3 Hz).

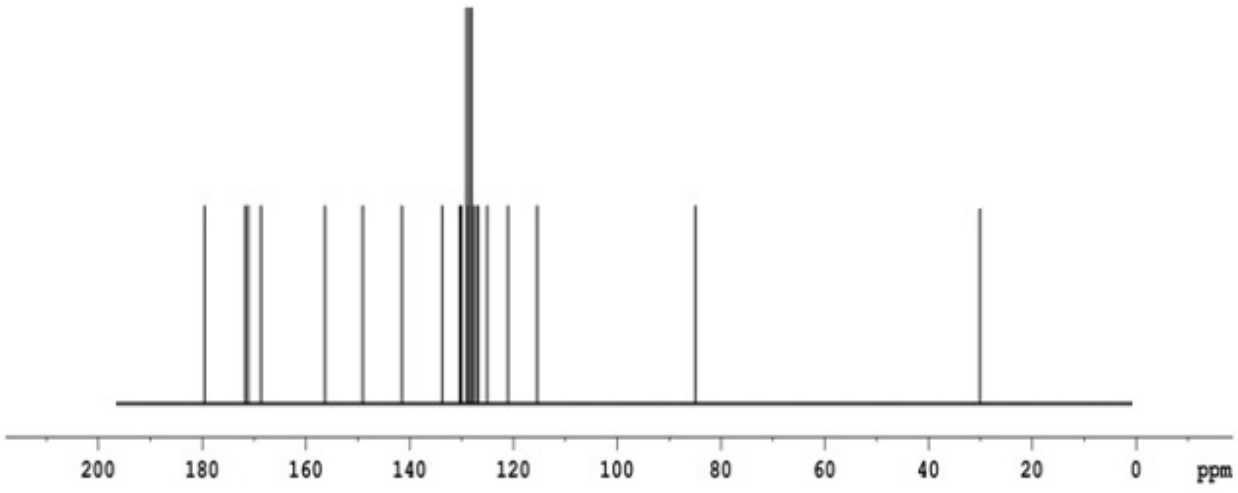


Figure S8. ^{13}CNMR spectra of compound **8a**

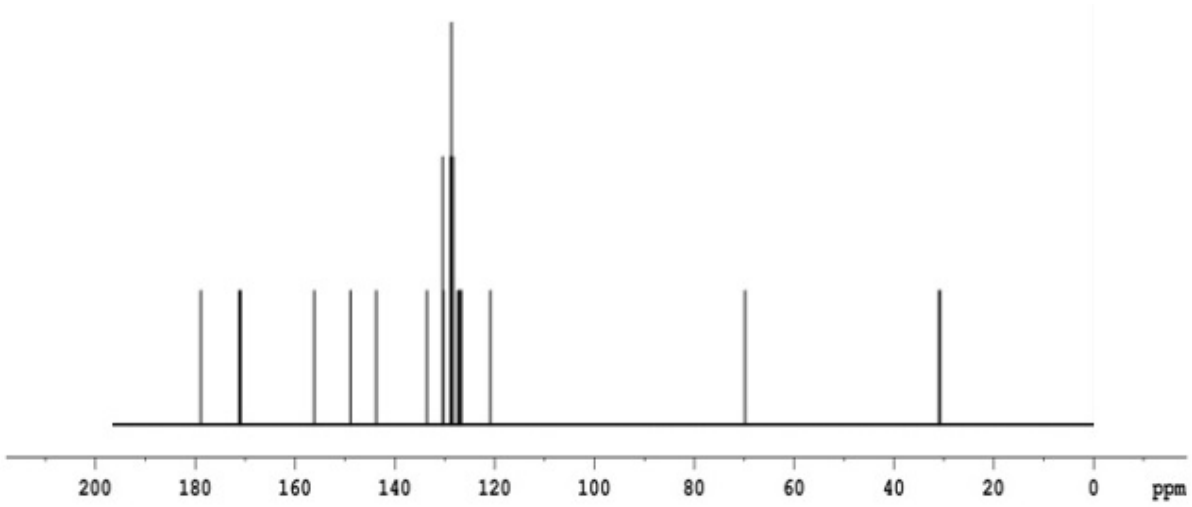


Figure S9. ^{13}CNMR spectra of compound **9a**

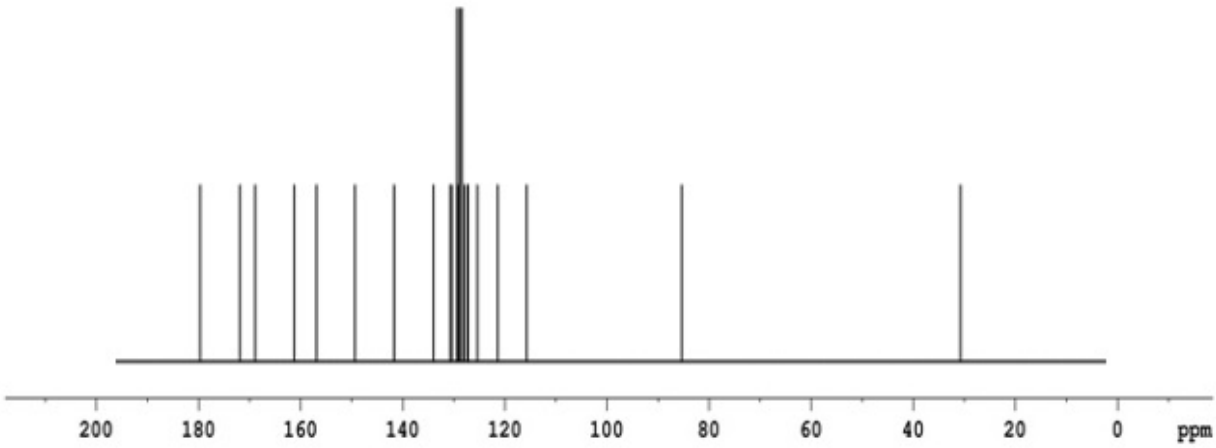


Figure S10. ^{13}CNMR spectra of compound **10a**

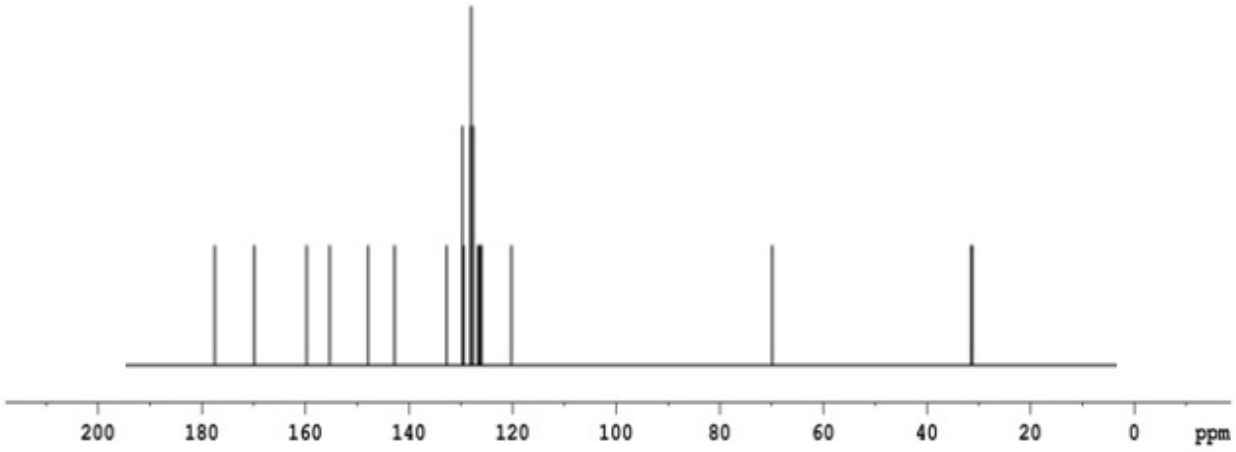
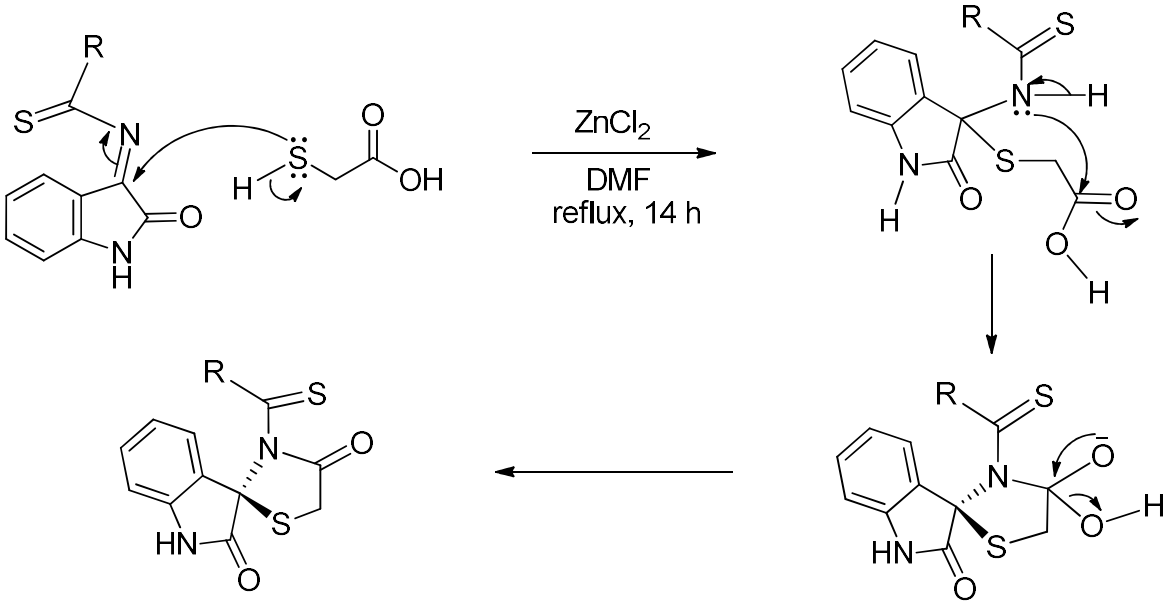


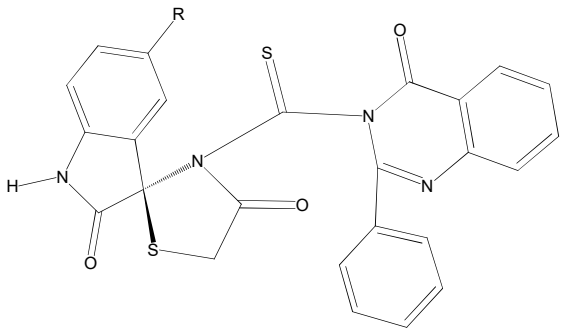
Figure S11. ^{13}CNMR spectra of compound **11a**

Proposed mechanism for the formation of Spiro compounds

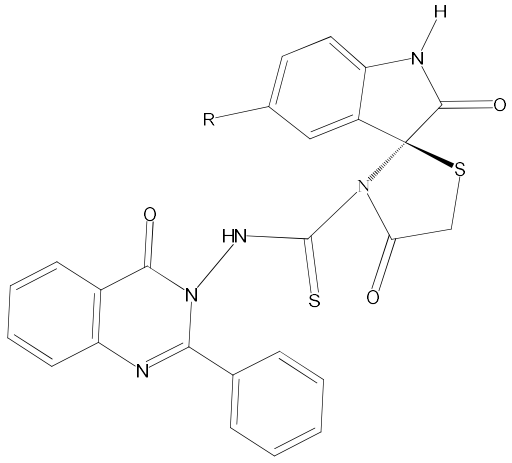


Scheme S1: Mechanism of formation of Spiro compounds

Role of zinc chloride (a good Lewis acid) in the reaction is to enhance the leaving ability of -OH group by forming complex with it.



Compound 8



Compound 10

Scheme 2: Stereochemistry of Spiro compounds 8 and 10

It is proposed that the synthesized spiro derivatives prefer one enantiomer over the other. As during cyclization there is considerable amount of steric repulsion due to bulkier nature of suphur atom over nitrogen atom. The sulphur atom of the thioglycolic acid preferentially attack the imine carbon from the front side and the already attached nitrogen is pushed back such that the nitrogen occupies an alpha (α) orientation in order to achieve minimum steric repulsion.