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Supplementary Information

Novel Quinazolinone–Isoxazoline Hybrids: Synthesis, Spectroscopic Characterization, and DFT Mechanistic Study

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Contents

1. Chemical reagents and instruments

All chemicals used were of analytical grade and were purchased from commercial suppliers. The progress of the reac- tions was monitored by TLC (Merck, silica gel 60 F254), and spots were visualized under UV light (VILBER LOUR- MAT, VL-215.LC). Column chromatography was performed using Merck silica gel (70-230 mesh) and n-hexane/ethyl acetate mixture as eluent. The melting points were determined with an uncertainty of ± 2°C using a KOFLER BENCH. The IR spectra were recorded in the range of 450–4000 cm^{-1} on a BRUKER VERTEX 70 FT-IR Spectrometer, and wave- numbers are given in cm^{-1}. The NMR spectra (^{1}H and ^{13}C) were recorded at room temperature on a BRUKER AVANCE II 300 Ultra-Shield (300 MHz for ^{1}H and 75 MHz for ^{13}C) spectrometer using $CDCl_3$ as solvent. The chemicalshifts are expressed in ppm and the coupling constants J are expressed in Hertz (Hz). The spin multiplicities are re- ported as singlet (s), doublet (d), triplet (t), multiplet (m), doublet of doublets (dd), doublet of triplets (dt) and broad (br). High-resolution mass spectra were recorded on a Waters/Vion IMS-QTOF: Spectrometer–, equipped with an electrospray ionization (ESI), source operating in either positive and negative ion mode.

2. FT-IR, 1H, 13C NMR and HRMS spectra of synthesized compounds

i. Quinazolin-4(3H)-one (1)

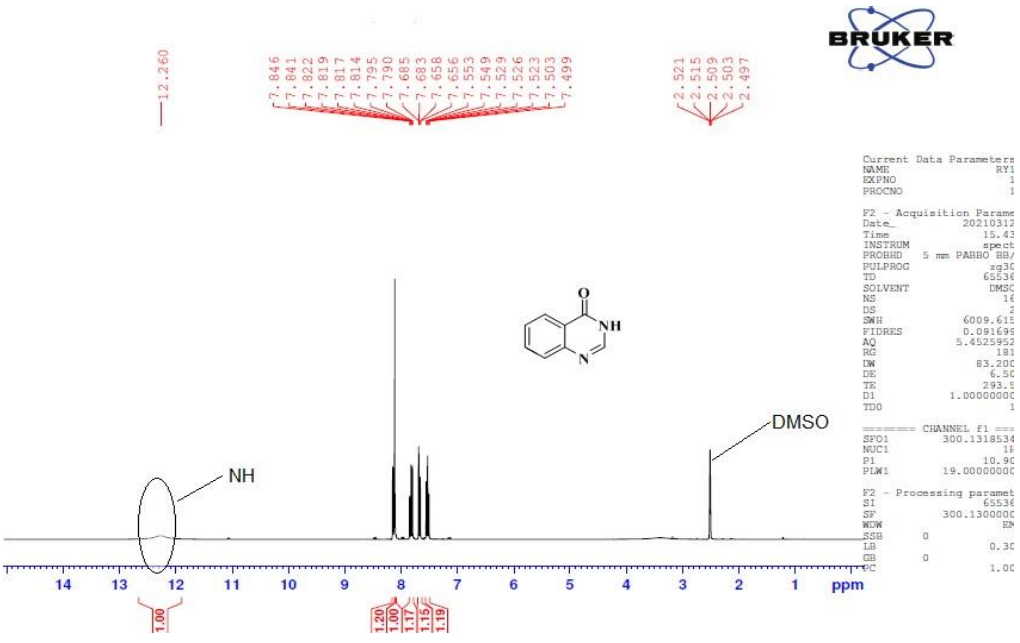

Figure S1.1H NMR spectrum (300 MHz, DMSO) of compound (1)

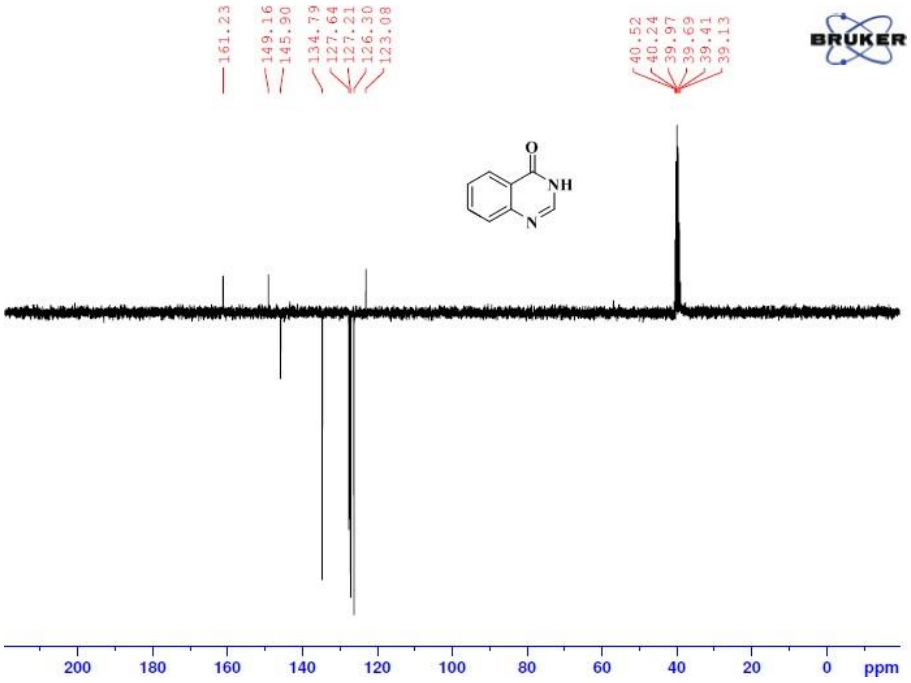

Figure S2. ^{13}C NMR spectrum (75 MHz, DMSO) of compound (**1**)

ii. N-allylquinazolin-4(3H)-one (2)

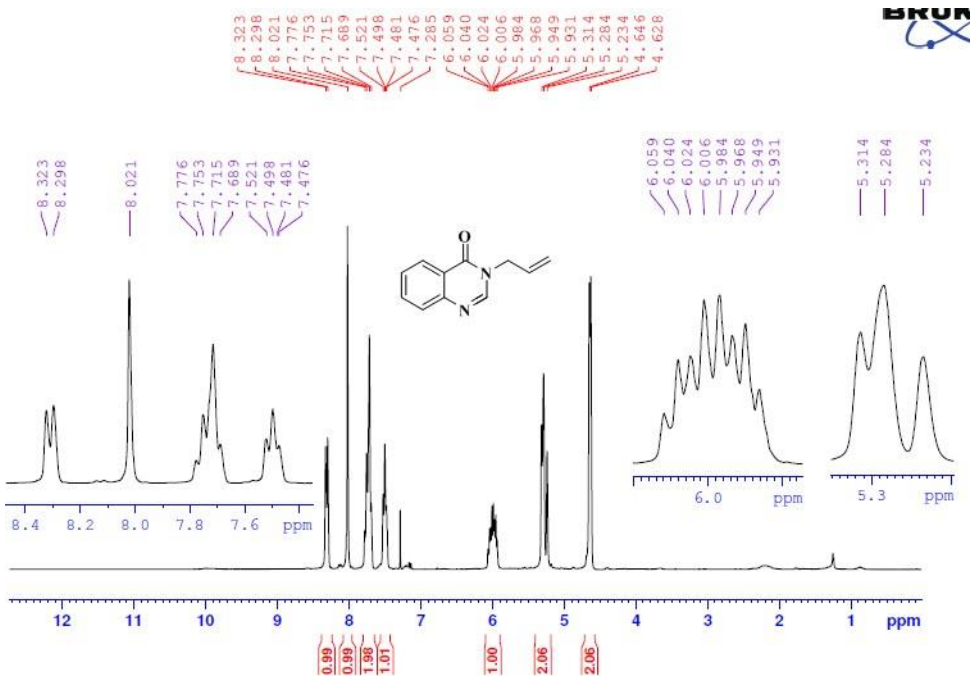

Figure S3. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound (**2**)

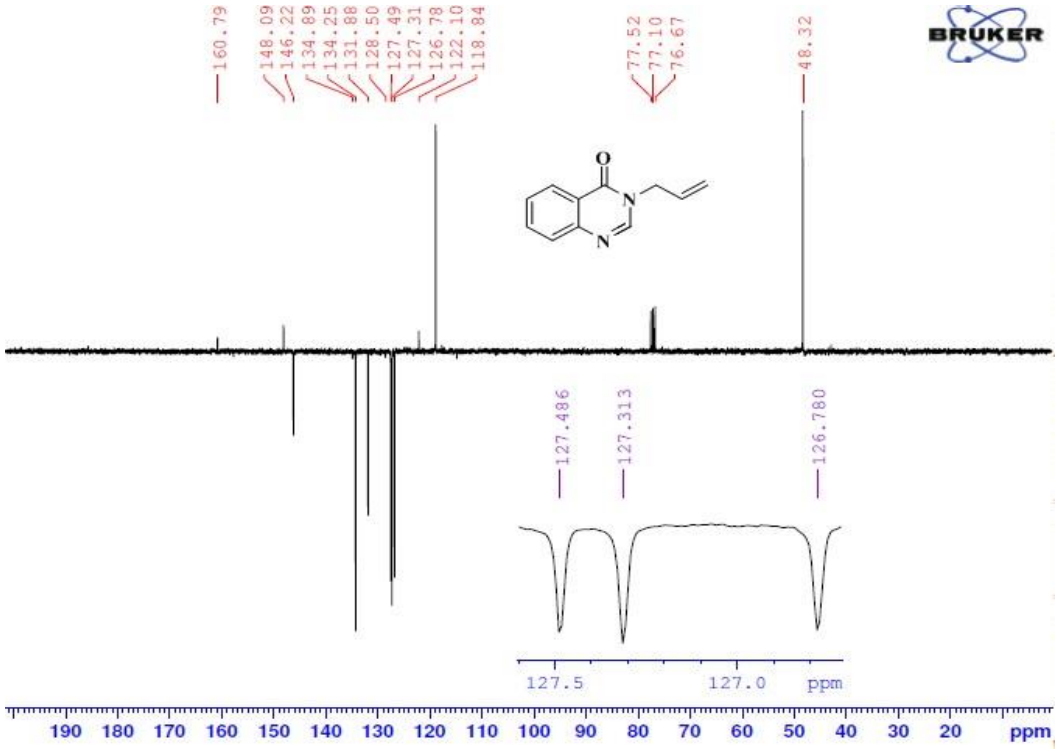

Figure S4. ^{13}C NMR spectrum (75 MHz, CDCl3) of compound (**2**)

iii. Hybrid Compounds Containing the Quinazolinone and Isoxazoline Nucleus (4a-h)

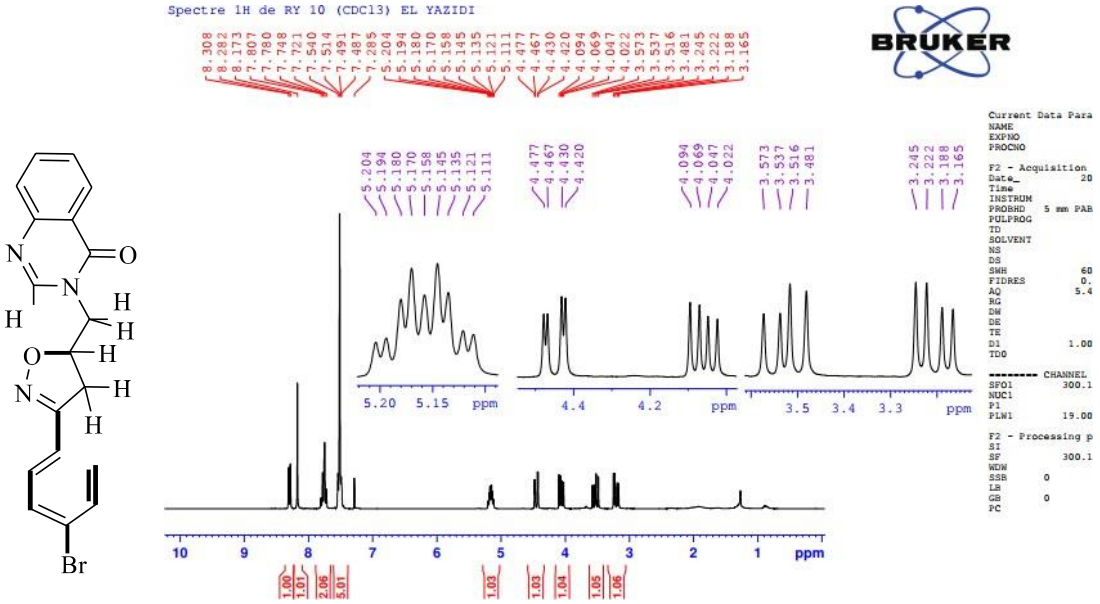

Figure S5. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound (**4a**)

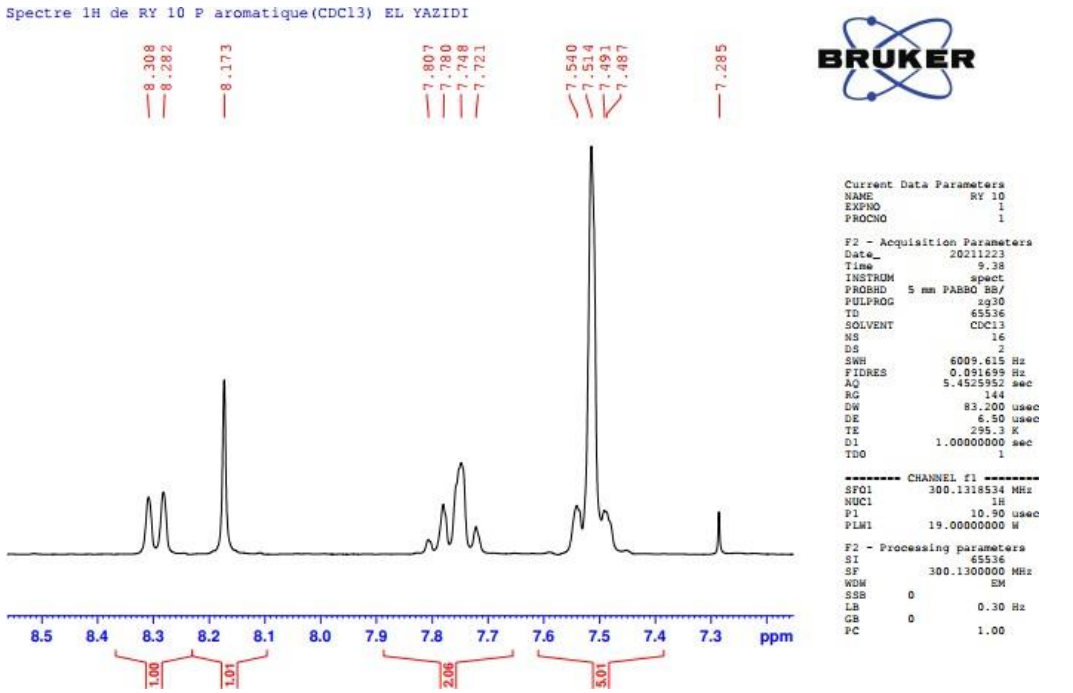

Figure S6. Aromatic enlarged region of 1H NMR spectrum of compound (4a)

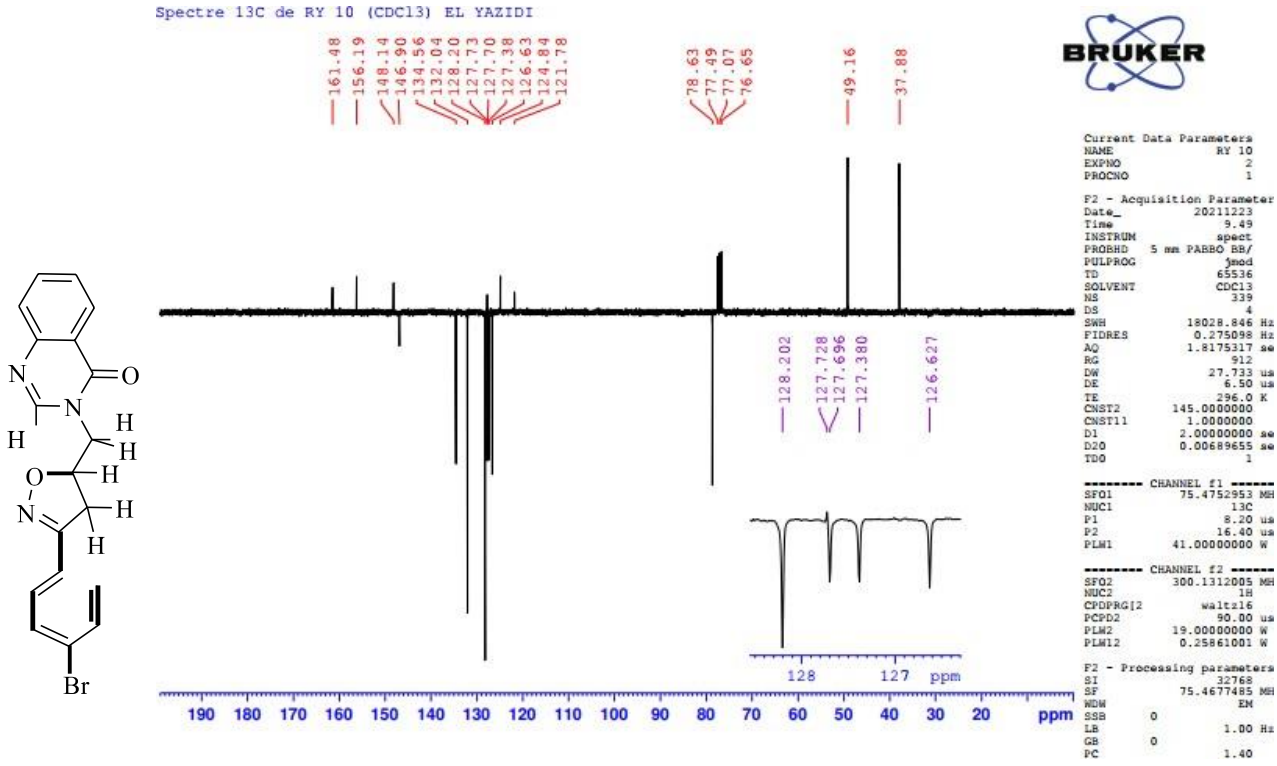

Figure S7. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound (**4a**)

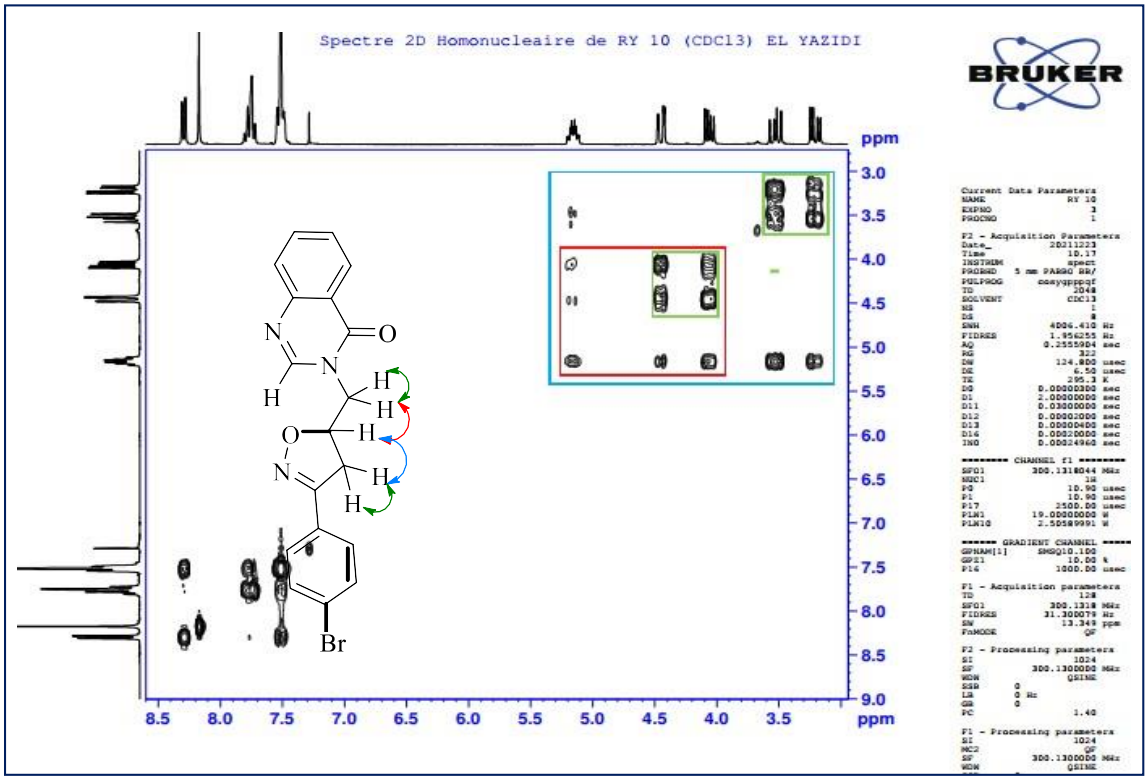

Figure S8. 2D-COSY NMR spectrum of compound 4a showing the coupling signals for hydrogen atoms.

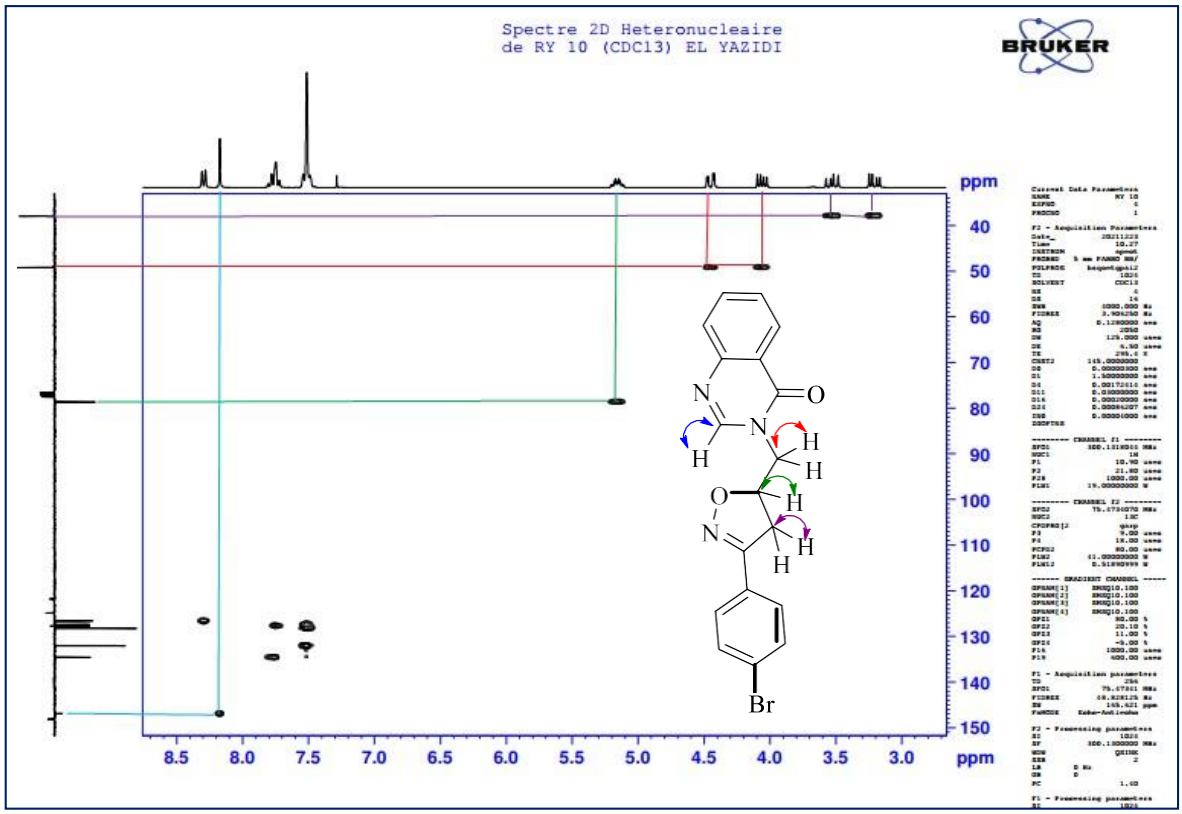

Figure S9. 2D-HSQC NMR spectrum of compound **4a** showing the identification of methine **C**$_5$ and meth-ylene **C**$_4$ carbons of isoxazoline, exocyclic methylene carbon **C**H_2 and **C**H of quinazolinone.

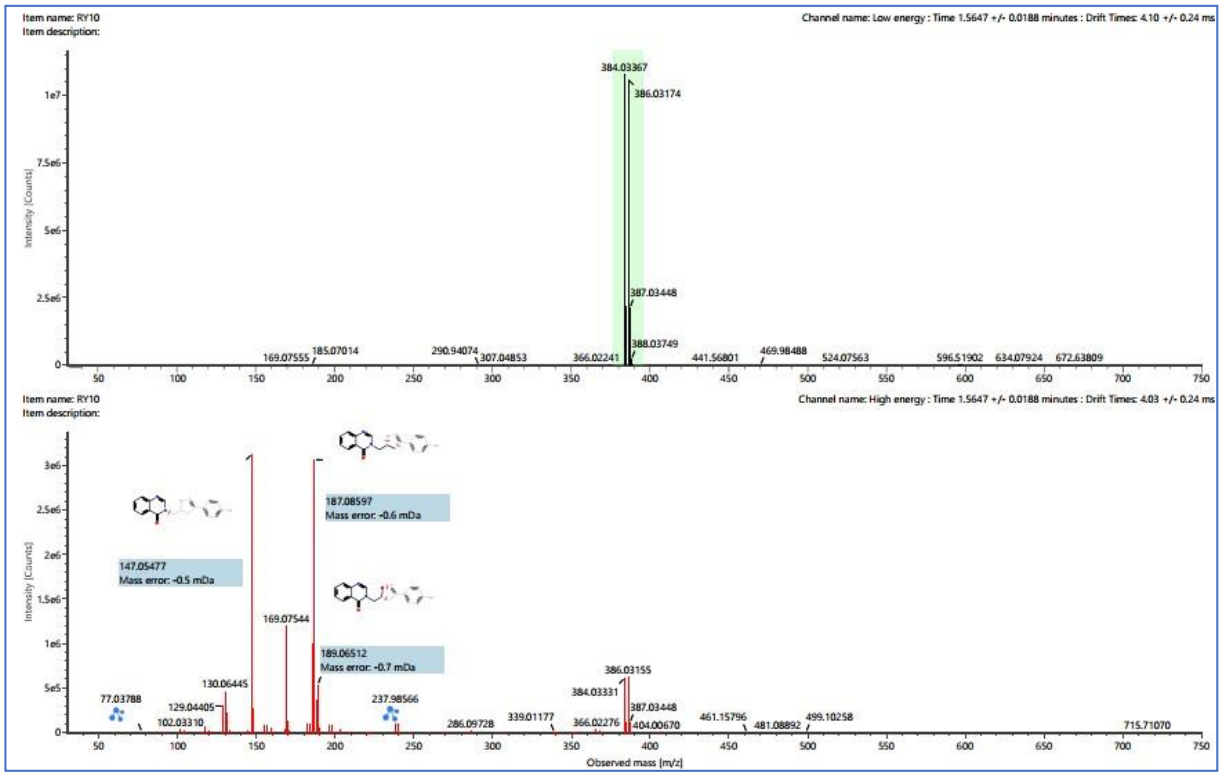

Figure S10. Mass spectrum of compound (**4a**)

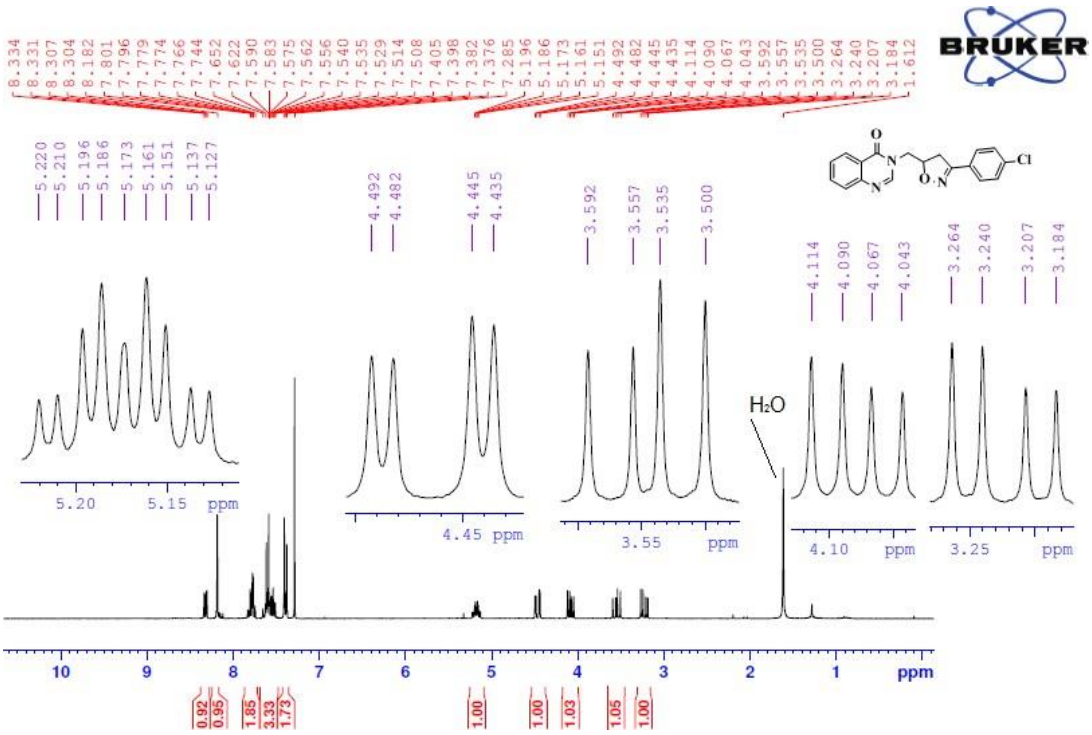

Figure S11. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound (**4b**)

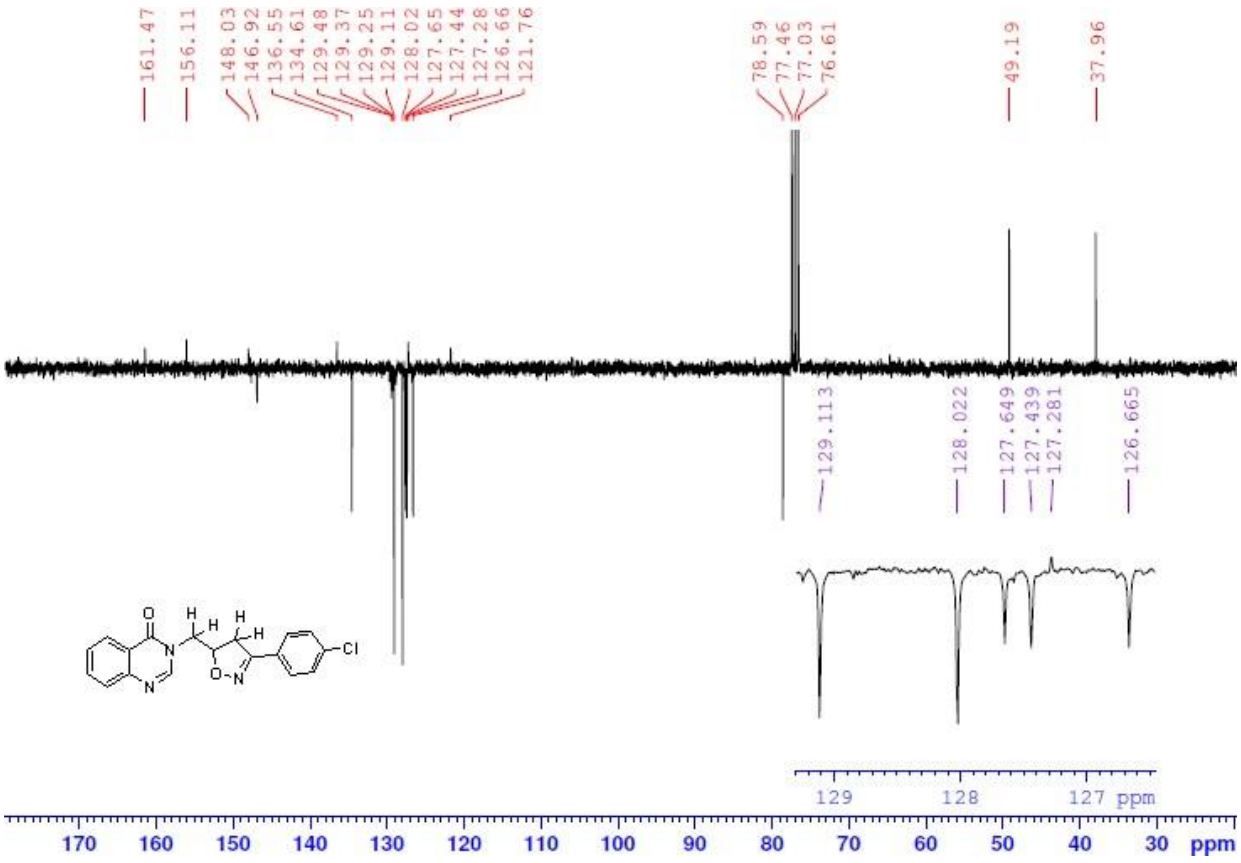

Figure S12. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound (**4b**)

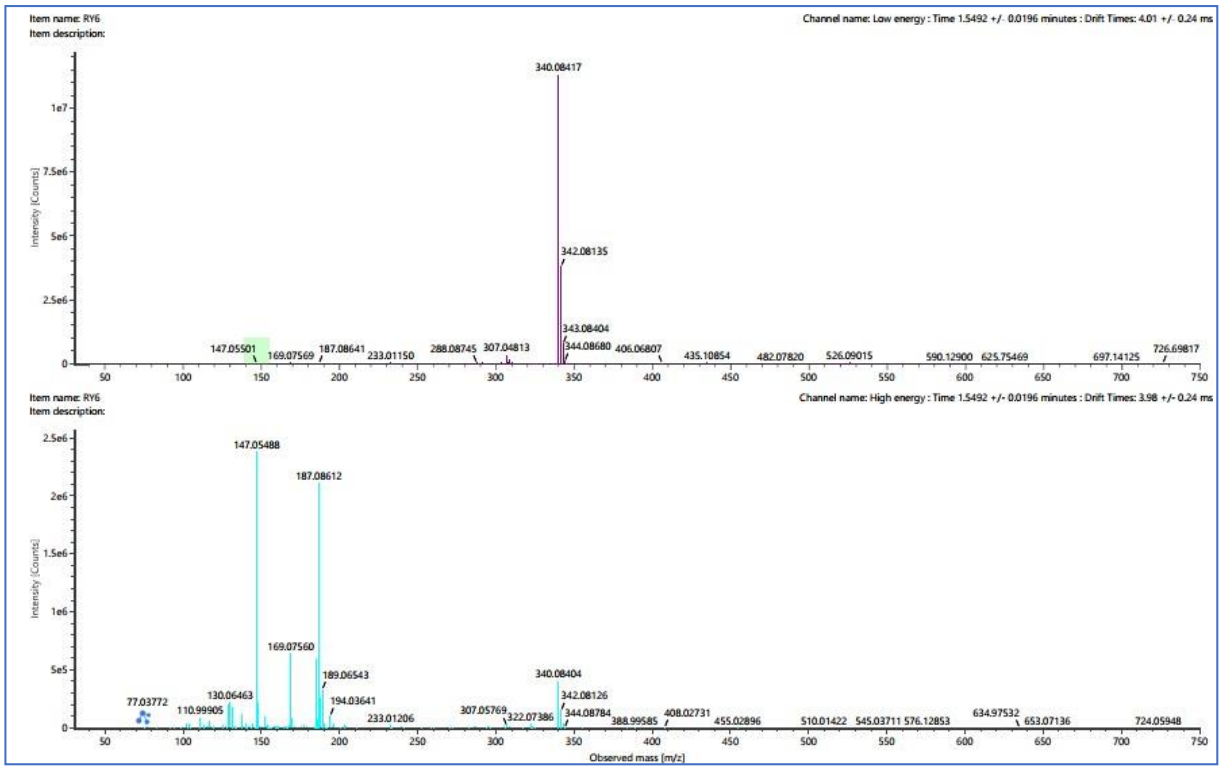

Figure S13. Mass spectrum of compound (**4b**)

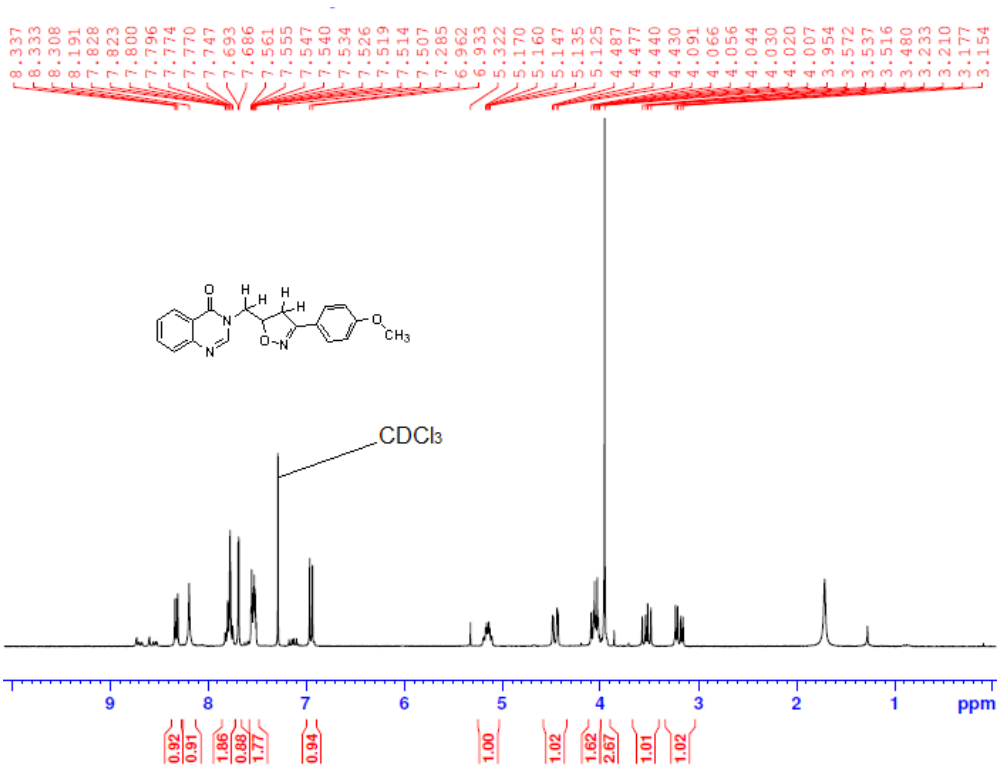

Figure S14. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **(4c)**

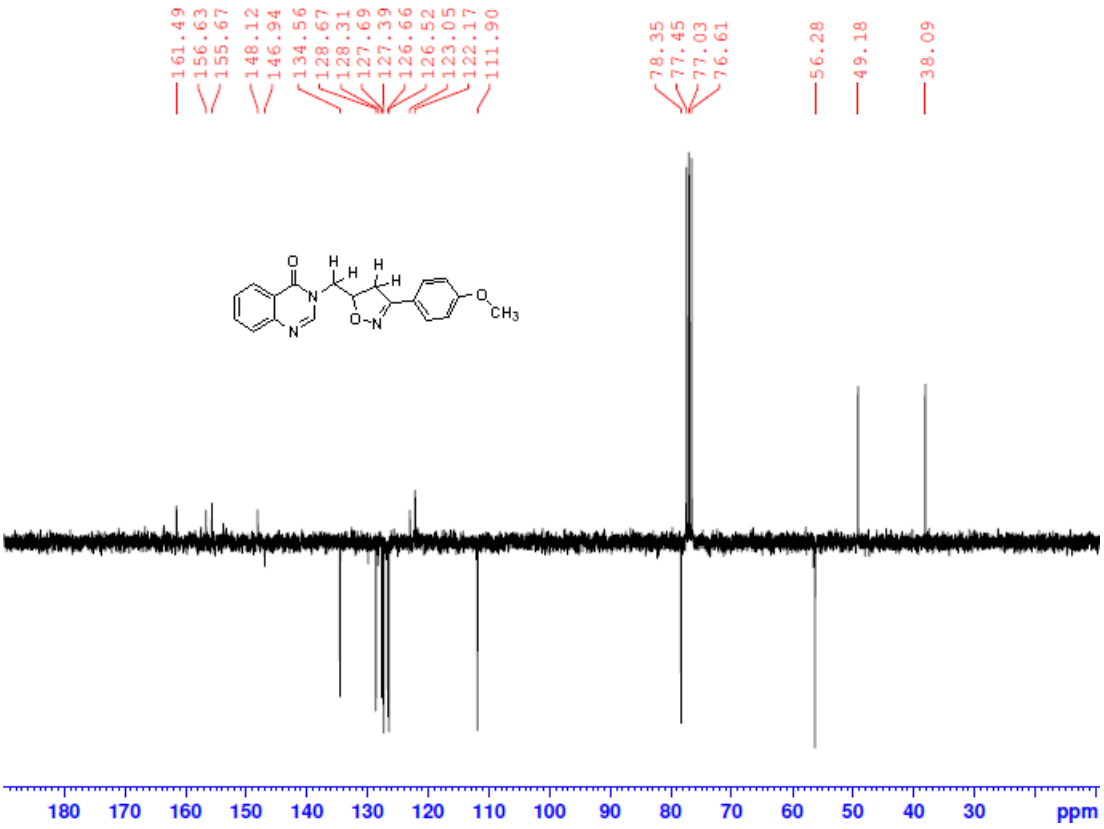

Figure S15. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound (**4c**)

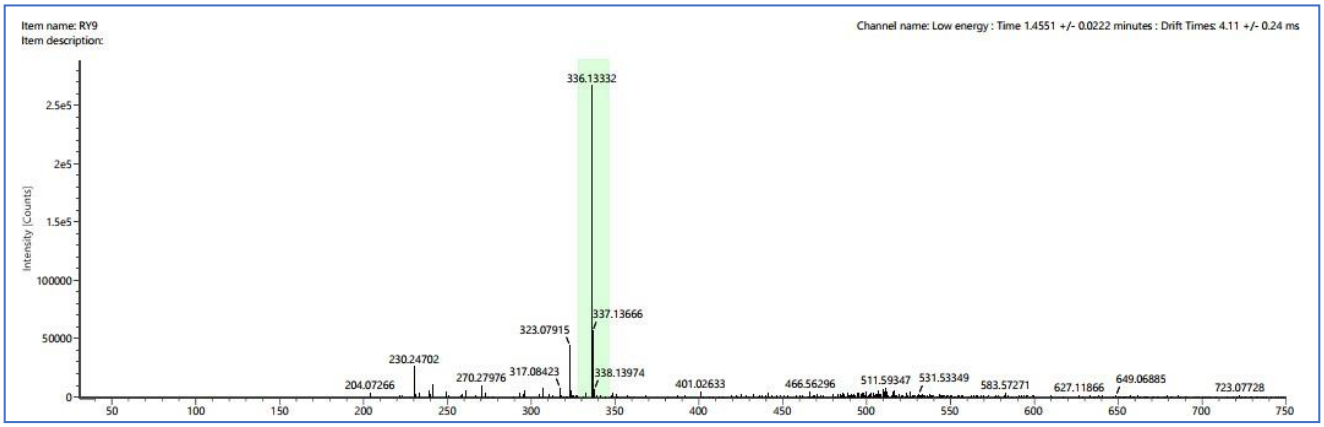

Figure S 16. Mass spectrum of compound (**4c**)

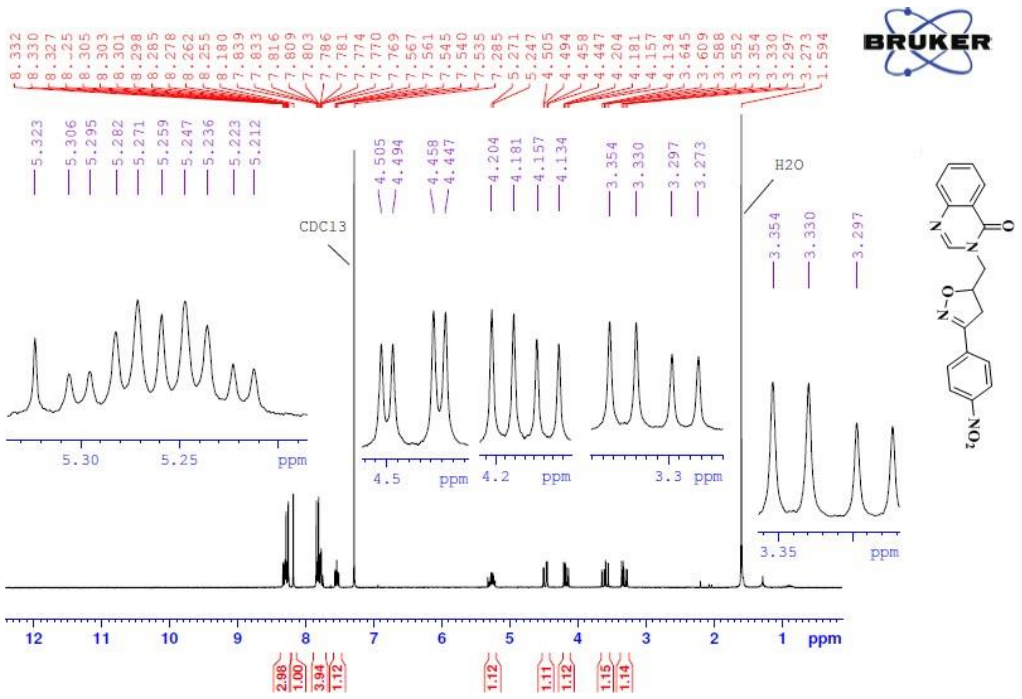

Figure S17. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **(4d)**

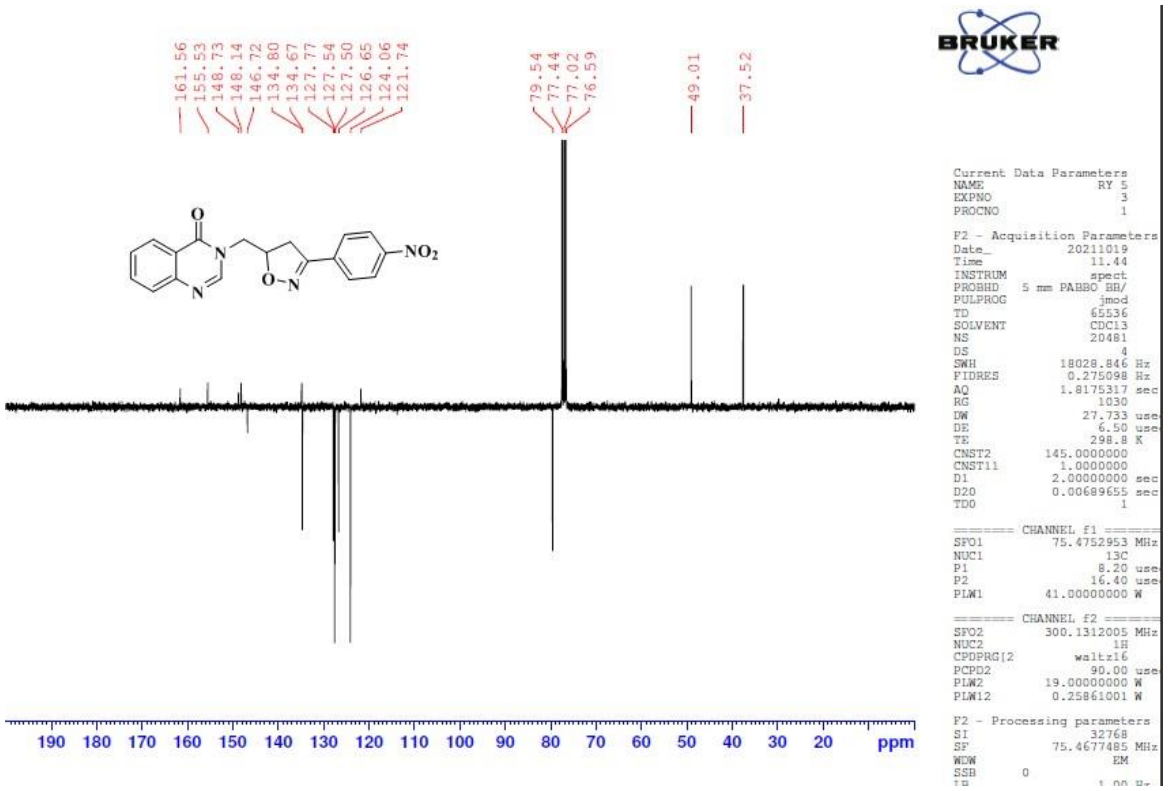

Figure S18. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound (**4d**)

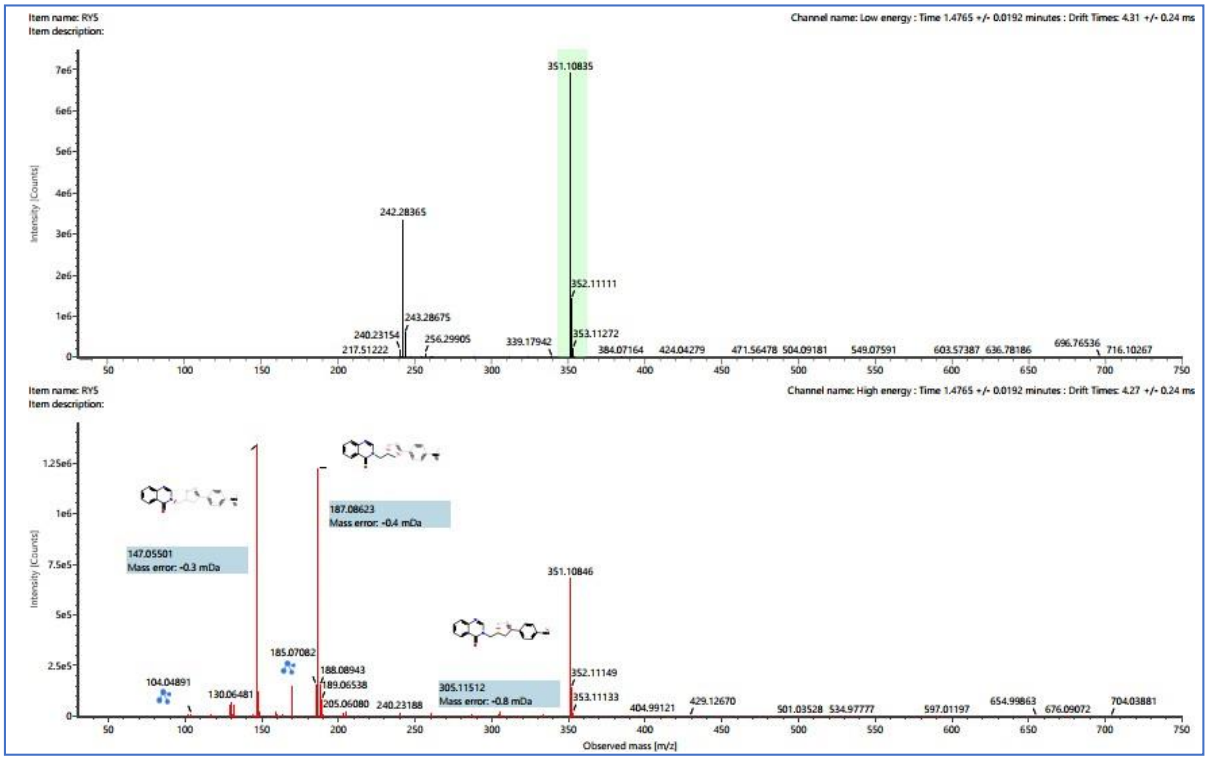

Figure S19. Mass spectrum of compound (**4d**)

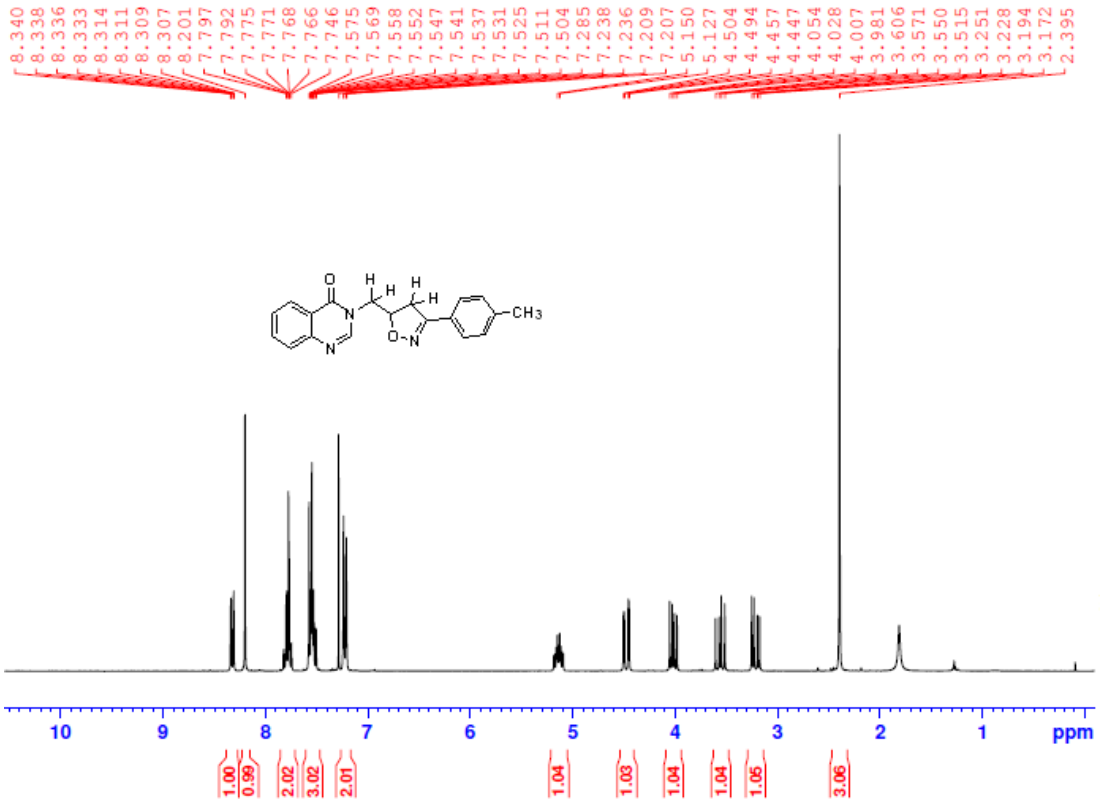

Figure S20. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **(4e)**

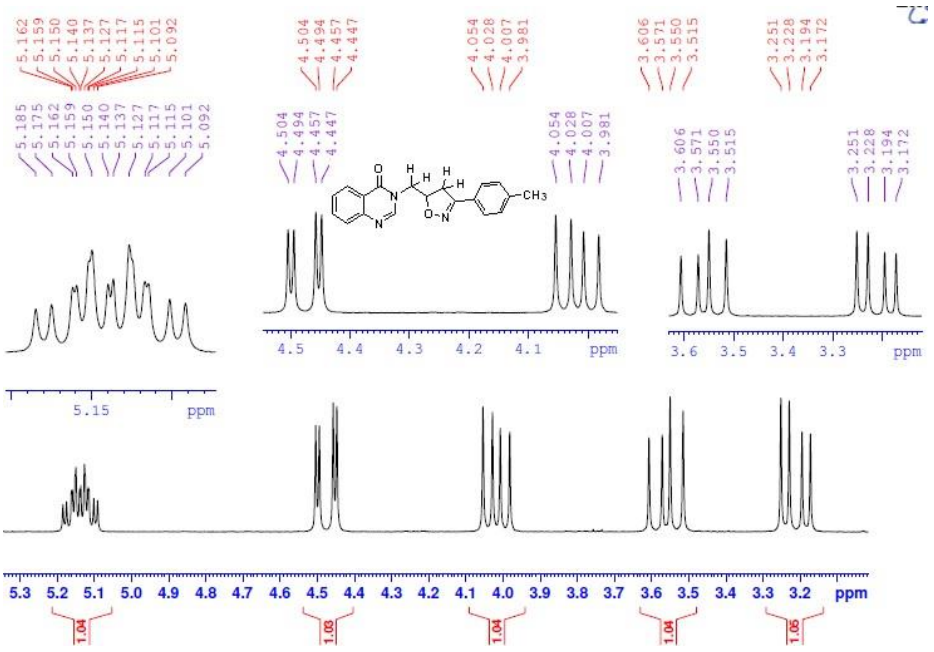

Figure S21. Aliphatic enlarged region of 1H NMR spectrum of compound (4e)

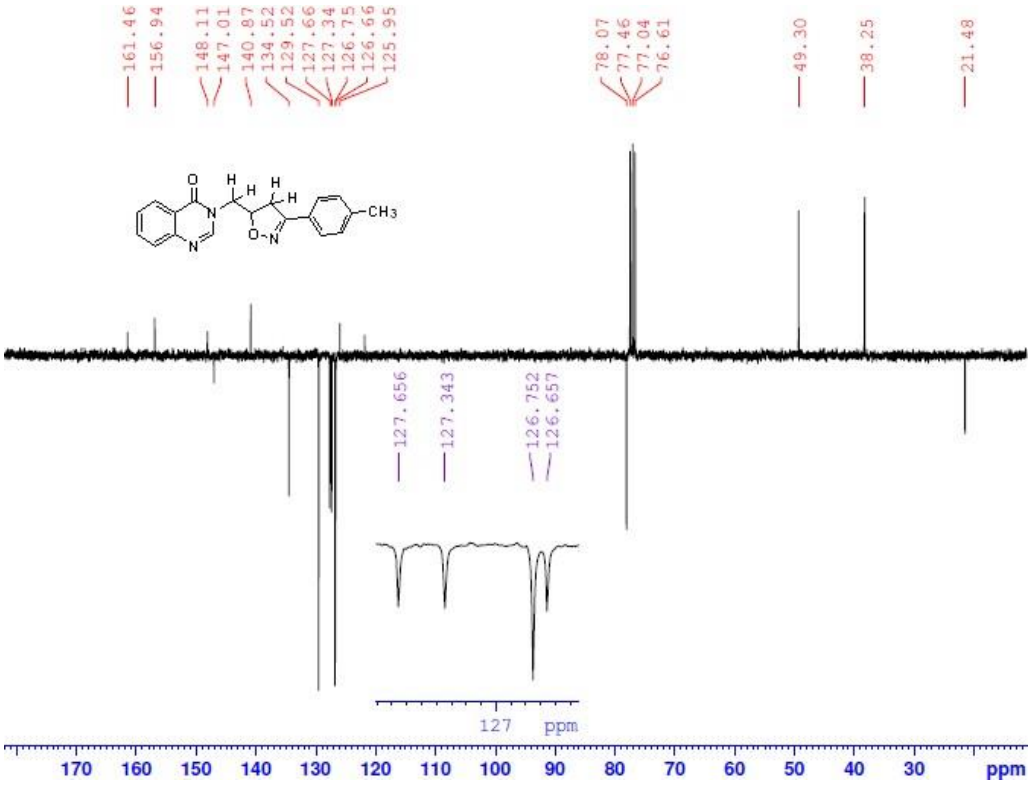

Figure S22. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound **(4e)**

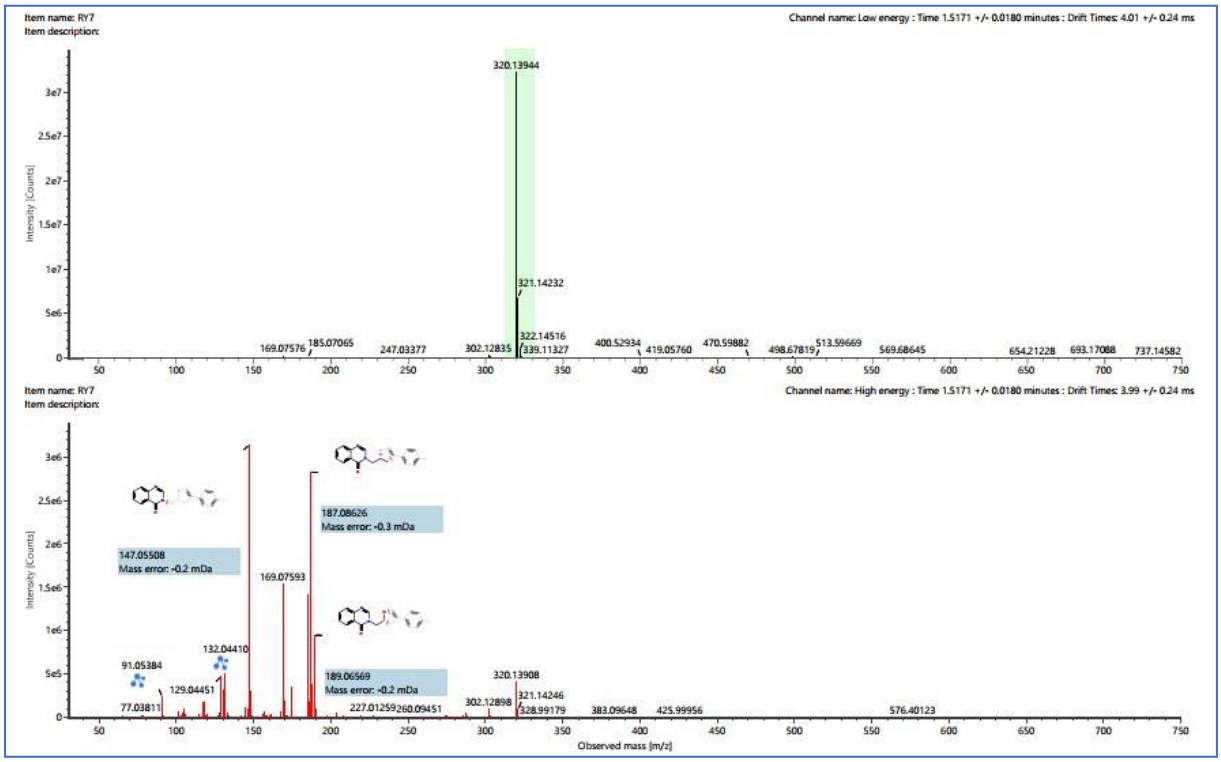

Figure S23. Mass spectrum of compound (**4e**)

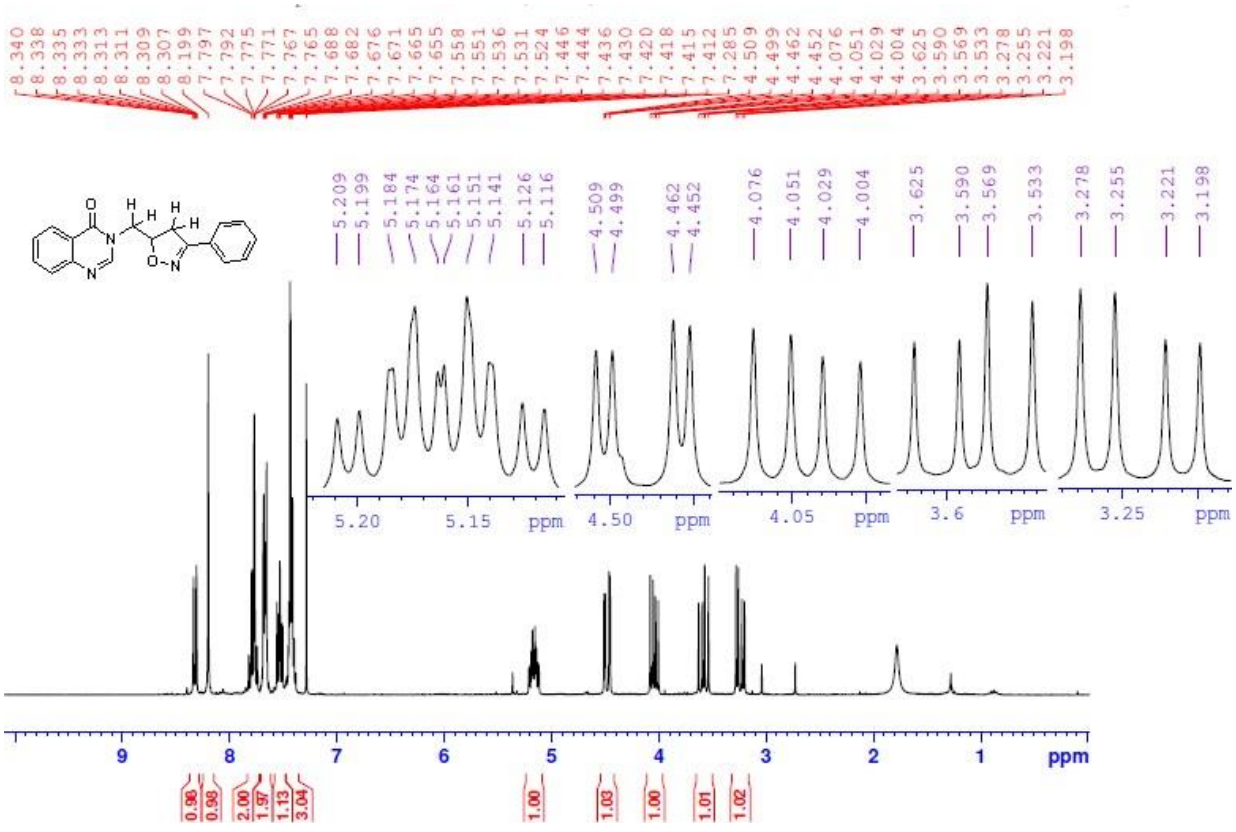

Figure S24. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **(4f)**

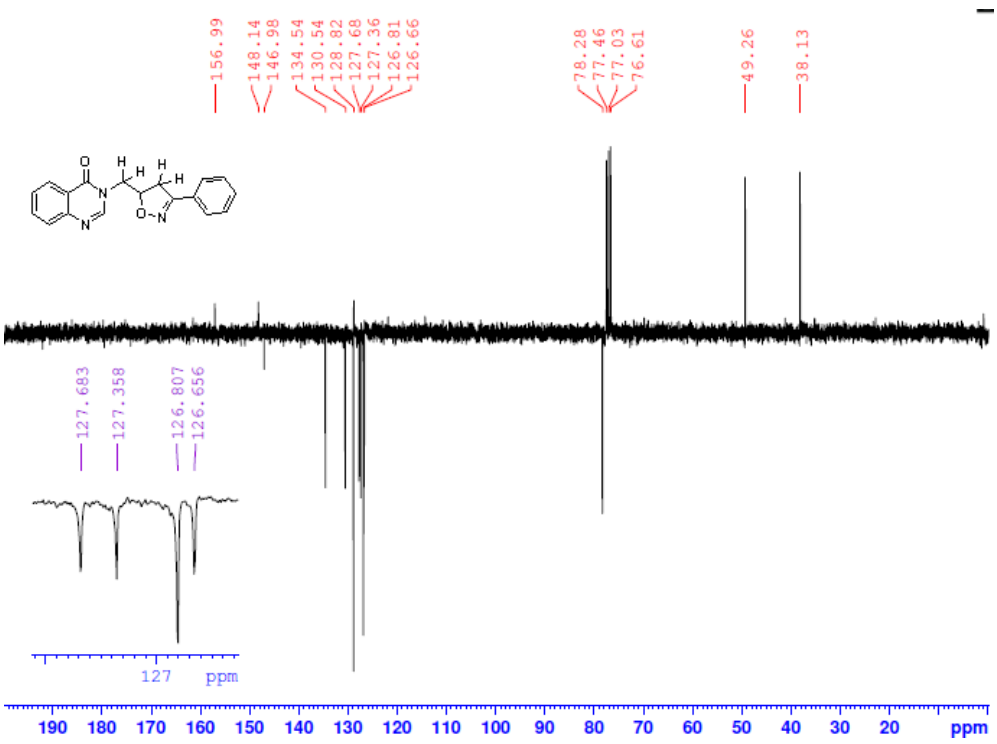

Figure S25. ^{13}C NMR spectrum (75 MHz, CDCl3) of compound **(4f)**

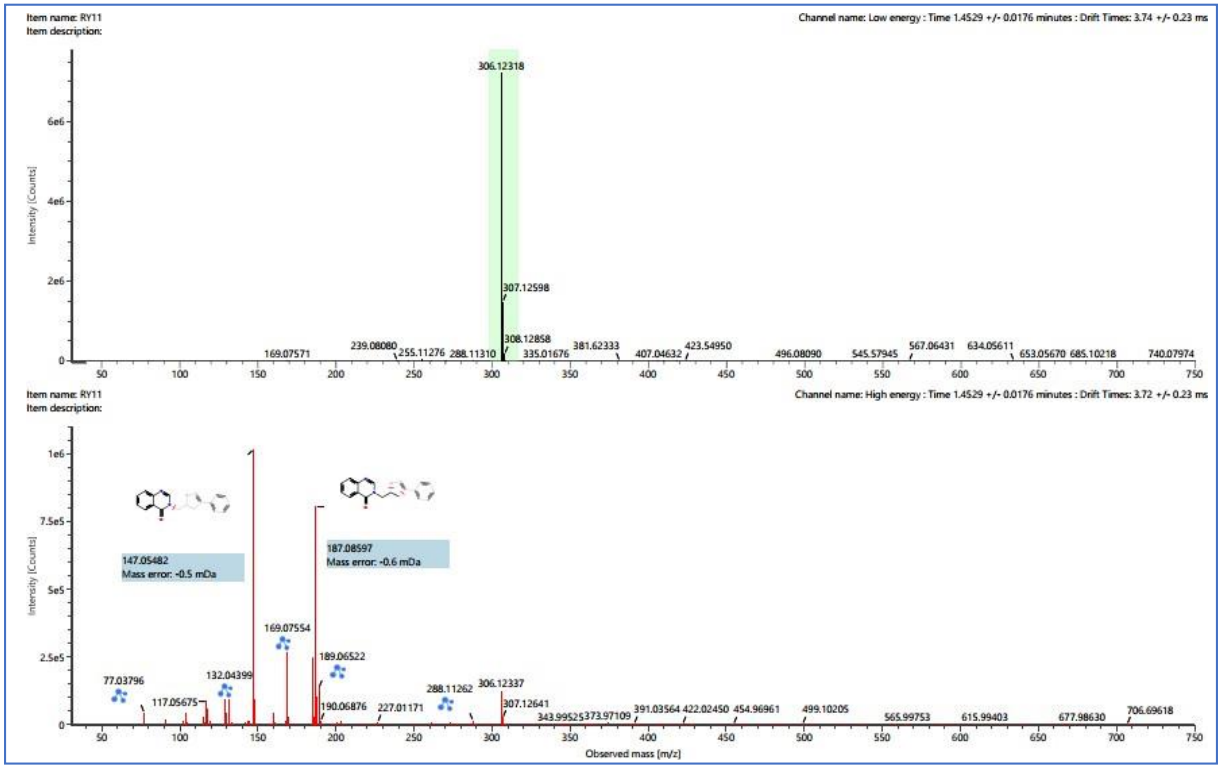

Figure S26. Mass spectrum of compound (**4f**)

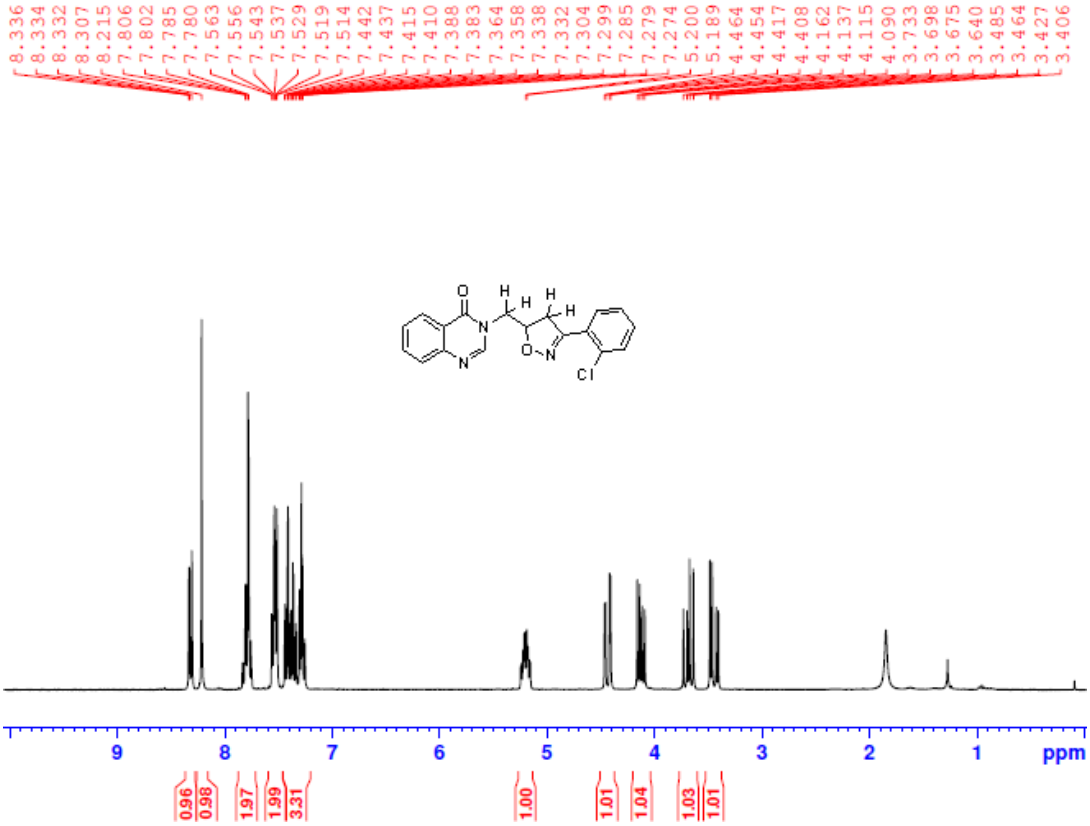

Figure S27. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **(4g)**

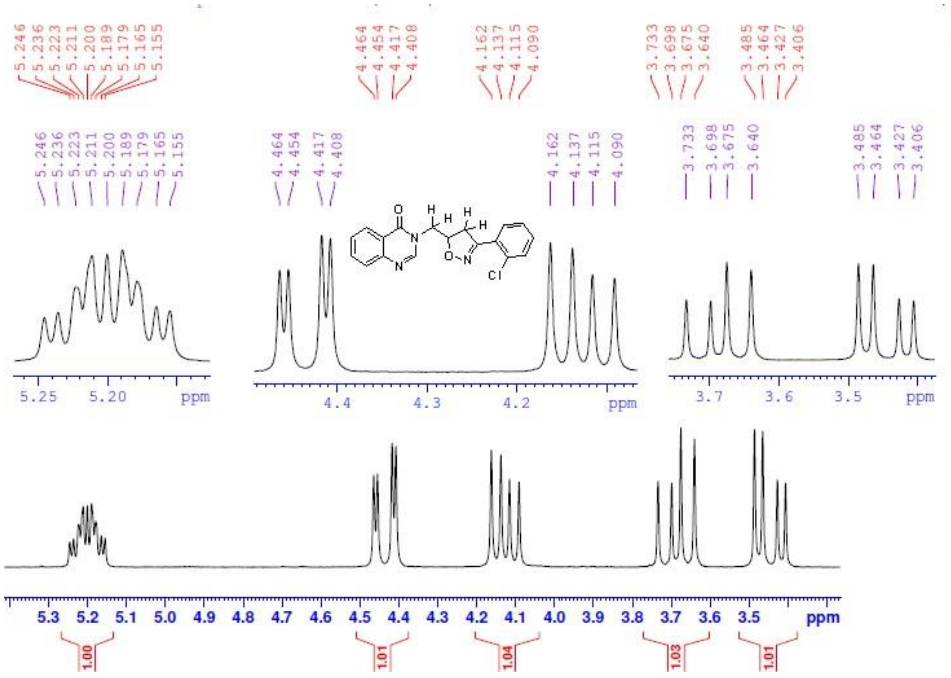

Figure S28. Aliphatic enlarged region of ^{1}H NMR spectrum of compound **(4g)**

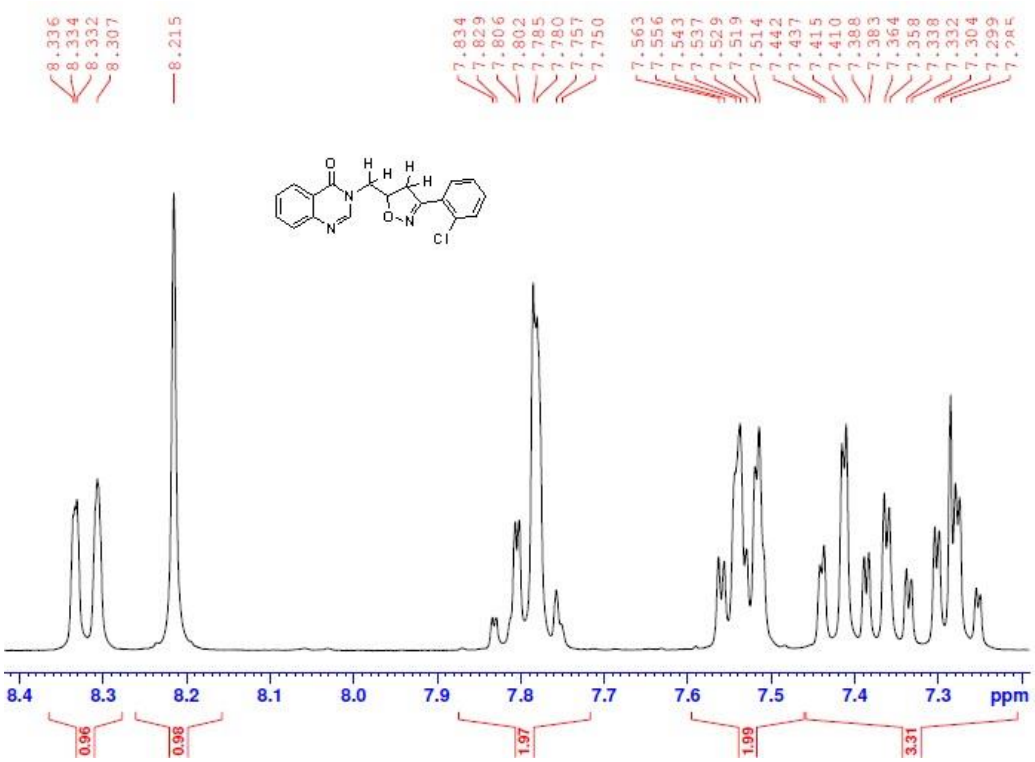

Figure S29. Aromatic enlarged region of ^{1}H NMR spectrum of compound **(4g)**

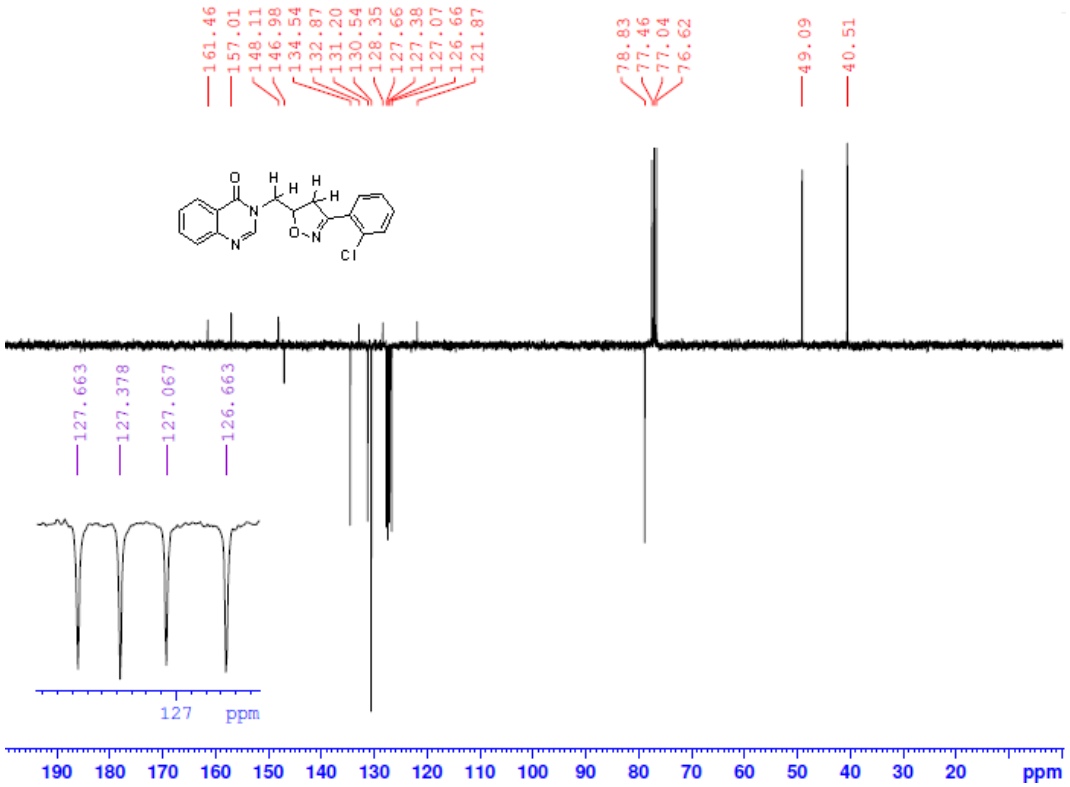

Figure S30. ^{13}C NMR spectrum (75 MHz, $CDCl_3$) of compound **(4g)**

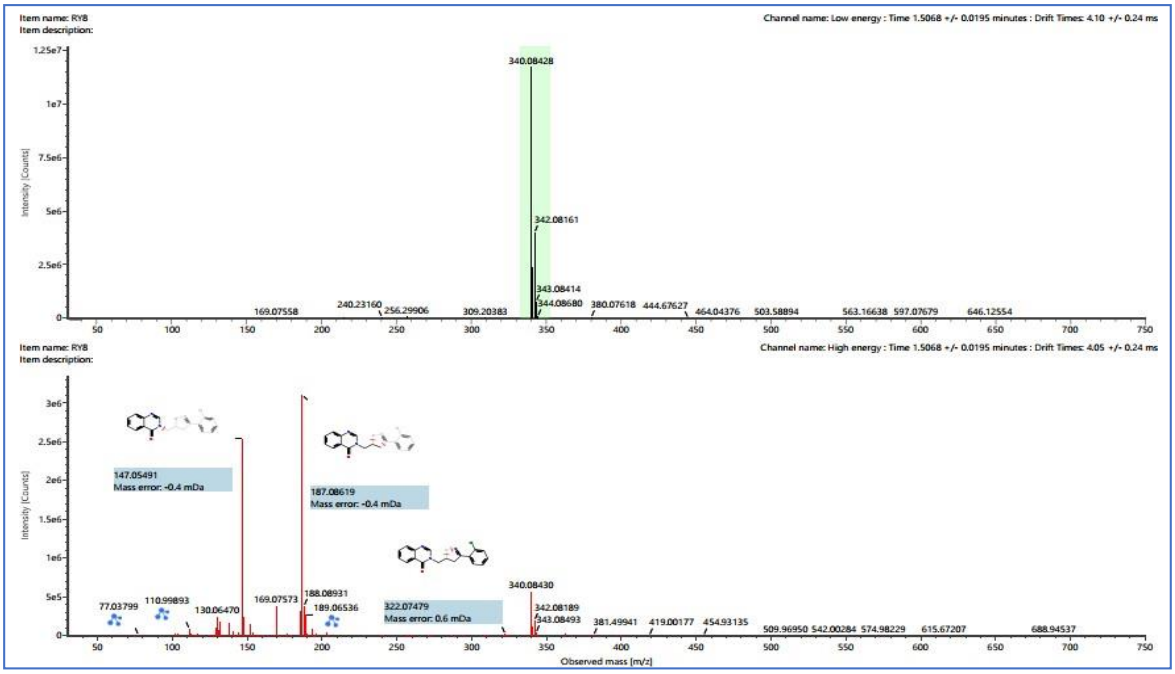

Figure S31. Mass spectrum of compound (**4g**)