

Supplementary Material

Unexpected Products from Mesoionic 1,3-Thiazinium or Oxazinium Olates: A novel Access to 3,5-Diaryl-1,3-thiazinane-2,4,6-trione and Alkoxy-3,5-diphenyl-3H-1,3-oxazine-2,6-dione Derivatives

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Contents: Figure S1-S18: GC-MS and NMR data

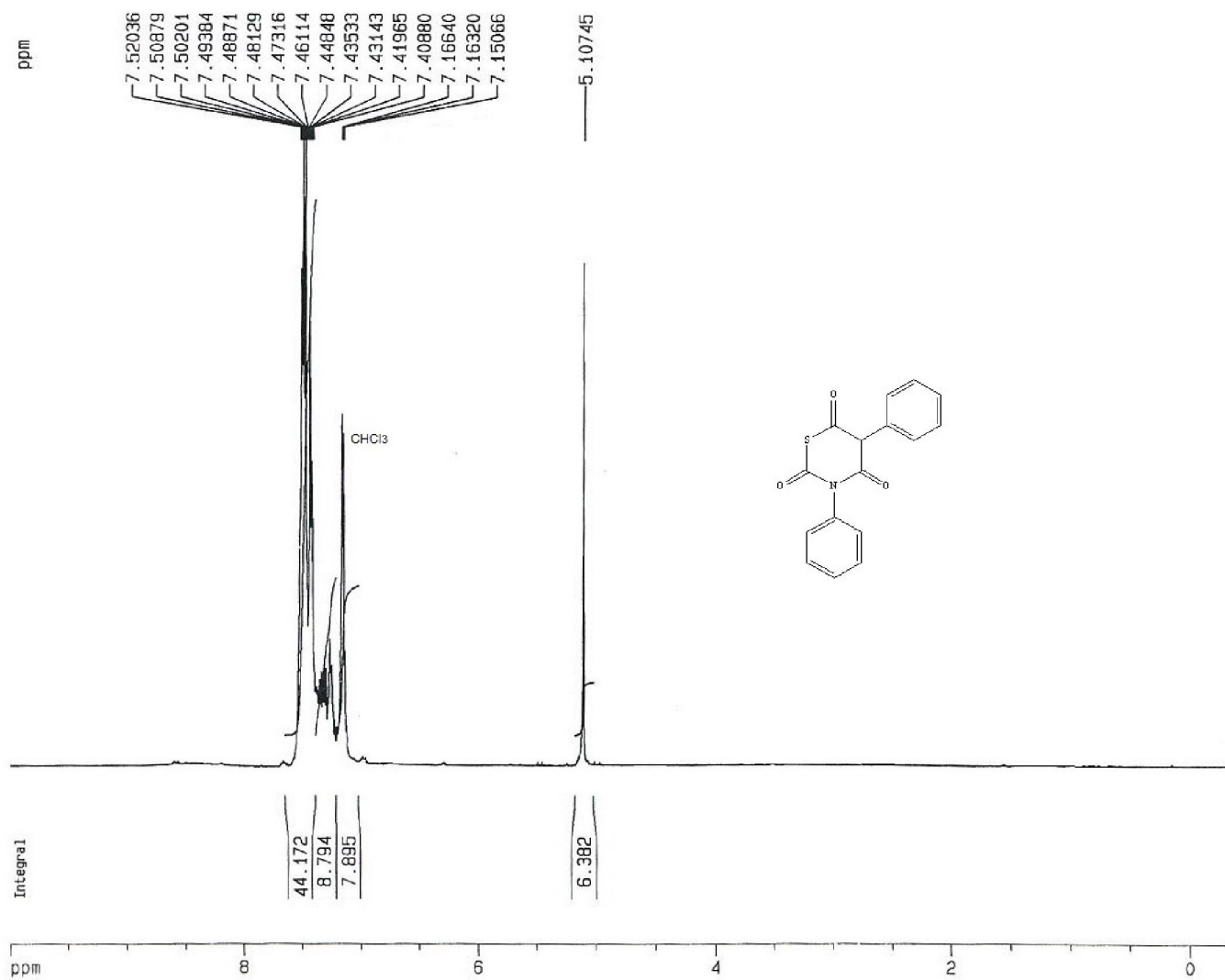


Figure S1. ¹H NMR spectrum of 3,5-diphenyl-1,3-thiazinane-2,4,6-trione **3a**

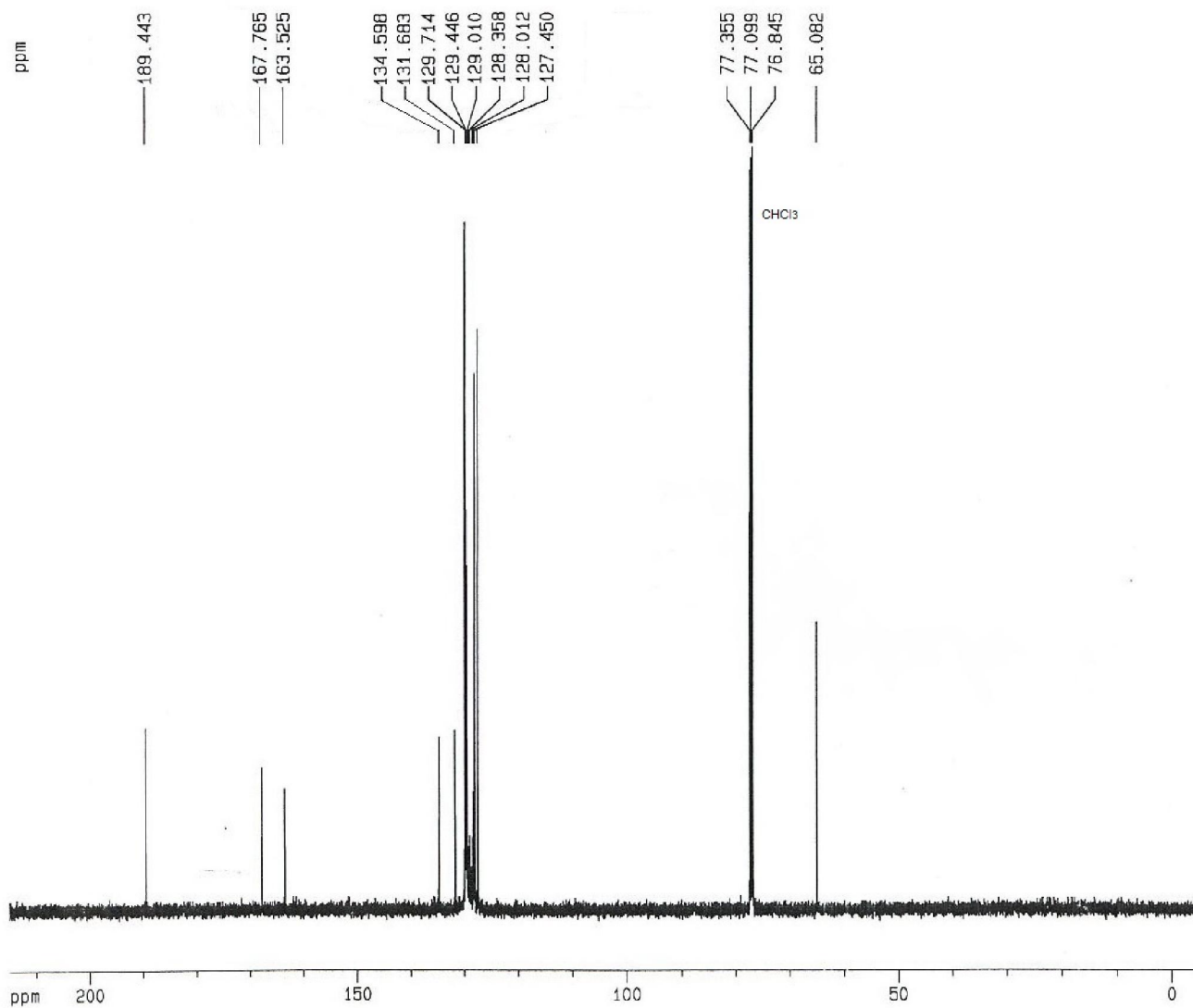


Figure S2. ¹³C NMR spectrum of 3,5-diphenyl-1,3-thiazinane-2,4,6-trione **3a**

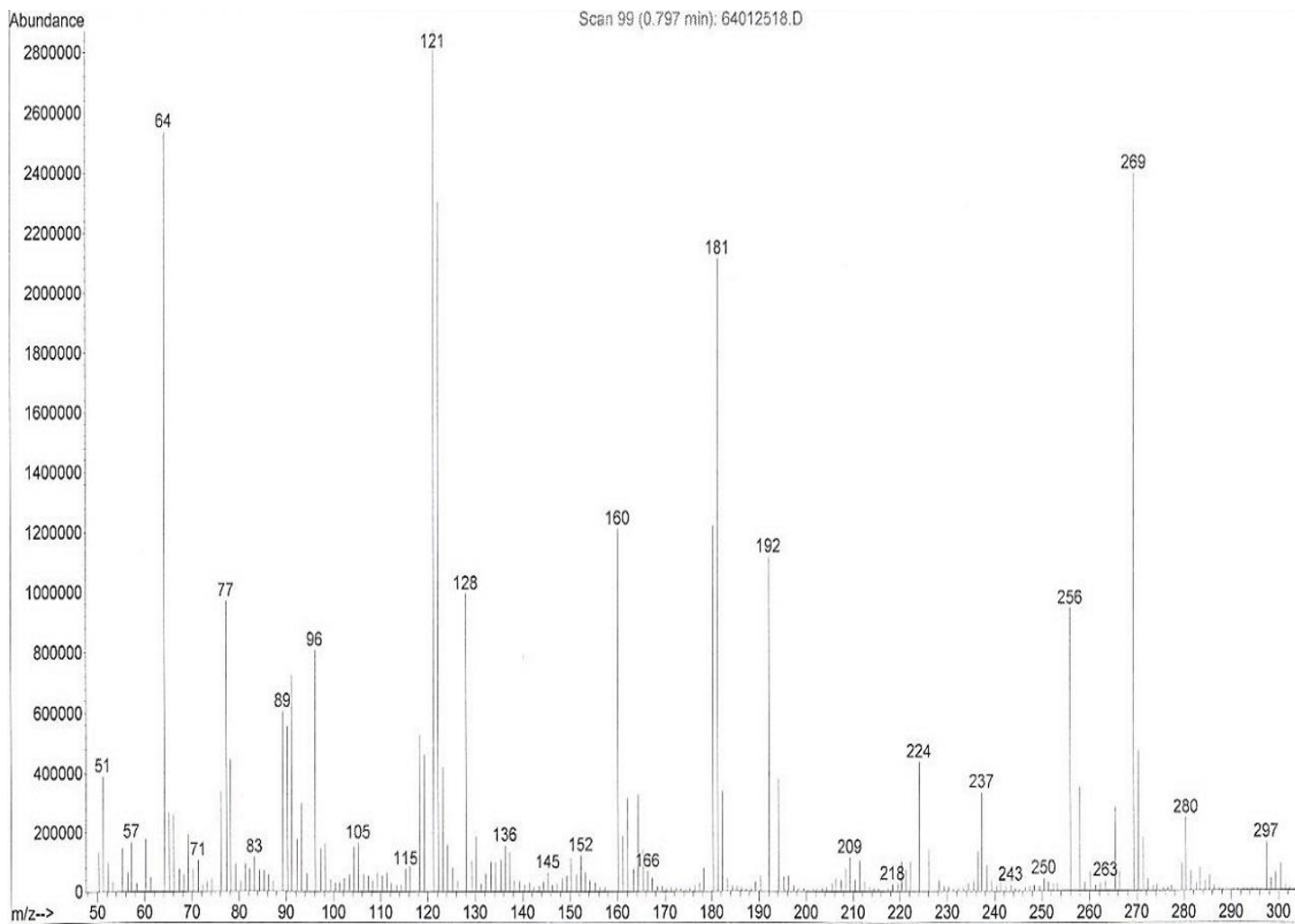


Figure S3. Mass spectrum of 3,5-diphenyl-1,3-thiazinane-2,4,6-trione **3a**

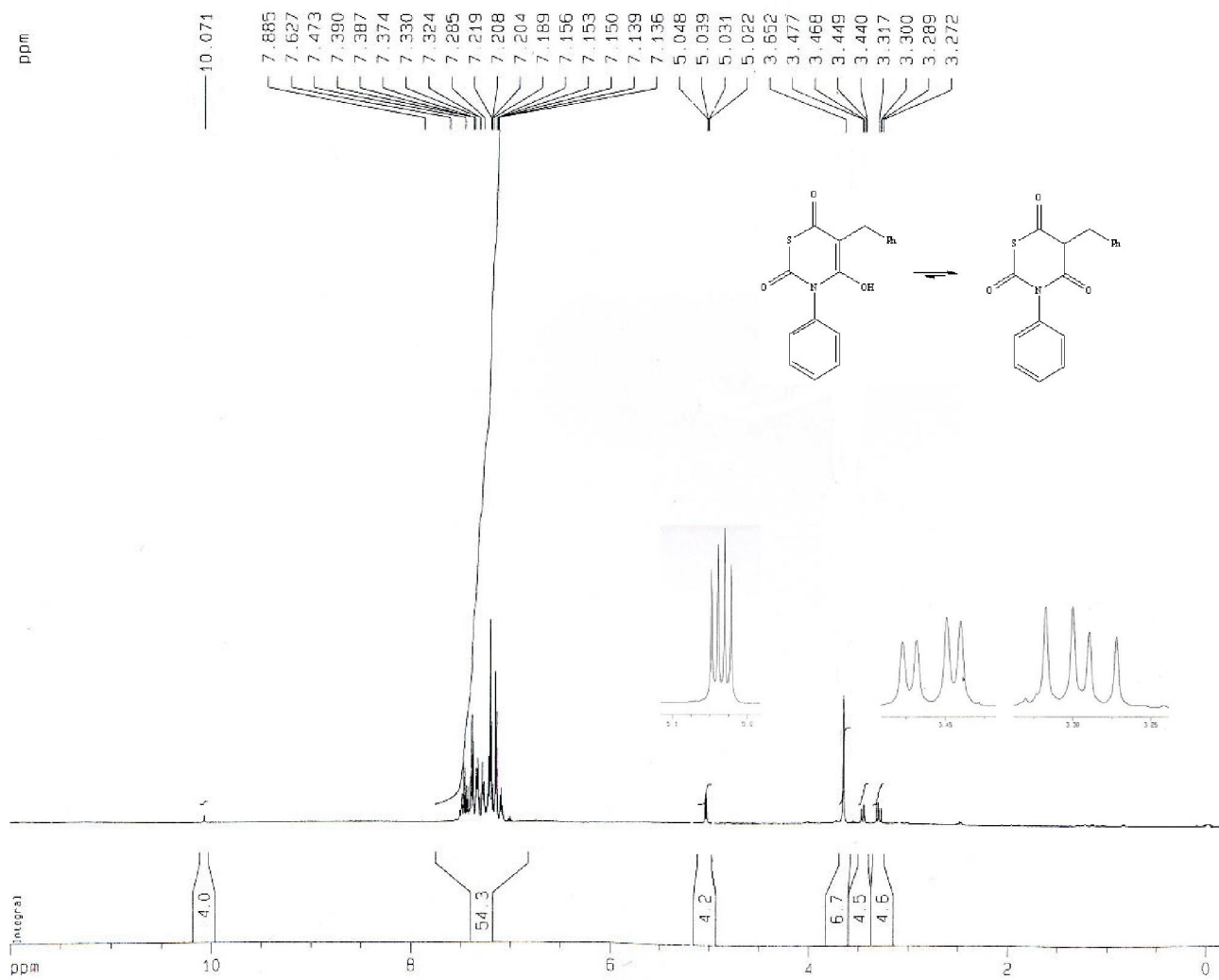


Figure S4. ¹H NMR spectrum of 5-benzyl-3-phenyl-1,3-thiazinane-2,4,6-trione **3b**

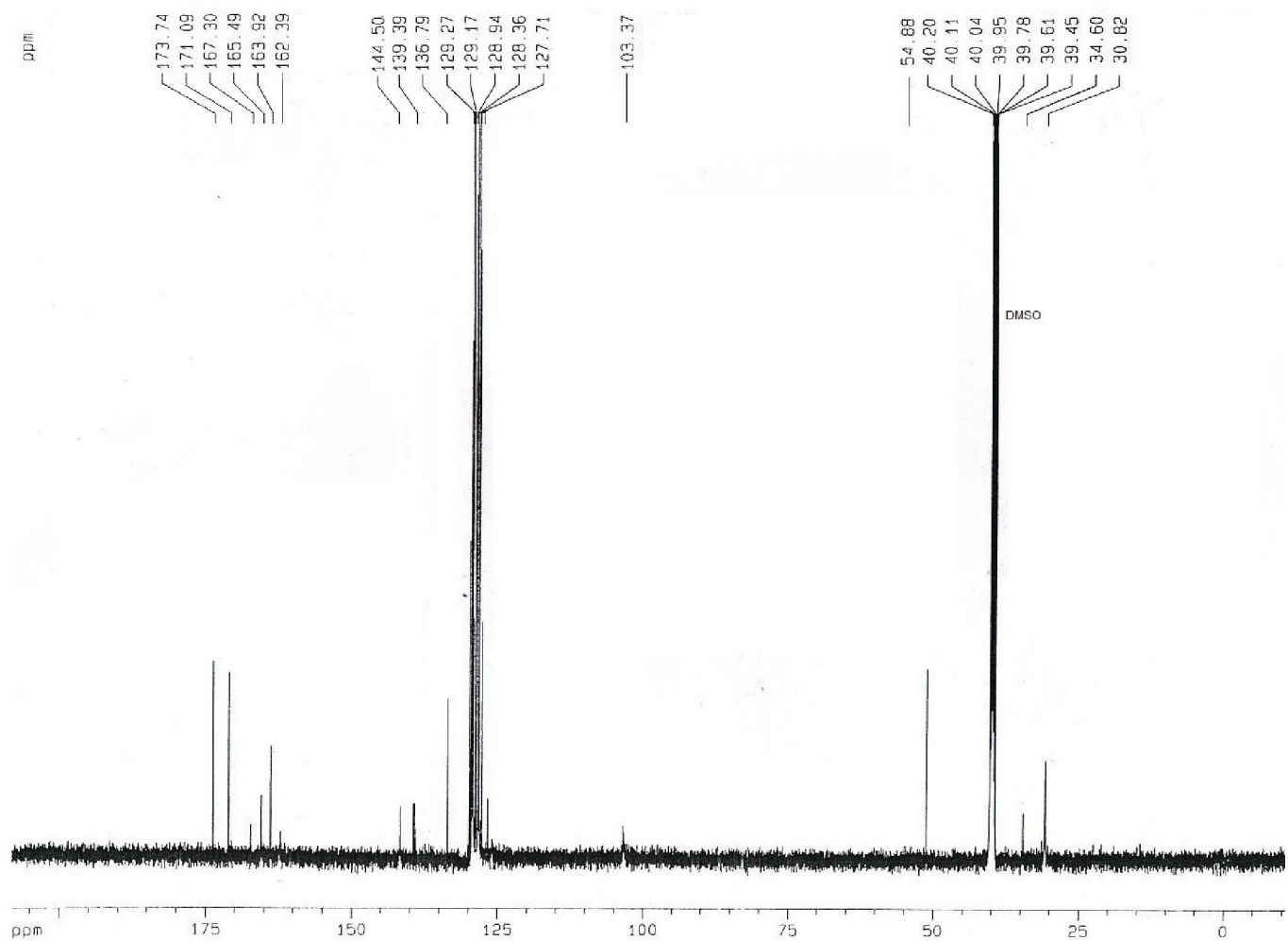


Figure S5. ^{13}C NMR spectrum of 5-benzyl-3-phenyl-1,3-thiazinane-2,4,6-trione **3b**

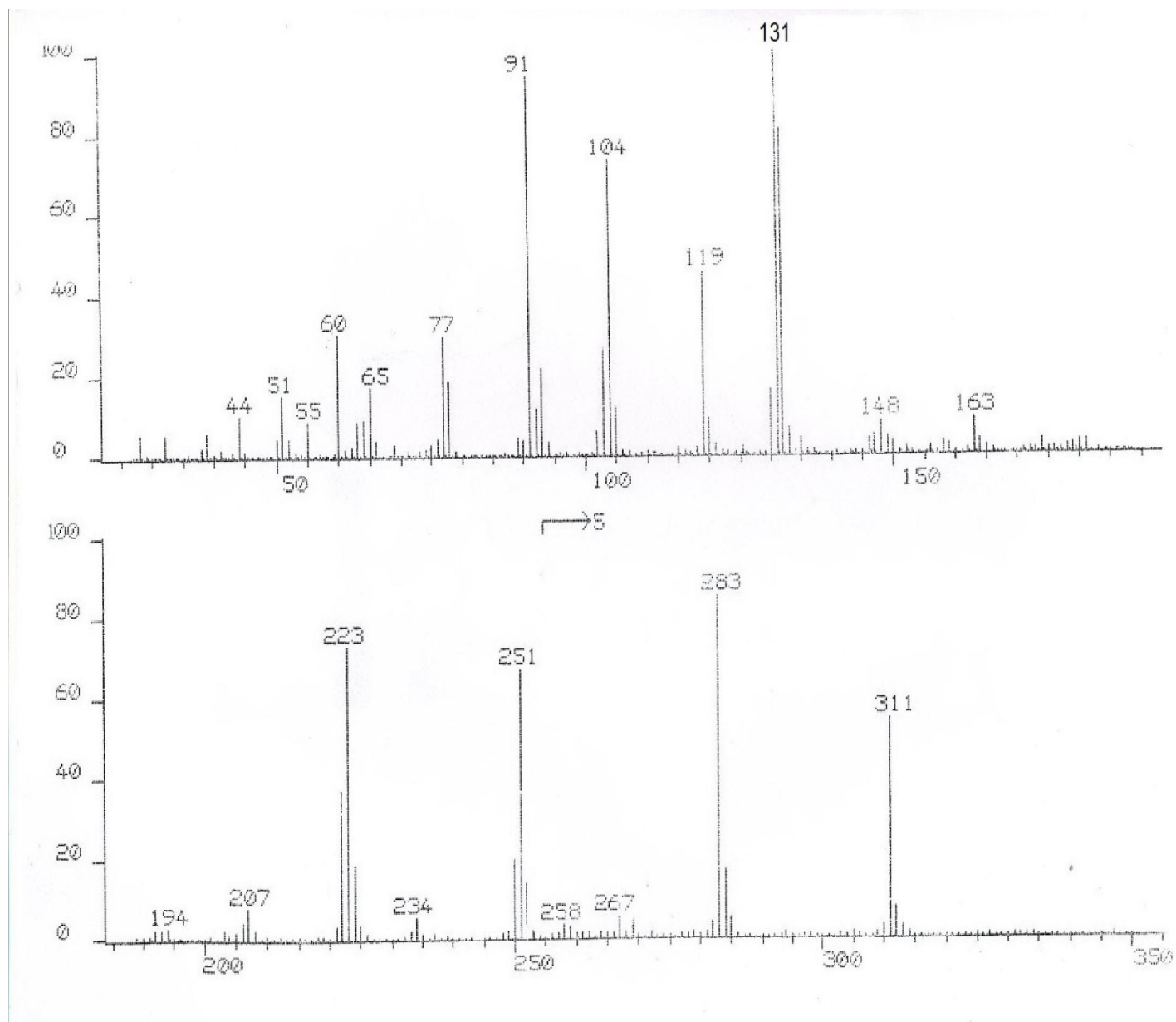


Figure S6. Mass spectrum of 5-benzyl-3-phenyl-1,3-thiazinane-2,4,6-trione **3b**

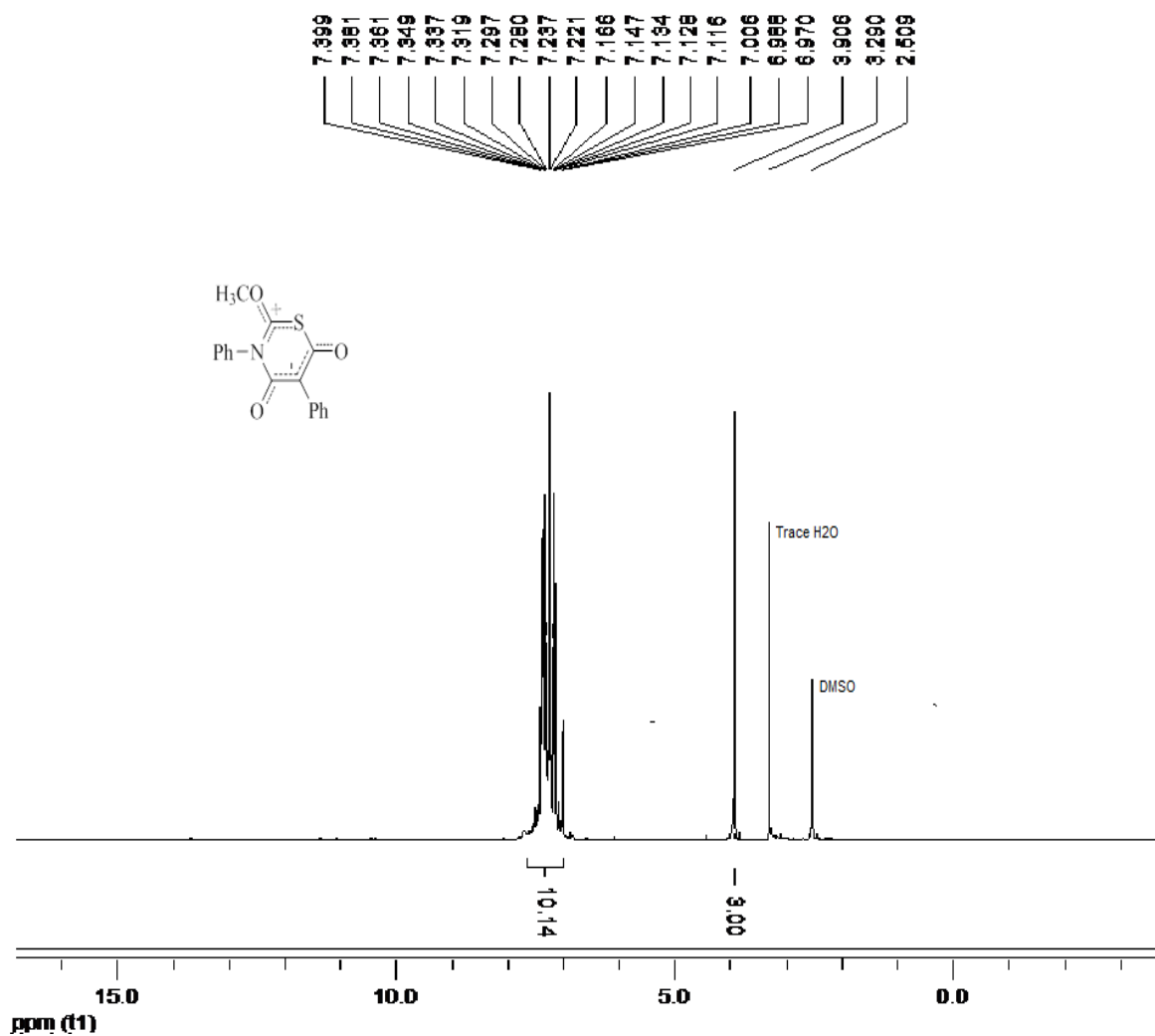


Figure S7. ¹H NMR spectrum of 2-methoxy-6-oxo-3,5-diphenyl-6H-1,3-thiazin-3-ium-4-olate **5**

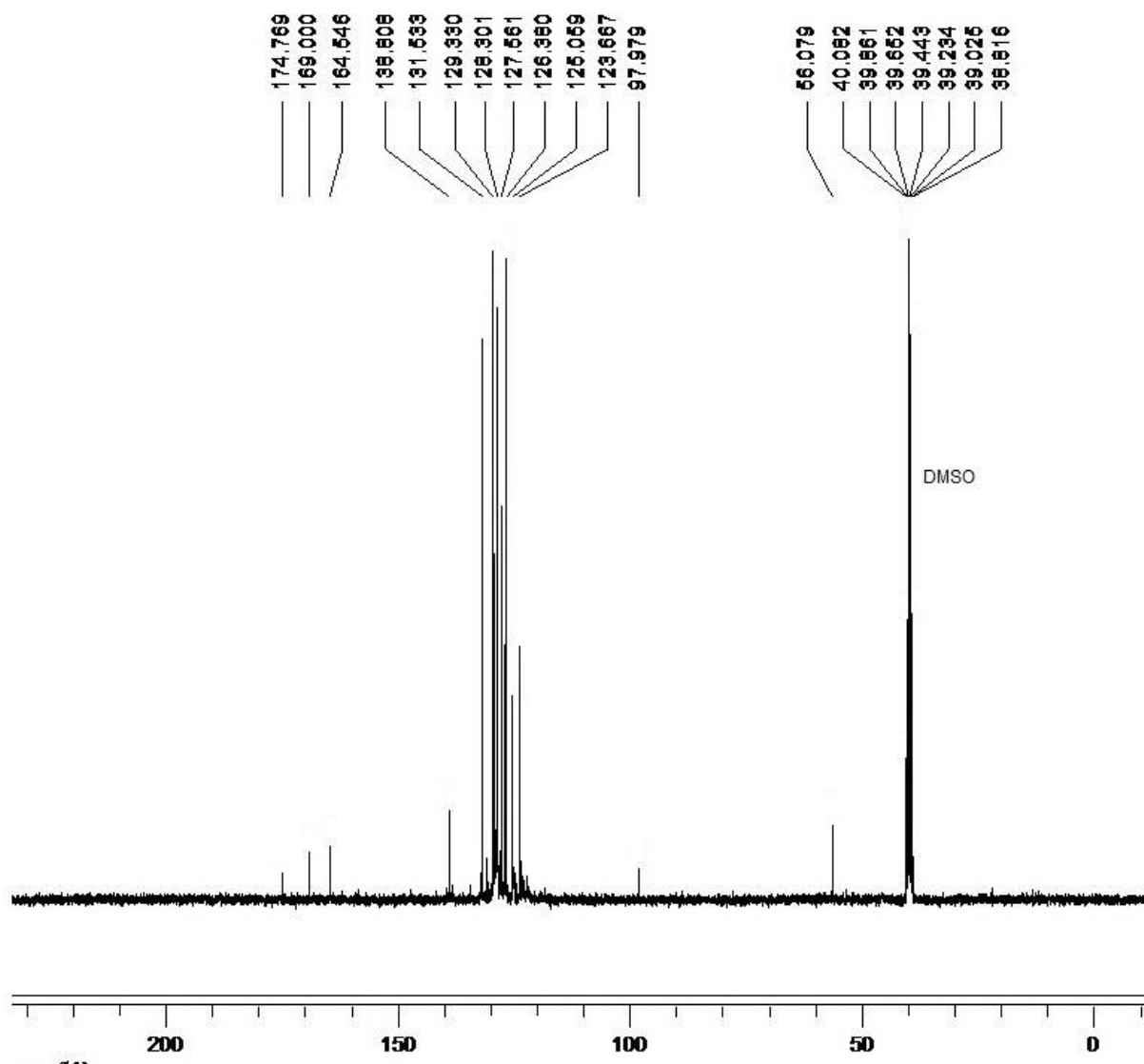


Figure S8. ^{13}C NMR spectrum of 2-methoxy-6-oxo-3,5-diphenyl-6H-1,3-thiazin-3-ium-4-olate **5**

Abundance

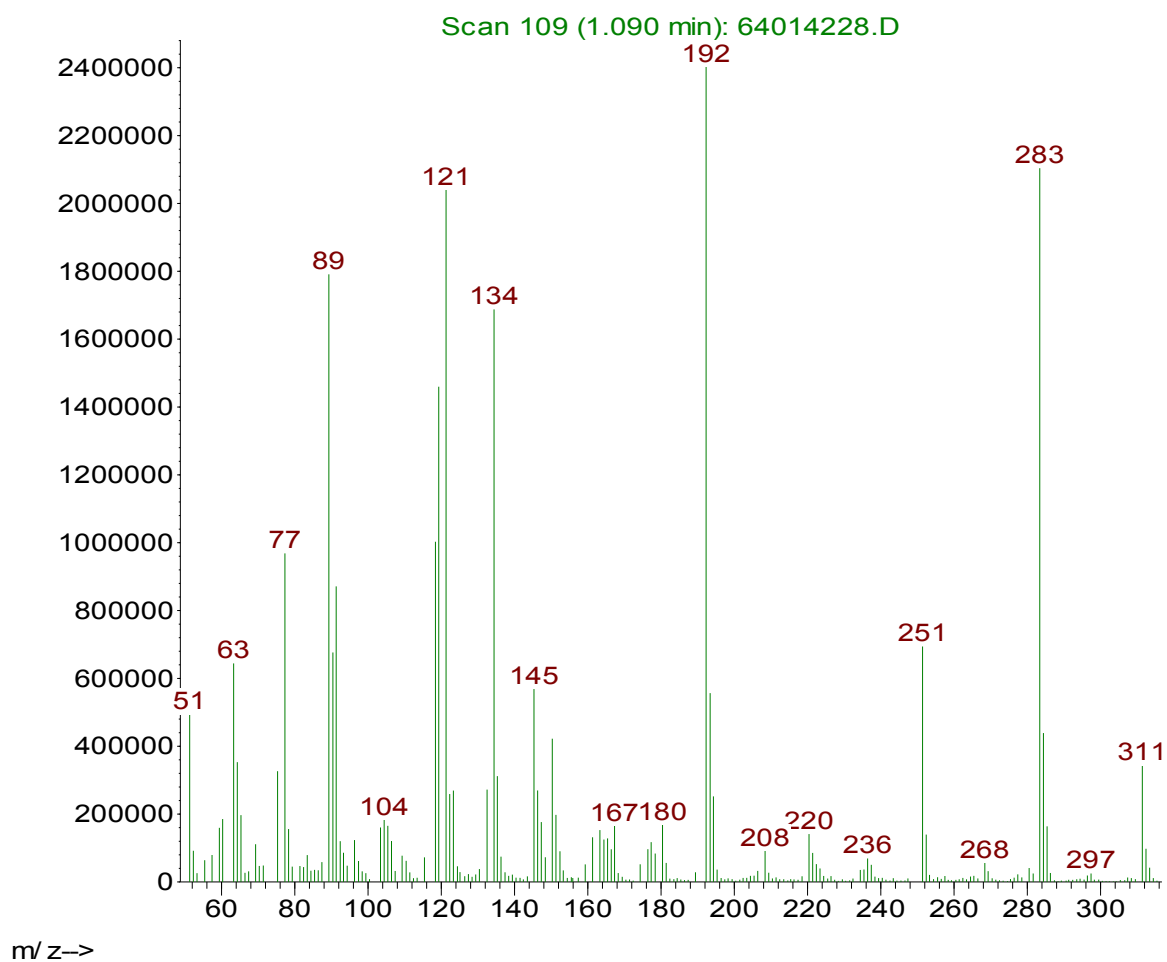


Figure S9. Mass spectrum of 2-methoxy-6-oxo-3,5-diphenyl-6H-1,3-thiazin-3-ium-4-olate **5**

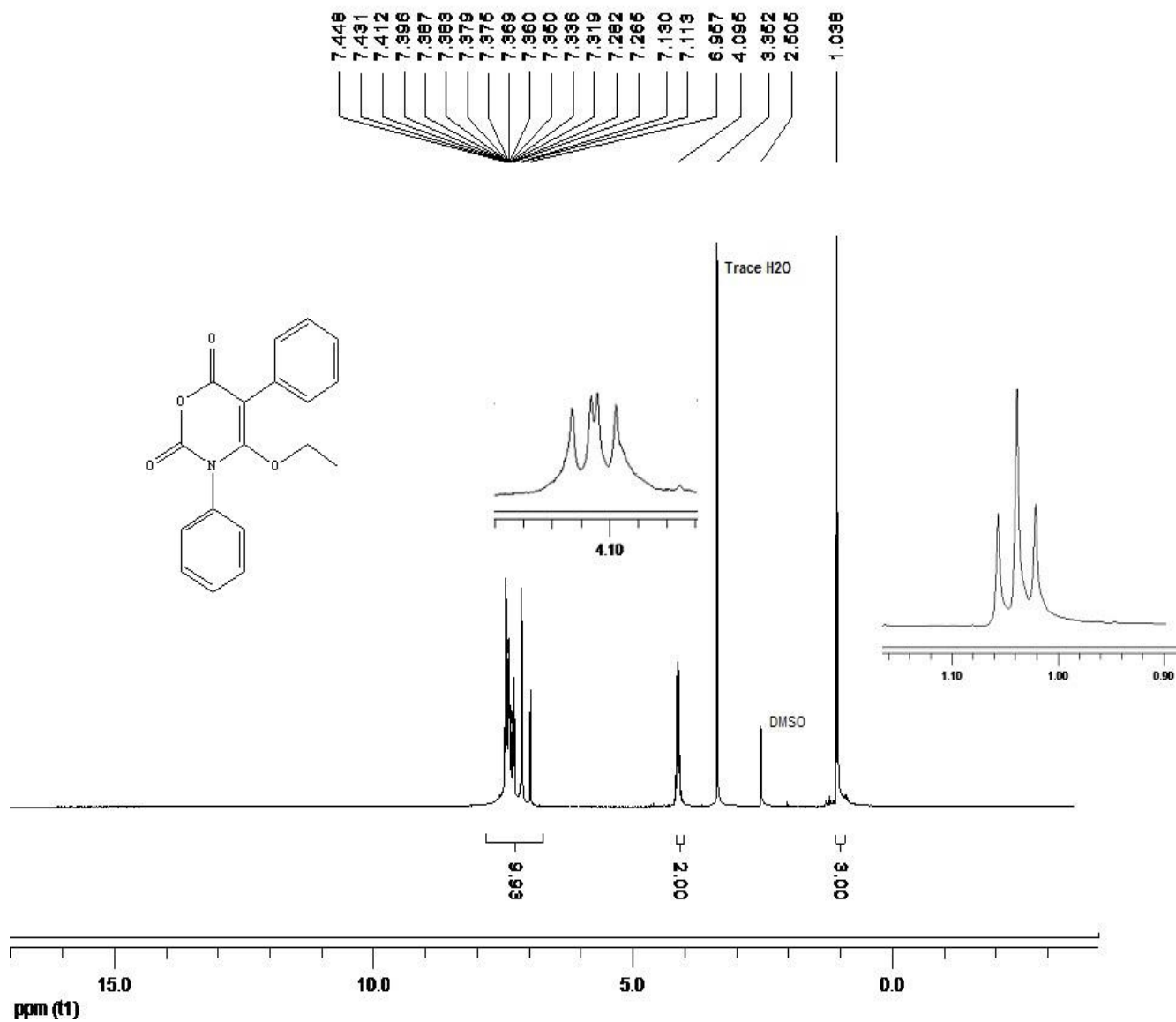


Figure S10. ¹H NMR spectrum of 4-ethoxy-3,5-diphenyl-2H-1,3-oxazine-2,6(3H)-dione **7a**

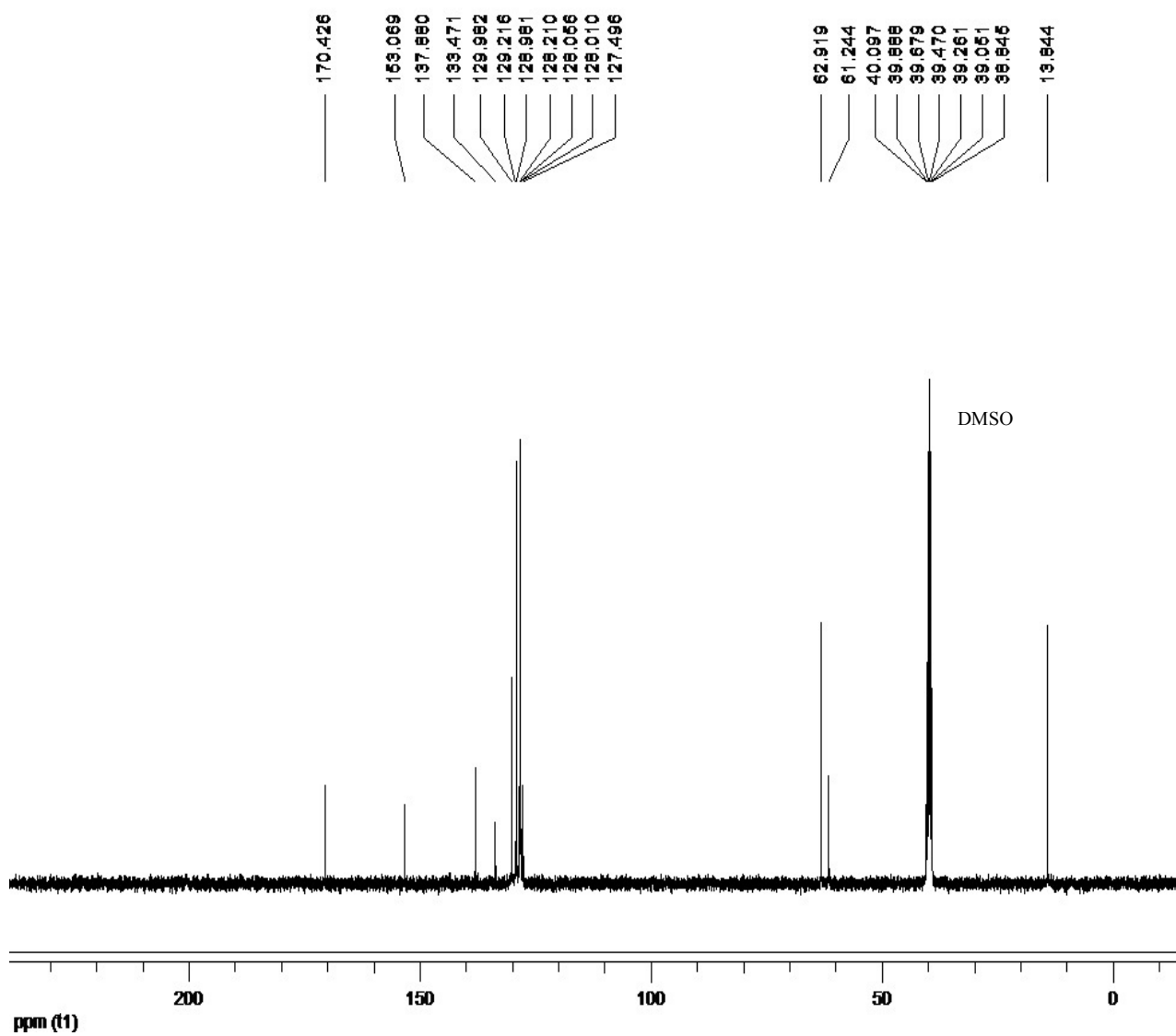


Figure S11. ^{13}C NMR spectrum of 4-ethoxy-3,5-diphenyl-2H-1,3-oxazine-2,6(3H)-dione **7a**

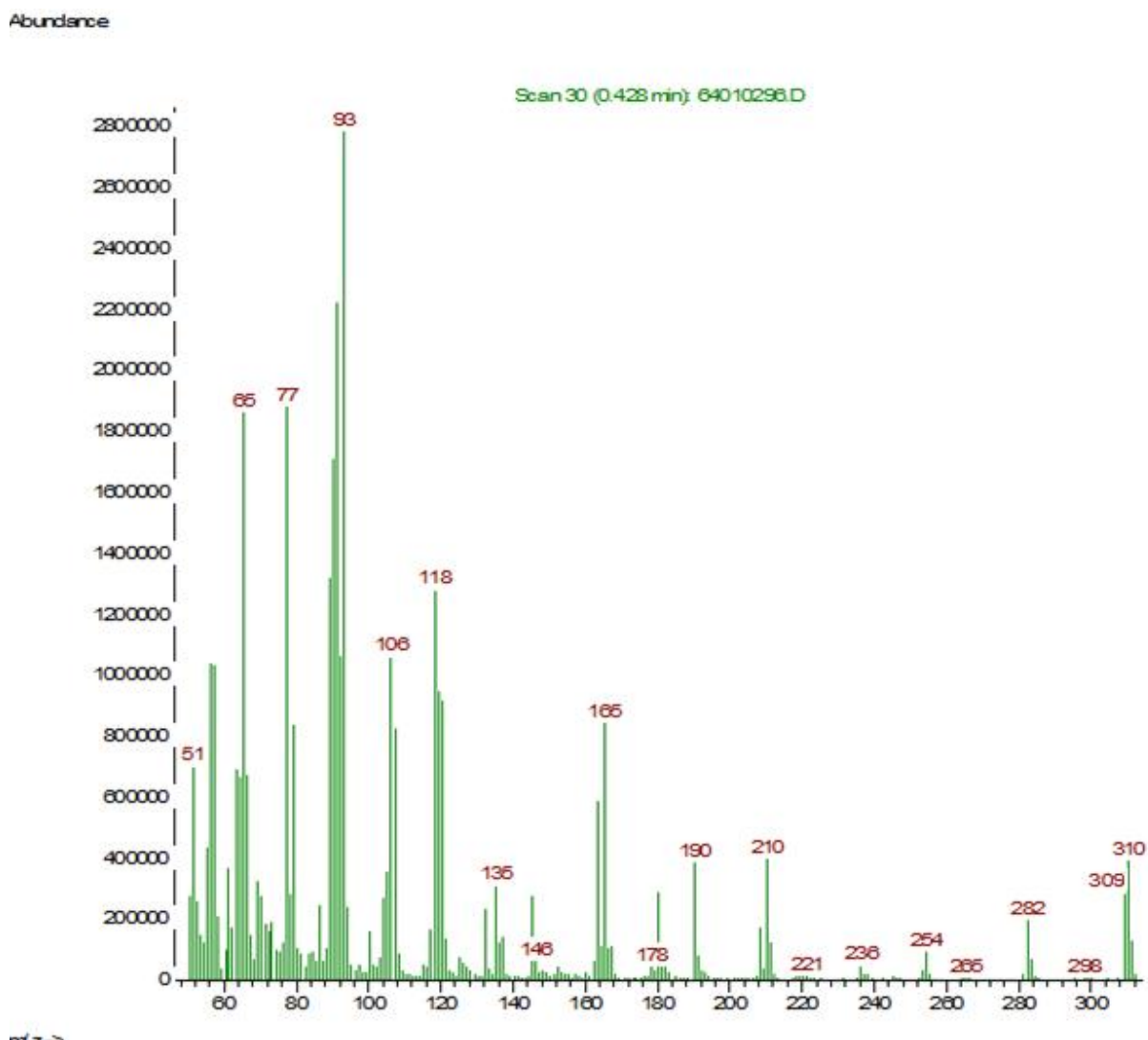


Figure S12. Mass spectrum of 4-ethoxy-3,5-diphenyl-2H-1,3-oxazine-2,6(3H)-dione **7a**

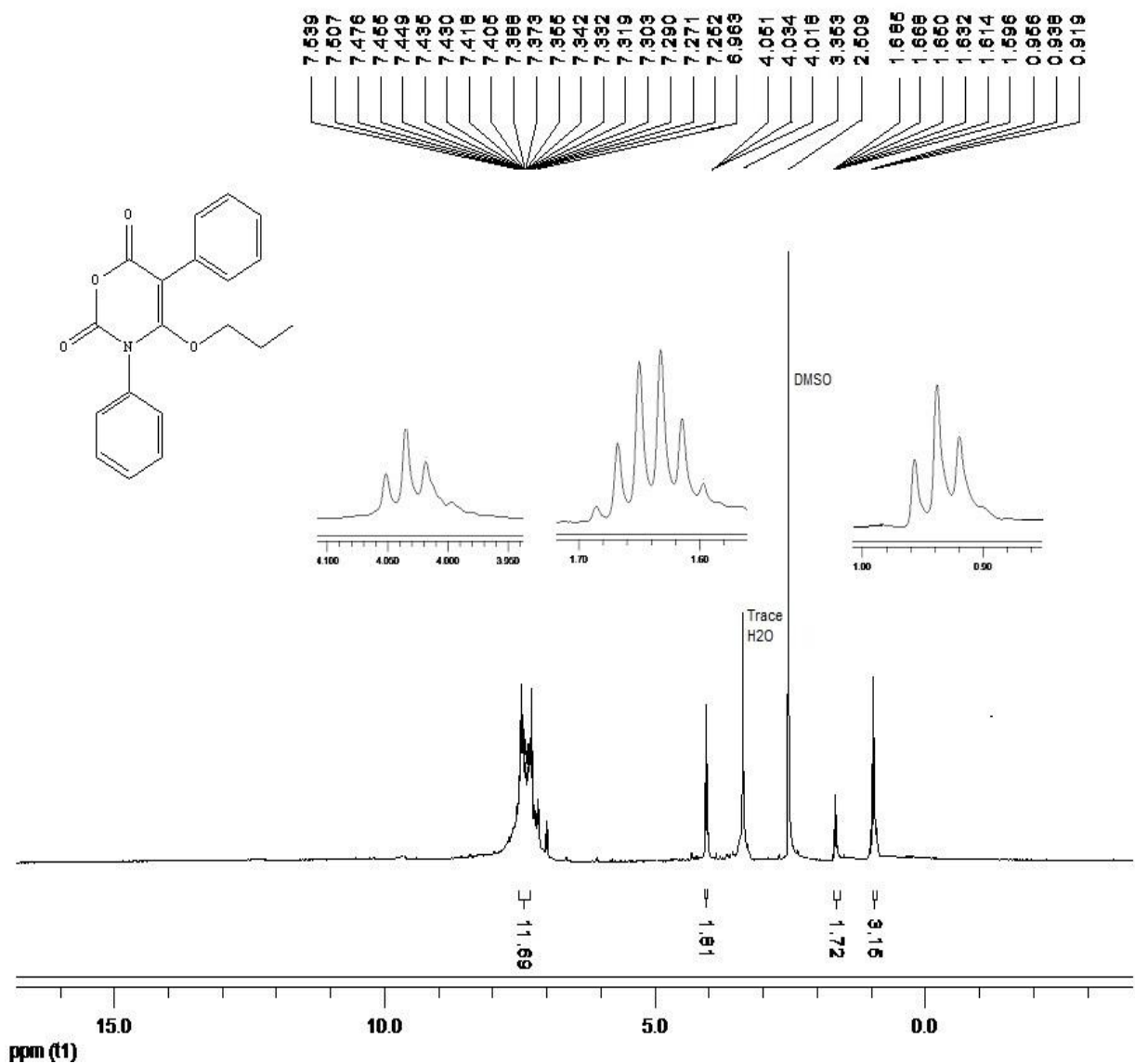


Figure S13. ¹H NMR spectrum 3,5-diphenyl-4-propoxy-2H-1,3-oxazine-2,6(3H)-dione **7b**

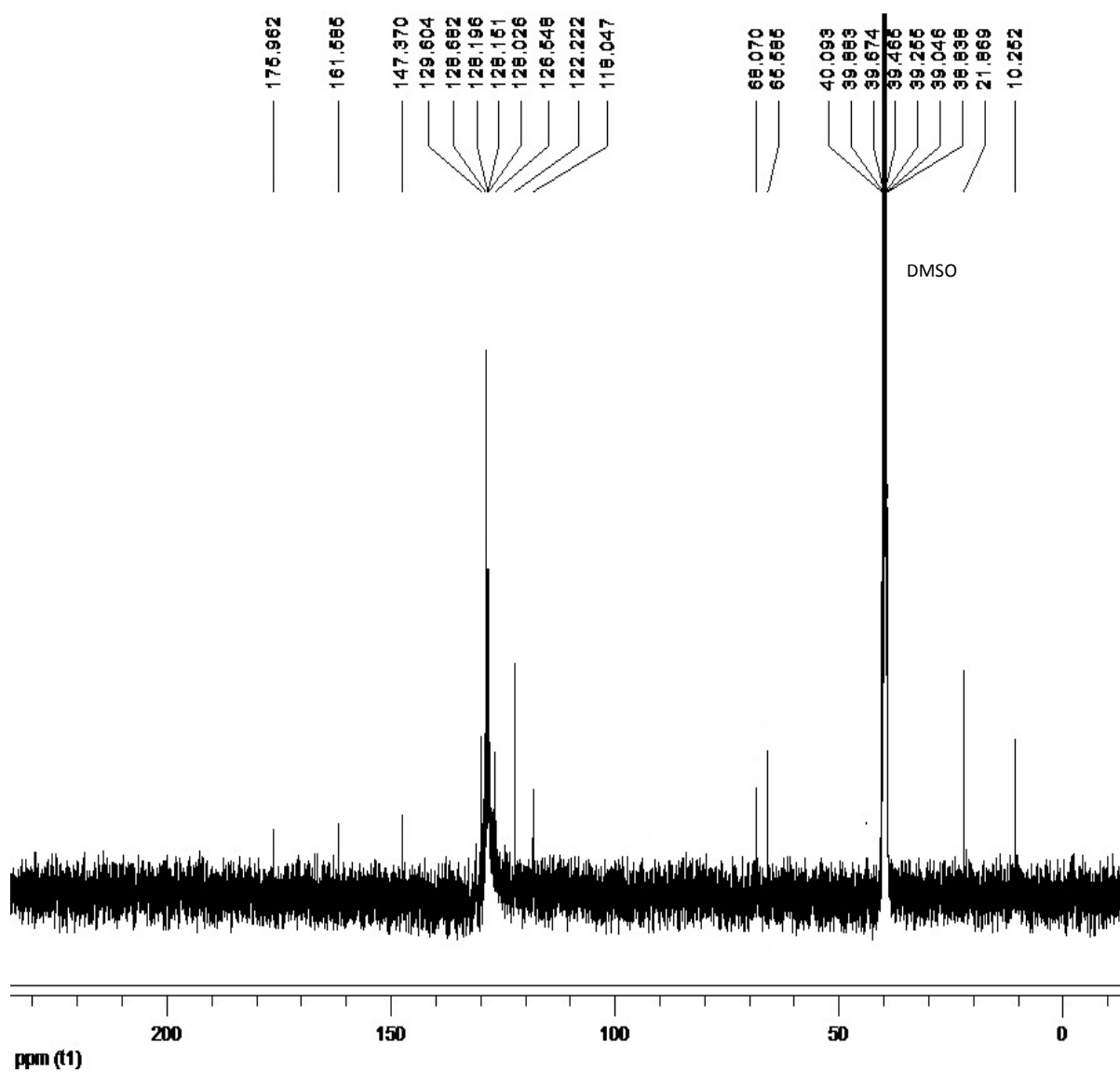


Figure S14. ^{13}C NMR spectrum of 3,5-diphenyl-4-propoxy-2H-1,3-oxazine-2,6(3H)-dione **7b**

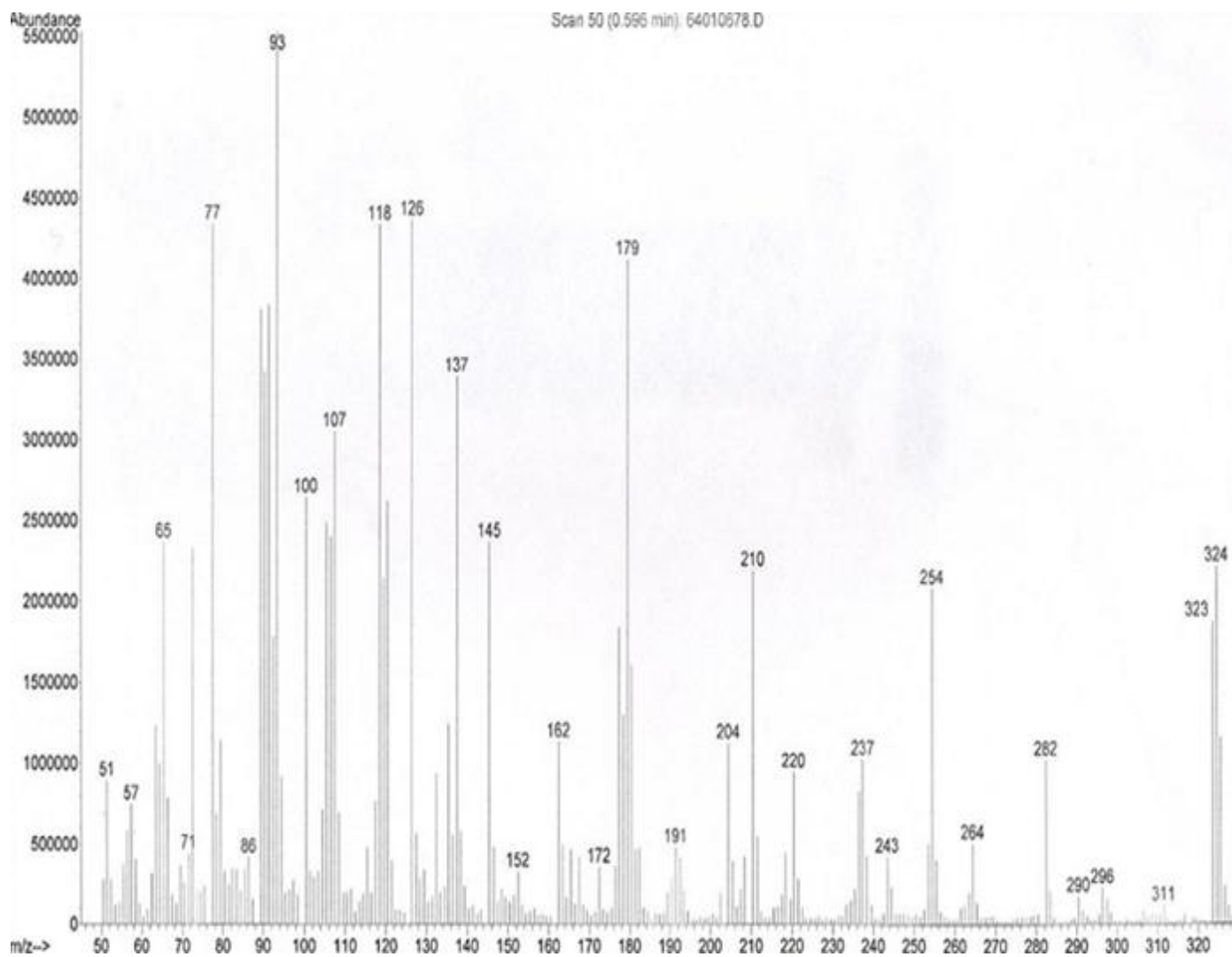


Figure S15. Mass spectrum of 3,5-diphenyl-4-propoxy-2H-1,3-oxazine-2,6(3H)-dione **7b**

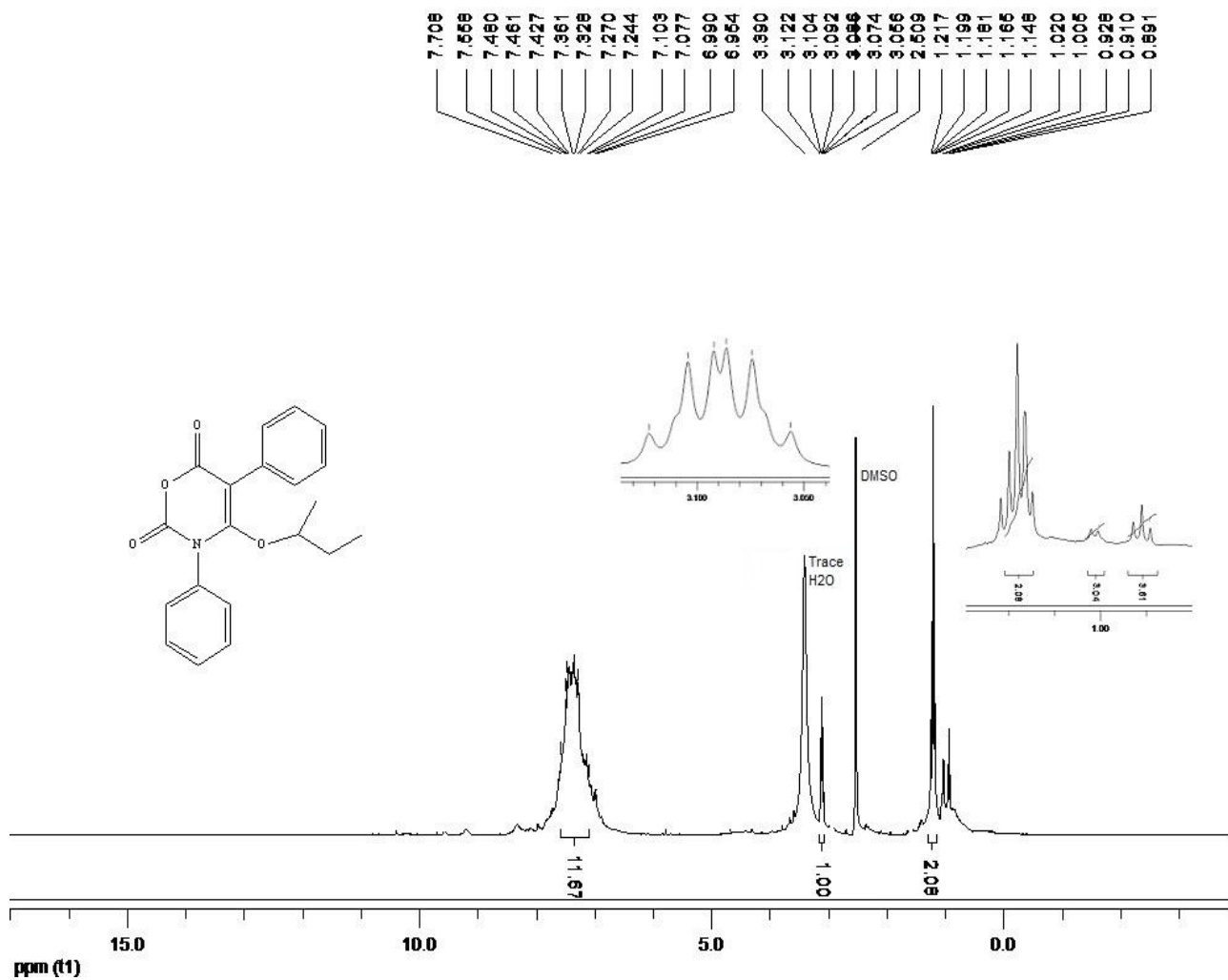


Figure S16. ¹H NMR spectrum 4-(sec-butoxy)-3,5-diphenyl-2H-1,3-oxazine-2,6(3H)-dione **7c**

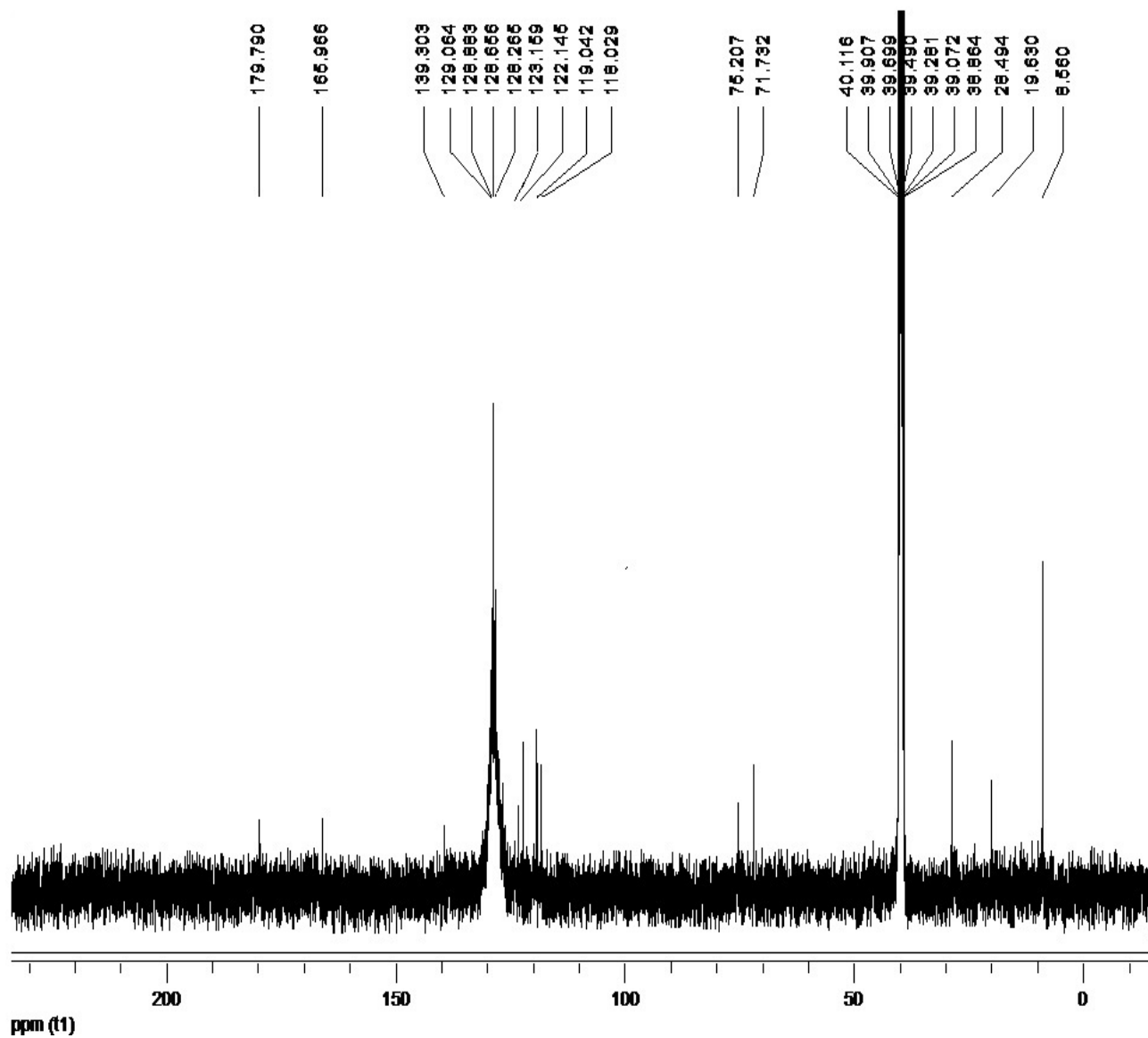


Figure S17. ^{13}C NMR spectrum of 4-(sec-butoxy)-3,5-diphenyl-2H-1,3-oxazine-2,6(3H)-dione **7c**

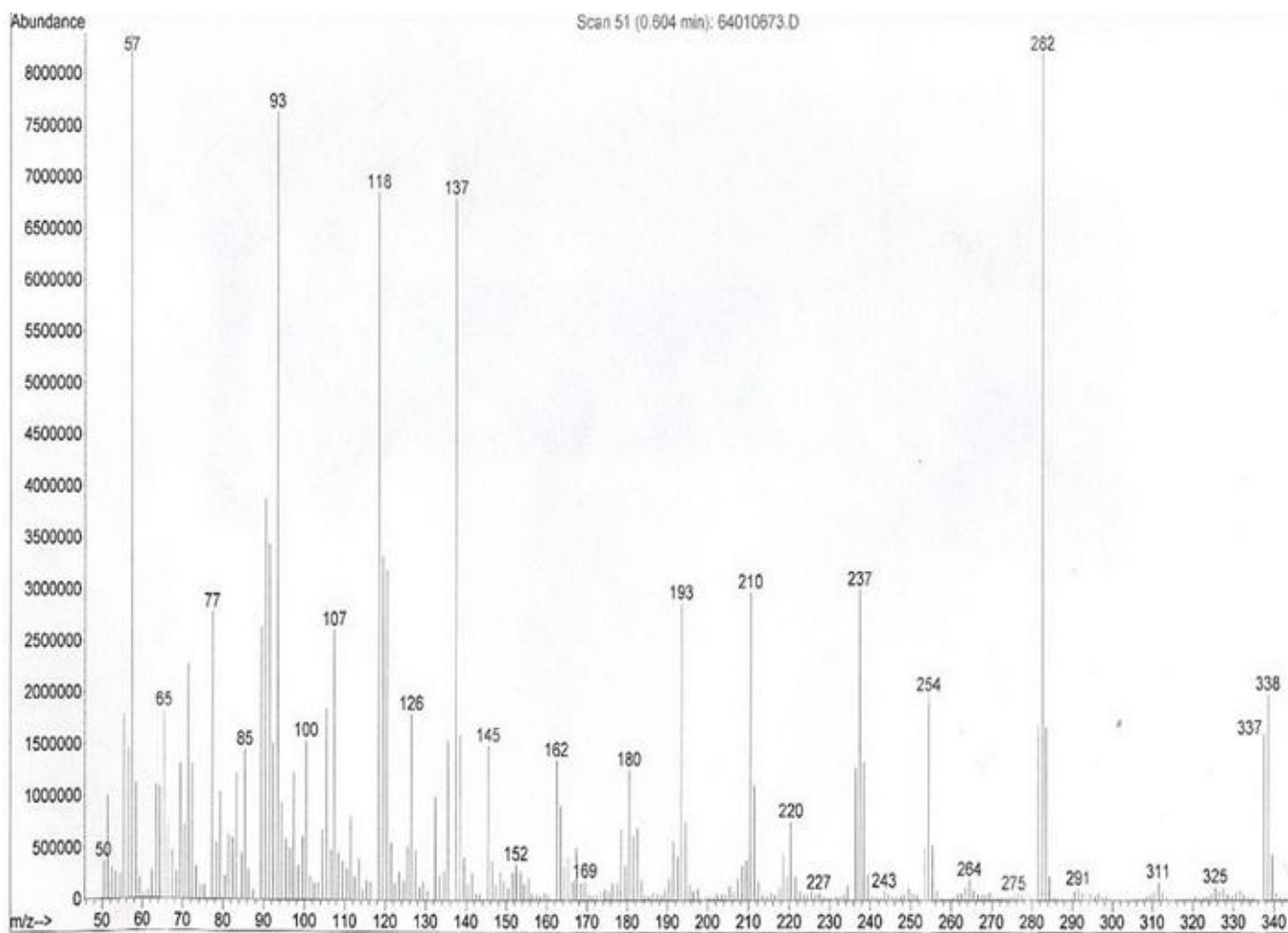


Figure S18. Mass spectrum of 4-(sec-butoxy)-3,5-diphenyl-2H-1,3-oxazine-2,6(3H)-dione **7c**