

# **Thiazole-Chalcone Hybrids as prospective antitubercular and antiproliferative agents: Design, synthesis, biological, molecular docking studies and in-silico ADME evaluation**

Ashok Babu Kasetti, Indrajeet Singhvi, Ravindra Nagasuri, Richie R. Bhandare and Afzal B. Shaik

## **FT-IR, $^1\text{H}$ NMR, $^{13}\text{C}$ NMR & Mass Spectra**

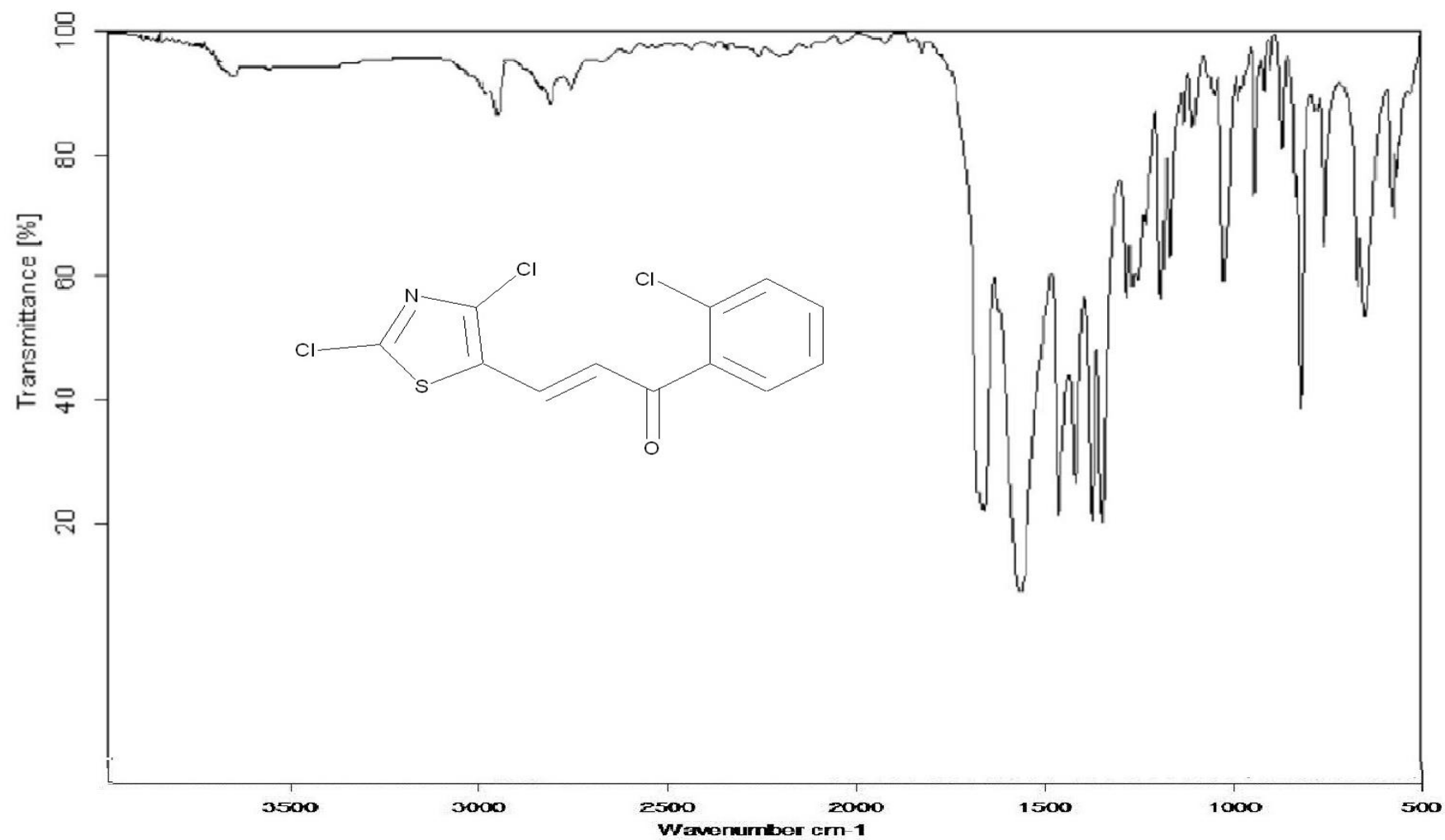


Figure S1. FT-IR Spectrum of compound 1

1 <sup>1</sup>H CDCl<sub>3</sub>

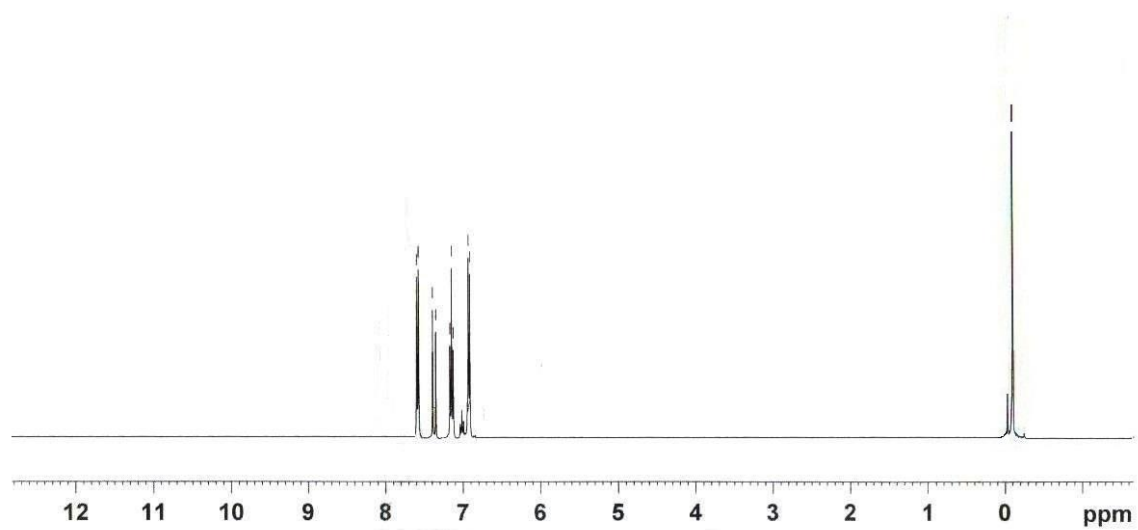
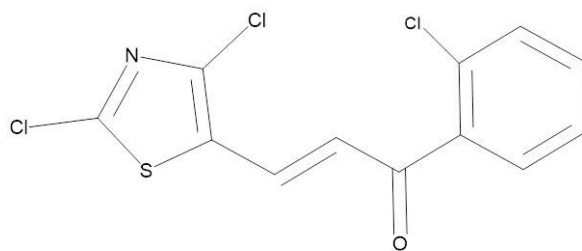


Figure S2. <sup>1</sup>H NMR Spectrum of compound 1

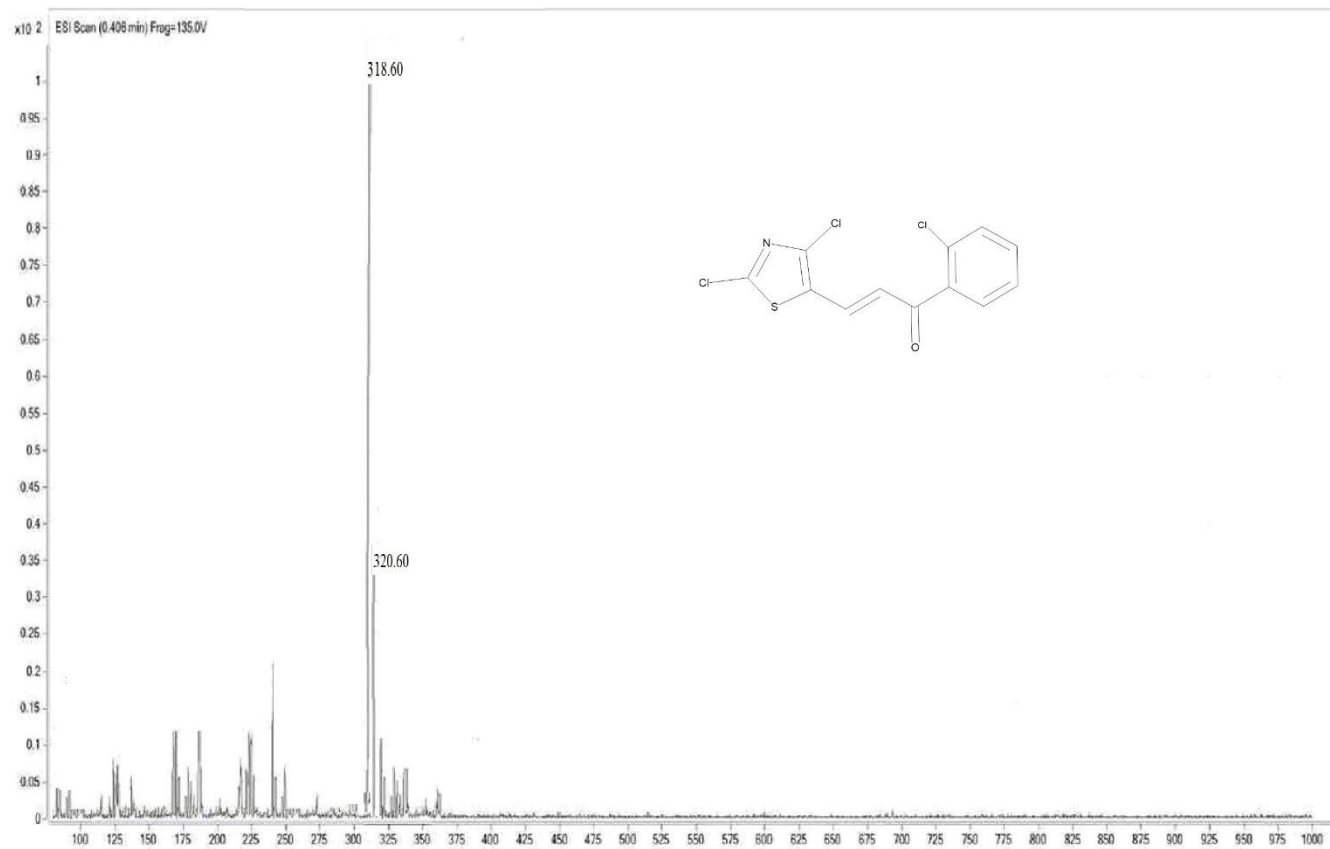


Figure S3. Mass Spectrum of compound 1

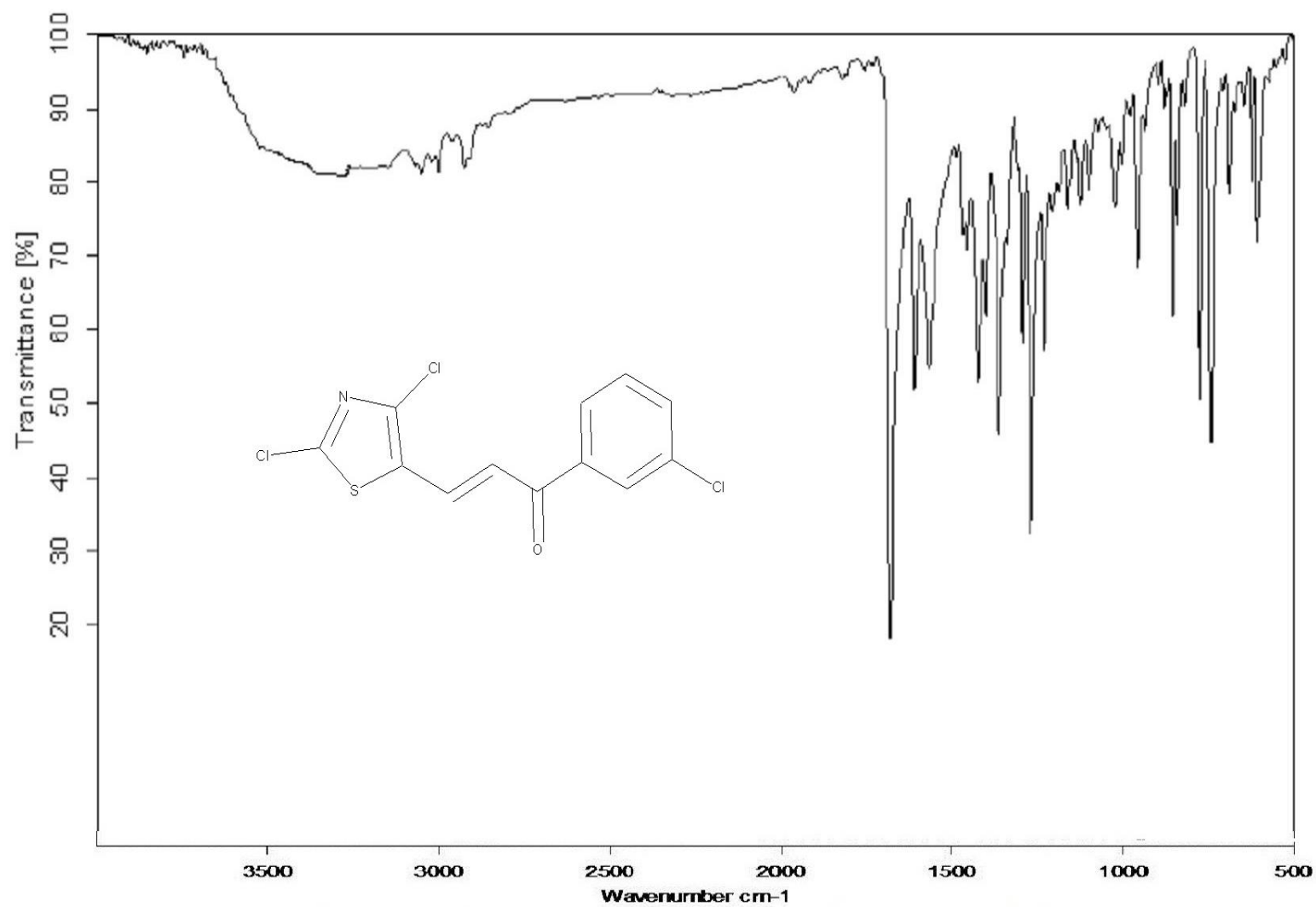


Figure S4. FT-IR Spectrum of compound 2

2 1H CDCl3

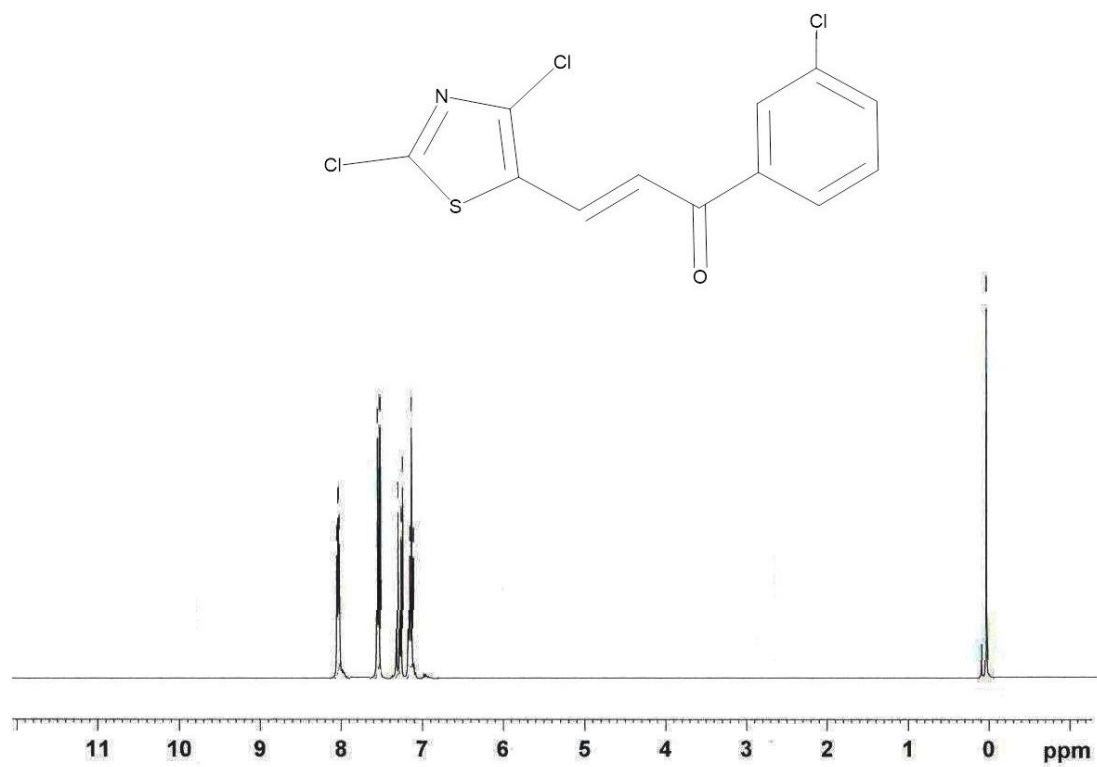


Figure S5. <sup>1</sup>H NMR Spectrum of compound 2

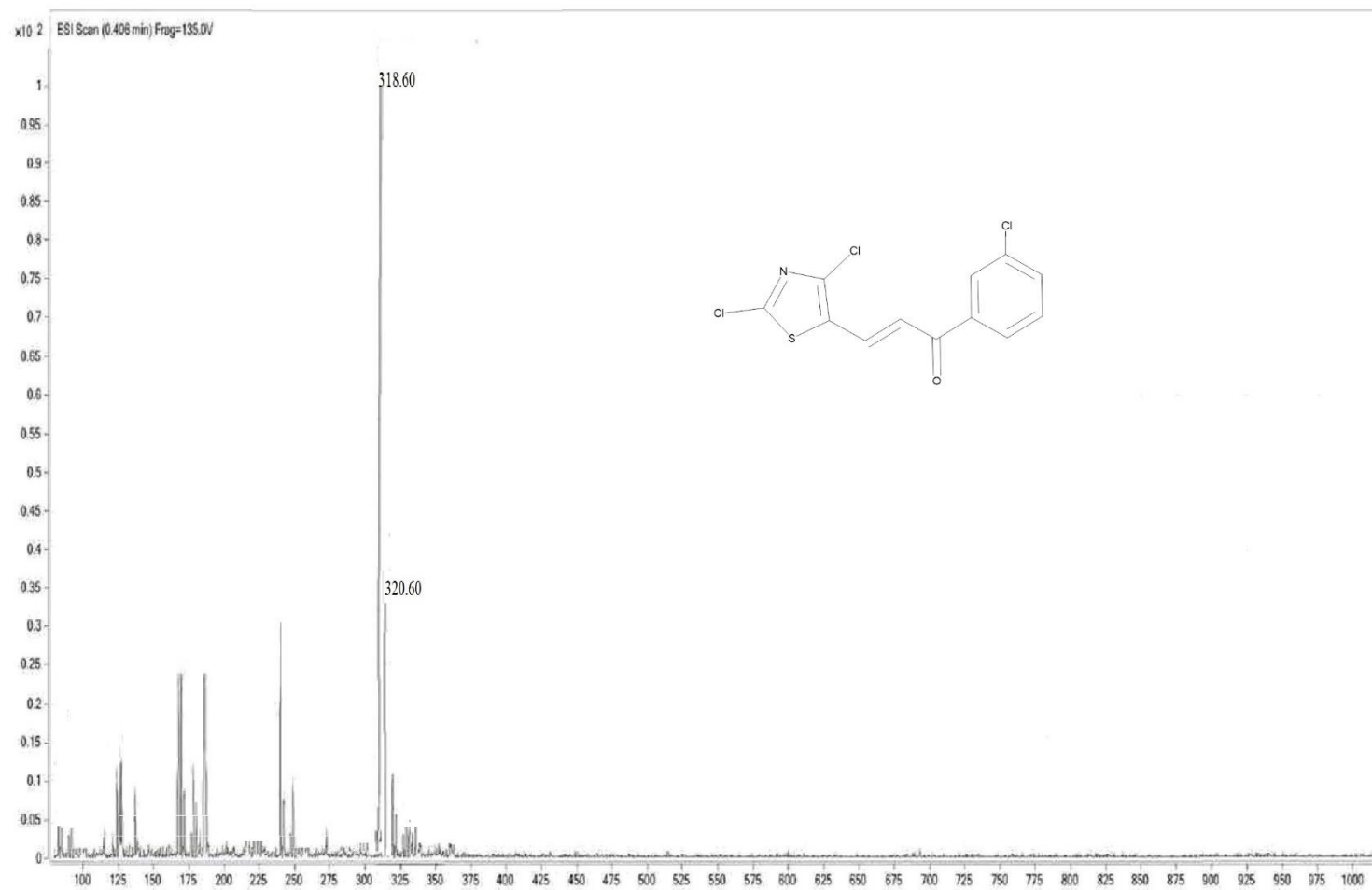


Figure S6. Mass Spectrum of compound 2

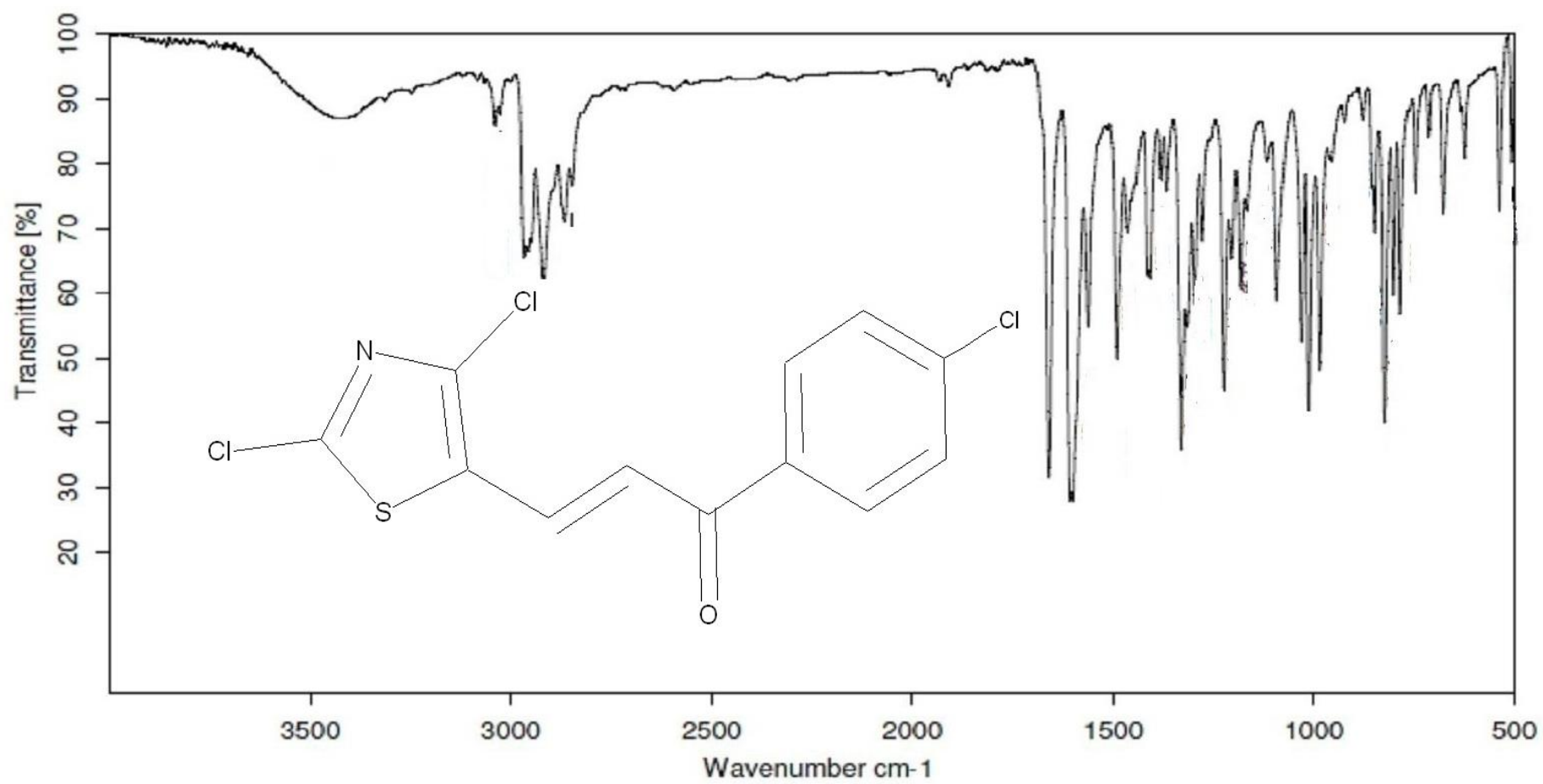


Figure S7. FT-IR Spectrum of compound 3



3  $^1\text{H}$   $\text{CDCl}_3$

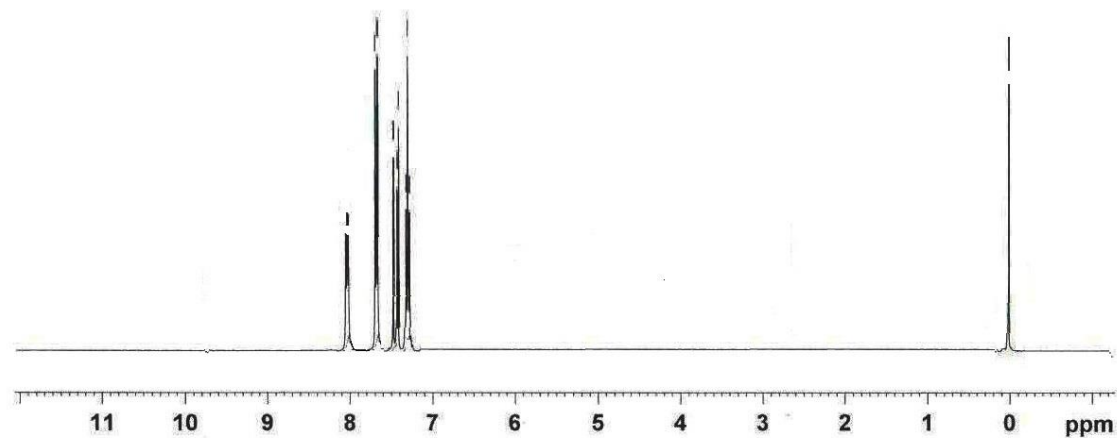
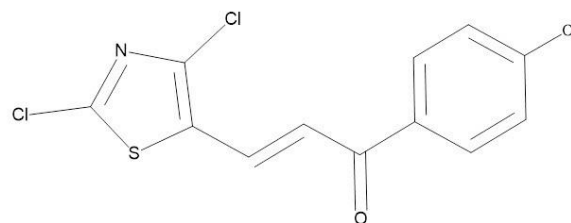


Figure S8.  $^1\text{H}$  NMR Spectrum of compound 3

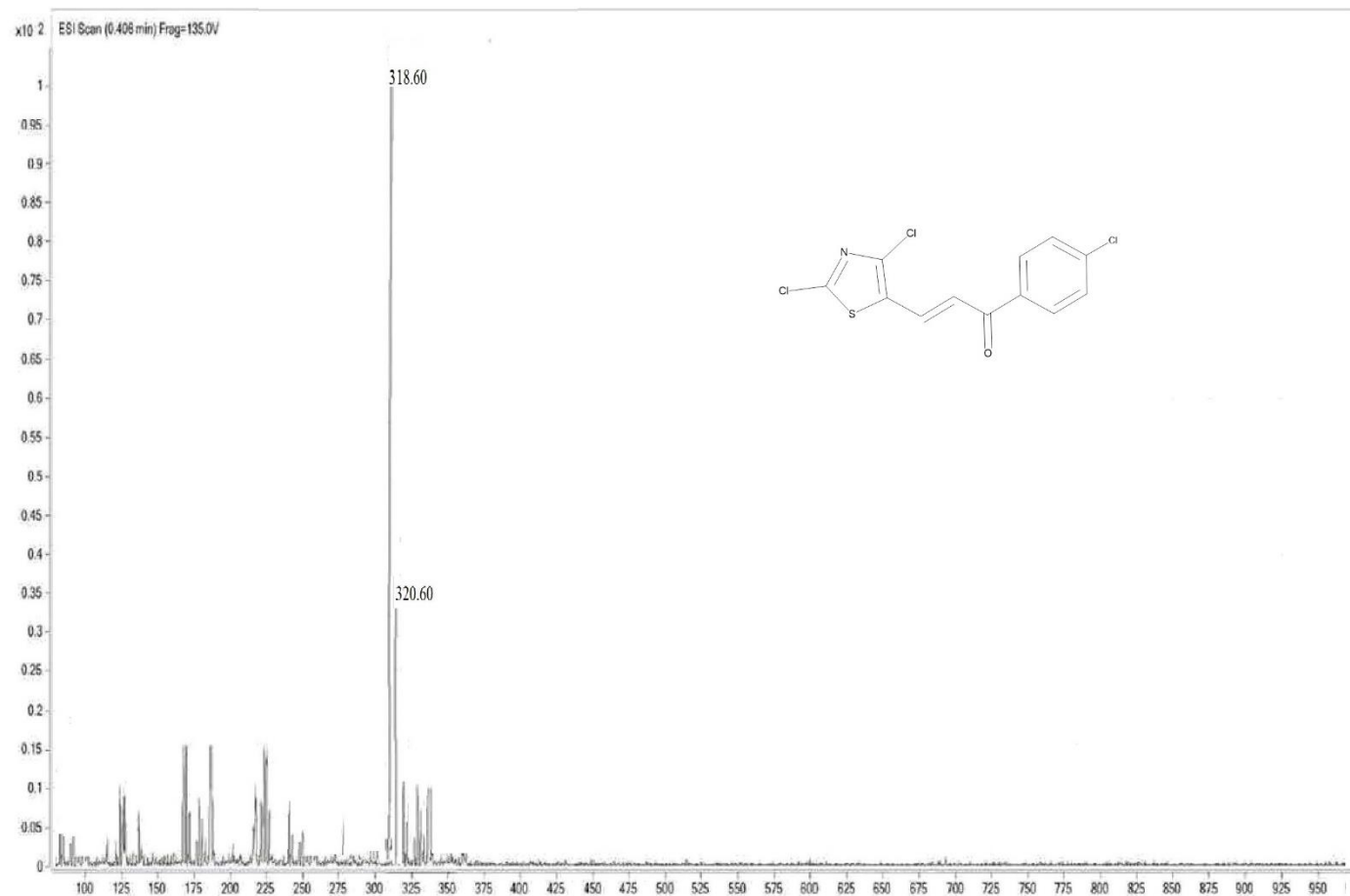


Figure S9. Mass Spectrum of compound 3

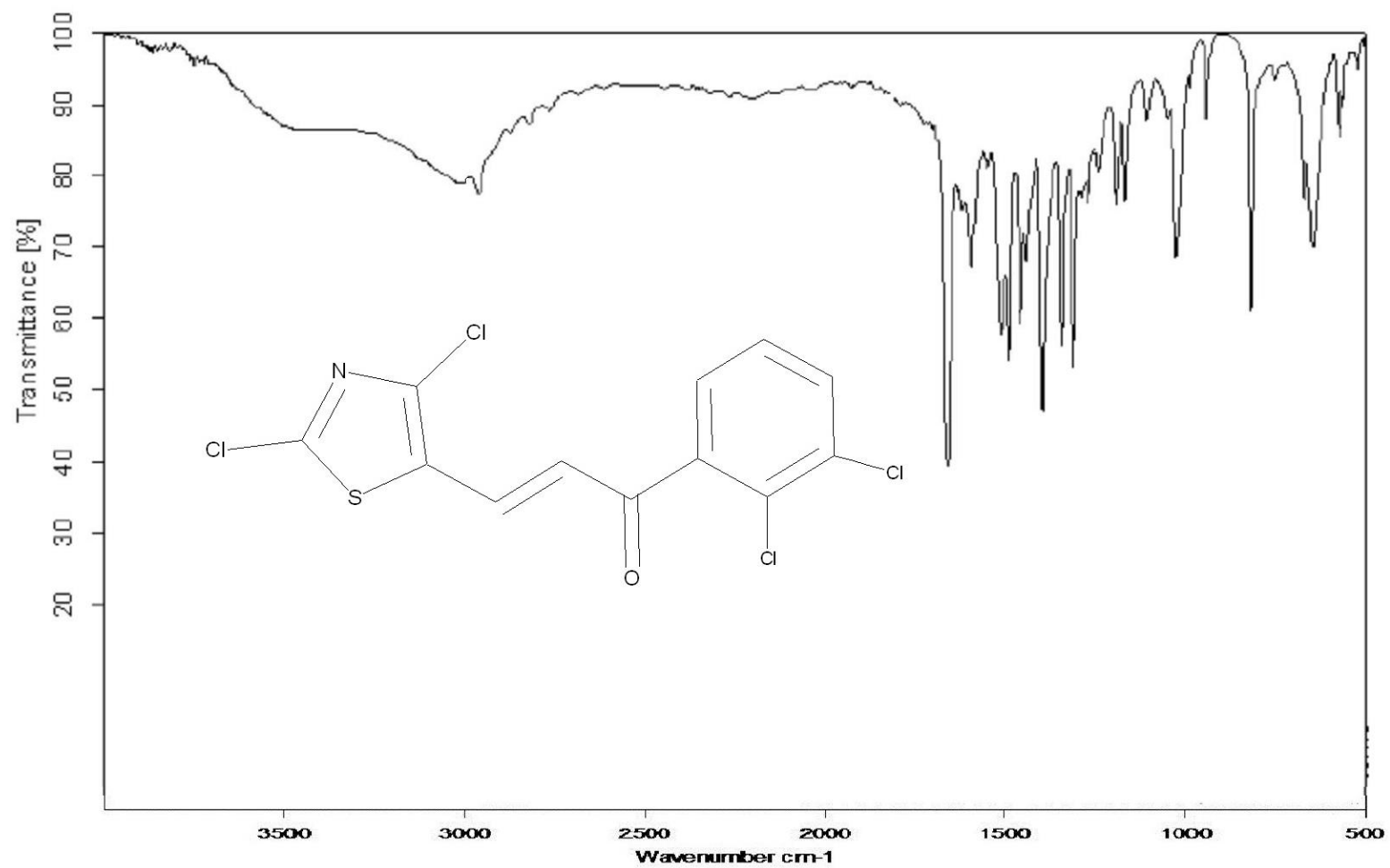


Figure S10. FT-IR Spectrum of compound 4

4 1H CDC13

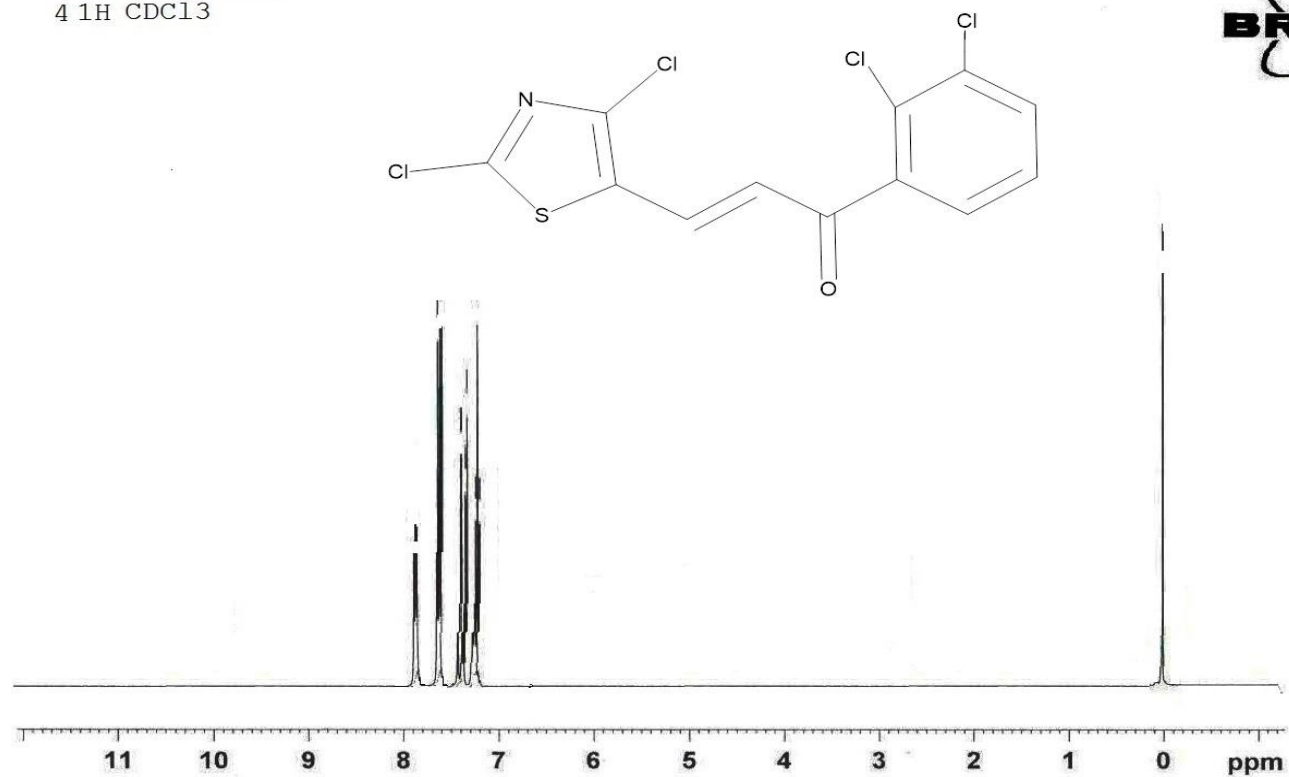


Figure S11. <sup>1</sup>H NMR Spectrum of compound 4

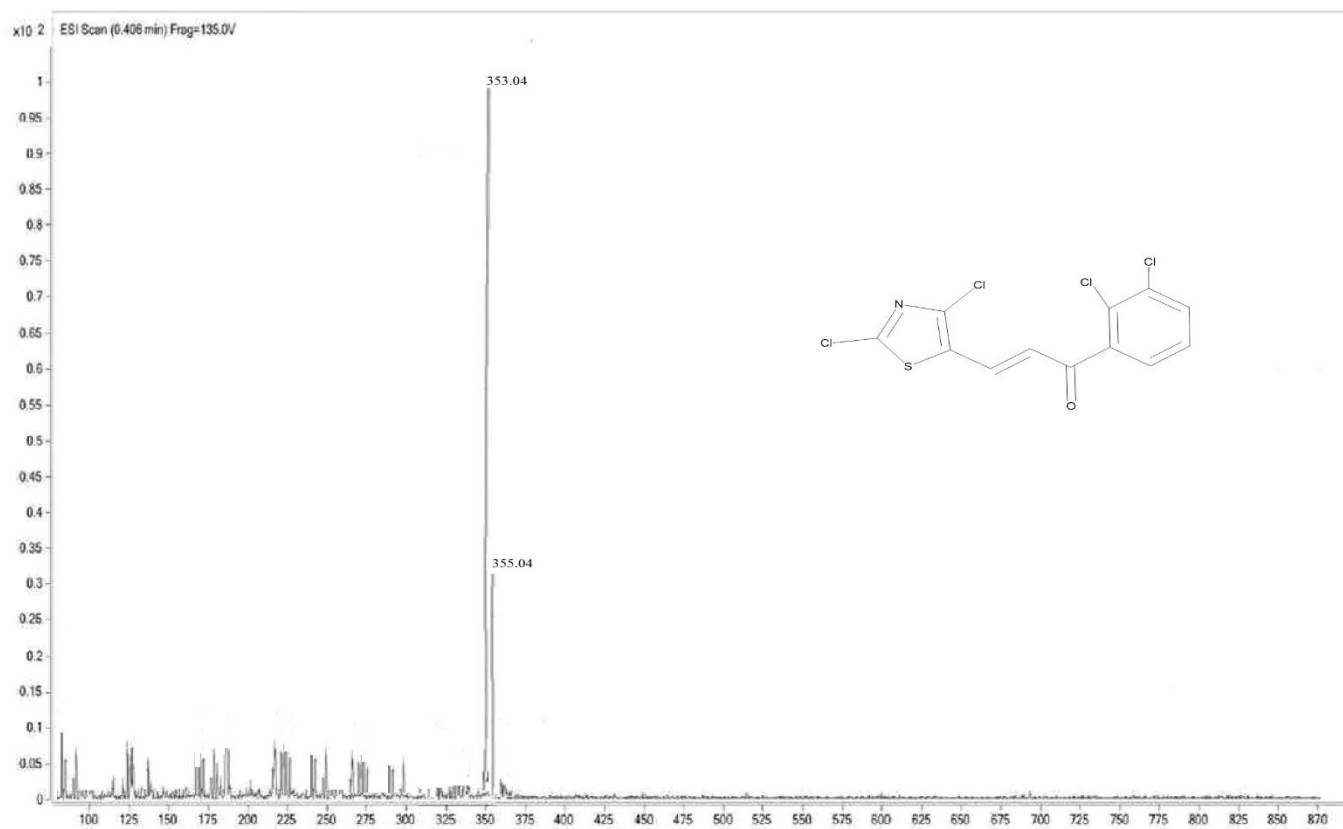


Figure S12. Mass Spectrum of compound 4

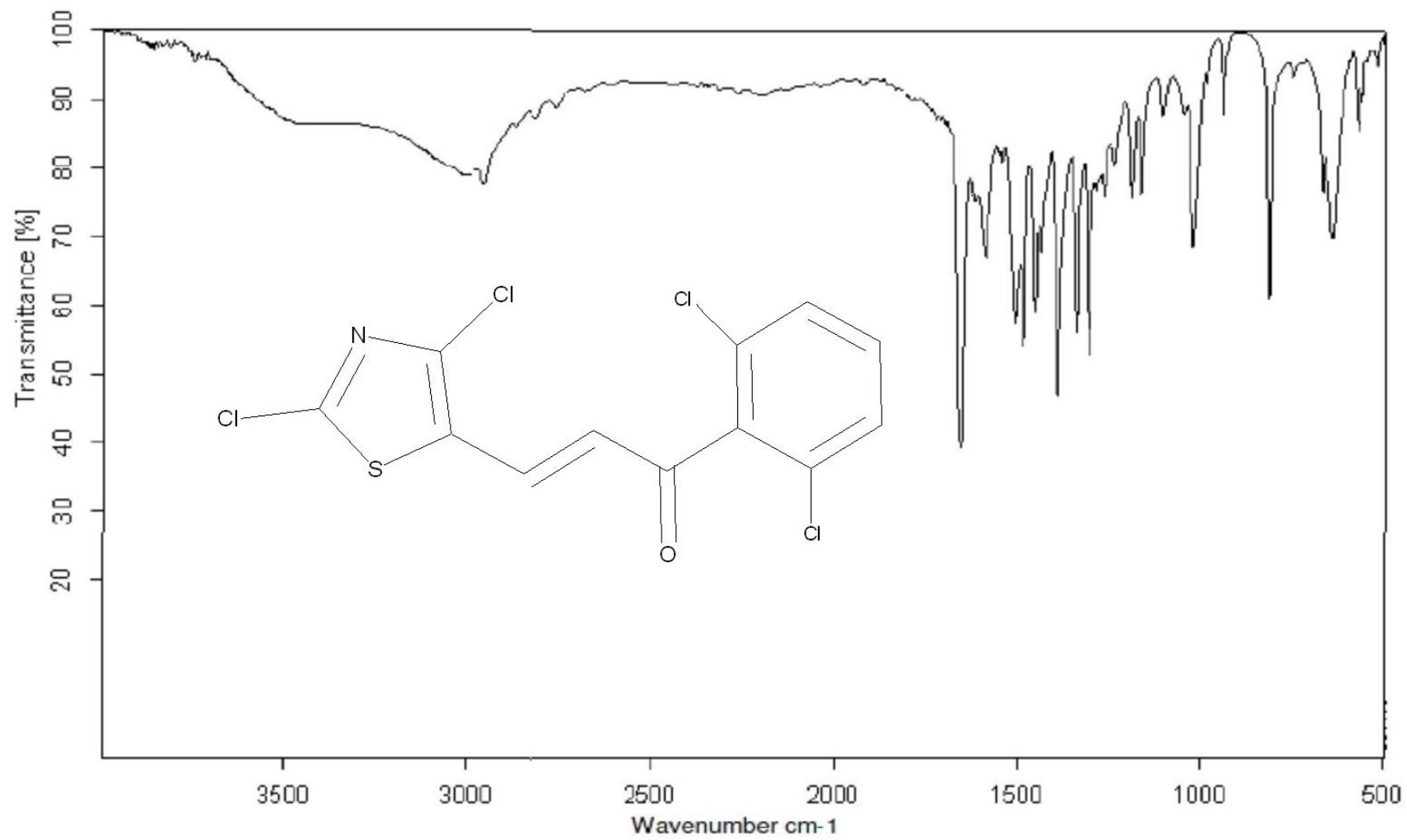


Figure S13. FT-IR Spectrum of compound 5

5 <sup>1</sup>H CDCl<sub>3</sub>

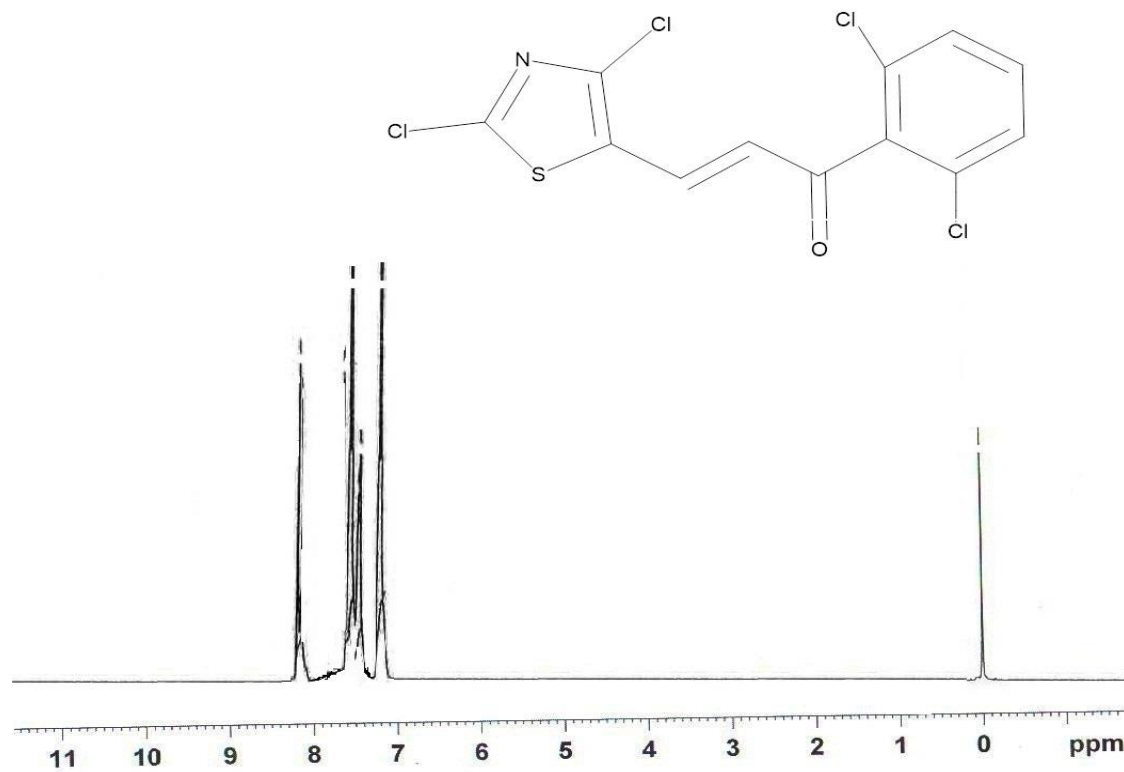


Figure S14. <sup>1</sup>H NMR Spectrum of compound 5

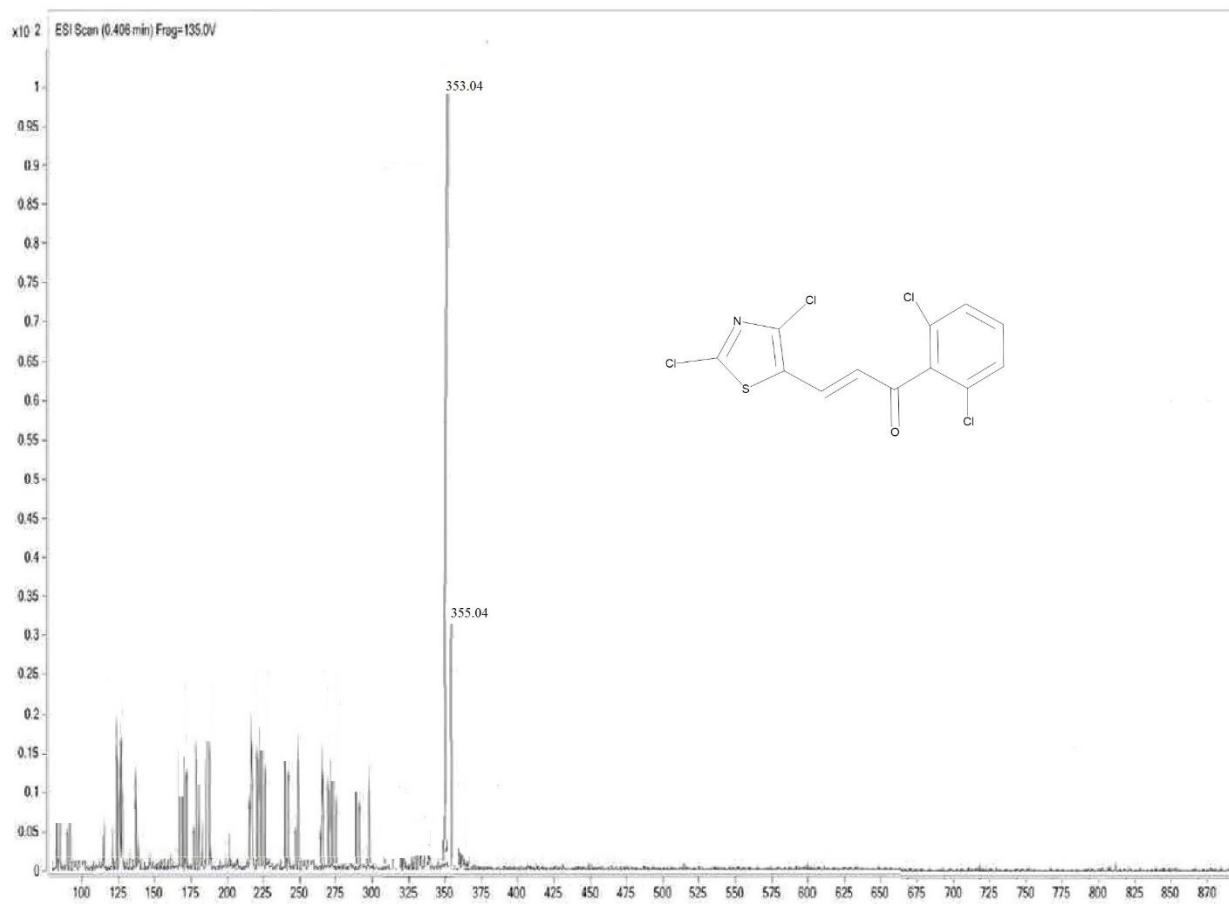


Figure S15. Mass Spectrum of compound 5



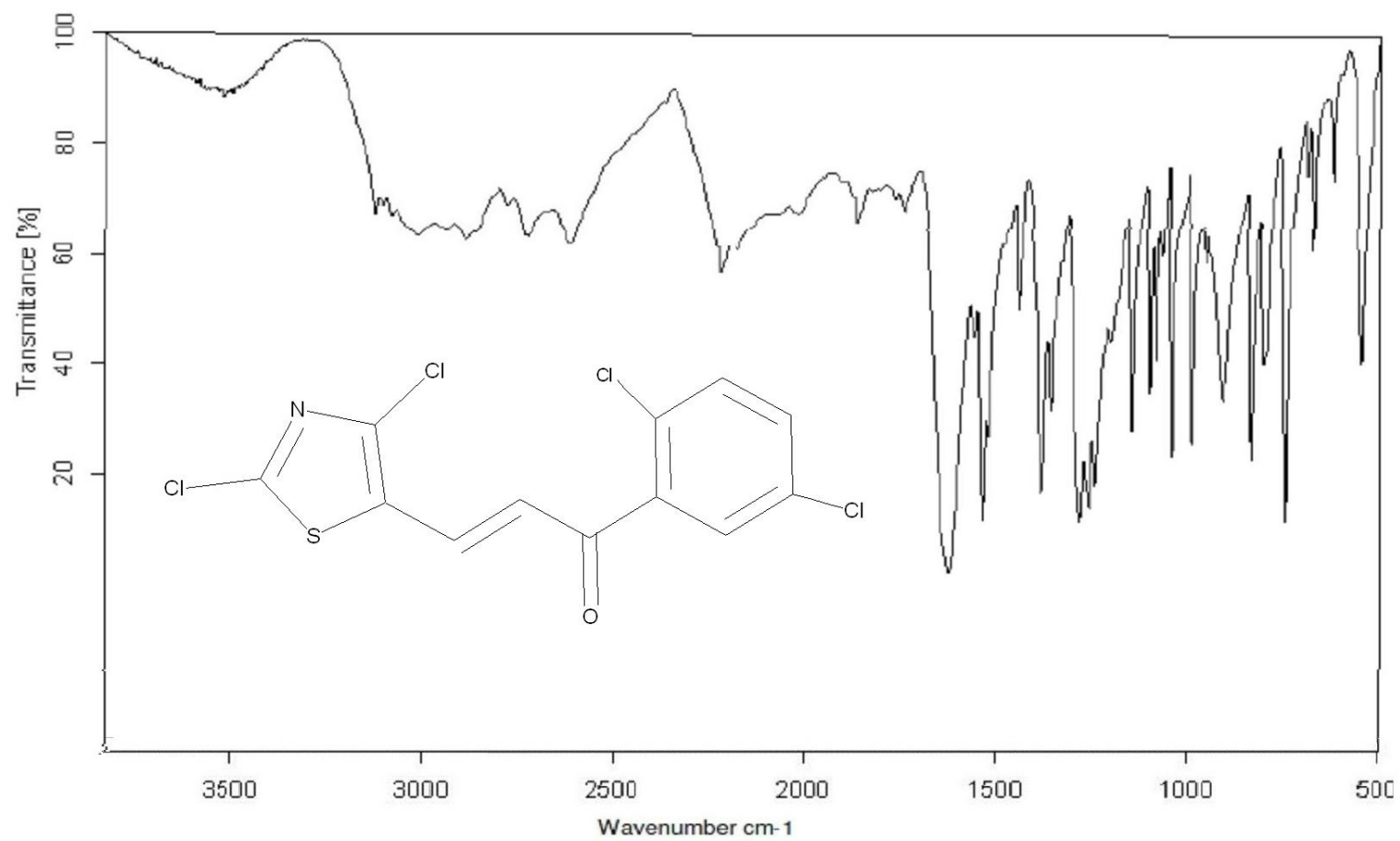


Figure S16. FT-IR Spectrum of compound 6

6 <sup>1</sup>H CDCl<sub>3</sub>

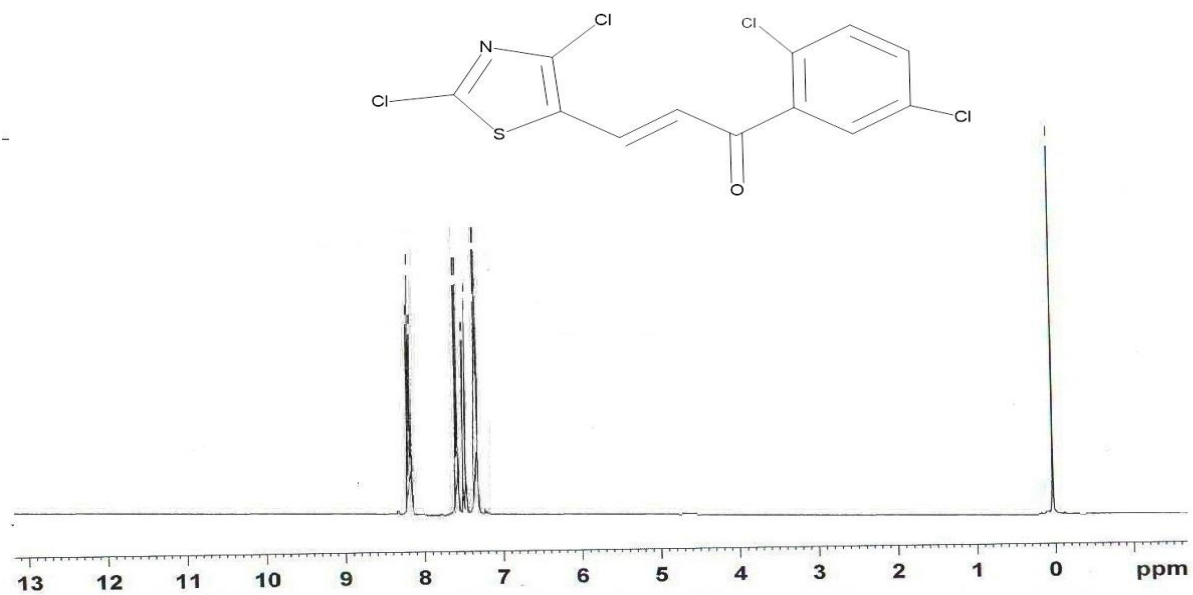


Figure S17. <sup>1</sup>H NMR Spectrum of compound 6

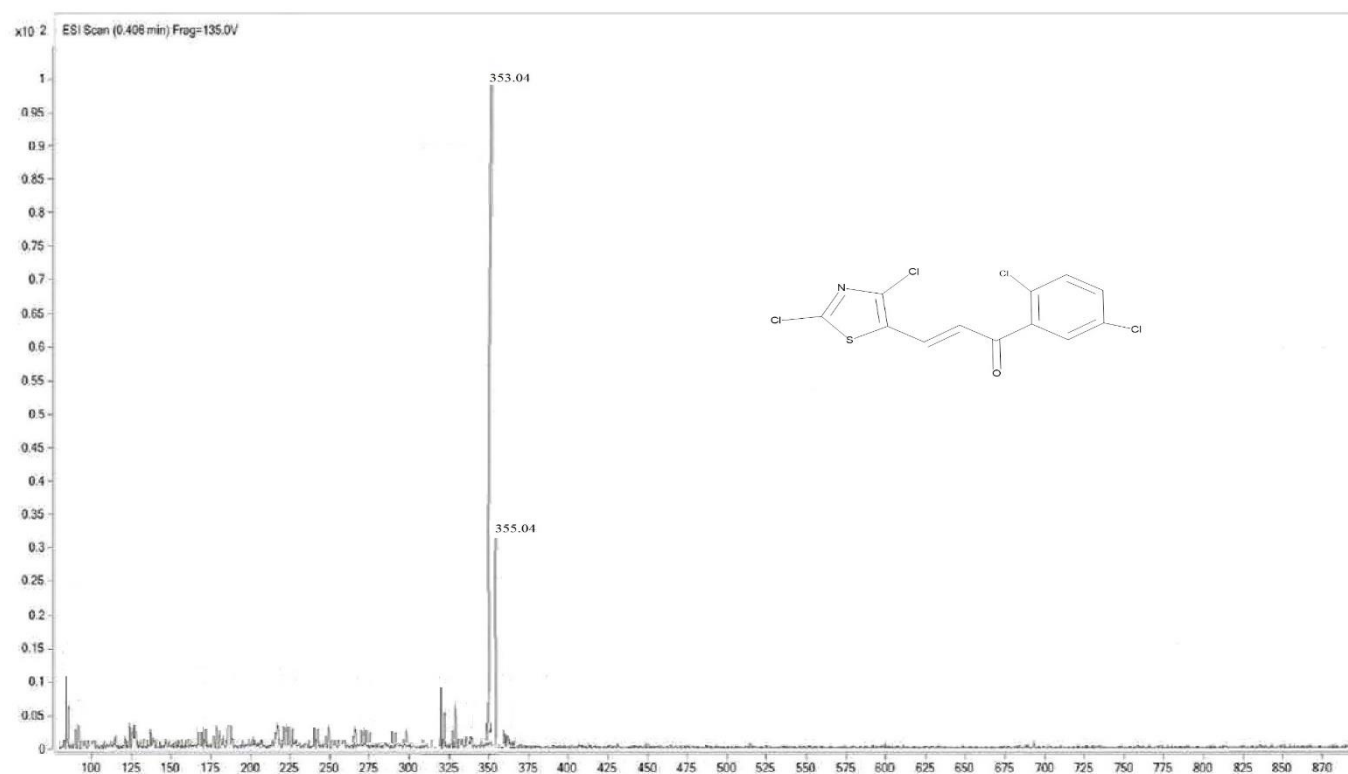


Figure S18. Mass Spectrum of compound 6

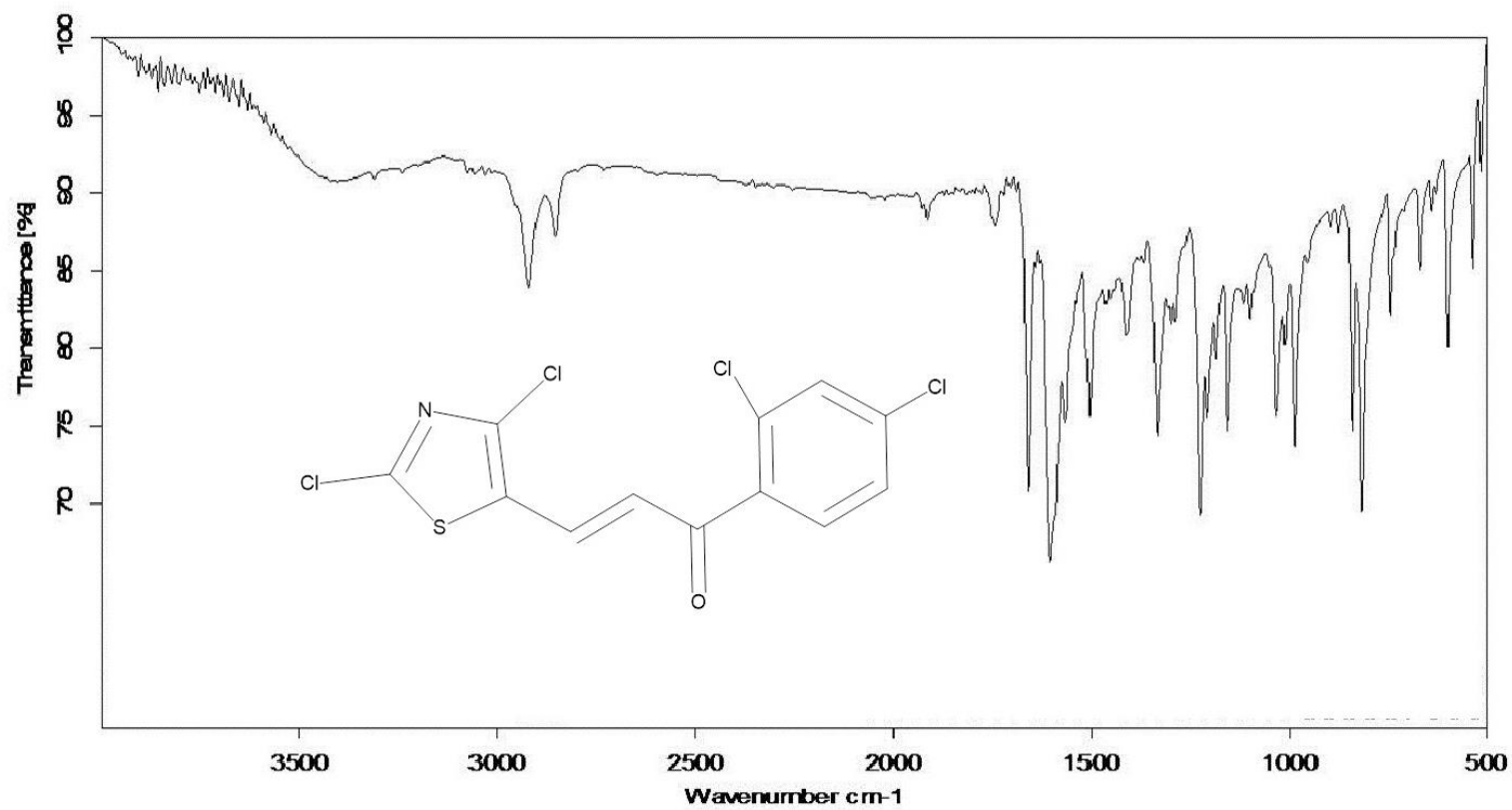


Figure S19. FT-IR Spectrum of compound 7

7 <sup>1</sup>H CDCl<sub>3</sub>

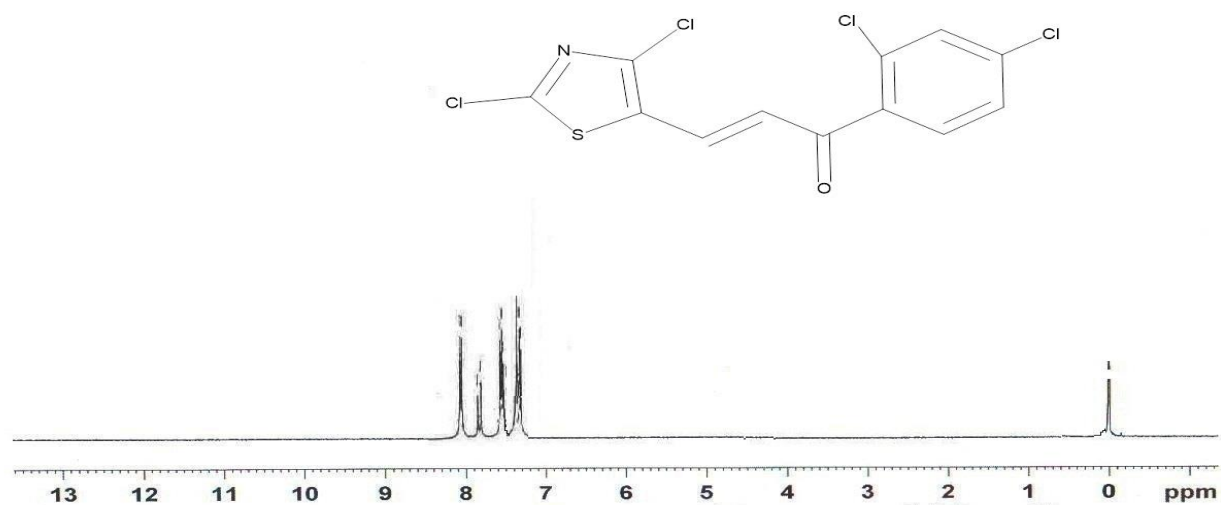


Figure S20. <sup>1</sup>H NMR Spectrum of compound 7

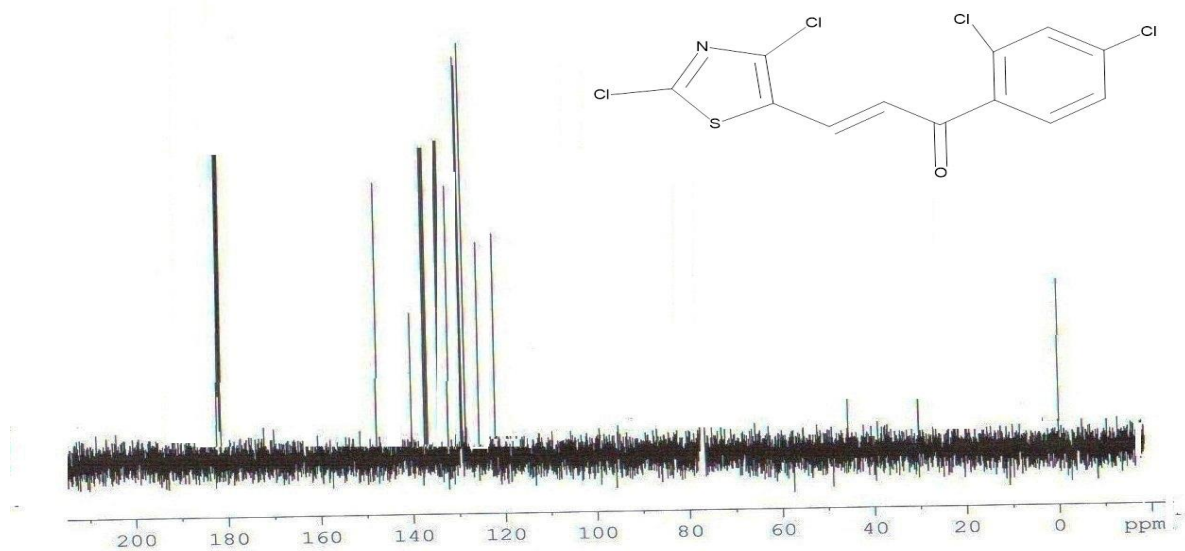


Figure S21.  $^{13}\text{C}$  NMR Spectrum of compound 7

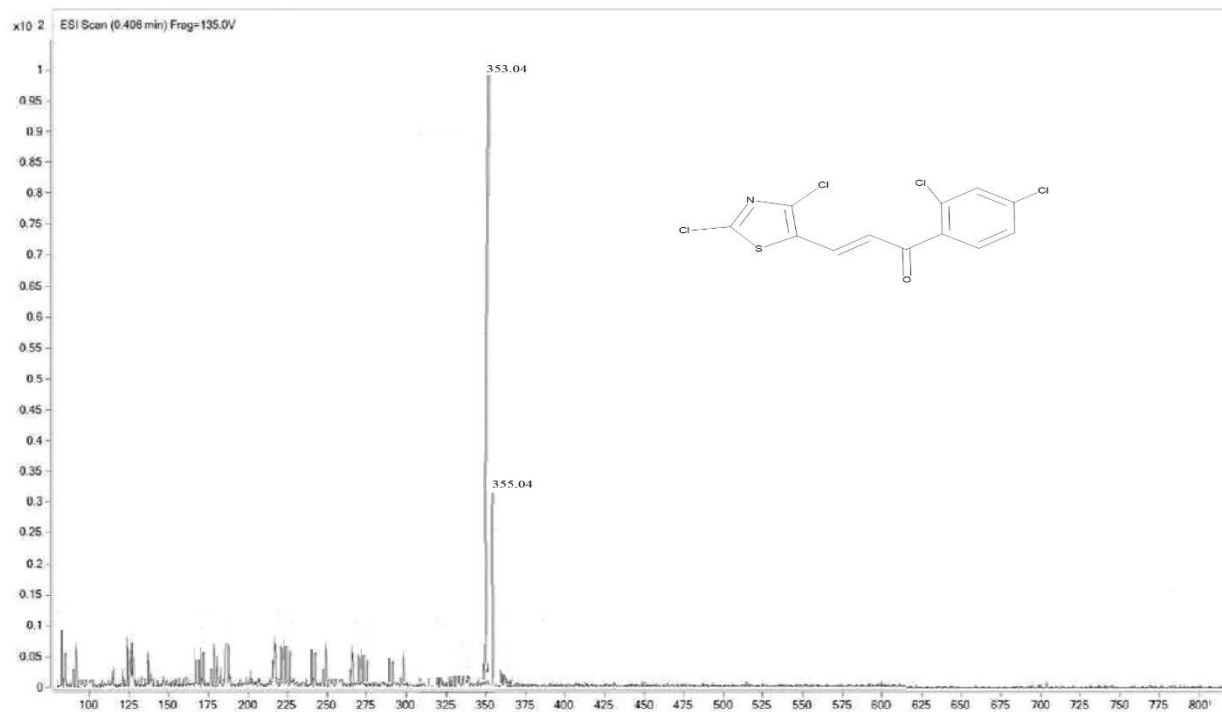


Figure S22. Mass Spectrum of compound 7

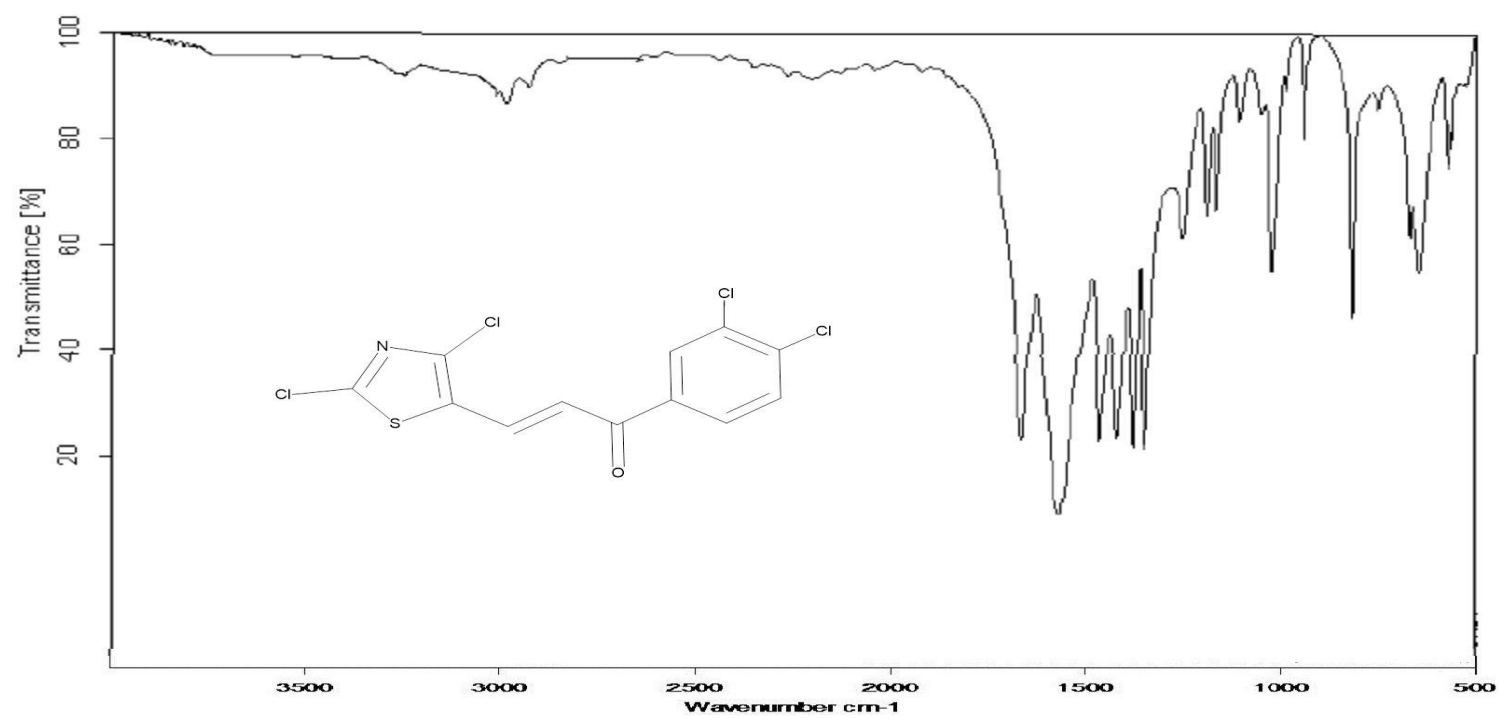


Figure 23. FT-IR Spectrum of compound 8



81H CDC13

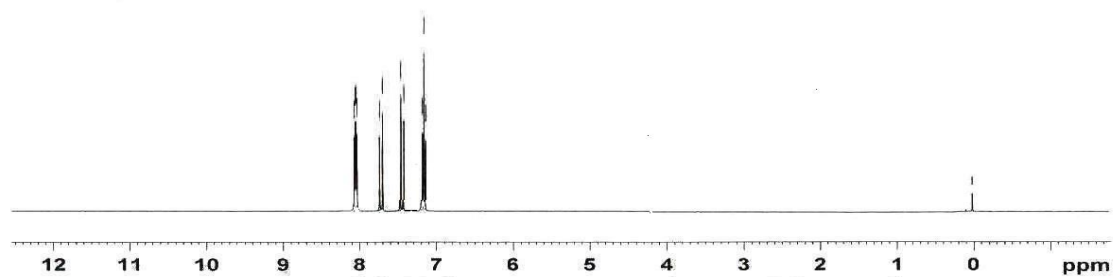
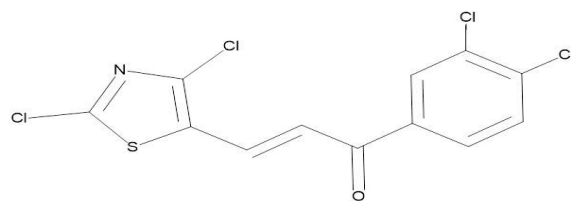


Figure S24. <sup>1</sup>H NMR Spectrum of compound 8

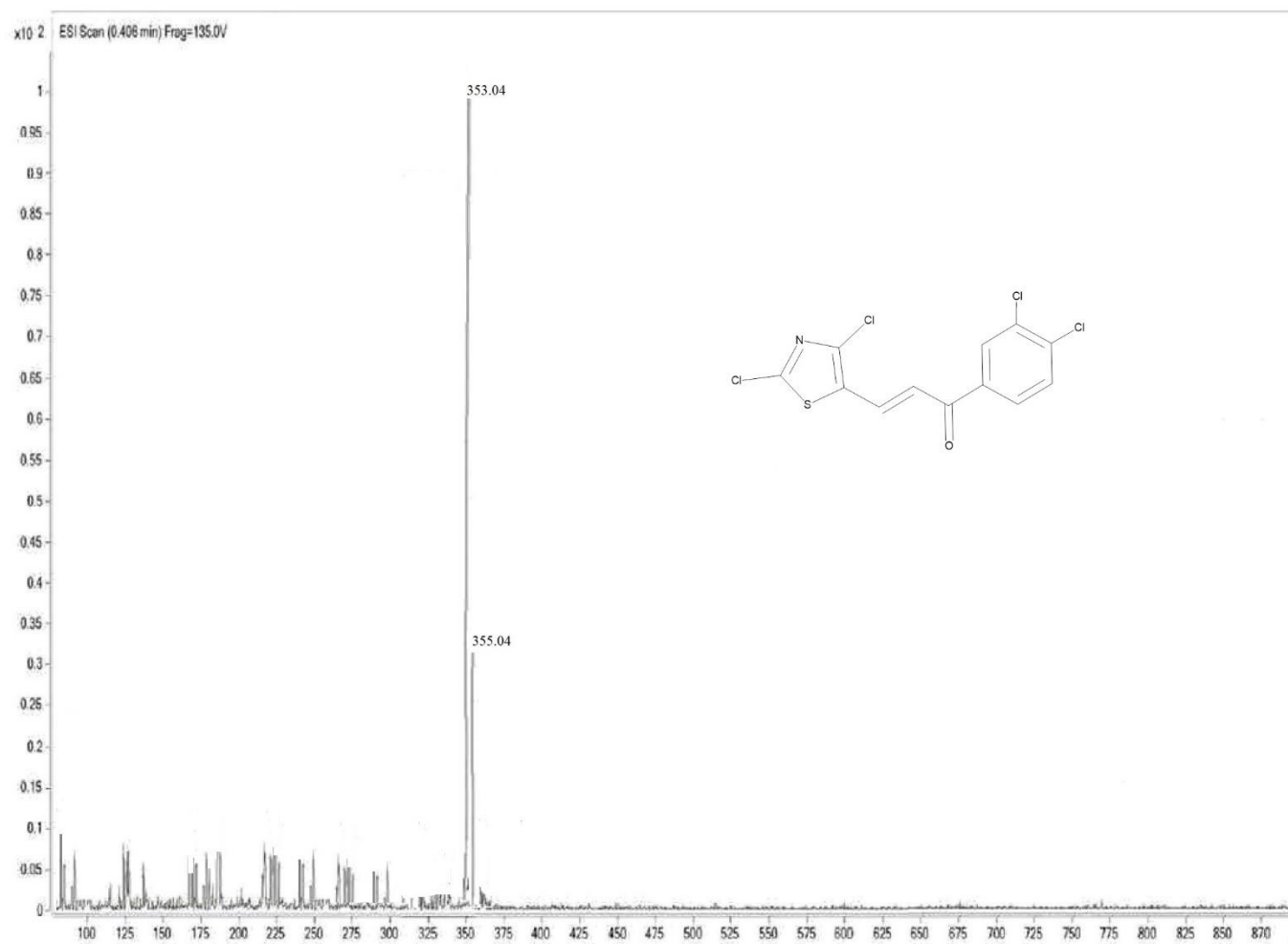


Figure S25. Mass Spectrum of compound 8

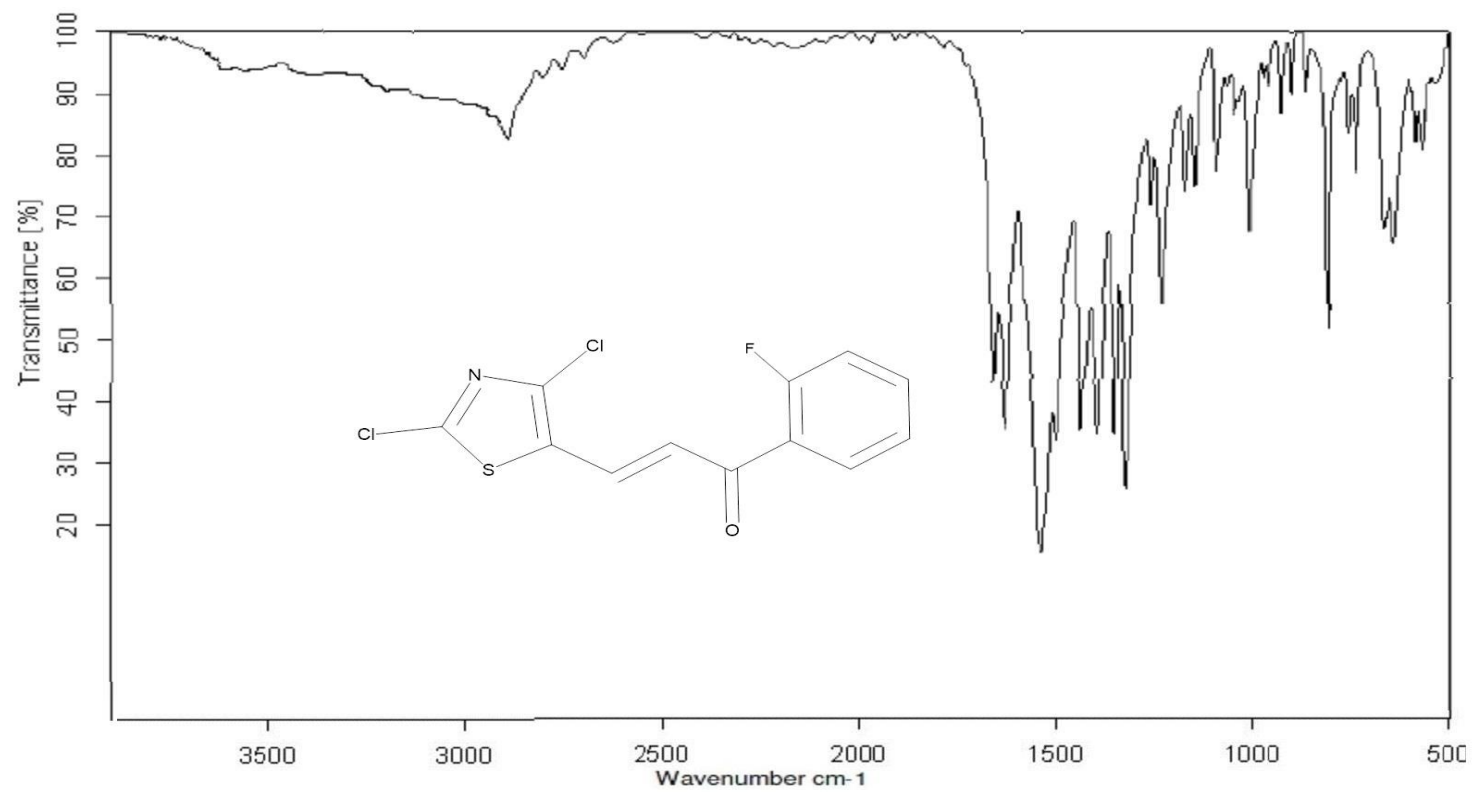


Figure S26. FT-IR Spectrum of compound 9

9 1H CDCl3

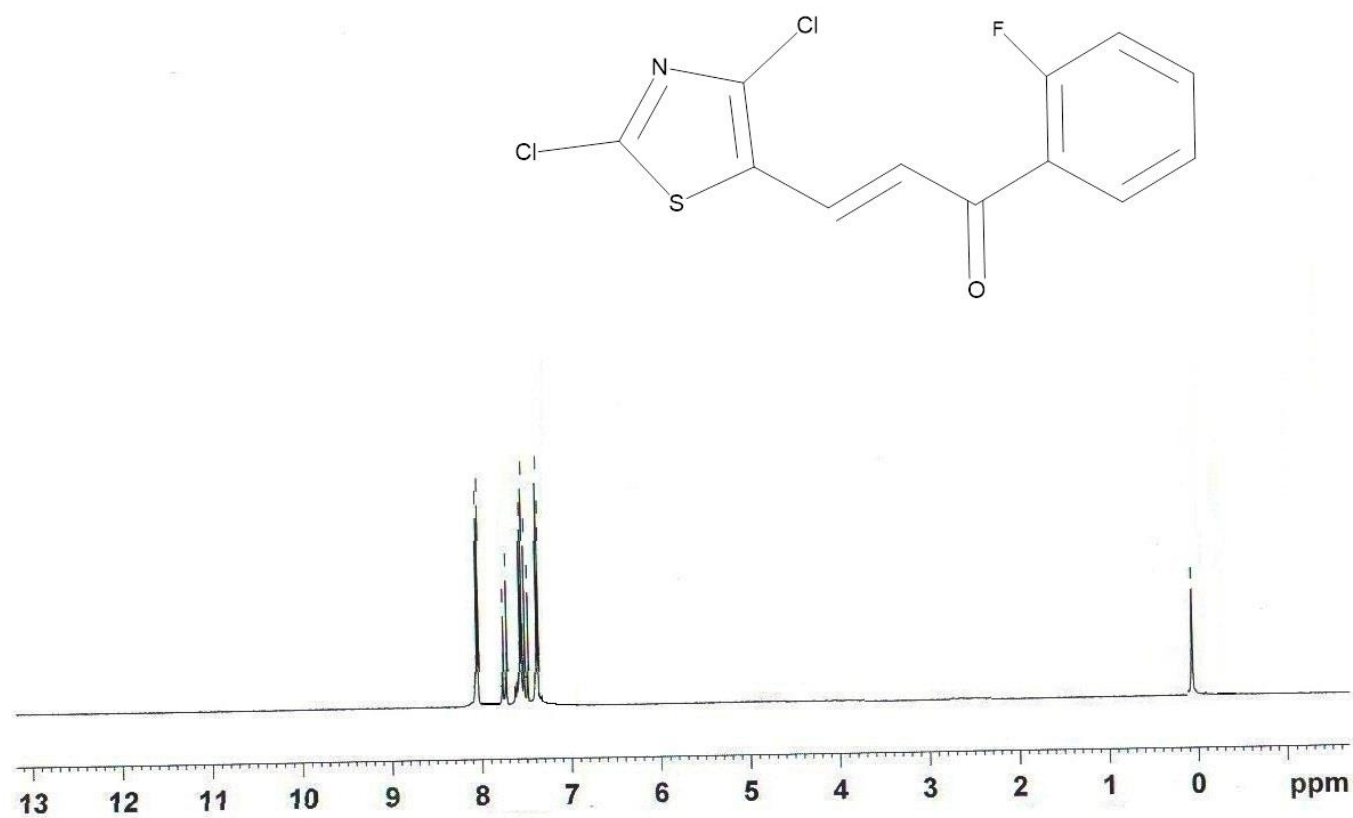


Figure S27. <sup>1</sup>H NMR Spectrum of compound 9

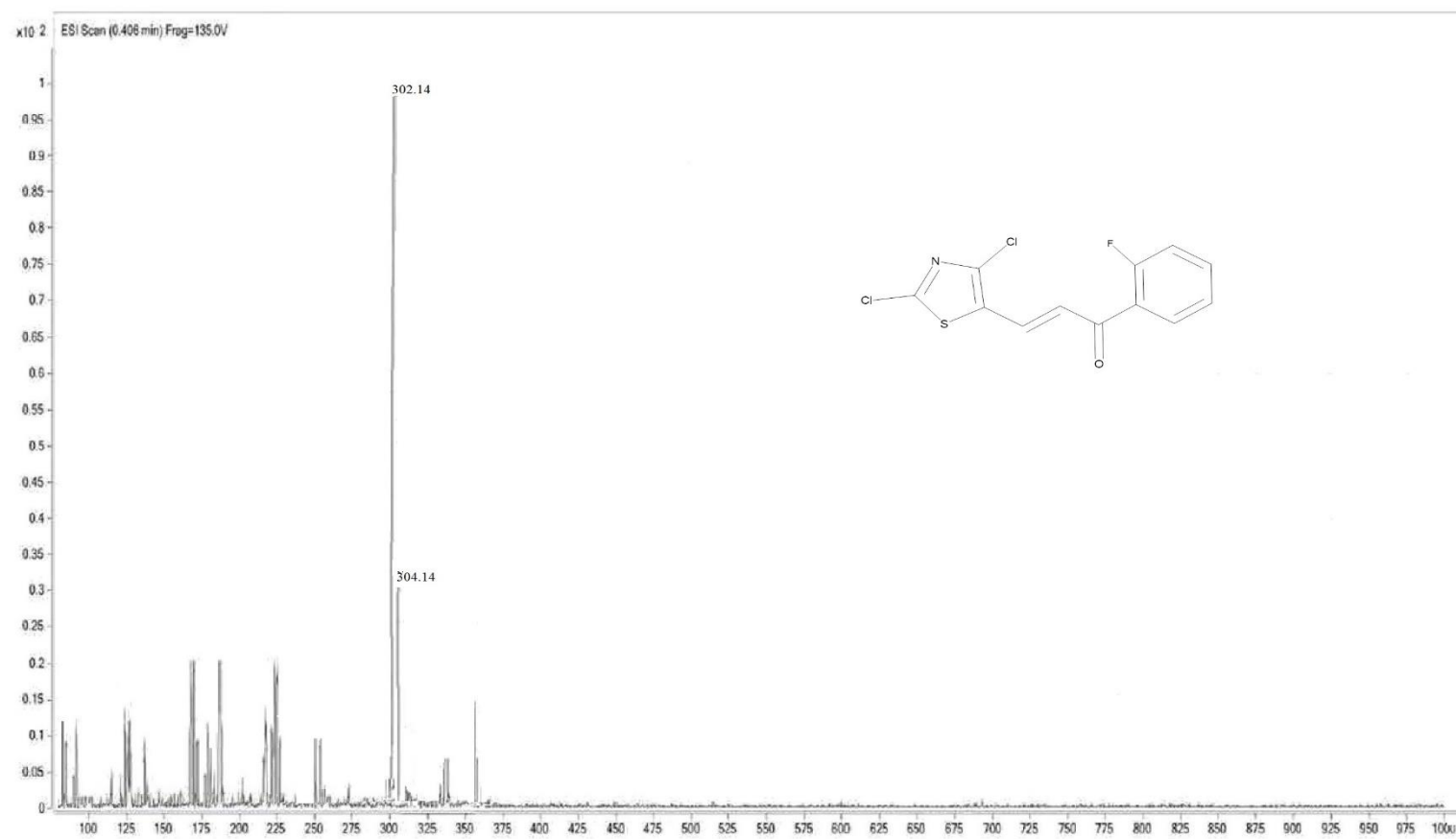


Figure S28. Mass Spectrum of compound 9

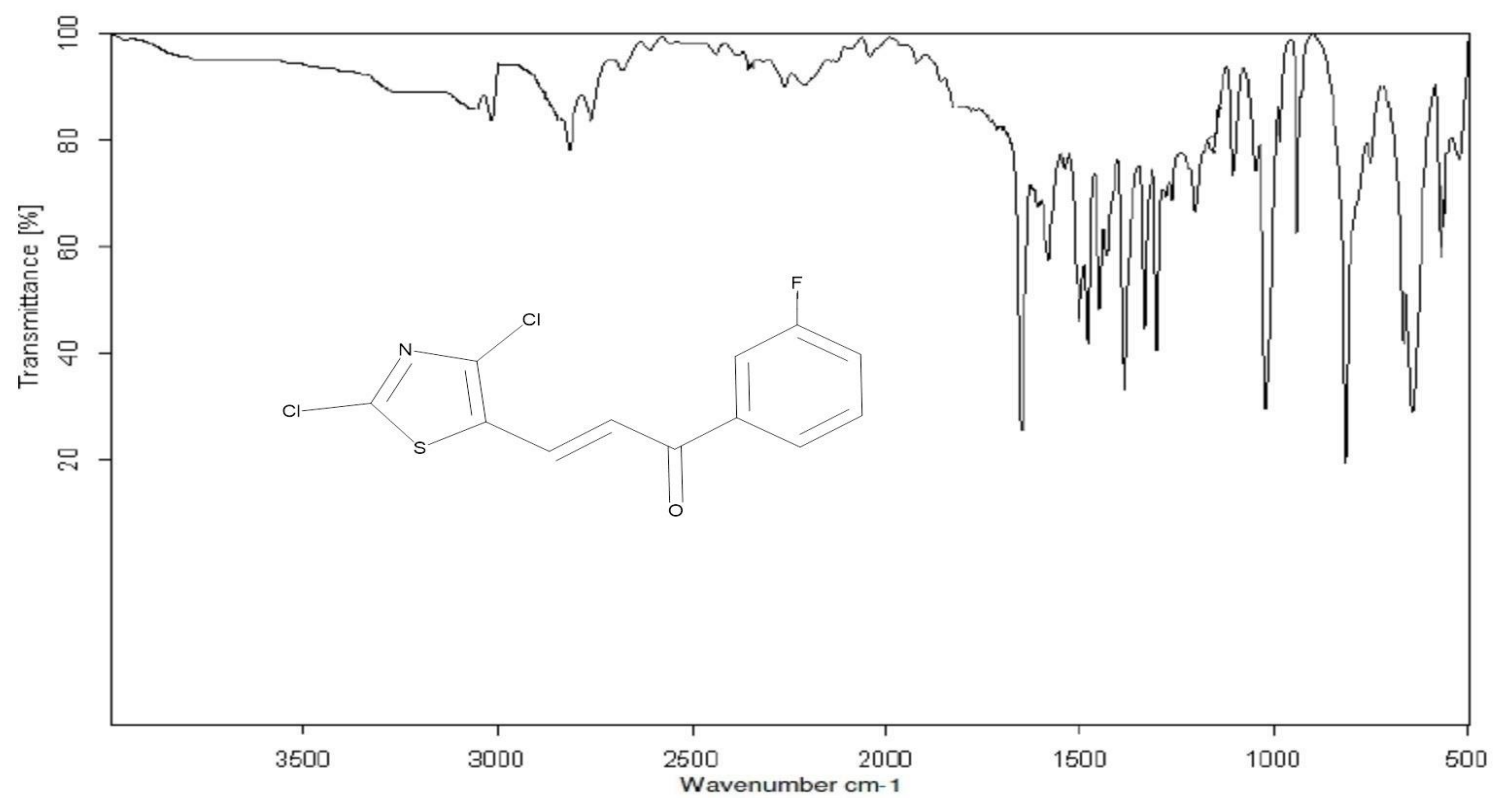


Figure S29. FT-IR Spectrum of compound 10

10  $^1\text{H}$   $\text{CDCl}_3$

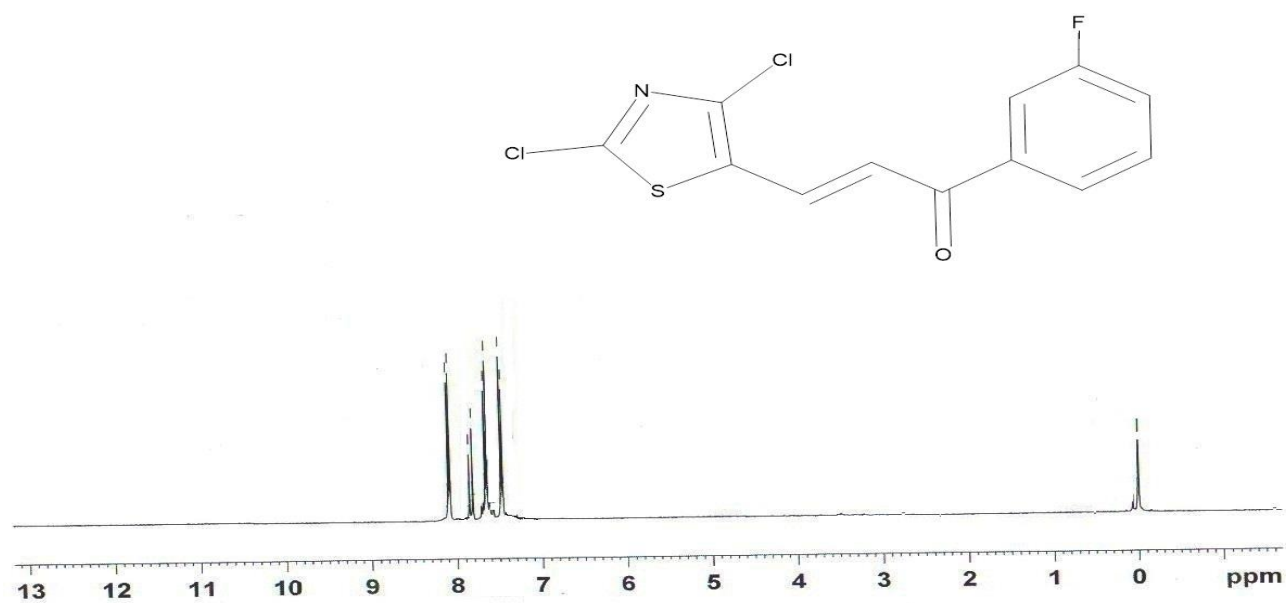


Figure S30.  $^1\text{H}$  NMR Spectrum of compound 10

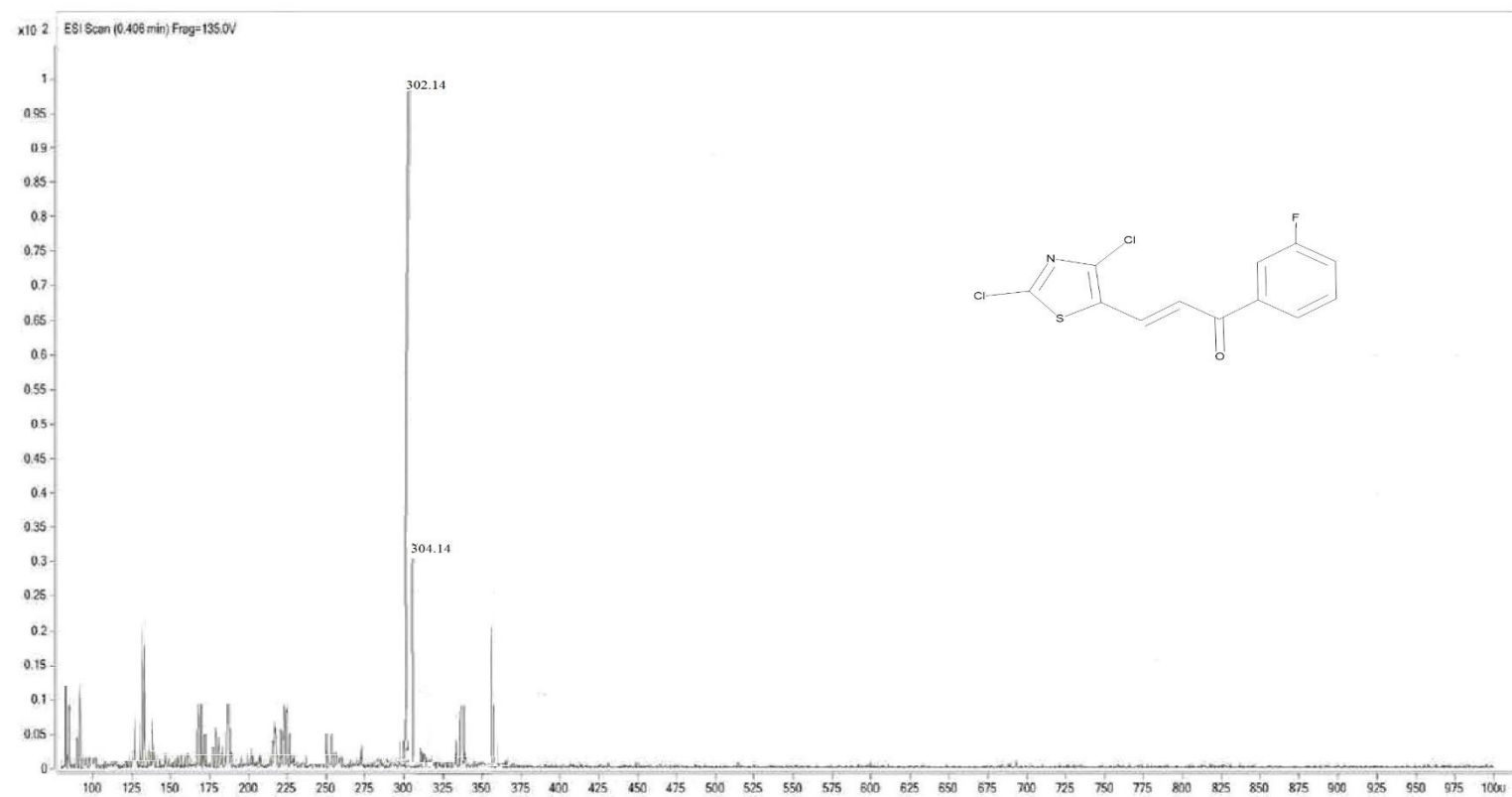


Figure S31. Mass Spectrum of compound 10



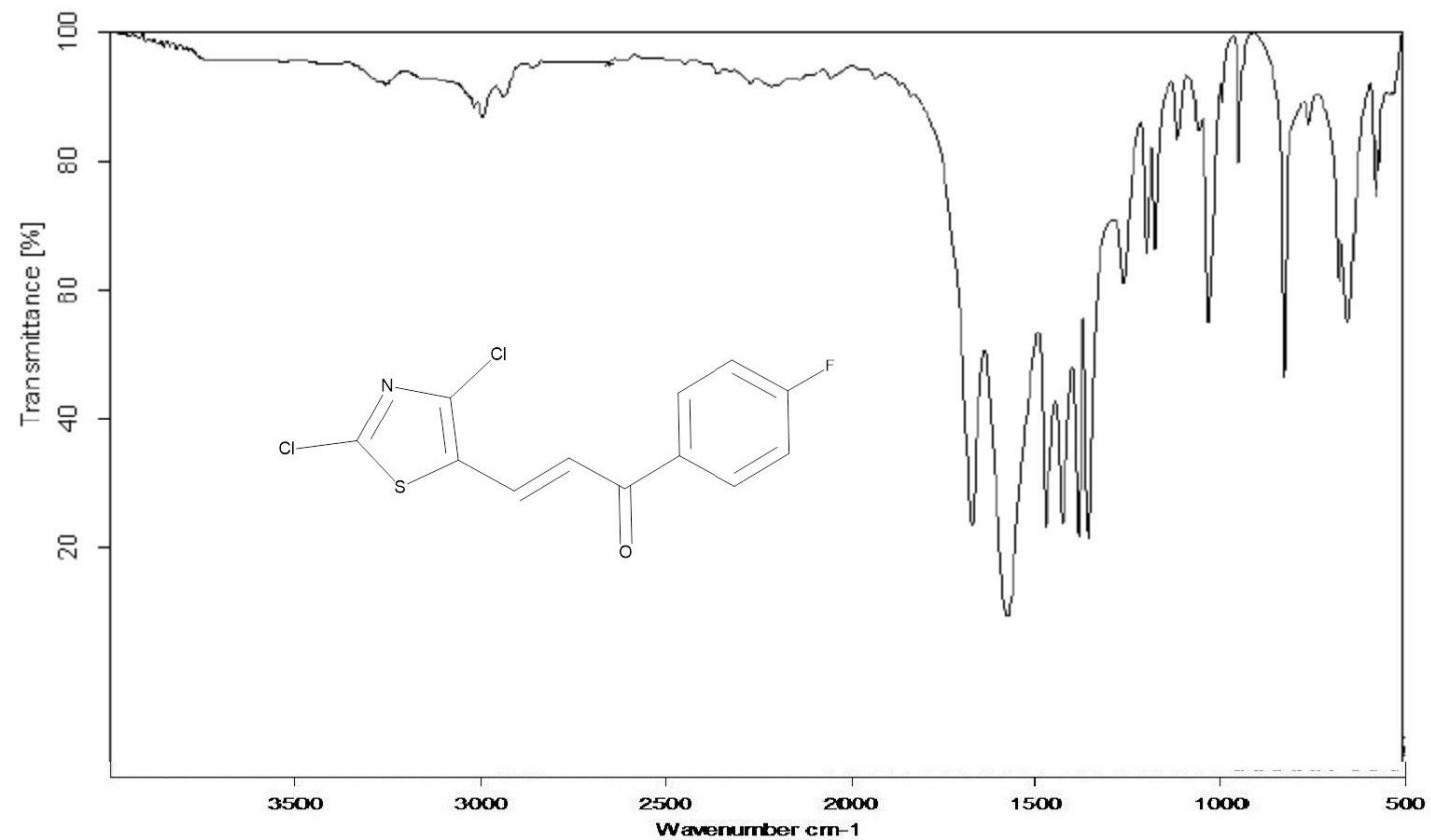


Figure S32. FT-IR Spectrum of compound 11

11 <sup>1</sup>H CDCl<sub>3</sub>

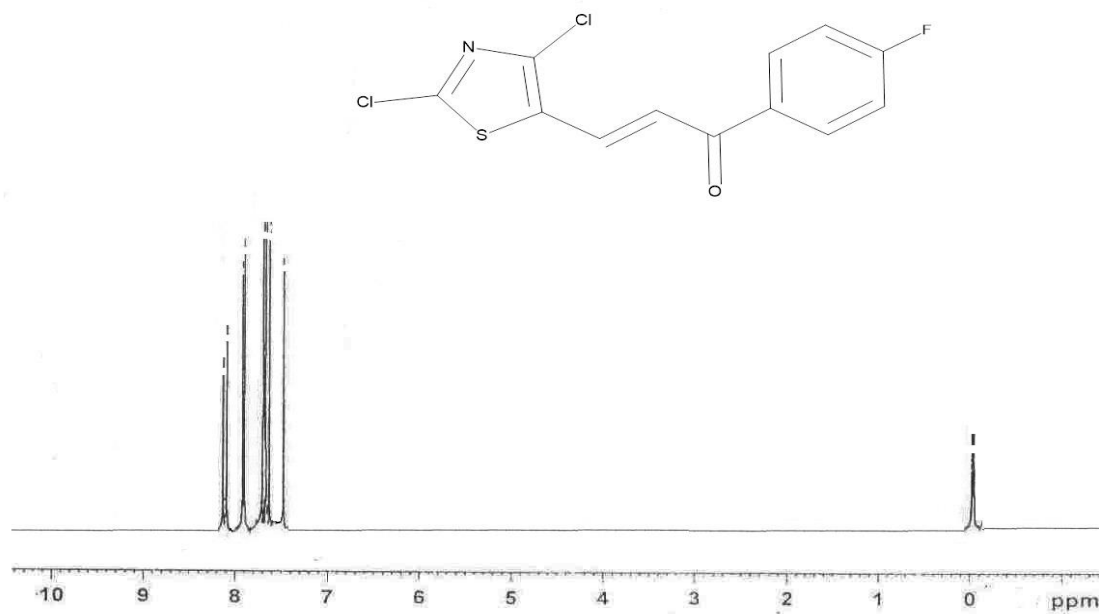


Figure S33. <sup>1</sup>H NMR Spectrum of compound 11

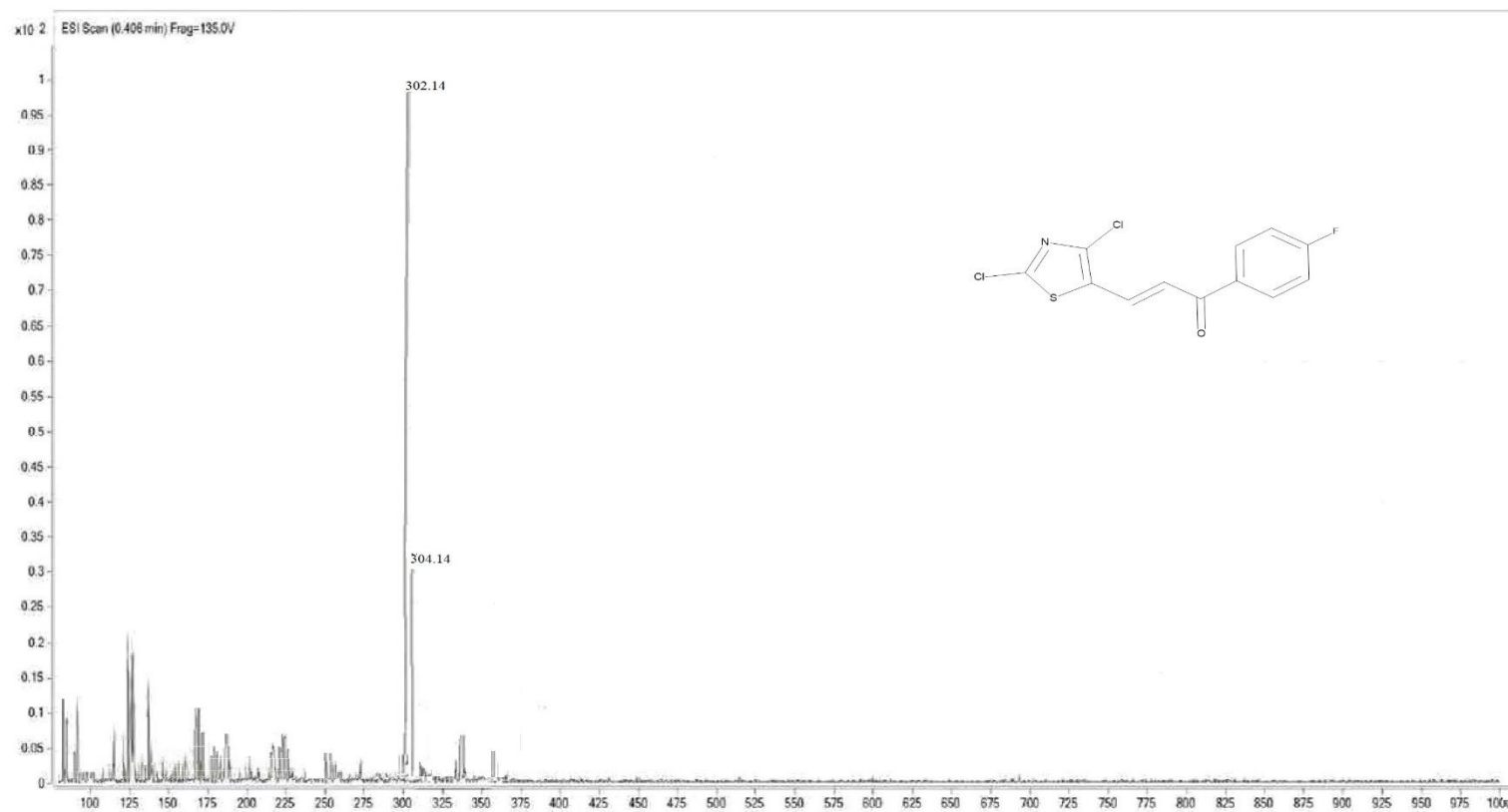


Figure S34. Mass Spectrum of compound 11

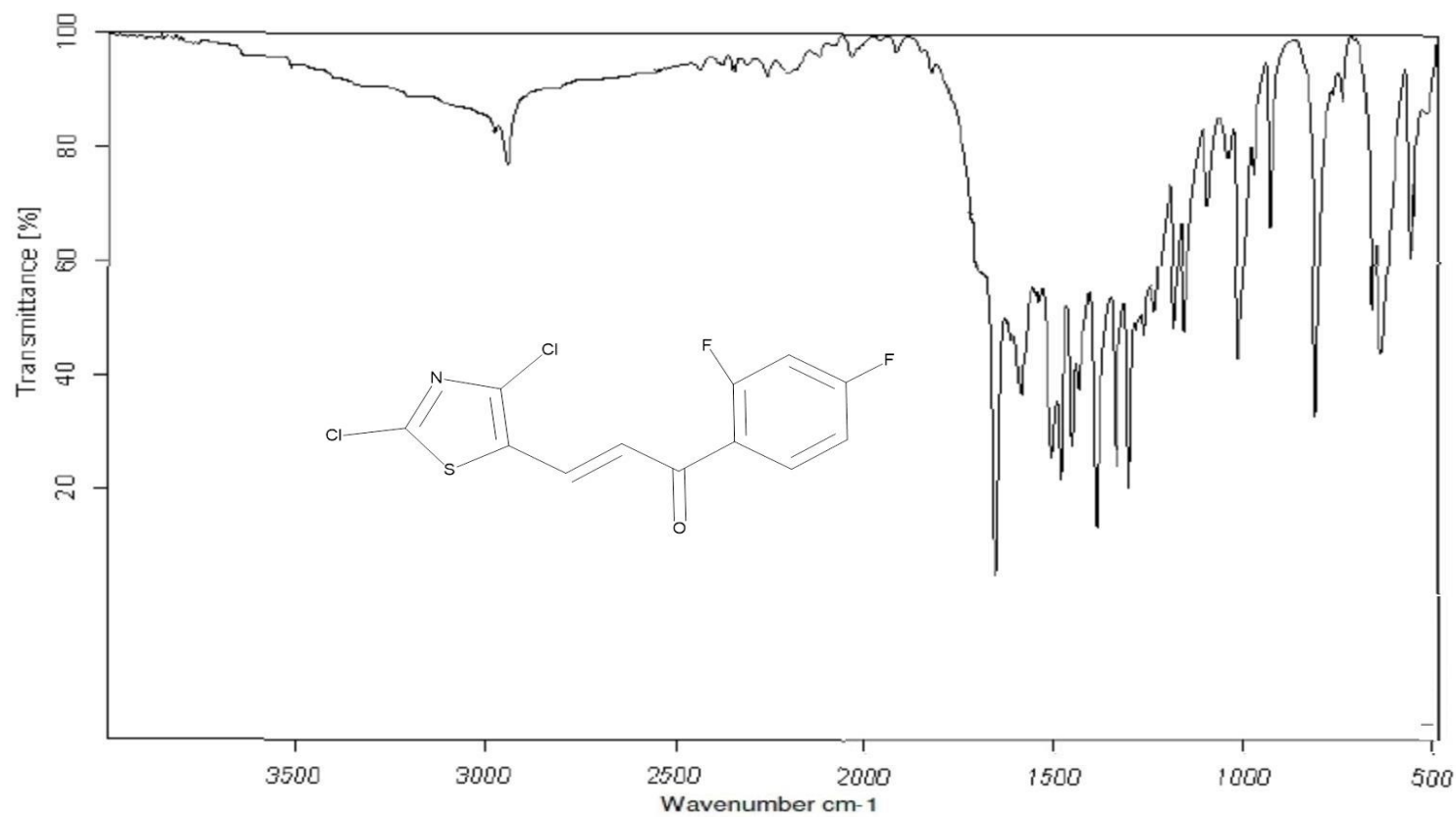


Figure S35. FT-IR Spectrum of compound 12

12 1H CDC13

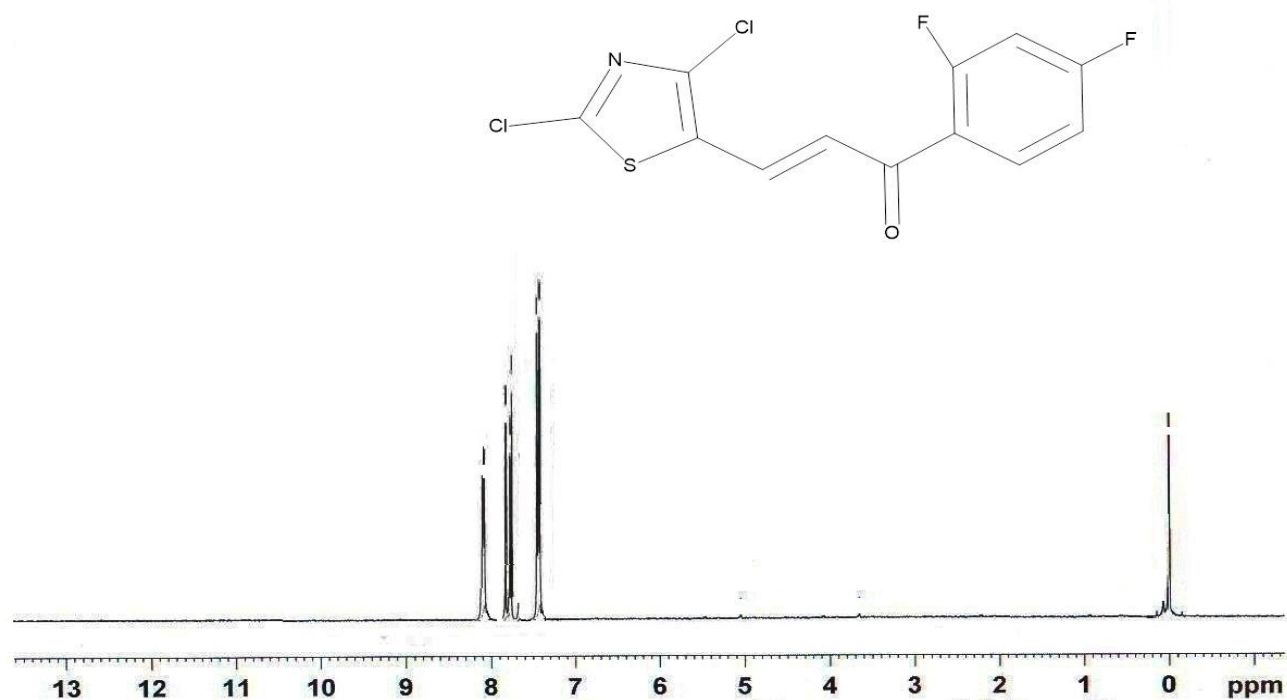


Figure S36. <sup>1</sup>H NMR Spectrum of compound 12

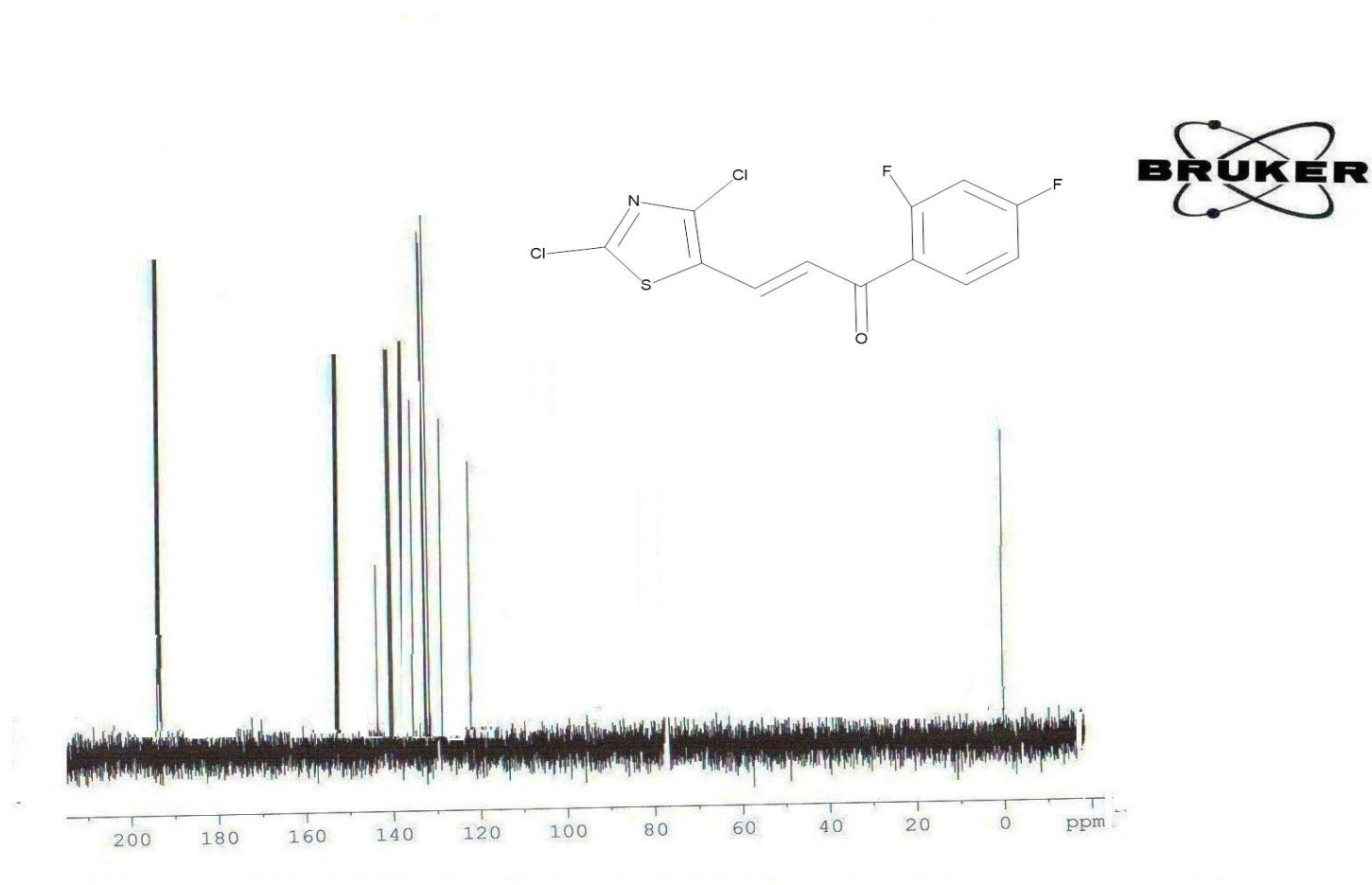


Figure S37.  $^{13}\text{C}$  NMR Spectrum of compound 12

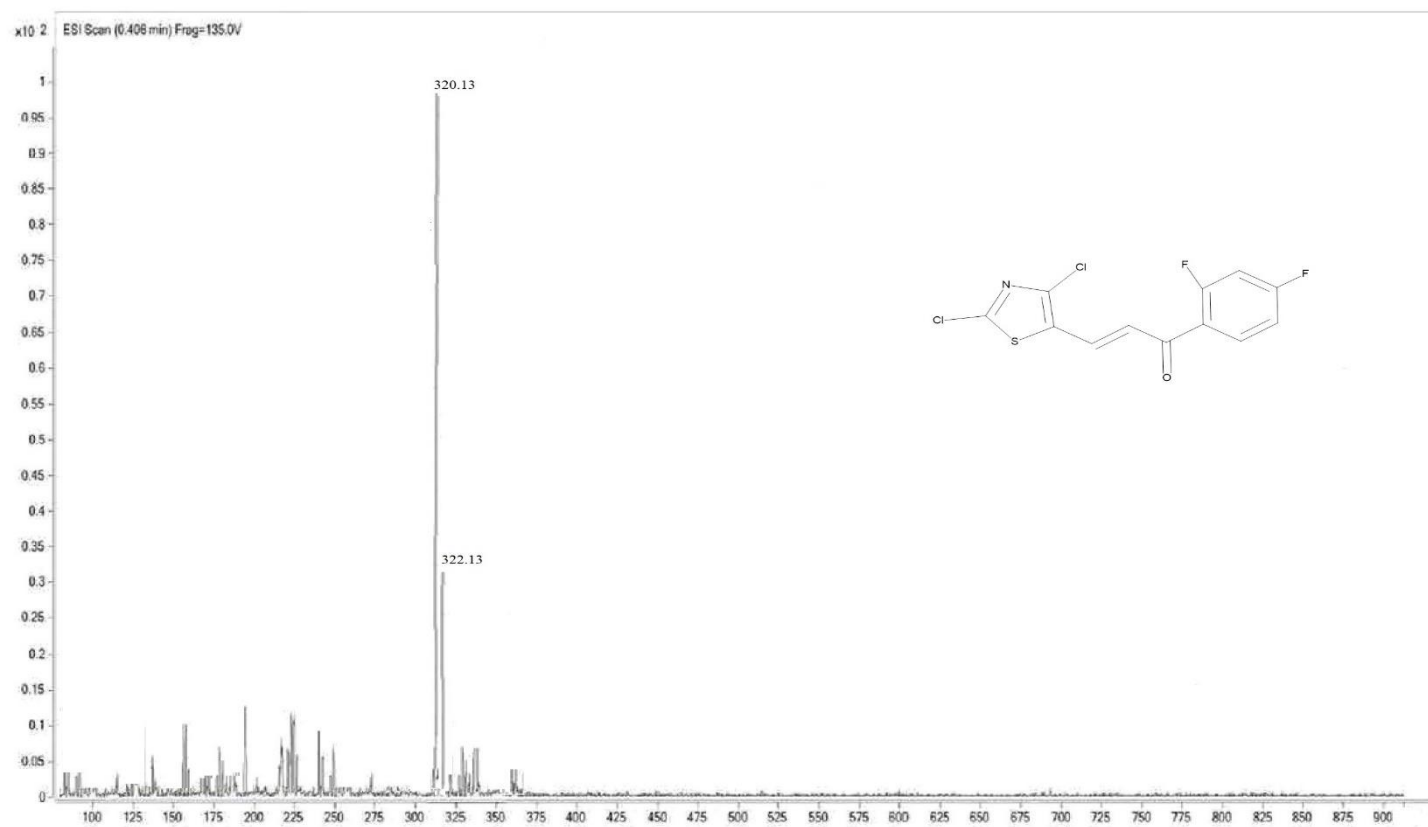


Figure S38. Mass Spectrum of compound 12

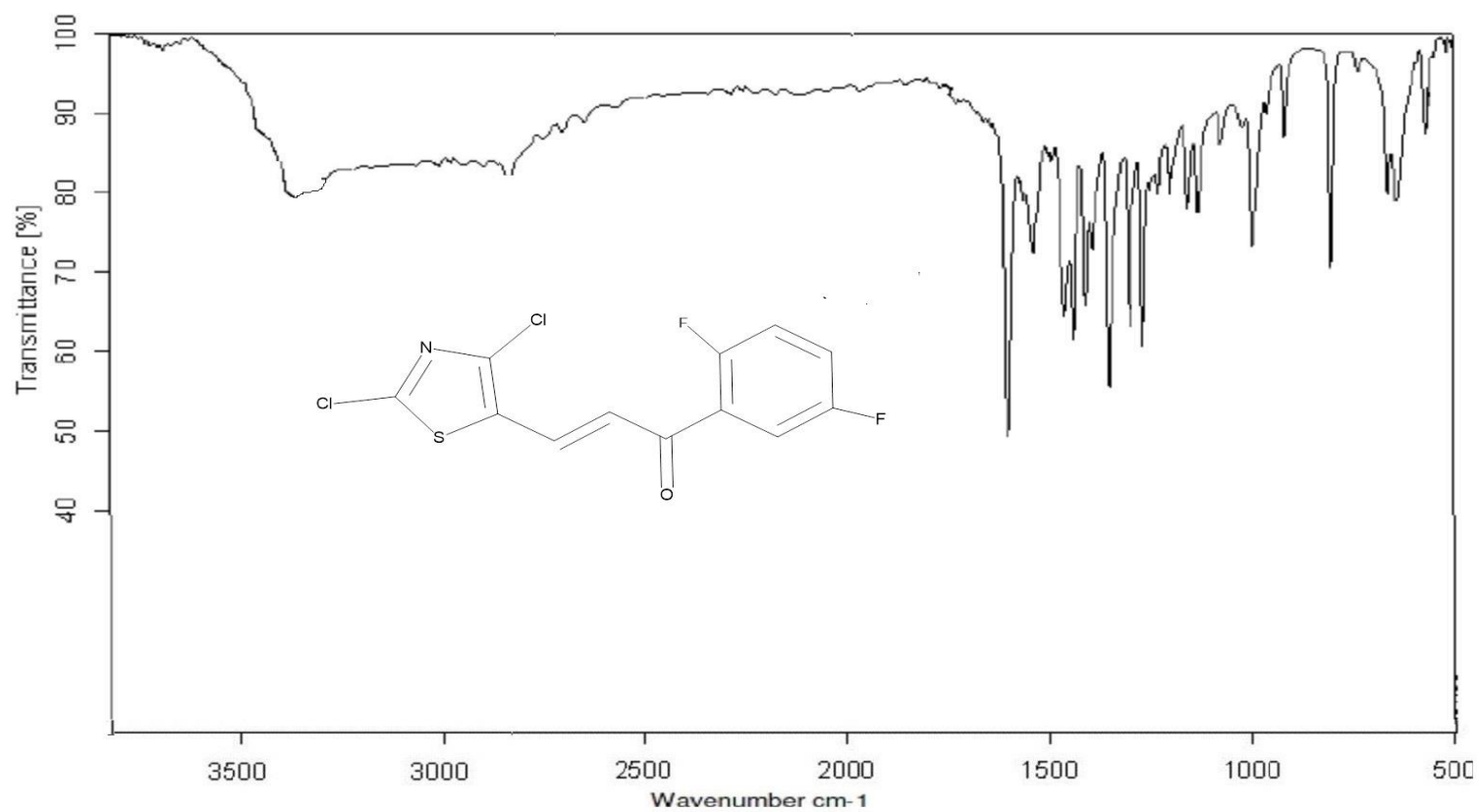


Figure S39. FT-IR Spectrum of compound 13



13 <sup>1</sup>H CDCl<sub>3</sub>

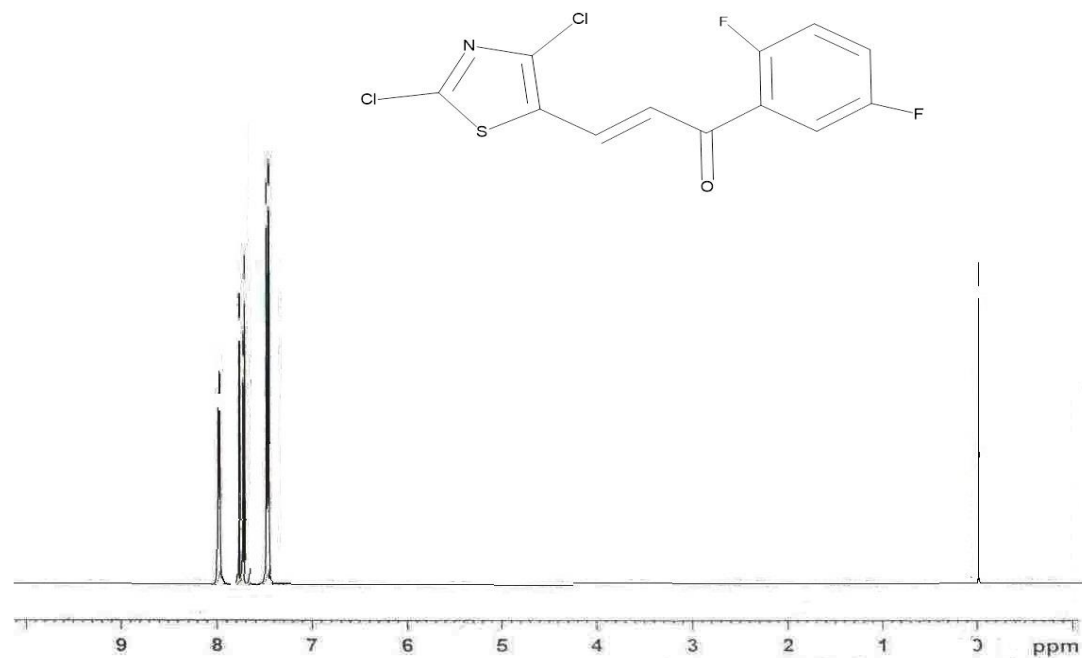


Figure S40. <sup>1</sup>H NMR Spectrum of compound 13

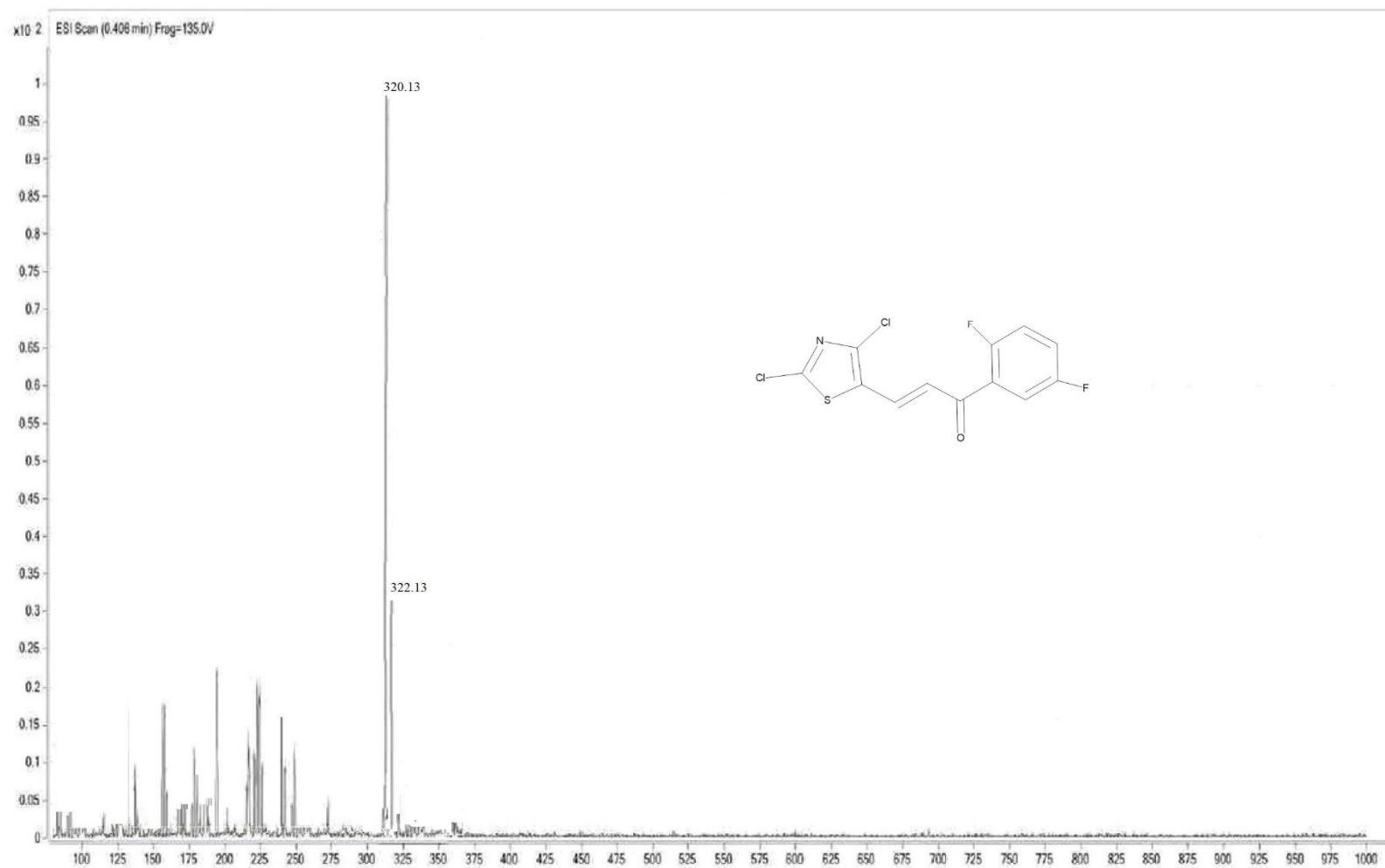


Figure S41. Mass Spectrum of compound 13

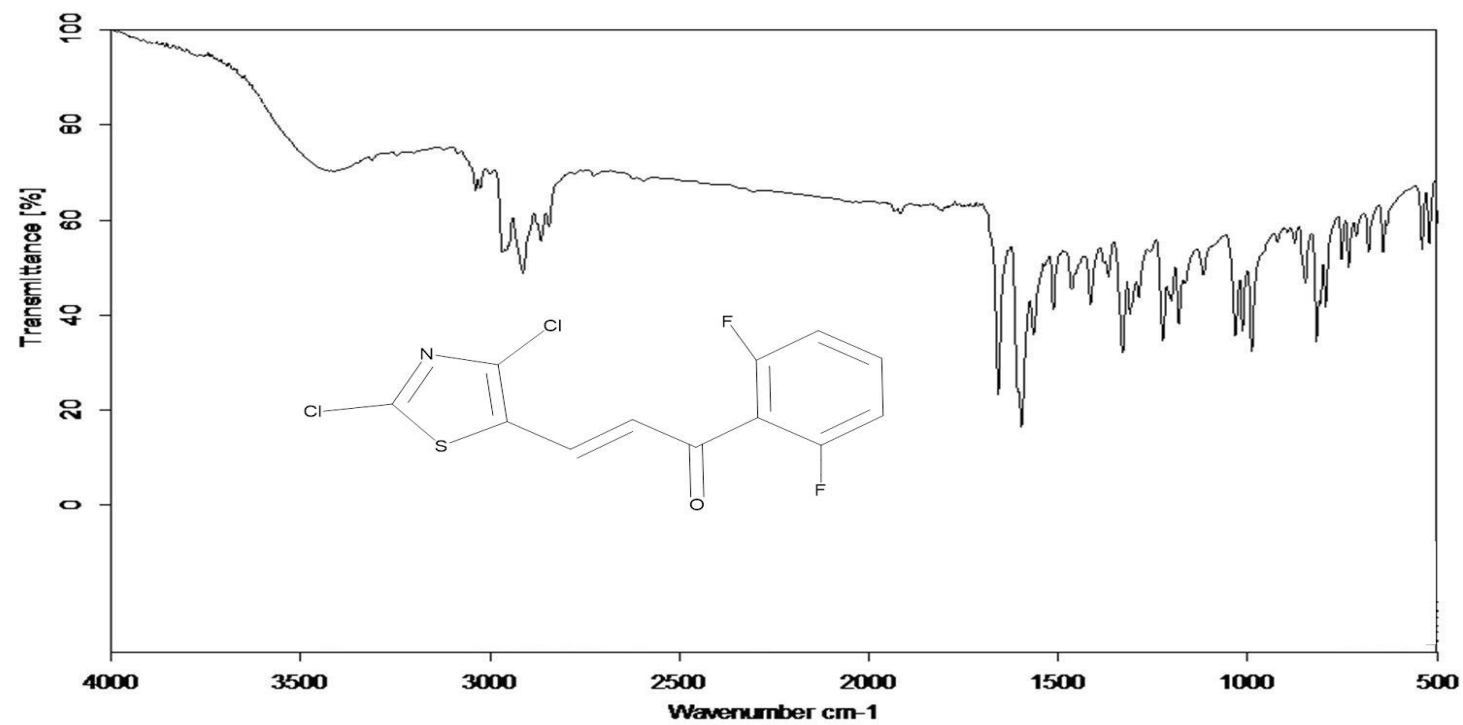


Figure S42. FT-IR Spectrum of compound 14

14 1H CDCl3

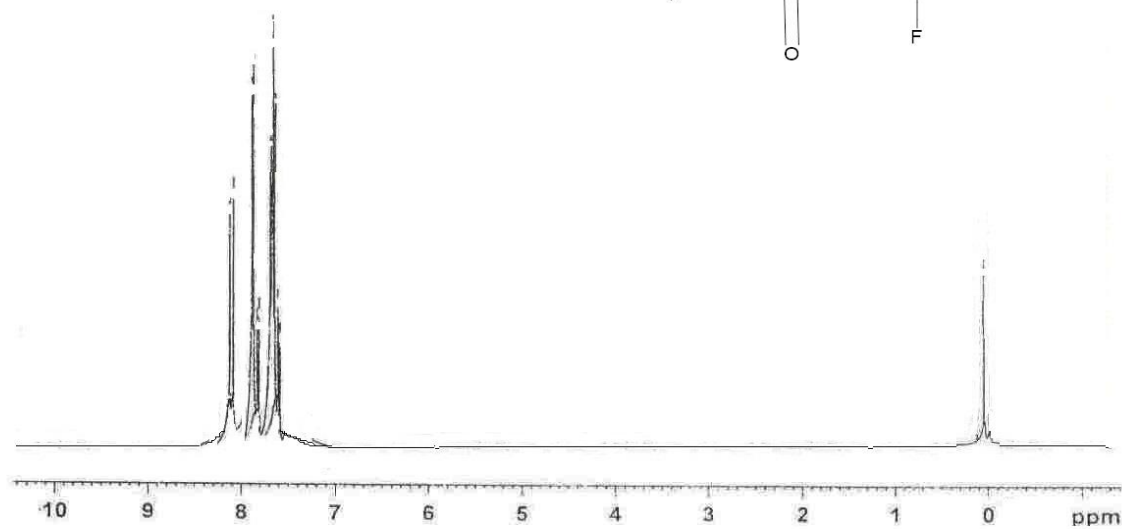
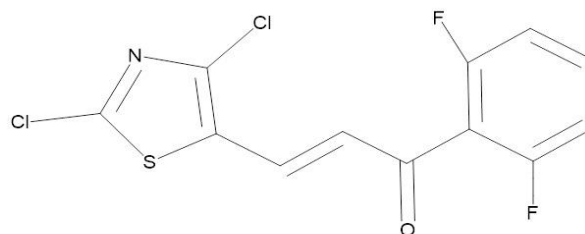


Figure S43. <sup>1</sup>H NMR Spectrum of compound 14

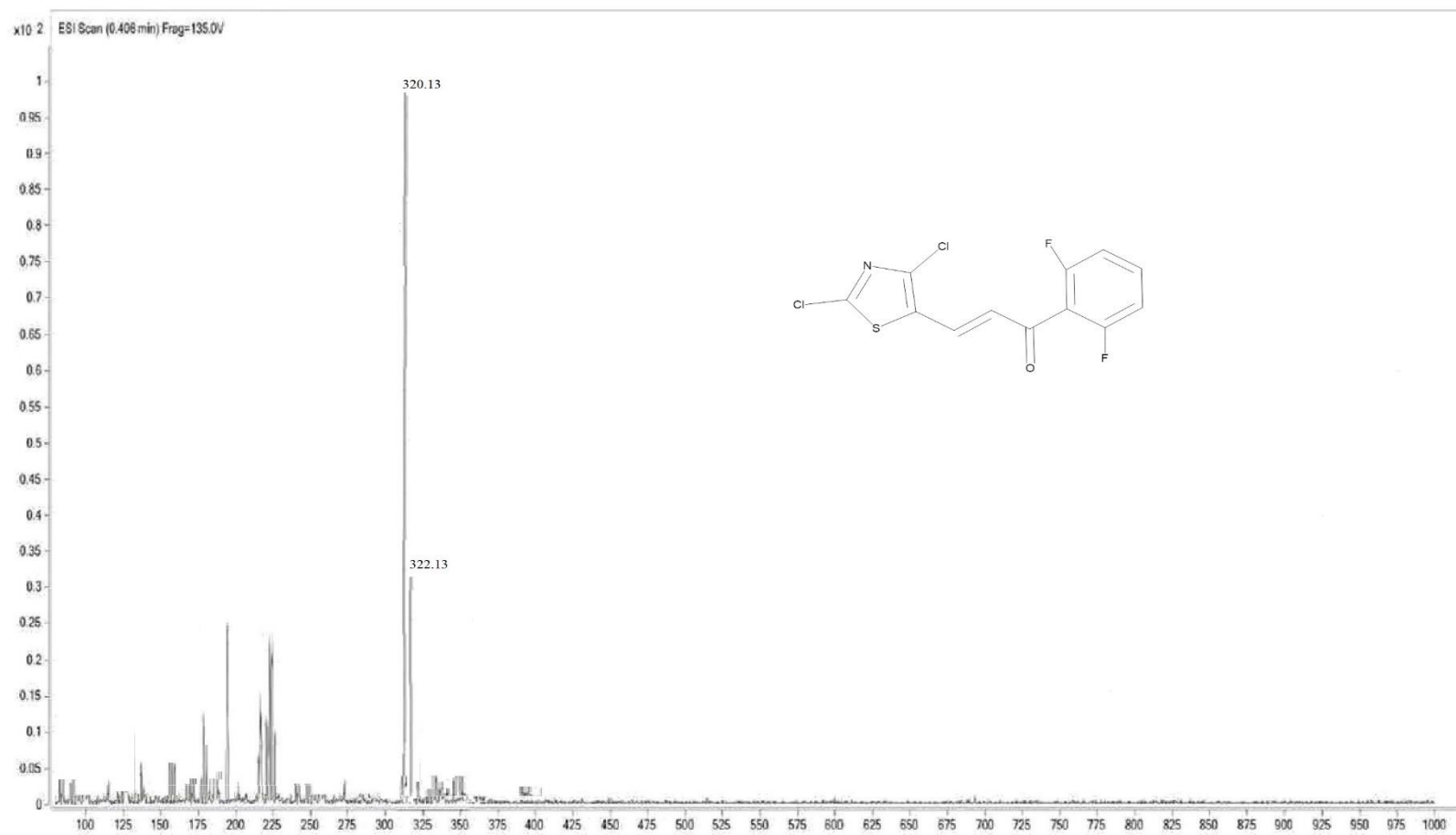


Figure S44. Mass Spectrum of compound 14

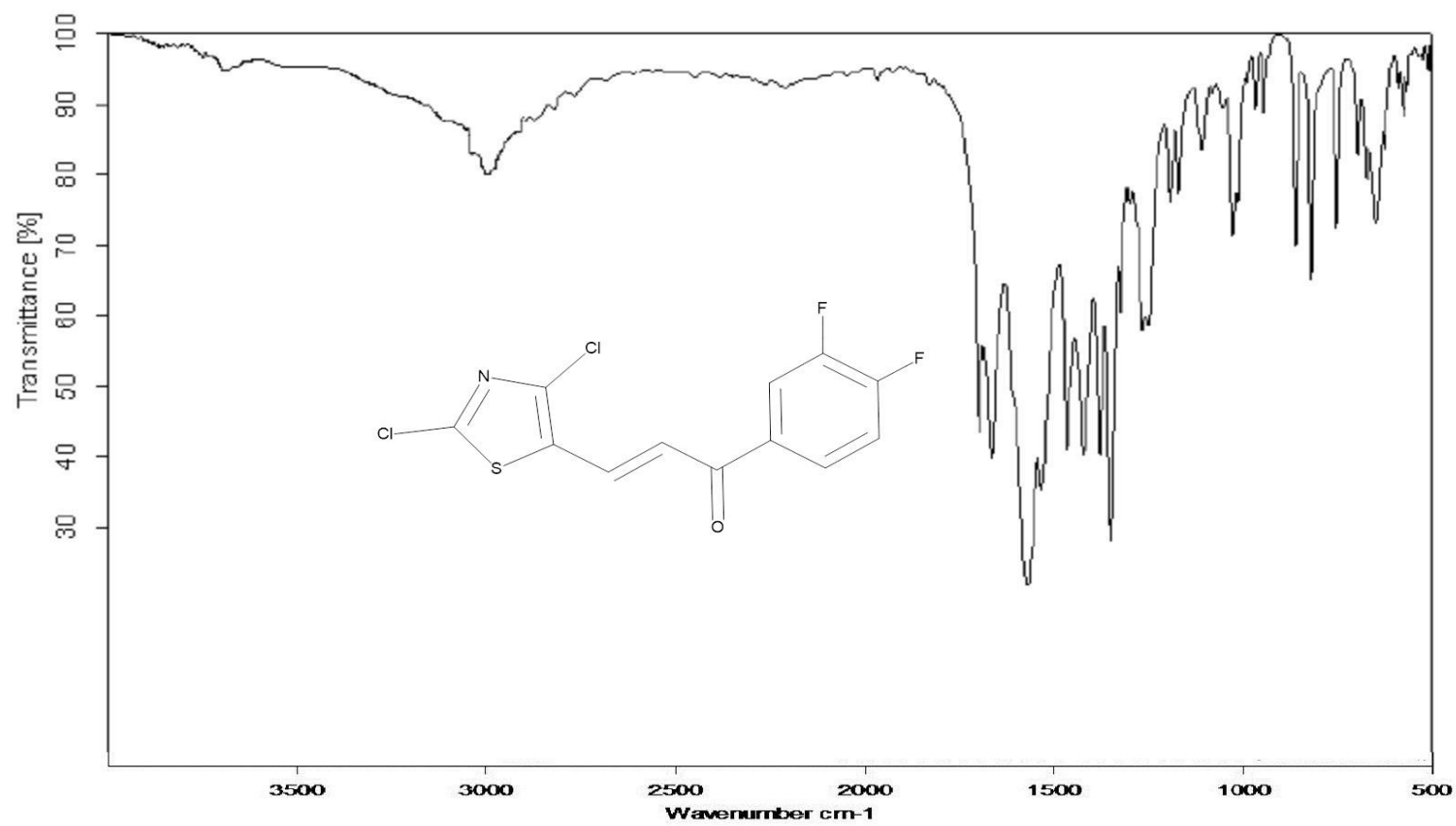


Figure S45. FT-IR Spectrum of compound 15

15 <sup>1</sup>H CDCl<sub>3</sub>

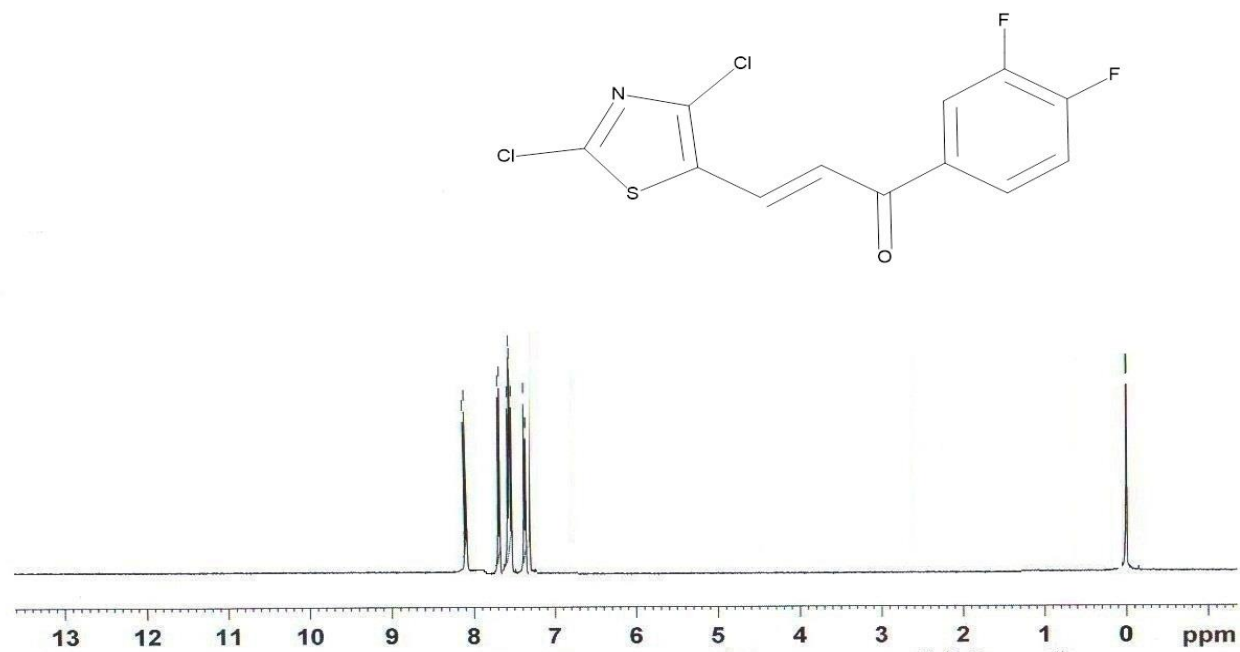


Figure S46. <sup>1</sup>H NMR Spectrum of compound 15

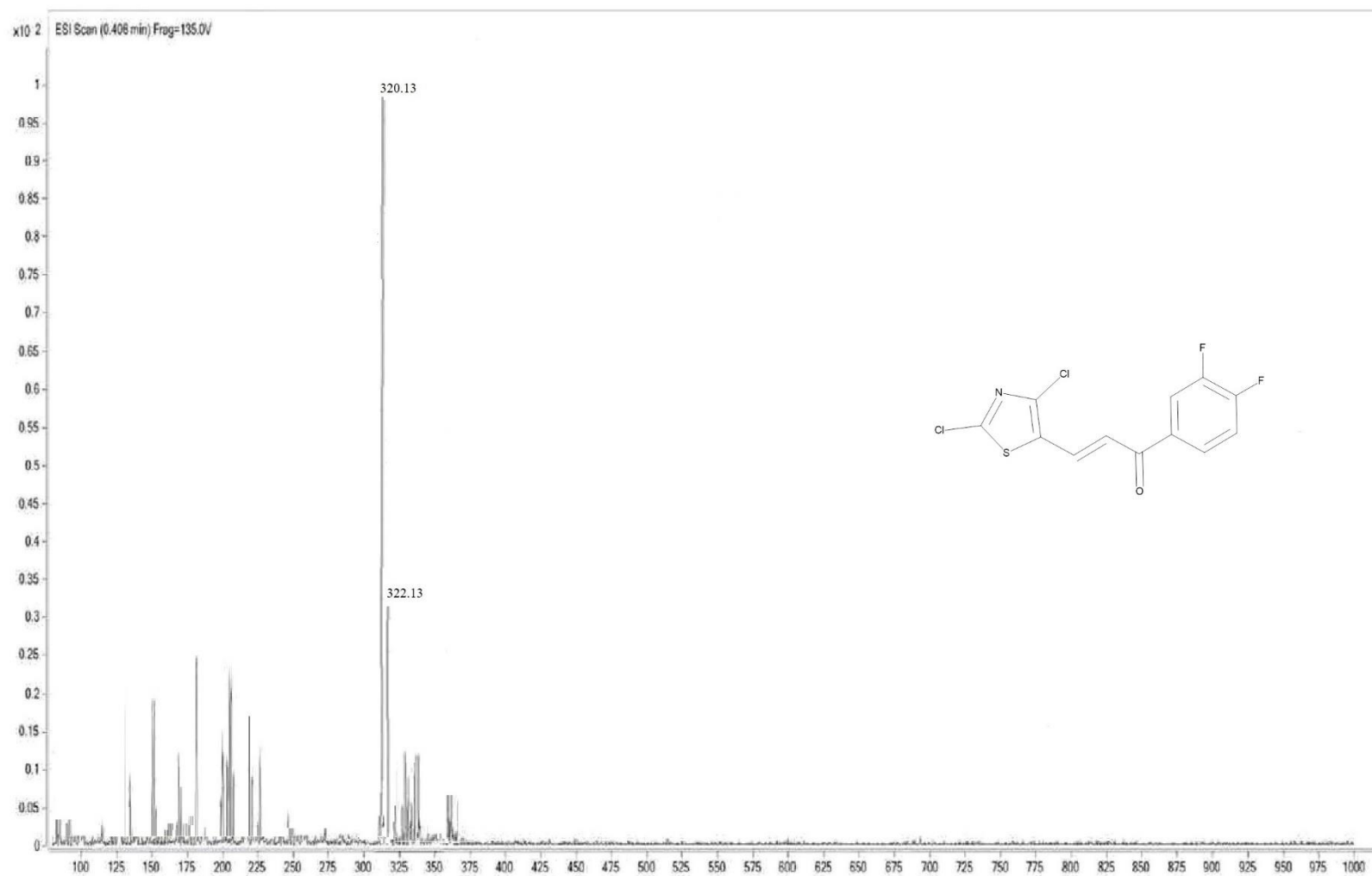


Figure S47. Mass Spectrum of compound 15



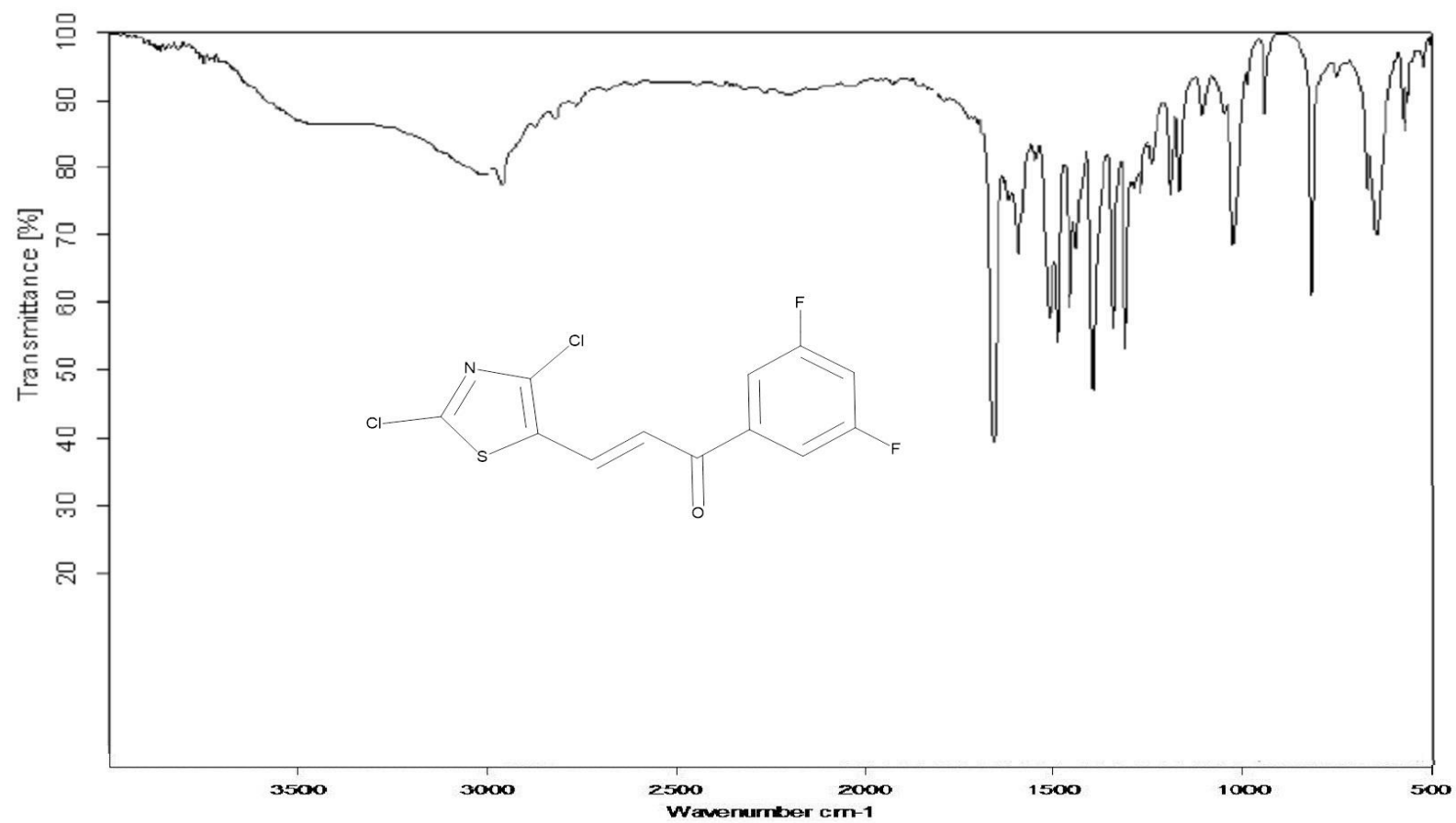


Figure S48. FT-IR Spectrum of compound 16

16 <sup>1</sup>H CDCl<sub>3</sub>

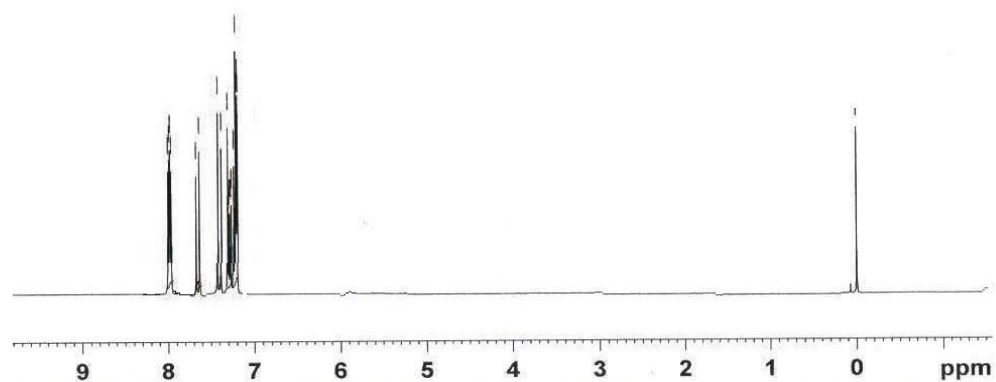
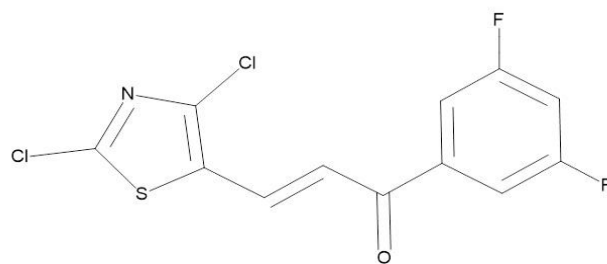


Figure S49. <sup>1</sup>H NMR Spectrum of compound 16

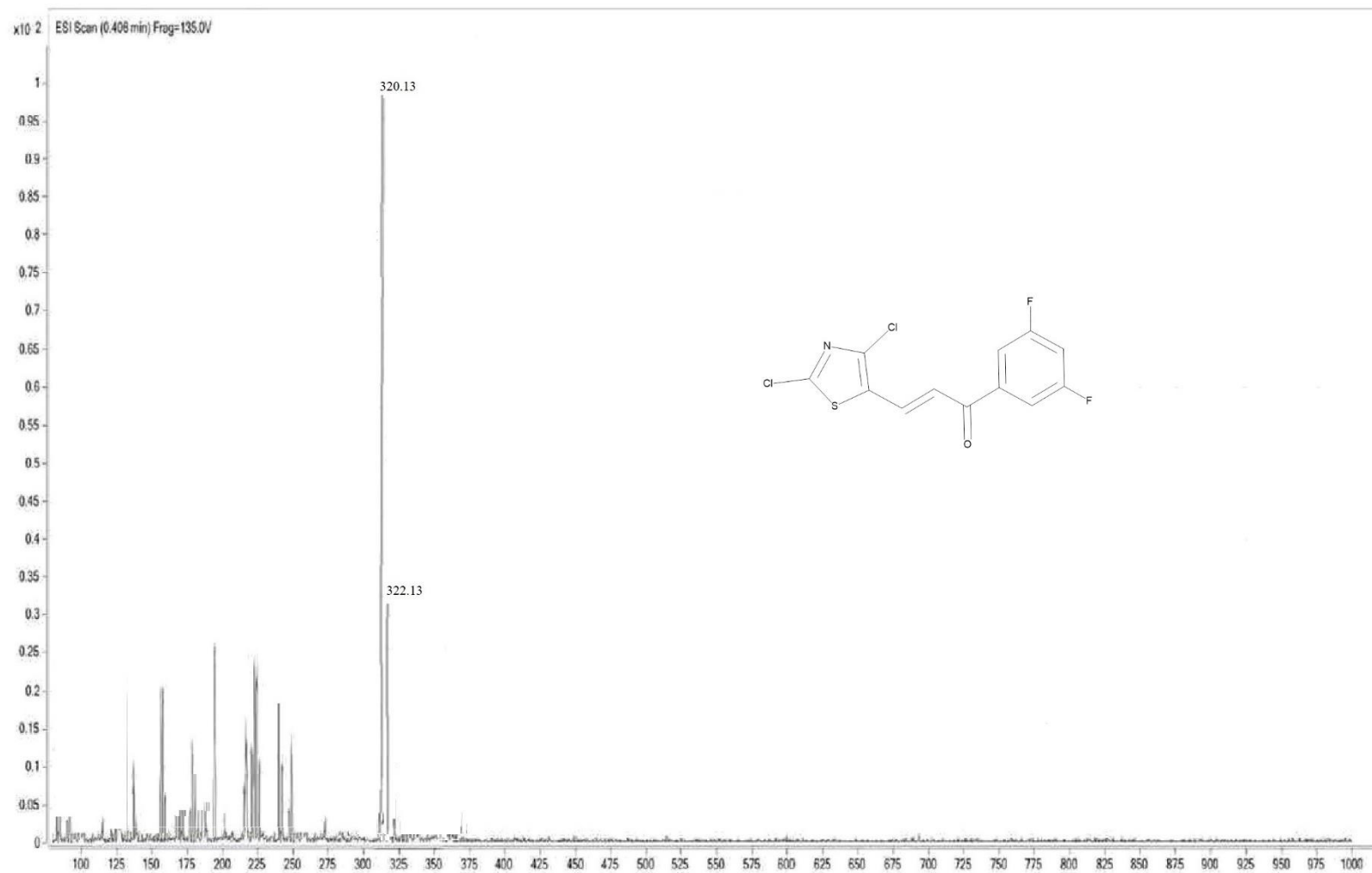


Figure S50. Mass Spectrum of compound 16

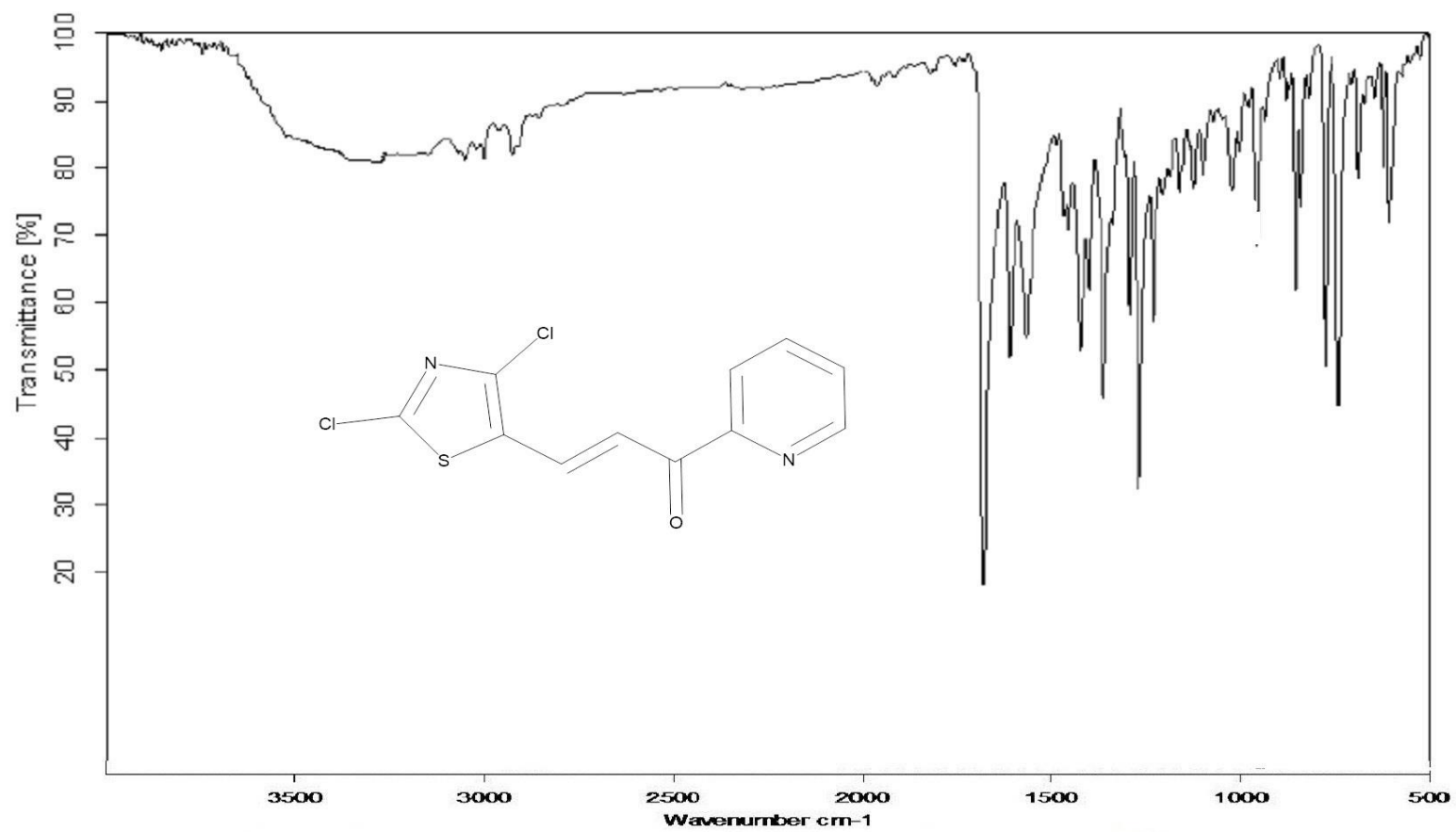


Figure S51. FT-IR Spectrum of compound 17

17 <sup>1</sup>H CDCl<sub>3</sub>

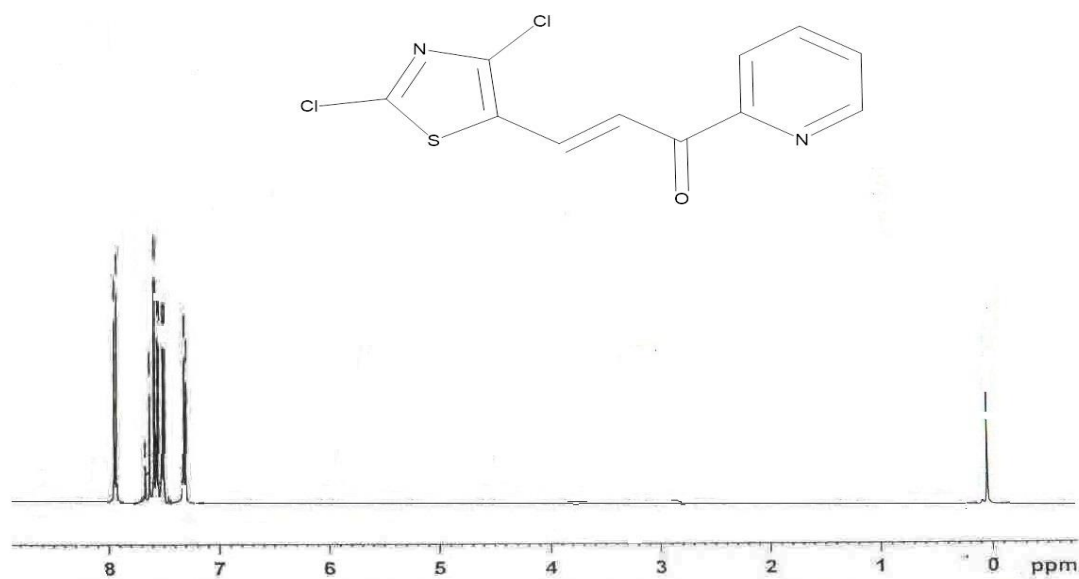


Figure S52. <sup>1</sup>H NMR Spectrum of compound 17

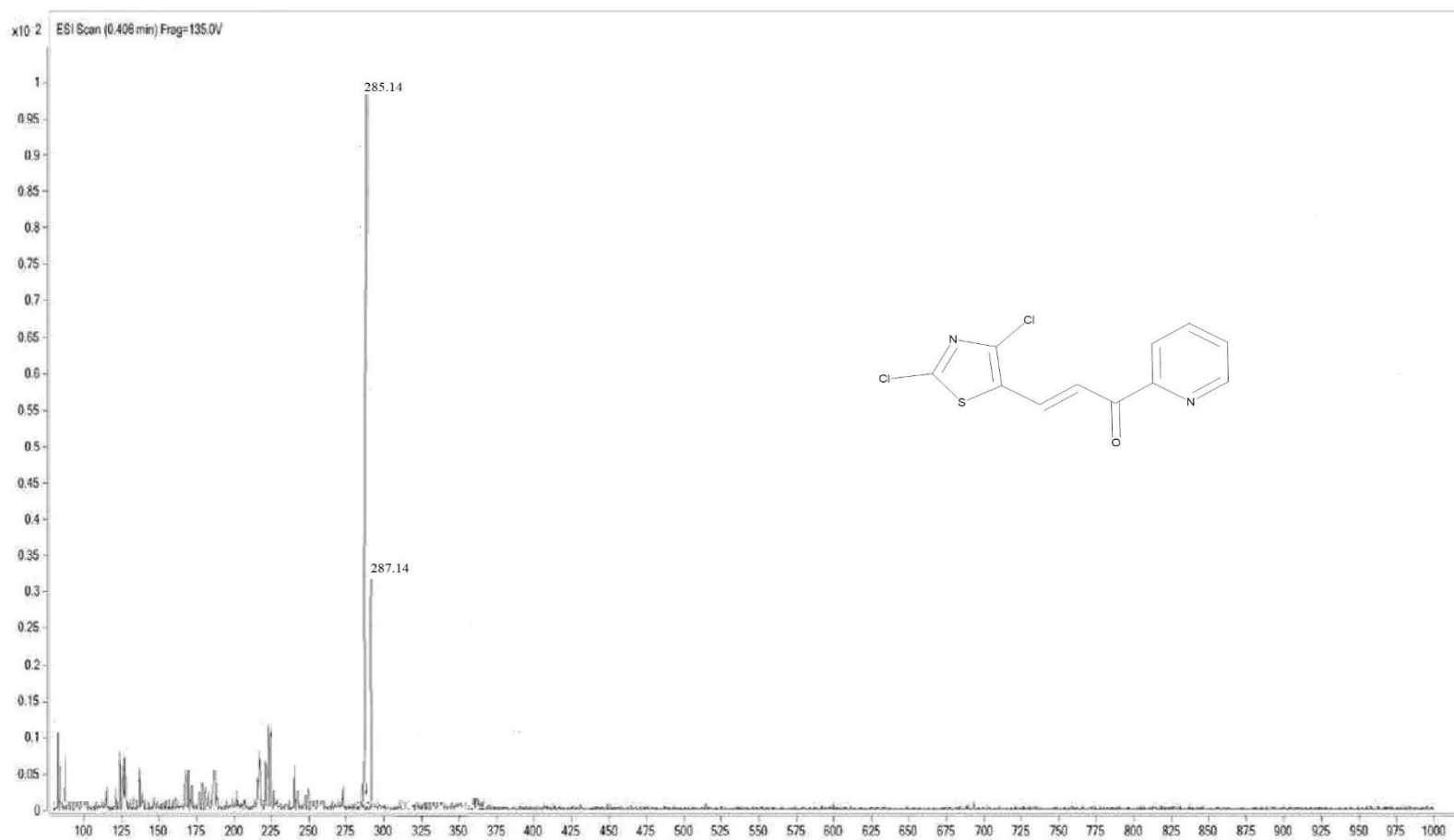


Figure S53. Mass Spectrum of compound 17

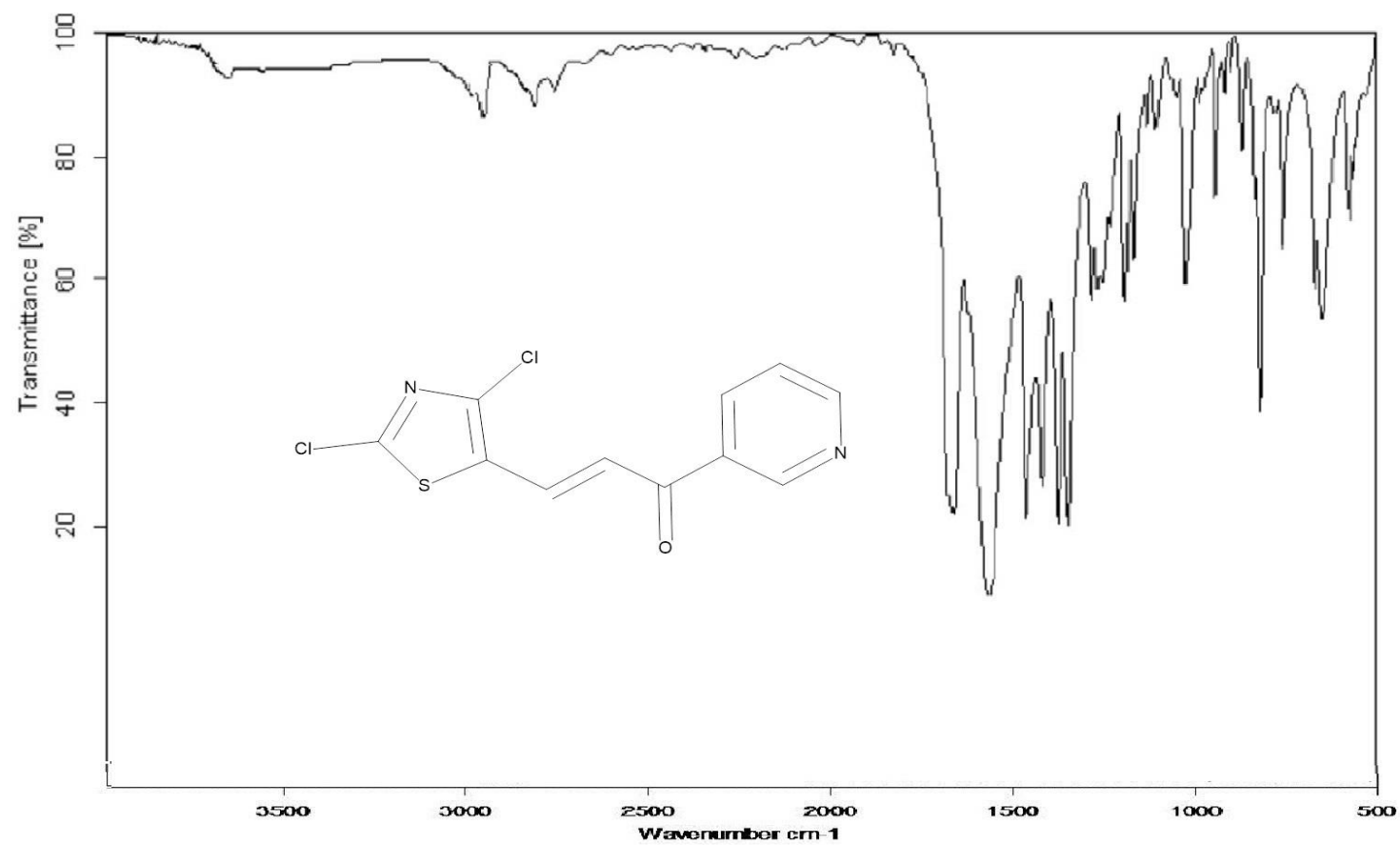


Figure S54. FT-IR Spectrum of compound 18

18 <sup>1</sup>H CDCl<sub>3</sub>

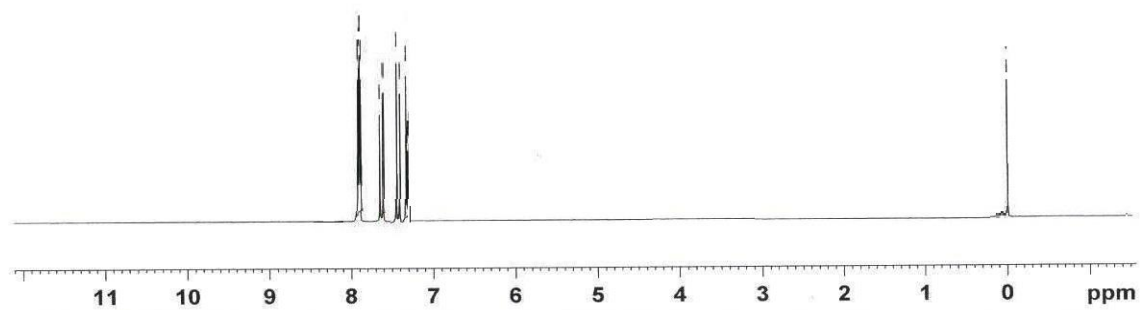
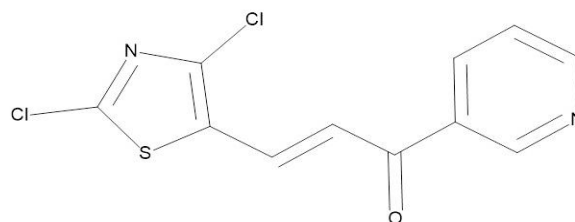


Figure S55. <sup>1</sup>H NMR Spectrum of compound 18



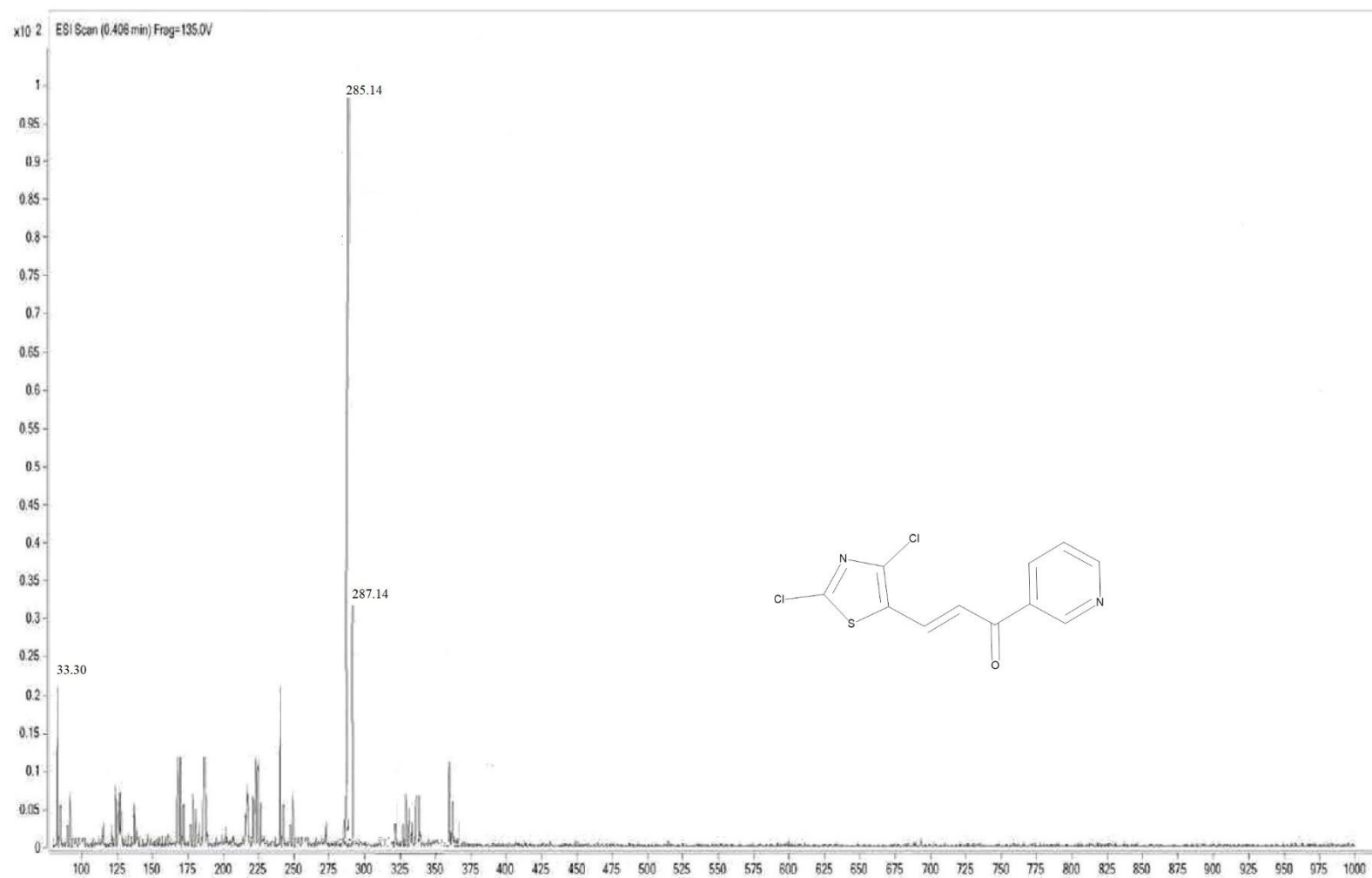


Figure S56. Mass Spectrum of compound 18

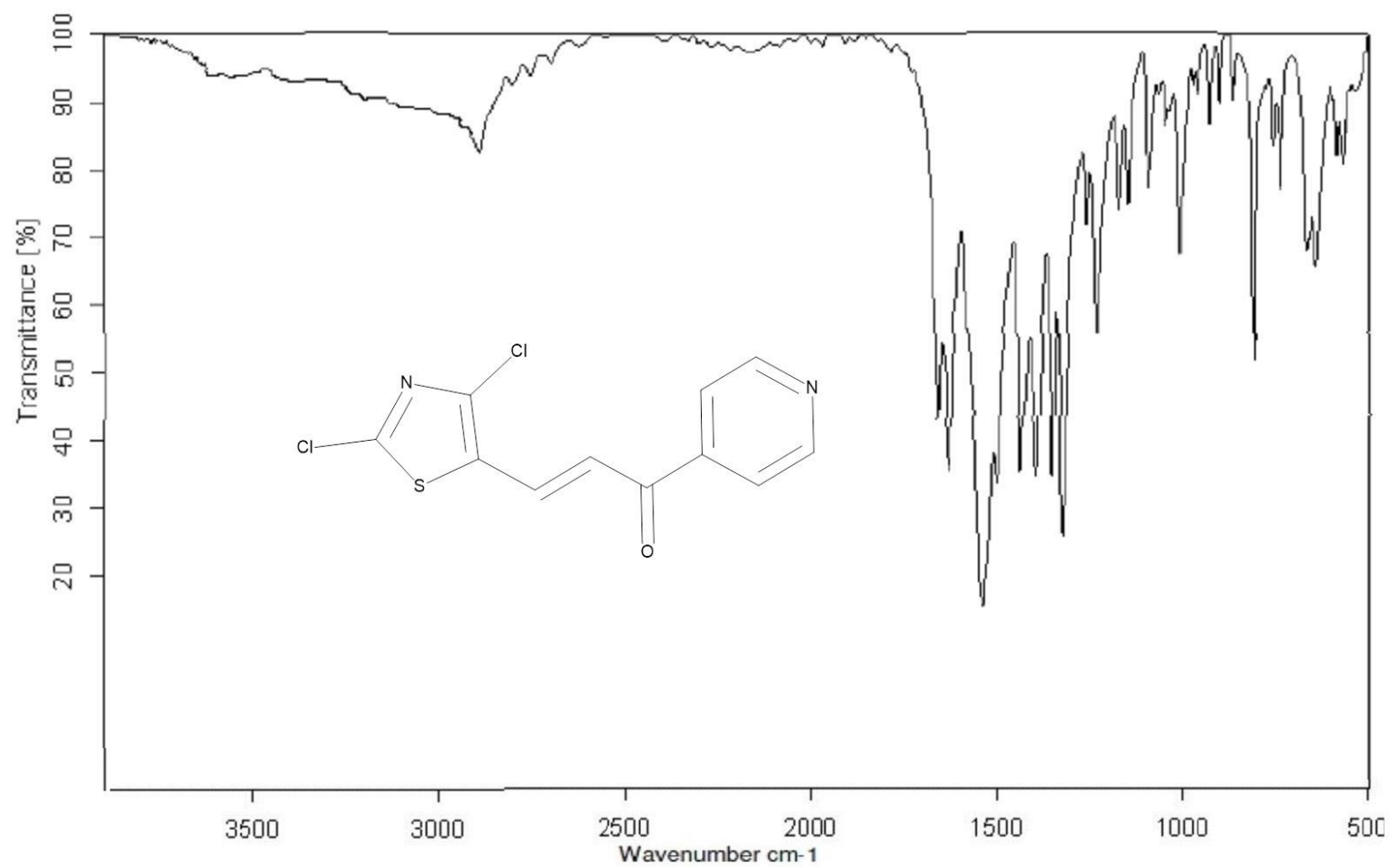


Figure S57. FT-IR Spectrum of compound 19

19 <sup>1</sup>H CDCl<sub>3</sub>

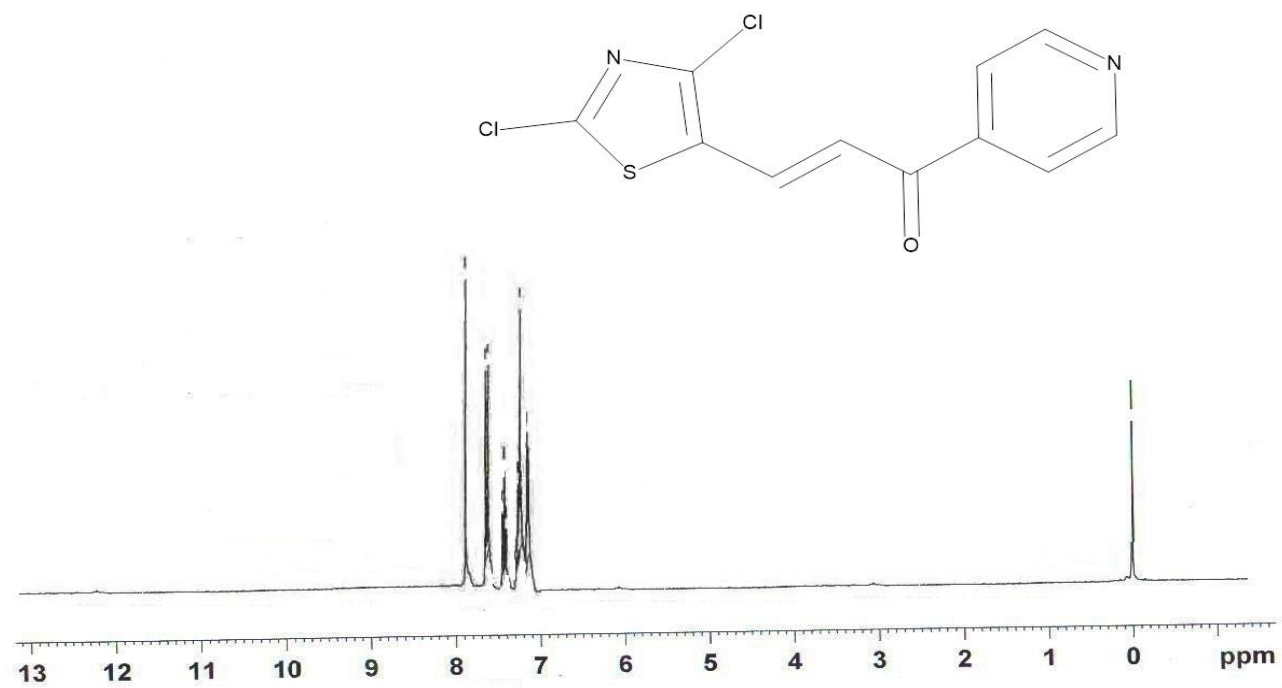


Figure S58. <sup>1</sup>H NMR Spectrum of compound 19

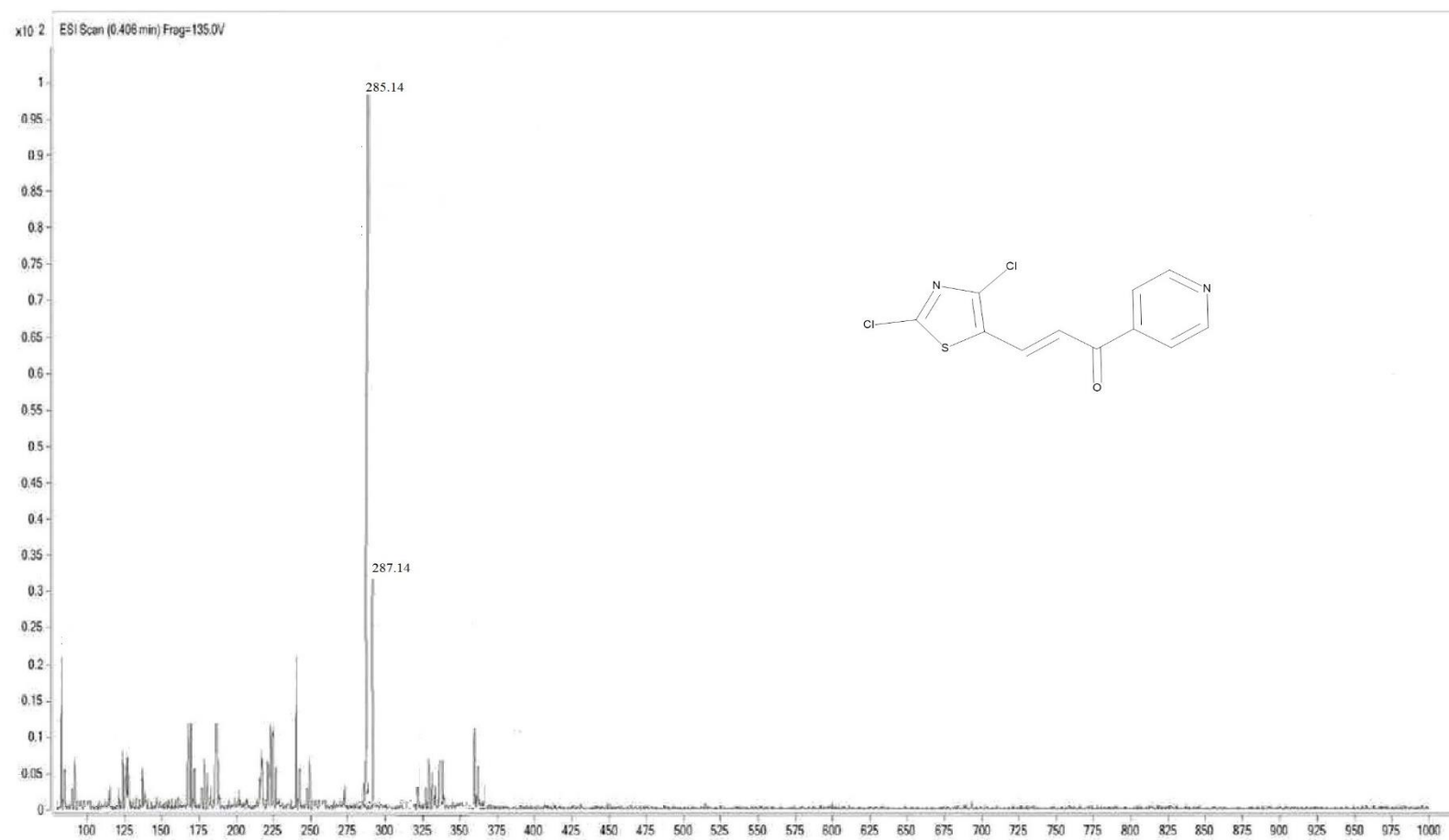


Figure S59. Mass Spectrum of compound 19

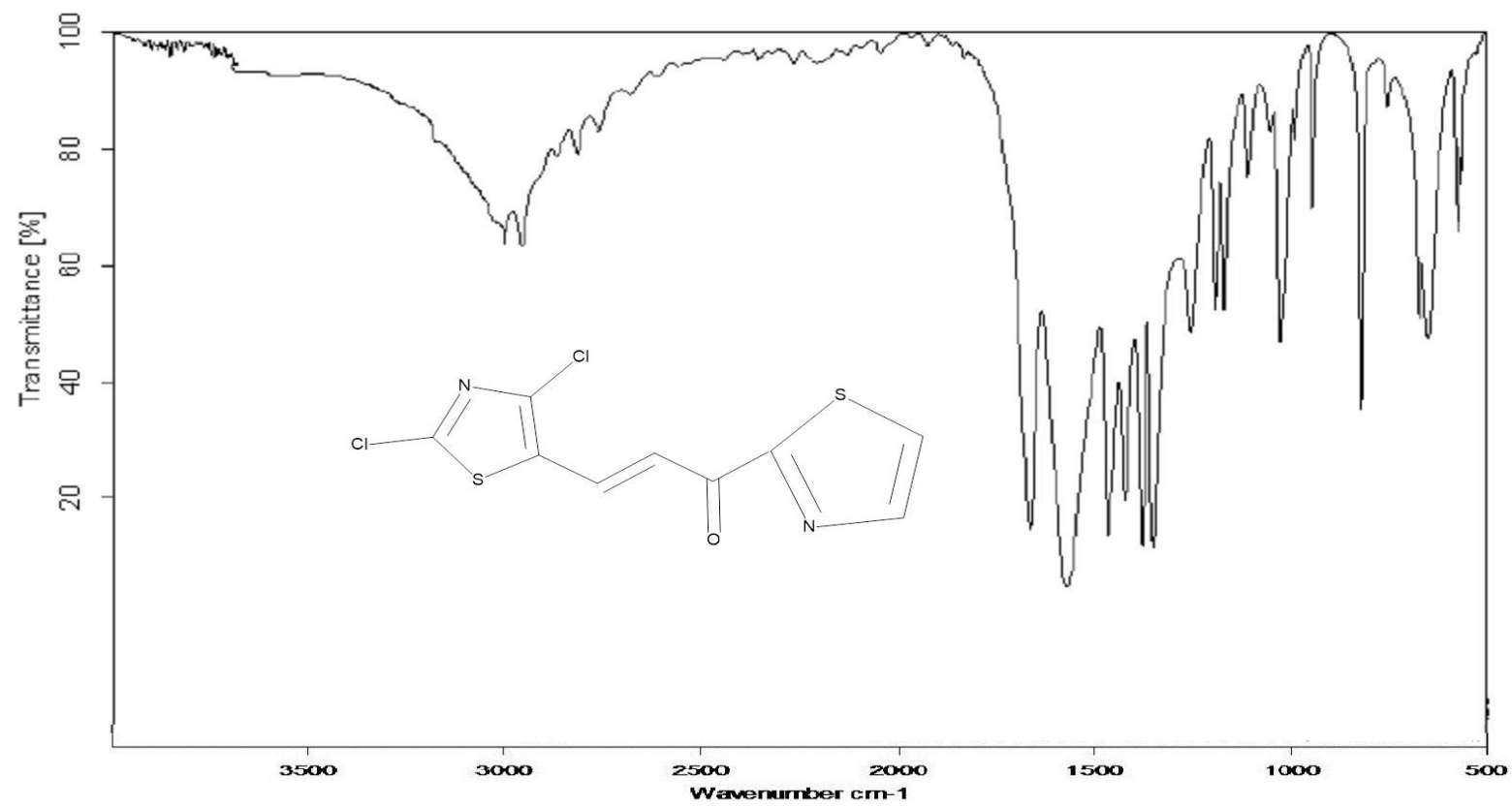


Figure S60. FT-IR Spectrum of compound 20

121H CDCl<sub>3</sub>

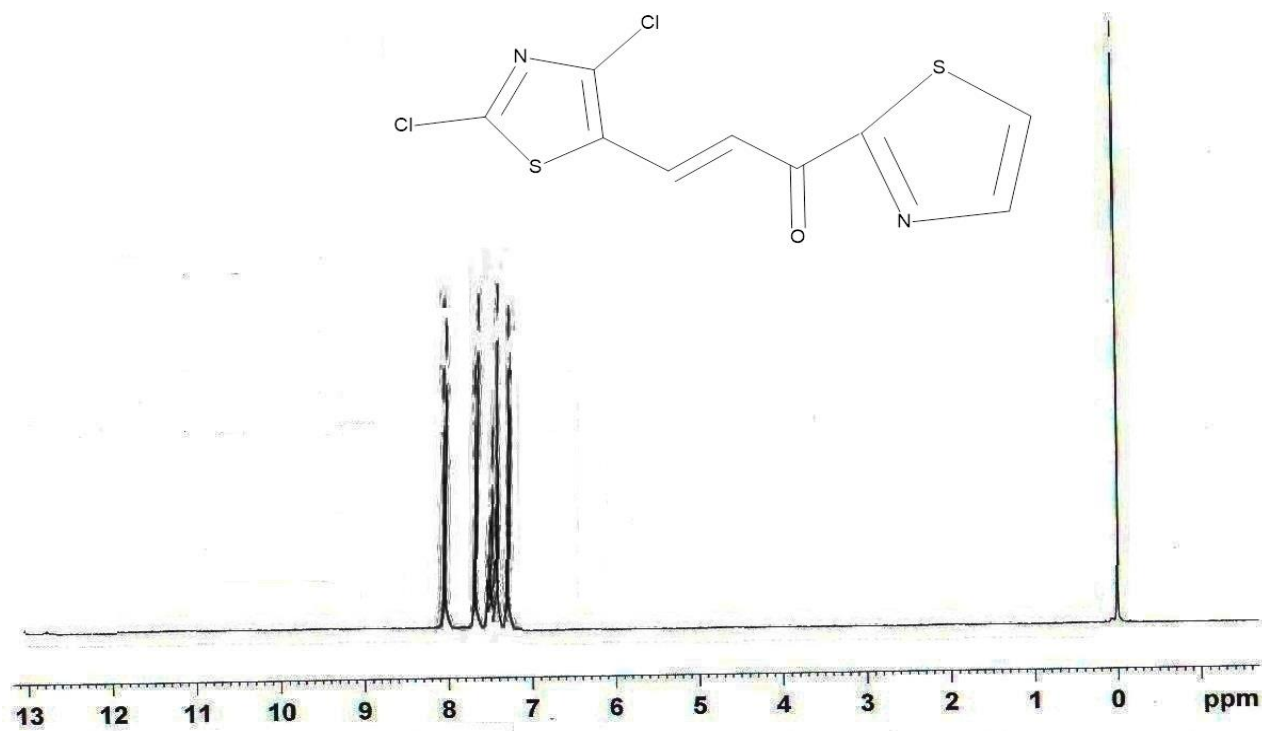


Figure S61. <sup>1</sup>H NMR Spectrum of compound 20

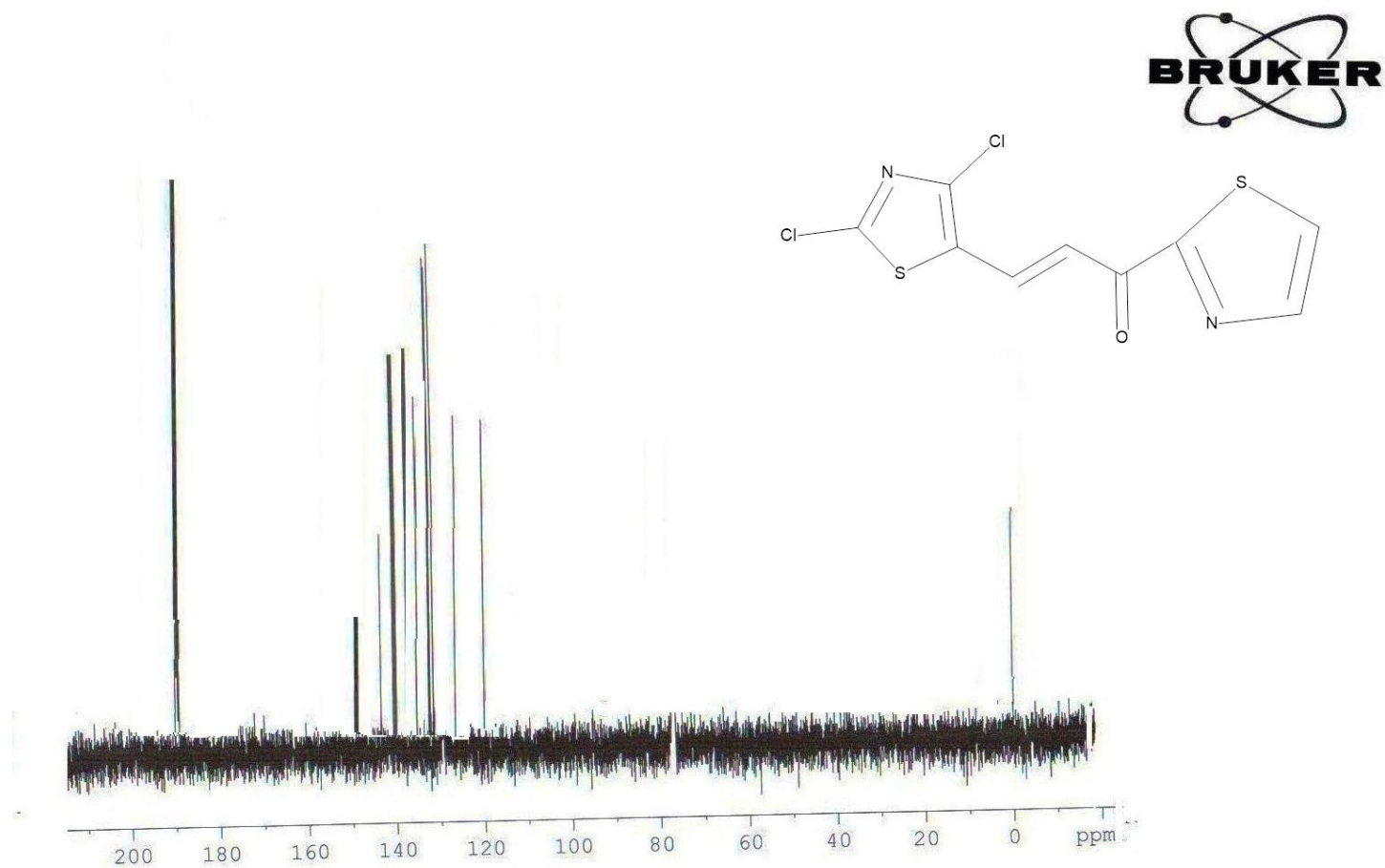


Figure S62.  $^{13}\text{C}$  NMR Spectrum of compound 20

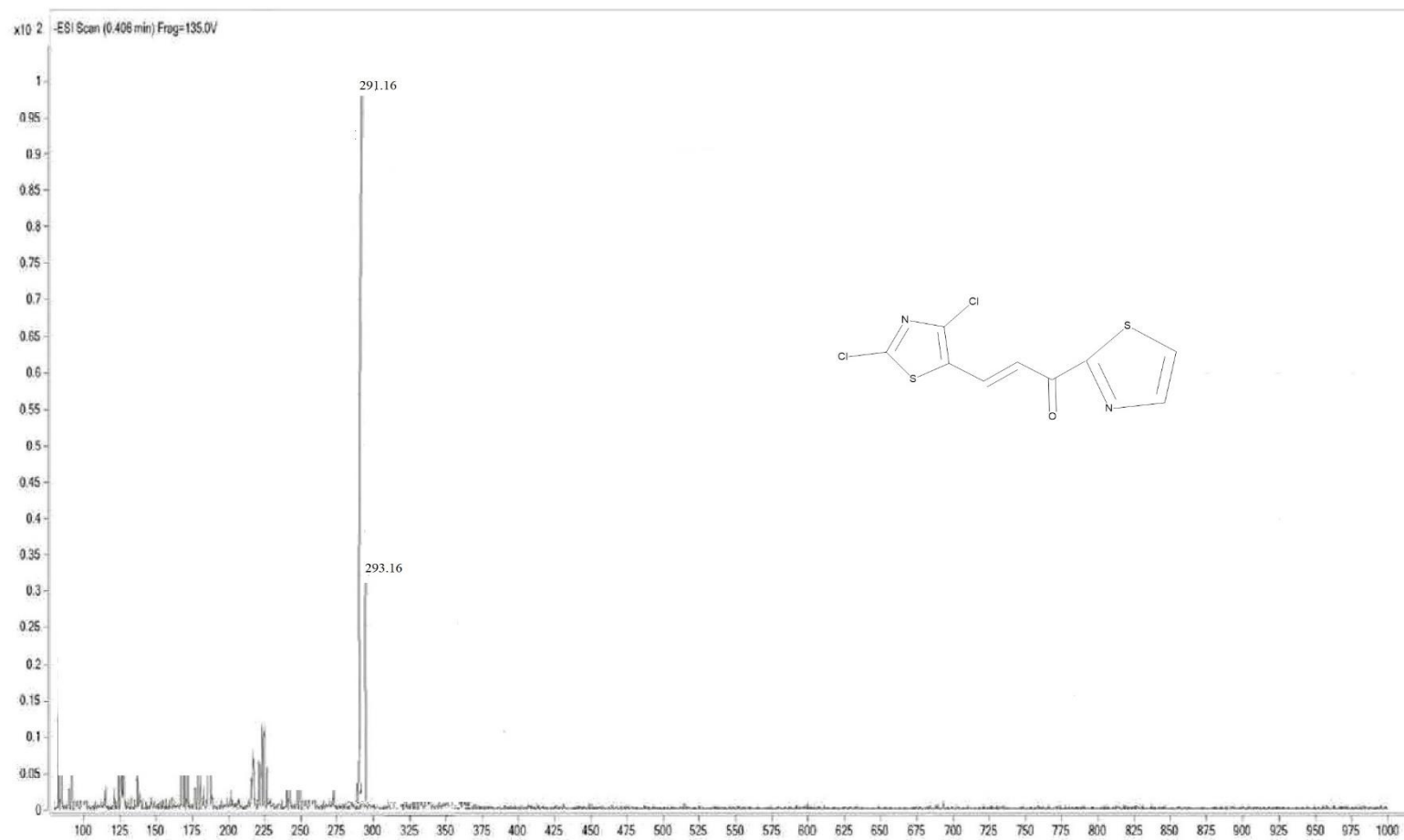


Figure S63. Mass Spectrum of compound 20