

SUPPORTING INFORMATION

Design, Synthesis and Evaluation of Novel Trichloromethyl Dichlorophenyl Triazole Derivatives as Potential Safener

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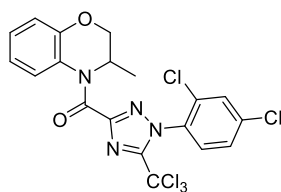
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[†] These authors contributed equally to this work.

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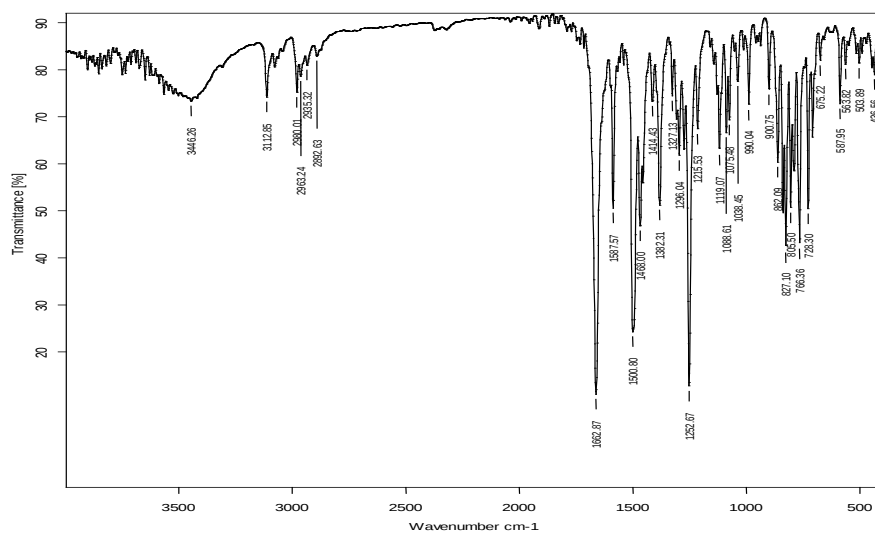
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1. The molecular structure and spectra of representative compound **5a**

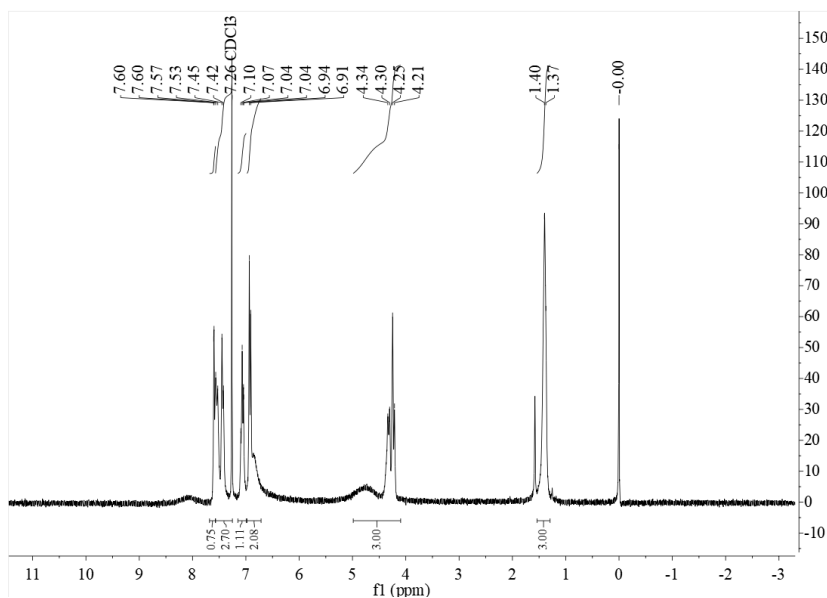


(1-(2,4-dichlorophenyl)-5-(trichloromethyl)-1H-1,2,4-triazol-3-yl)(3-methyl-2,3-dihydro-4H-benzo[*b*][1,4]oxazin-4-yl)methanone

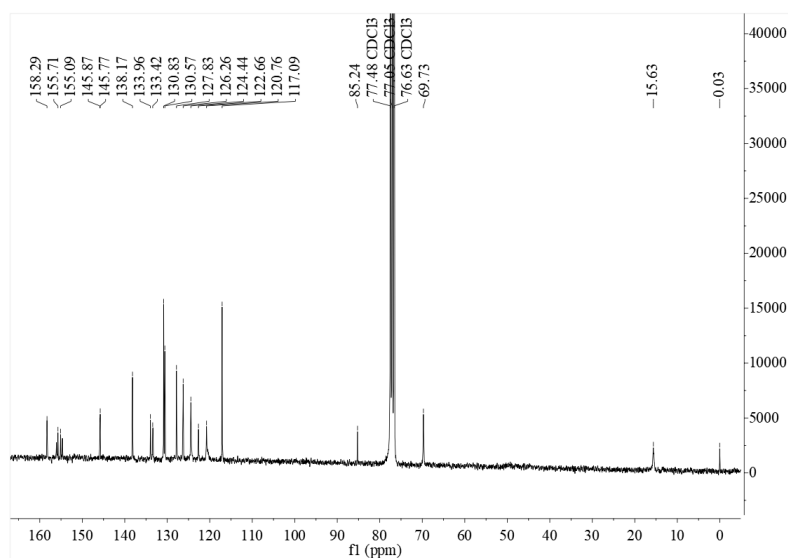
$C_{19}H_{13}Cl_5N_4O_2$



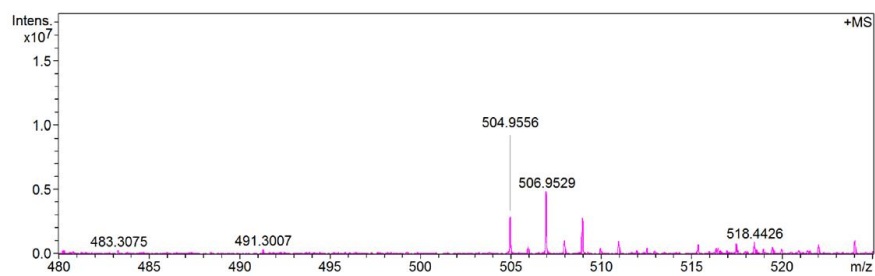
The IR spectrum of compound **5a**



The 1H NMR spectrum of compound **5a**

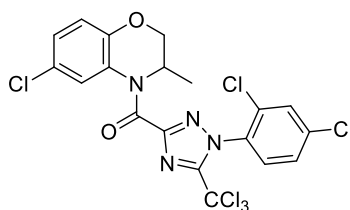


The ^{13}C NMR spectrum of compound **5a**



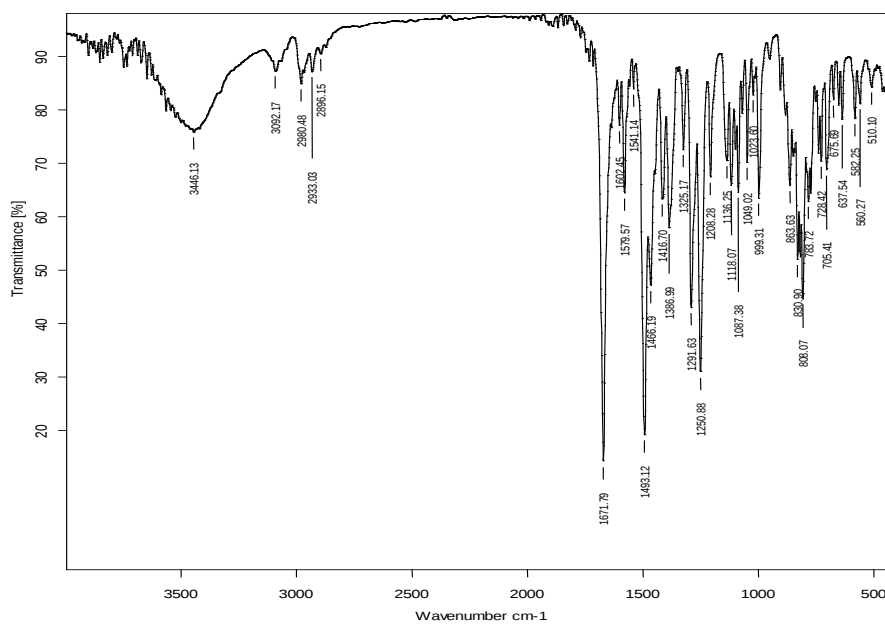
The HRMS spectrum of compound **5a**

2. The molecular structure and spectra of representative compound **5b**

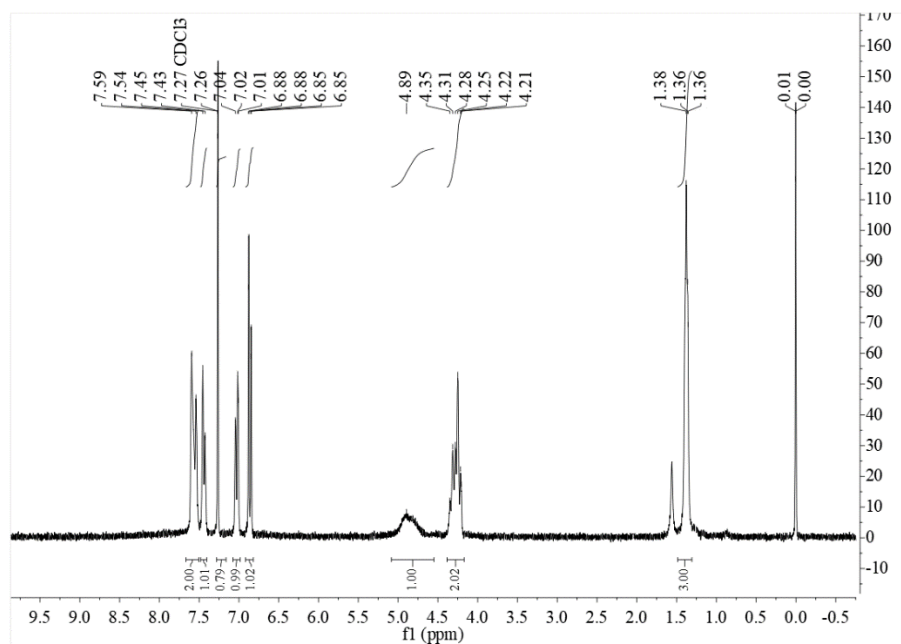


(6-chloro-3-methyl-2,3-dihydro-4*H*-benzo[*b*][1,4]oxazin-4-yl)(1-(2,4-dichlorophenyl)-5-(trichloromethyl)-1*H*-1,2,4-triazol-3-yl)methanone

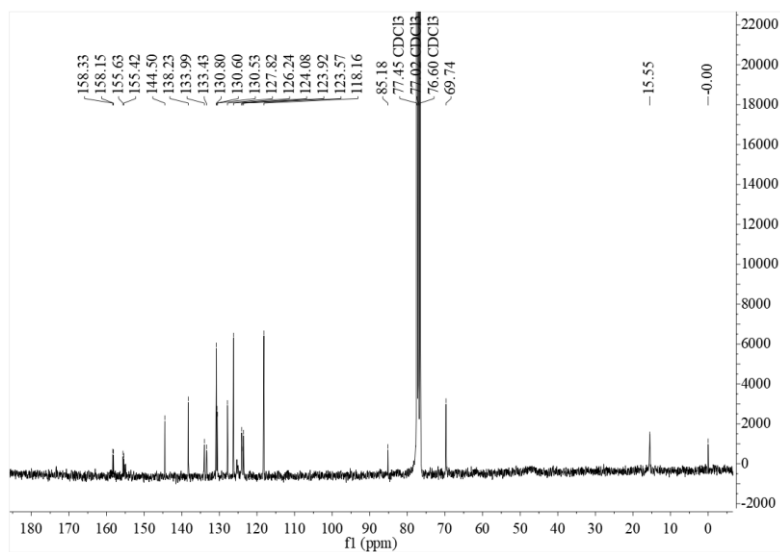
$C_{19}H_{12}Cl_6N_4O_2$



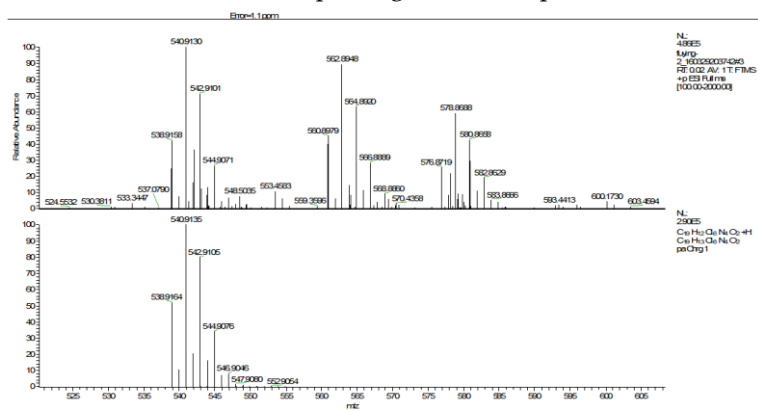
The IR spectrogram of compound **5b**



The 1H NMR spectrogram of compound **5b**

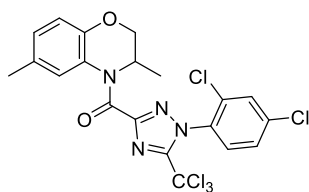


The ¹³C NMR spectrum of compound **5b**

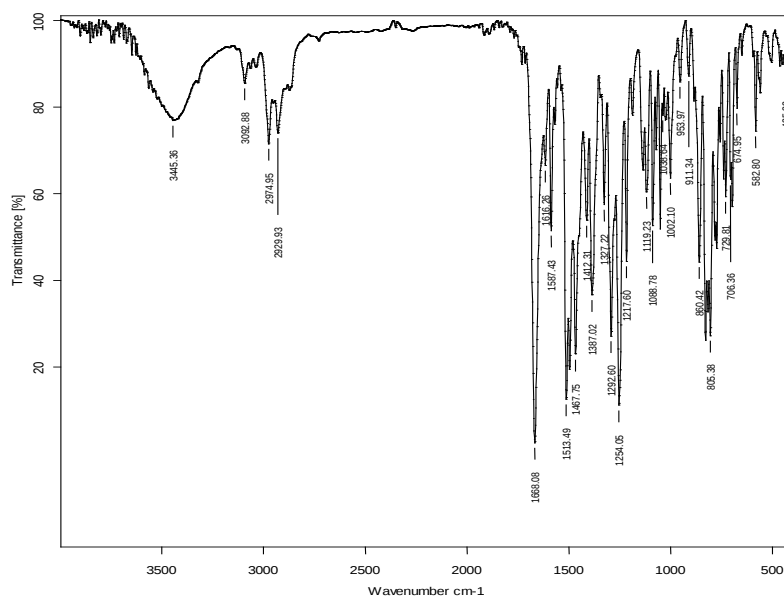


The HRMS spectrum of compound **5b**

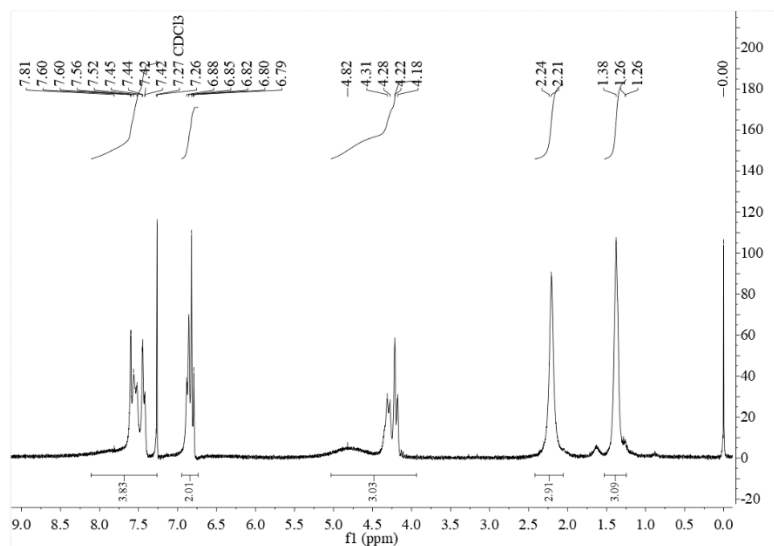
3. The molecular structure and spectra of representative compound **5c**



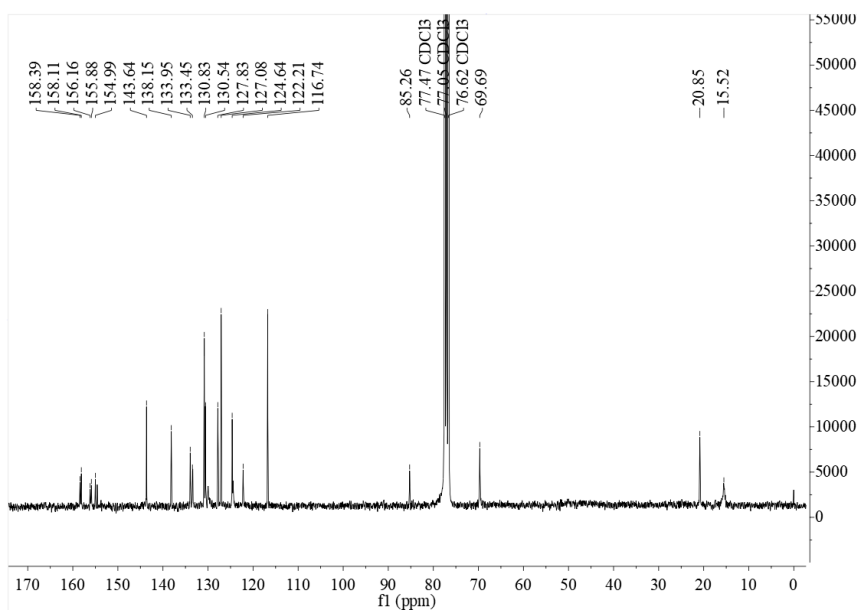
(1-(2,4-dichlorophenyl)-5-(trichloromethyl)-1H-1,2,4-triazol-3-yl)(3,6-dimethyl-2,3-dihydro-4H-benzo[b][1,4]oxazin-4-yl)methanone



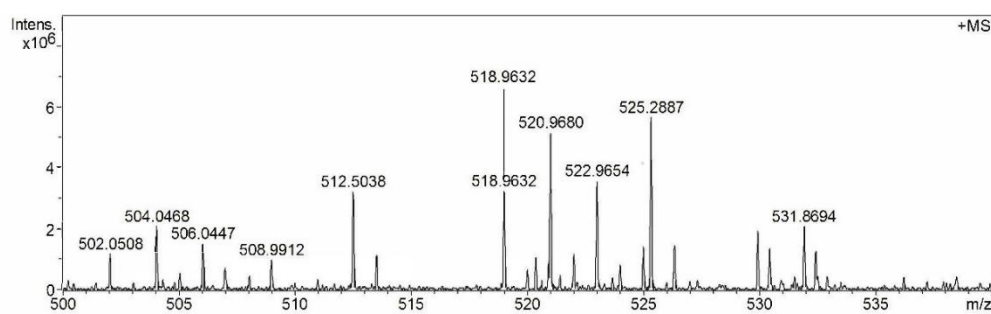
The IR spectrogram of compound **5c**



The 1H NMR spectrogram of compound **5c**

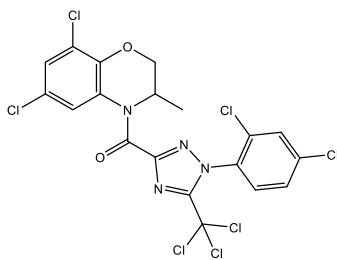


The ¹³C NMR spectrogram of compound **5c**

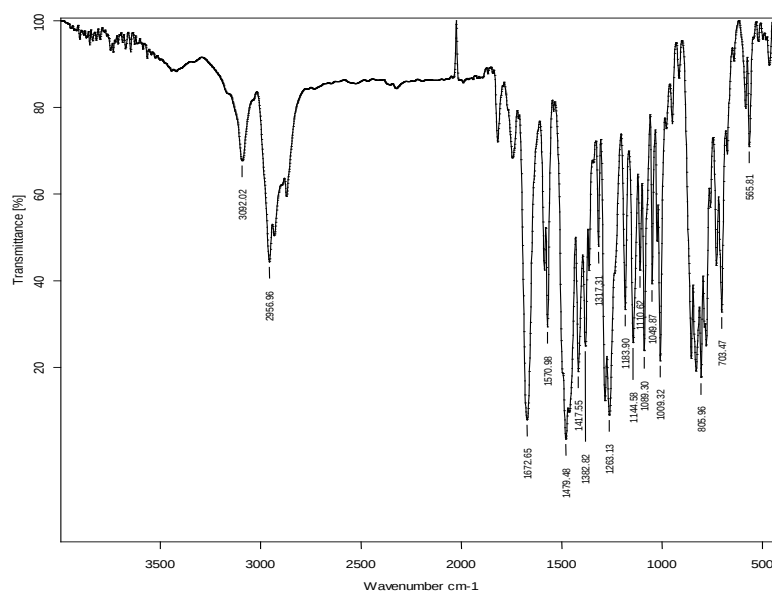


The HRMS spectrogram of compound **5c**

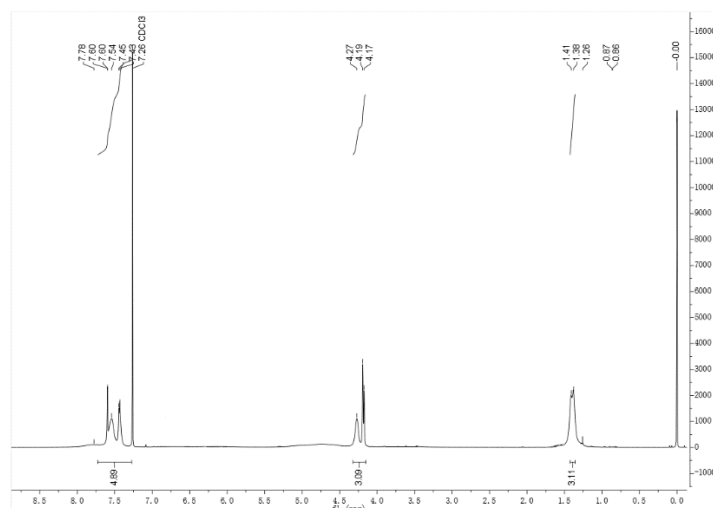
4. The molecular structure and spectra of representative compound **5d**



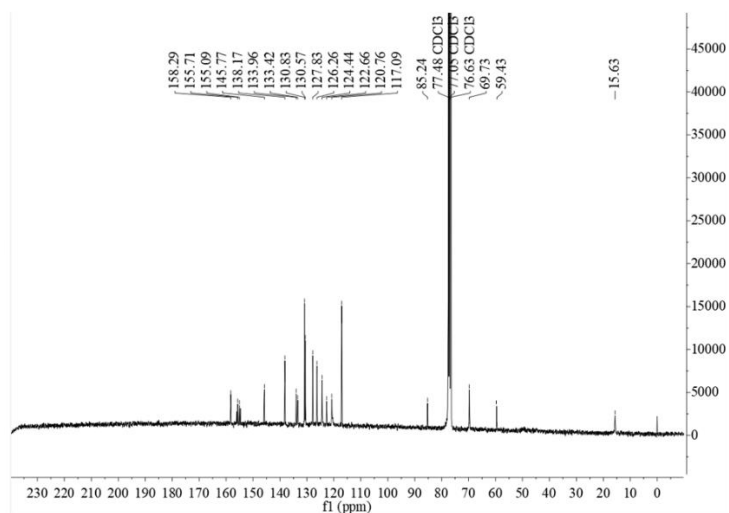
(6,8-dichloro-3-methyl-2,3-dihydro-4*H*-benzo[*b*][1,4]oxazin-4-yl)(1-(2,4-dichlorophenyl)-5-(trichloromethyl)-1*H*-1,2,4-triazol-3-yl)methanone
 $C_{19}H_{11}Cl_7N_4O_2$



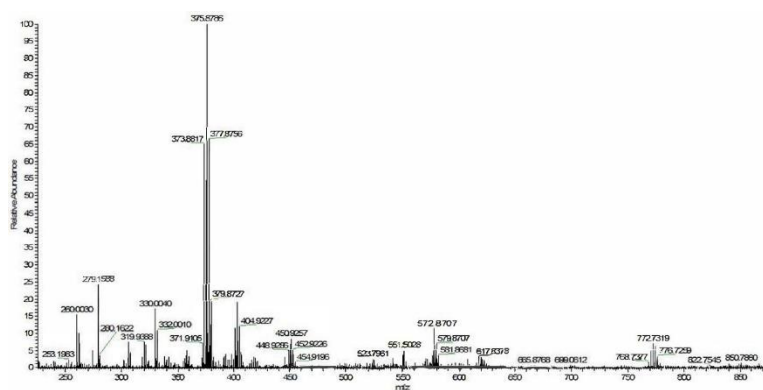
The IR spectrogram of compound **5d**



The 1H NMR spectrogram of compound **5d**

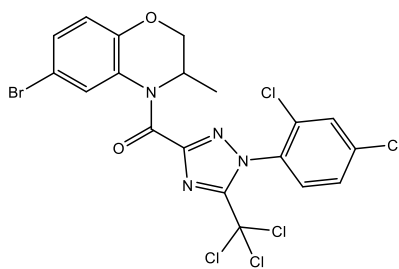


The ^{13}C NMR spectrogram of compound **5d**

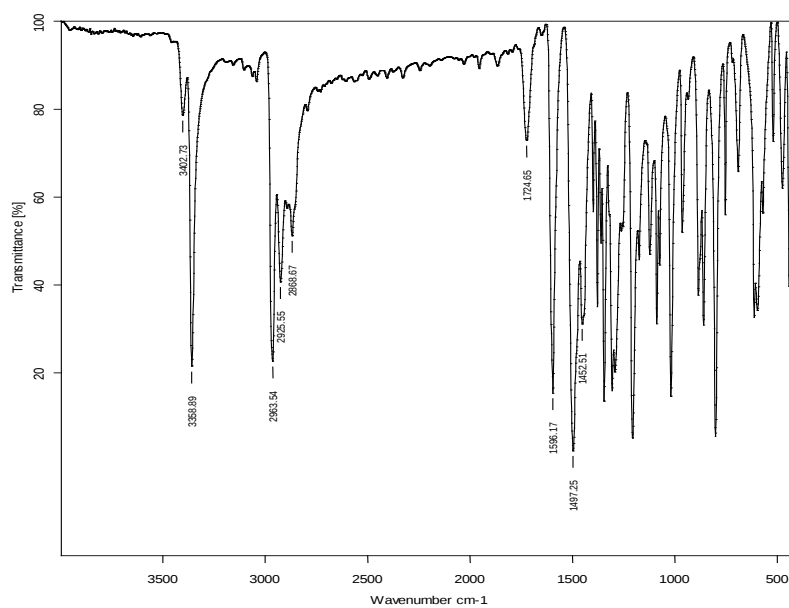


The HRMS spectrogram of compound **5d**

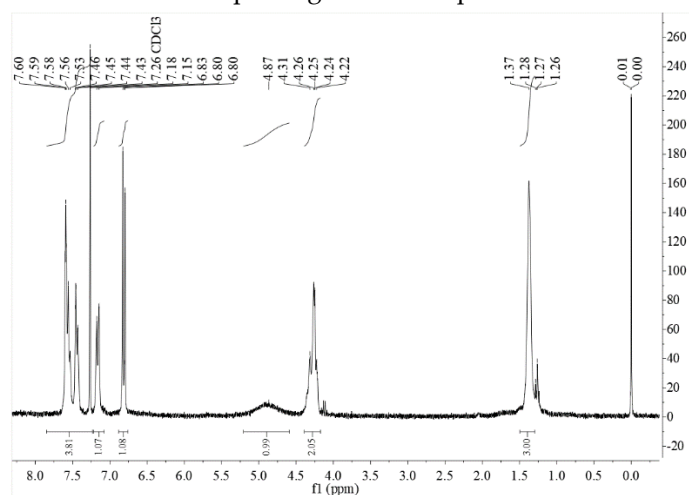
5. The molecular structure and spectra of representative compound **5e**



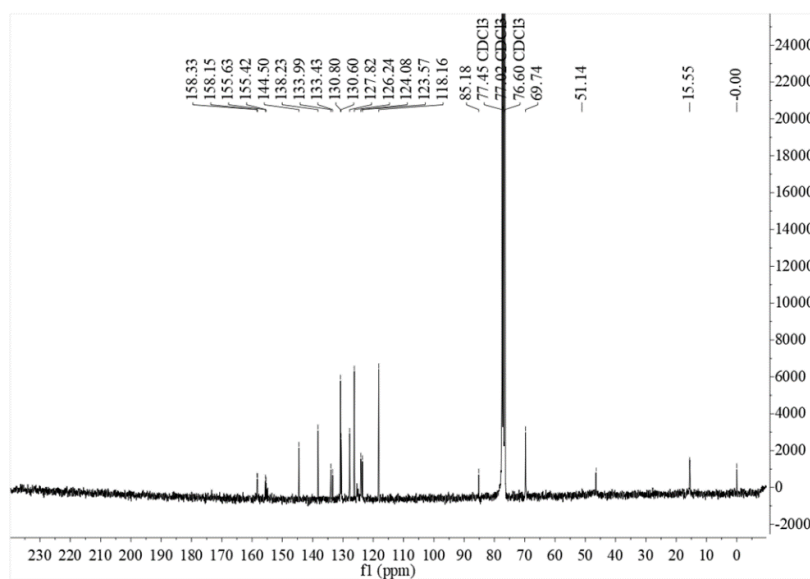
(6-bromo-3-methyl-2,3-dihydro-4H-benzo[*b*][1,4]oxazin-4-yl)(1-(2,4-dichlorophenyl)-5-(trichloromethyl)-1H-1,2,4-triazol-3-yl)methanone
 $C_{19}H_{12}BrCl_5N_4O_2$



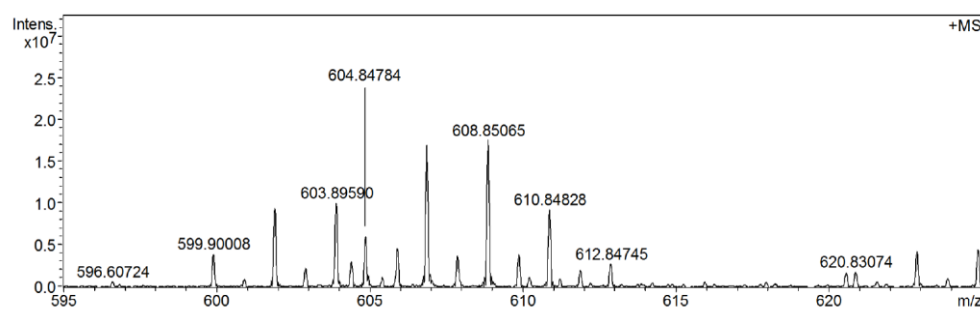
The IR spectrogram of compound **5e**



The 1H NMR spectrogram of compound **5e**

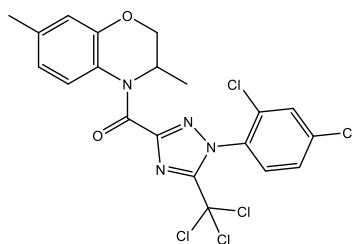


The ¹³C NMR spectrogram of compound **5e**

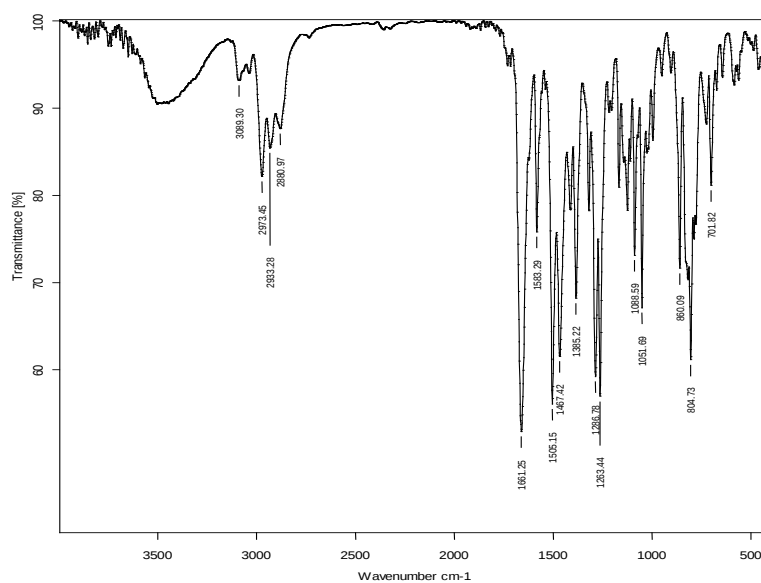


The HRMS spectrogram of compound **5e**

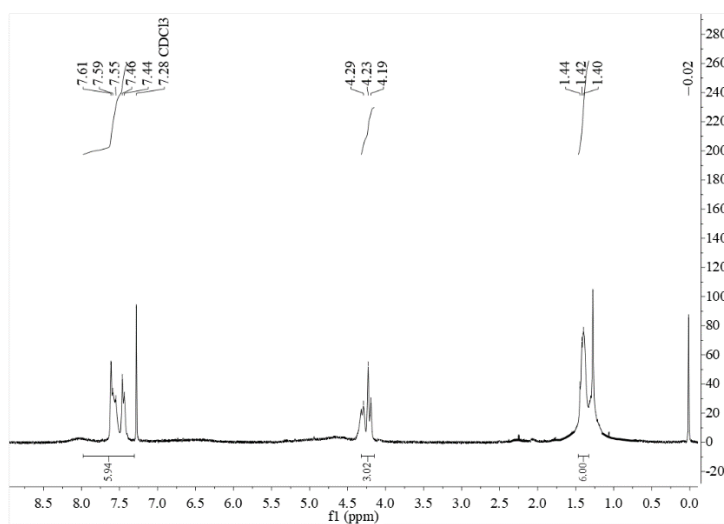
6. The molecular structure and spectra of representative compound **5f**



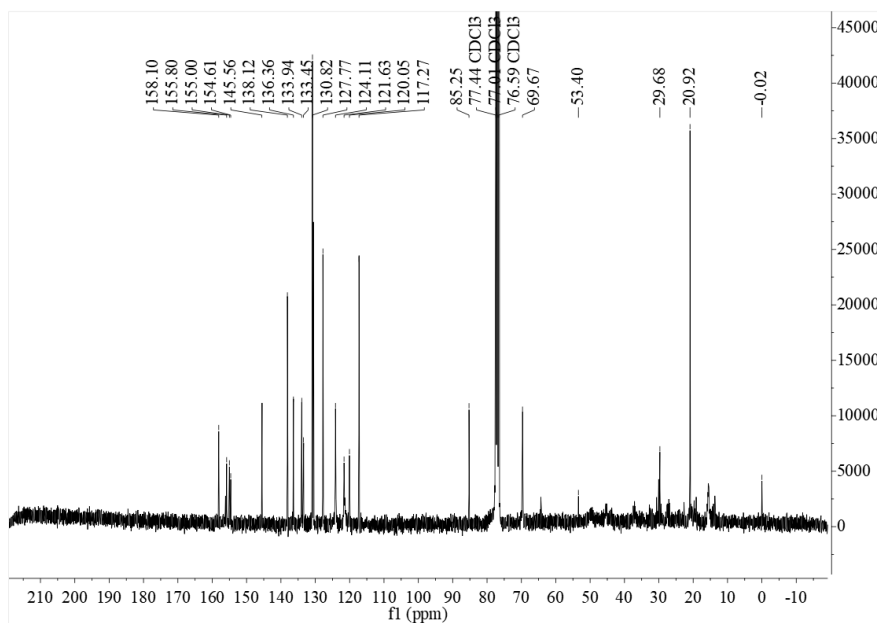
(1-(2,4-dichlorophenyl)-5-(trichloromethyl)-1H-1,2,4-triazol-3-yl)(3,7-dimethyl-2,3-dihydro-4H-benzo[b][1,4]oxazin-4-yl)methanone
 $C_{20}H_{15}Cl_5N_4O_2$



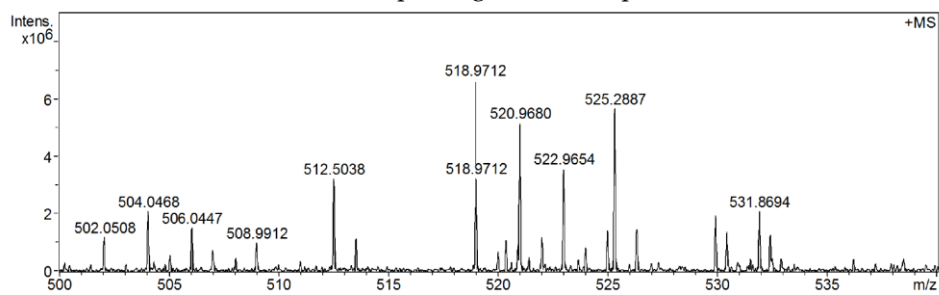
The IR spectrogram of compound **5f**



The 1H NMR spectrogram of compound **5f**

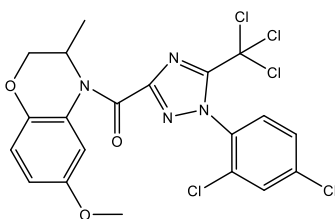


The ¹³C NMR spectrum of compound **5f**

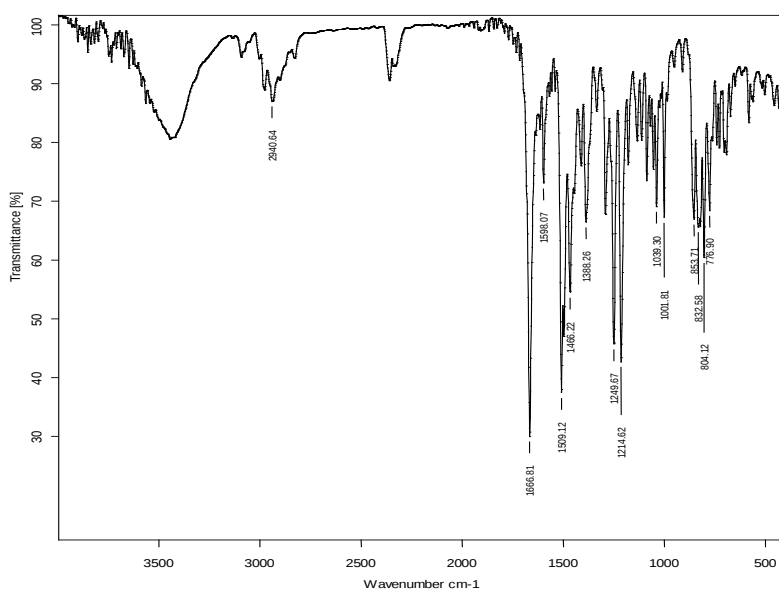


The HRMS spectrum of compound **5f**

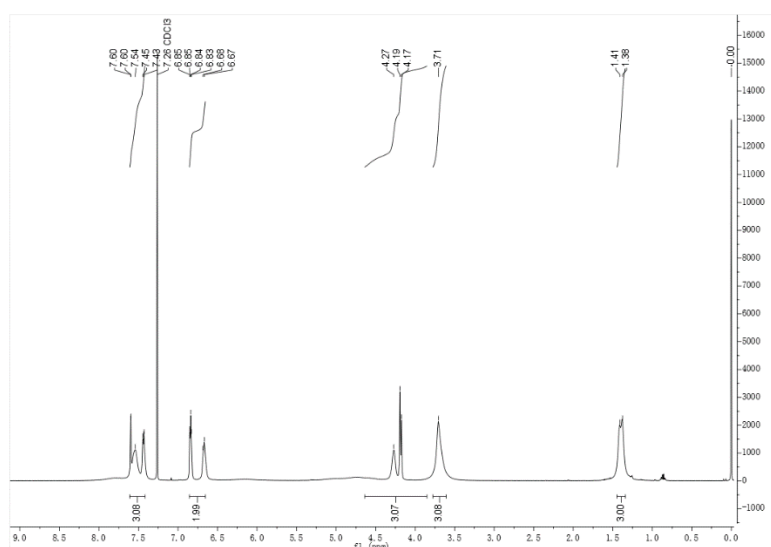
7. The molecular structure and spectra of representative compound **5g**



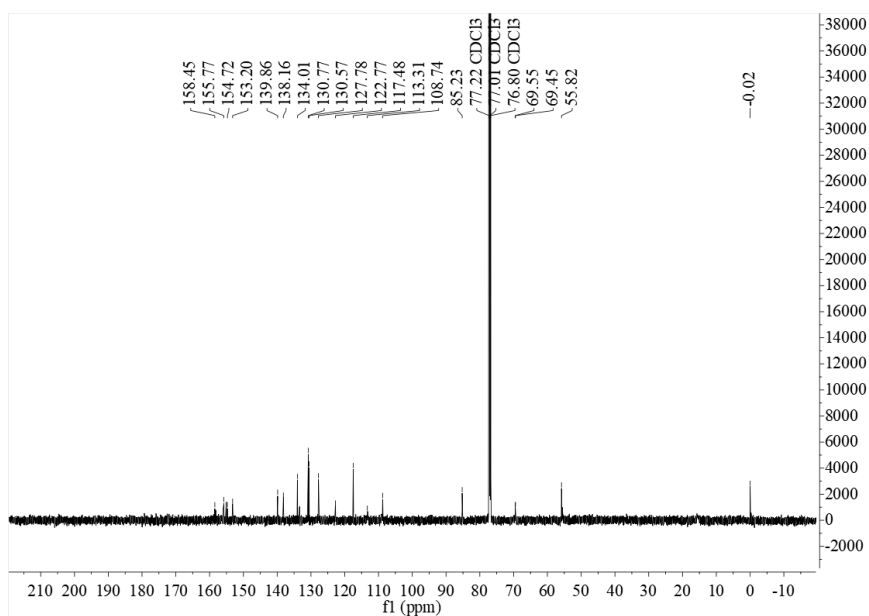
(1-(2,4-dichlorophenyl)-5-(trichloromethyl)-1H-1,2,4-triazol-3-yl)(6-methoxy-3-methyl-2,3-dihydro-4H-benzo[b][1,4]oxazin-4-yl)methanone



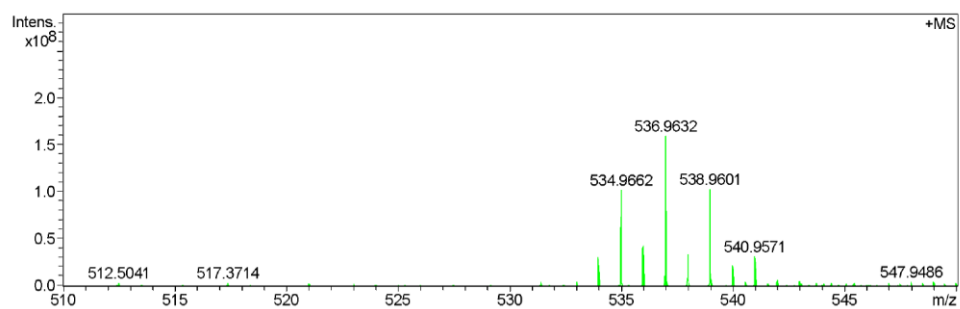
The IR spectrogram of compound **5g**



The 1H NMR spectrogram of compound **5g**

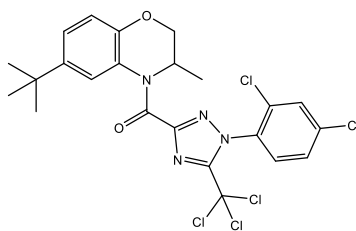


The ¹³C NMR spectrogram of compound **5g**



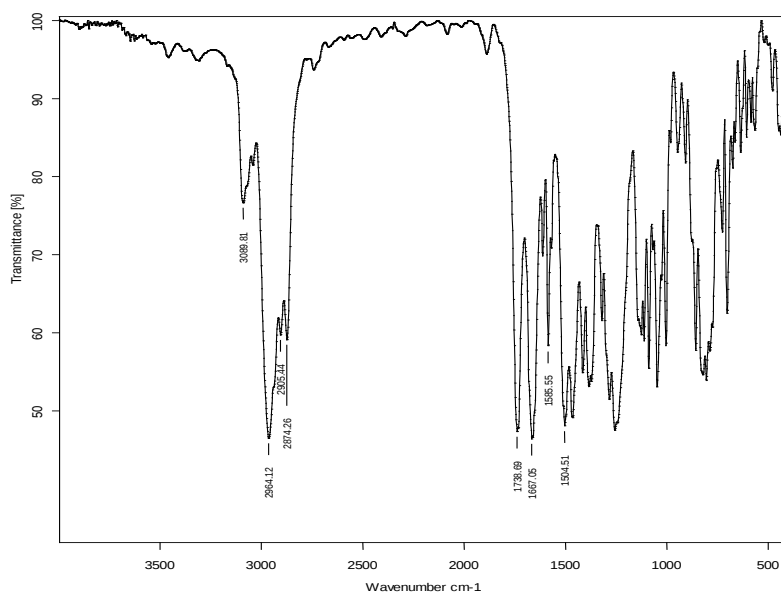
The HRMS spectrogram of compound **5g**

8. The molecular structure and spectra of representative compound **5h**

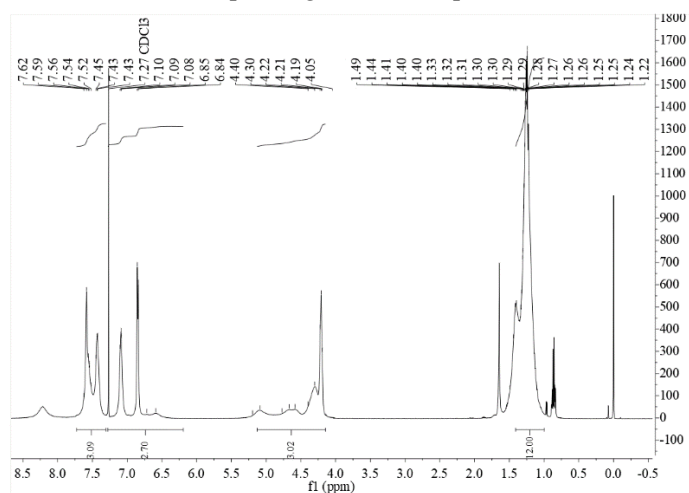


(6-(*tert*-butyl)-3-methyl-2,3-dihydro-4*H*-benzo[*b*][1,4]oxazin-4-yl)(1-(2,4-dichlorophenyl)-5-(trichloromethyl)-1*H*-1,2,4-triazol-3-yl)methanone

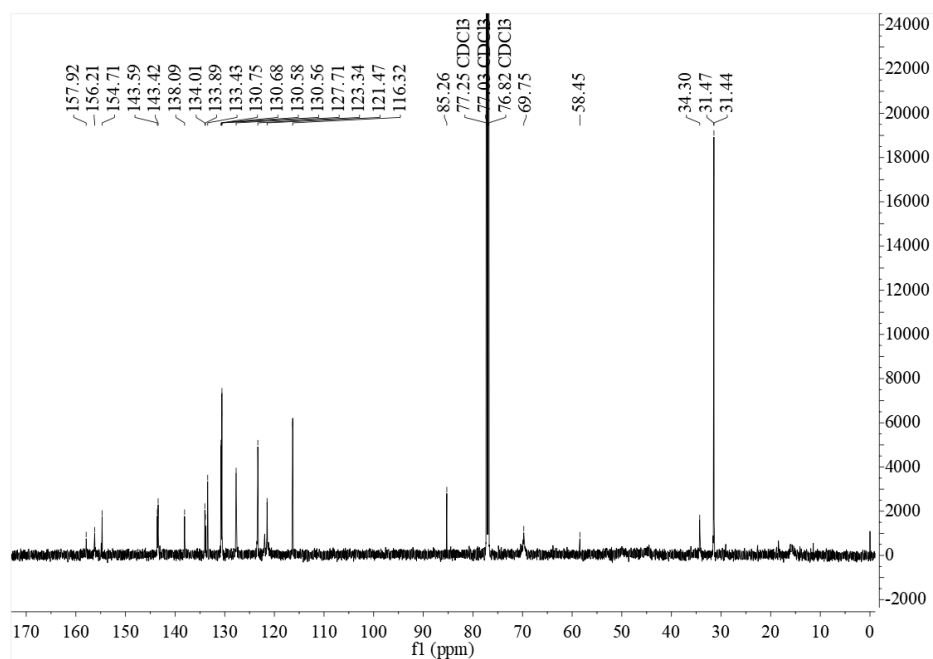
$C_{23}H_{21}Cl_5N_4O_2$



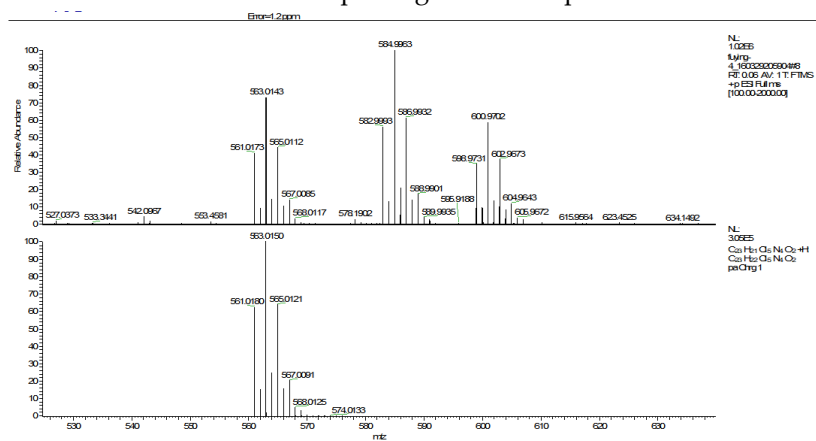
The IR spectrogram of compound **5h**



The 1H NMR spectrogram of compound **5h**

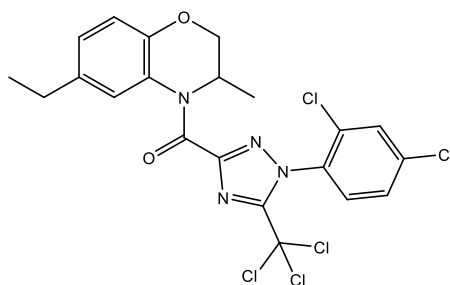


The ¹³C NMR spectrogram of compound **5h**

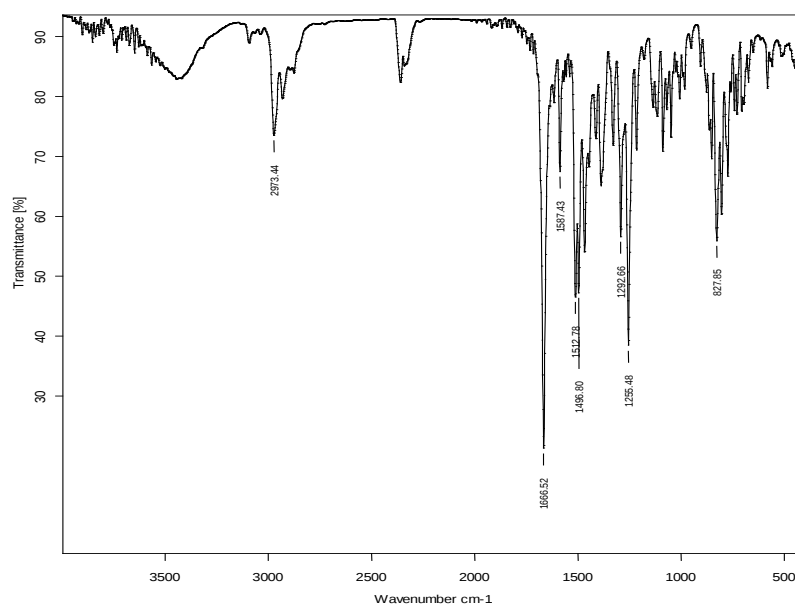


The HRMS spectrogram of compound **5h**

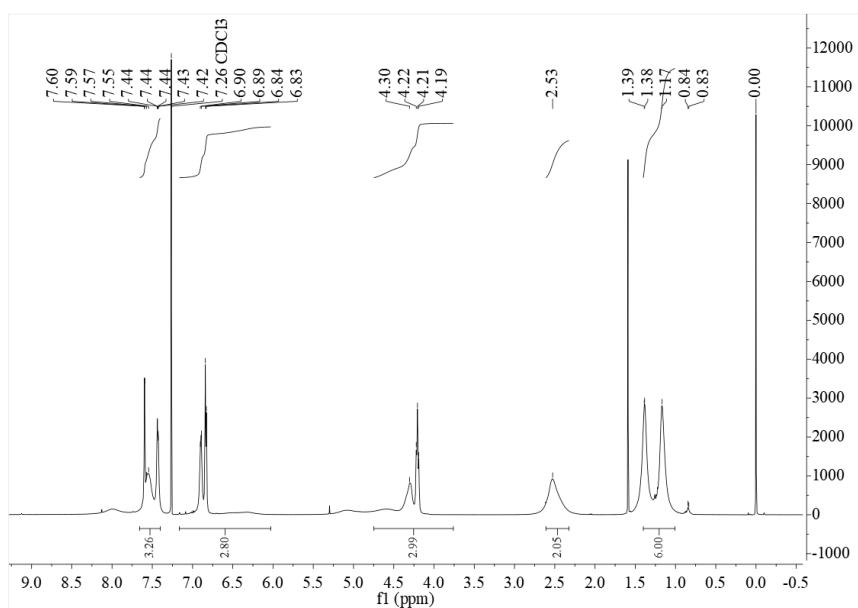
9. The molecular structure and spectra of representative compound **5i**



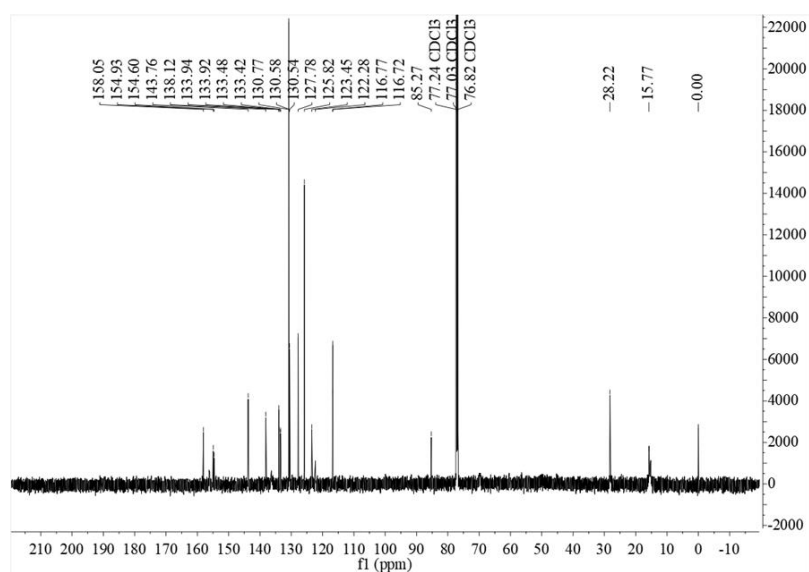
(1-(2,4-dichlorophenyl)-5-(trichloromethyl)-1H-1,2,4-triazol-3-yl)(6-ethyl-3-methyl-2,3-dihydro-4H-benzo[b][1,4]oxazin-4-yl)methanone



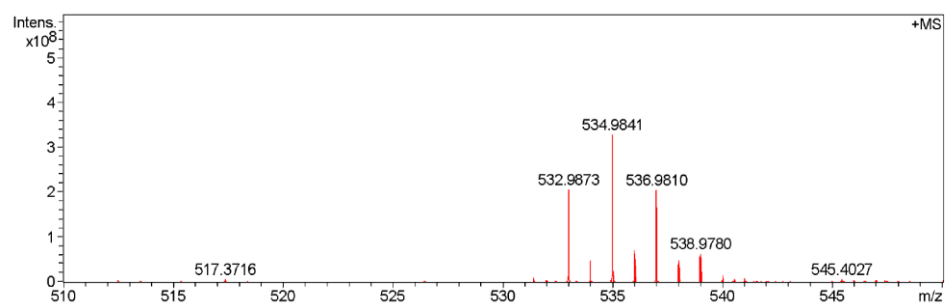
The IR spectrogram of compound **5i**



The 1H NMR spectrogram of compound **5i**

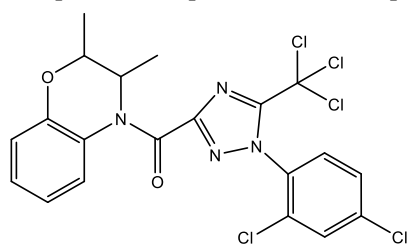


The ¹³C NMR spectrum of compound **5i**

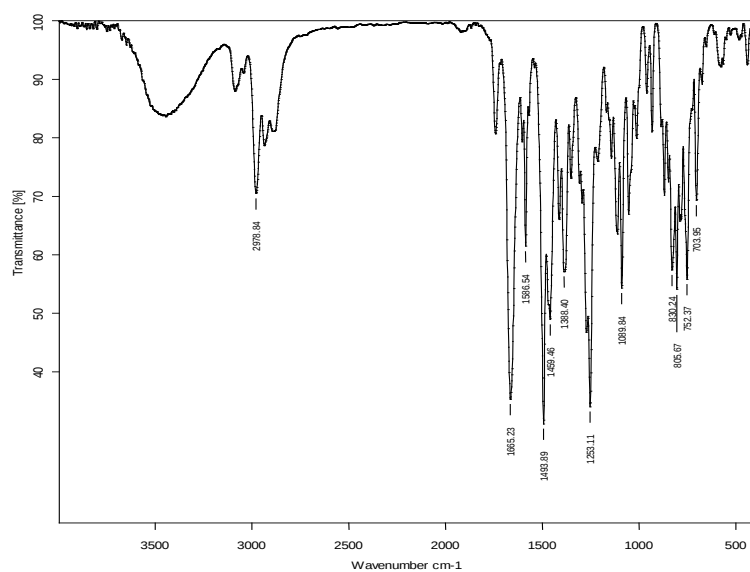


The HRMS spectrum of compound **5i**

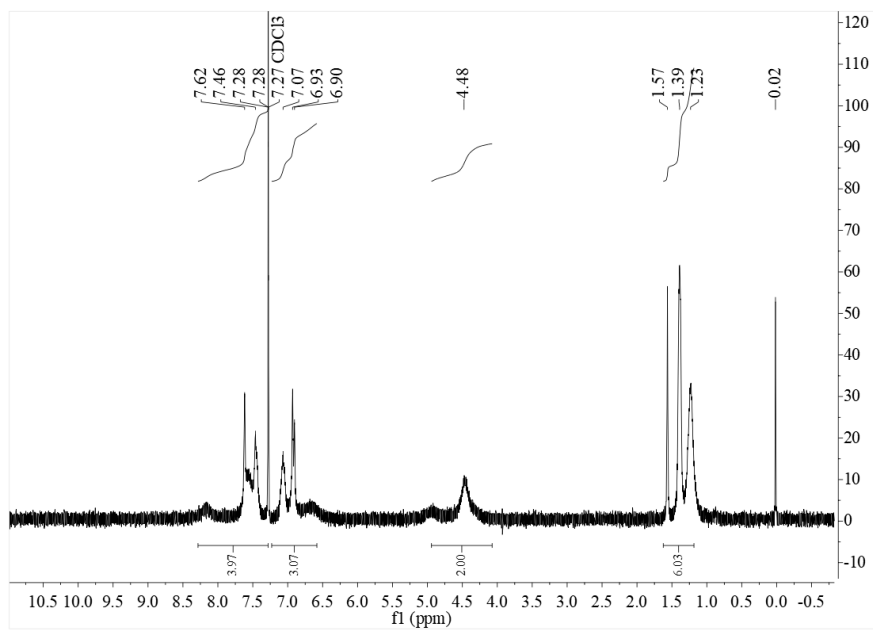
10. The molecular structure and spectra of representative compound **5j**



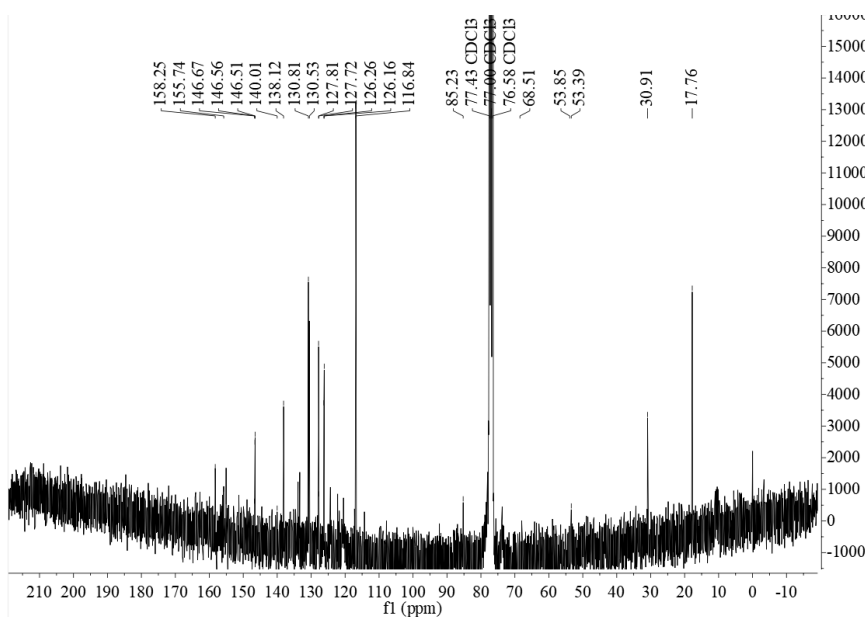
(1-(2,4-dichlorophenyl)-5-(trichloromethyl)-1H-1,2,4-triazol-3-yl)(2,3-dimethyl-2,3-dihydro-4H-benzo[b][1,4]oxazin-4-yl)methanone



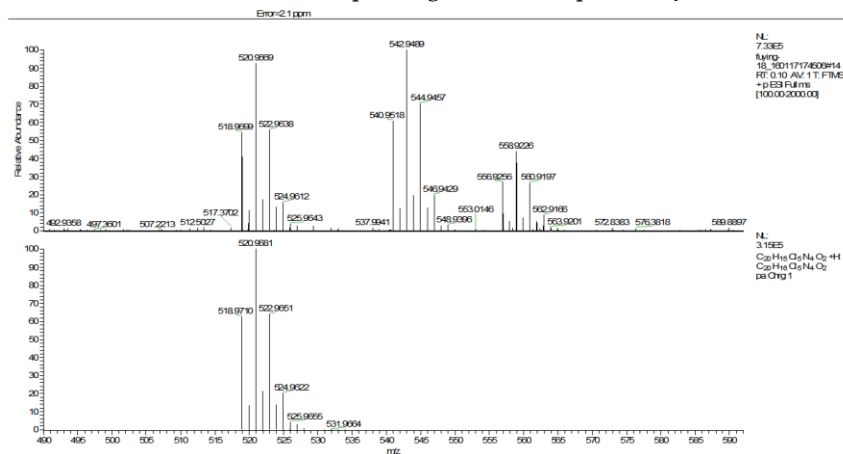
The IR spectrogram of compound **5j**



The 1H NMR spectrogram of compound **5j**

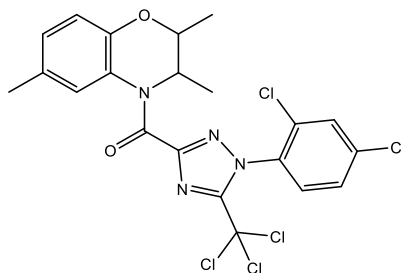


The ¹³C NMR spectrogram of compound **5j**

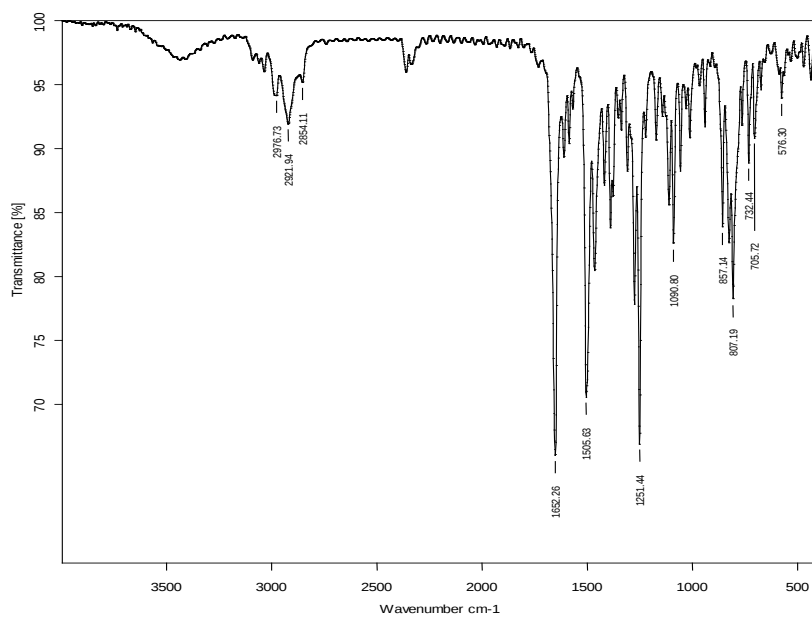


The HRMS spectrogram of compound **5j**

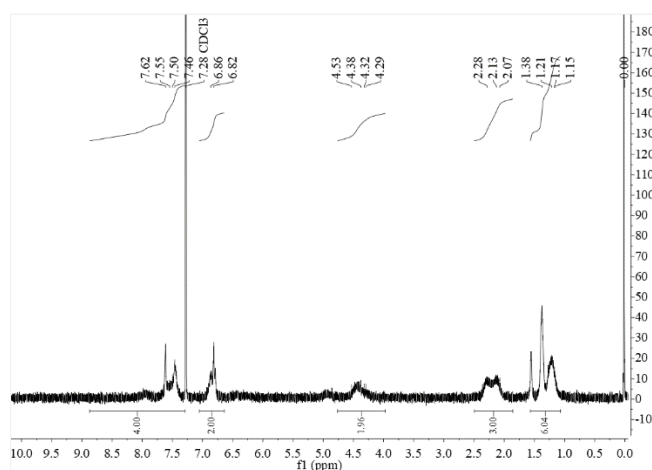
11. The molecular structure and spectra of representative compound **5k**



(1-(2,4-dichlorophenyl)-5-(trichloromethyl)-1H-1,2,4-triazol-3-yl)(2,3,6-trimethyl-2,3-dihydro-4H-benzo[b][1,4]oxazin-4-yl)methanone
 $C_{21}H_{17}Cl_5N_4O_2$

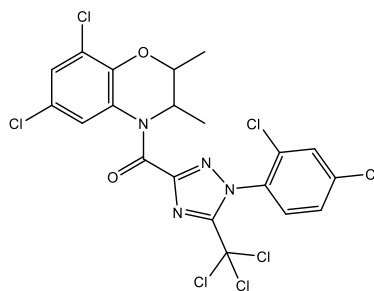


The IR spectrum of compound **5k**

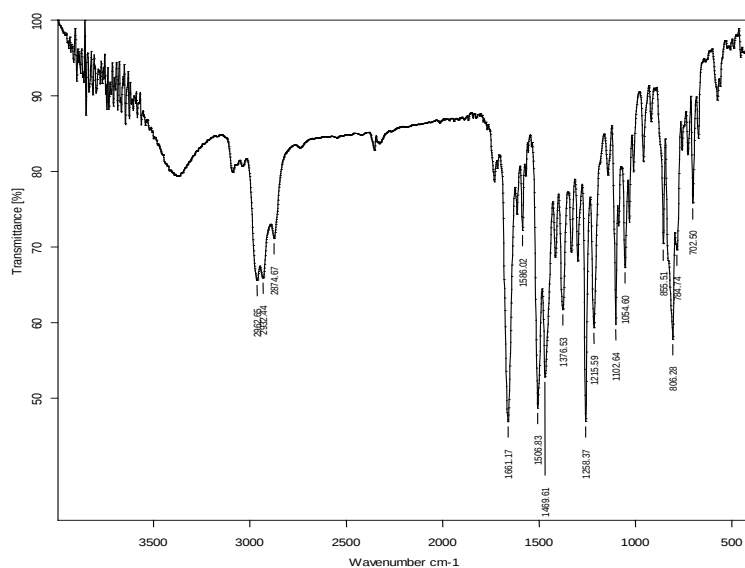


The 1H NMR spectrum of compound **5k**

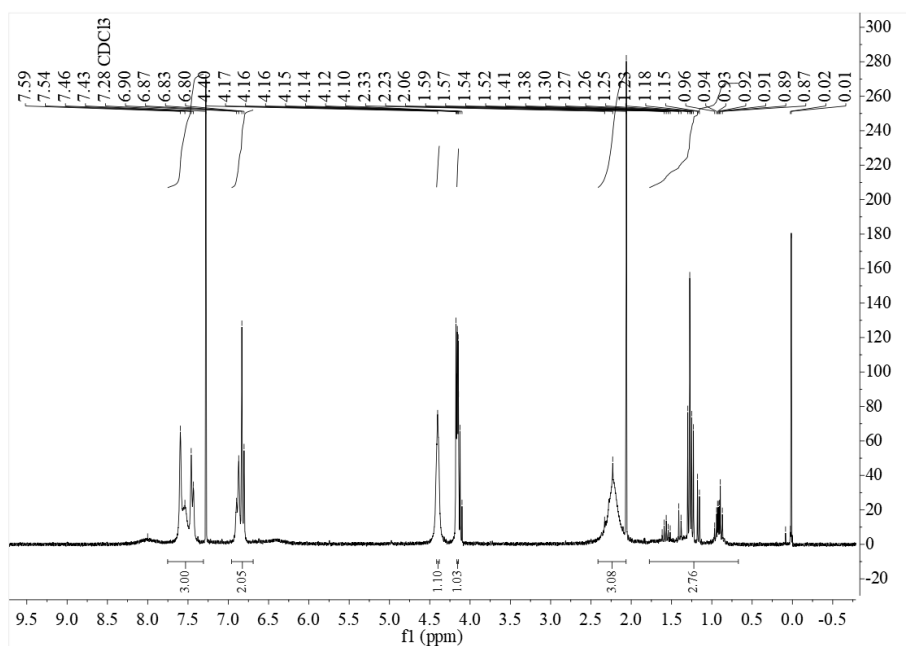
12. The molecular structure and spectra of representative compound **51**



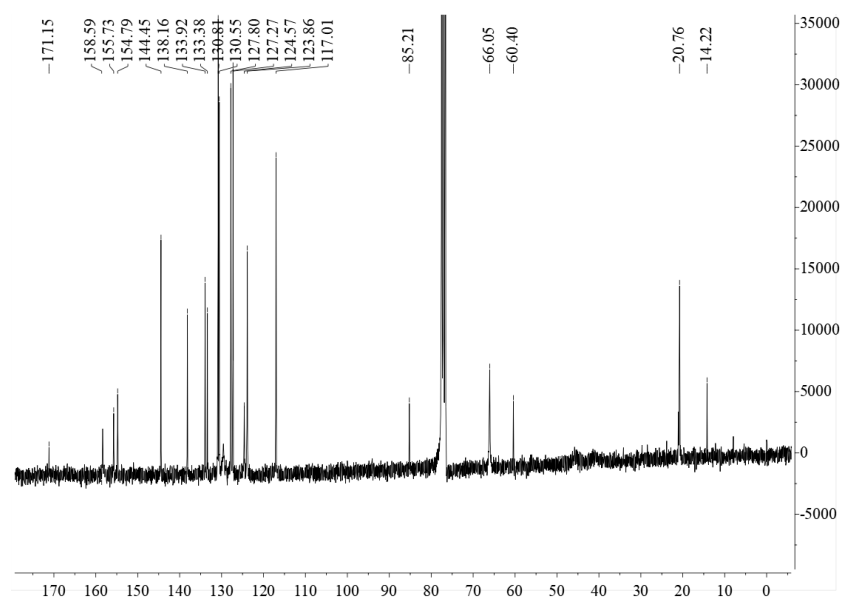
(6,8-dichloro-2,3-dimethyl-2,3-dihydro-4H-benzo[b][1,4]oxazin-4-yl)(1-(2,4-dichlorophenyl)-5-(trichloromethyl)-1H-1,2,4-triazol-3-yl)methanone



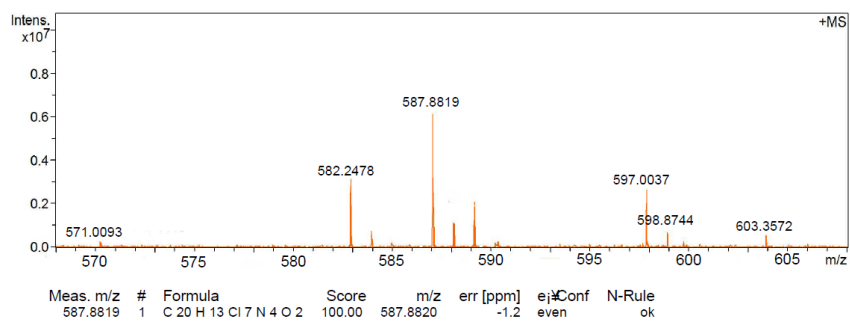
The IR spectrum of compound **51**



The 1H NMR spectrum of compound **51**

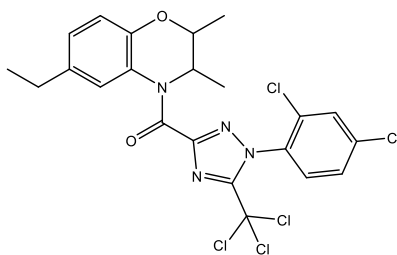


The ^{13}C NMR spectrum of compound **51**

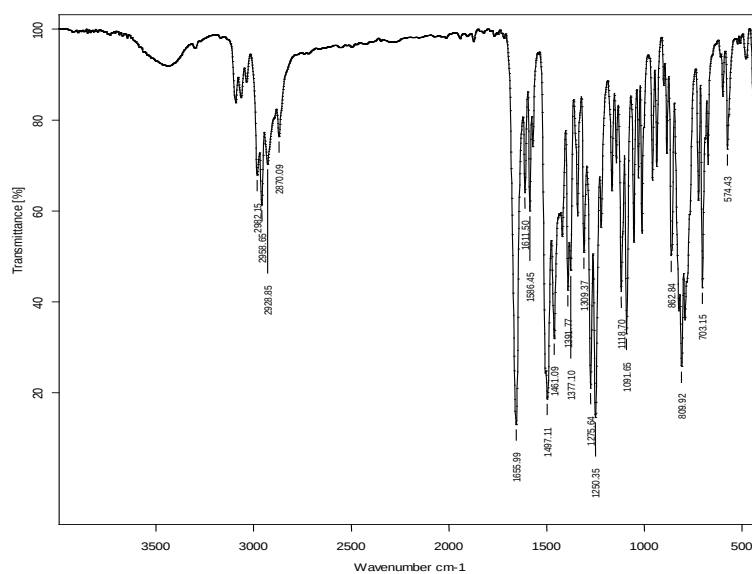


The HRMS spectrum of compound **51**

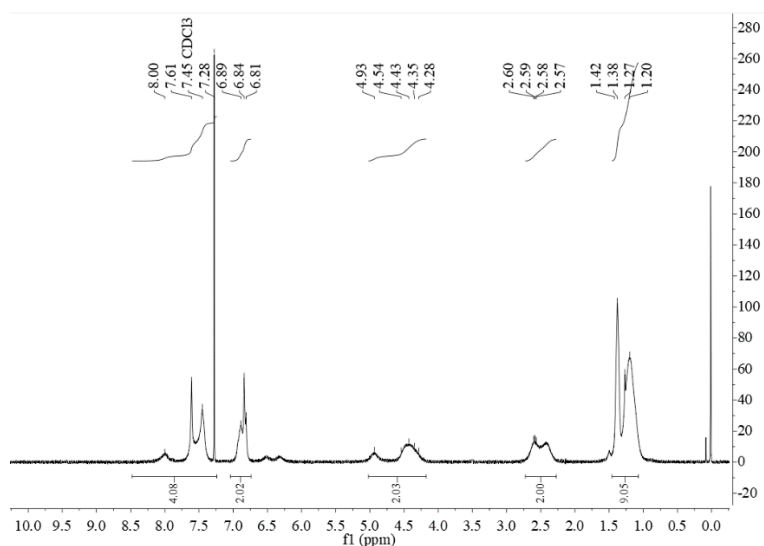
13. The molecular structure and spectra of representative compound **5m**



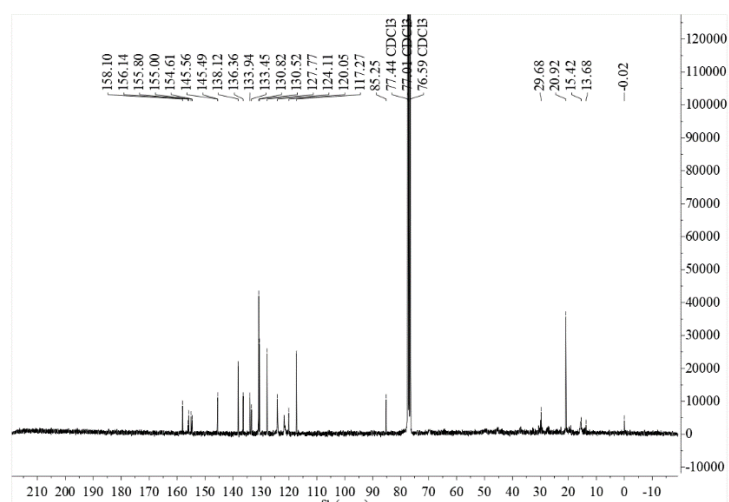
(1-(2,4-dichlorophenyl)-5-(trichloromethyl)-1H-1,2,4-triazol-3-yl)(6-ethyl-2,3-dimethyl-2,3-dihydro-4H-benzo[b][1,4]oxazin-4-yl)methanone
 $C_{22}H_{19}Cl_5N_4O_2$



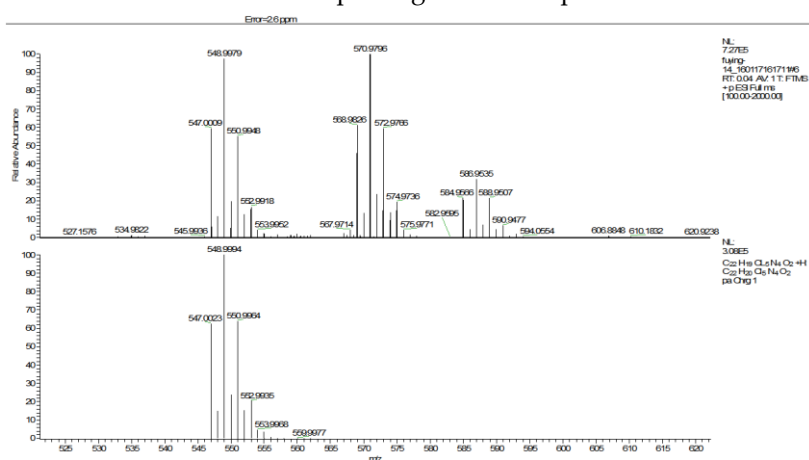
The IR spectrogram of compound **5m**



The 1H NMR spectrogram of compound **5m**

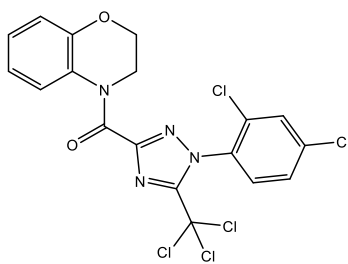


The ¹³C NMR spectrogram of compound **5m**

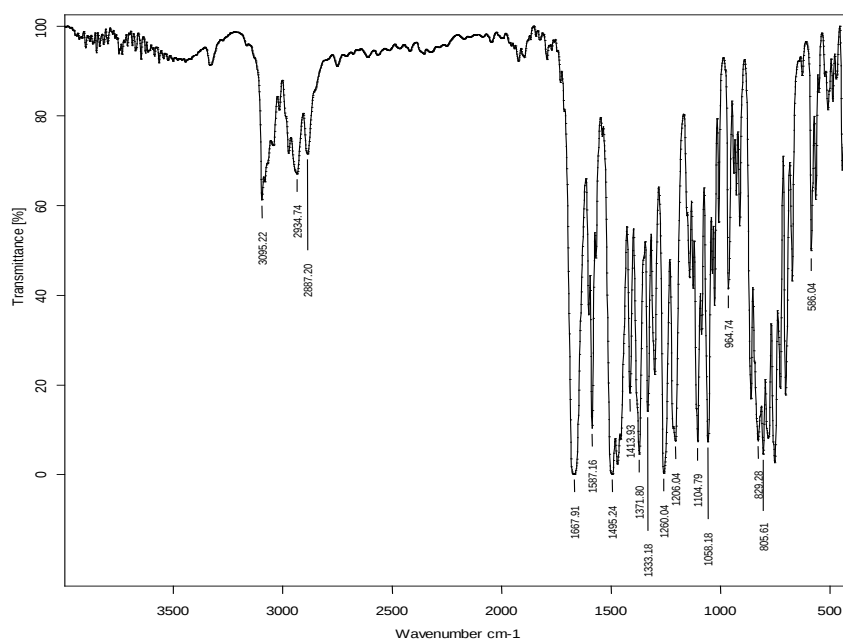


The HRMS spectrogram of compound **5m**

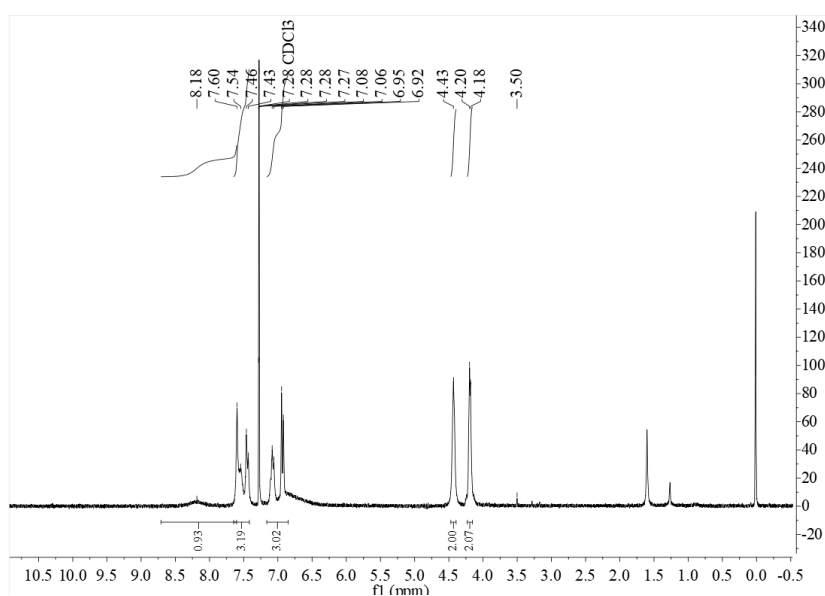
14. The molecular structure and spectra of representative compound **5n**



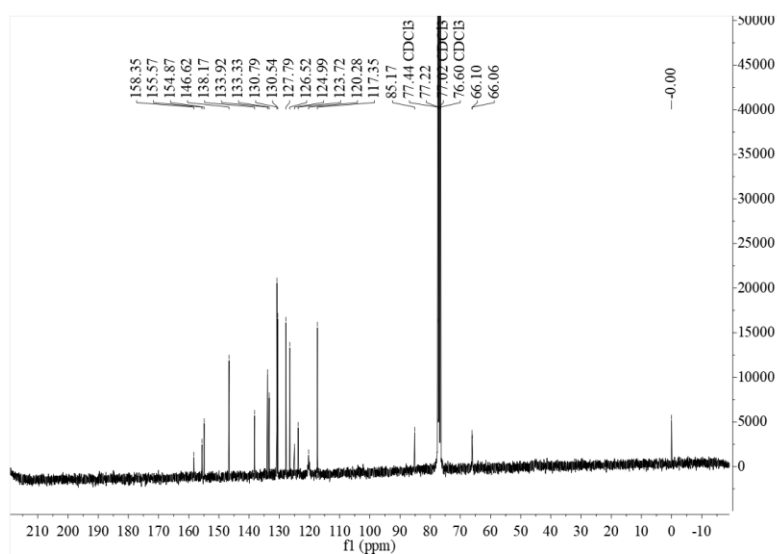
(1-(2,4-dichlorophenyl)-5-(trichloromethyl)-1H-1,2,4-triazol-3-yl)(2,3-dihydro-4H-benzo[b][1,4]oxazin-4-yl)methanone
 $C_{18}H_{11}Cl_5N_4O_2$



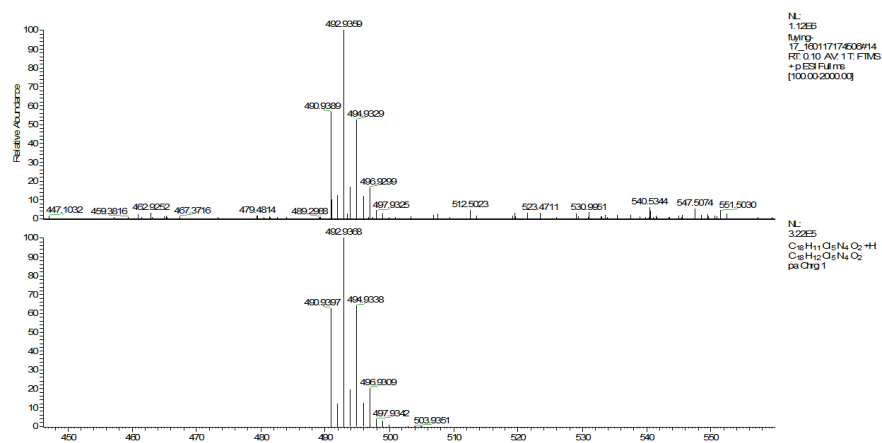
The IR spectrum of compound **5n**



The 1H NMR spectrum of compound **5n**

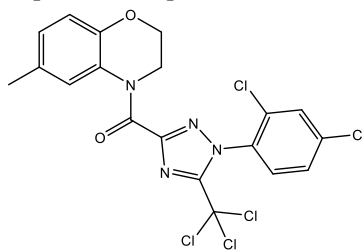


The ¹³C NMR spectrogram of compound **5n**

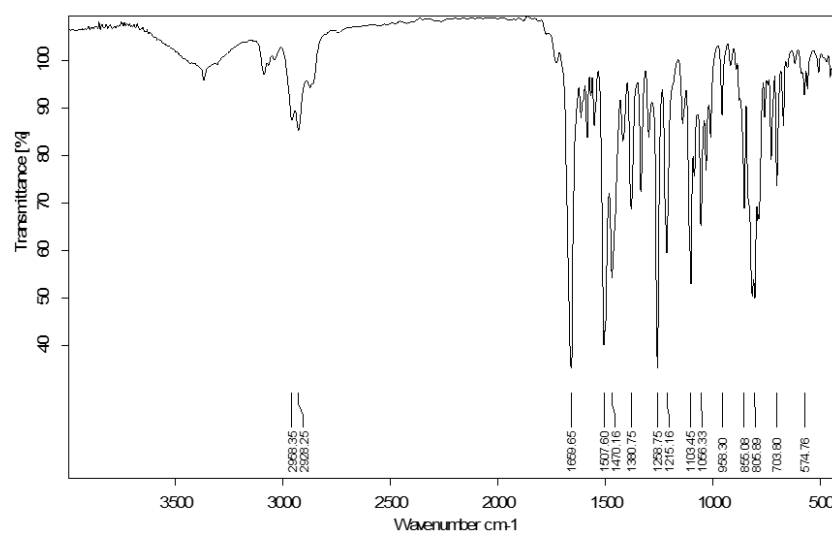


The HRMS spectrogram of compound **5n**

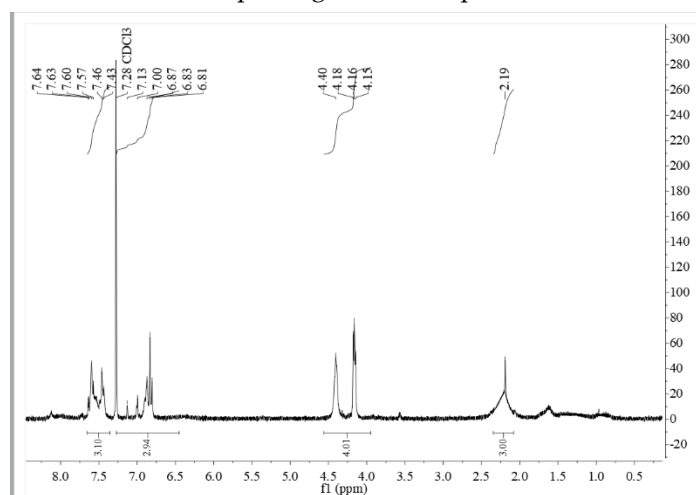
15. The molecular structure and spectra of representative compound **5o**



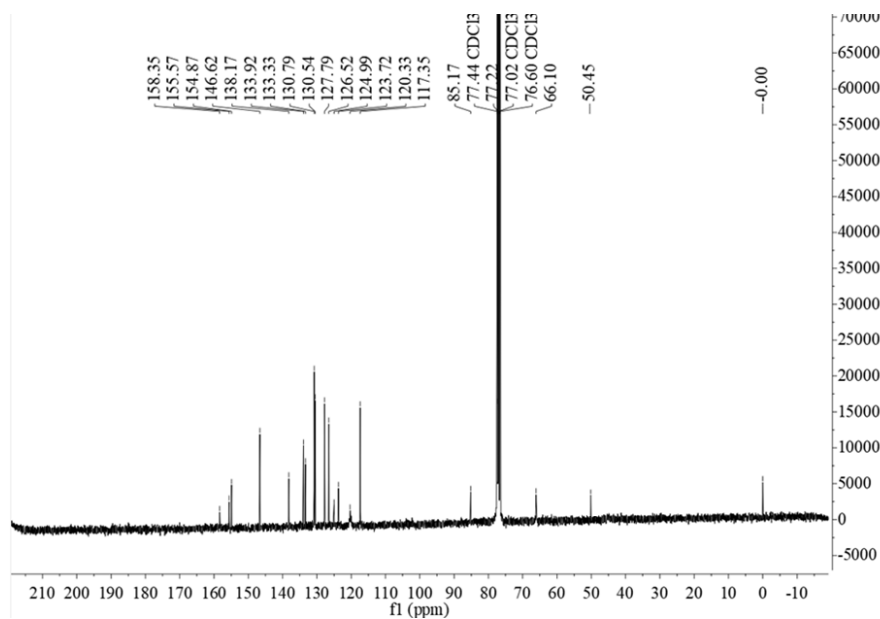
(1-(2,4-dichlorophenyl)-5-(trichloromethyl)-1H-1,2,4-triazol-3-yl)(6-methyl-2,3-dihydro-4H-benzo[b][1,4]oxazin-4-yl)methanone



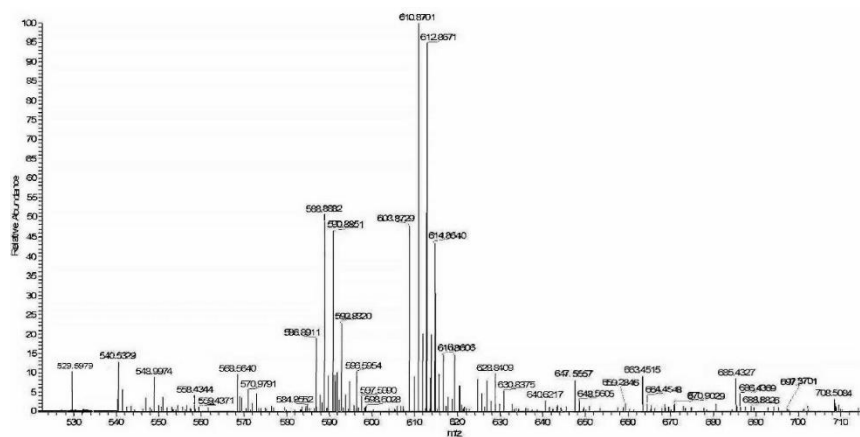
The IR spectrum of compound **5o**



The 1H NMR spectrum of compound **5o**

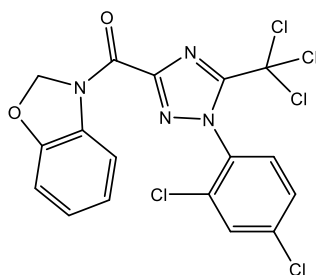


The ¹³C NMR spectrogram of compound **5o**

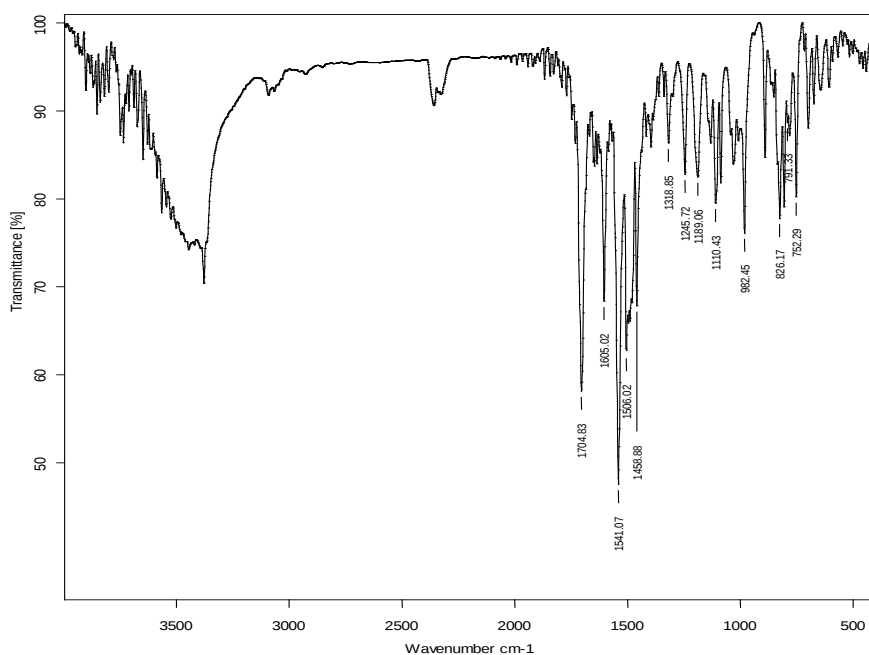


The HRMS spectrogram of compound **5o**

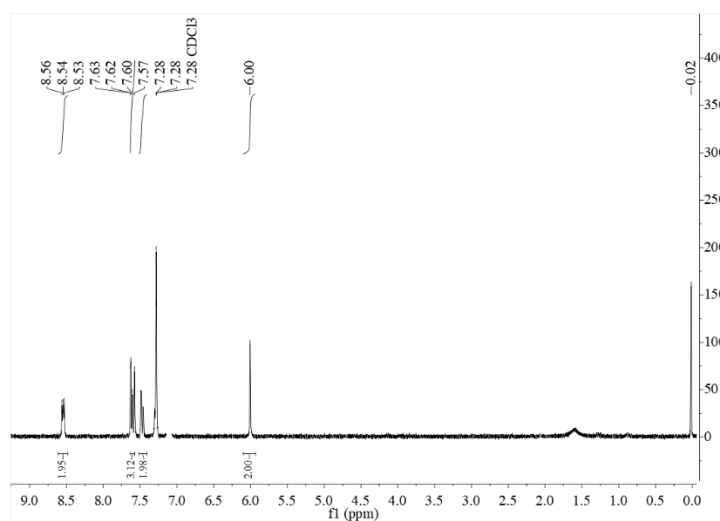
16. The molecular structure and spectra of representative compound **5p**



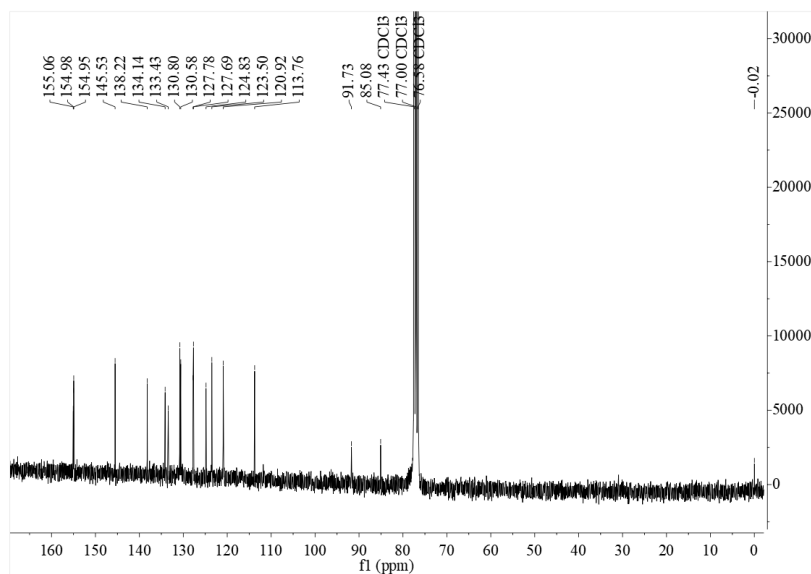
benzo[d]oxazol-3(2H)-yl(1-(2,4-dichlorophenyl)-5-(trichloromethyl)-1H-1,2,4-triazol-3-yl)methanone
 $C_{17}H_9Cl_5N_4O_2$



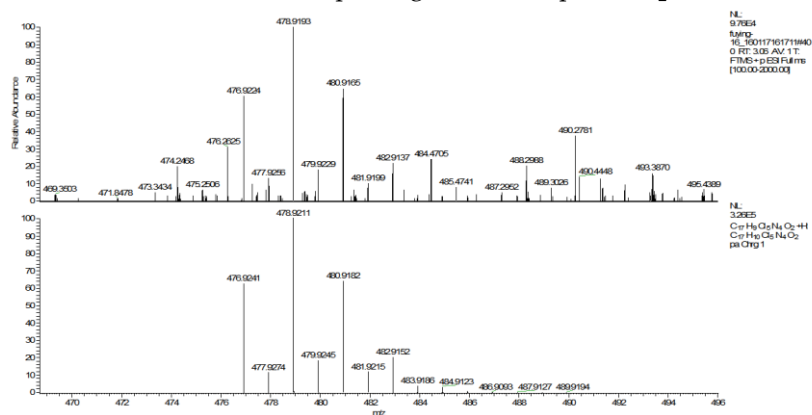
The IR spectrogram of compound **5p**



The 1H NMR spectrogram of compound **5p**

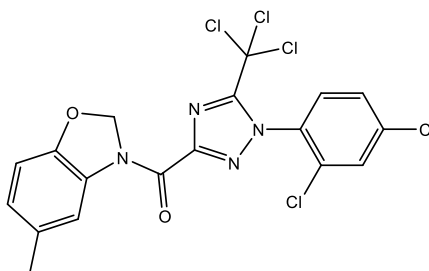


The ¹³C NMR spectrum of compound **5p**

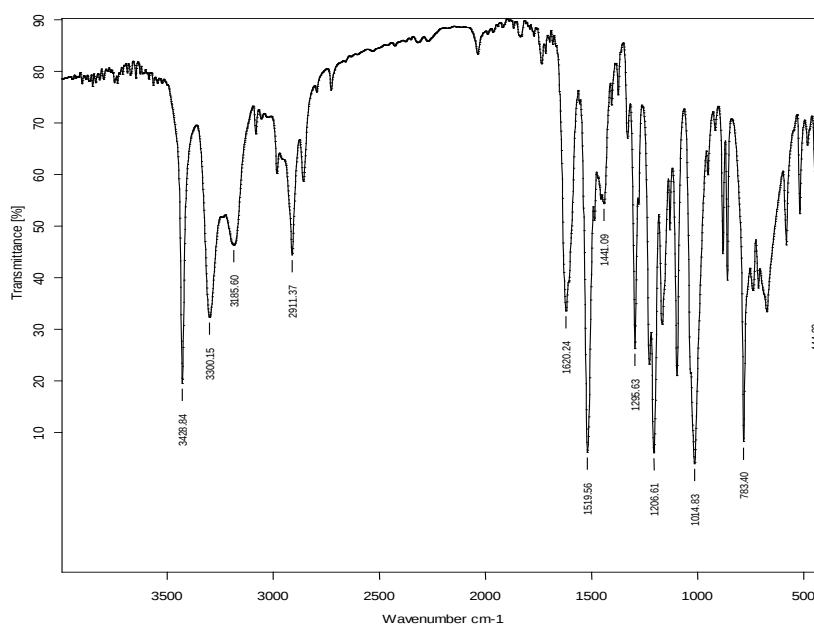


The HRMS spectrum of compound **5p**

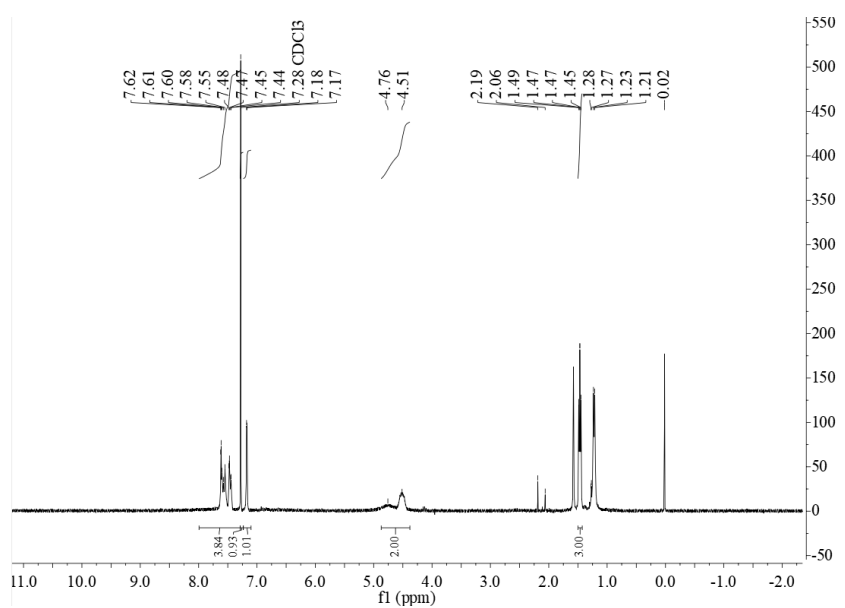
17. The molecular structure and spectra of representative compound **5q**



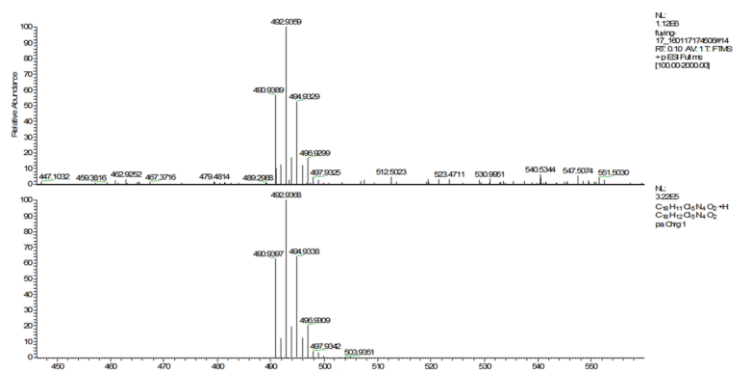
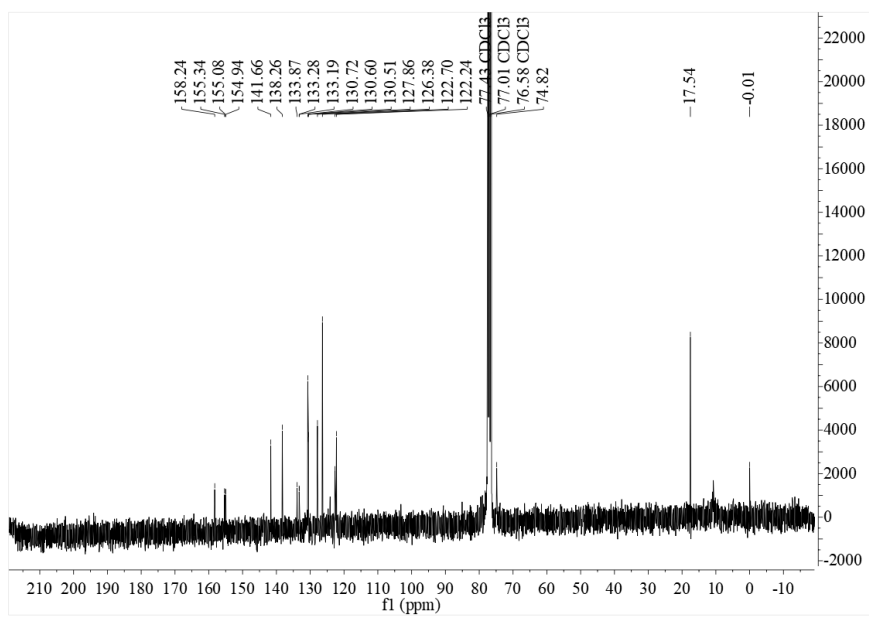
(1-(2,4-dichlorophenyl)-5-(trichloromethyl)-1H-1,2,4-triazol-3-yl)(5-methylbenzo[d]oxazol-3(2H)-yl)methanone
 $C_{18}H_{11}Cl_5N_4O_2$



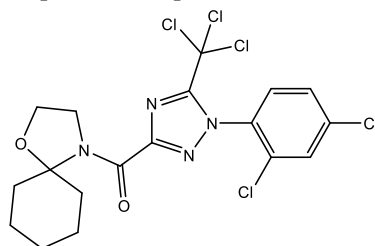
The IR spectrogram of compound **5q**



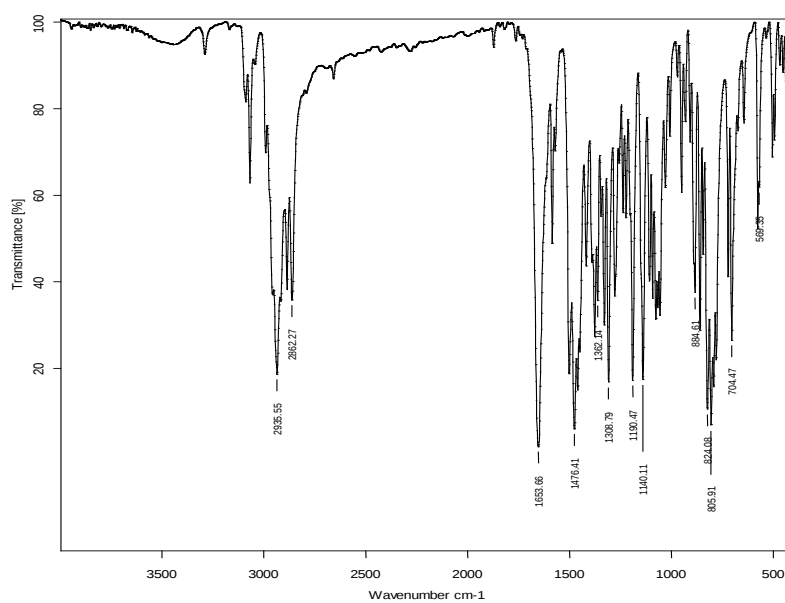
The 1H NMR spectrogram of compound **5q**



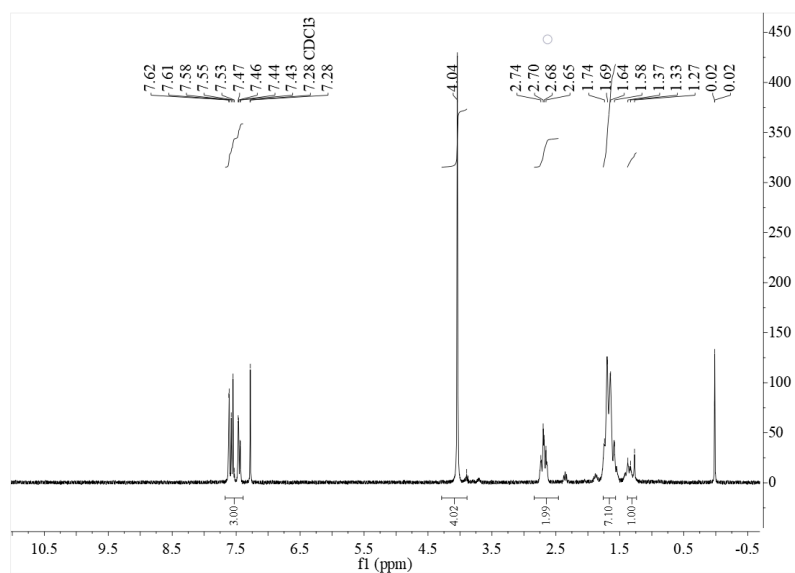
18. The molecular structure and spectra of representative compound **5r**



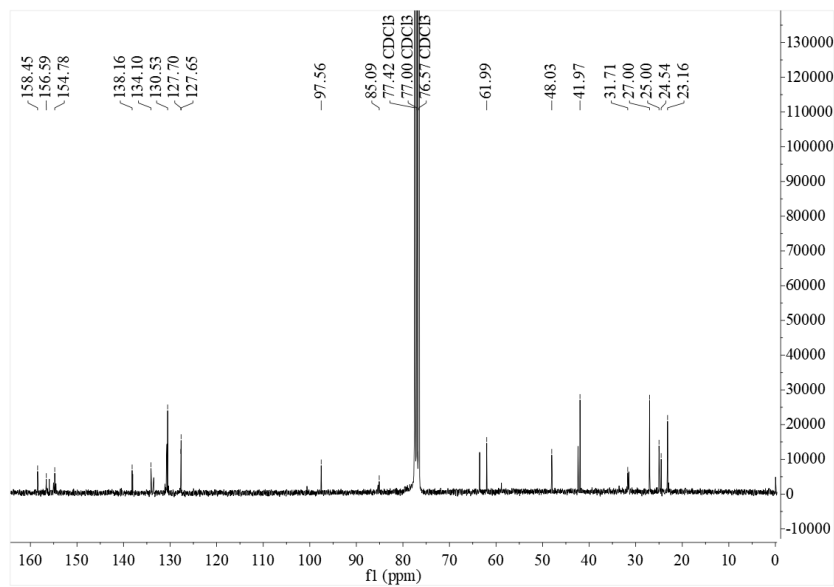
(1-(2,4-dichlorophenyl)-5-(trichloromethyl)-1H-1,2,4-triazol-3-yl)(1-oxa-4-azaspiro[4.5]decan-4-yl)methanone
 $C_{18}H_{17}Cl_5N_4O_2$



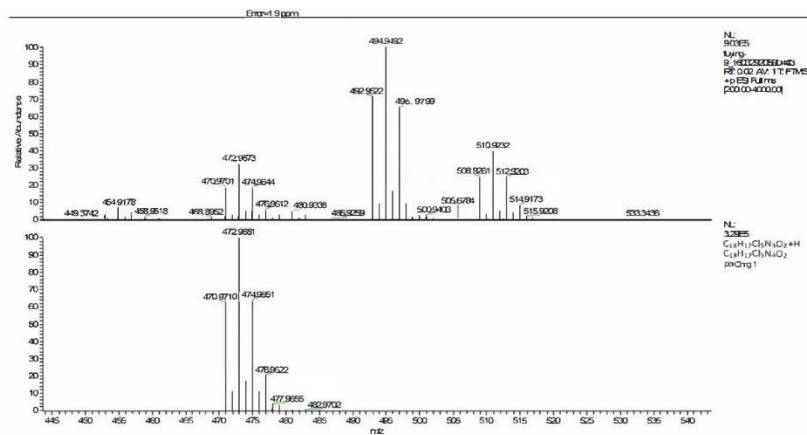
The IR spectrum of compound **5r**



The 1H NMR spectrum of compound **5r**

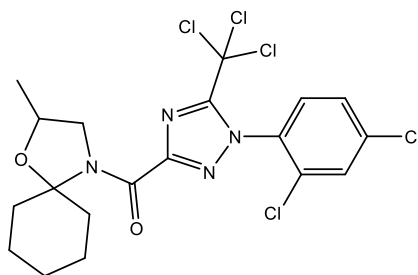


The ¹³C NMR spectrogram of compound **5r**

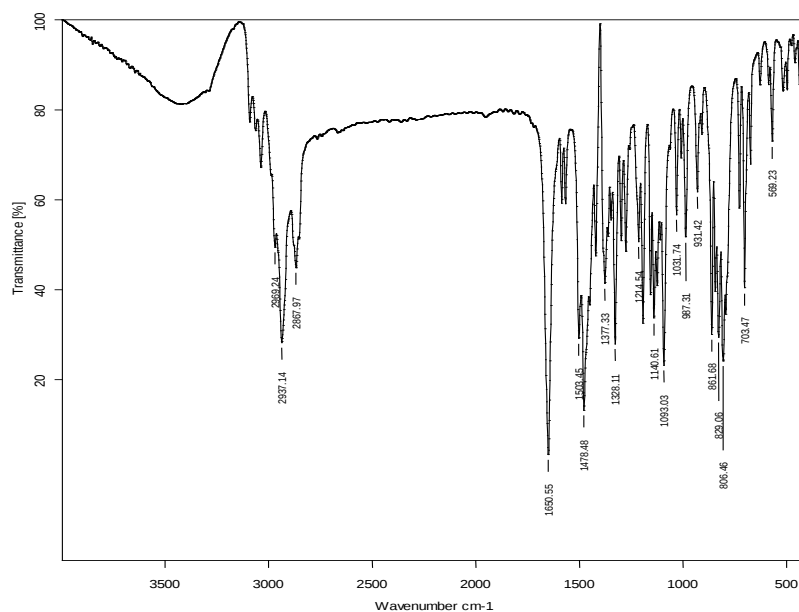


The HRMS spectrogram of compound **5r**

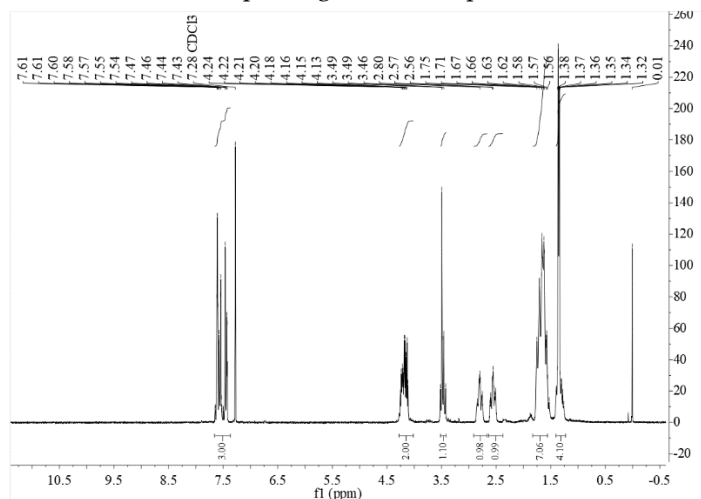
19. The molecular structure and spectra of representative compound **5s**



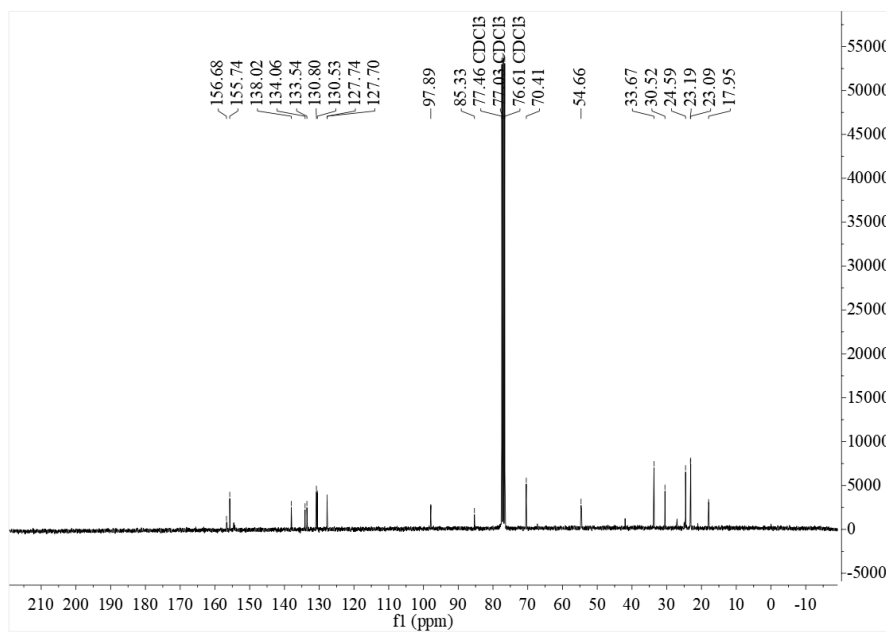
(1-(2,4-dichlorophenyl)-5-(trichloromethyl)-1*H*-1,2,4-triazol-3-yl)(2-methyl-1-oxa-4-azaspiro[4.5]decan-4-yl)methanone
C₁₉H₁₉Cl₅N₄O₂



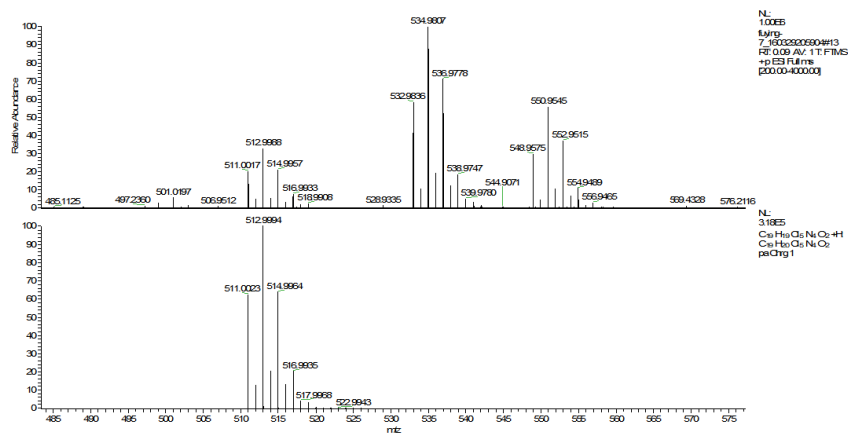
The IR spectrum of compound **5s**



The ¹H NMR spectrum of compound **5s**

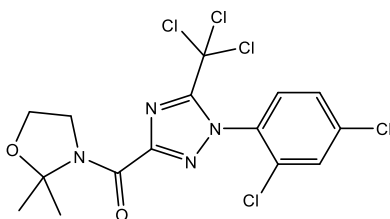


The ^{13}C NMR spectrogram of compound **5s**

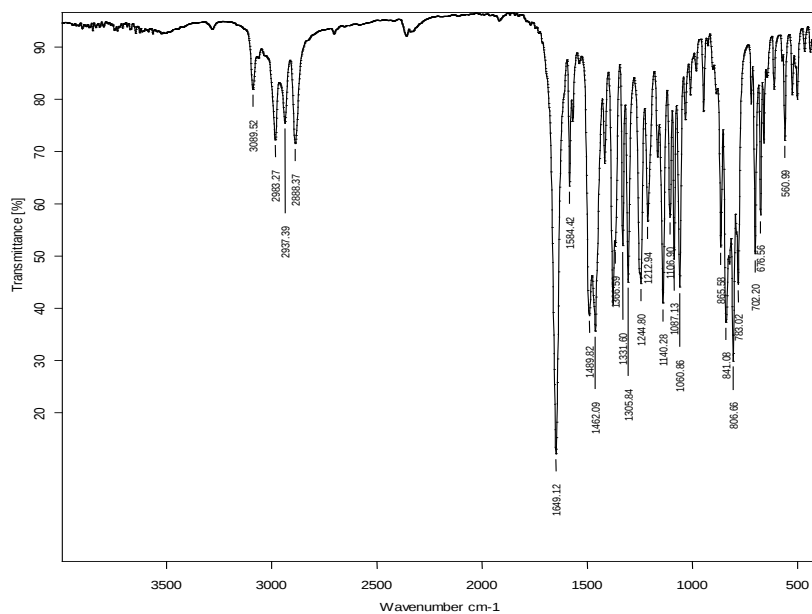


The HRMS spectrogram of compound **5s**

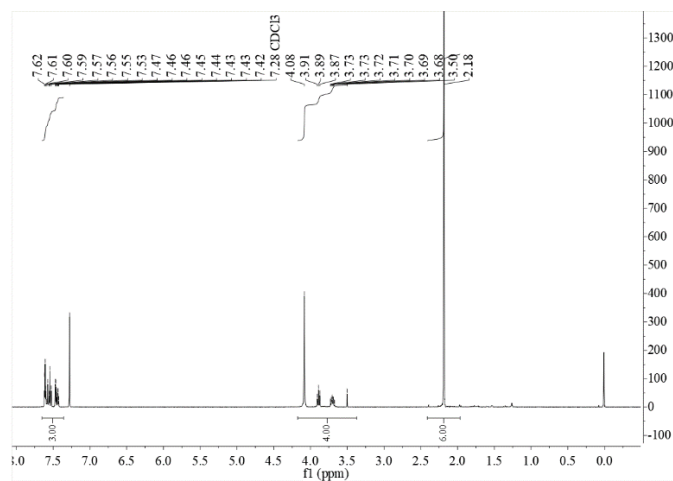
20. The molecular structure and spectra of representative compound **5t**



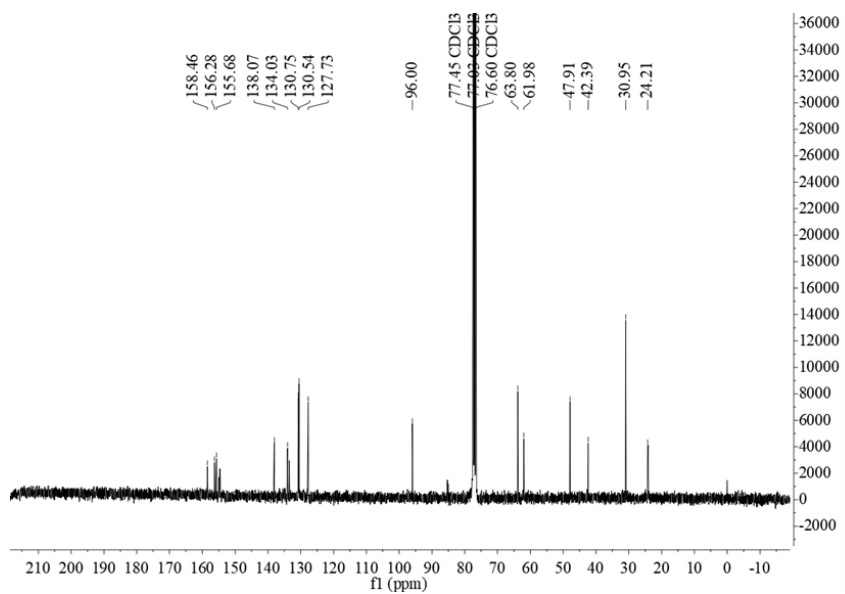
(1-(2,4-dichlorophenyl)-5-(trichloromethyl)-1H-1,2,4-triazol-3-yl)(2,2-dimethyloxazolidin-3-yl)methanone
 $C_{15}H_{13}Cl_5N_4O_2$



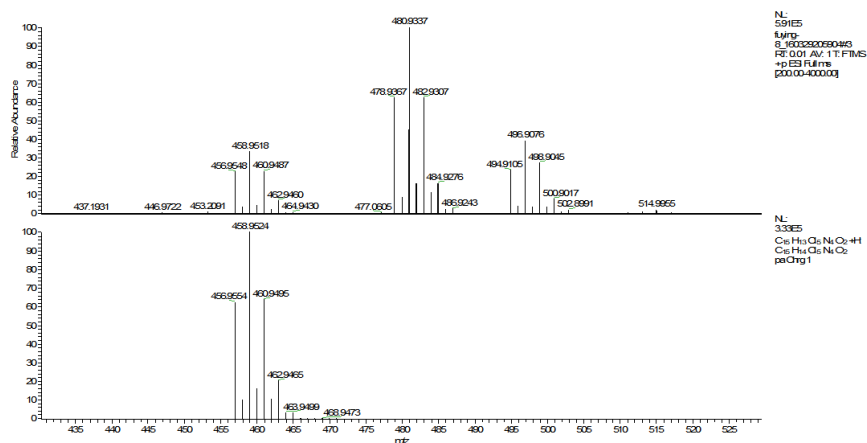
The IR spectrogram of compound **5t**



The 1H NMR spectrogram of compound **5t**

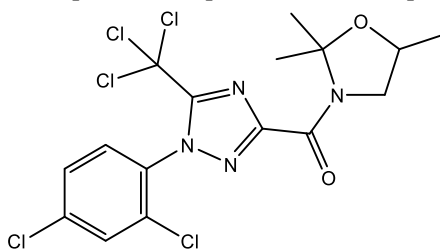


The ¹³C NMR spectrogram of compound **5t**

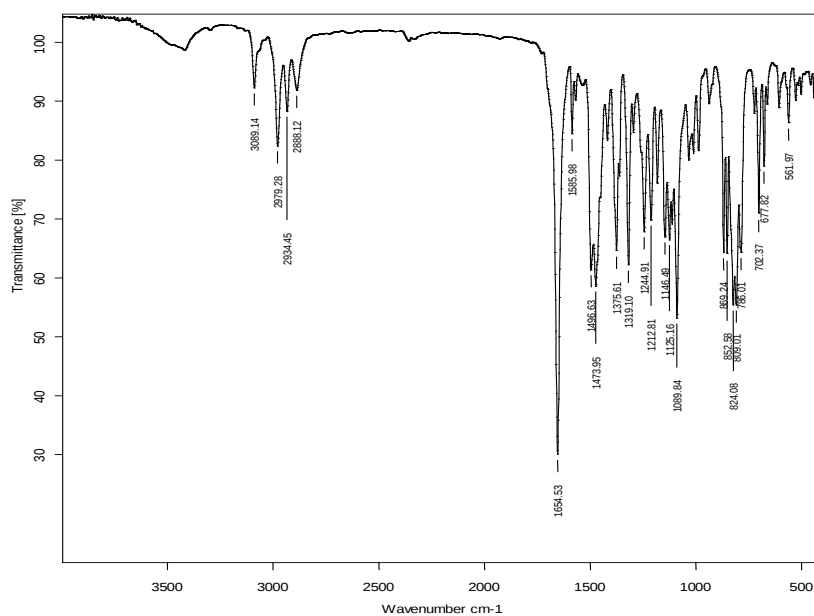


The HRMS spectrogram of compound **5t**

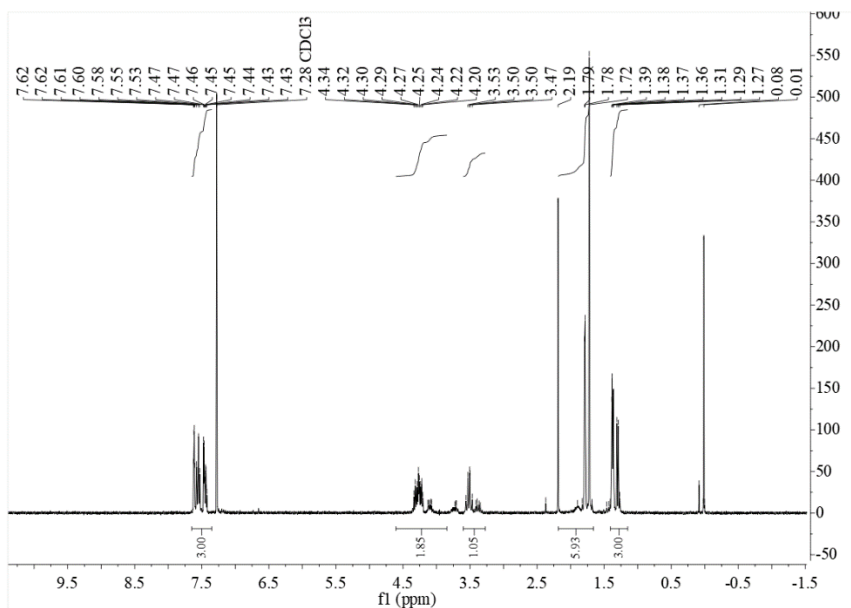
21. The molecular structure and spectra of representative compound **5u**



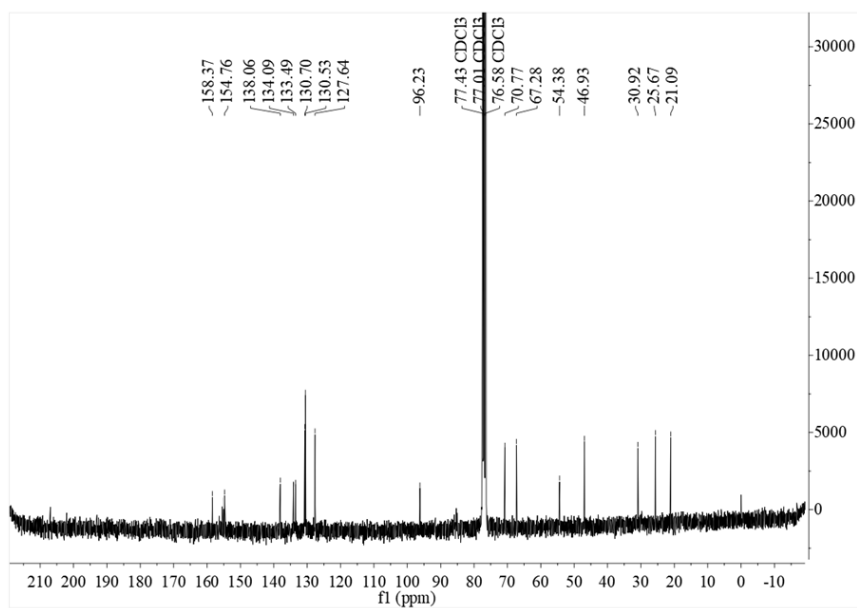
(1-(2,4-dichlorophenyl)-5-(trichloromethyl)-1H-1,2,4-triazol-3-yl)(2,2,5-trimethyloxazolidin-3-yl)methanone
 $C_{16}H_{15}Cl_5N_4O_2$



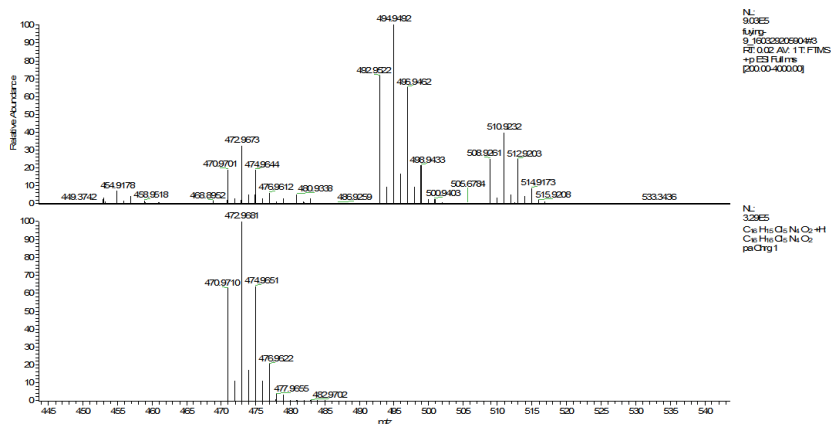
The IR spectrogram of compound **5u**



The 1H NMR spectrogram of compound **5u**



The ¹³C NMR spectrogram of compound **5u**



The HRMS spectrogram of compound **5u**