

Supplementary Materials: Synthesis and Antifungal Activity of Novel Myrtenal-Based 4-Methyl-1,2,4-triazole-thioethers

Gui-Shan Lin, Wen-Gui Duan, Lin-Xiao Yang, Min Huang and Fu-Hou Lei

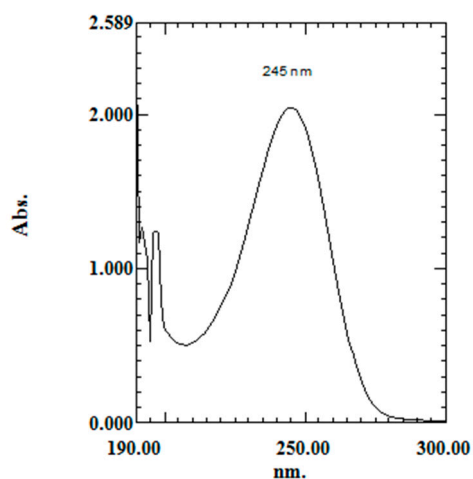


Figure S1. UV-vis spectrum of myrtenal (2) in EtOH.

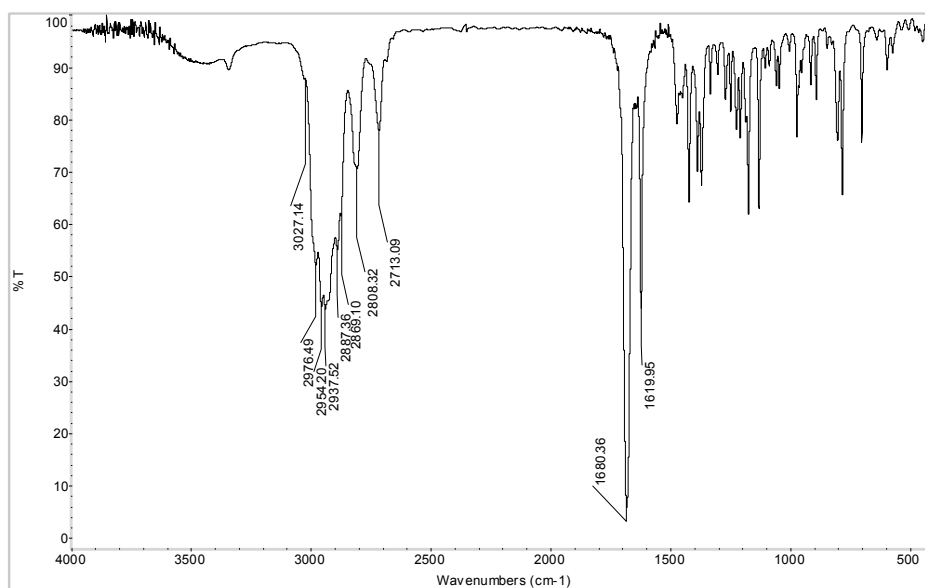


Figure S2. FTIR spectrum of myrtenal (2).

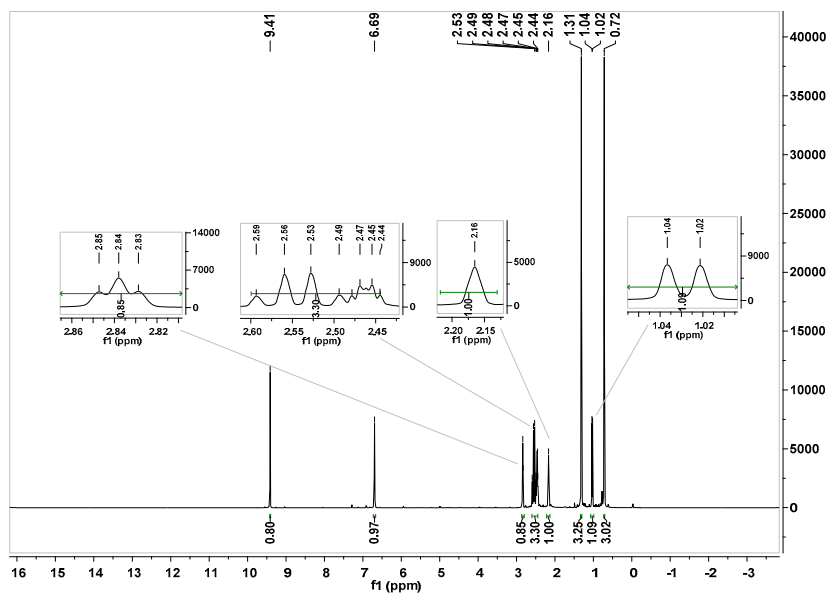


Figure S3. $^1\text{H-NMR}$ spectrum of myrtenal (2) in CDCl_3 .

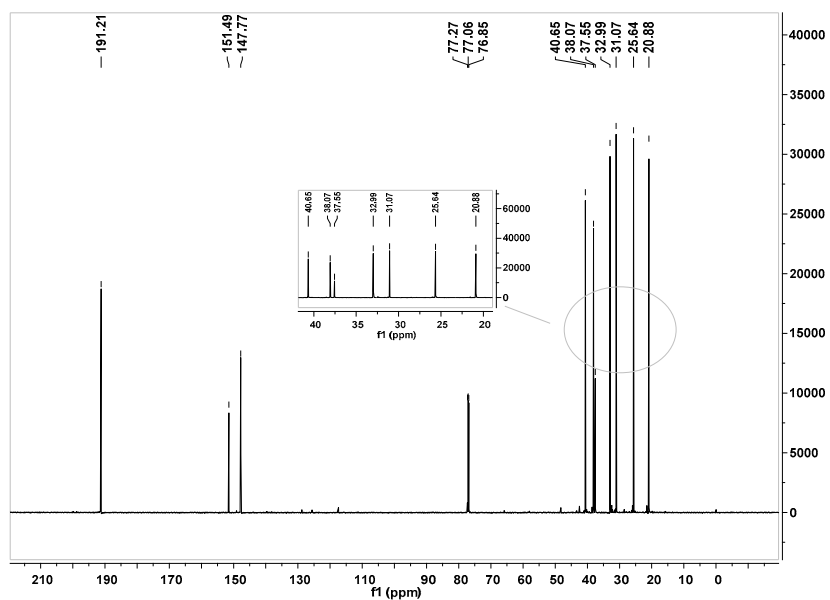


Figure S4. $^{13}\text{C-NMR}$ spectrum of myrtenal (2) in CDCl_3 .

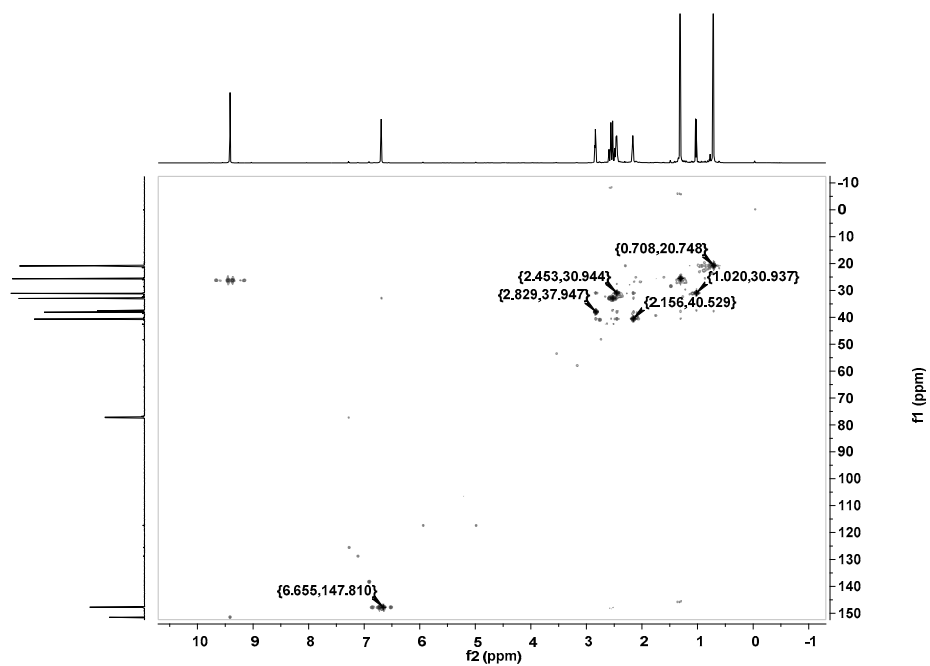


Figure S5a. HMQC spectrum of myrtenal (2) in CDCl₃.

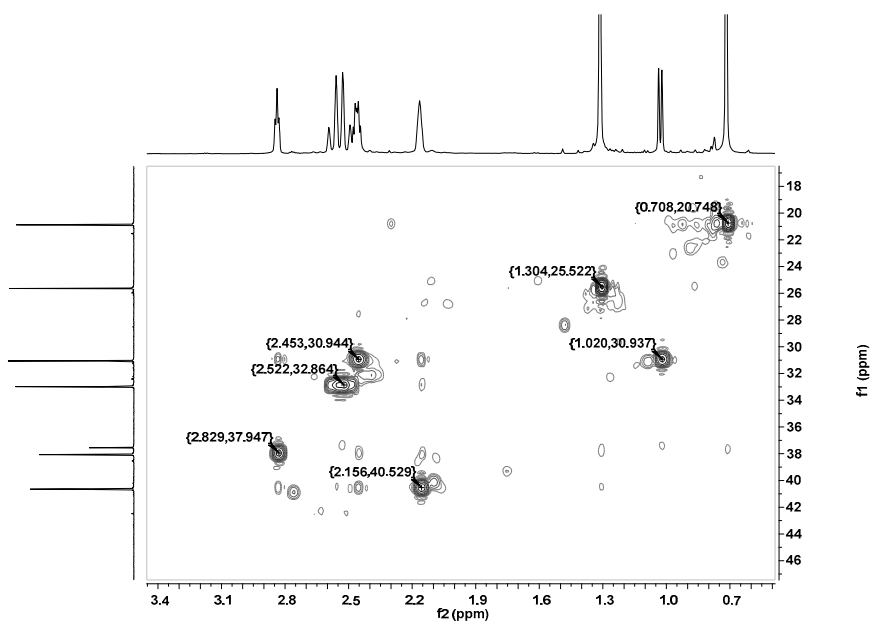


Figure S5b. Expanded HMQC spectrum of myrtenal (2) in CDCl₃.

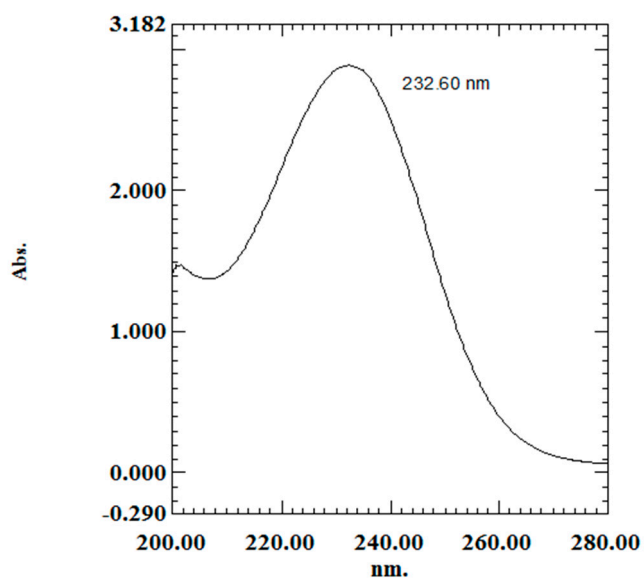


Figure S6. UV-vis spectrum of myrtenic acid (3) in EtOH.

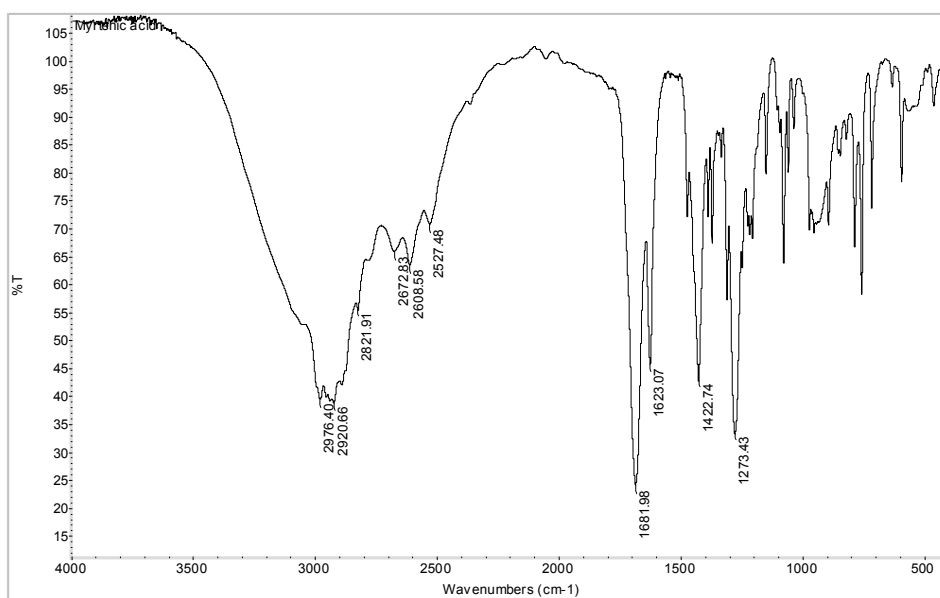


Figure S7. FTIR spectrum of myrtenic acid (3).

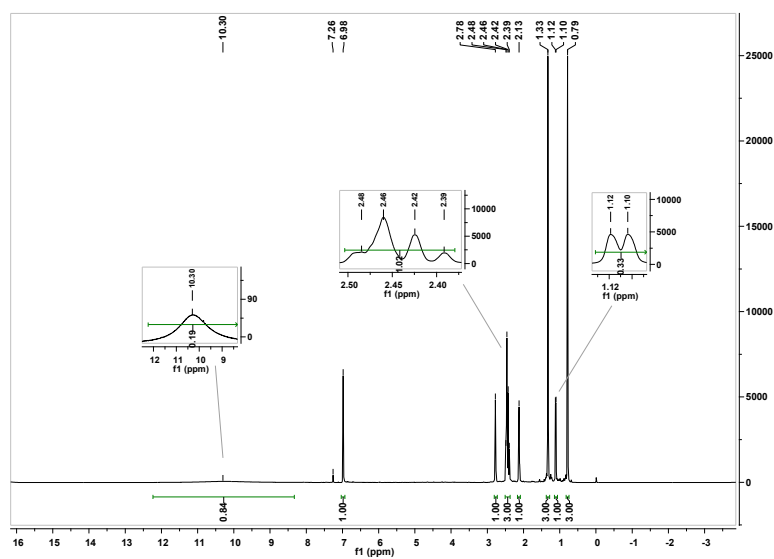
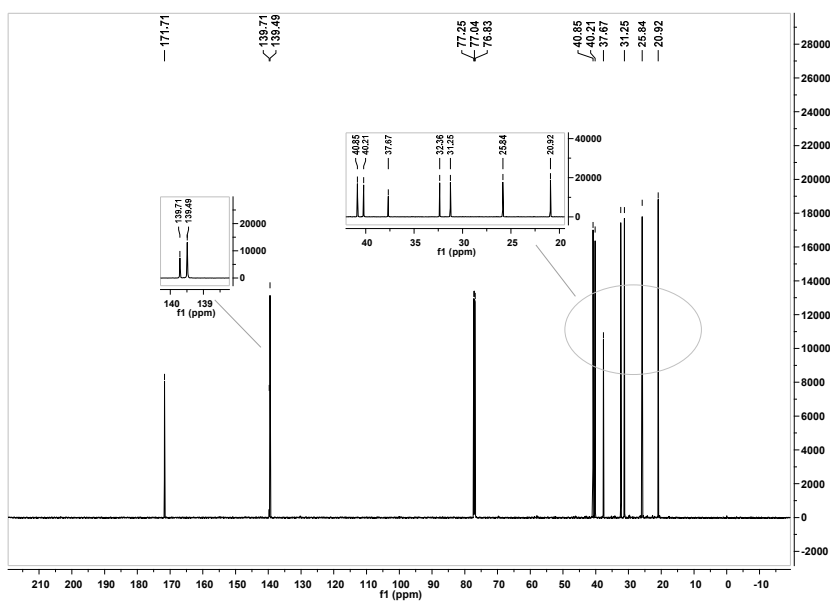
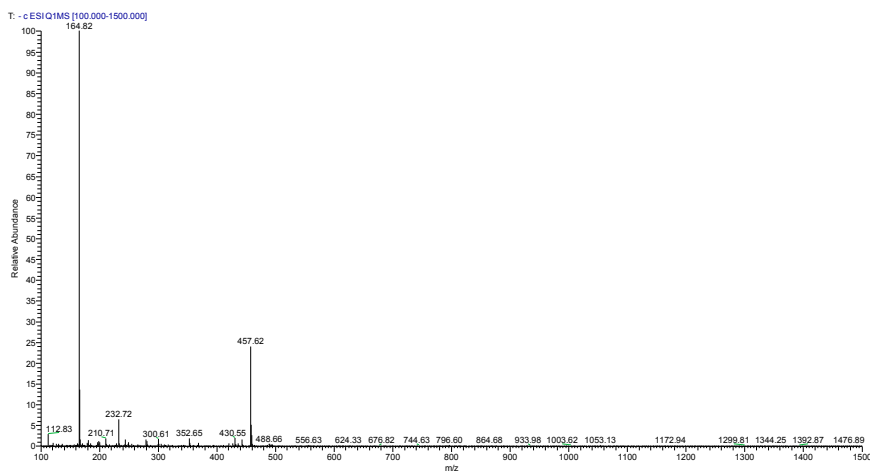
Figure S8. ^1H -NMR spectrum of myrtenic acid (3) in CDCl_3 .Figure S9. ^{13}C -NMR spectrum of myrtenic acid (3) in CDCl_3 .

Figure S10. ESI-MS spectrum of myrtenic acid (3).

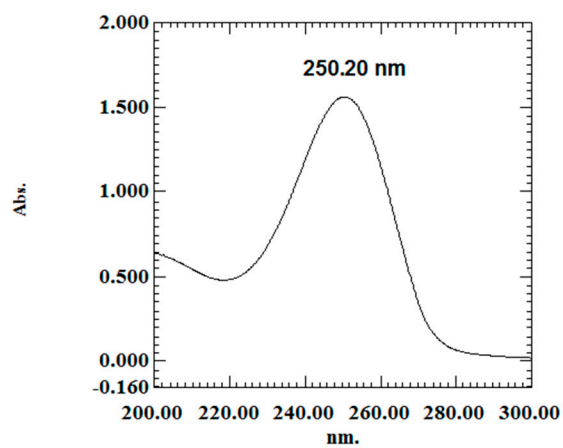


Figure S11. UV-vis spectrum of myrtenyl chloride (4) in cyclohexane.

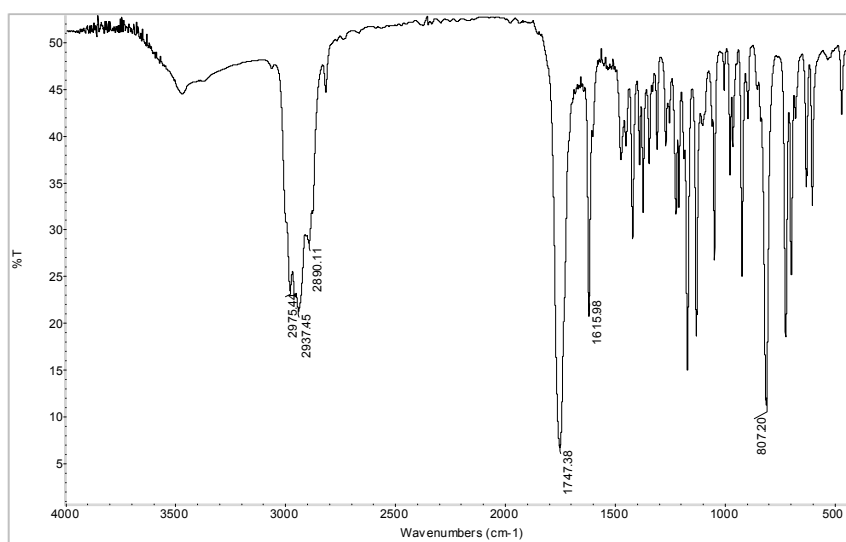
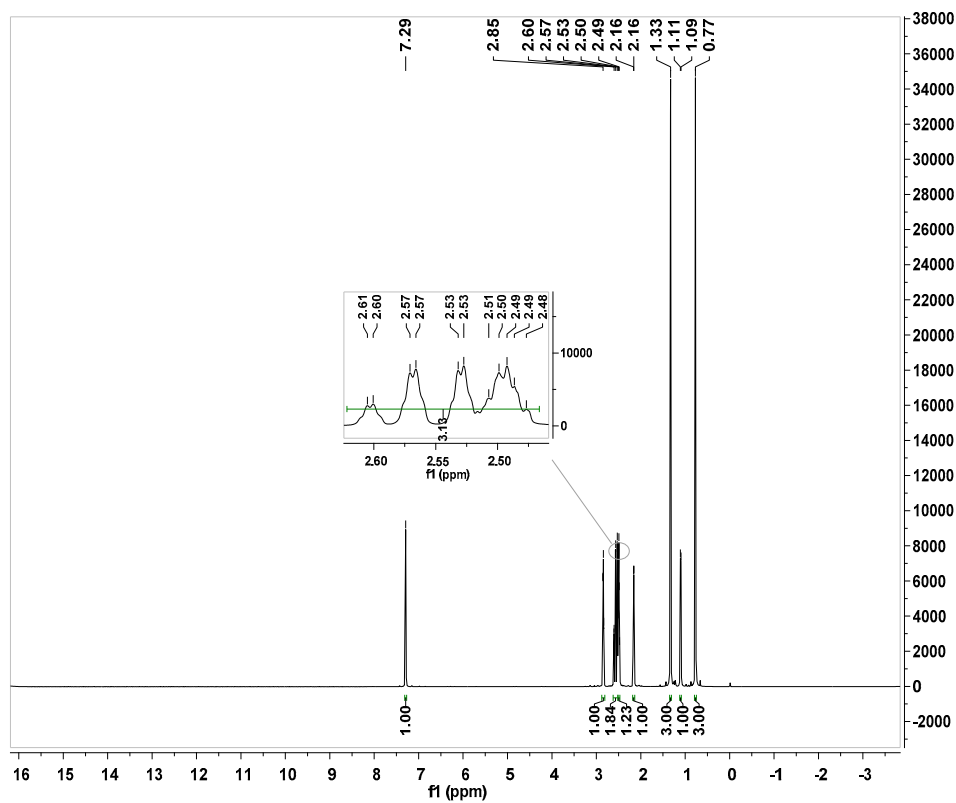
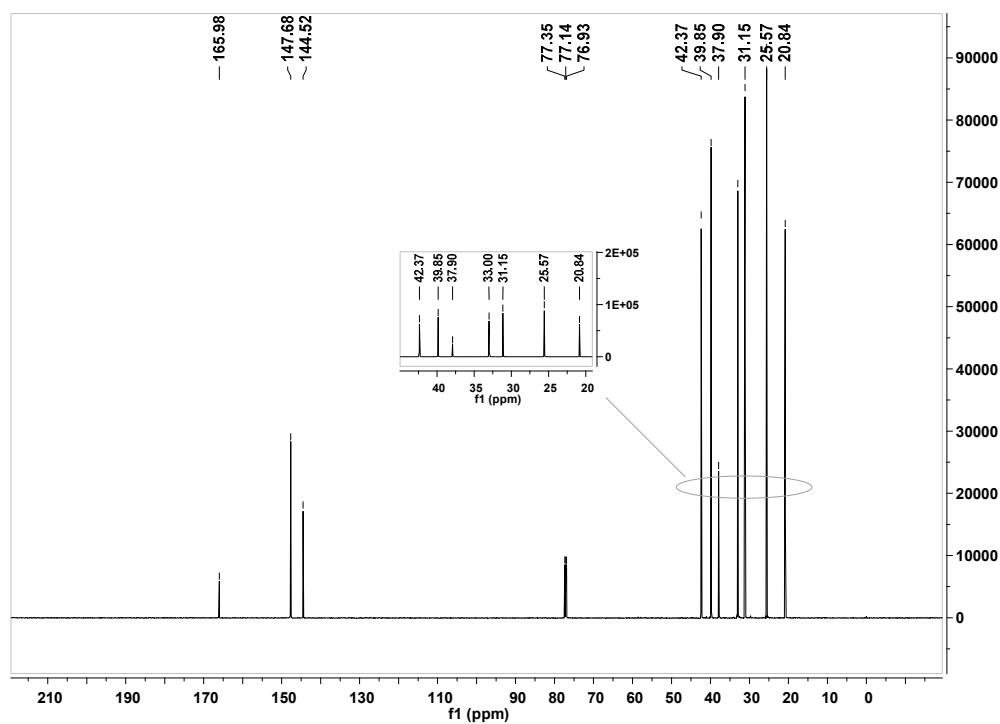


Figure S12. FTIR spectrum of myrtenyl chloride (4).

Figure S13. ^1H -NMR spectrum of myrtenyl chloride (4) in CDCl_3 .Figure S14. ^{13}C -NMR spectrum of myrtenyl chloride (4) in CDCl_3 .

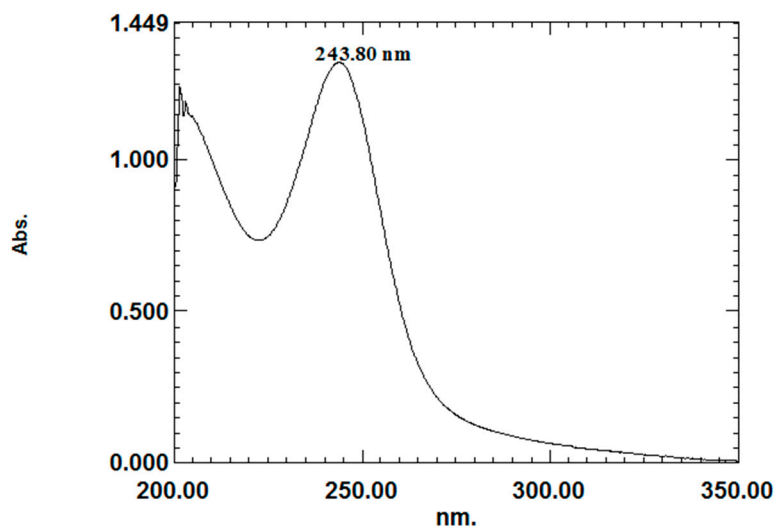


Figure S15. UV-vis spectrum of (5) in EtOH.

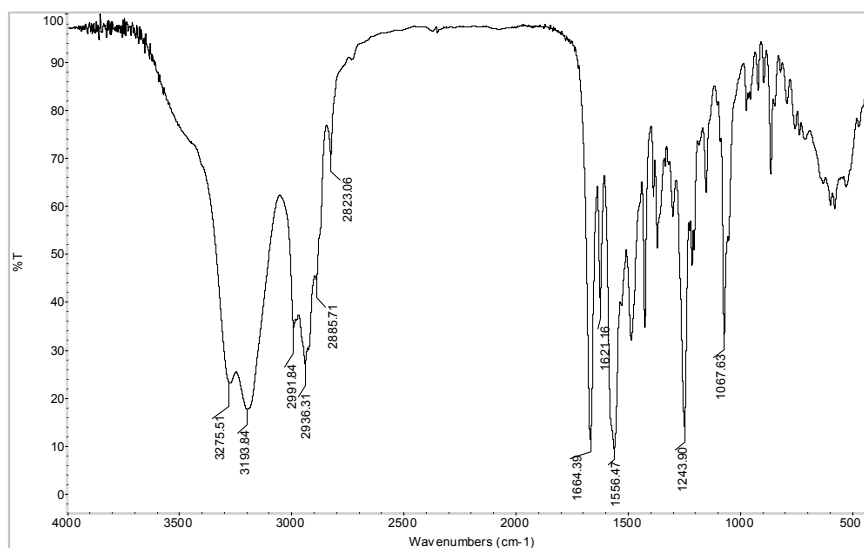


Figure S16. FTIR spectrum of 2-(myrtenoic carbonyl)-*N*-methylhydrazinecarbothioamide (5).

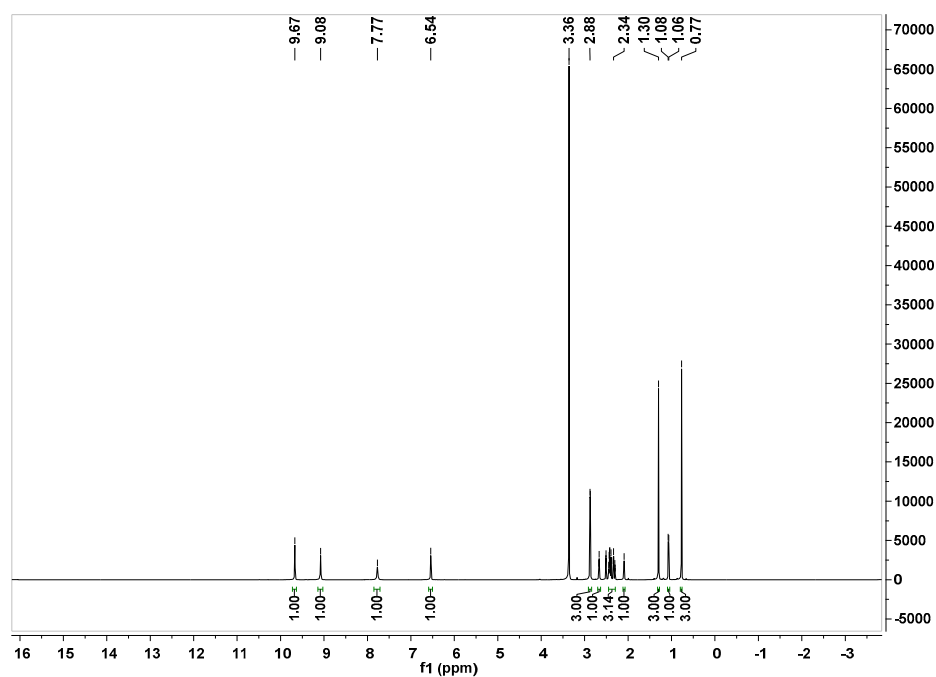


Figure S17. $^1\text{H-NMR}$ 2-(myrtenoic carbonyl)-*N*-methylhydrazinecarbothioamide (5) in CDCl_3 .

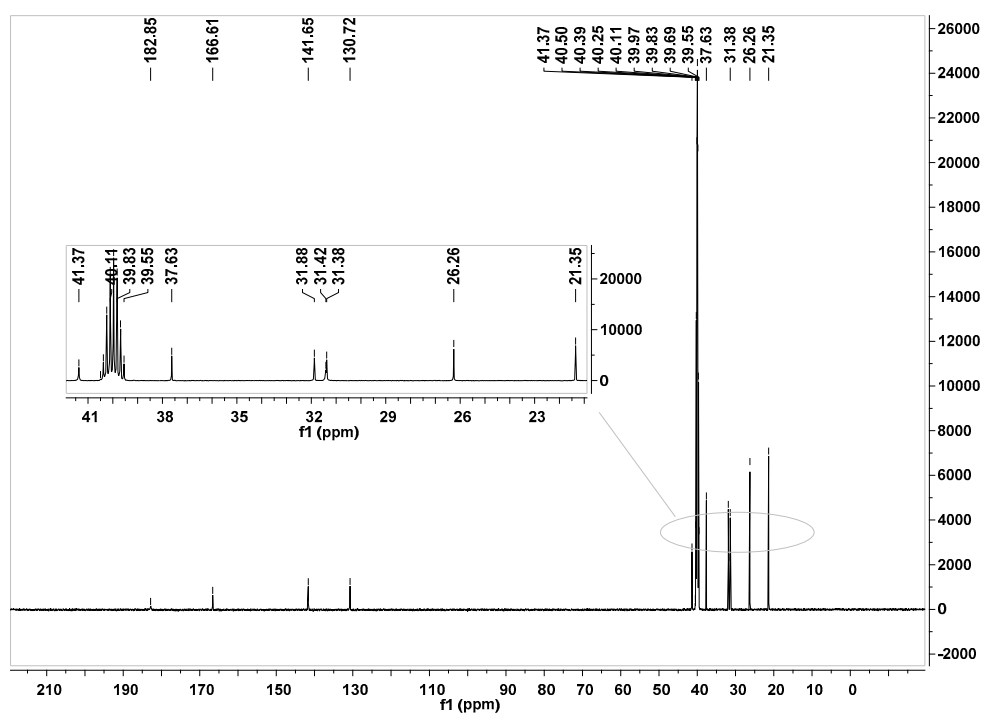


Figure S18. $^{13}\text{C-NMR}$ spectrum of 2-(myrtenoic carbonyl)-*N*-methylhydrazinecarbothioamide (5) in CDCl_3 .

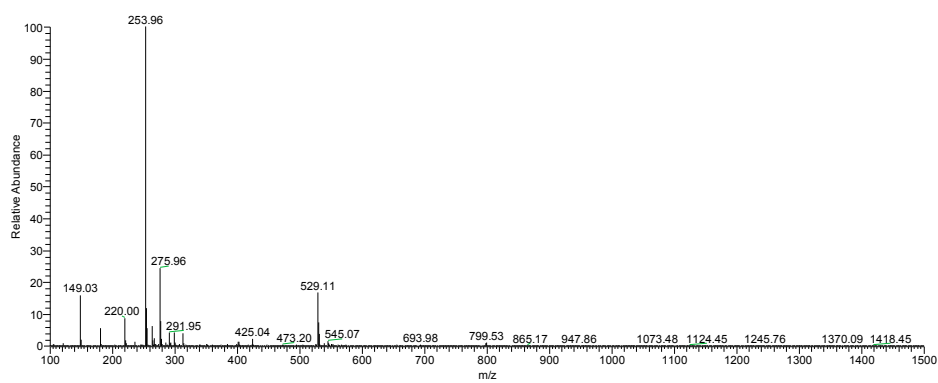


Figure S19. ESI-MS spectrum of (5).

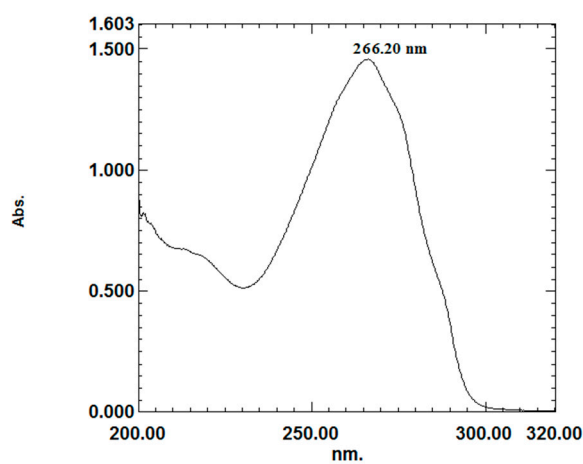


Figure S20. UV-vis spectrum of the target compound 6a in cyclohexane.

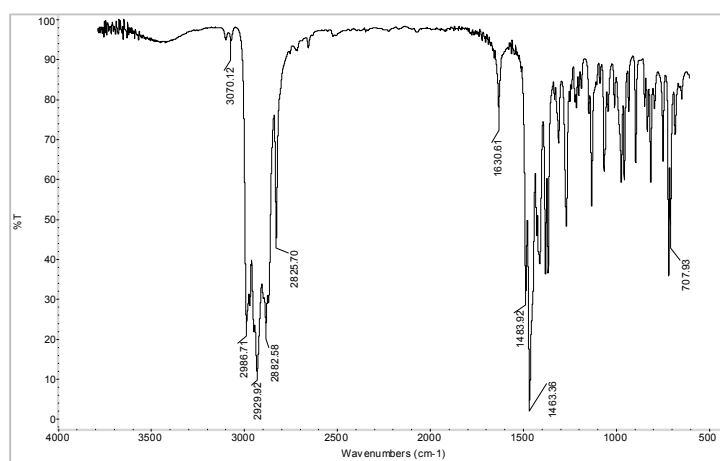


Figure S21. FTIR spectrum of the target compound 6a.

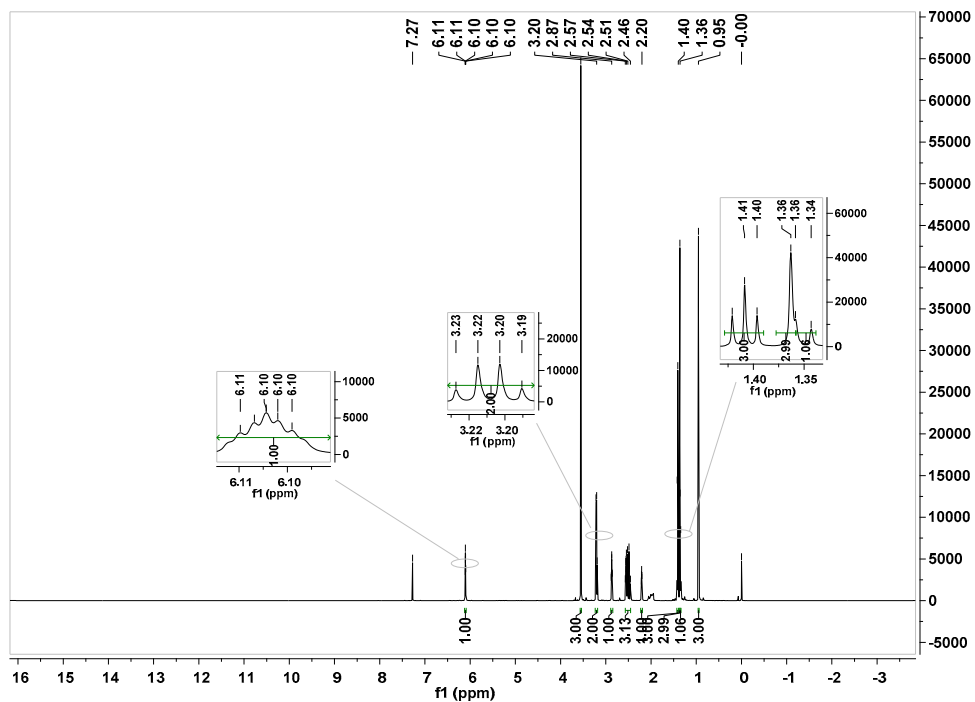
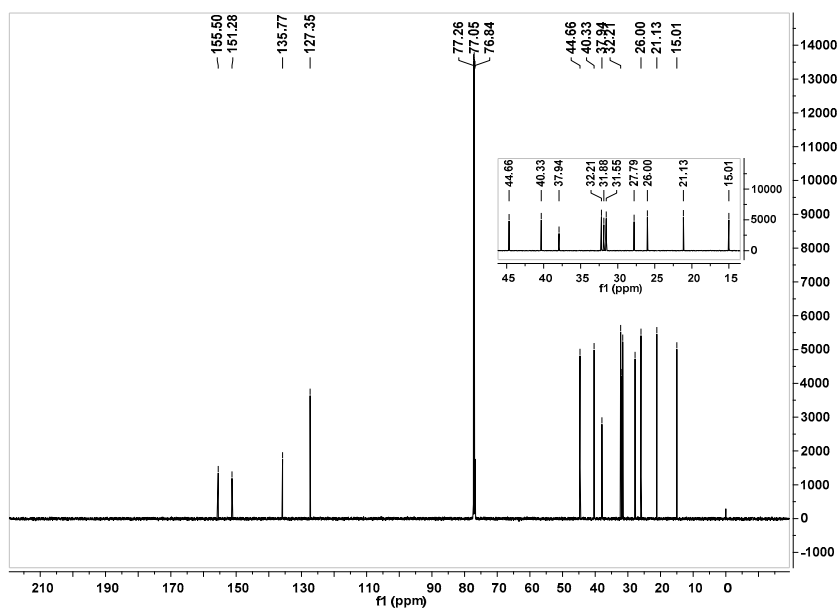
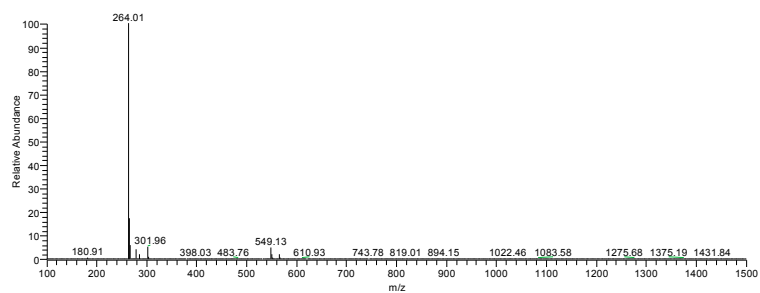
Figure S22. ^1H -NMR spectrum of the target compound **6a** in CDCl_3 .Figure S23. ^{13}C -NMR spectrum of the target compound **6a** in CDCl_3 .

Figure S24. ESI-MS spectrum of the target compound 6a.

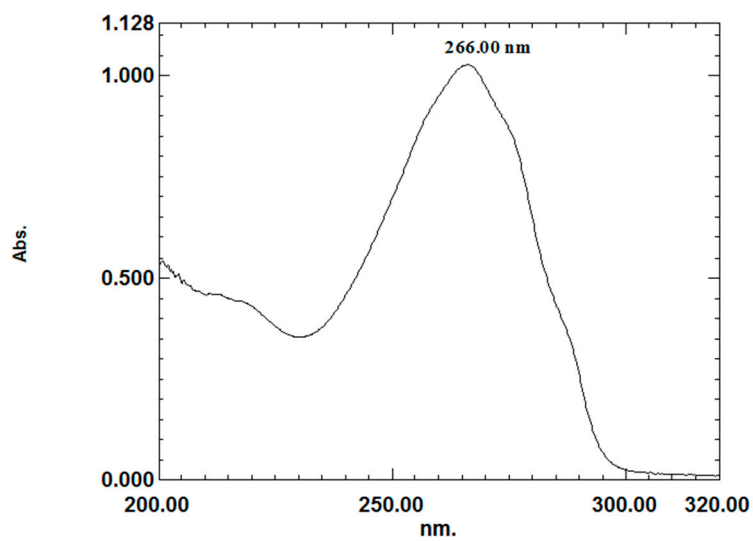


Figure S25. UV-vis spectrum of the target compound 6b in cyclohexane.

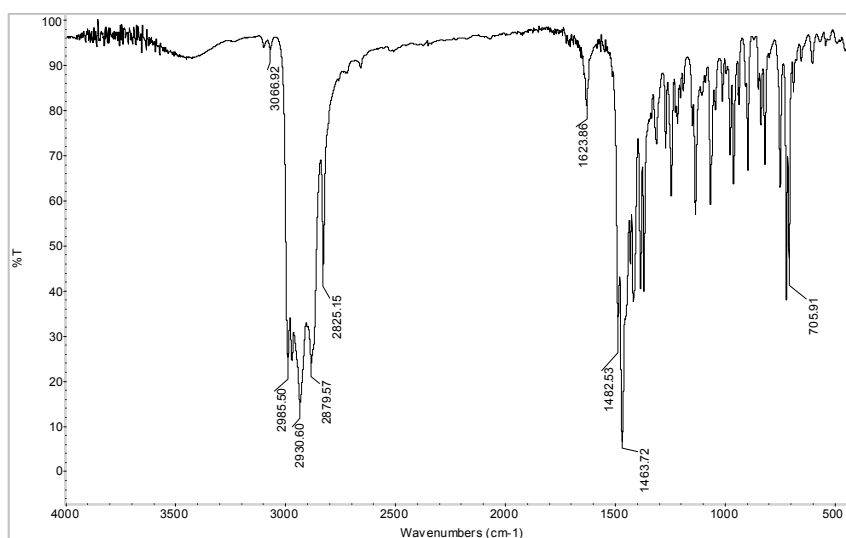


Figure S26. FTIR spectrum of the target compound 6b.

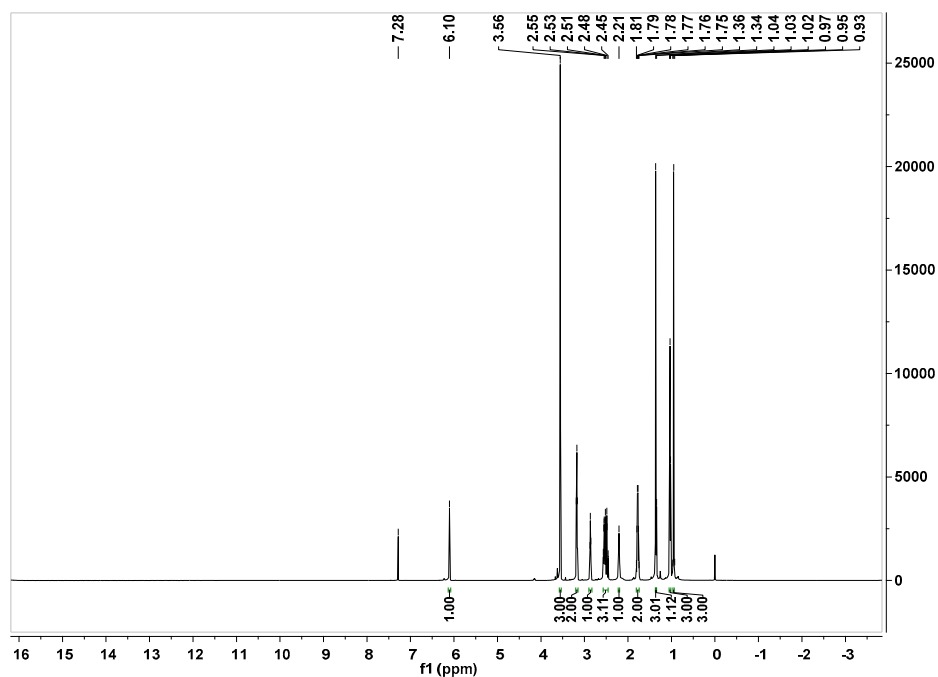
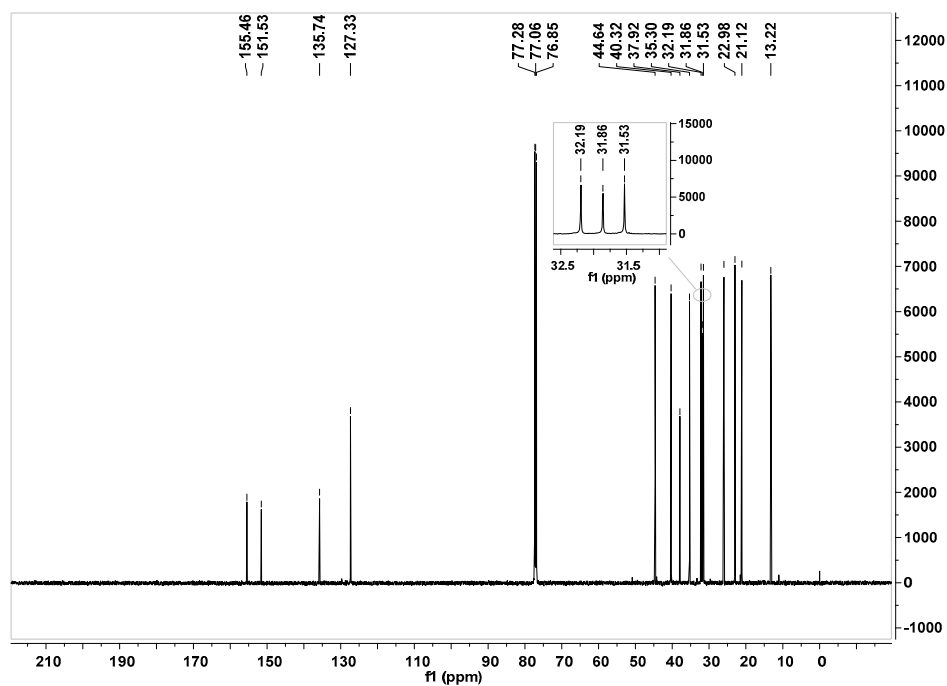
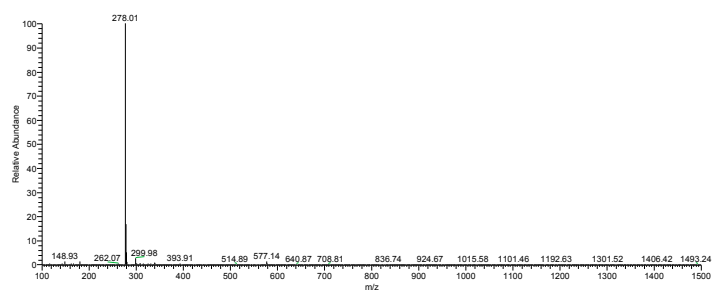
Figure S27. $^1\text{H-NMR}$ spectrum of the target compound **6b** in CDCl_3 .Figure S28. $^{13}\text{C-NMR}$ spectrum of the target compound **6b** in CDCl_3 .

Figure S29. ESI-MS spectrum of the target compound 6b.

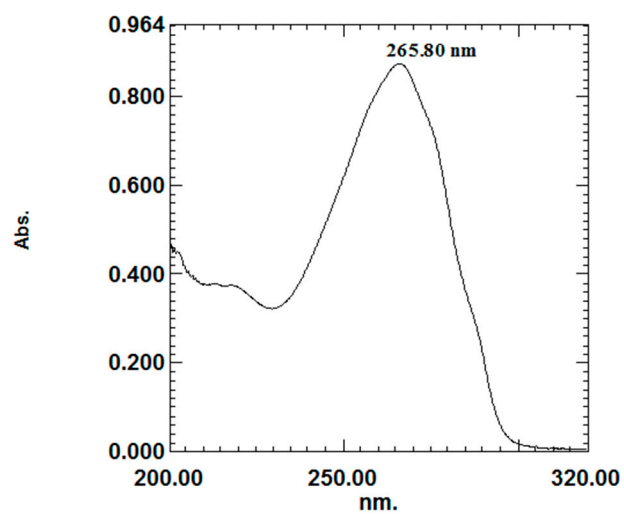


Figure S30. UV-vis spectrum of the target compound 6c in cyclohexane.

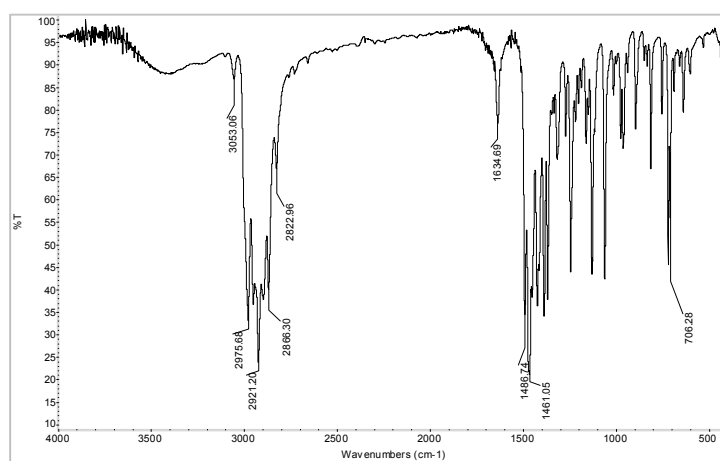


Figure S31. FTIR spectrum of the target compound 6c.

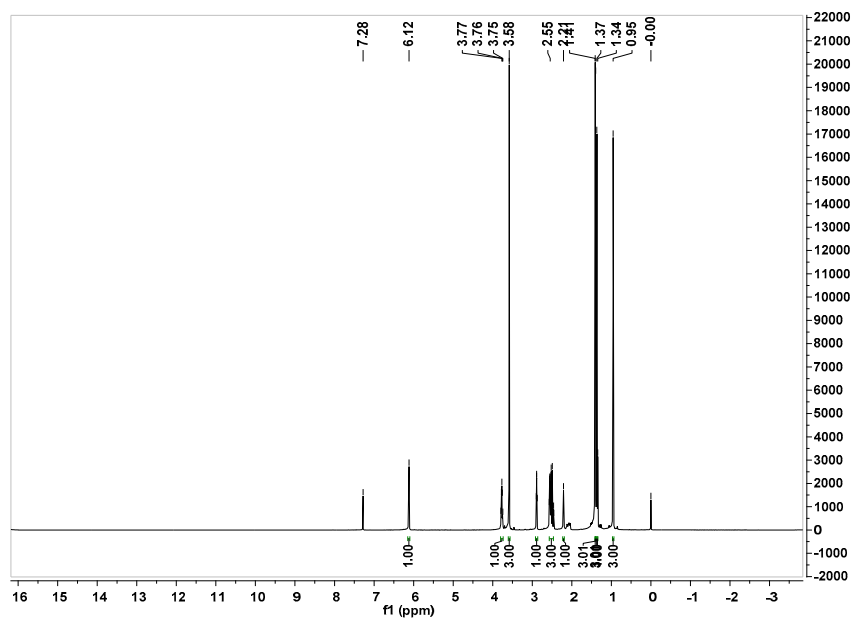


Figure S32. $^1\text{H-NMR}$ spectrum of the target compound **6c** in CDCl_3 .

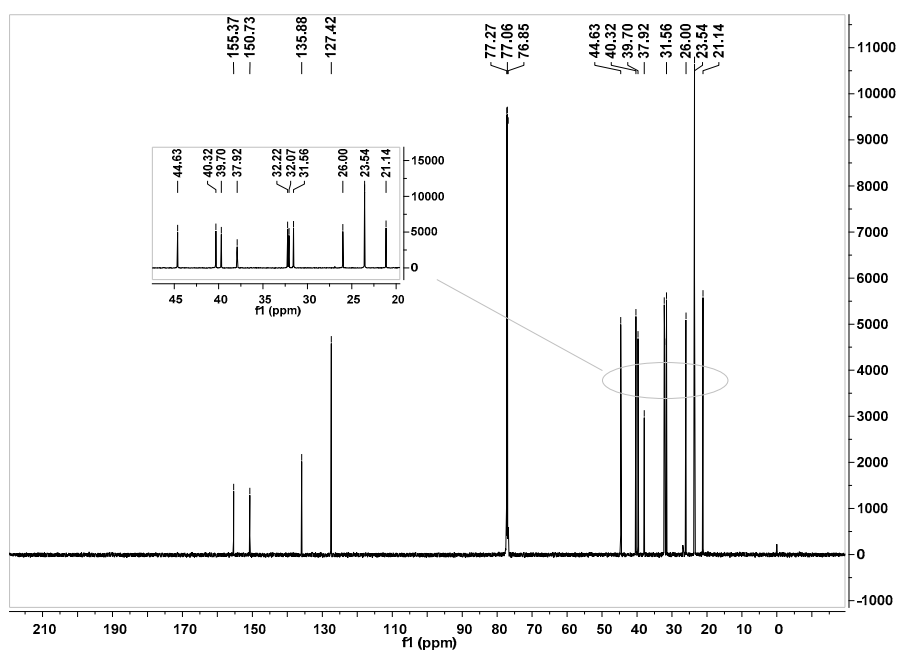


Figure S33. $^{13}\text{C-NMR}$ spectrum of the target compound **6c** in CDCl_3 .

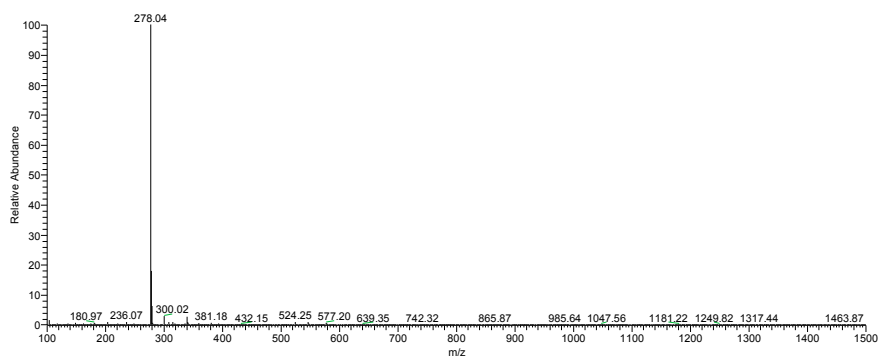


Figure S34. ESI-MS spectrum of the target compound 6c.

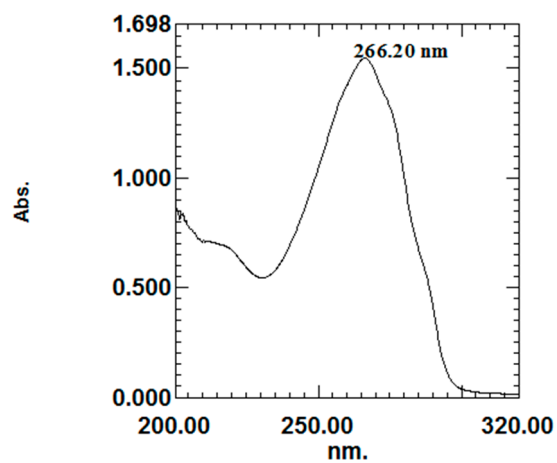


Figure S35. UV-vis spectrum of the target compound 6d in cyclohexane.

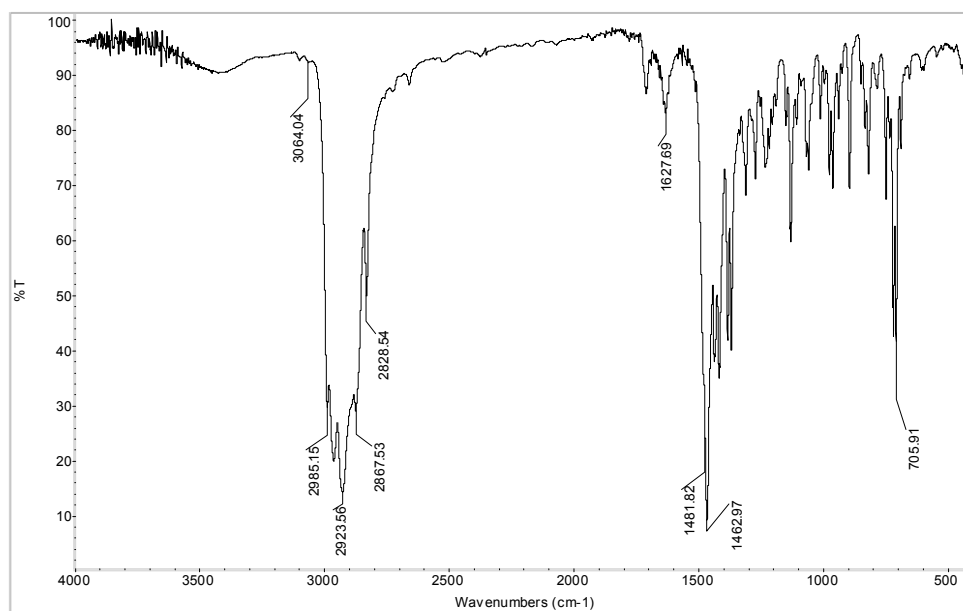


Figure S36. FTIR spectrum of the target compound 6d.

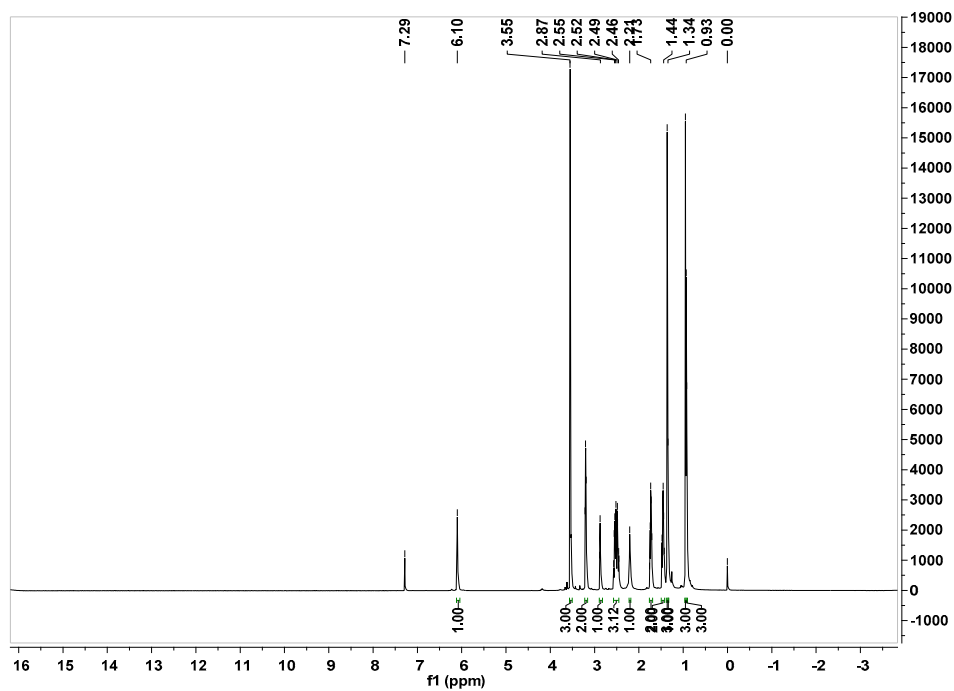
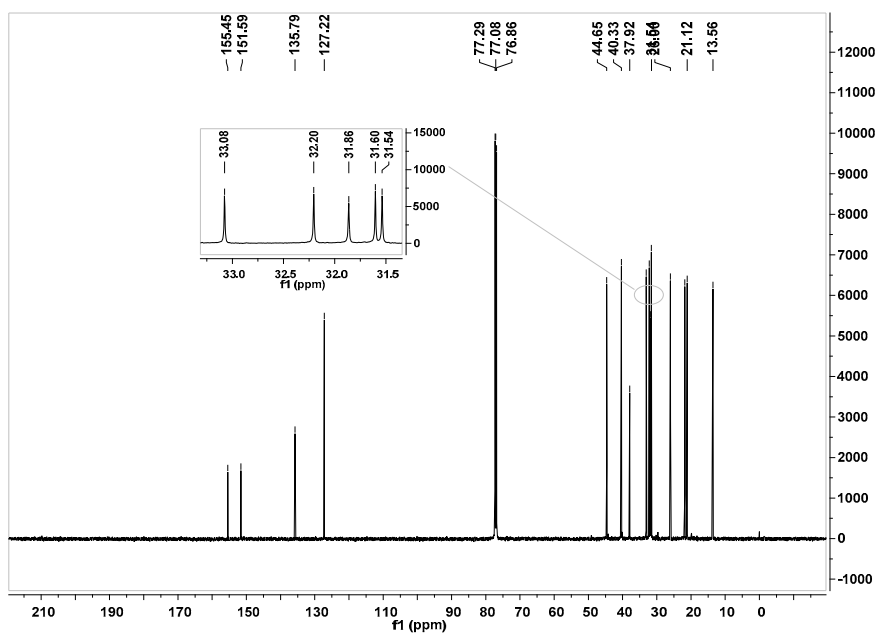
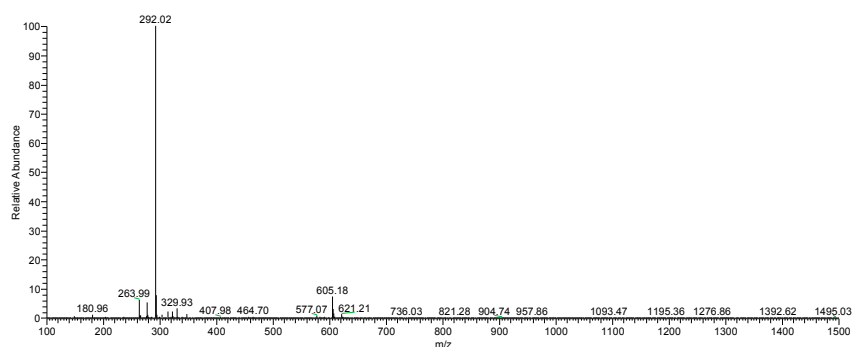
Figure S37. $^1\text{H-NMR}$ spectrum of the target compound **6d** in CDCl_3 .Figure S38. $^{13}\text{C-NMR}$ spectrum of the target compound **6d** in CDCl_3 .

Figure S39. ESI-MS spectrum of the target compound 6d.

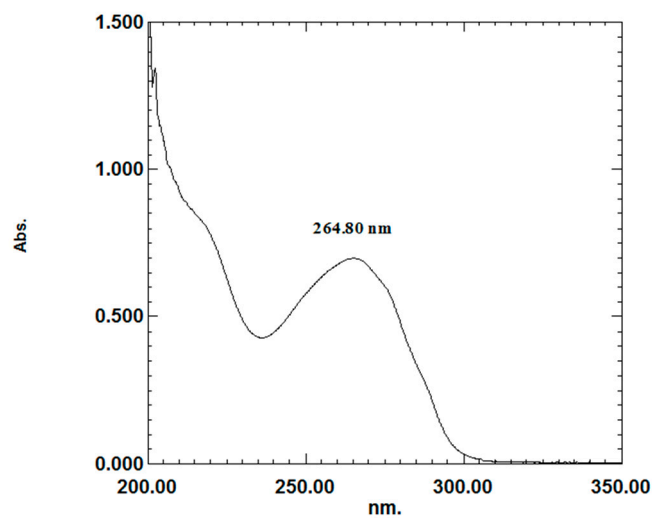


Figure S40. UV-vis spectrum of the target compound 6e in cyclohexane.

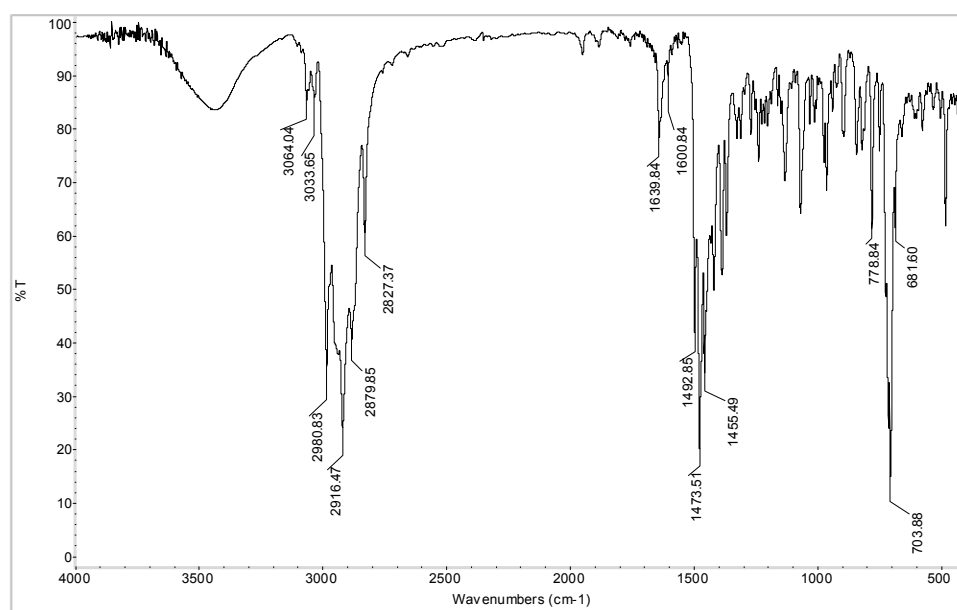
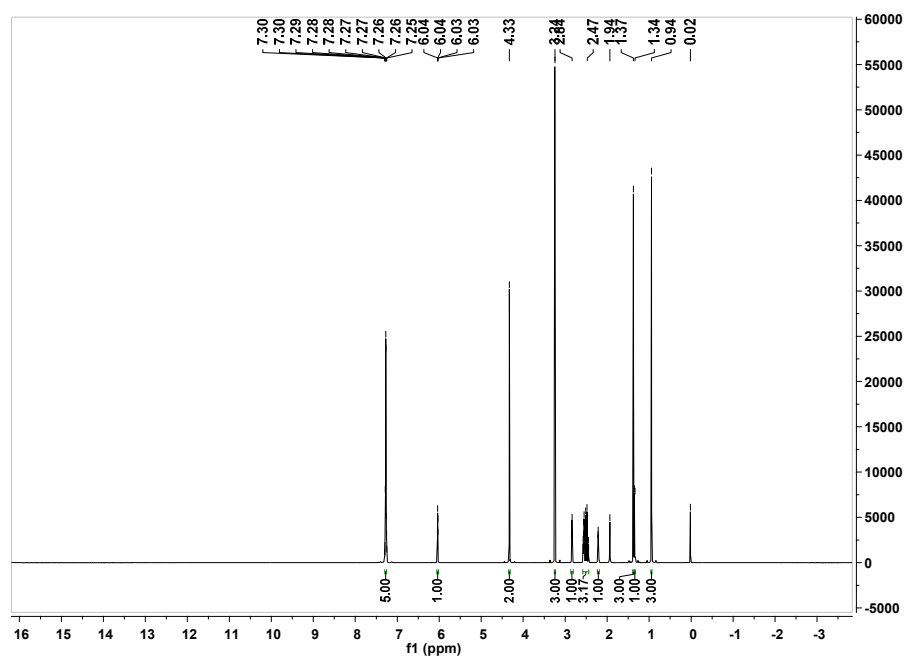
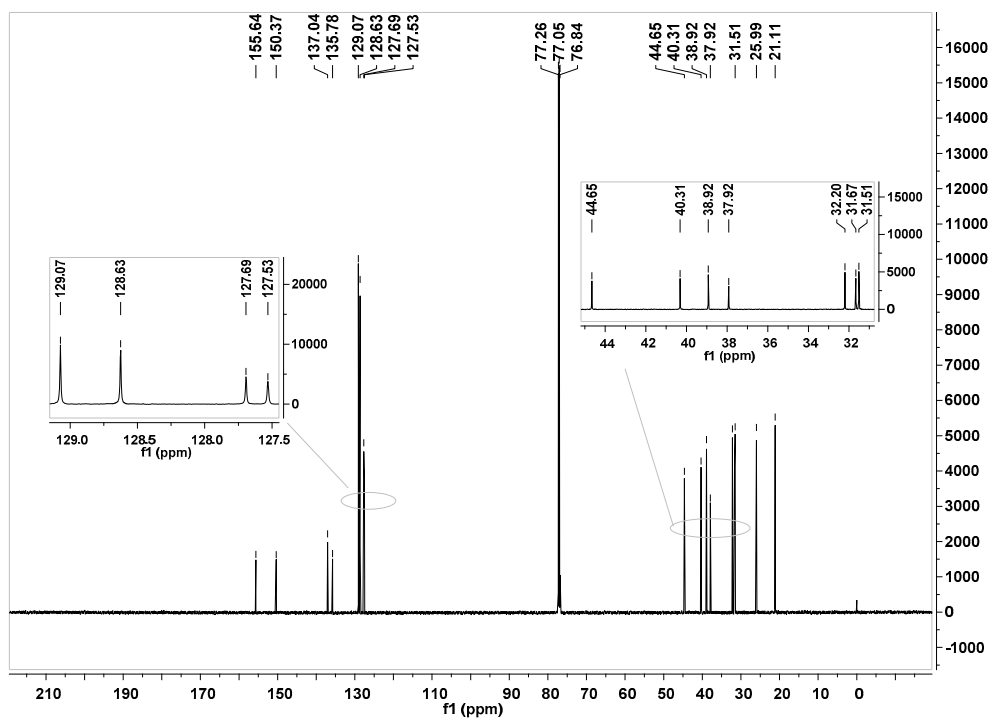


Figure S41. FTIR spectrum of the target compound 6e.

Figure S42. ¹H-NMR spectrum of the target compound 6e in CDCl₃.Figure S43. ¹³C-NMR spectrum of the target compound 6e in CDCl₃.

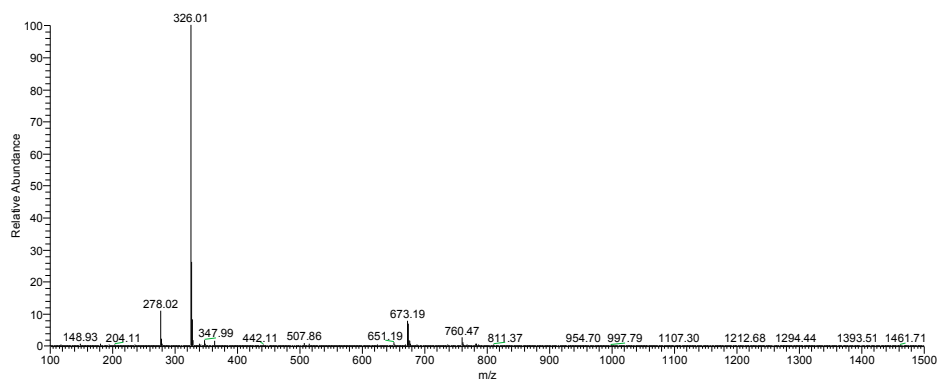


Figure S44. ESI-MS spectrum of the target compound 6e.

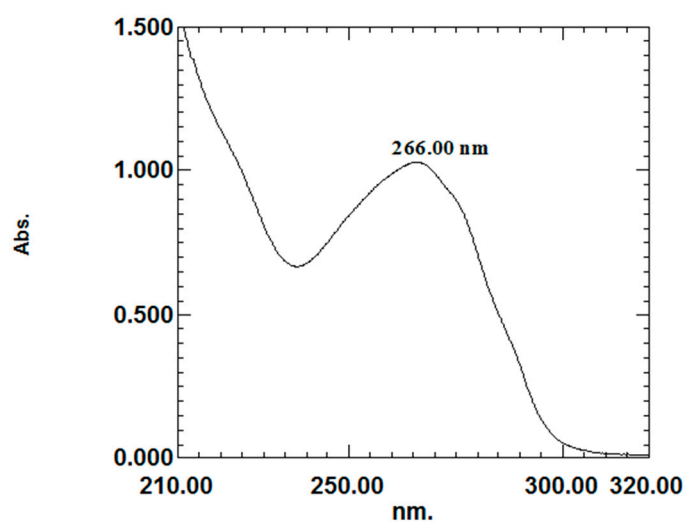


Figure S45. UV-vis spectrum of the target compound 6f in cyclohexane.

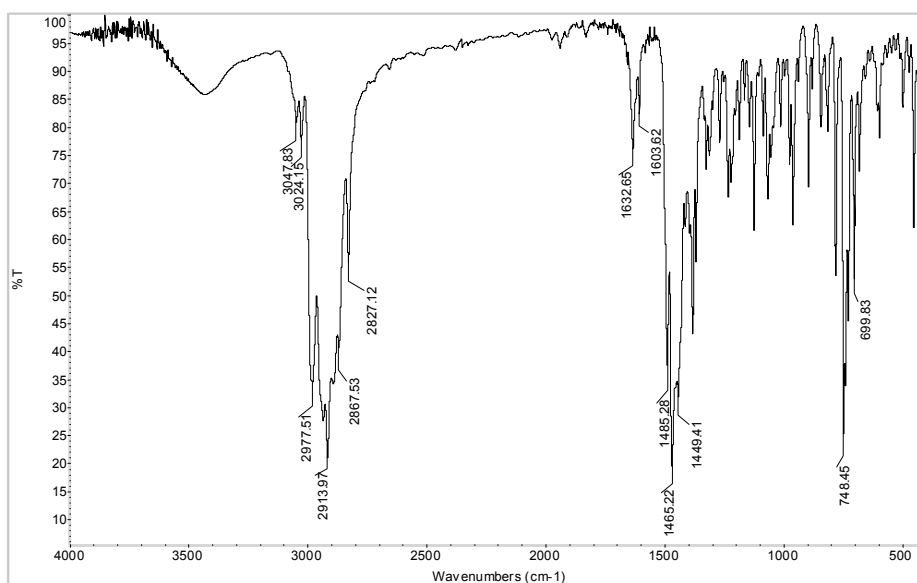


Figure S46. FTIR spectrum of the target compound 6f.

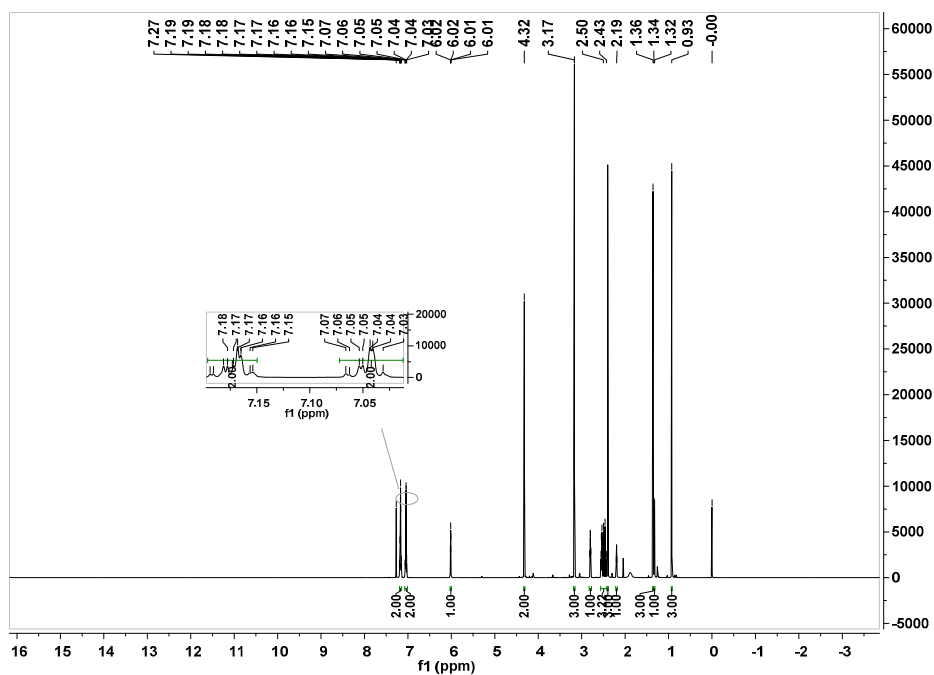


Figure S47. ^1H -NMR spectrum of the target compound **6f** in CDCl_3 .

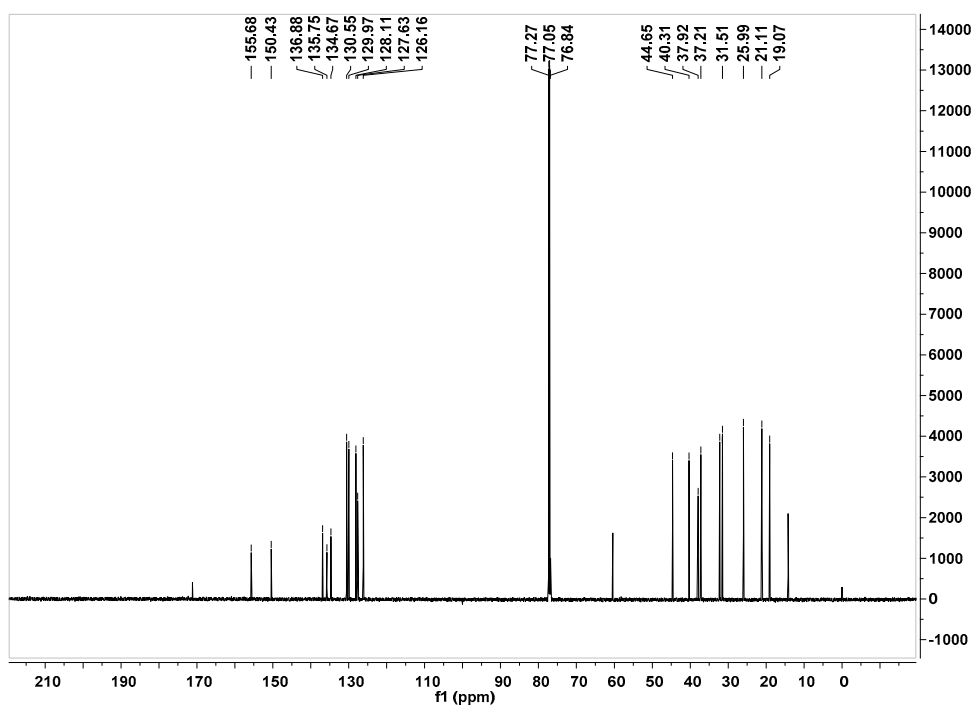


Figure S48. ^{13}C -NMR spectrum of the target compound **6f** in CDCl_3 .

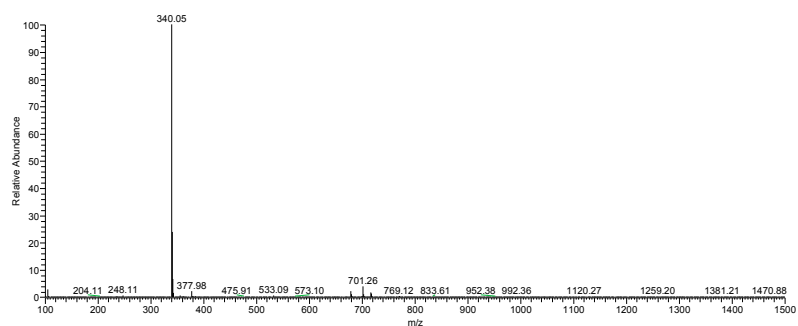


Figure S49. ESI-MS spectrum of the target compound 6f.

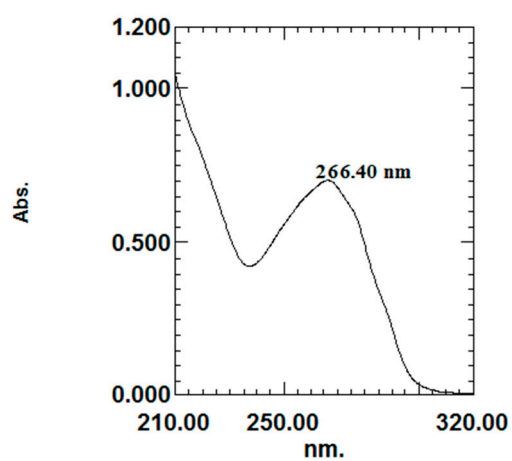


Figure S50. UV-vis spectrum of the target compound 6g in cyclohexane.

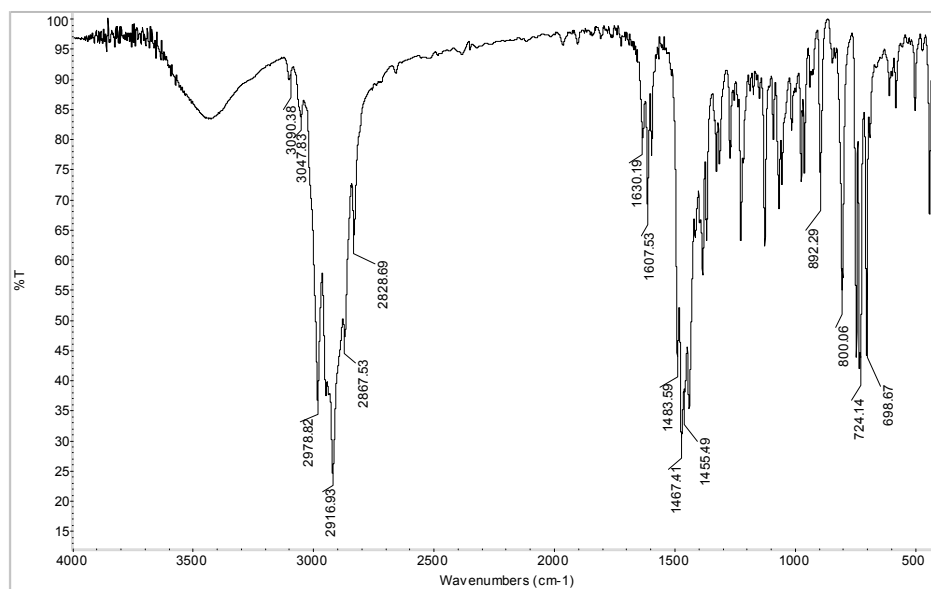


Figure S51. FTIR spectrum of the target compound 6g.

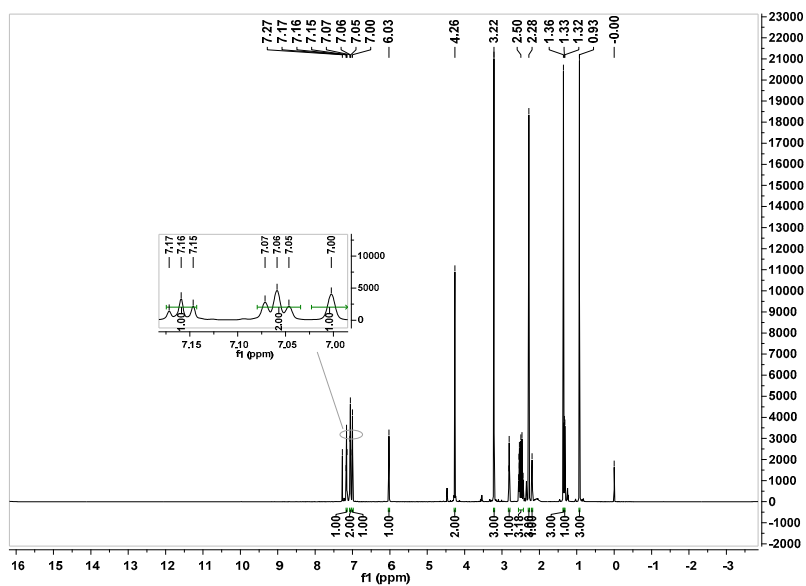


Figure S52. $^1\text{H-NMR}$ spectrum of the target compound **6g** in CDCl_3 .

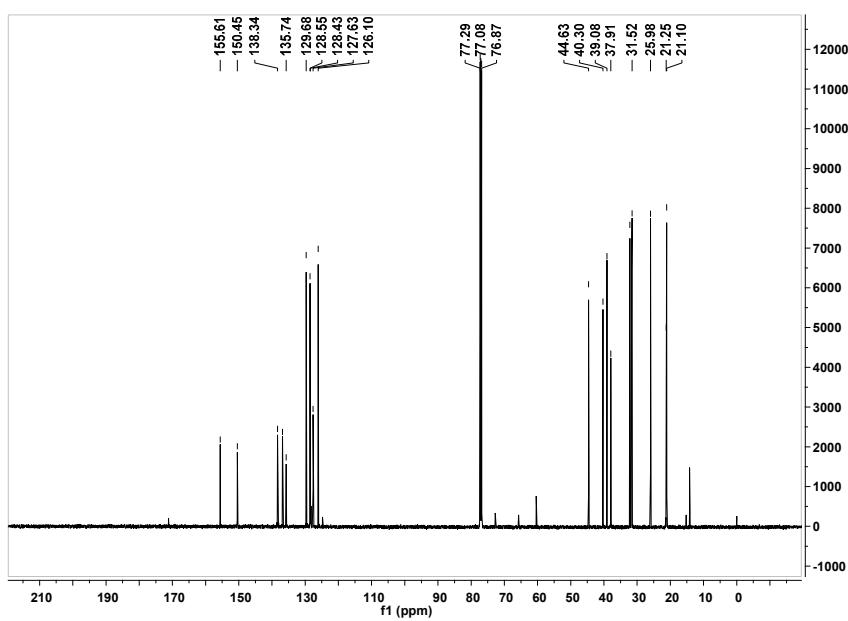


Figure S53. $^{13}\text{C-NMR}$ spectrum of the target compound **6g** in CDCl_3 .

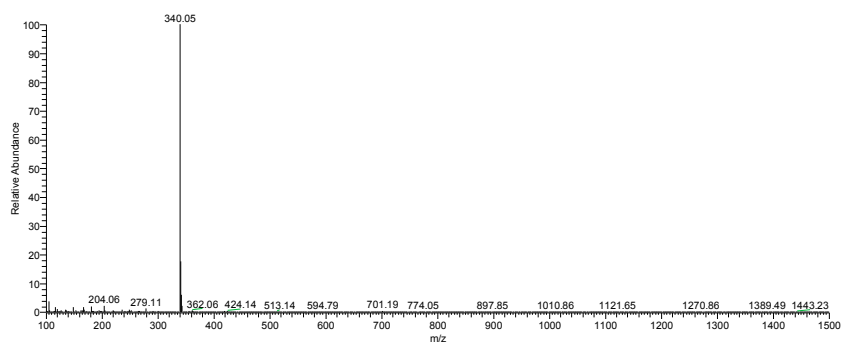


Figure S54. ESI-MS spectrum of the target compound **6g**.

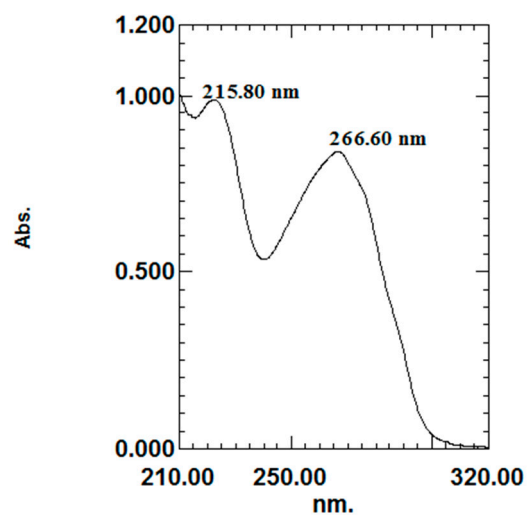


Figure S55. UV-vis spectrum of the target compound **6h** in cyclohexane.

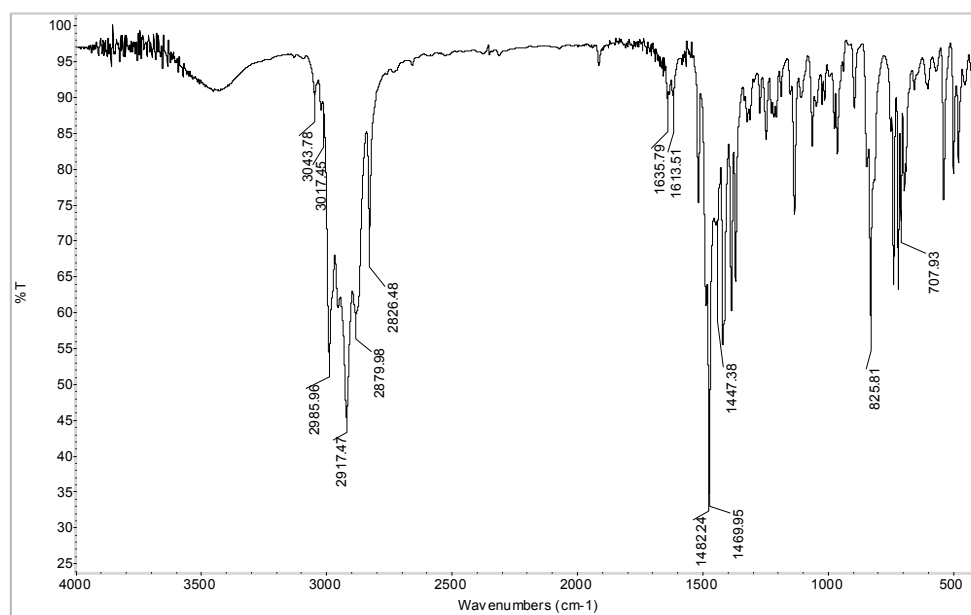
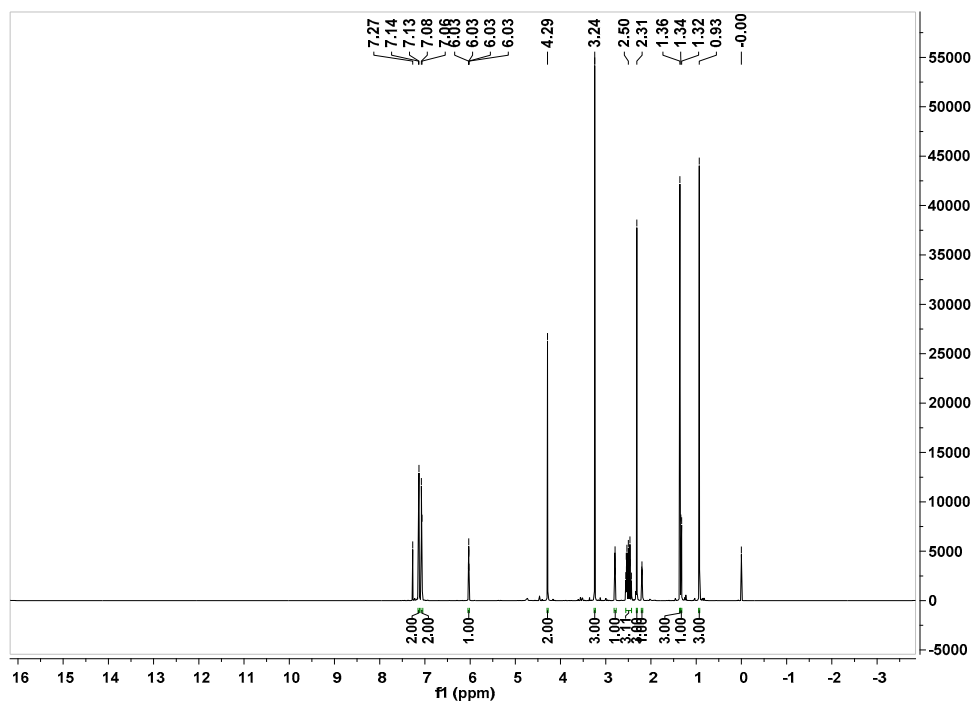
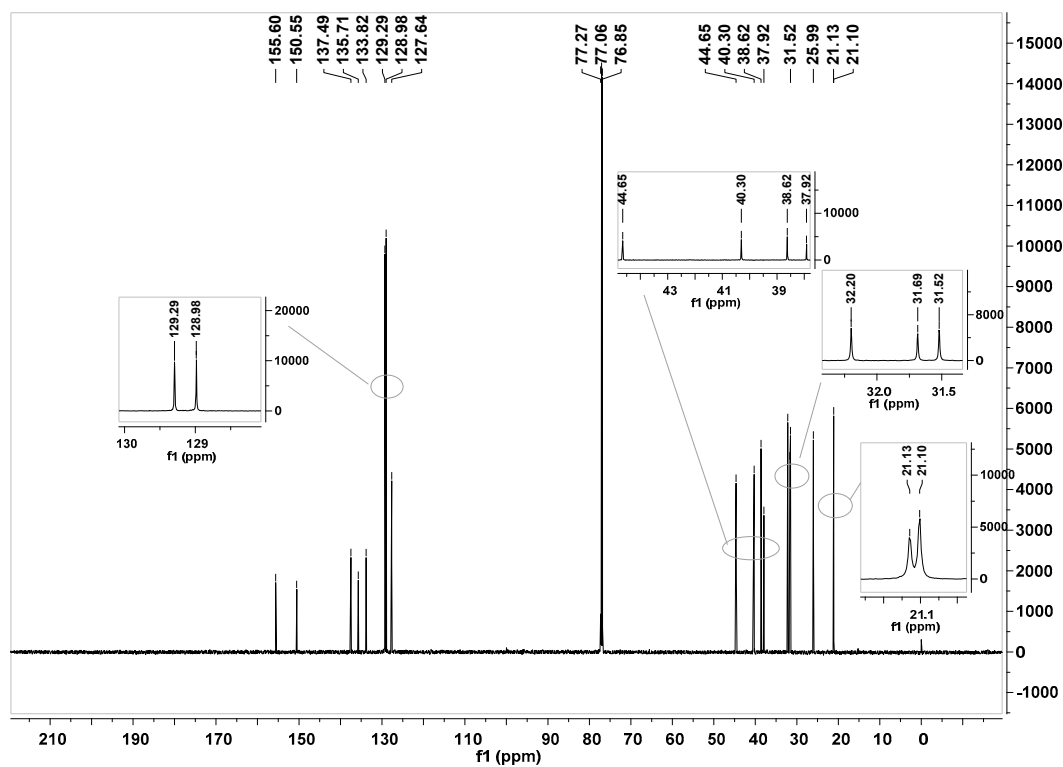


Figure S56. FTIR spectrum of the target compound **6h**.

Figure S57. ¹H-NMR spectrum of the target compound **6h** in CDCl₃.Figure S58. ¹³C-NMR spectrum of the target compound **6h** in CDCl₃.

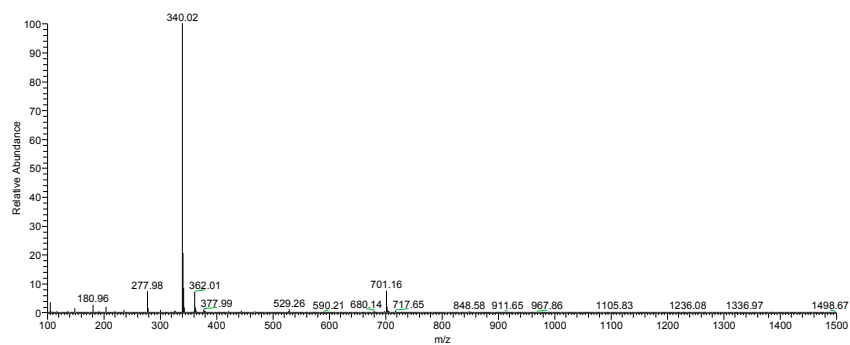


Figure S59. ESI-MS spectrum of the target compound **6h**.

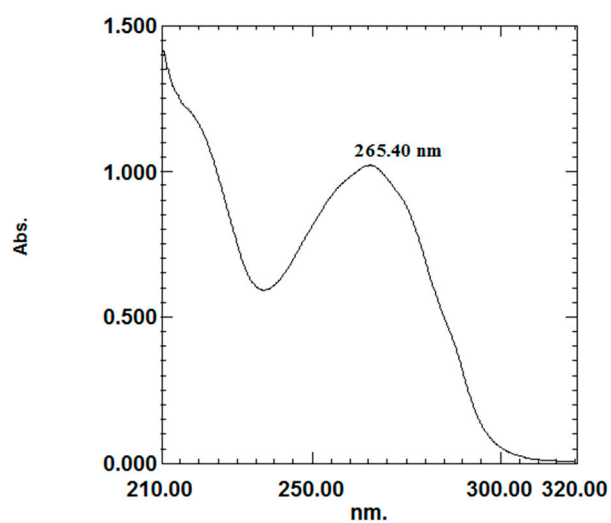


Figure S60. UV-vis spectrum of the target compound **6i** in cyclohexane.

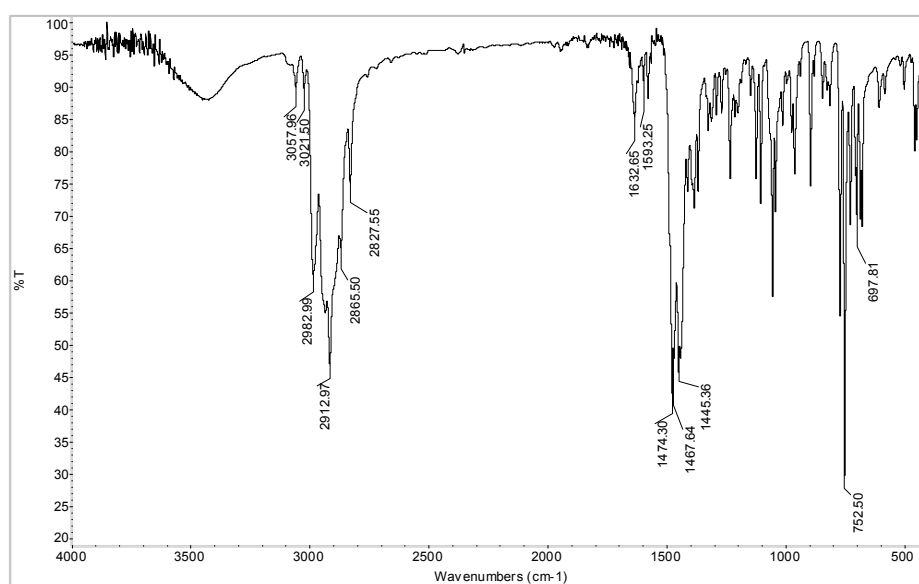


Figure S61. FTIR spectrum of the target compound **6i**.

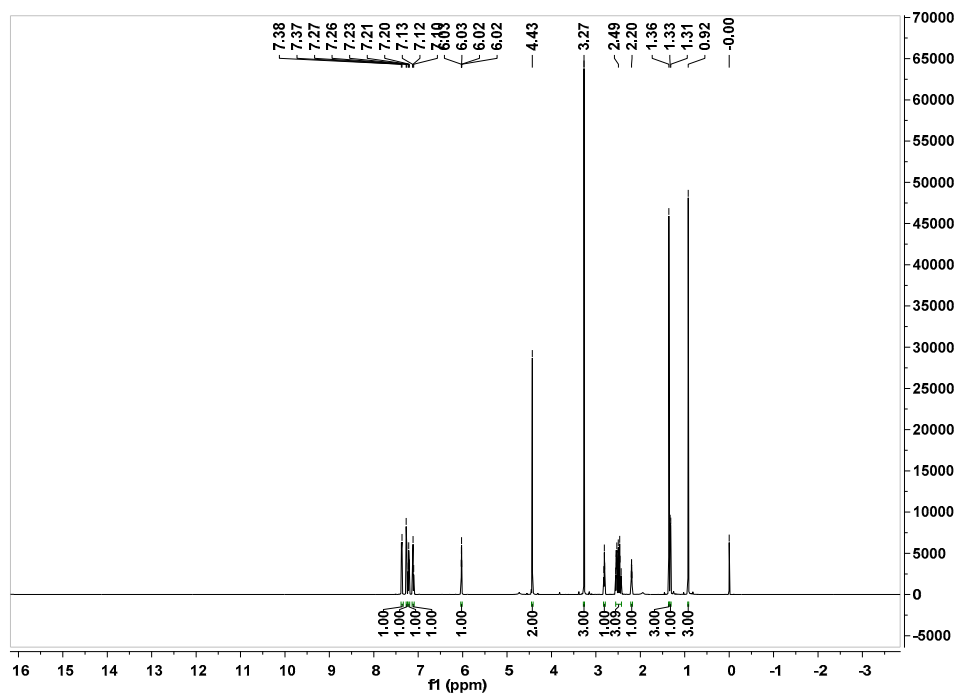


Figure S62. ¹H-NMR spectrum of the target compound **6i** in CDCl₃.

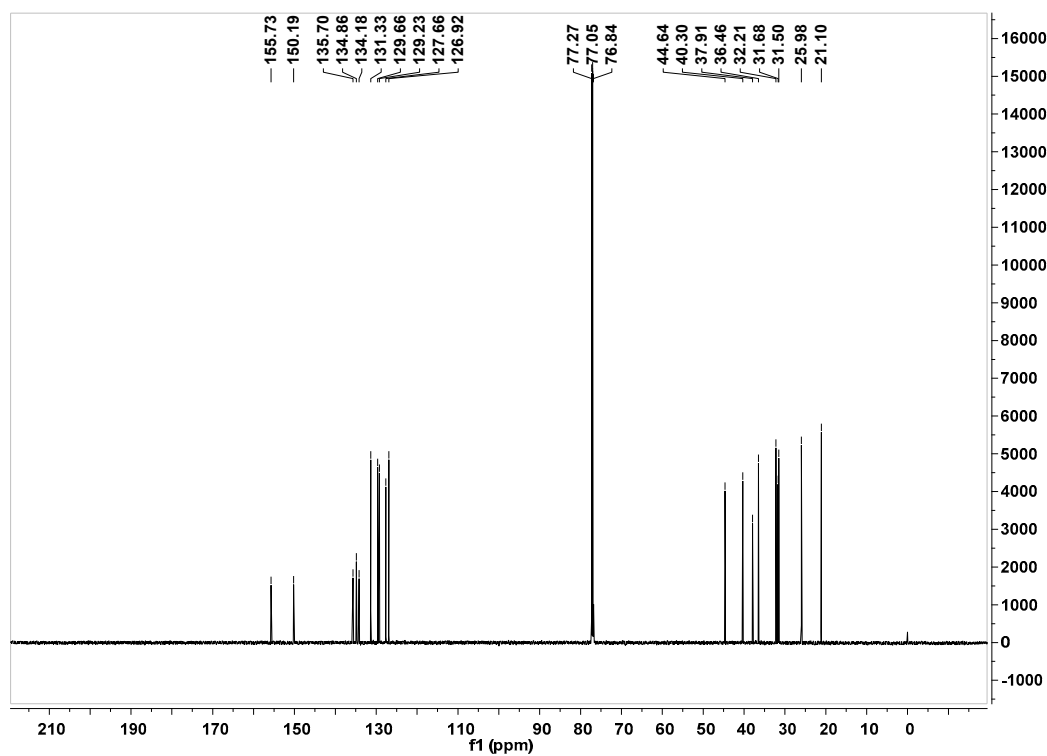


Figure S63. ¹³C-NMR spectrum of the target compound **6i** in CDCl₃.

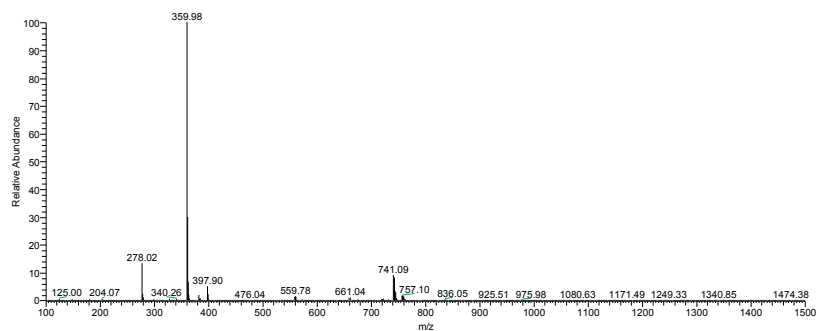


Figure S64. ESI-MS spectrum of the target compound 6i.

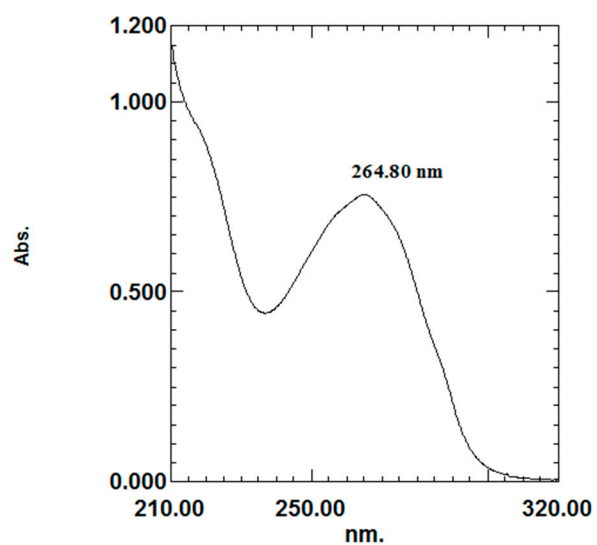


Figure S65. UV-vis spectrum of the target compound 6j in cyclohexane.

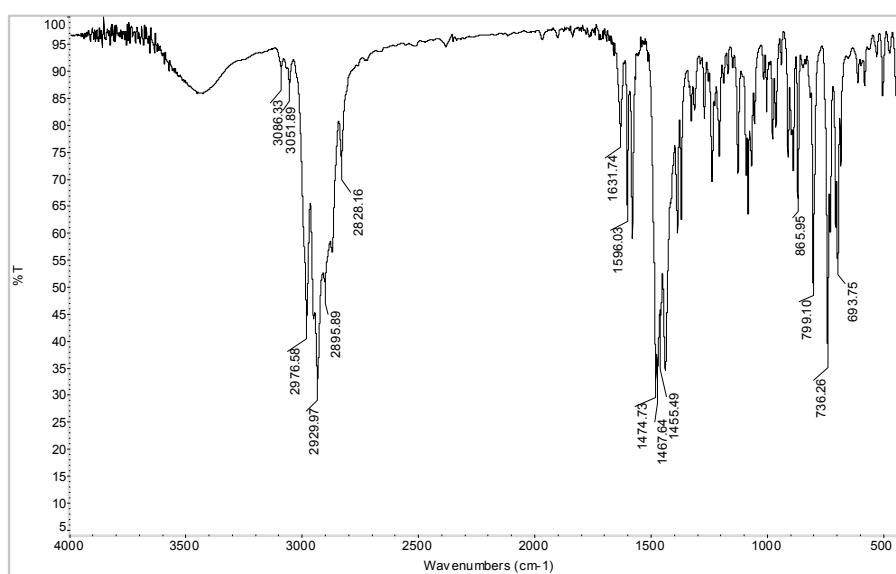
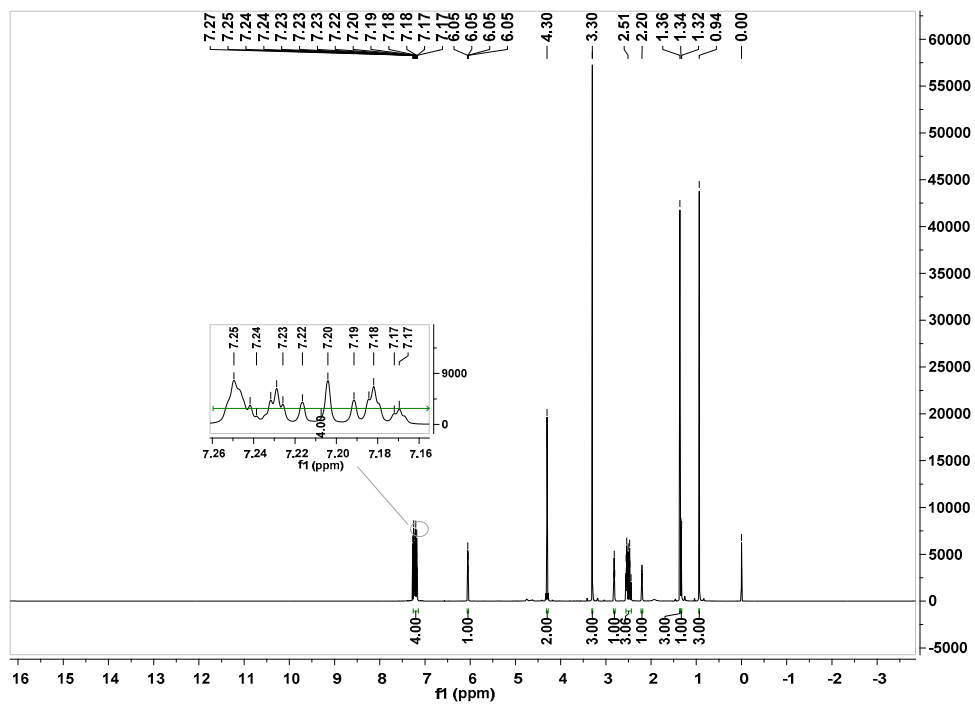
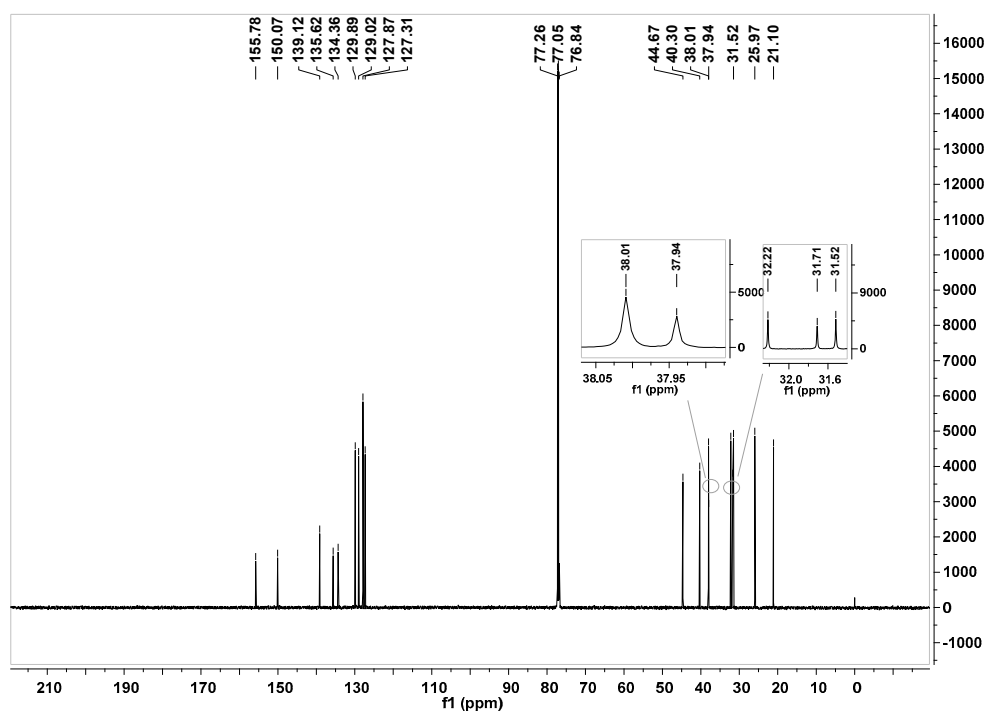


Figure S66. FTIR spectrum of the target compound 6j.

Figure S67. ¹H-NMR spectrum of the target compound **6j** in CDCl₃.Figure S68. ¹³C-NMR spectrum of the target compound **6j** in CDCl₃.

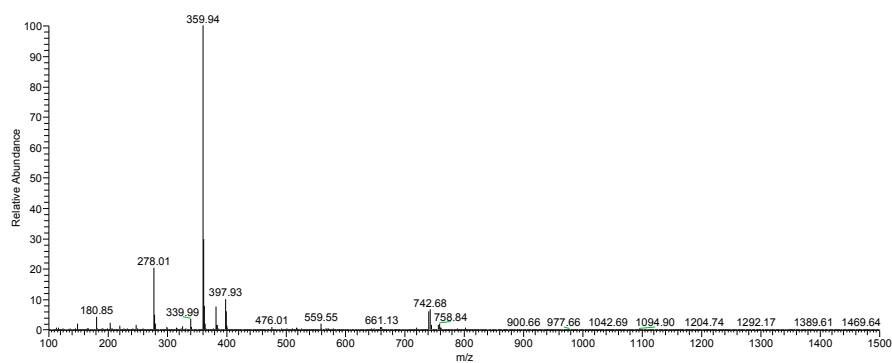


Figure S69. ESI-MS spectrum of the target compound 6j.

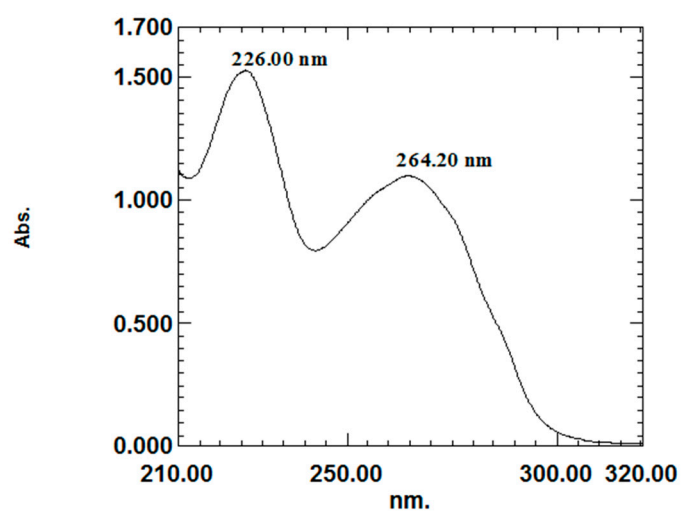


Figure S70. UV-vis spectrum of the target compound 6k in cyclohexane.

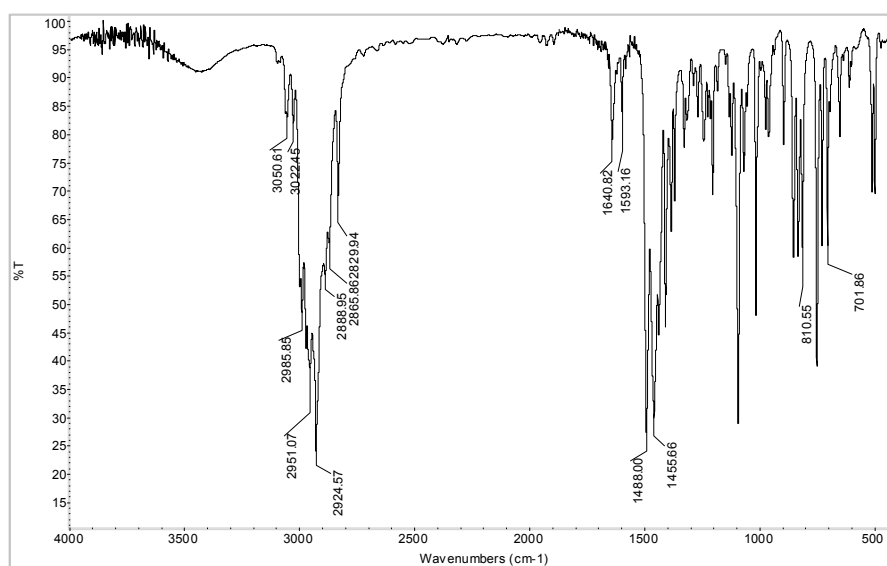


Figure S71. FTIR spectrum of the target compound 6k.

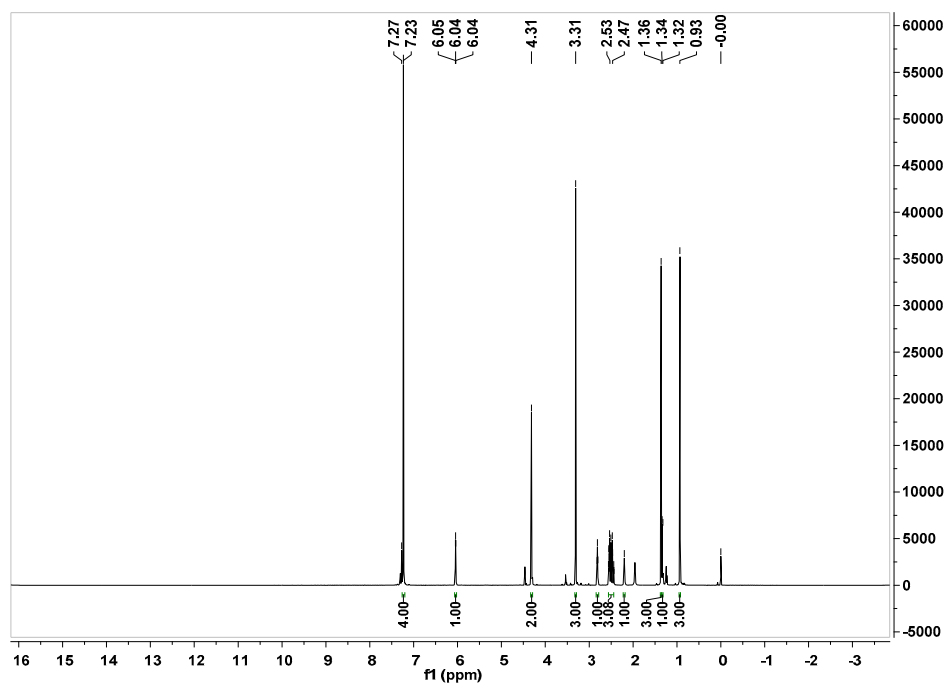
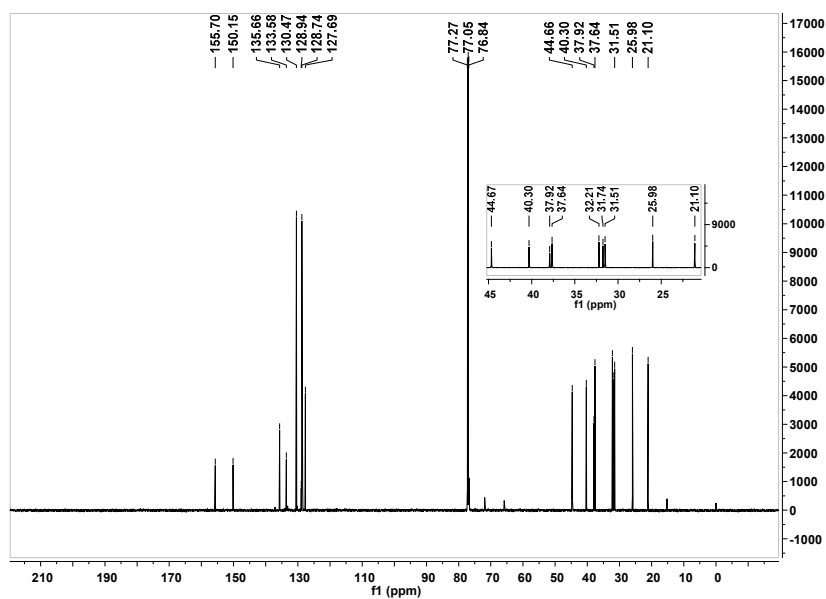
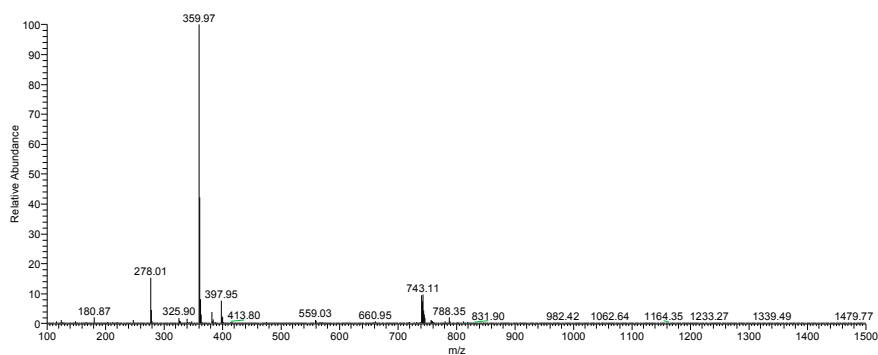
Figure S72. ^1H -NMR spectrum of the target compound **6k** in CDCl_3 .Figure S73. ^{13}C -NMR spectrum of the target compound **6k** in CDCl_3 .

Figure S74. ESI-MS spectrum of the target compound 6k.

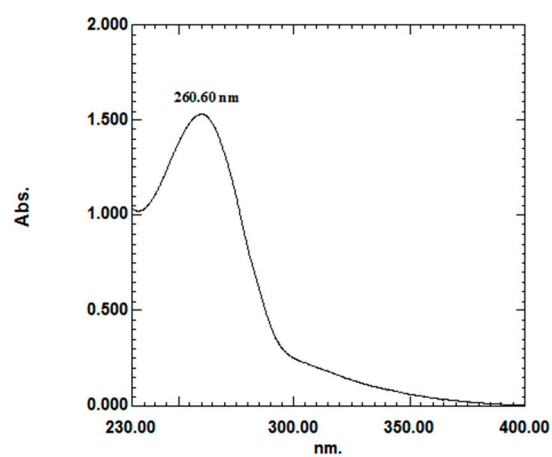


Figure S75. UV-vis spectrum of the target compound 6l in EtOH.

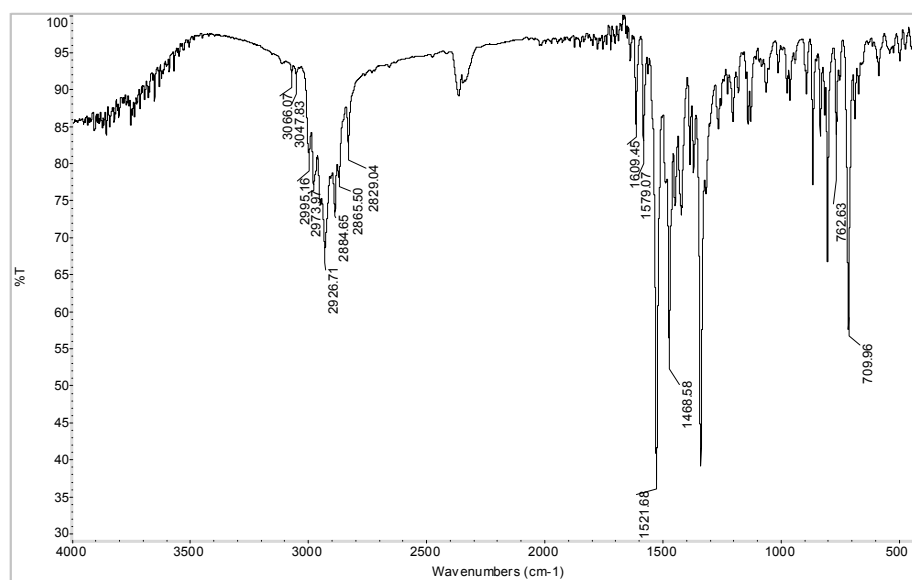
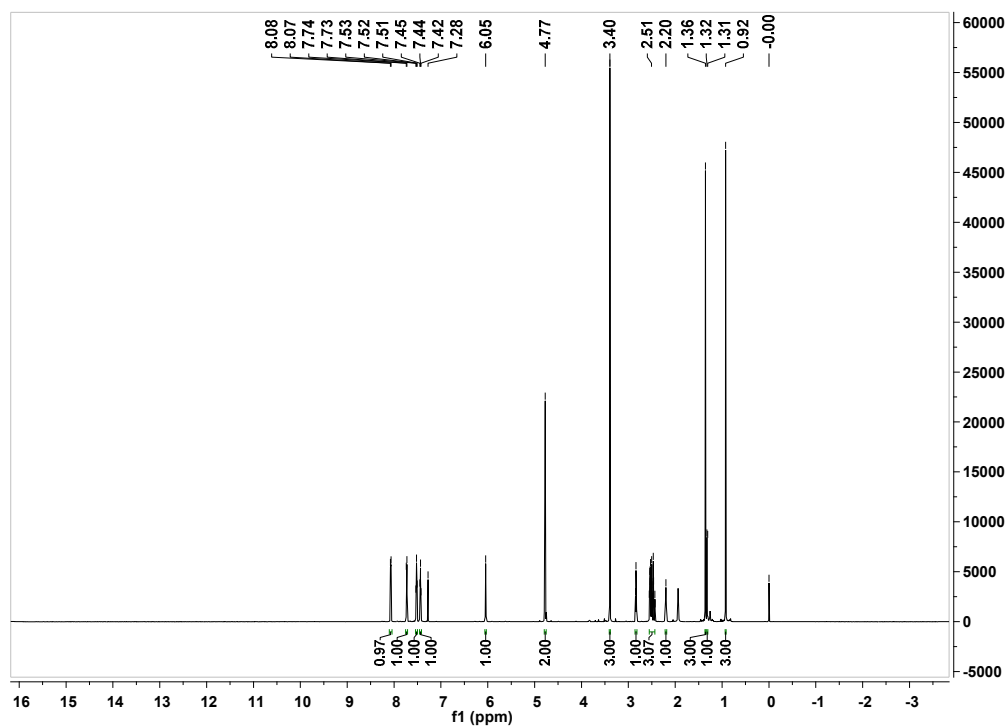
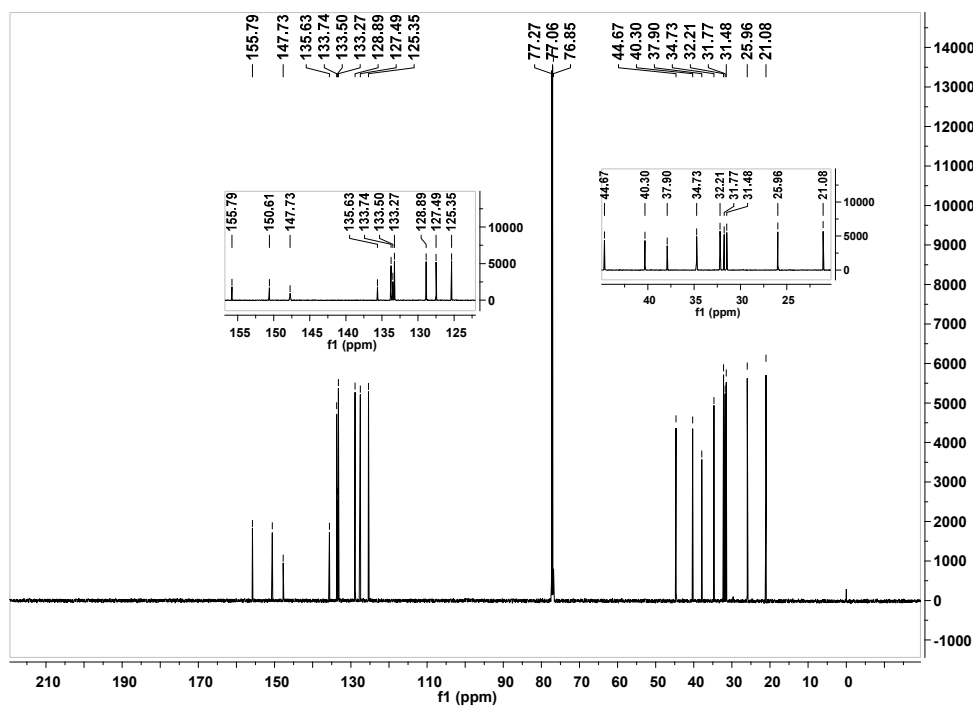


Figure S76. FTIR spectrum of the target compound 6l.

Figure S77. ¹H-NMR spectrum of the target compound **6l** in CDCl₃.Figure S78. ¹³C-NMR spectrum of the target compound **6l** in CDCl₃.

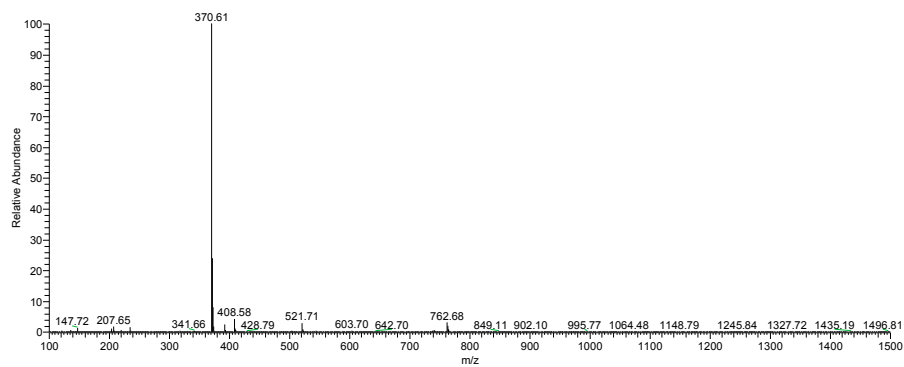


Figure S79. ESI-MS spectrum of the target compound 6l.

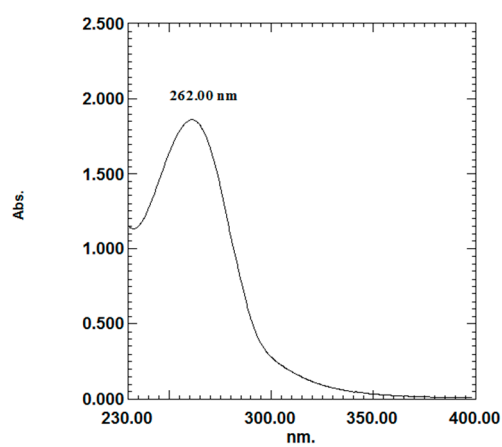


Figure S80. UV-vis spectrum of the target compound 6m in EtOH.

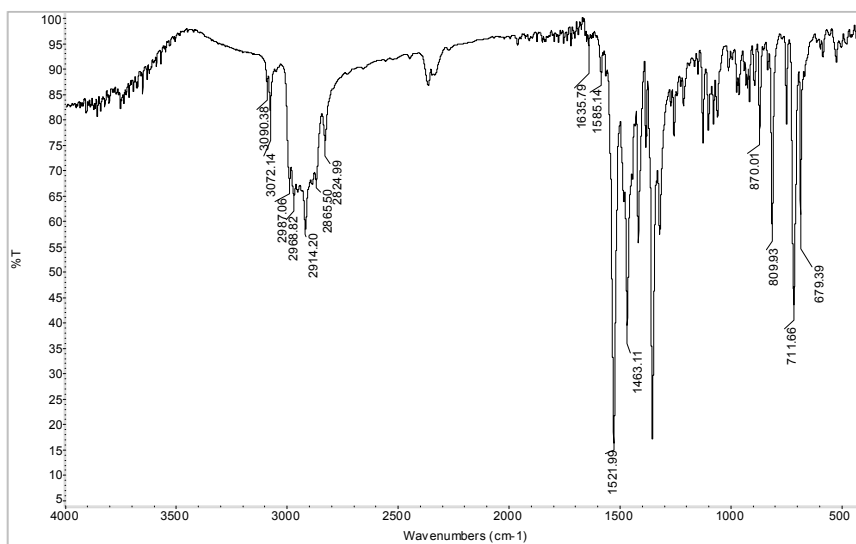
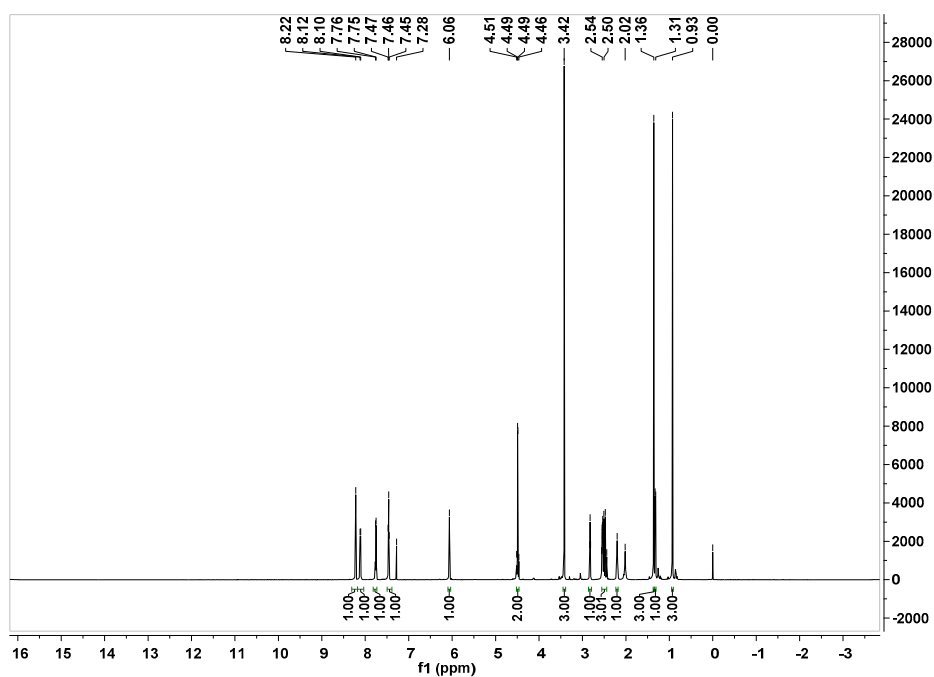
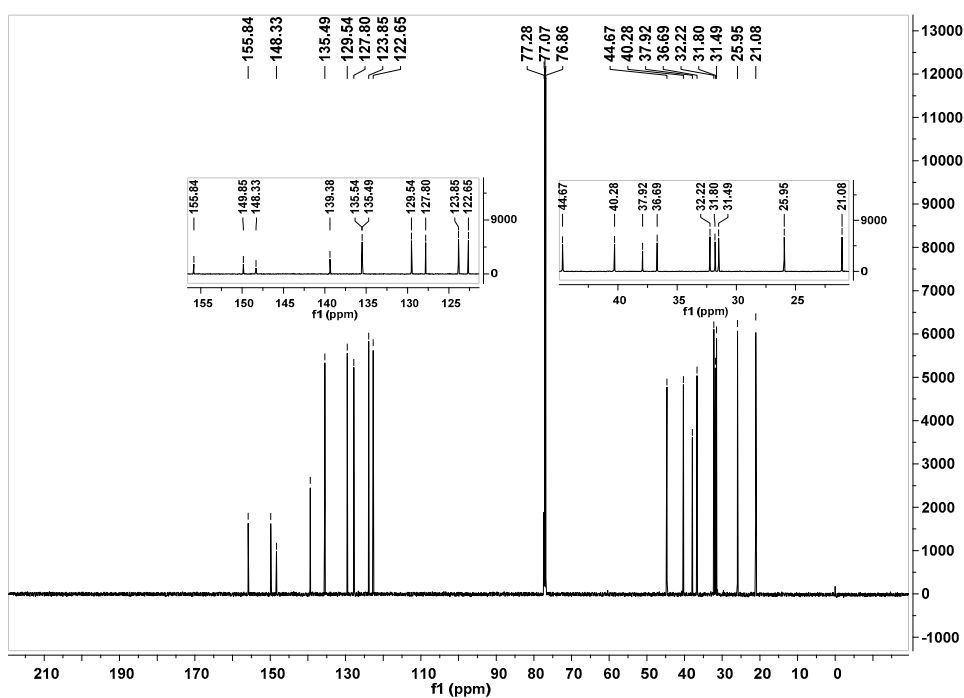


Figure S81. FTIR spectrum of the target compound 6m.

Figure S82. ¹H-NMR spectrum of the target compound **6m** in CDCl₃.Figure S83. ¹³C-NMR spectrum of the target compound **6m** in CDCl₃.

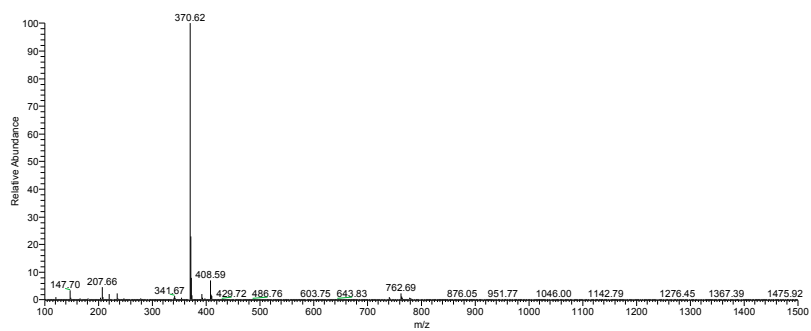


Figure S84. ESI-MS spectrum of the target compound 6m.

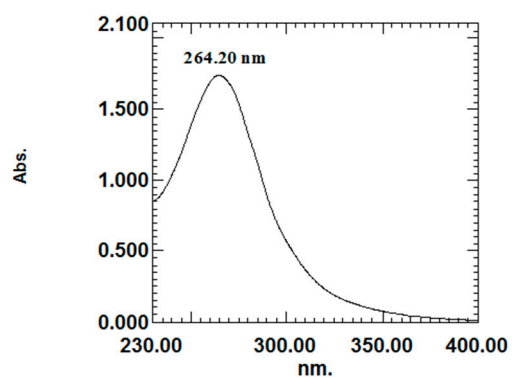


Figure S84. UV-vis spectrum of the target compound 6n in EtOH.

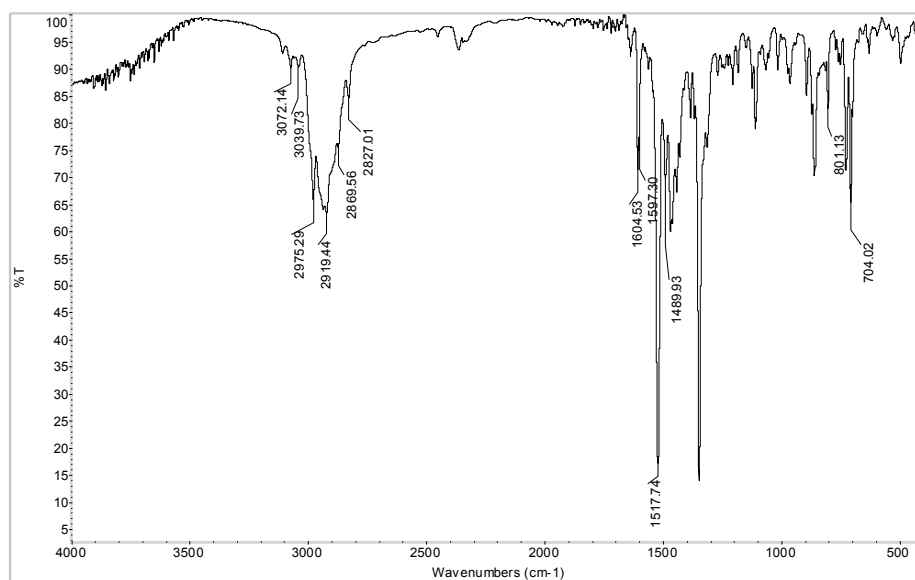
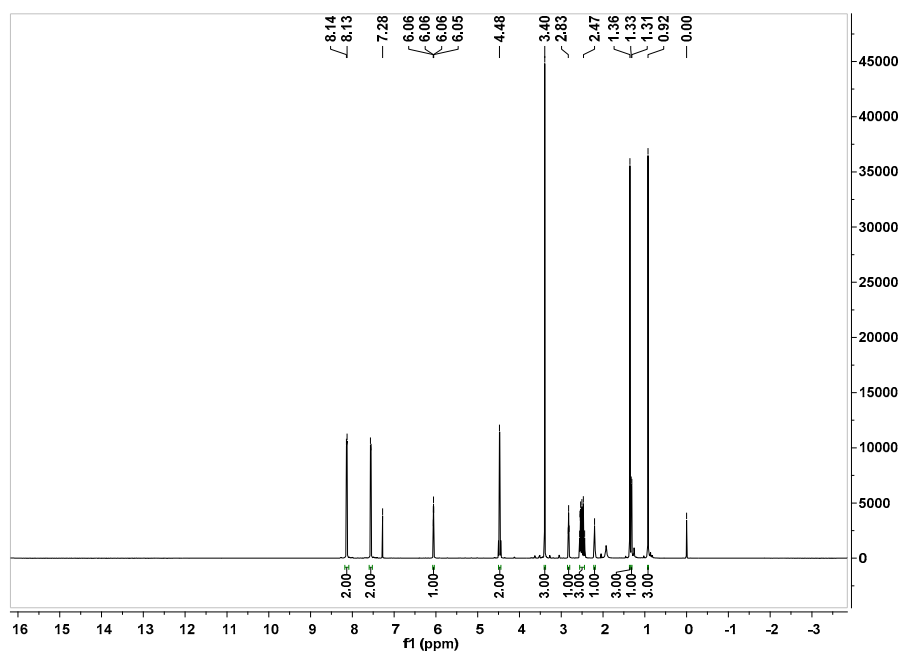
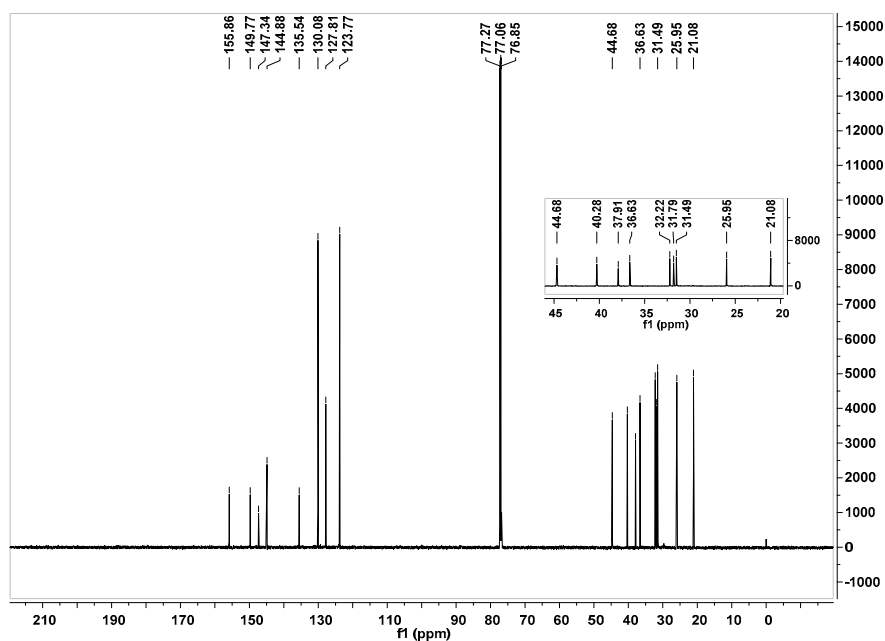
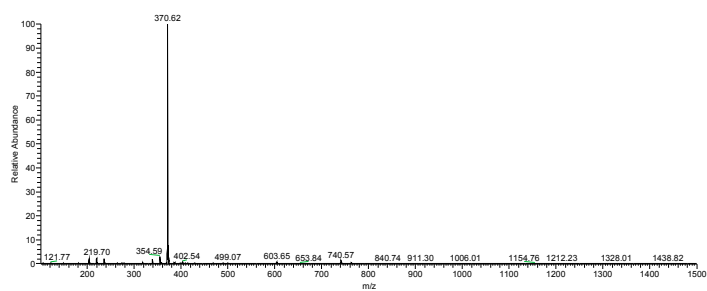


Figure S86. FTIR spectrum of the target compound 6n.

Figure S87. ^1H -NMR spectrum of the target compound **6n** in CDCl_3 .Figure S88. ^{13}C -NMR spectrum of the target compound **6n** in CDCl_3 .Figure S89. ESI-MS spectrum of the target compound **6n**.