MJCCA9 –

Received: March 17, 2026
Accepted: August 4, 2026

ISSN 1857-5552
e-ISSN 1857-5625
DOI: 10.20450/mjcce.2026.3489
Original scientific paper

SUPPLEMENTARY MATERIAL

MICROWAVE SOLVENT-FREE SYNTHESIS OF ANTIPYRINE-BASED TRIARYLMETHANES AND EVALUATION OF THEIR PHARMACOLOGICAL PROPERTIES

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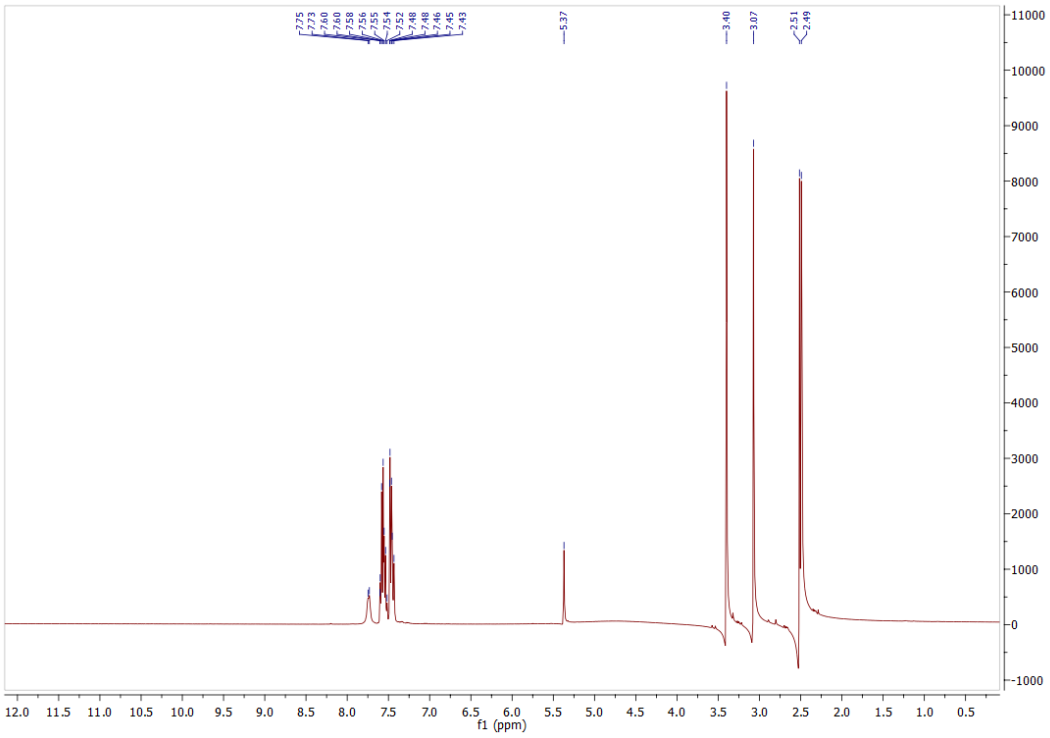


Figure S1. ^{1}H NMR spectrum of **3a**

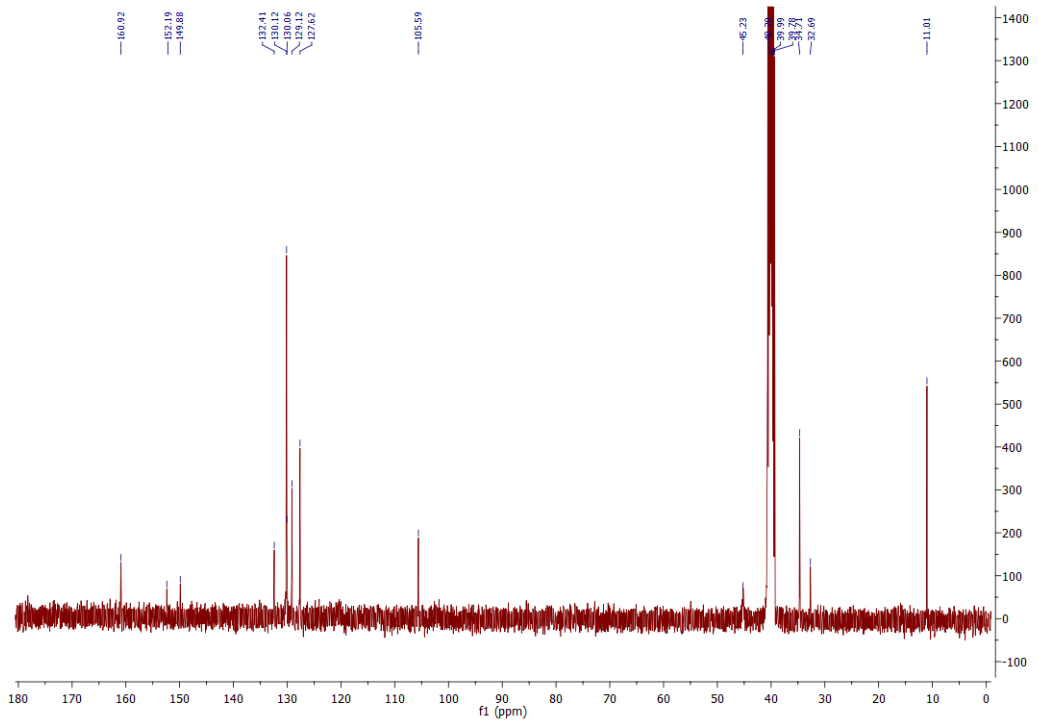


Figure S2. ^{13}C NMR spectrum of **3a**

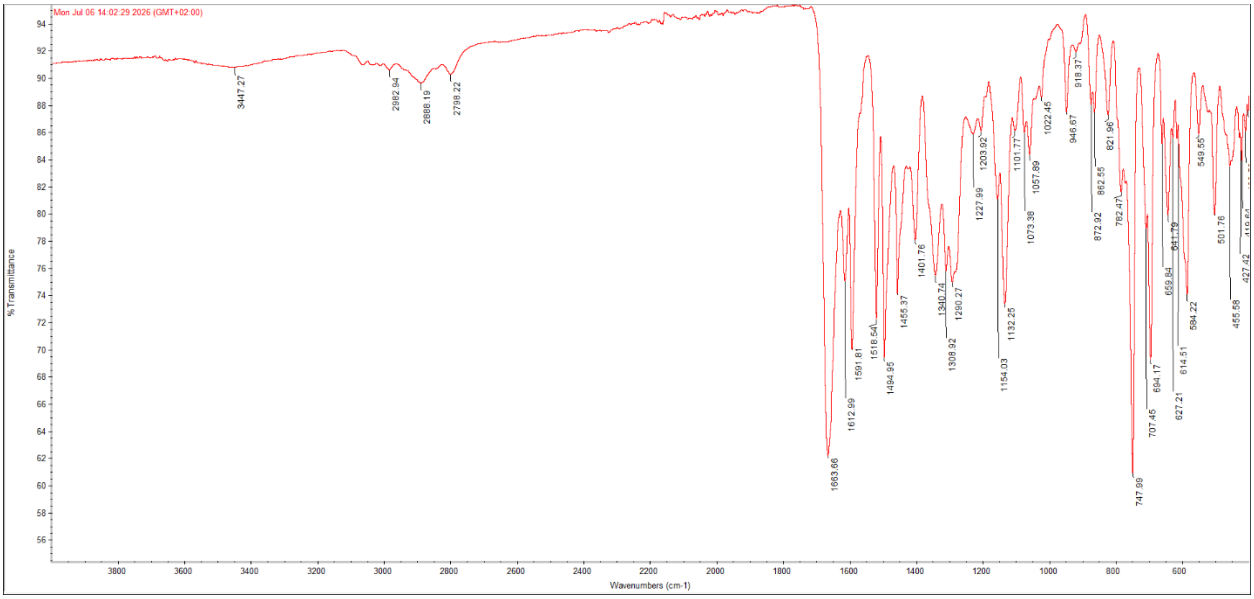


Figure S3. FTIR spectrum of **3a**

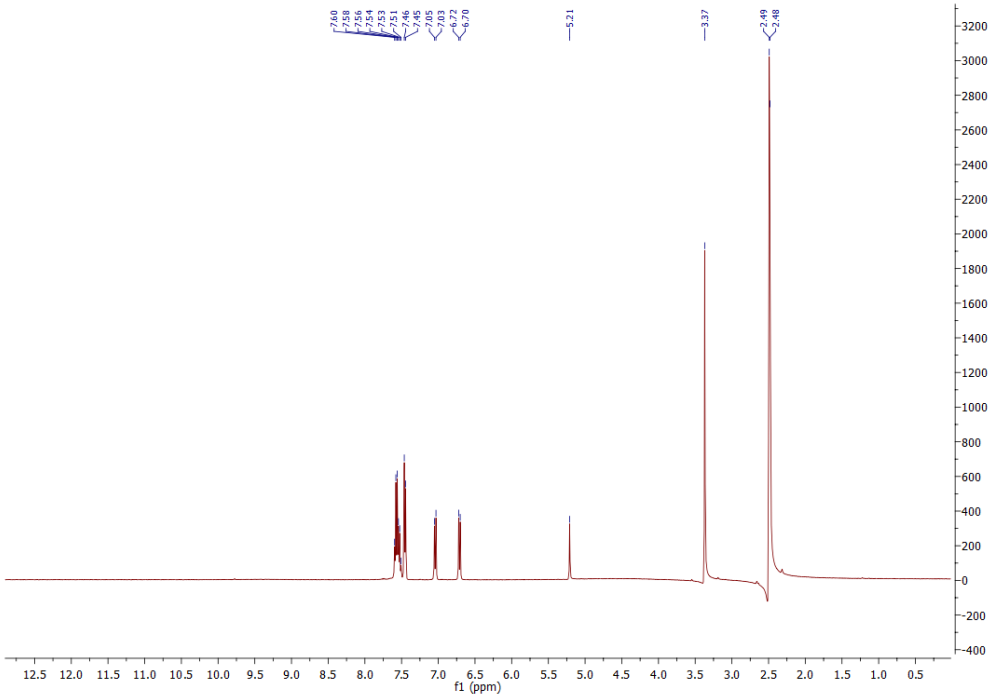


Figure S4. ^{1}H NMR spectrum of **3b**

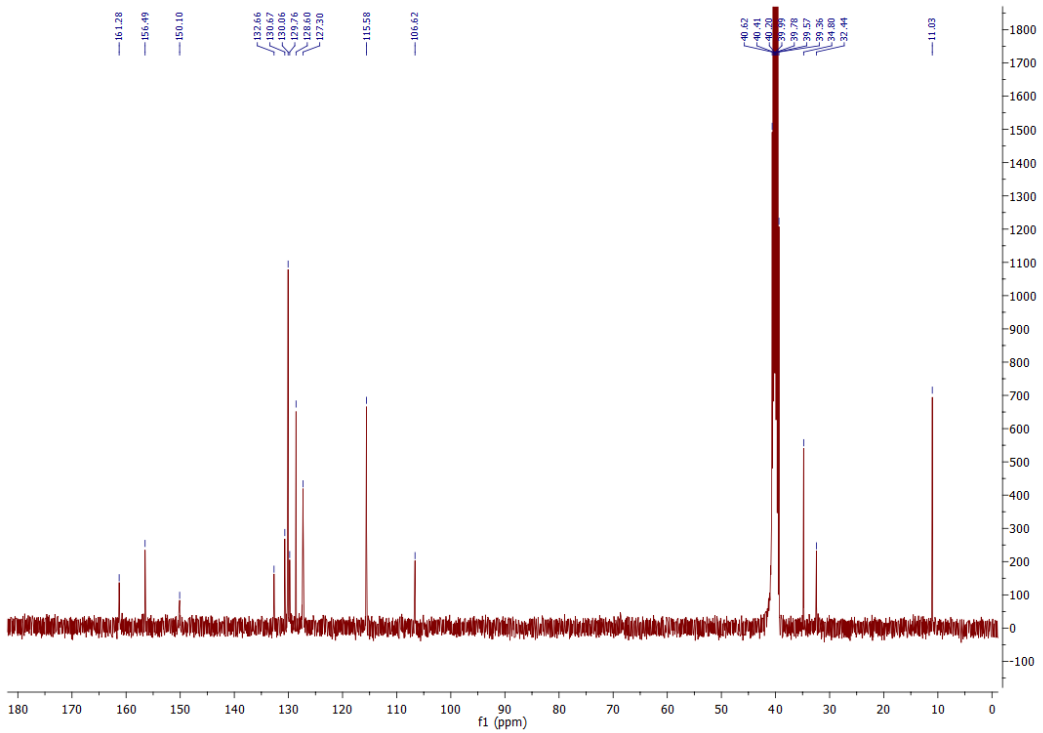


Figure S5. ^{13}C NMR spectrum of **3b**

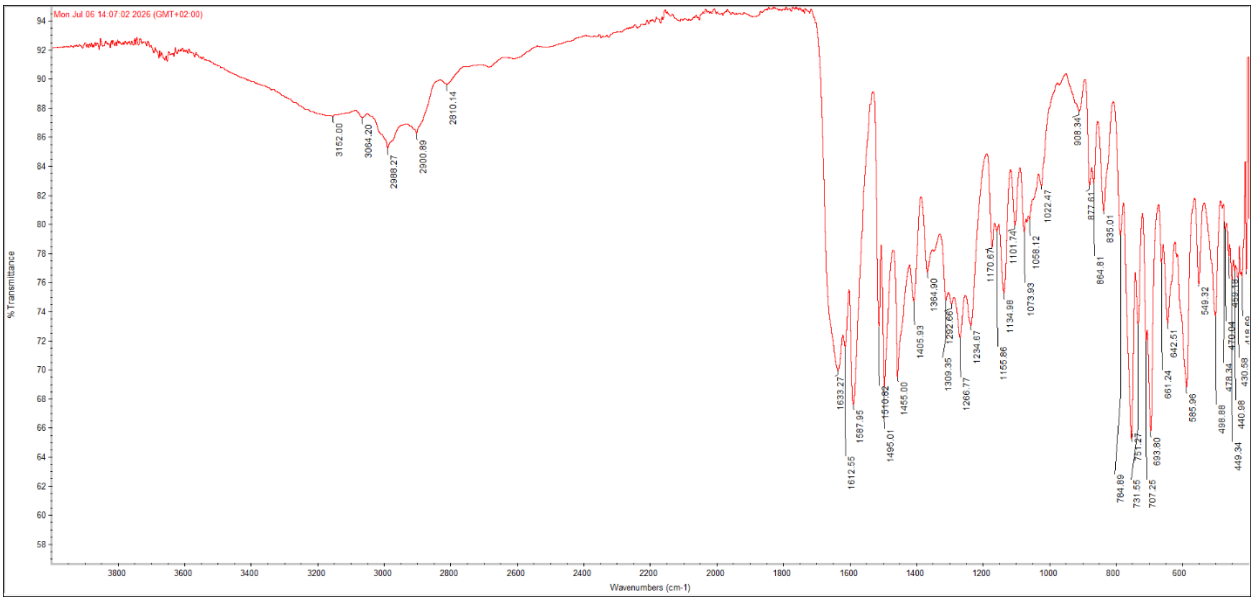


Figure S6. FTIR spectrum of **3b**

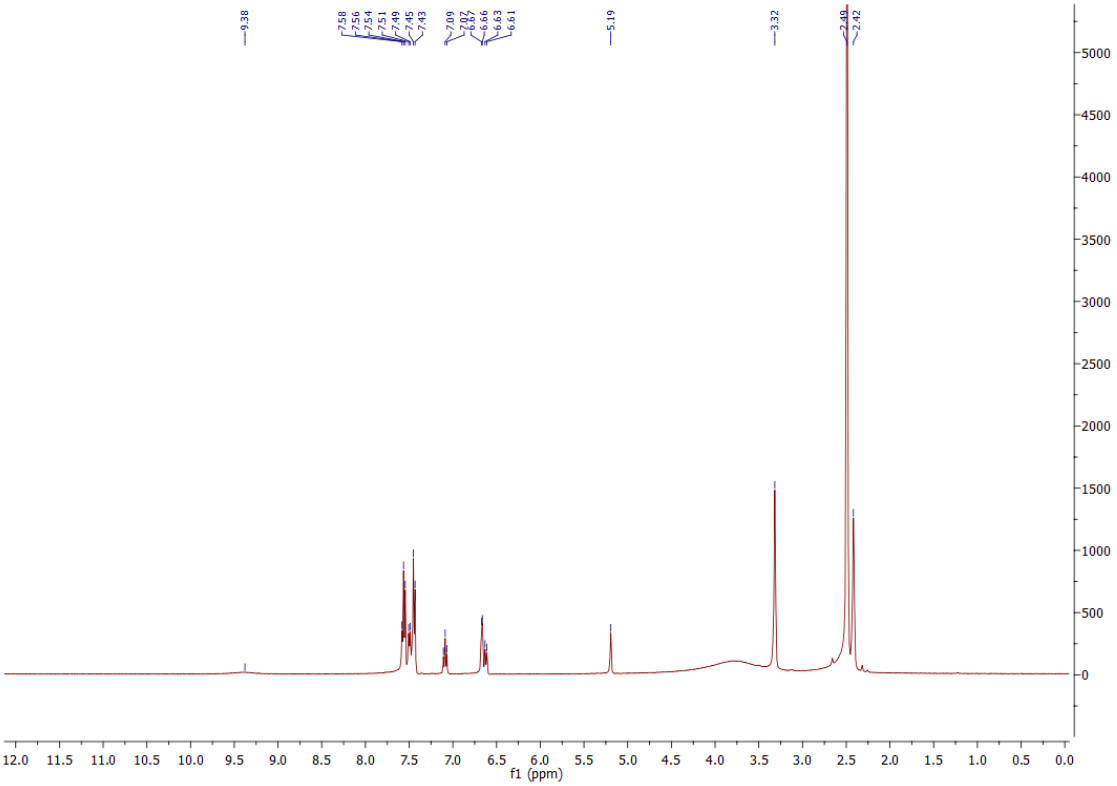


Figure S7. ^{1}H NMR spectrum of **3c**

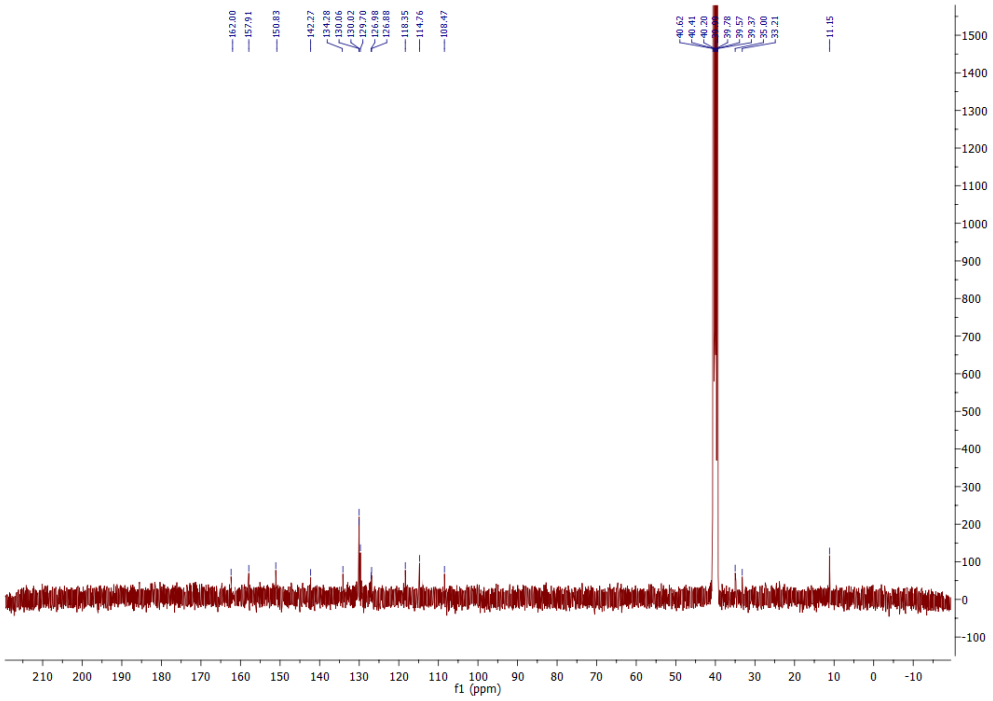


Figure S8. ^{13}C NMR spectrum of **3c**

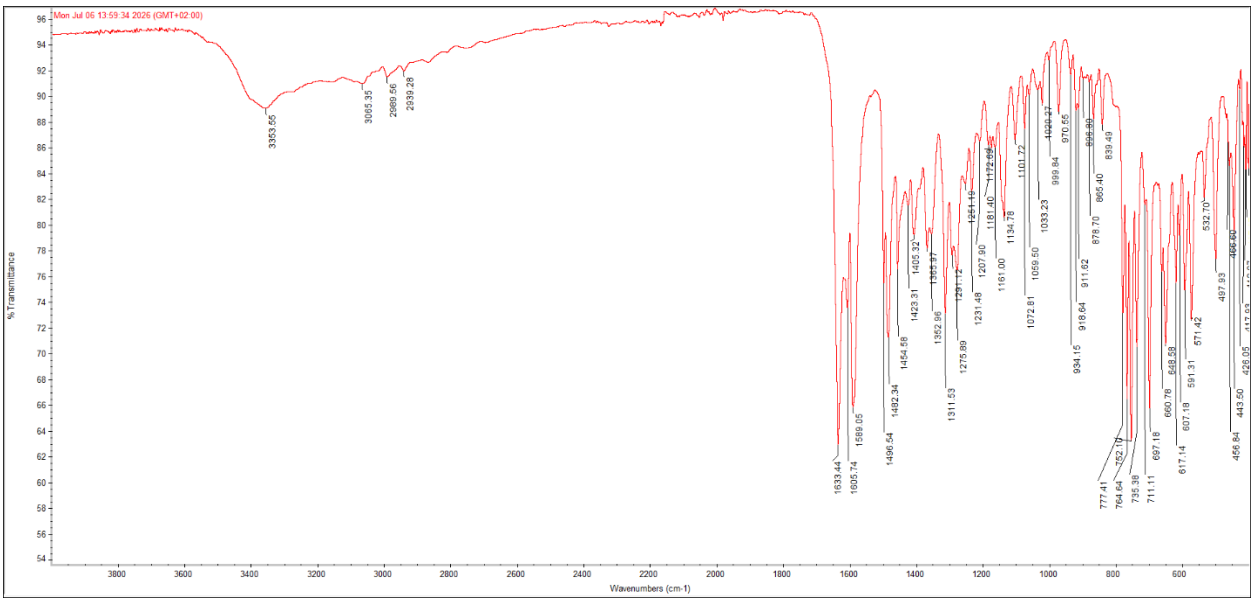


Figure S9. FTIR spectrum of **3c**

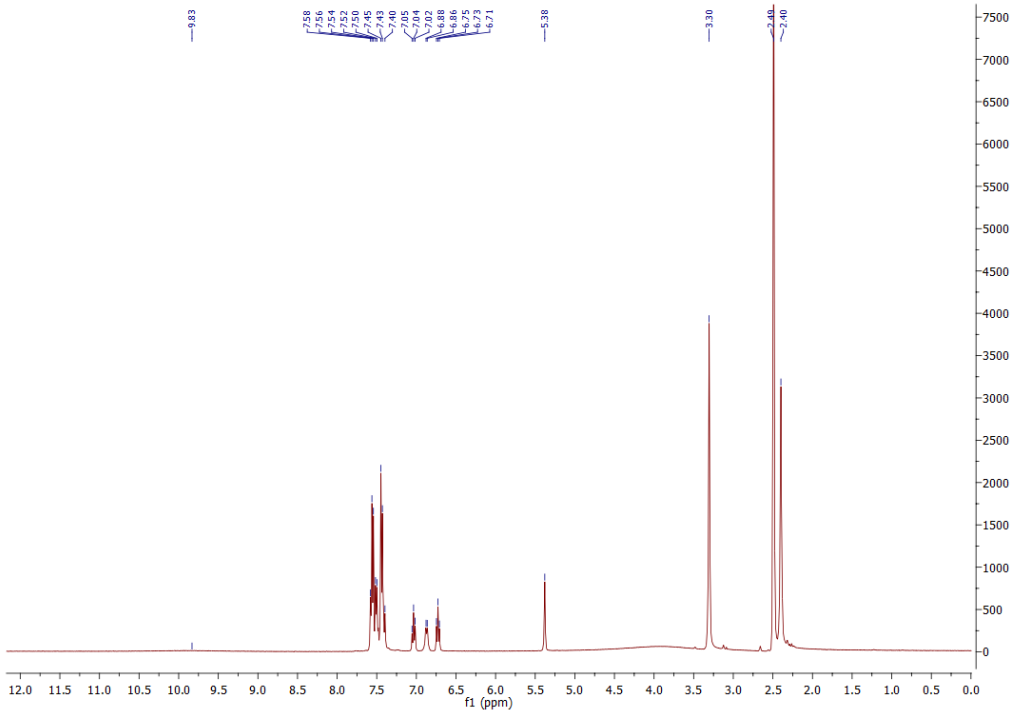


Figure S10. ^{1}H NMR spectrum of **3d**

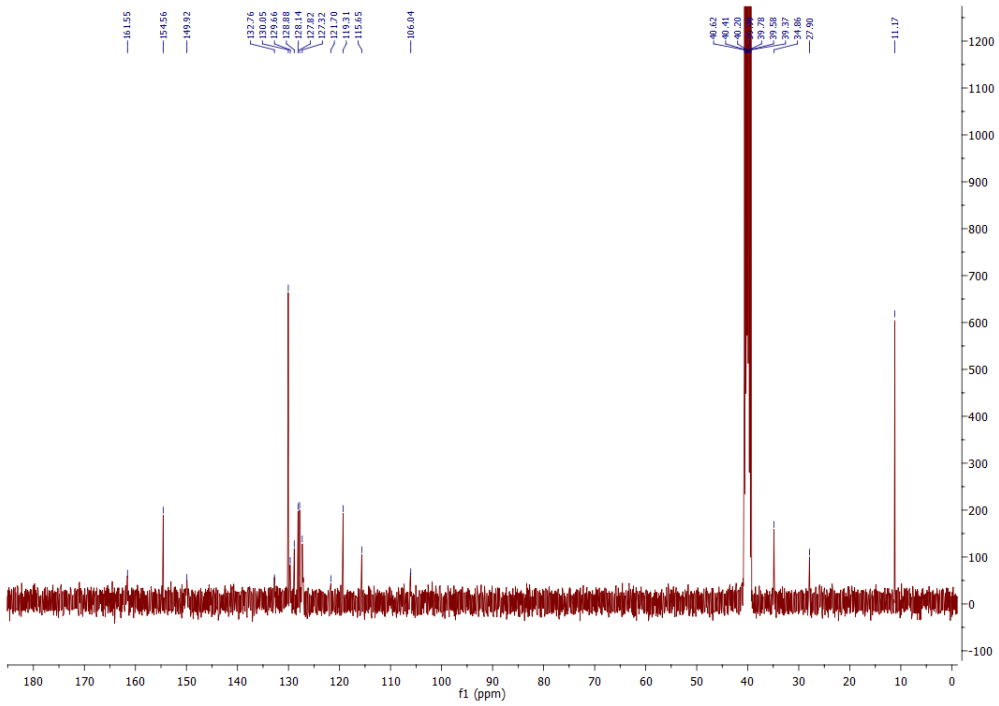


Figure S11. ^{13}C NMR spectrum of **3d**



Figure S12. FTIR spectrum of **3d**

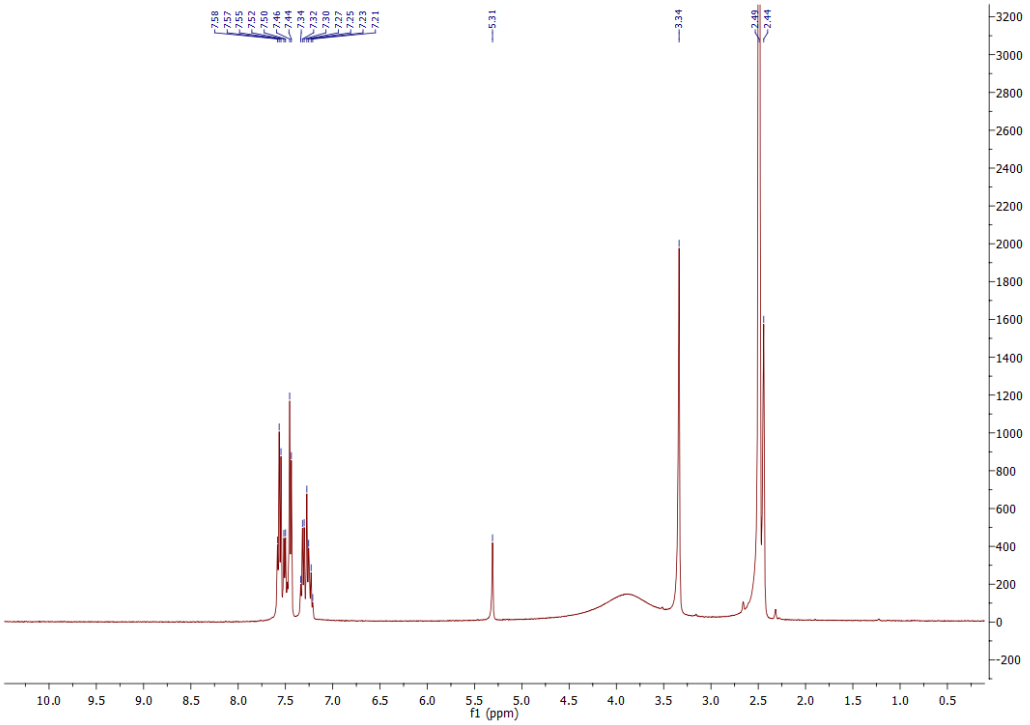


Figure S13. ^{1}H NMR spectrum of **3e**

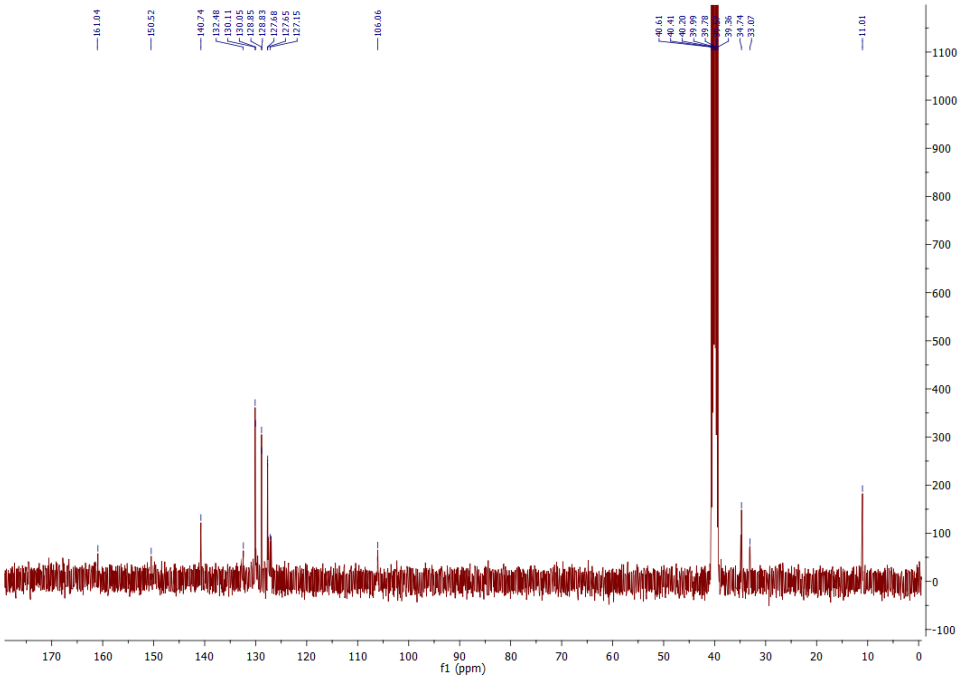


Figure S14. ^{13}C NMR spectrum of **3e**

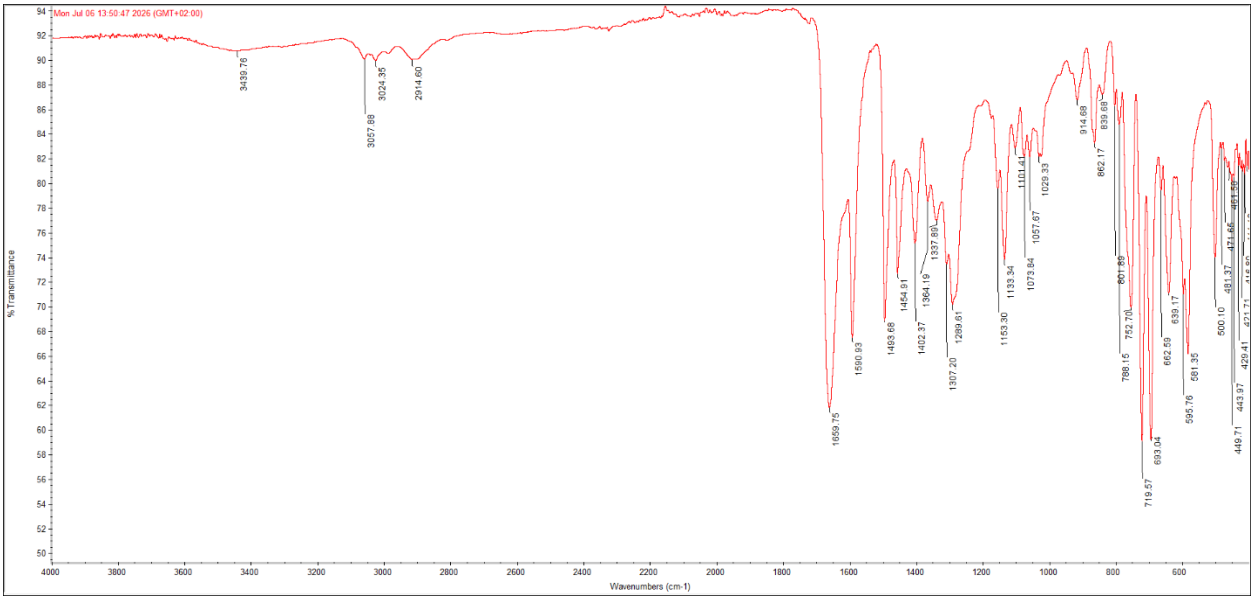


Figure S15. FTIR spectrum of **3e**

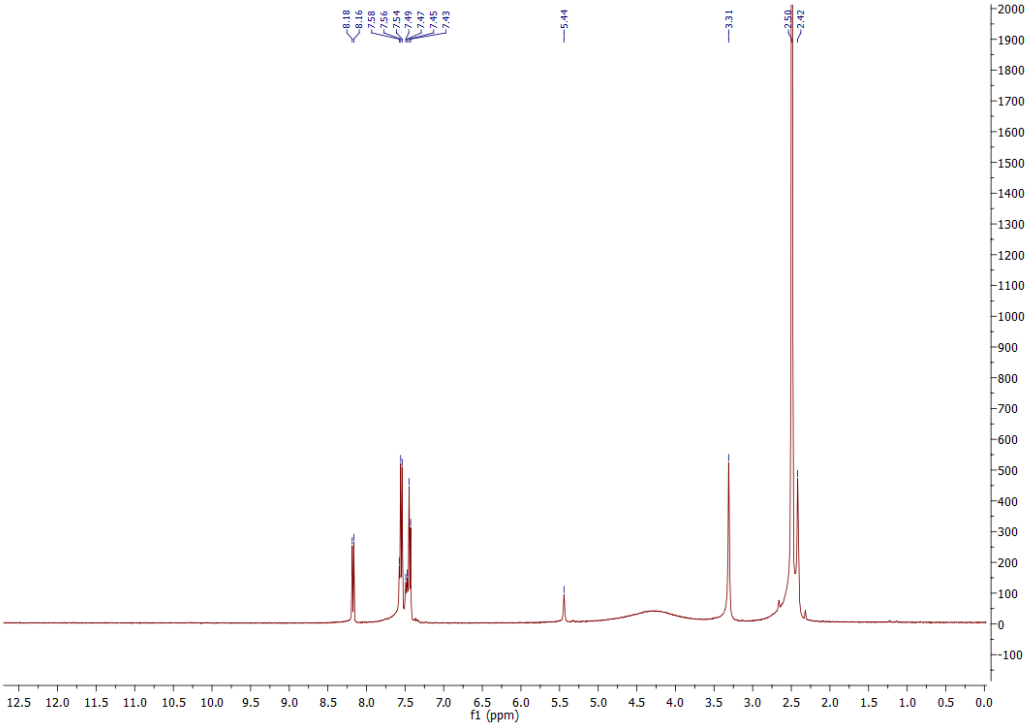


Figure S16. ^{1}H NMR spectrum of **3f**

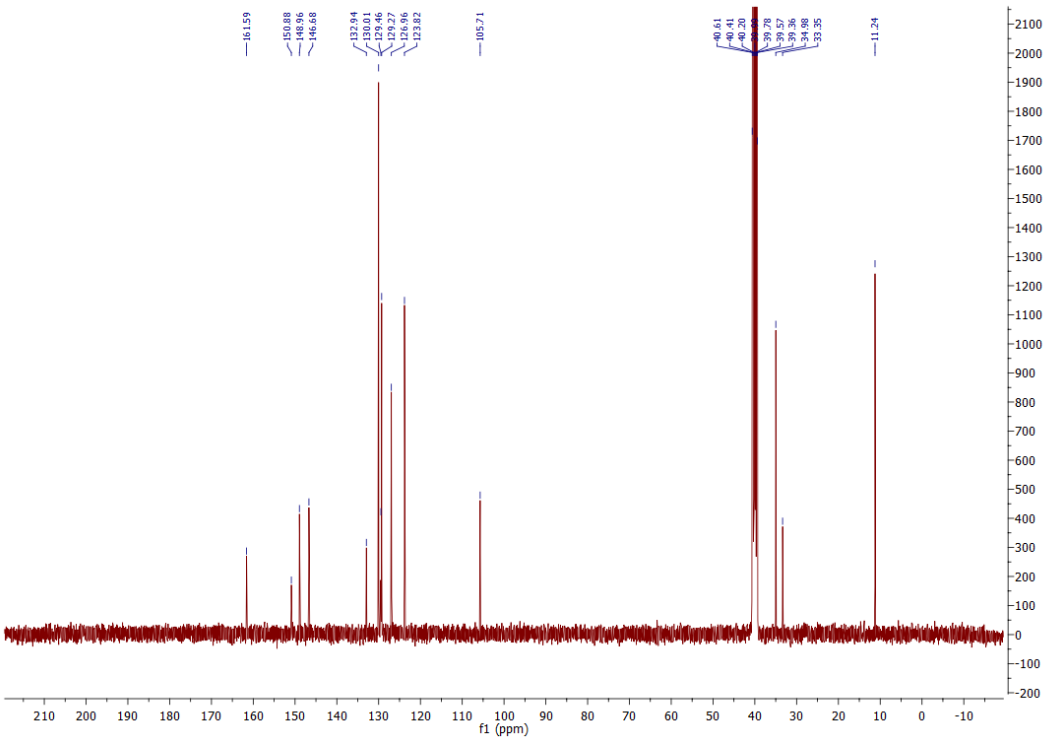


Figure S17. ^{13}C NMR spectrum of **3f**

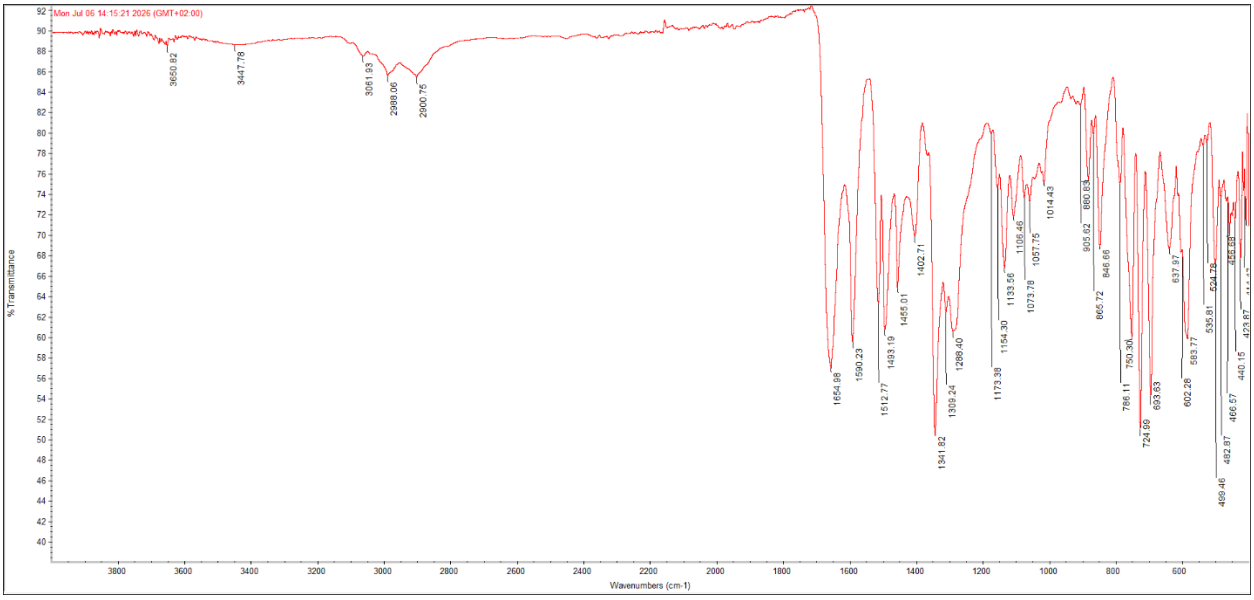


Figure S18. FTIR spectrum of **3f**

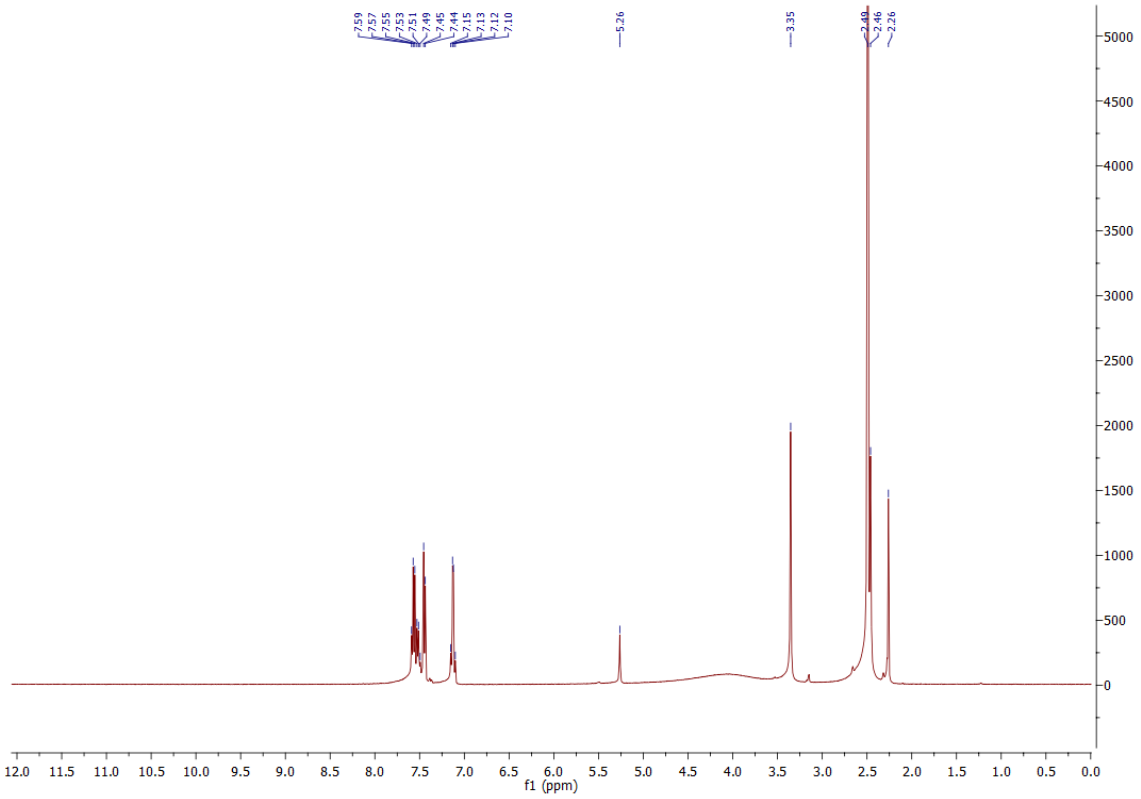


Figure S19. ^{1}H NMR spectrum of **3g**

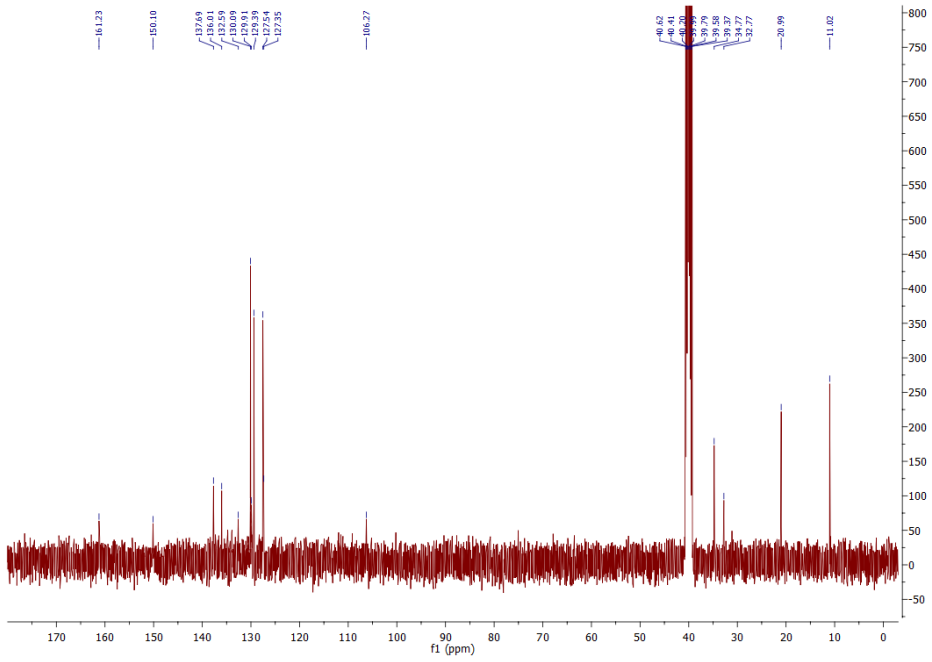


Figure S20. ^{13}C NMR spectrum of **3g**

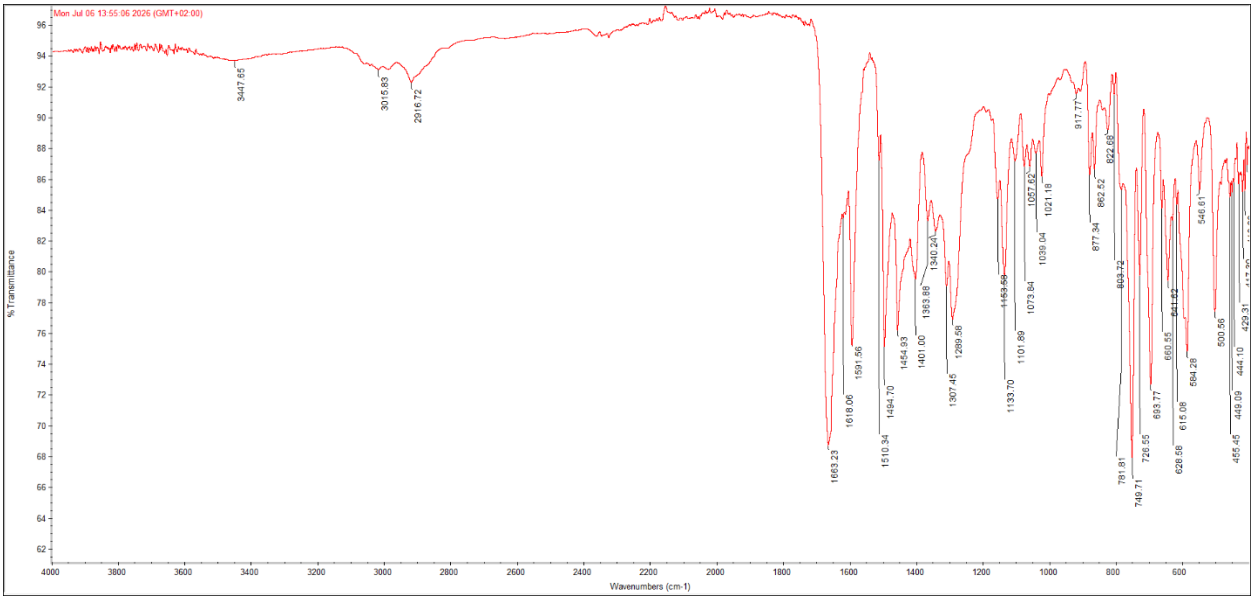


Figure S21. ^{13}C NMR spectrum of **3g**

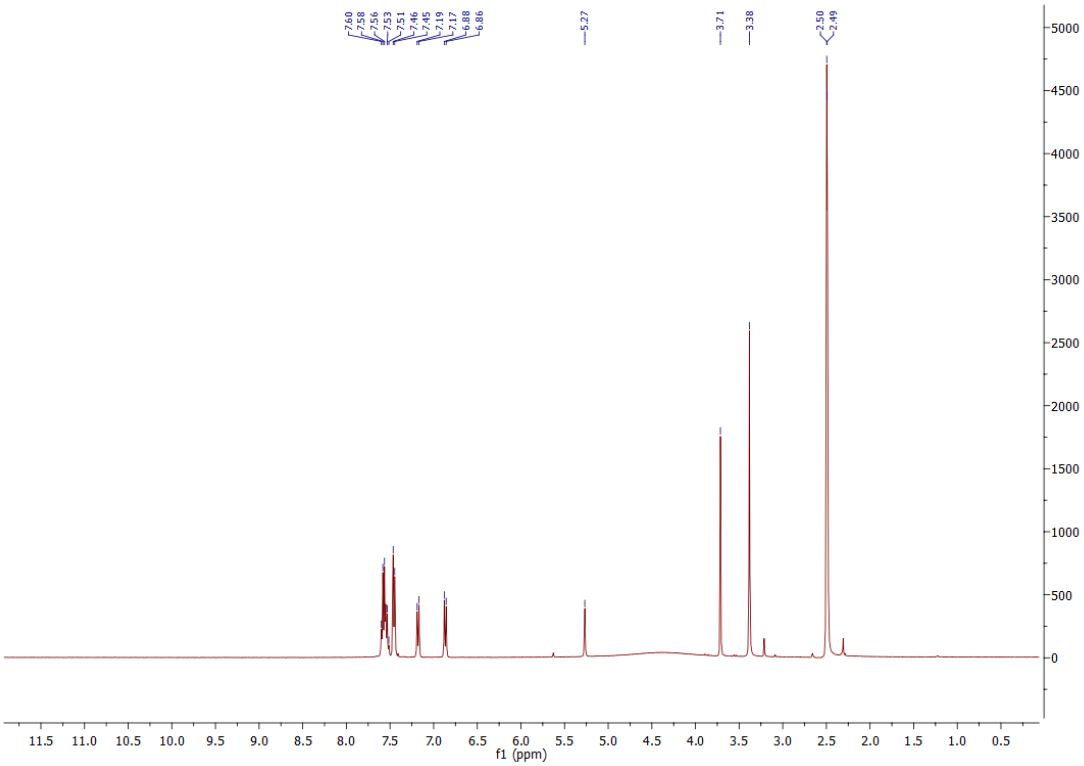


Figure S22. ^{1}H NMR spectrum of **3h**

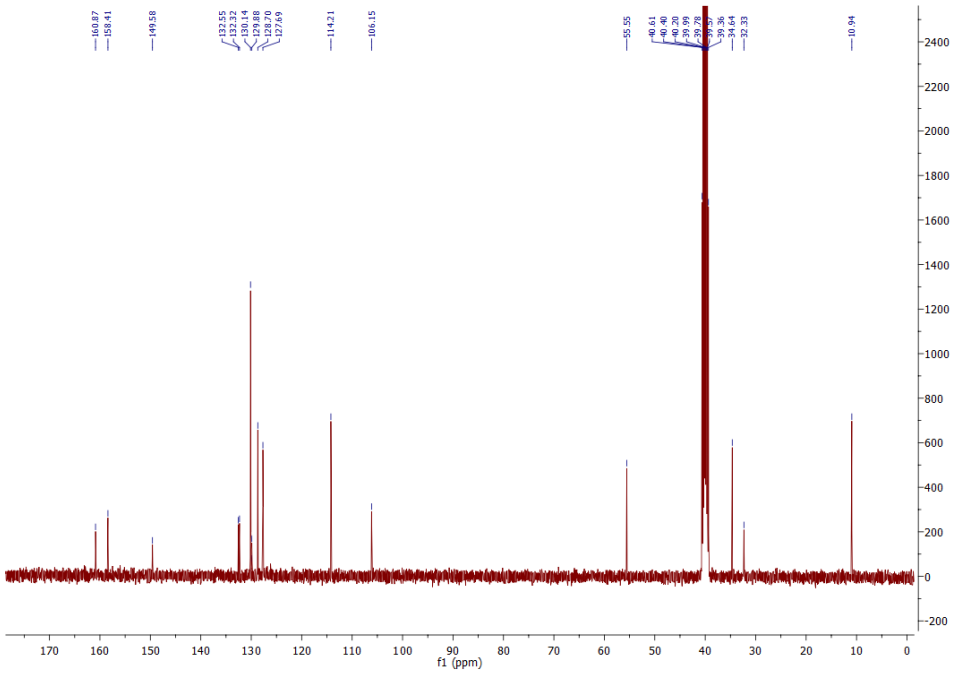


Figure S23. ^{13}C NMR spectrum of **3h**

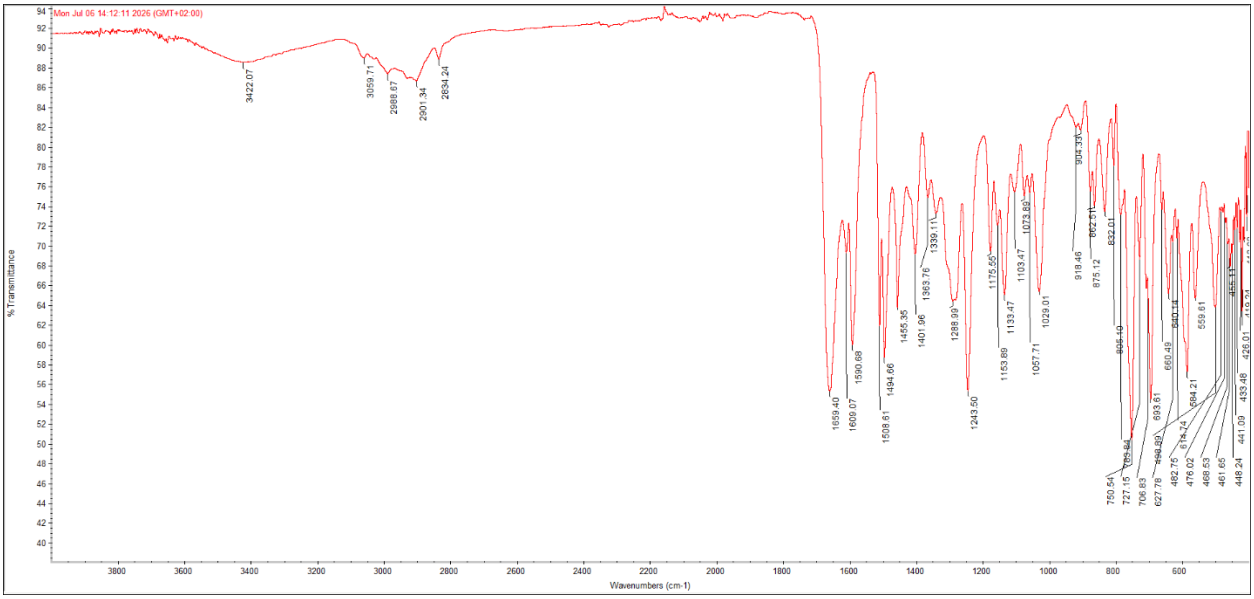


Figure S24. FTIR spectrum of **3h**

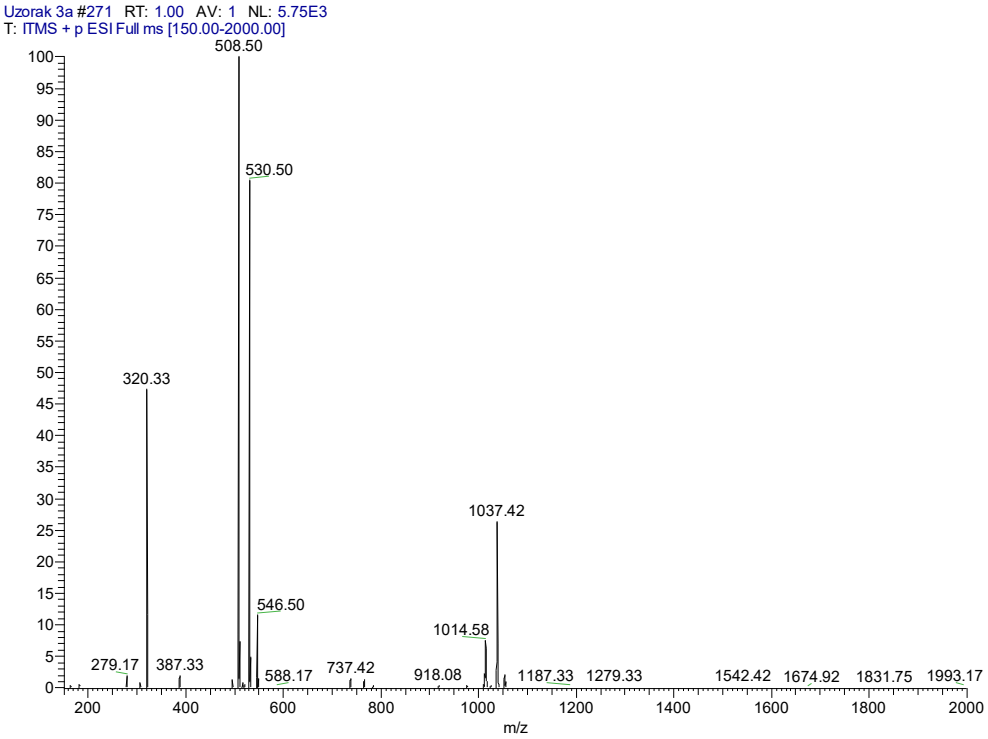
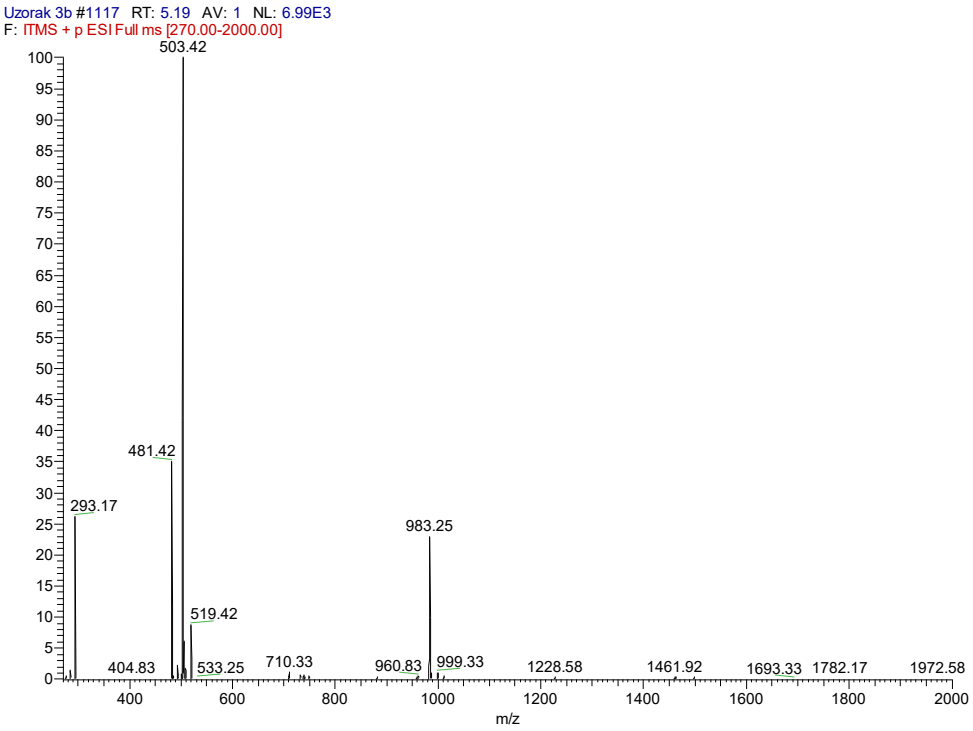
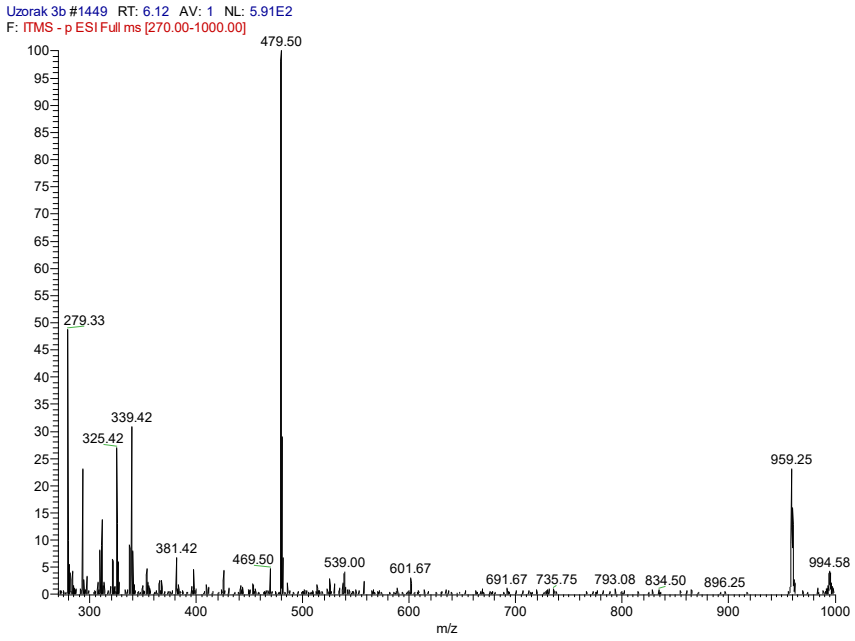


Figure S25. Full MS spectra of **3a**: *m/z* =508.50 – $[M+H]^+$, *m/z* = 530.50 – $[M+Na]^+$, *m/z* = 546.50 – $[M+K]^+$, *m/z* = 1037.42 – $[2M+Na]^+$

a)



b)



c)

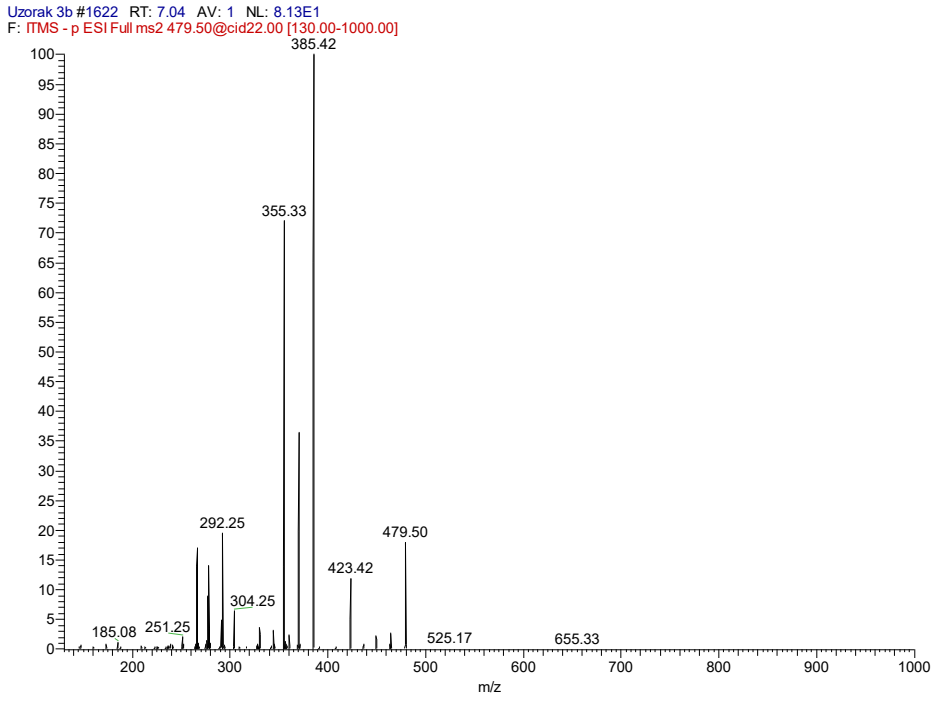
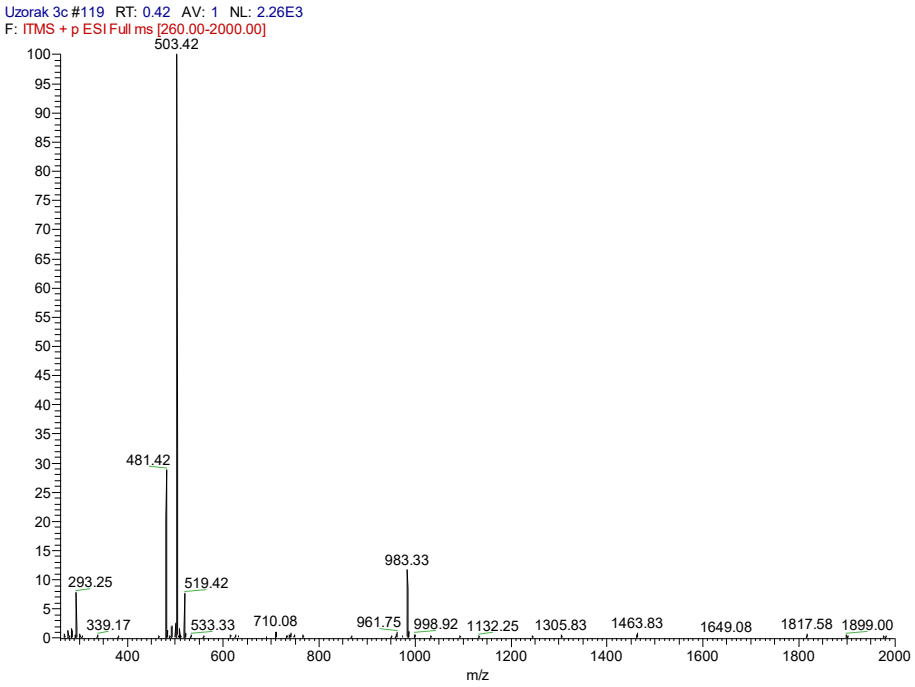
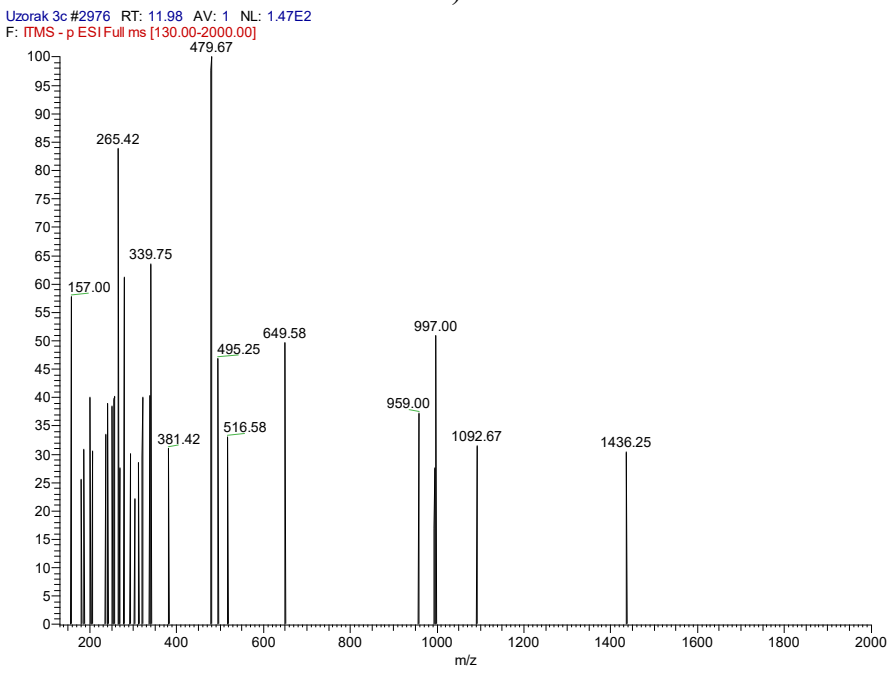


Figure S26. Full MS spectra of **3b** in positive mode (a): *m/z* = 481.42 – $[M+H]^+$, *m/z* = 503.42 – $[M+Na]^+$, *m/z* = 519.42 – $[M+K]^+$, *m/z* = 983.25 – $[2M+Na]^+$; in negative mode (b): *m/z* = 479.50 – $[M–H]^–$; and (c) MS^2 spectrum

a)


Uzorak 3c #119 RT: 0.42 AV: 1 NL: 2.26E3
F: ITMS + p ESI Full ms [260.00-2000.00]
503.42
481.42
983.33
293.25
519.42
339.17
533.33
710.08
961.75
998.92
1132.25
1305.83
1463.83
1649.08
1817.58
1899.00
m/z

b)


Uzorak 3c #2976 RT: 11.98 AV: 1 NL: 1.47E2
F: ITMS - p ESI Full ms [130.00-2000.00]
479.67
265.42
339.75
157.00
649.58
997.00
495.25
959.00
516.58
381.42
1092.67
1436.25
m/z

c)

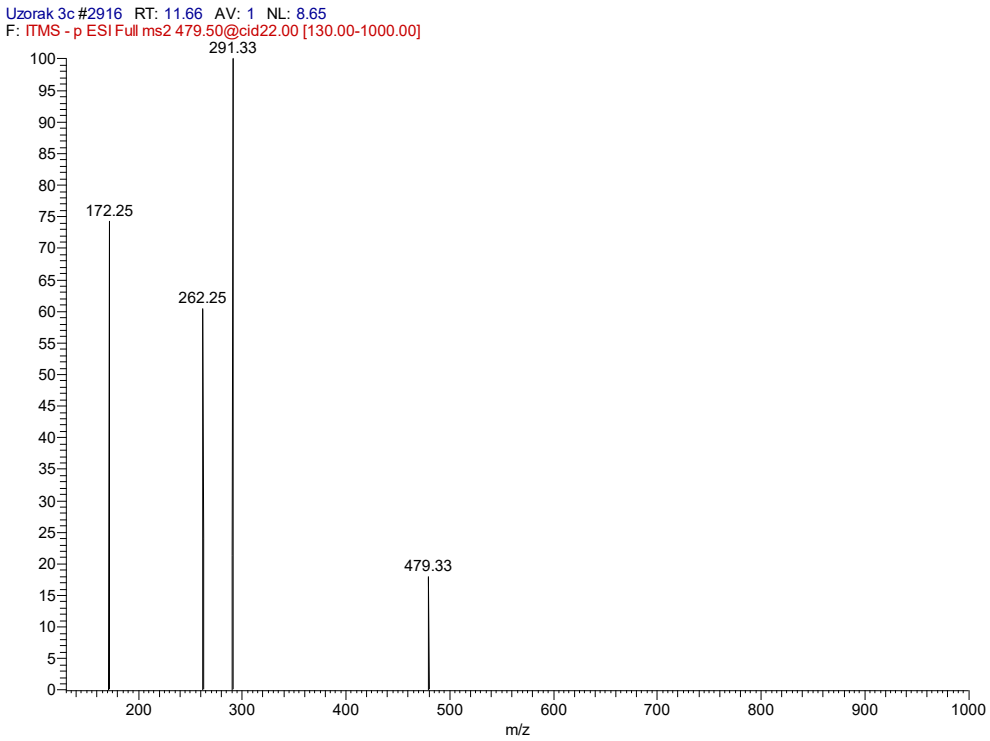
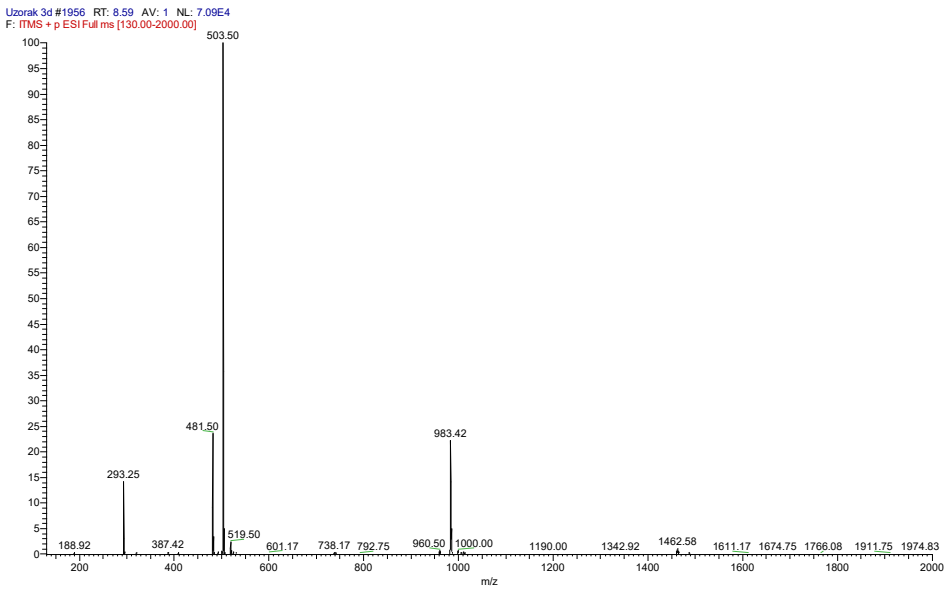
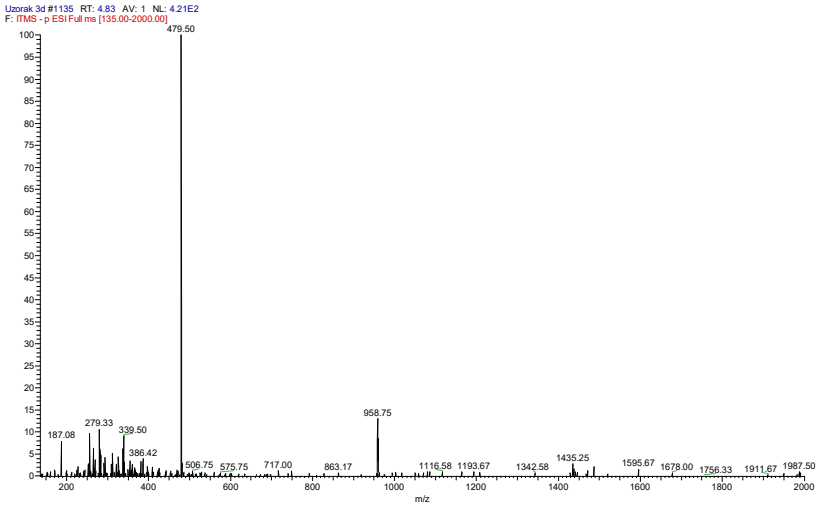


Figure S27. Full MS spectra of **3c** in positive mode (a): *m/z* = 481.42 – $[M+H]^+$, *m/z* = 503.42 – $[M+Na]^+$, *m/z* = 519.42 – $[M+K]^+$, *m/z* = 983.33 – $[2M+Na]^+$; in negative mode (b): *m/z* = 479.67 – $[M–H]^–$; and (c) MS^2 spectrum

a)



b)



c)

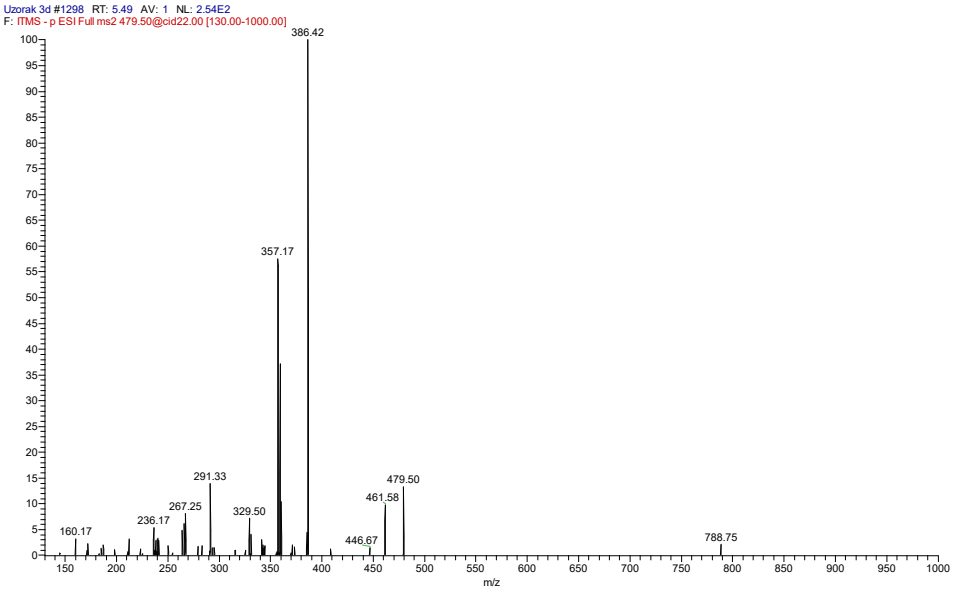


Figure S28. Full MS spectra of **3d** in positive mode (a): *m/z* = 481.50 – $[M+H]^+$, *m/z* = 503.50 – $[M+Na]^+$, *m/z* = 983.42 – $[2M+Na]^+$; in negative mode (b): *m/z* = 479.50 – $[M-H]^-$; and (c) MS^2 spectrum

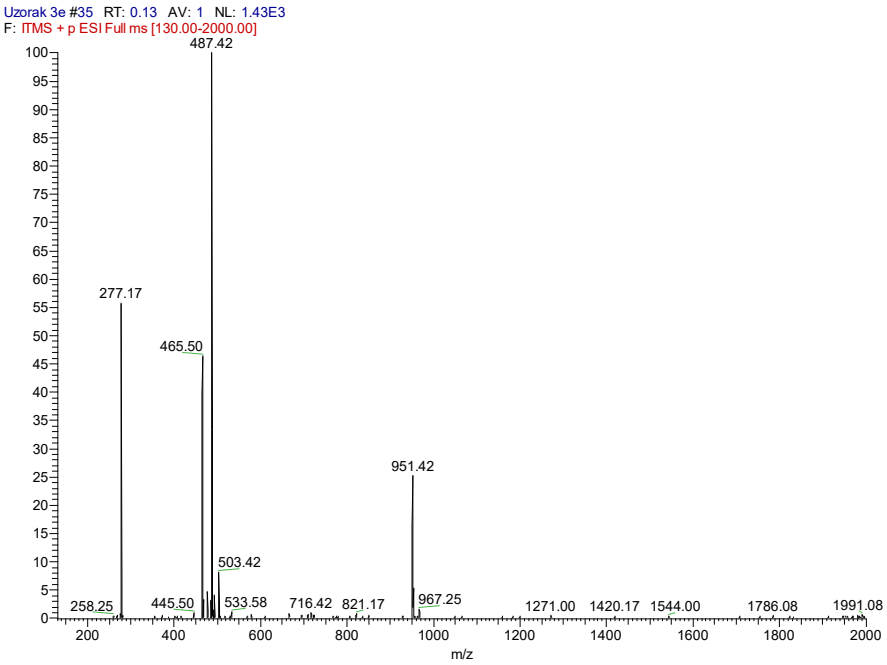


Figure S29. Full MS spectra of **3e** *m/z* = 465.50 – $[M+H]^+$, *m/z* = 487.42 – $[M+Na]^+$, *m/z* = 503.42 – $[M+K]^+$, *m/z* = 951.42 – $[2M+Na]^+$

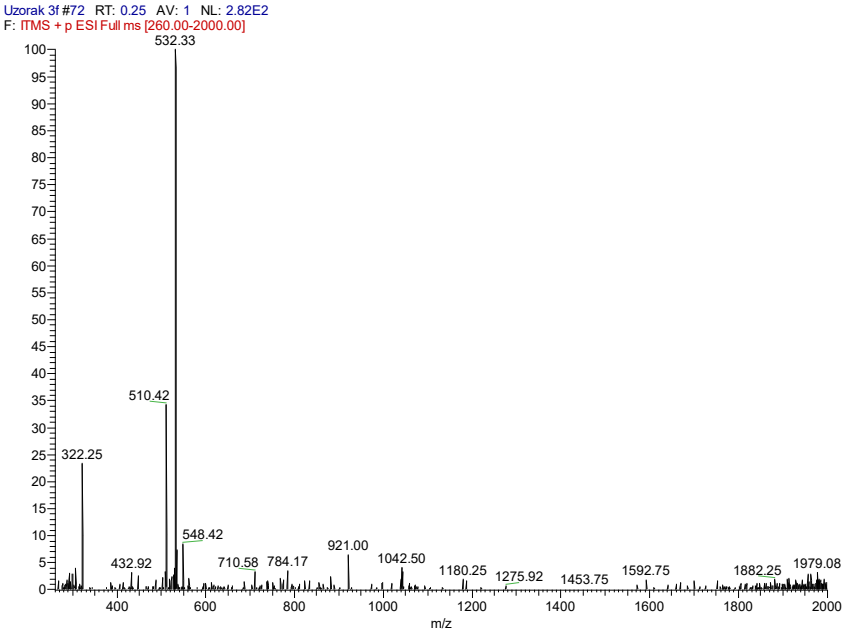


Figure S30. Full MS spectra of **3f** *m/z* = 510.42 – $[M+H]^+$, *m/z* = 532.33 – $[M+Na]^+$

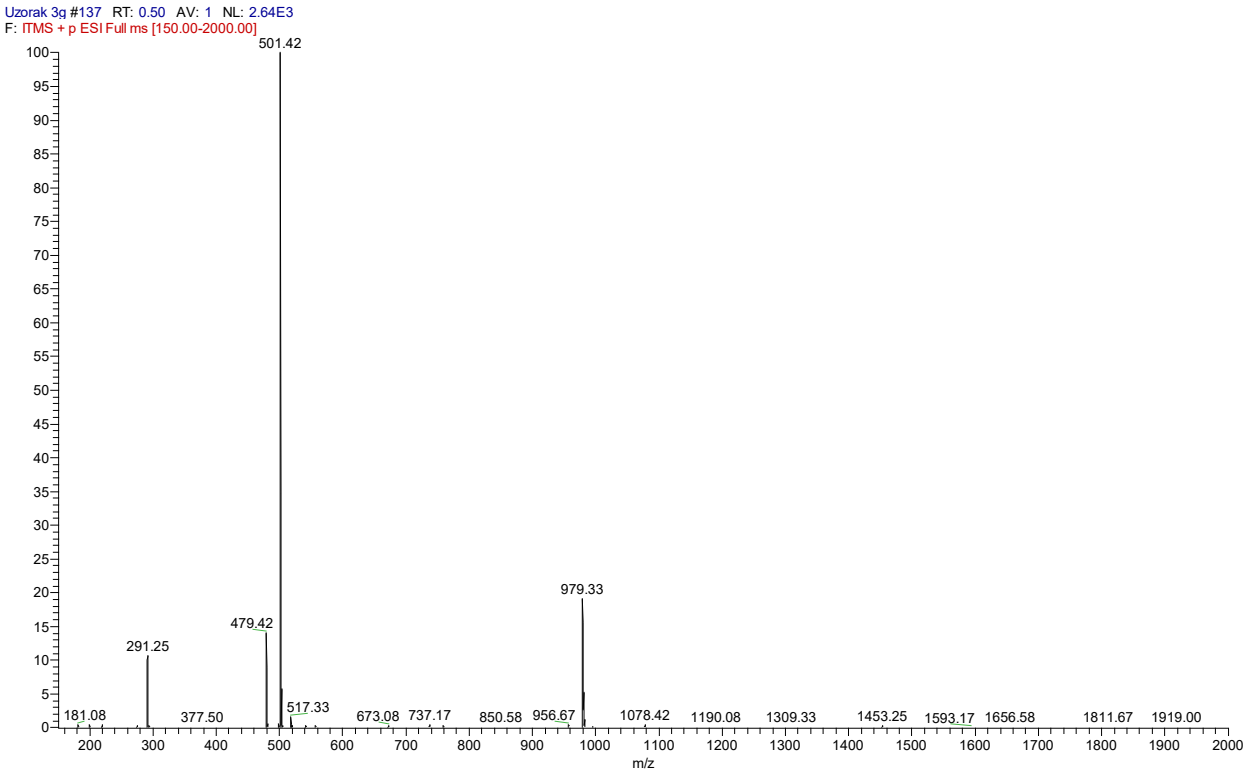


Figure S31. Full MS spectra of **3g** *m/z* = 479.42 – $[M+H]^+$, *m/z* = 501.42 – $[M+Na]^+$, *m/z* = 979.33 –$[2M+Na]^+$

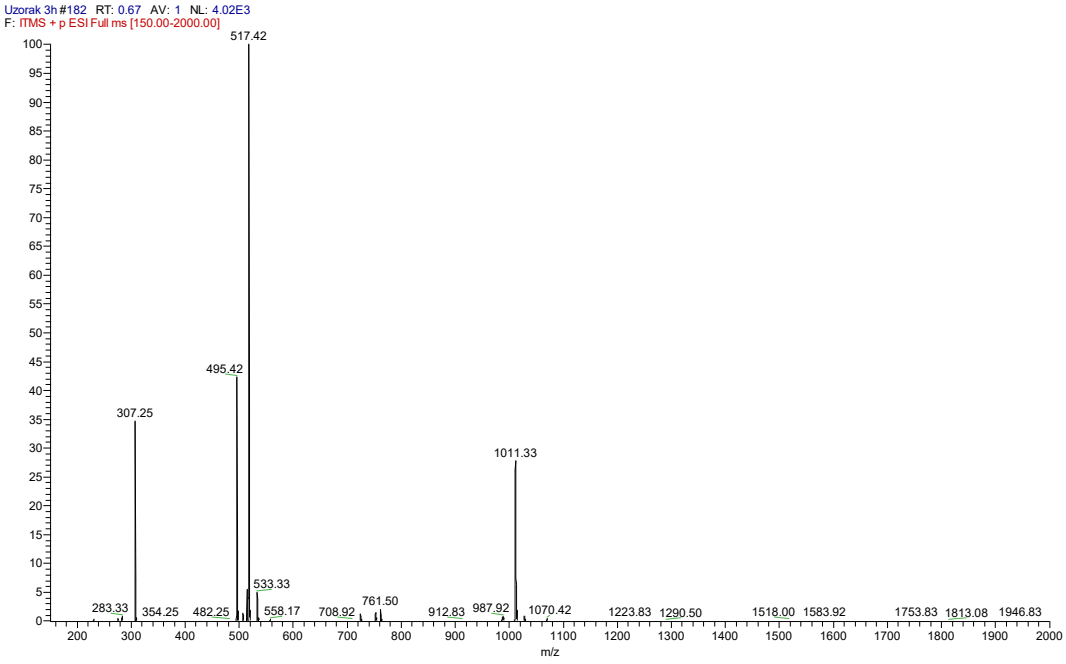


Figure S32. Full MS spectra of **3h** *m/z* = 495.42 – $[M+H]^+$, *m/z* = 517.42 – $[M+Na]^+$, *m/z* = 1011.33 –$[2M+Na]^+$

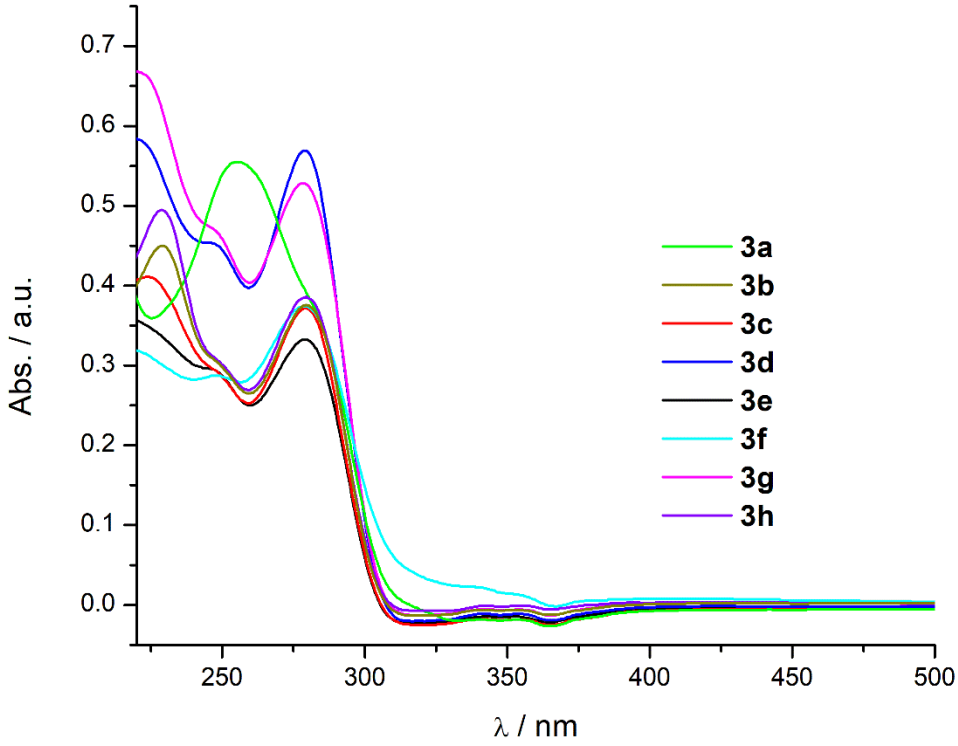


Figure S33. UV-Vis spectra of the compounds **3a**–**3h** in methanol.