Supplementary material

Novel 2,4-Disubstituted-1,3-Thiazole Derivatives: Synthesis, Anti-*Candida* Activity Evaluation and Interaction with Bovine Serum Albumine

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Table of contents

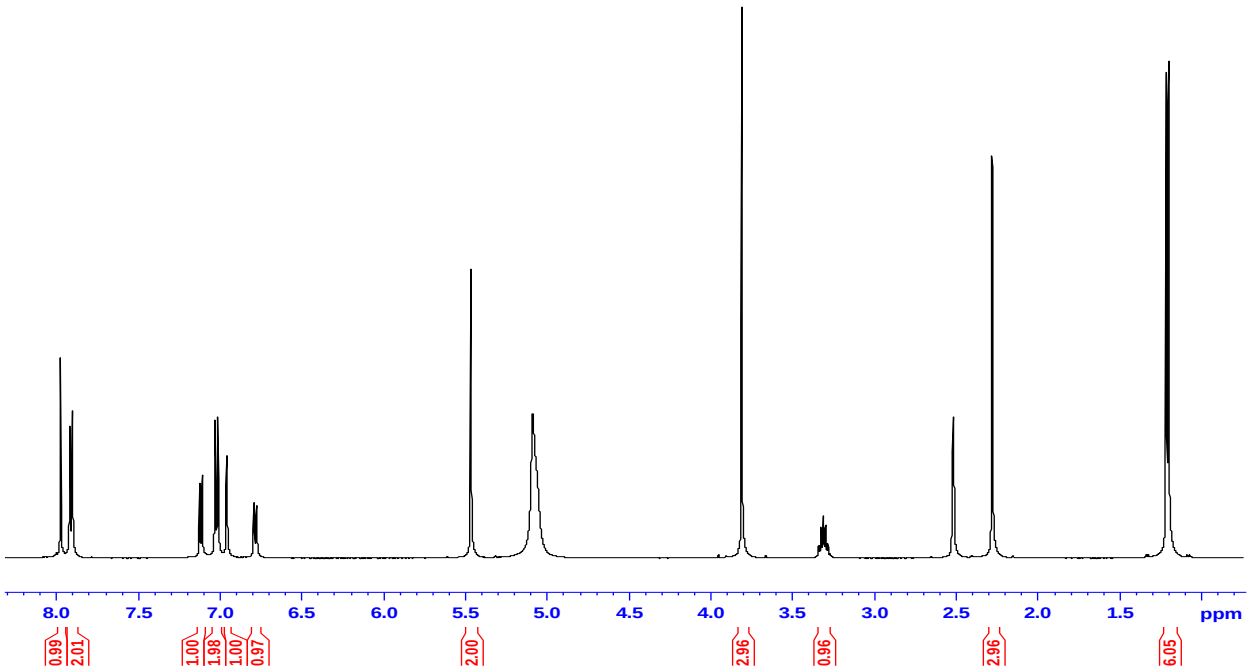


Figure 1. ^{1}H-NMR spectra of compound **4a**

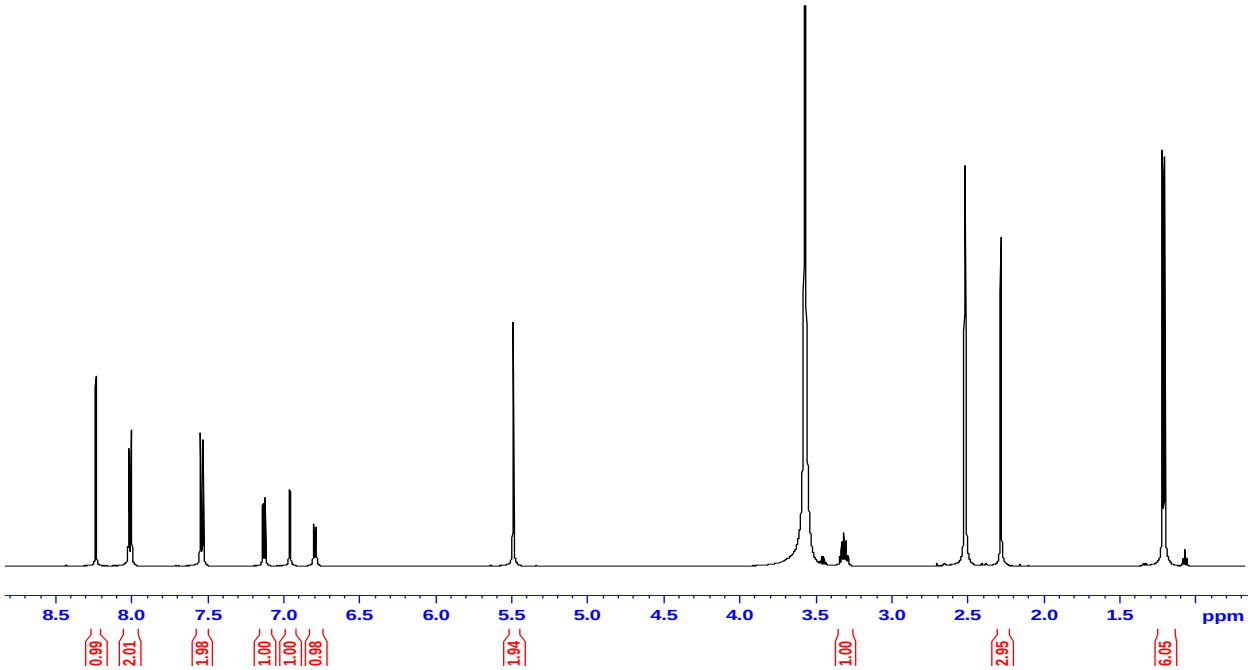


Figure 2. ^{1}H-NMR spectra of compound **4b**

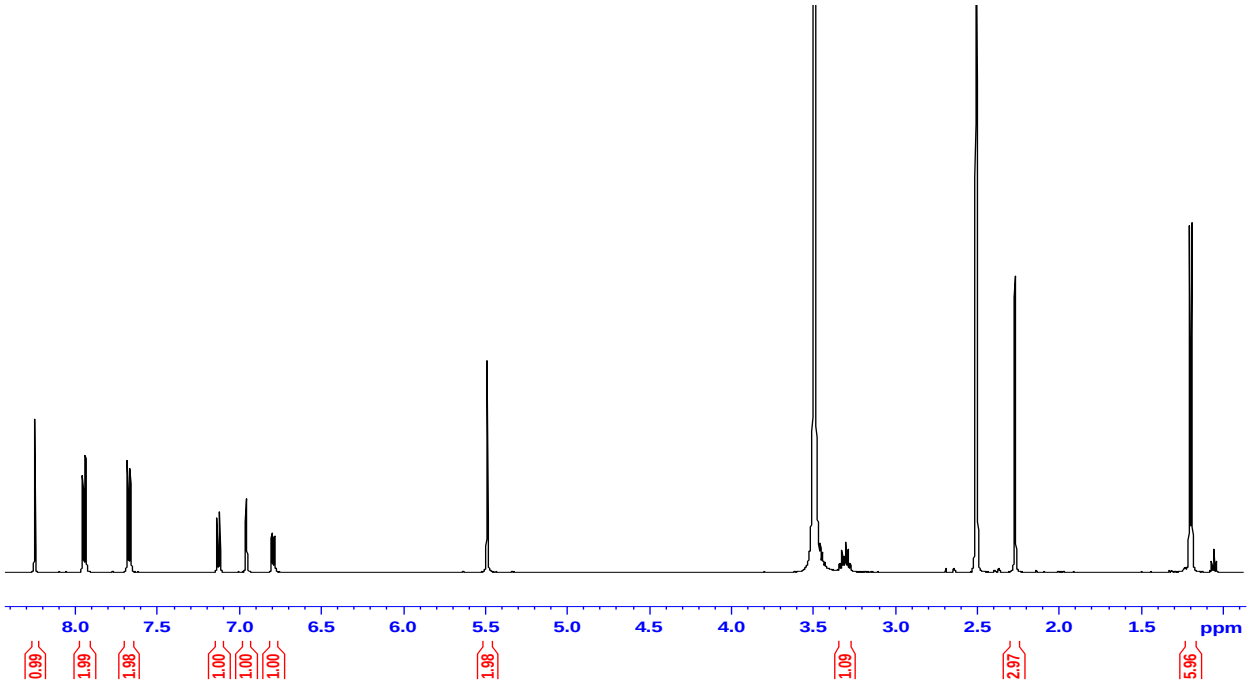


Figure 3. ^{1}H-NMR spectra of compound **4c**

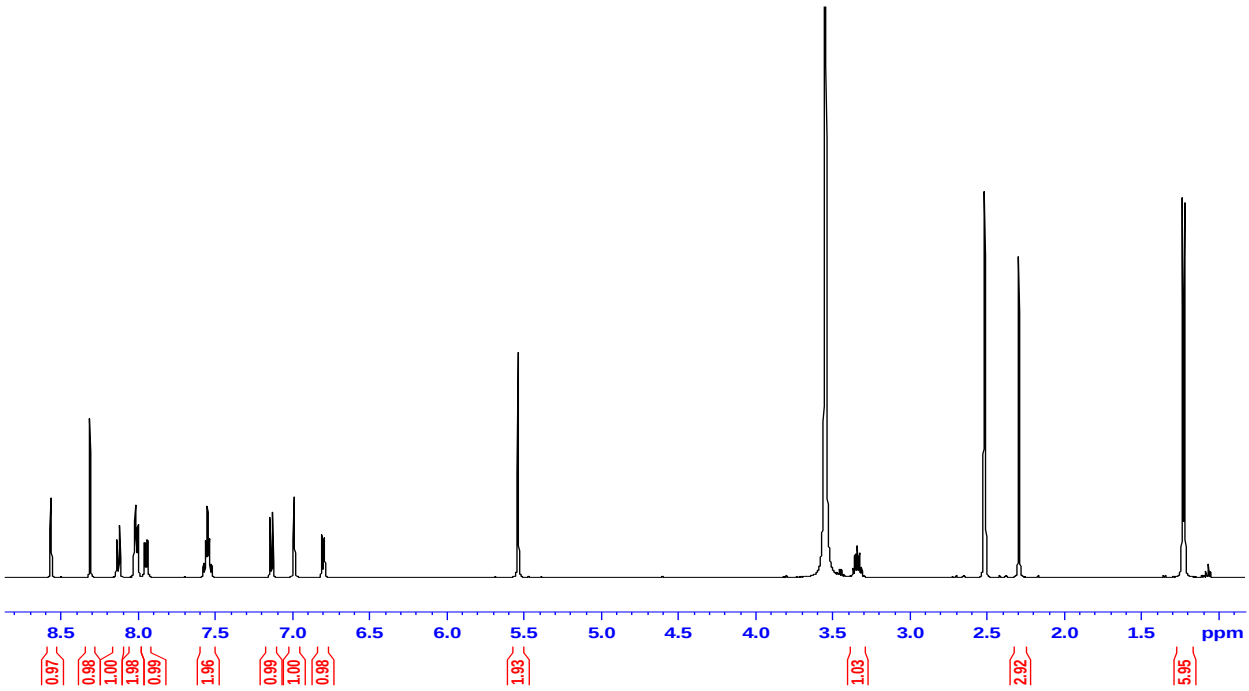


Figure 4. ^{1}H-NMR spectra of compound **4d**

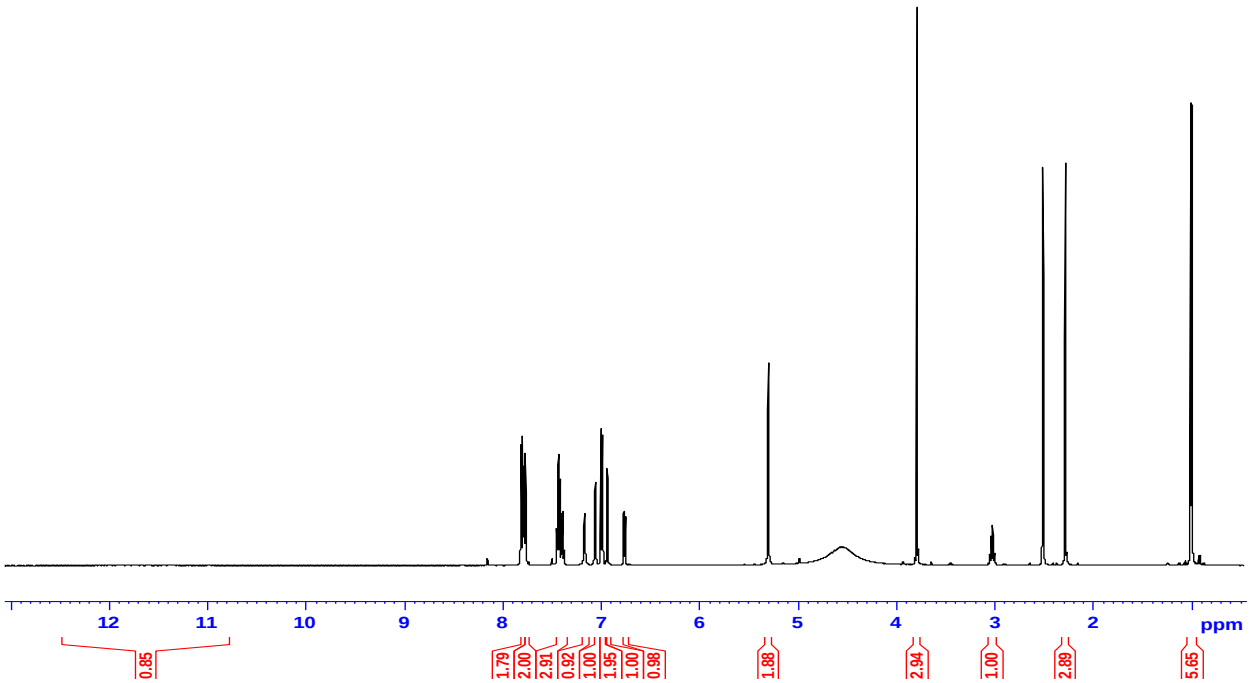


Figure 5. ^{1}H-NMR spectra of compound **7a**

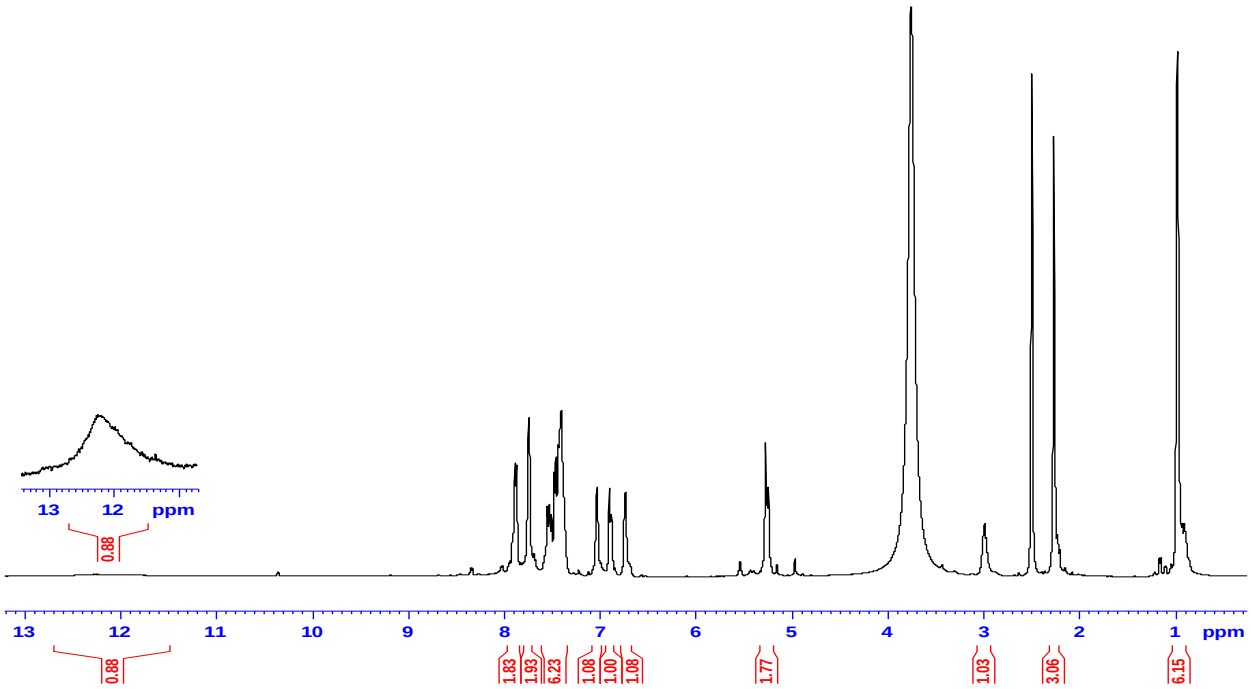


Figure 6. ^{1}H-NMR spectra of compound **7b**

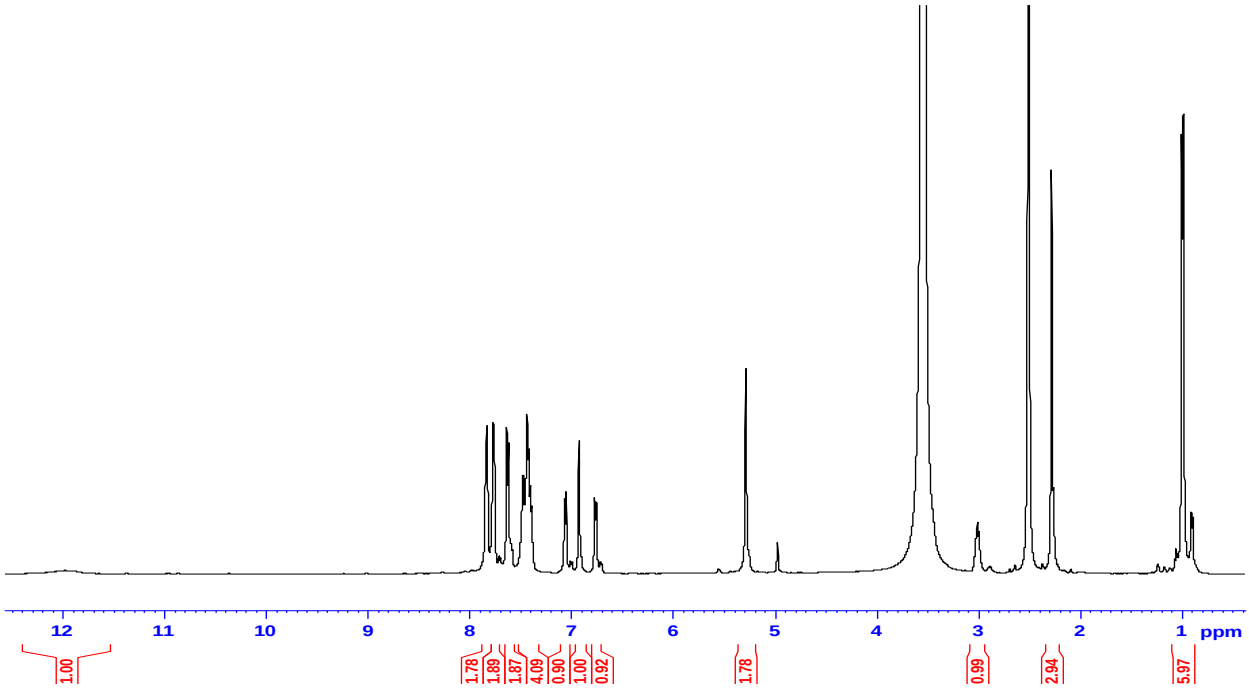


Figure 7. ^{1}H-NMR spectra of compound **7c**

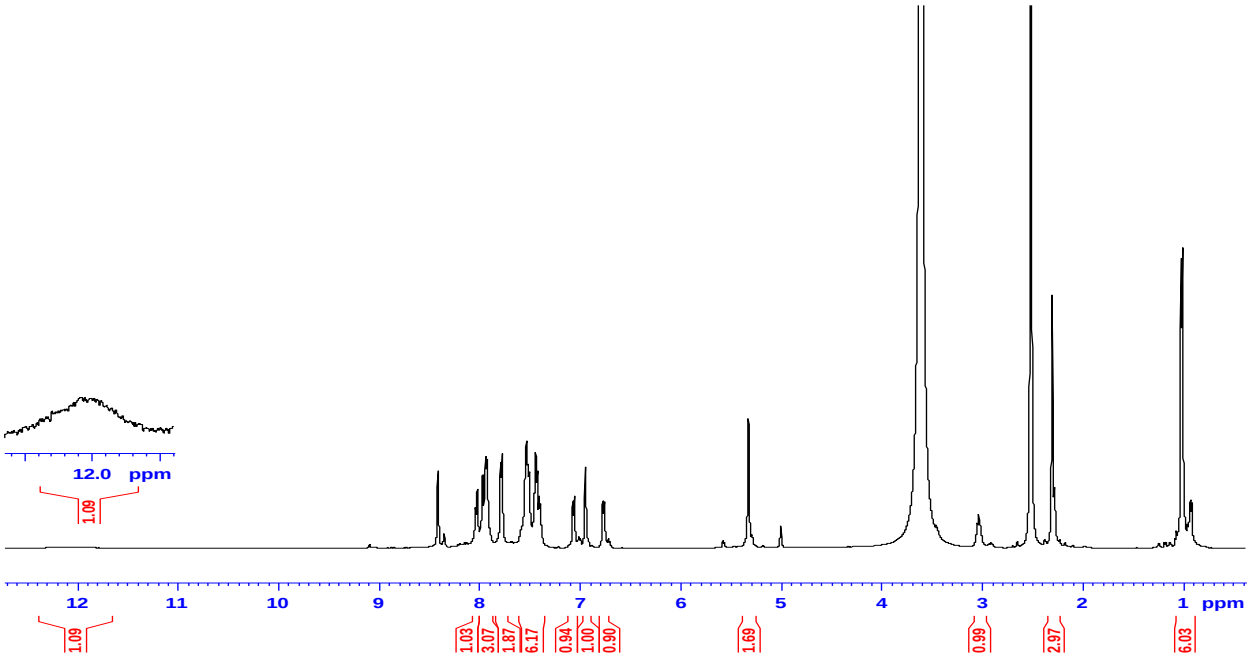


Figure 8. ^{1}H-NMR spectra of compound **7d**

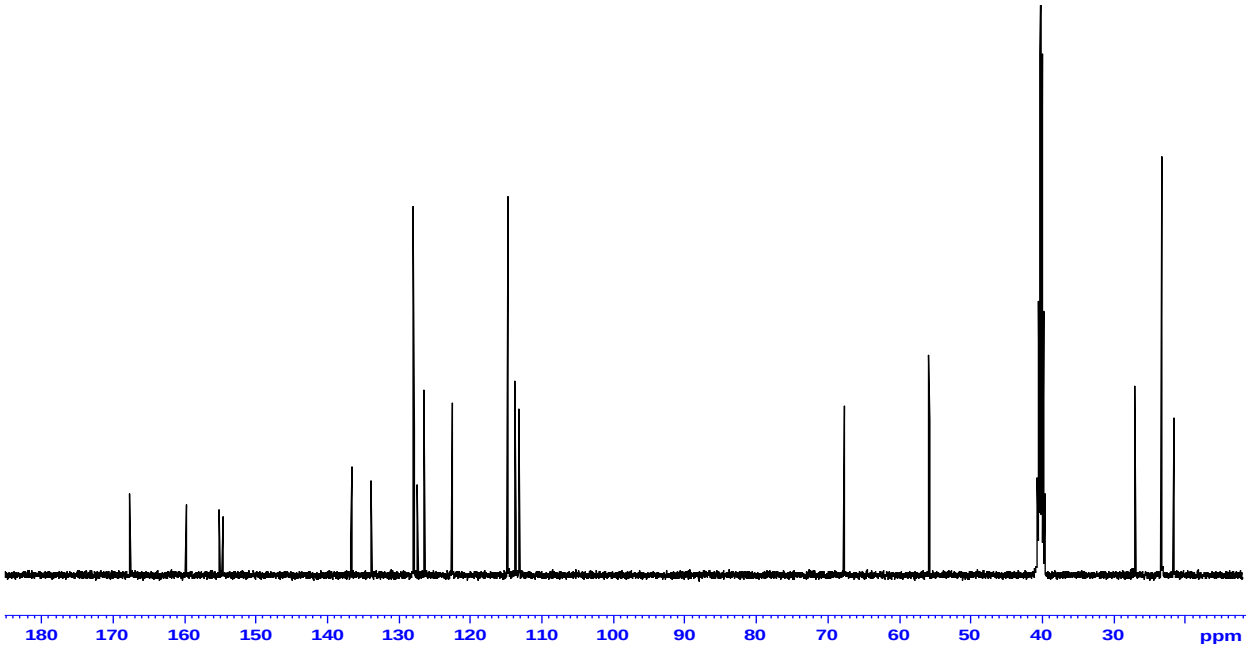


Figure 9. ^{13}C-NMR spectra of compound **4a**

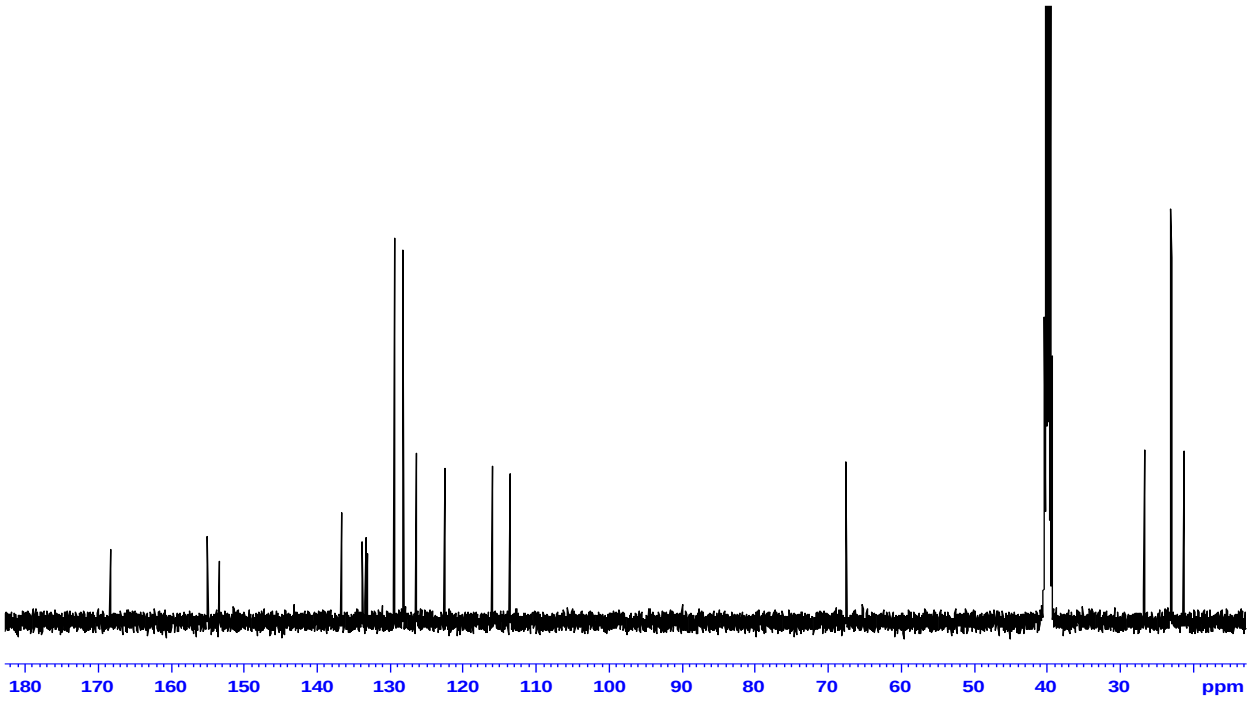


Figure 10. ^{13}C-NMR spectra of compound **4b**

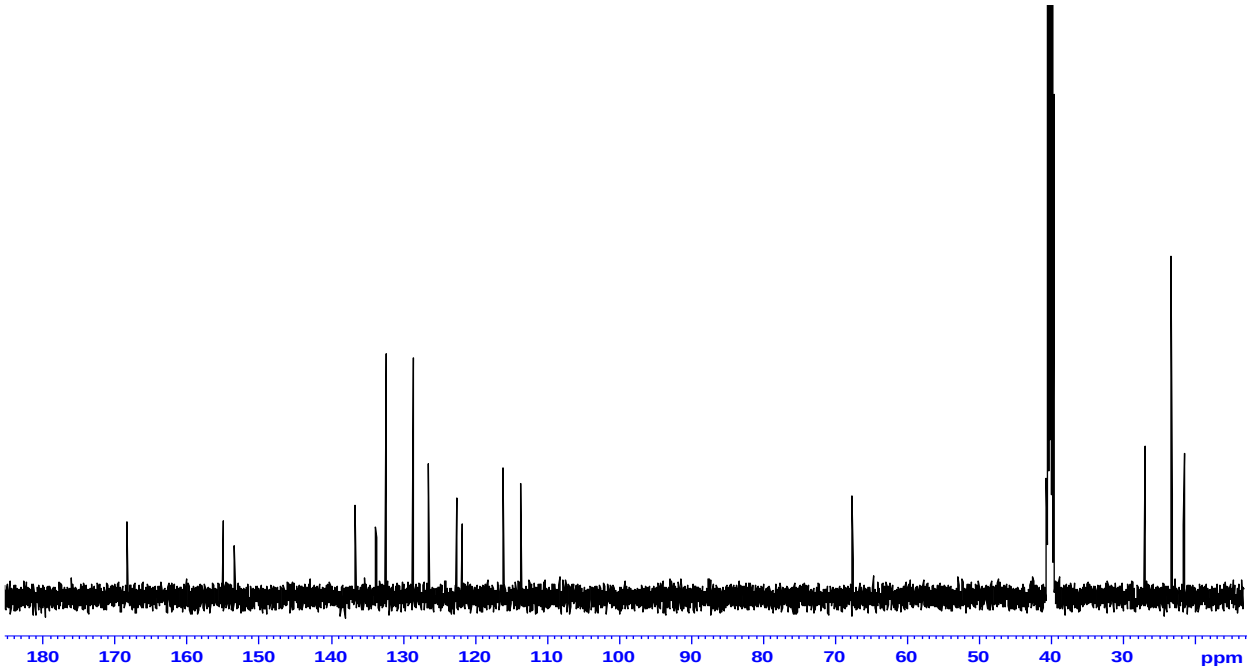


Figure 11. ^{13}C-NMR spectra of compound **4c**

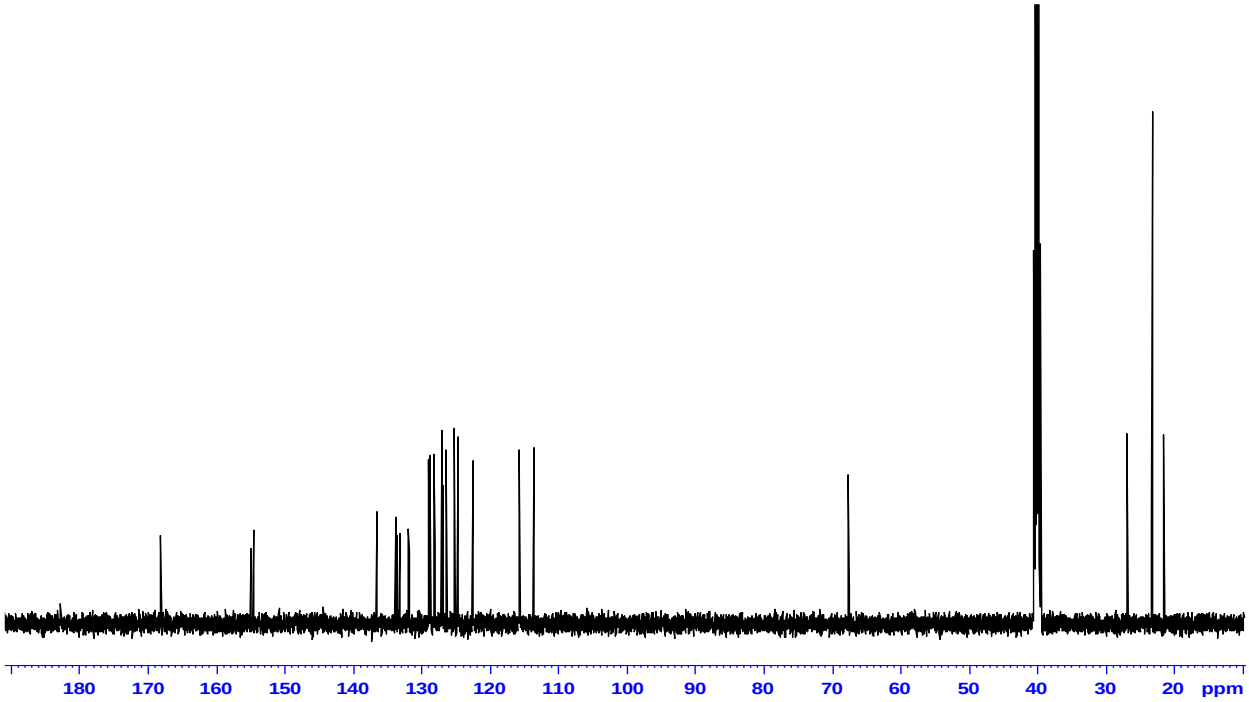


Figure 12. ^{13}C-NMR spectra of compound **4d**

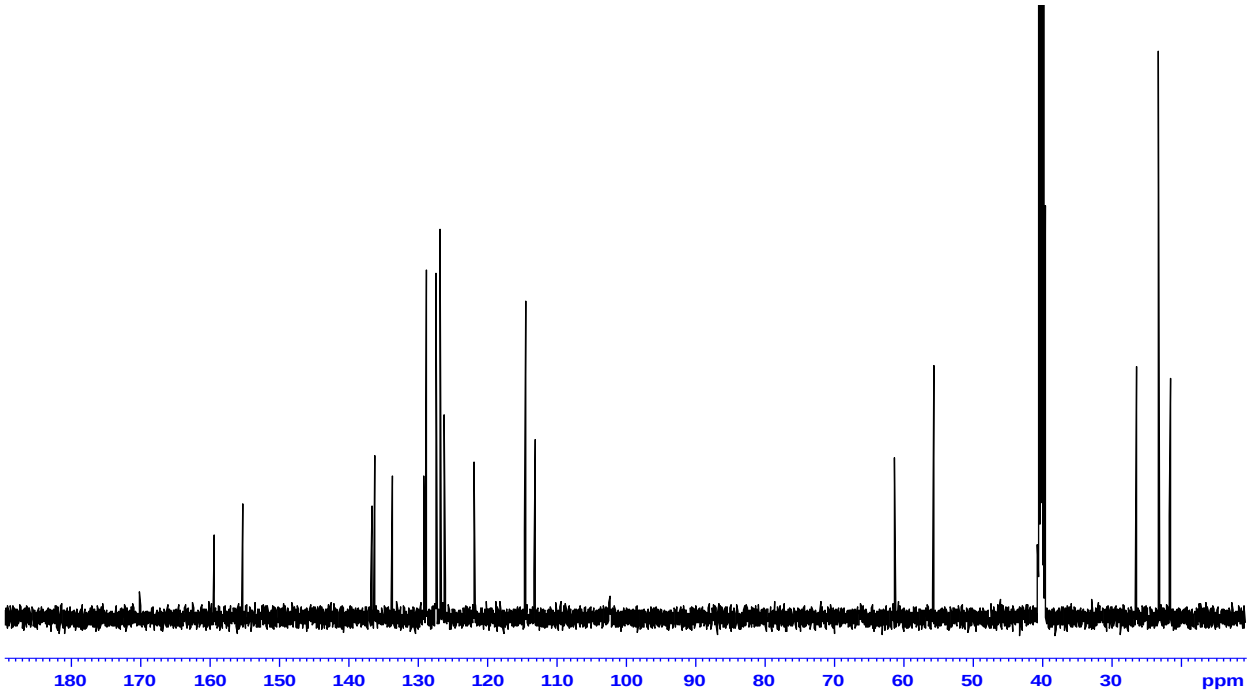


Figure 13. ^{13}C-NMR spectra of compound **7a**

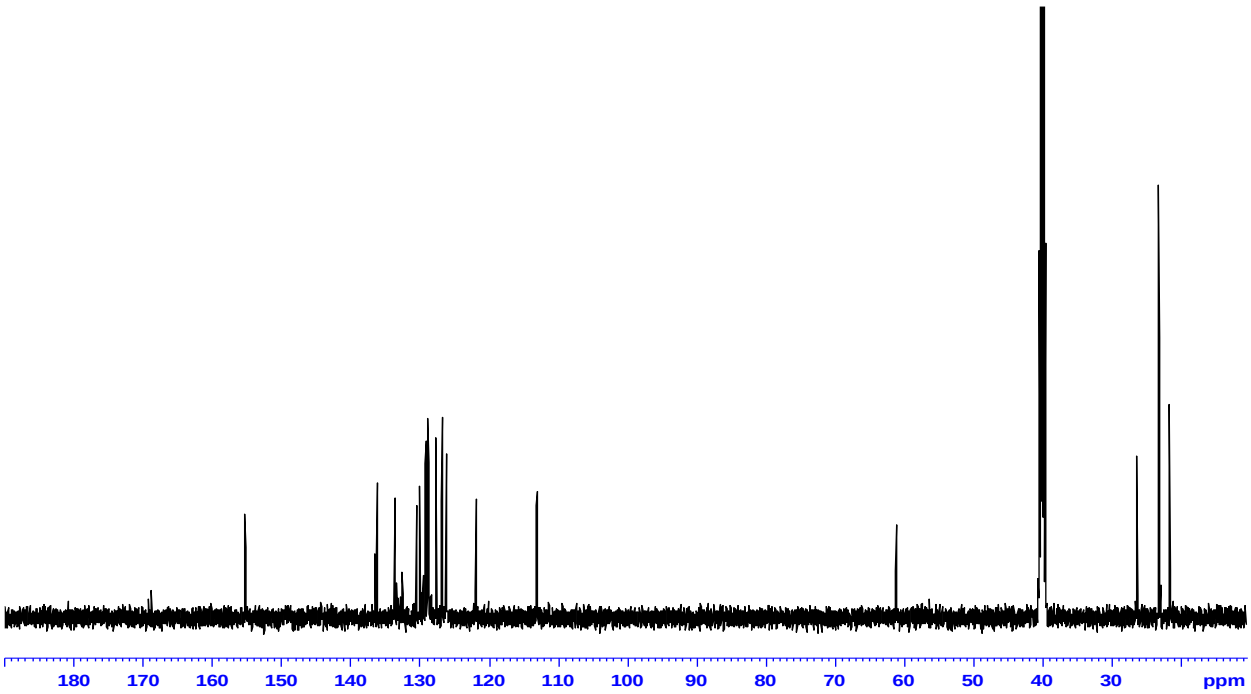


Figure 14. ^{13}C-NMR spectra of compound **7b**

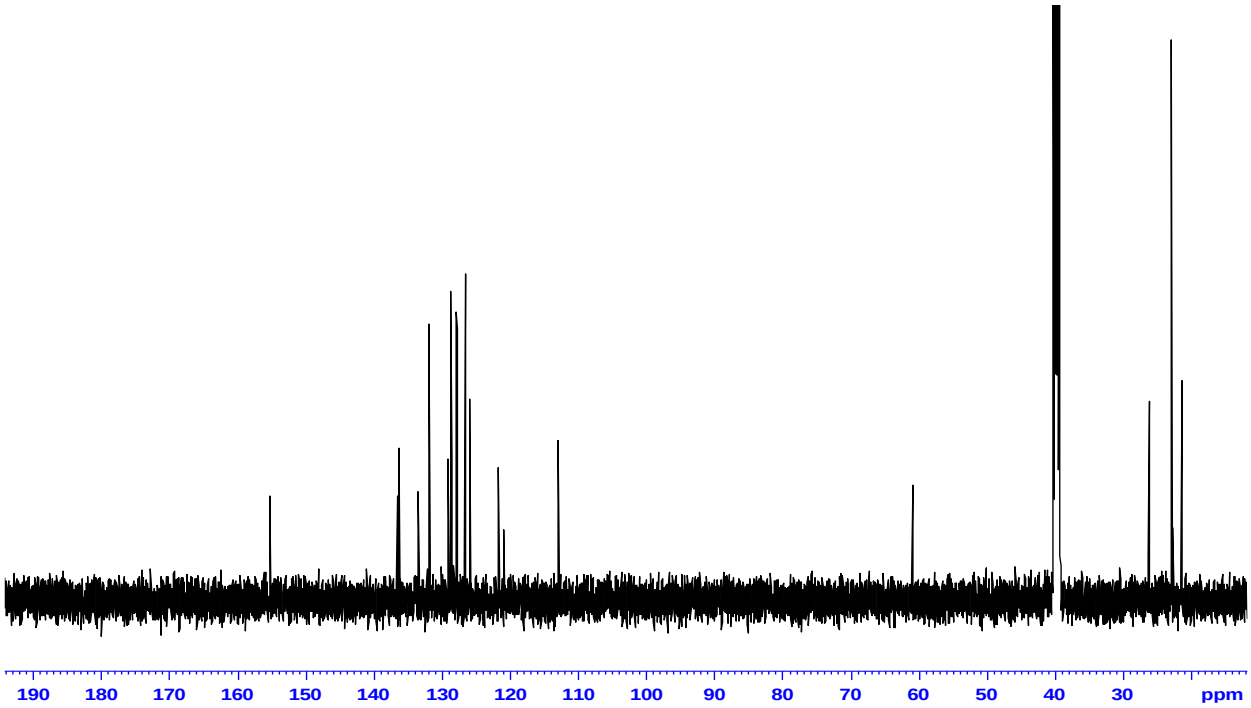


Figure 15. ^{13}C-NMR spectra of compound **7c**

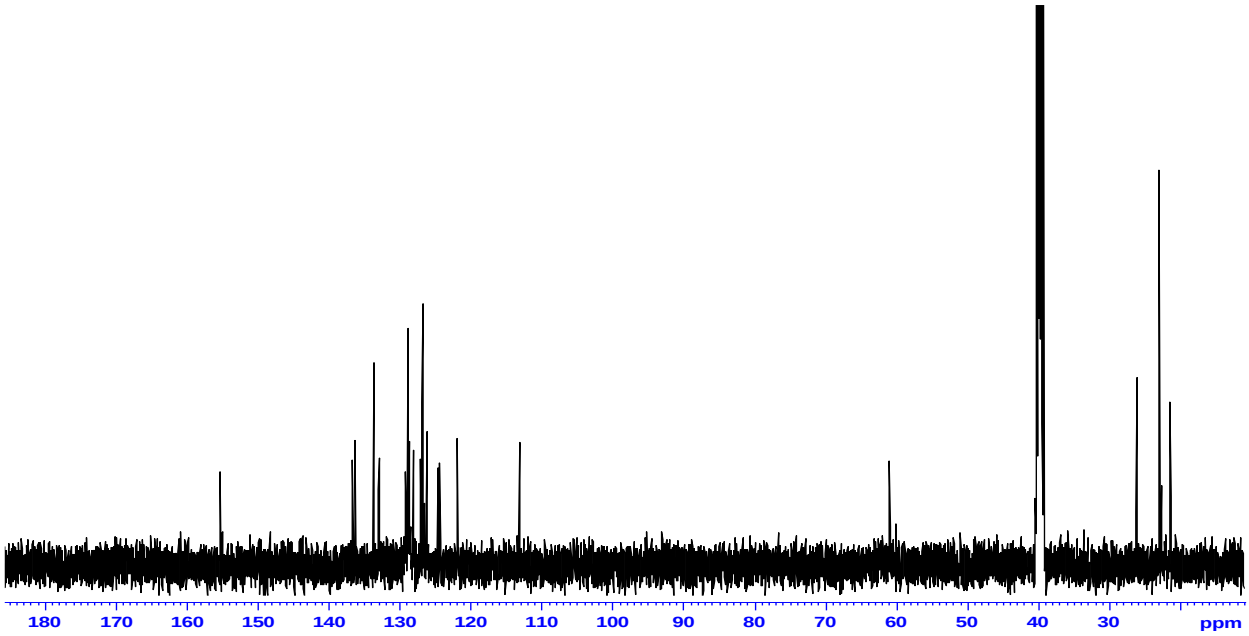


Figure 16. ^{13}C-NMR spectra of compound **7d**

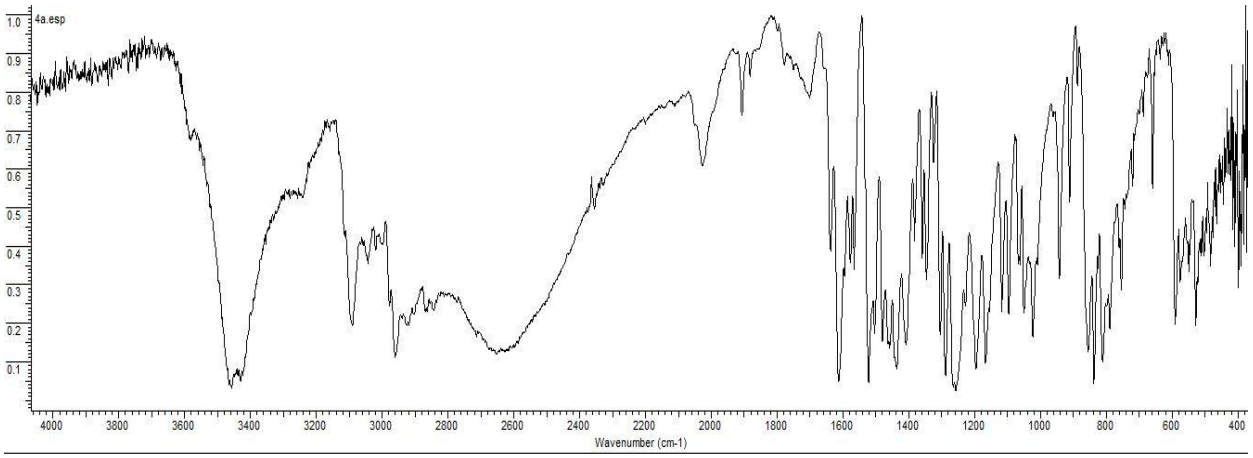


Figure 17. FT-IR spectra of compound **4a**

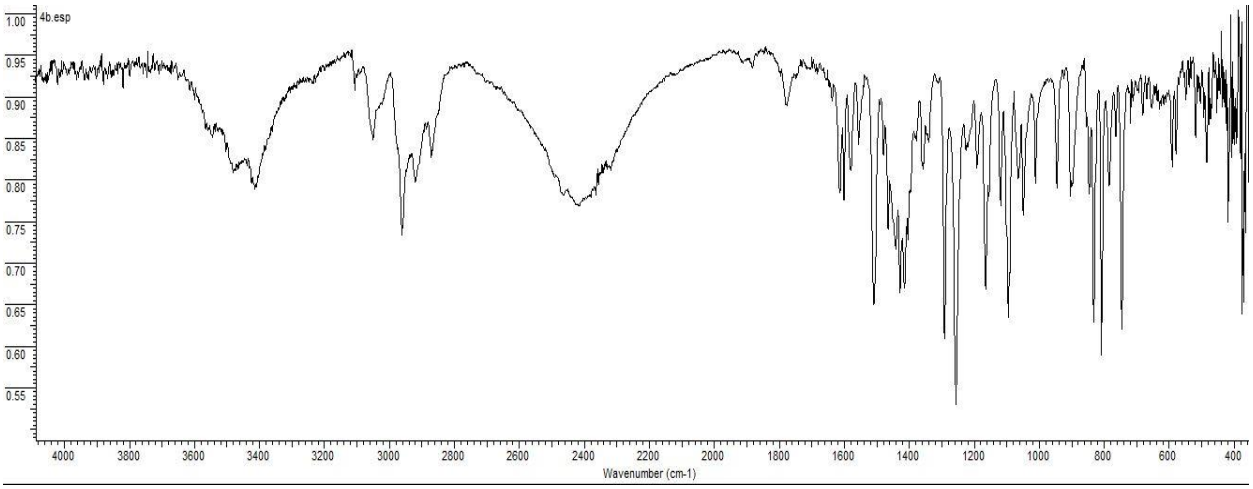


Figure 18. FT-IR spectra of compound **4b**

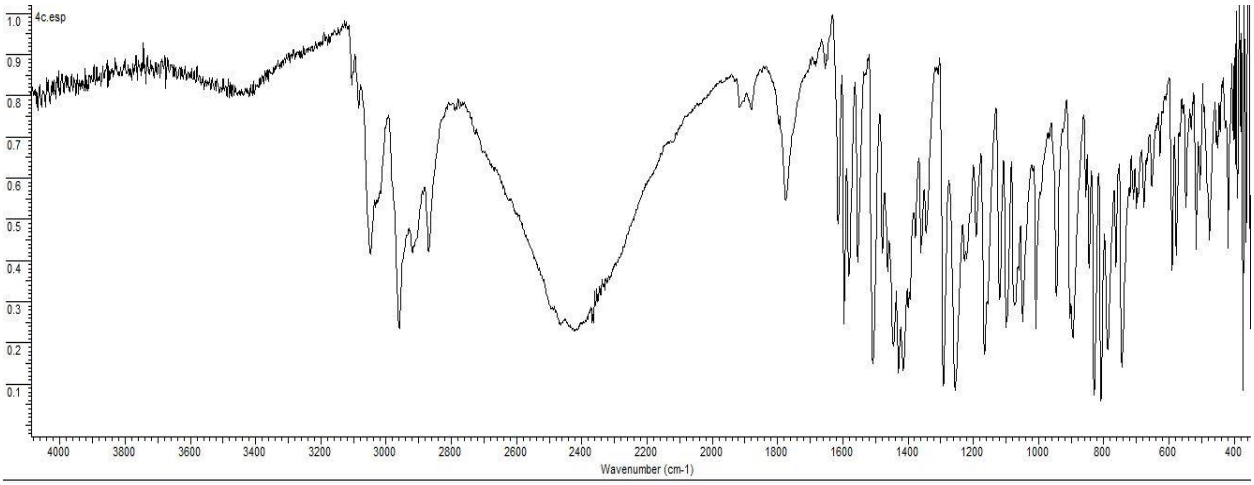


Figure 19. FT-IR spectra of compound **4c**

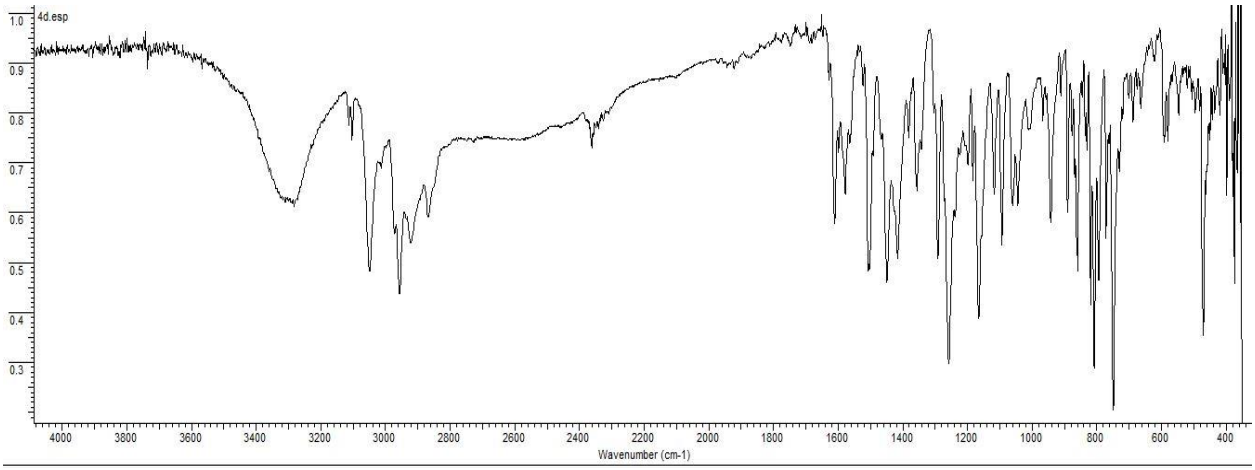


Figure 20. FT-IR spectra of compound **4d**

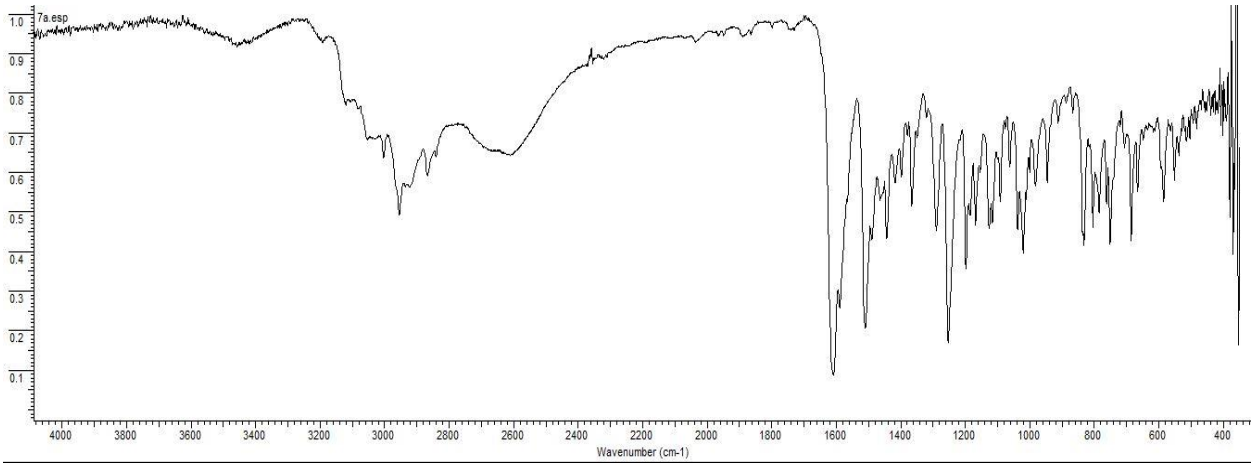


Figure 21. FT-IR spectra of compound **7a**

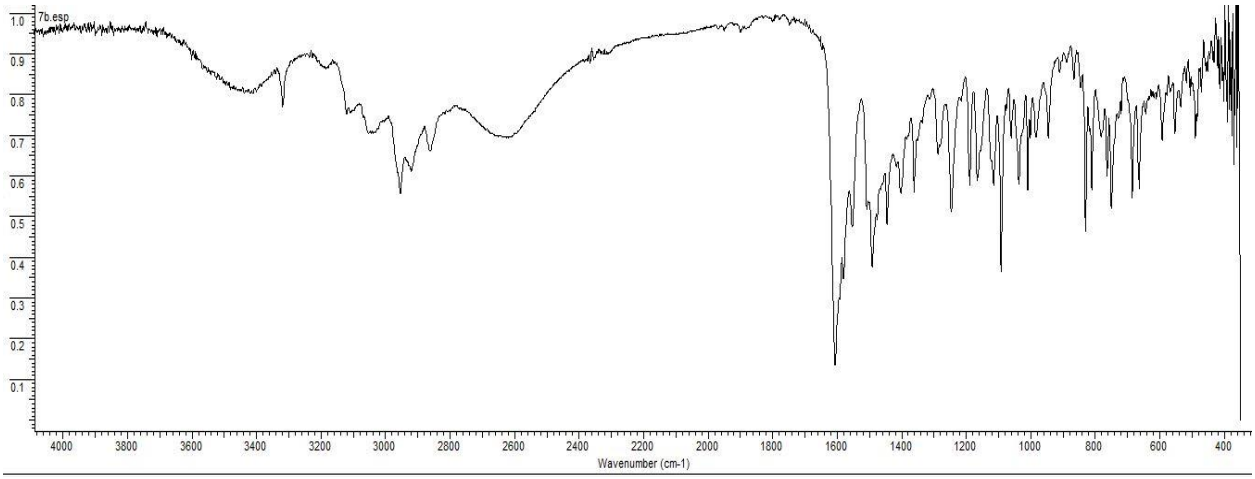


Figure 22. FT-IR spectra of compound **7b**

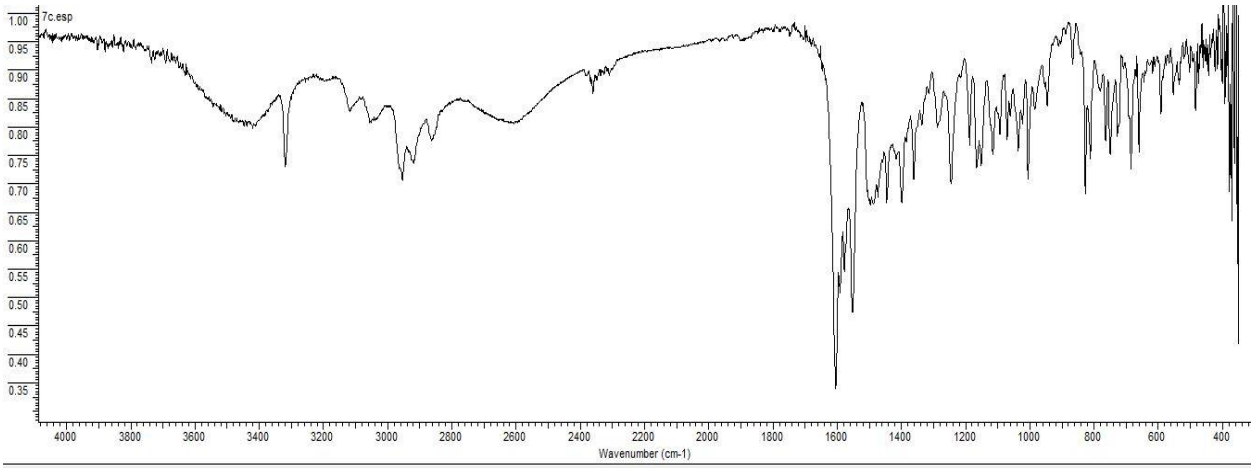


Figure 23. FT-IR spectra of compound **7c**

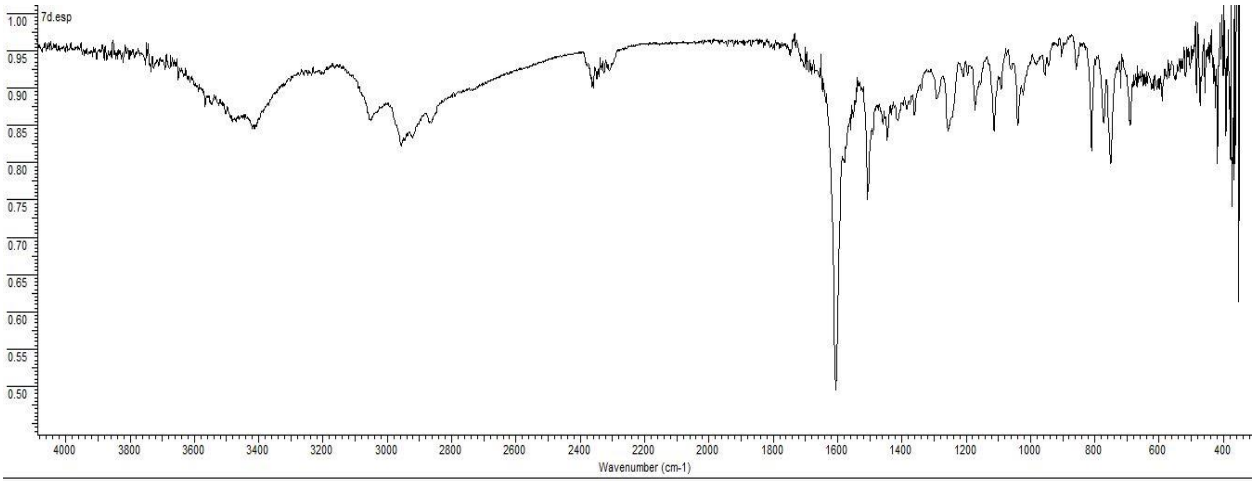
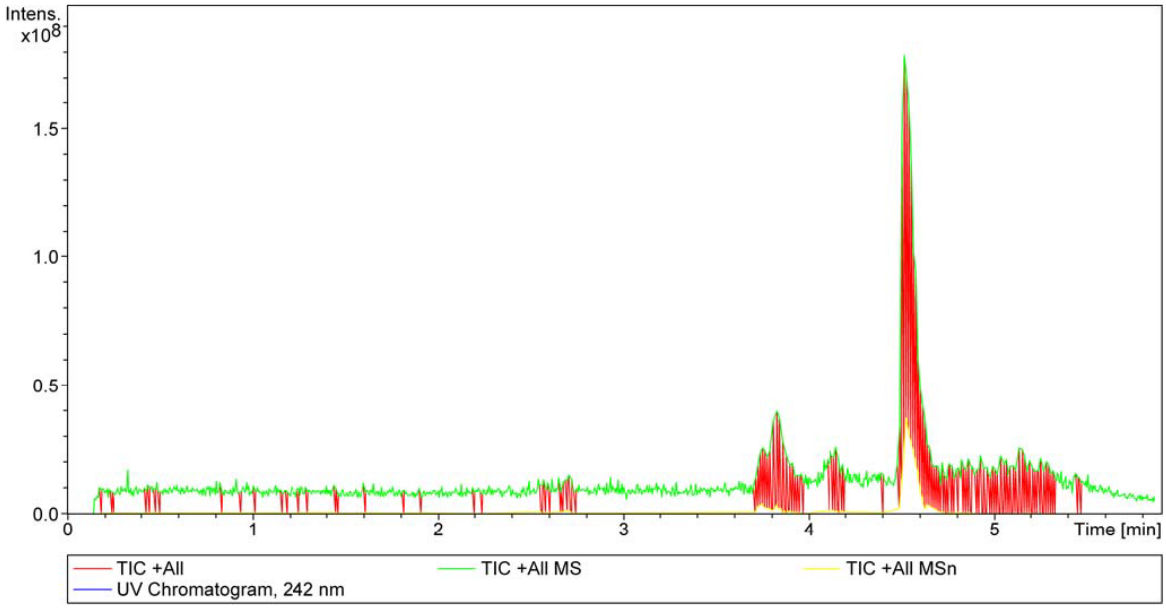


Figure 24. FT-IR spectra of compound **7d**

Acquisition Parameter:

Mass Range Mode	Std/Normal	Trap Drive	43.0	Scan Begin	105 m/z	Auto MS/MS	off
Ion Polarity	Positive	Octopole RF Amplitude	75.0 Vpp	Scan End	500 m/z		
Ion Source Type	ESI			Averages	1 Spectra		
Dry Temp (Set)	350 °C	Capillary Exit	95.5 Volt	Max. Accu Time	100000 µs		
Nebulizer (Set)	60.00 psi	Skimmer	40.0 Volt	ICC Target	40000		
Dry Gas (Set)	12.00 l/min	Oct 1 DC	12.00 Volt	Charge Control	on		
		Oct 2 DC	1.70 Volt				



Compound List:

#	RT [min]	Range [min]	MS(n) Isol. m/z
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n.a.	4.5	4.5	354.5

+MS, 4.5min #882

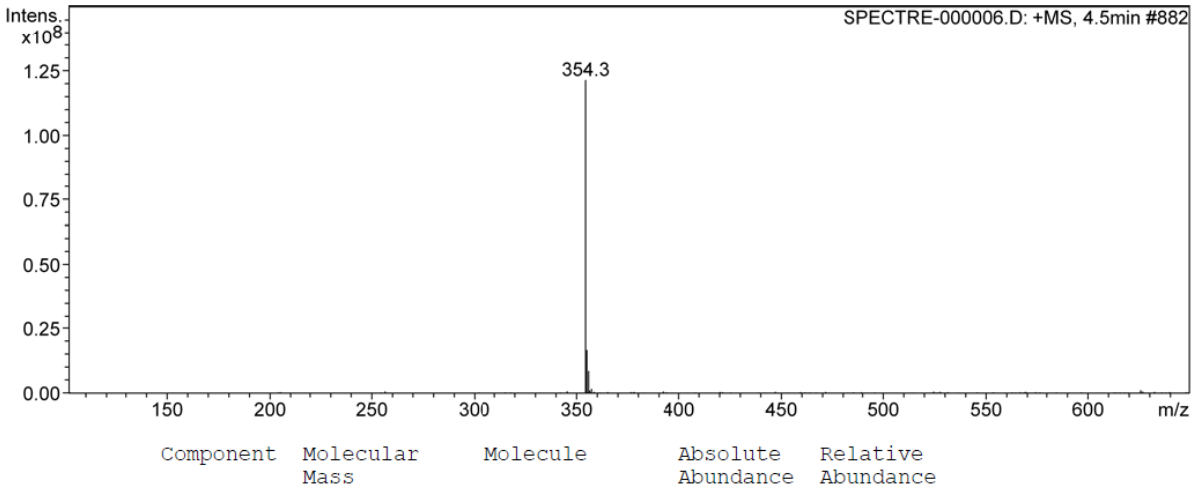
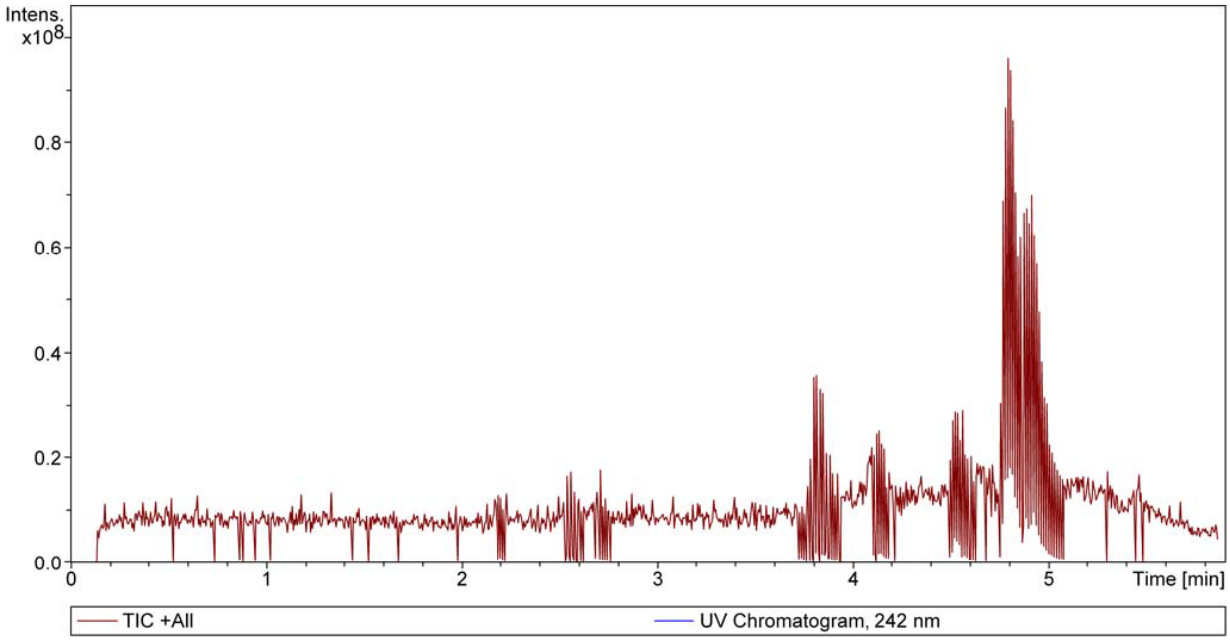


Figure 25. ESI-MS spectrum of compound **4a**

Acquisition Parameter:

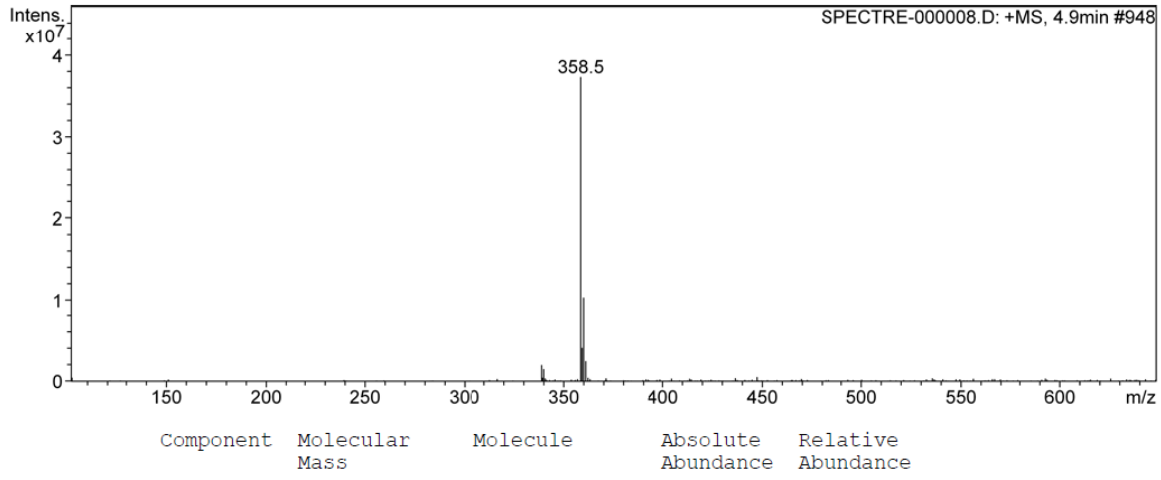
Mass Range Mode	Std/Normal	Trap Drive	43.0	Scan Begin	105 m/z	Auto MS/MS off
Ion Polarity	Positive	Octopole RF Amplitude	75.0 Vpp	Scan End	500 m/z	
Ion Source Type	ESI			Averages	1 Spectra	
Dry Temp (Set)	350 °C	Capillary Exit	95.5 Volt	Max. Accu Time	100000 µs	
Nebulizer (Set)	60.00 psi	Skimmer	40.0 Volt	ICC Target	40000	
Dry Gas (Set)	12.00 l/min	Oct 1 DC	12.00 Volt	Charge Control	on	
		Oct 2 DC	1.70 Volt			



Compound List:

#	RT [min]	Range [min]	MS(n) Isol. m/z
n.a.	4.9	4.9	
n.a.	4.9	4.9	358.9

+MS, 4.9min #948

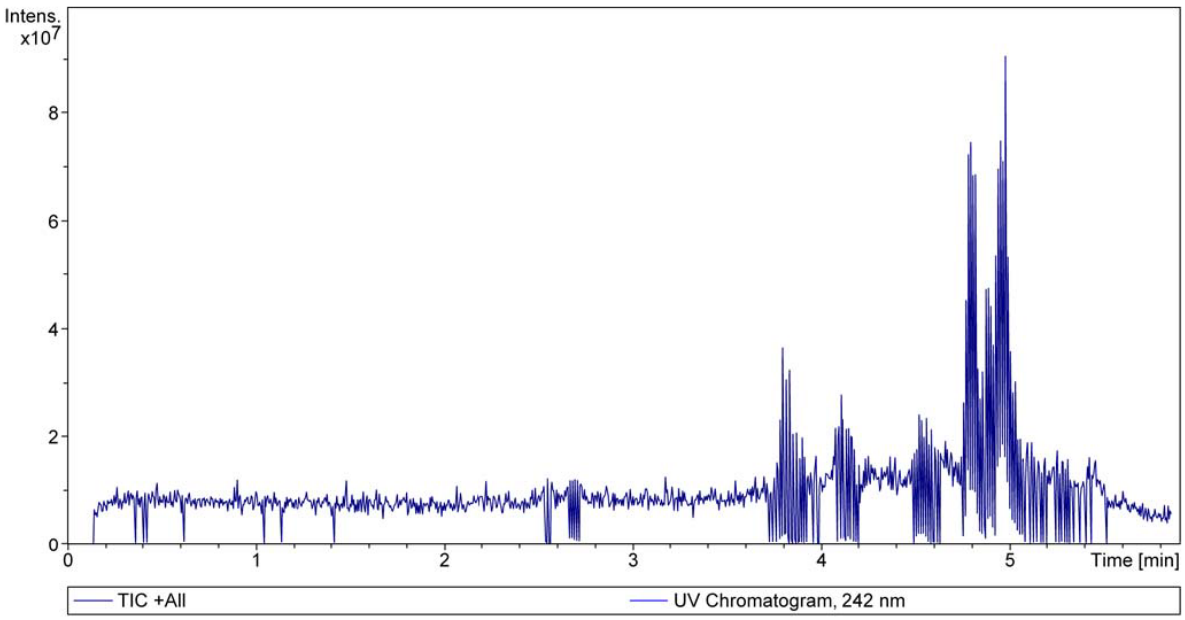


Component	Molecular Mass	Molecule	Absolute Abundance	Relative Abundance

Figure 26. ESI-MS spectrum of compound **4b**

Acquisition Parameter:

Mass Range Mode	Std/Normal	Trap Drive	43.0	Scan Begin	105 m/z	Auto MS/MS	off
Ion Polarity	Positive	Octopole RF Amplitude	75.0 Vpp	Scan End	500 m/z		
Ion Source Type	ESI			Averages	1 Spectra		
Dry Temp (Set)	350 °C	Capillary Exit	95.5 Volt	Max. Accu Time	100000 µs		
Nebulizer (Set)	60.00 psi	Skimmer	40.0 Volt	ICC Target	40000		
Dry Gas (Set)	12.00 l/min	Oct 1 DC	12.00 Volt	Charge Control	on		
		Oct 2 DC	1.70 Volt				



Compound List:

#	RT [min]	Range [min]	MS(n) Isol. m/z
n.a.	5.0	5.0	
n.a.	5.0	5.0	403.4

+MS, 5.0min #965

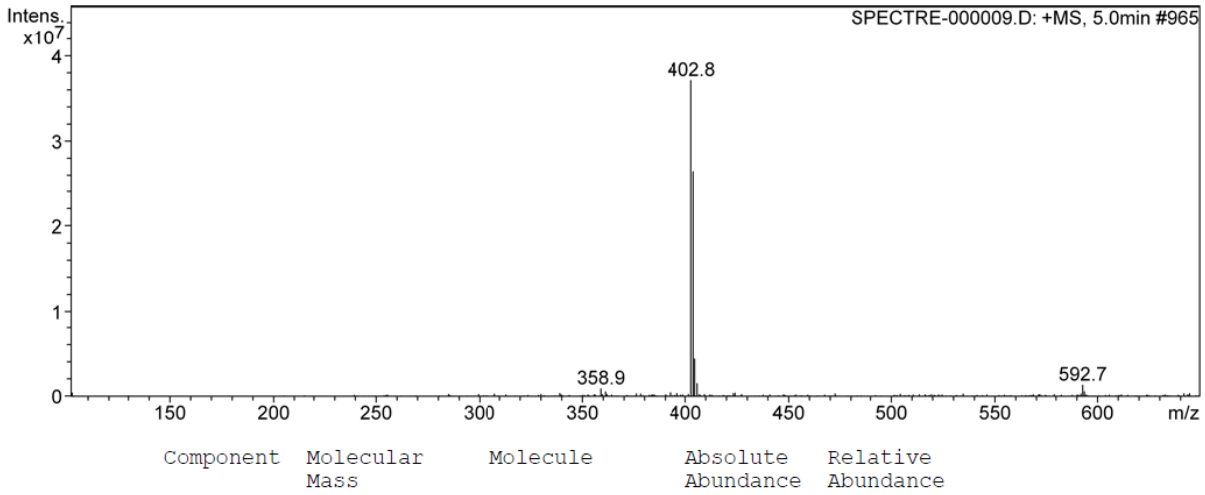
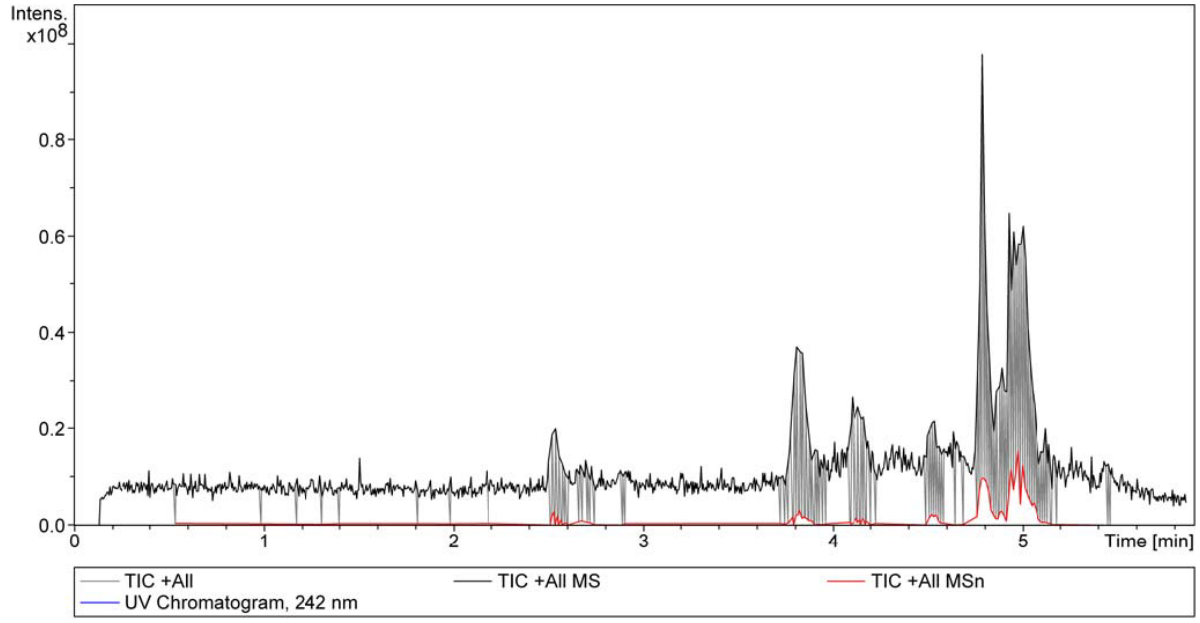


Figure 27. ESI-MS spectrum of compound **4c**

Acquisition Parameter:

Mass Range Mode	Std/Normal	Trap Drive	43.0	Scan Begin	105 m/z	Auto MS/MS off
Ion Polarity	Positive	Octopole RF Amplitude	75.0 Vpp	Scan End	500 m/z	
Ion Source Type	ESI			Averages	1 Spectra	
Dry Temp (Set)	350 °C	Capillary Exit	95.5 Volt	Max. Accu Time	100000 µs	
Nebulizer (Set)	60.00 psi	Skimmer	40.0 Volt	ICC Target	40000	
Dry Gas (Set)	12.00 l/min	Oct 1 DC	12.00 Volt	Charge Control	on	
		Oct 2 DC	1.70 Volt			



Compound List:

#	RT [min]	Range [min]	MS(n) Isol. m/z
n.a.	5.0	5.0	
n.a.	5.0	5.0	374.5

+MS, 5.0min #967

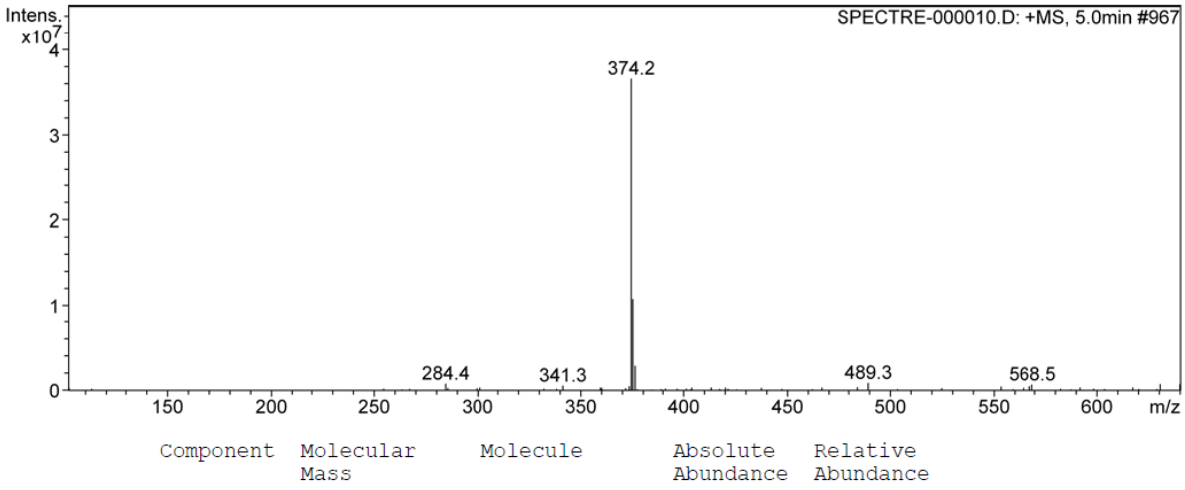
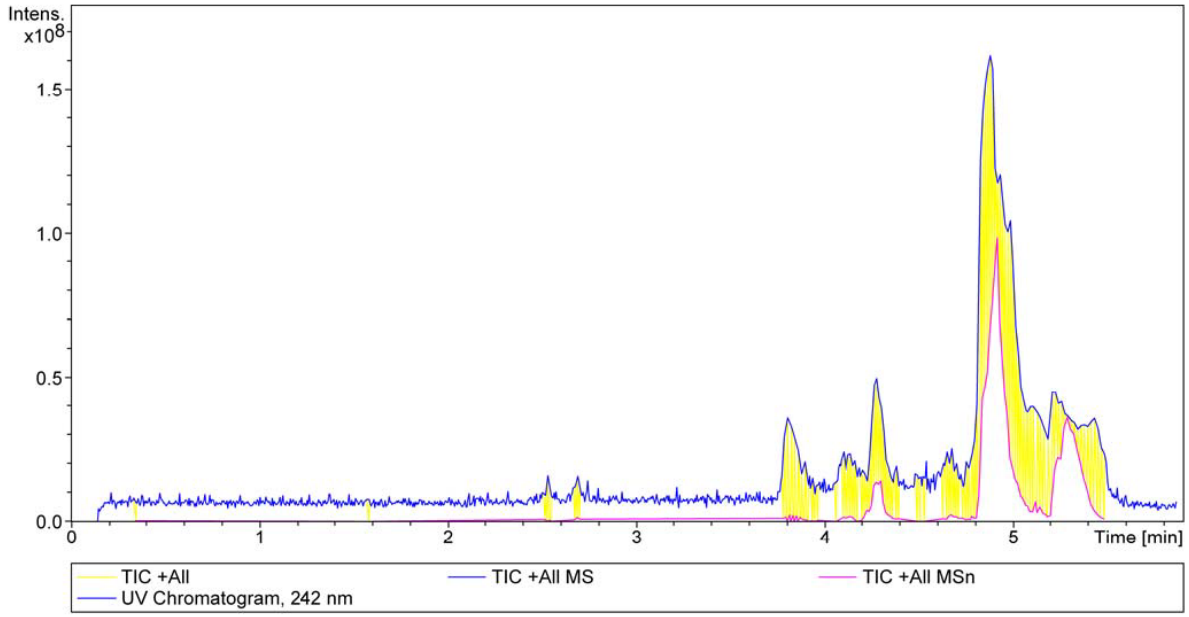


Figure 28. ESI-MS spectrum of compound **4d**

Acquisition Parameter:

Mass Range Mode	Std/Normal	Trap Drive	43.0	Scan Begin	105 m/z	Auto MS/MS off
Ion Polarity	Positive	Octopole RF Amplitude	75.0 Vpp	Scan End	500 m/z	
Ion Source Type	ESI			Averages	1 Spectra	
Dry Temp (Set)	350 °C	Capillary Exit	95.5 Volt	Max. Accu Time	100000 µs	
Nebulizer (Set)	60.00 psi	Skimmer	40.0 Volt	ICC Target	40000	
Dry Gas (Set)	12.00 l/min	Oct 1 DC	12.00 Volt	Charge Control	on	
		Oct 2 DC	1.70 Volt			



Compound List:

#	RT [min]	Range [min]	MS(n) Isol. m/z
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n.a.	4.9	4.9	472.7

+MS, 4.9min #943

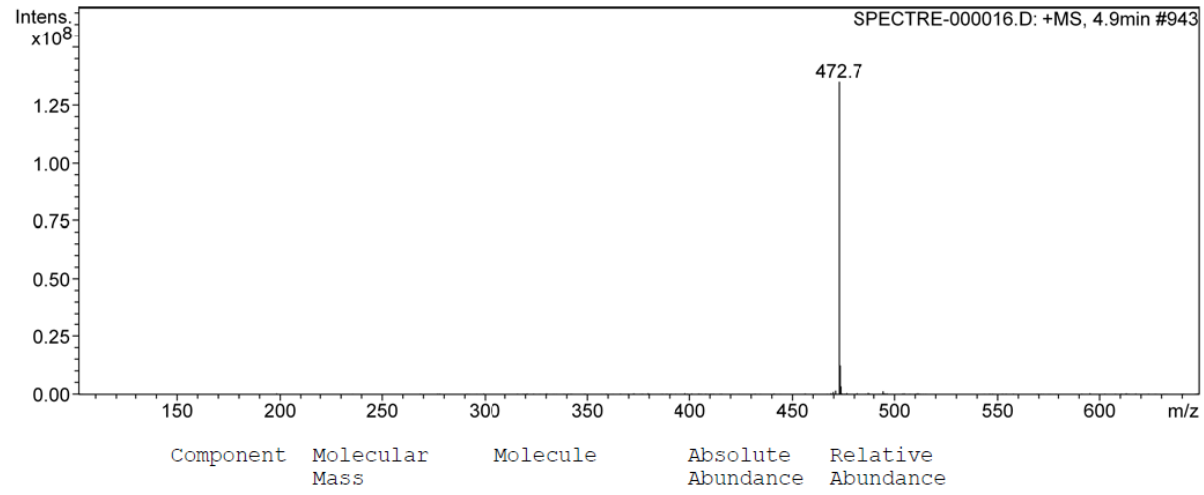
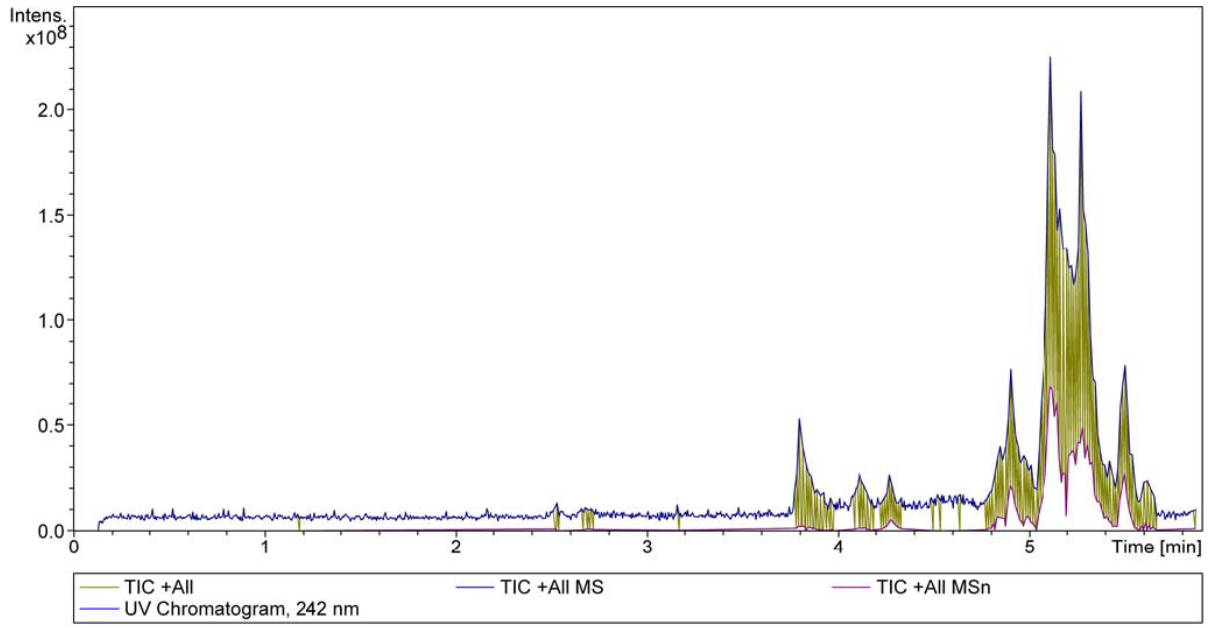


Figure 29. ESI-MS spectrum of compound **7a**

Acquisition Parameter:

Mass Range Mode	Std/Normal	Trap Drive	43.0	Scan Begin	105 m/z	Auto MS/MS	off
Ion Polarity	Positive	Octopole RF Amplitude	75.0 Vpp	Scan End	500 m/z		
Ion Source Type	ESI			Averages	1 Spectra		
Dry Temp (Set)	350 °C	Capillary Exit	95.5 Volt	Max. Accu Time	100000 µs		
Nebulizer (Set)	60.00 psi	Skimmer	40.0 Volt	ICC Target	40000		
Dry Gas (Set)	12.00 l/min	Oct 1 DC	12.00 Volt	Charge Control	on		
		Oct 2 DC	1.70 Volt				



Compound List:

#	RT [min]	Range [min]	MS(n) Isol. m/z
n.a.	5.3	5.3	
n.a.	5.3	5.3	476.8

+MS, 5.3min #1014

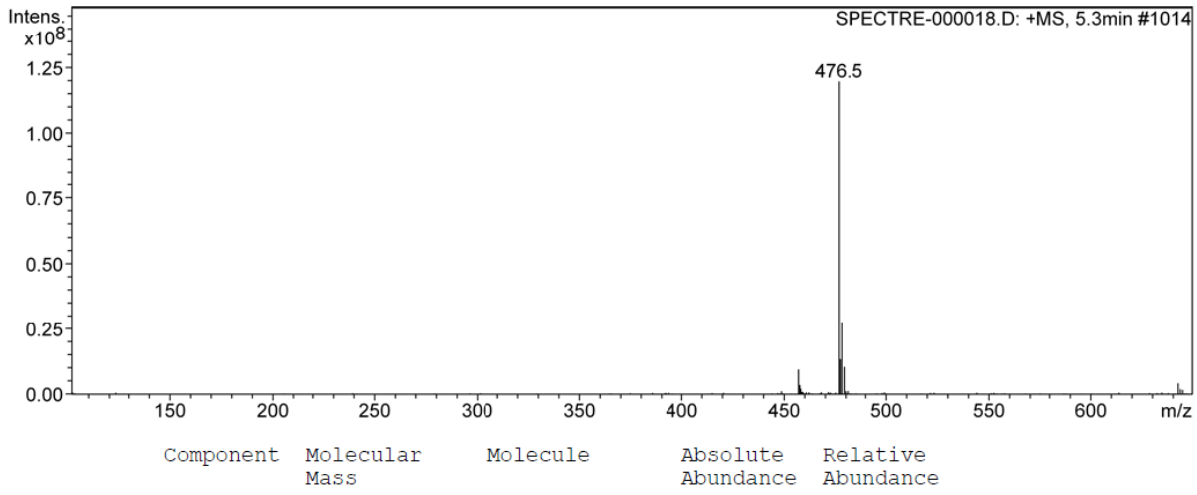
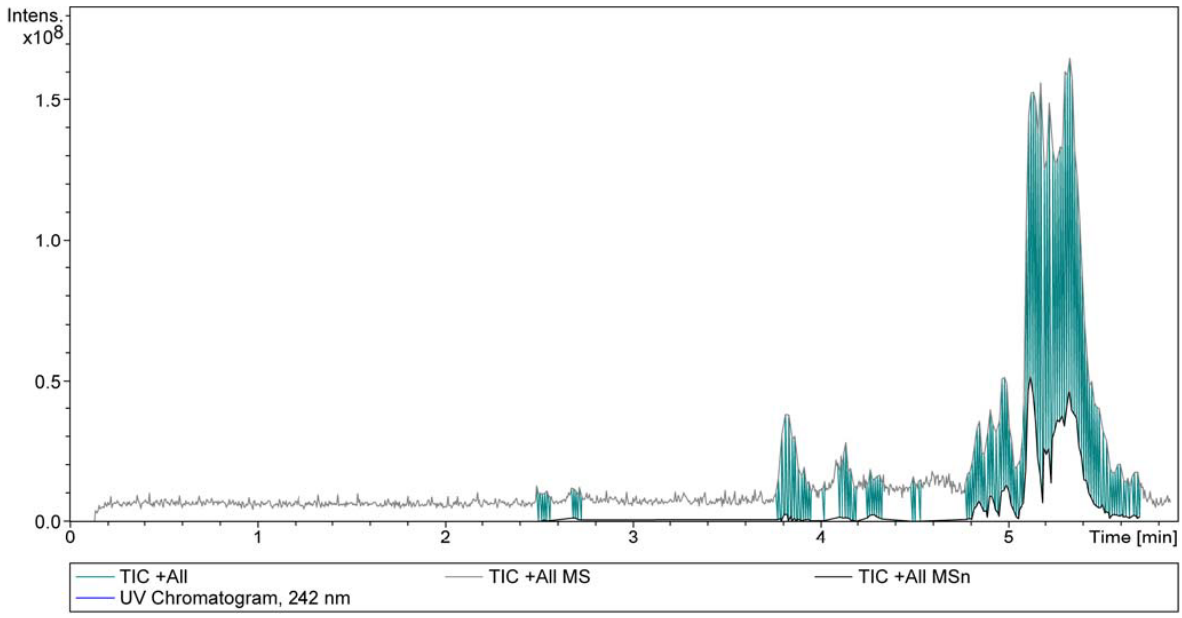


Figure 30. ESI-MS spectrum of compound **7b**

Acquisition Parameter:

Mass Range Mode	Std/Normal	Trap Drive	43.0	Scan Begin	105 m/z	Auto MS/MS off
Ion Polarity	Positive	Octopole RF Amplitude	75.0 Vpp	Scan End	500 m/z	
Ion Source Type	ESI			Averages	1 Spectra	
Dry Temp (Set)	350 °C	Capillary Exit	95.5 Volt	Max. Accu Time	100000 µs	
Nebulizer (Set)	60.00 psi	Skimmer	40.0 Volt	ICC Target	40000	
Dry Gas (Set)	12.00 l/min	Oct 1 DC	12.00 Volt	Charge Control	on	
		Oct 2 DC	1.70 Volt			



Compound List:

#	RT [min]	Range [min]	MS(n) Isol. m/z
n.a.	5.3	5.3	
n.a.	5.3	5.3	521.4

+MS, 5.3min #1021

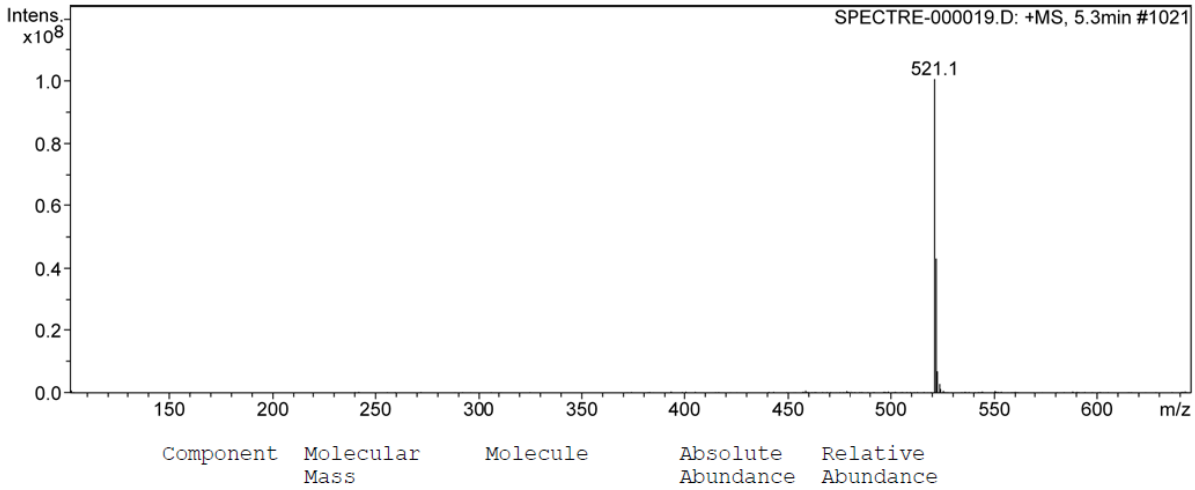
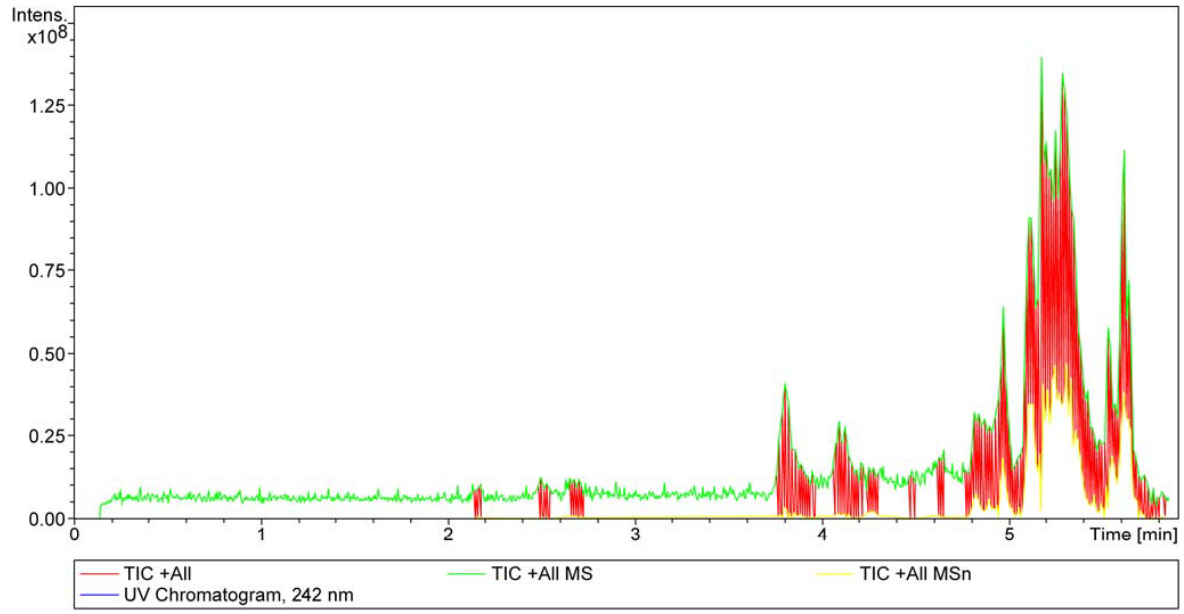


Figure 31. ESI-MS spectrum of compound **7c**

Acquisition Parameter:

Mass Range Mode	Std/Normal	Trap Drive	43.0	Scan Begin	105 m/z	Auto MS/MS off
Ion Polarity	Positive	Octopole RF Amplitude	75.0 Vpp	Scan End	500 m/z	
Ion Source Type	ESI			Averages	1 Spectra	
Dry Temp (Set)	350 °C	Capillary Exit	95.5 Volt	Max. Accu Time	100000 µs	
Nebulizer (Set)	60.00 psi	Skimmer	40.0 Volt	ICC Target	40000	
Dry Gas (Set)	12.00 l/min	Oct 1 DC	12.00 Volt	Charge Control	on	
		Oct 2 DC	1.70 Volt			



Compound List:

#	RT [min]	Range [min]	MS(n) Isol. m/z
n.a.	5.3	5.3	
n.a.	5.3	5.3	492.6

+MS, 5.3min #1019

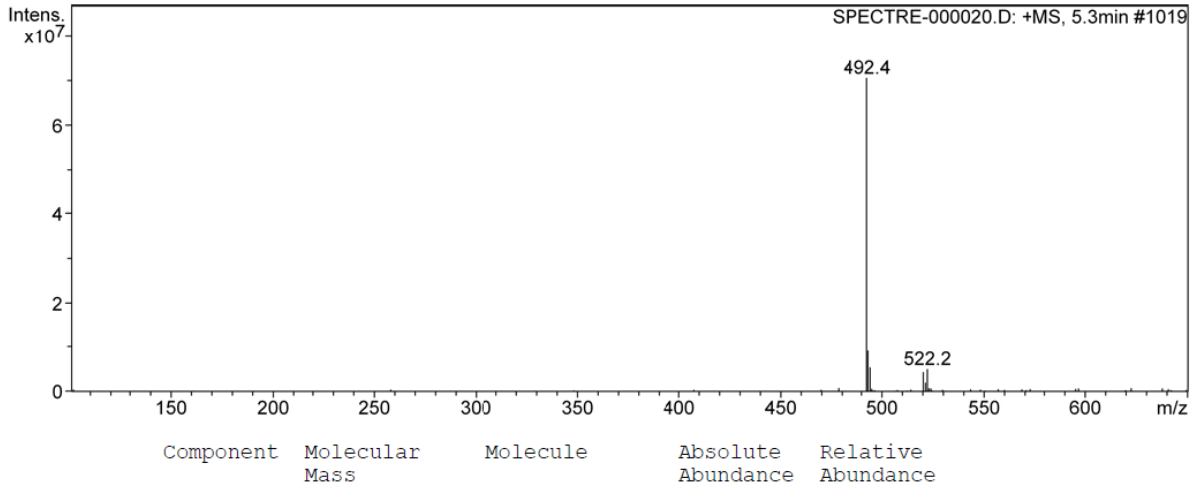


Figure 32. ESI-MS spectrum of compound **7d**