

Synthesis and Analytical characterization of cyclization products of 3-propargyloxy-5-benzyloxy-benzoic acid methyl ester

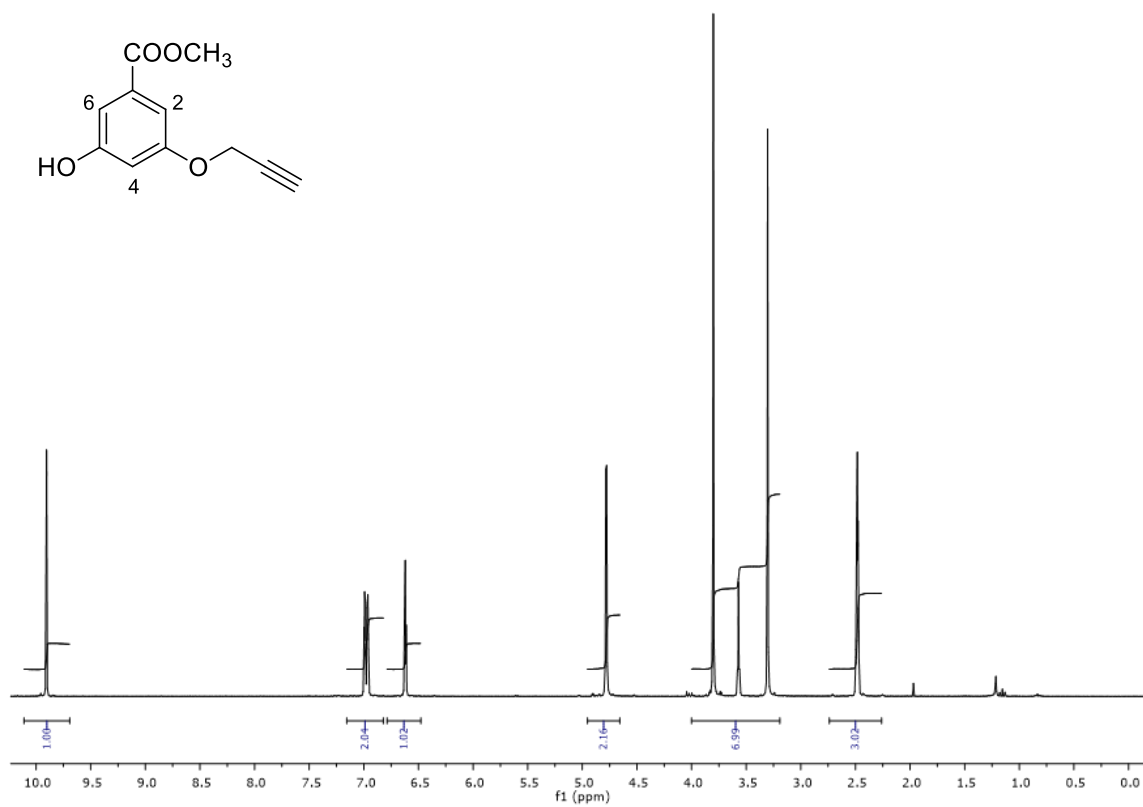
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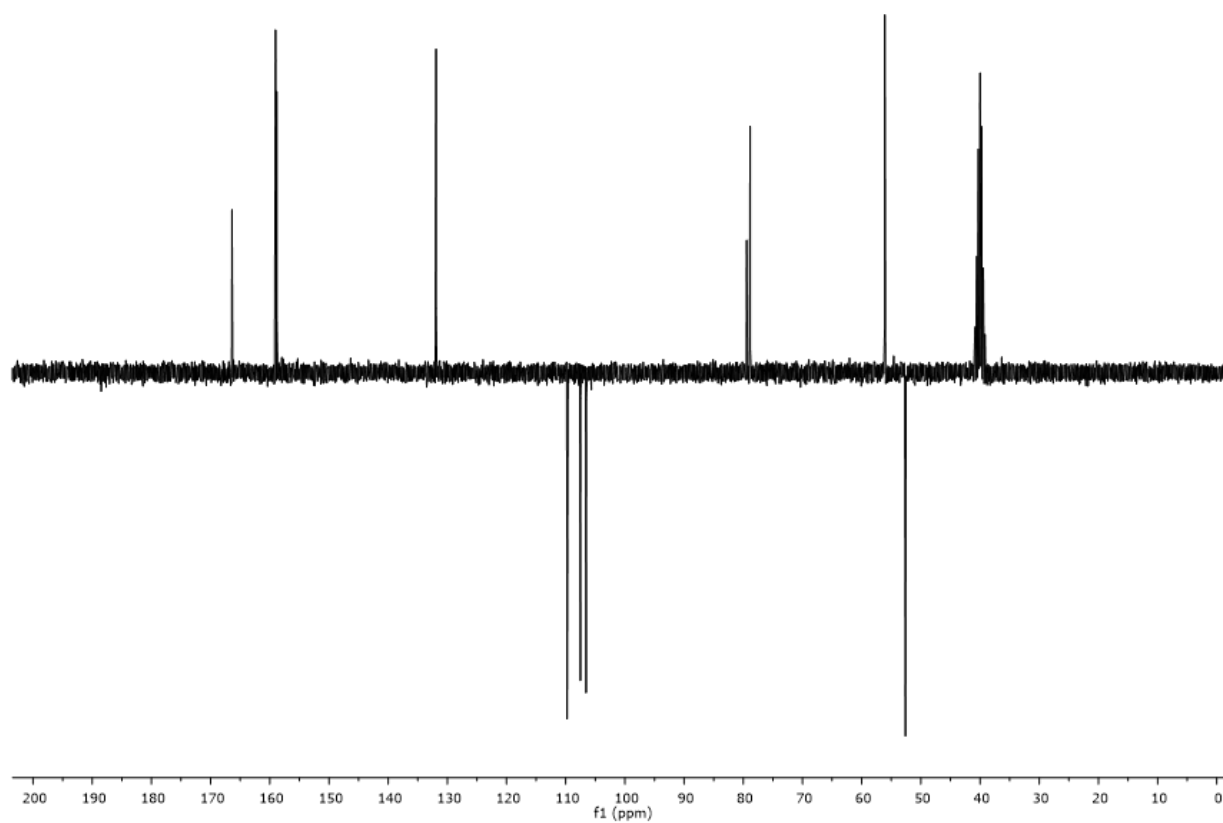
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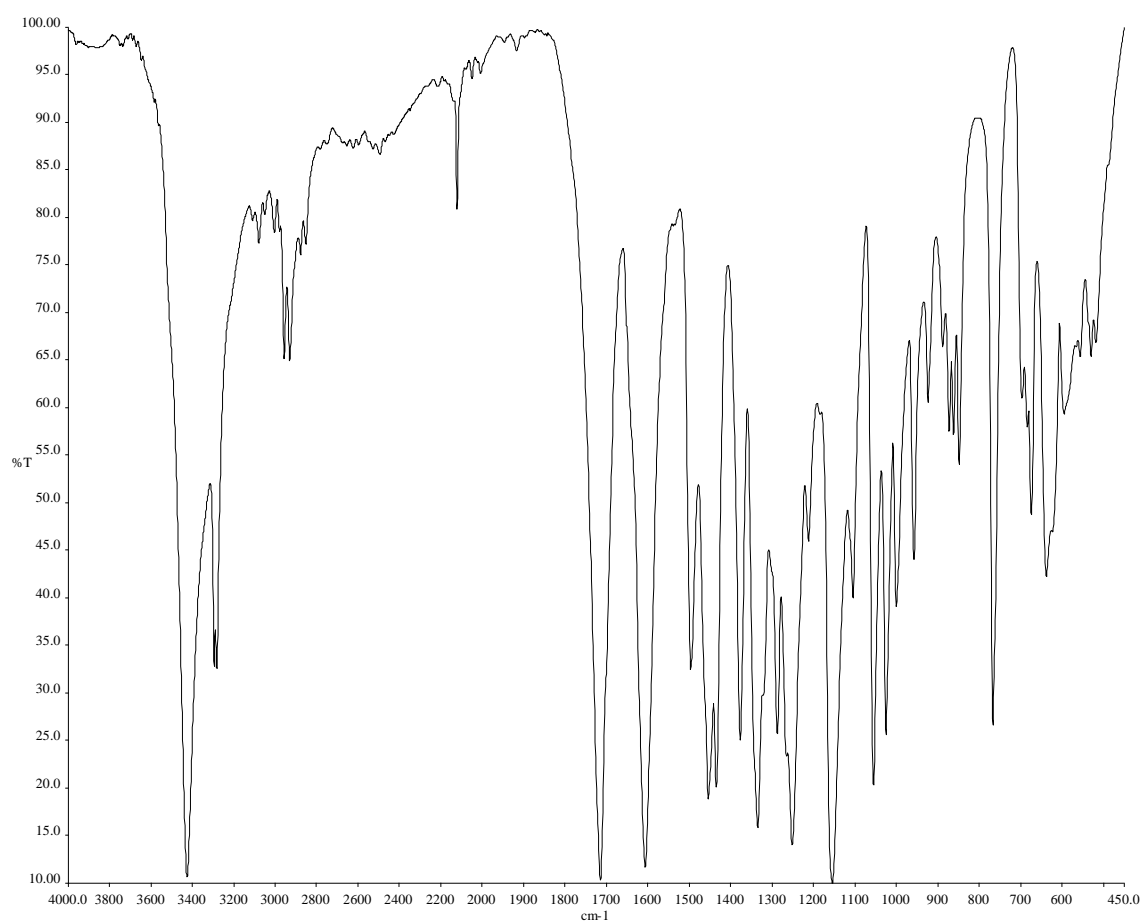
1. ^1H NMR spectrum of compound 1



2. ^{13}C NMR spectrum of compound 1

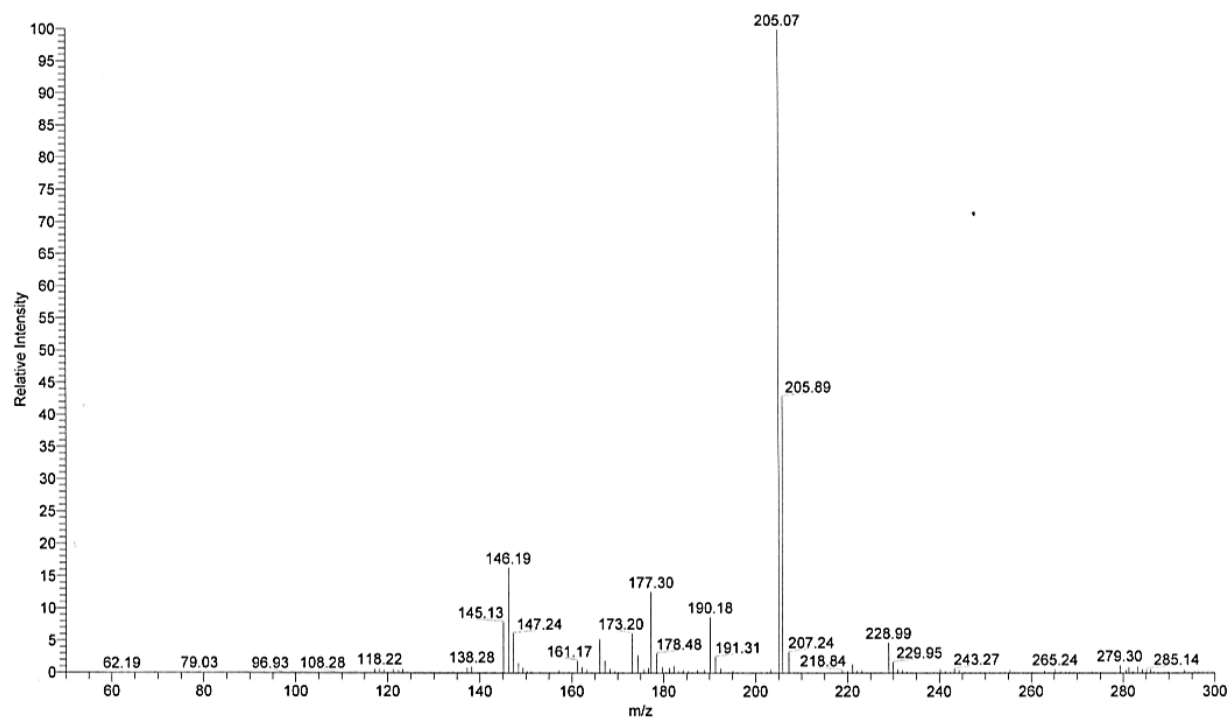


3. FT-IR spectrum of compound 1

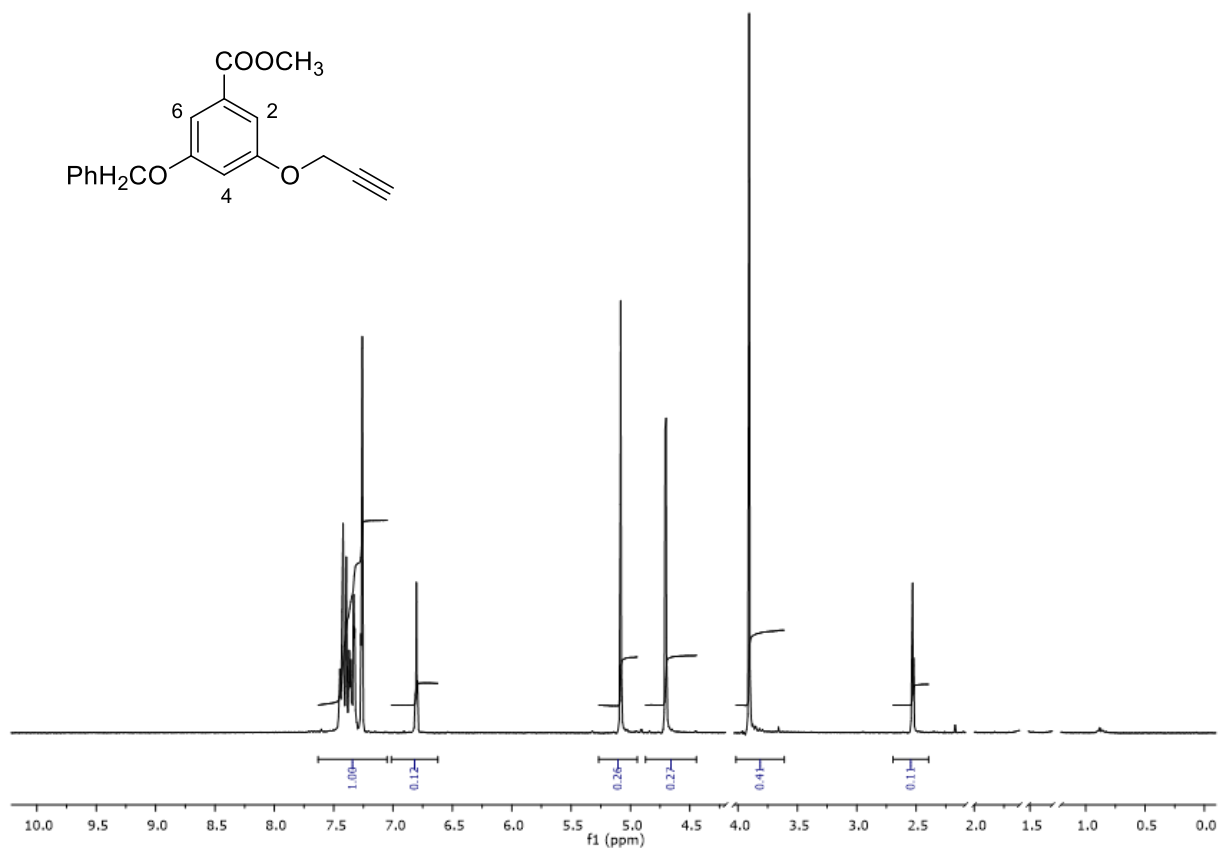


4. ESI-MS spectrum of compound 1

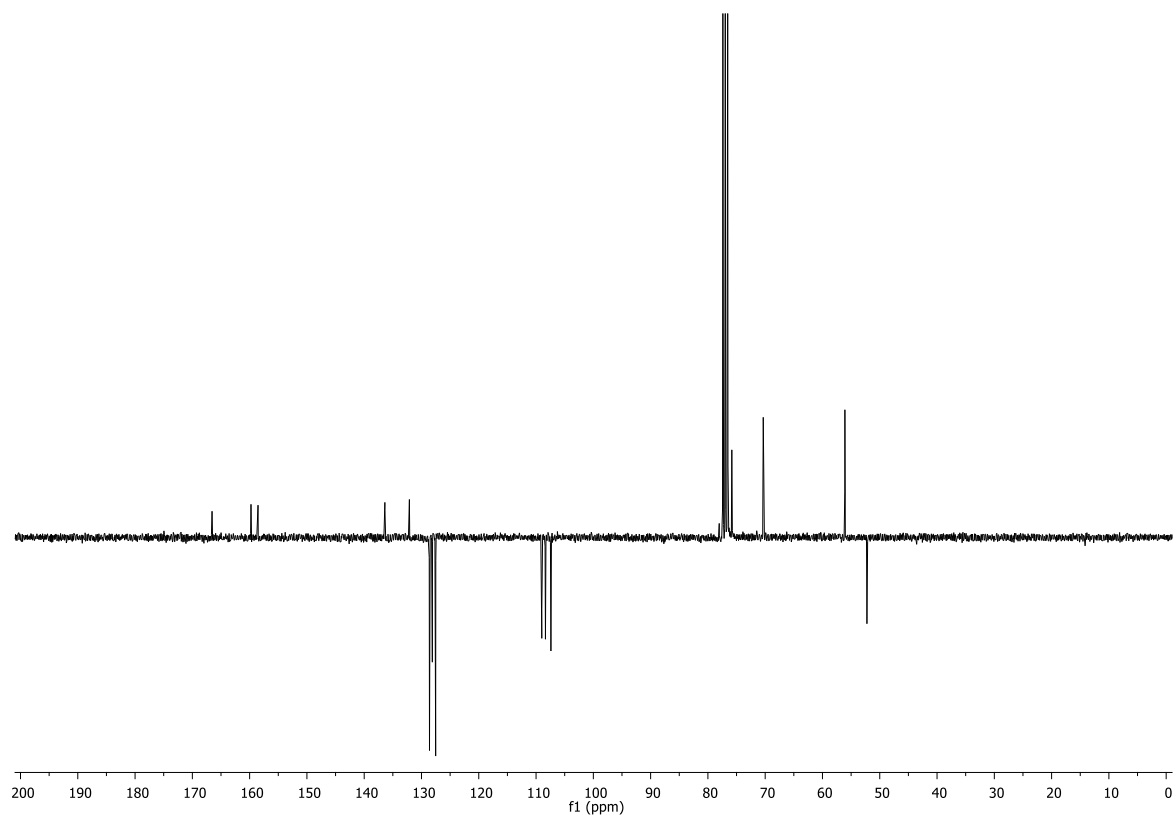
#14742 AV: 9 IT: 38.798 ST: 0.41 uS: 3 NL: 1.06E4
F: ITMS - c HESI Full ms [50.00-300.00]



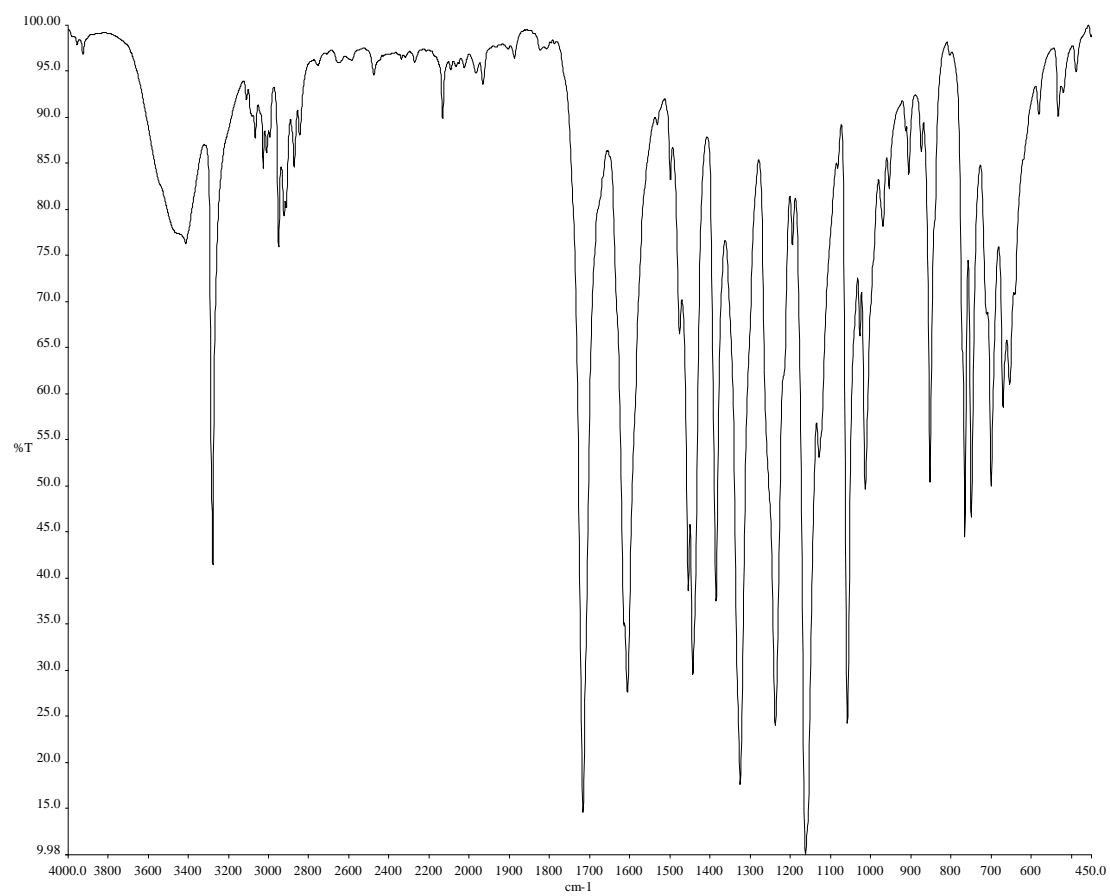
5. ^1H NMR spectrum of compound 2



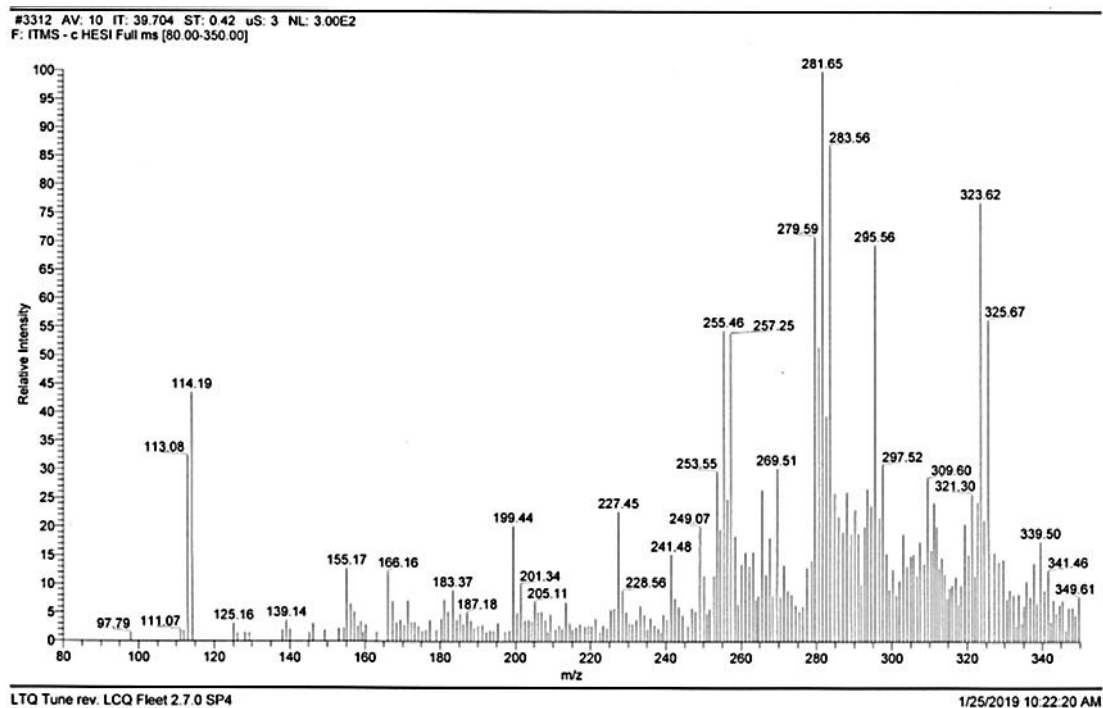
6. ^{13}C NMR spectrum of compound 2



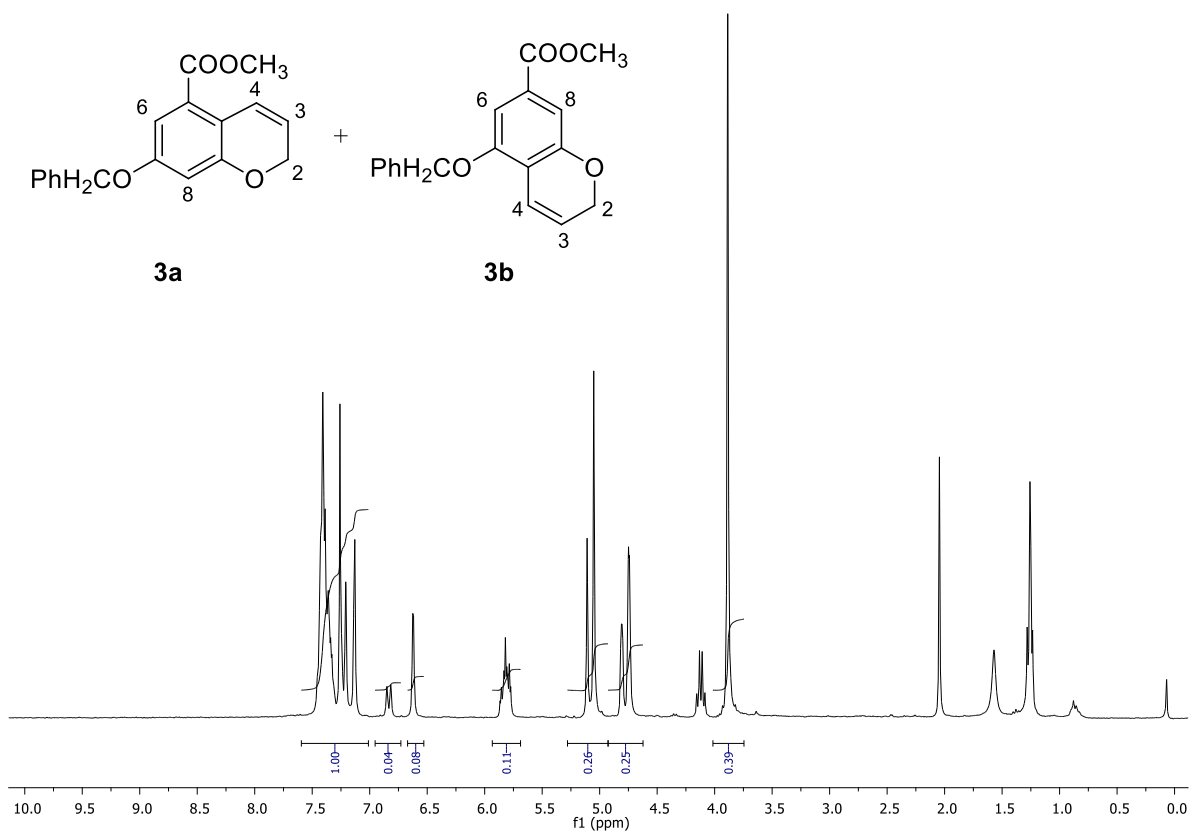
7. FT-IR spectrum of compound 2



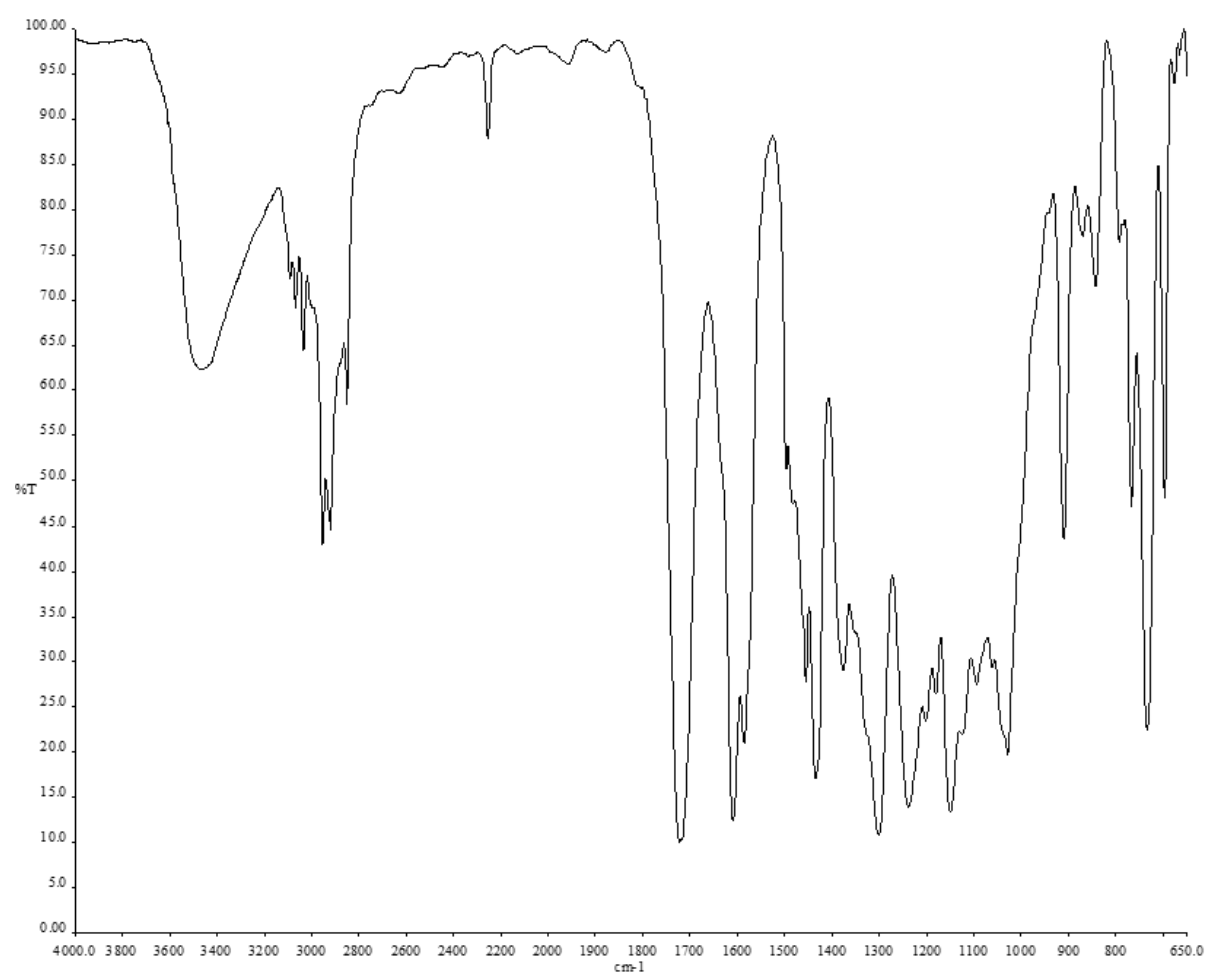
8. ESI-MS spectrum of compound 2



9. ^1H NMR of compounds mixture 3a and 3b

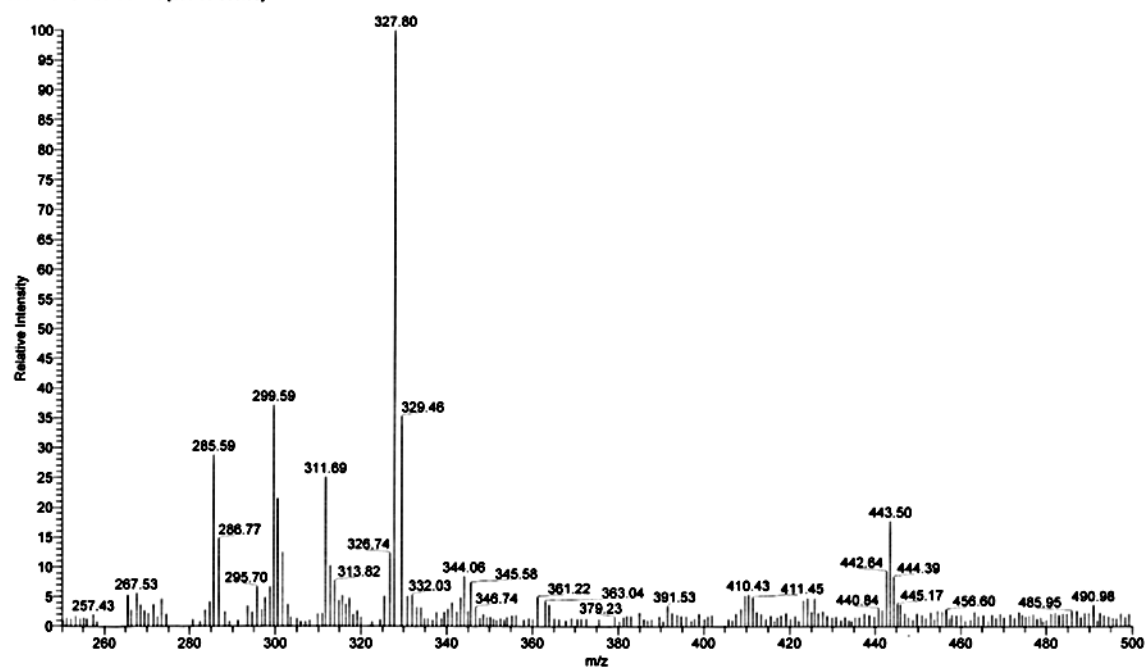


10. FT-IR of compounds mixture 3a and 3b

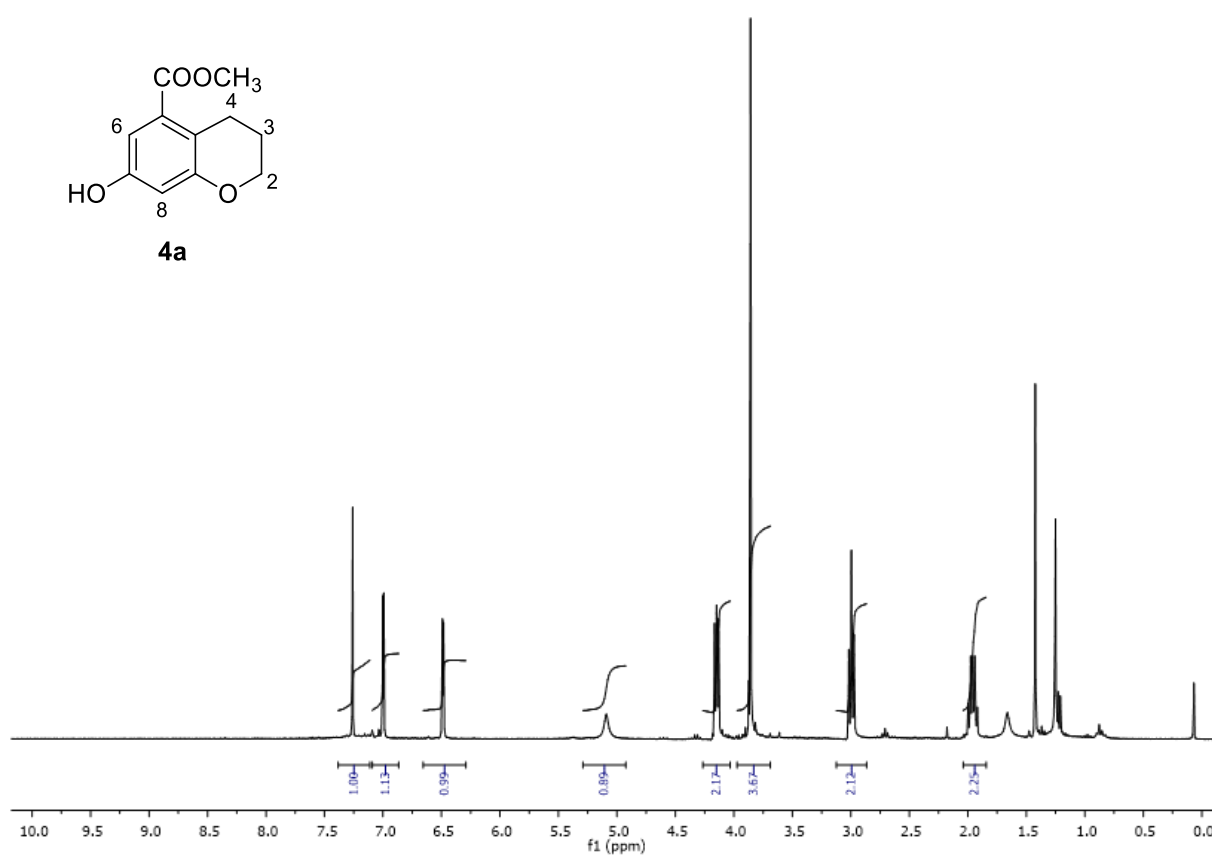


11. ESI-MS spectrum of compounds mixture 3a and 3b

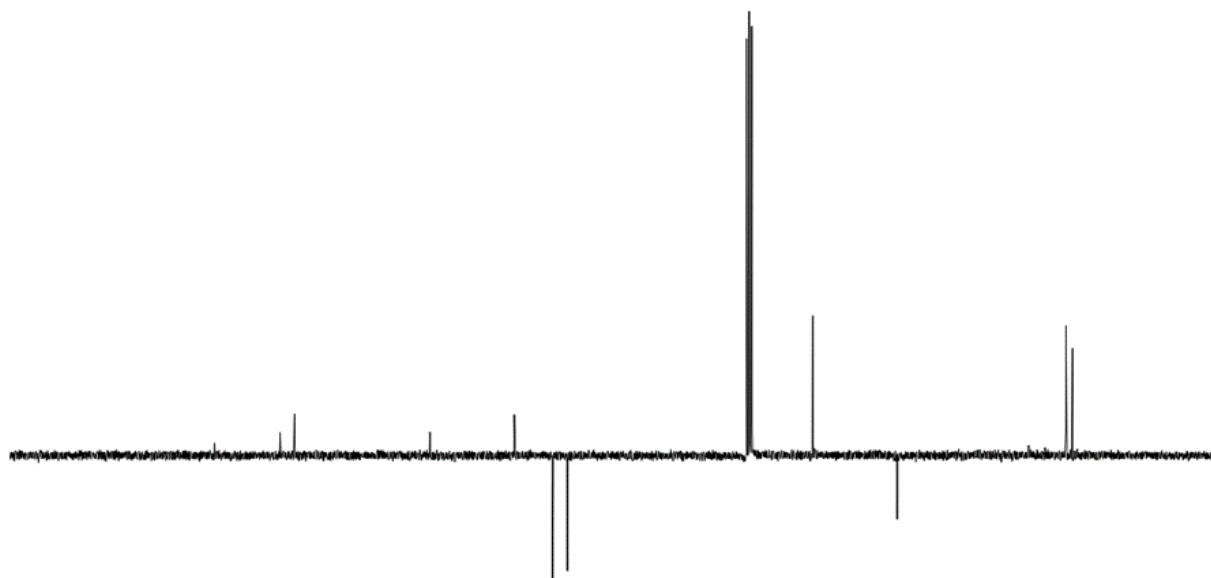
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F: ITMS - c HESI Full ms [250.00-500.00]



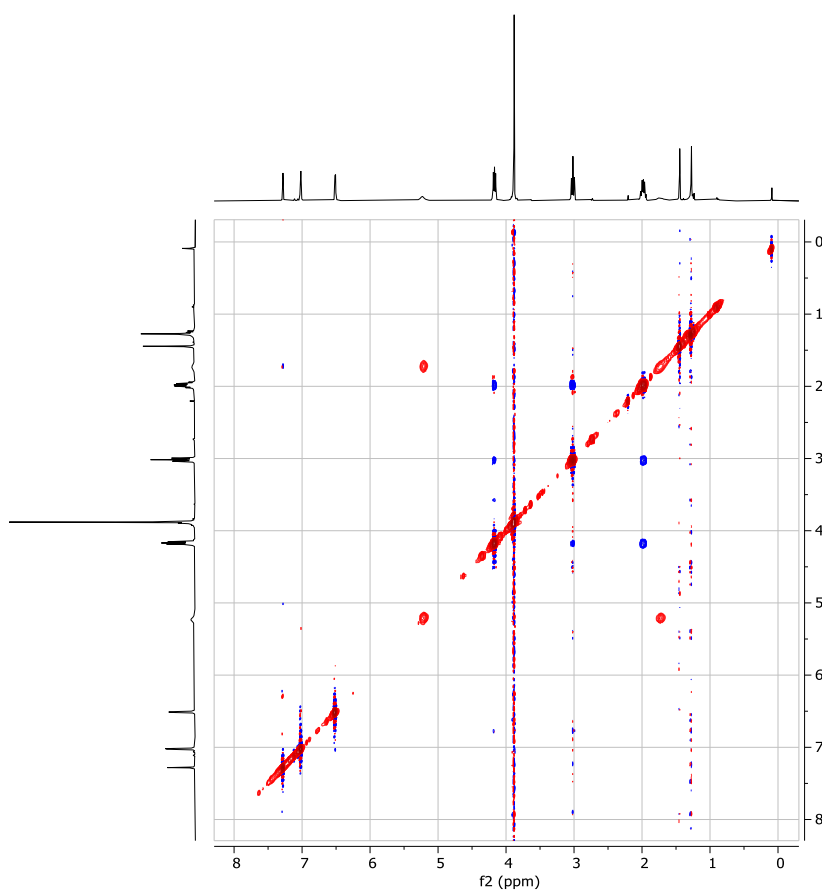
12. ^1H NMR spectrum of compound 4a



13. ^{13}C NMR spectrum of compound 4a

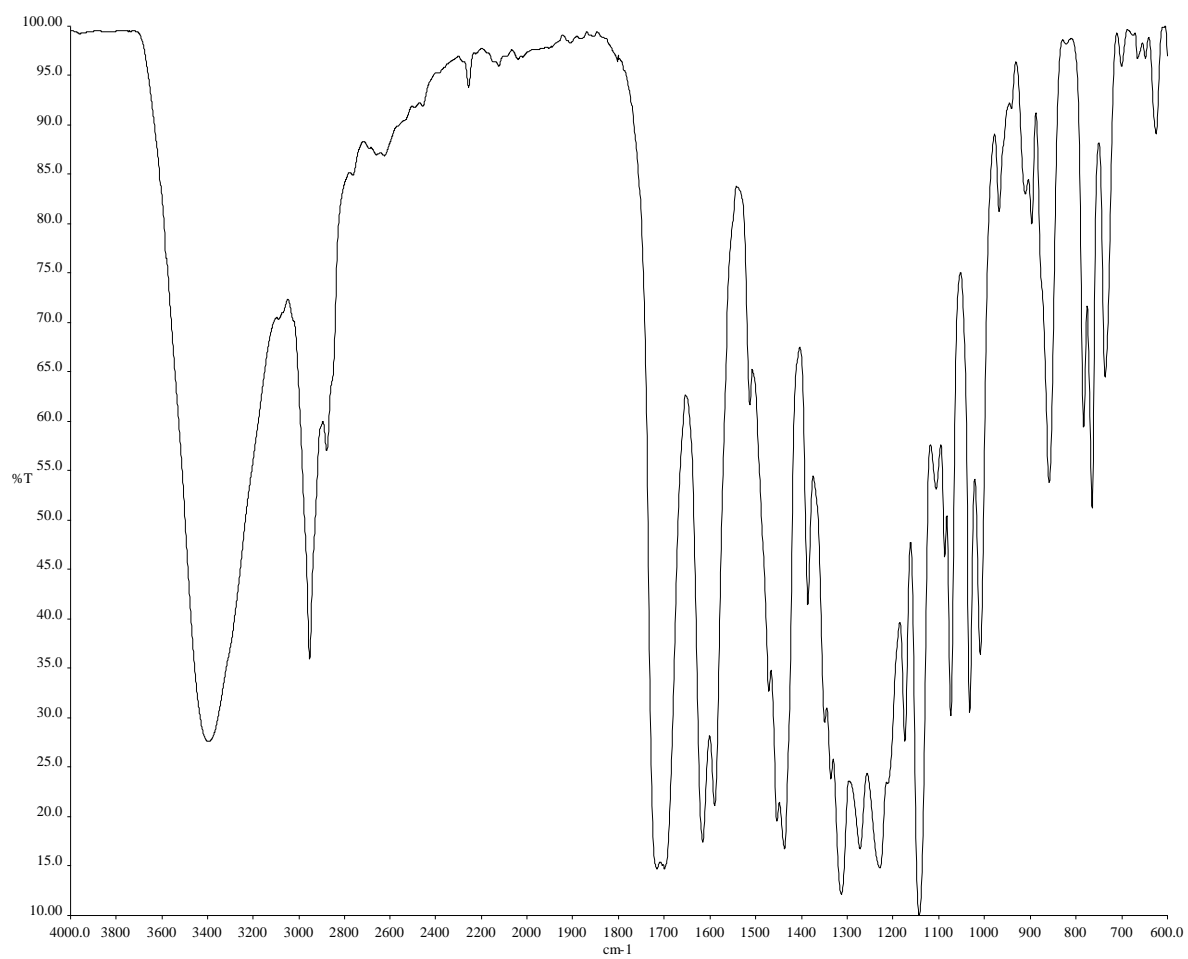


14. NOESY spectrum of compound 4a

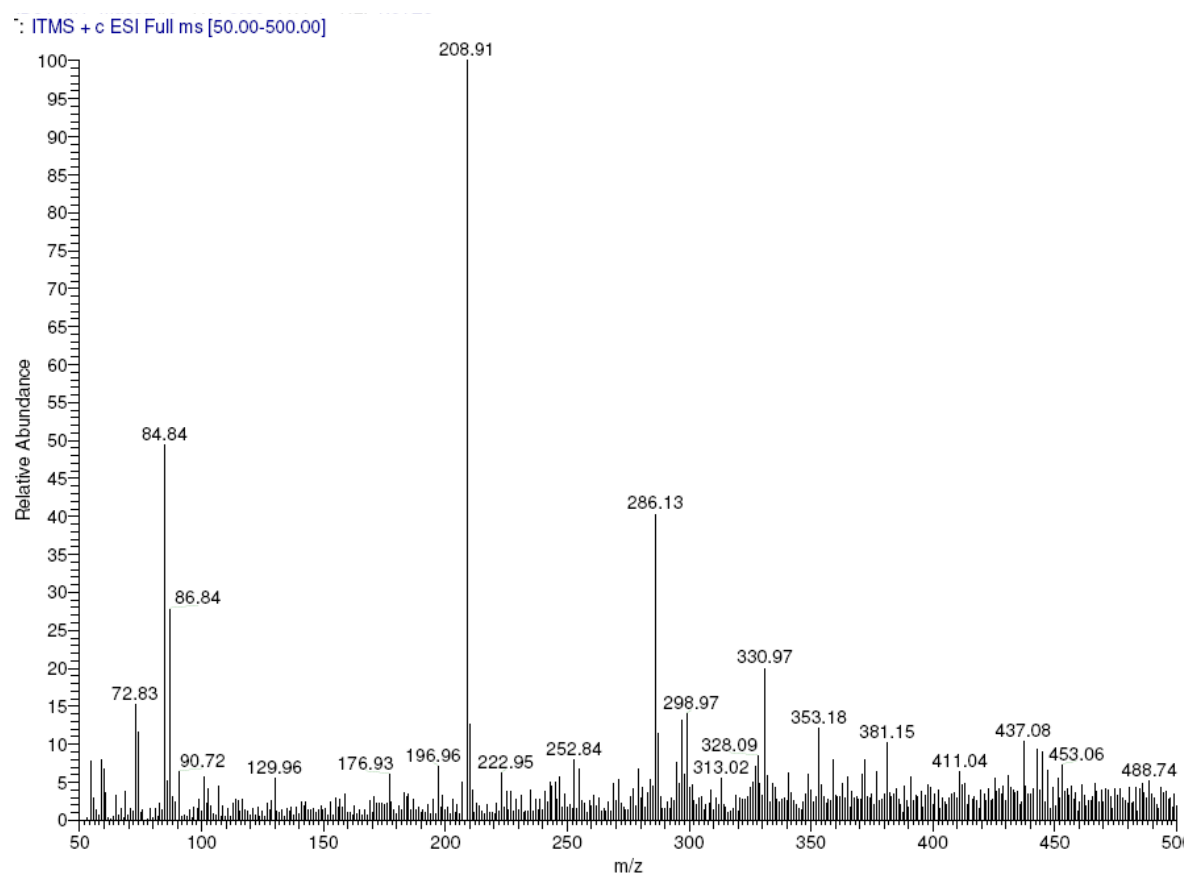


Parameter	Value (f2, f1)
Data File Name	C:/ Desktop/ NMR/ NMR 300MHz _ Am
Title	Compound 4b
Comment	4b NOESYph in CDCl3 a T=amb., tmix=1.2s
Origin	Bruker BioSpin GmbH
Owner	nmr
Site	
Spectrometer	spect
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	noesyph
Experiment	NOESY
Probe	5 mm QNP 1H/ 13C/ 31P/ 19F Z- grad Z8352/ 0036
Number of Scans	8
Receiver Gain	1820
Relaxation Delay	2.5000
Pulse Width	11.5000
Acquisition Time	0.3965
Acquisition Date	2019-02-18T14:24:34
Modification Date	2019-02-18T16:17:00
Class	
Spectrometer Frequency	(300.13, 300.13)
Spectral Width	(2582.6, 2582.7)
Lowest Frequency	(-93.5, -93.5)
Nucleus	(1H, 1H)
Acquired Size	(1024, 202)
Spectral Size	(2048, 2048)

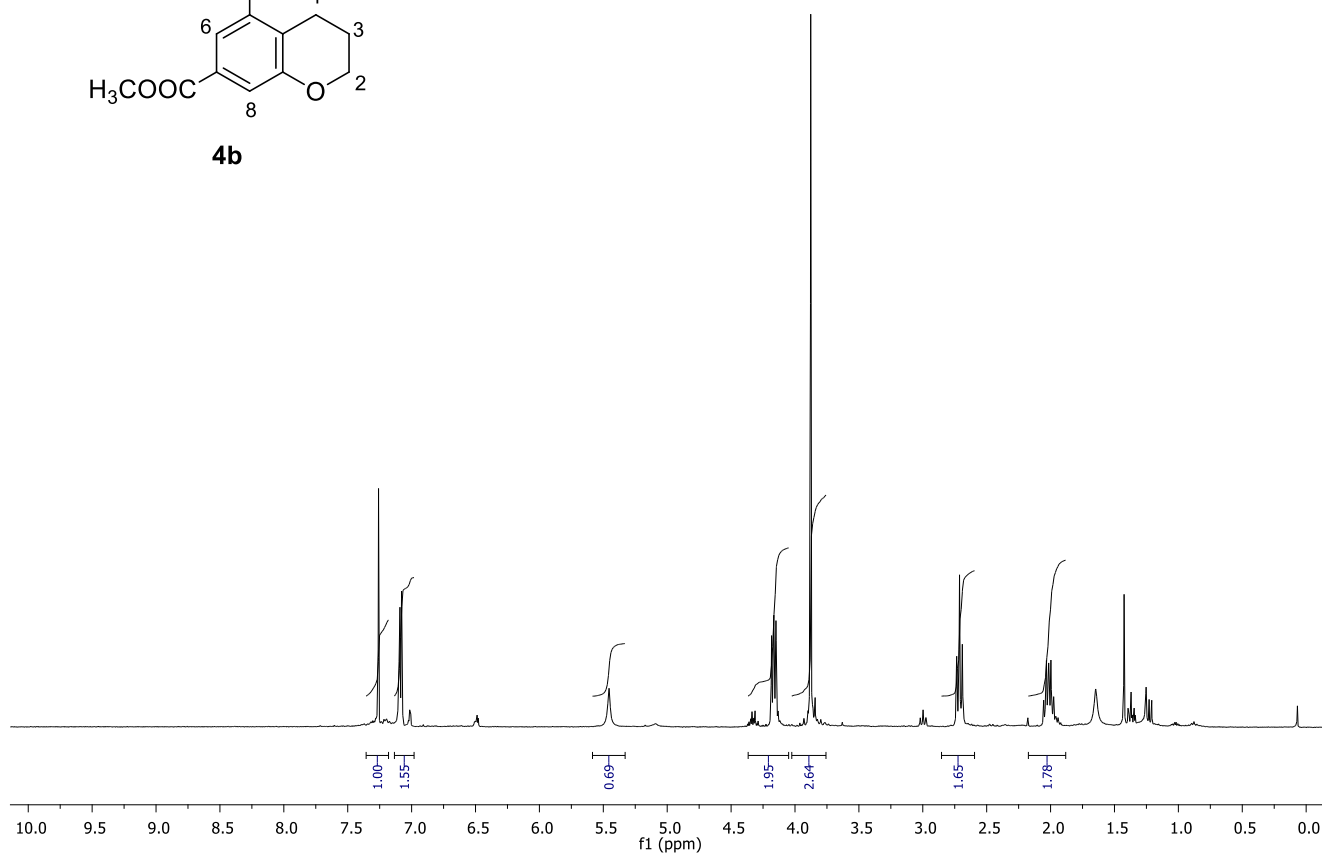
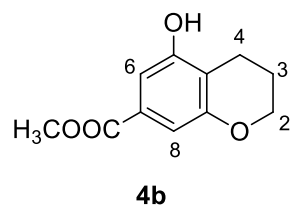
15. FT-IR spectrum of compound 4a



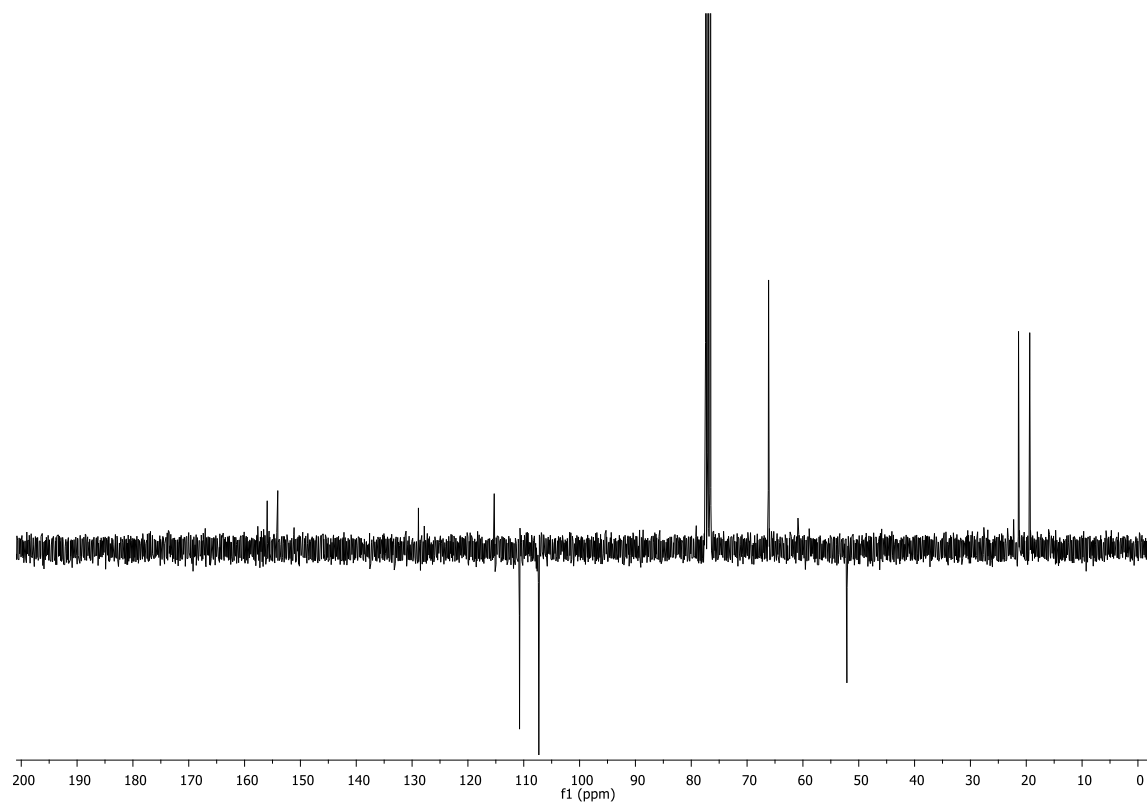
16. ESI MS spectrum of compound 4a



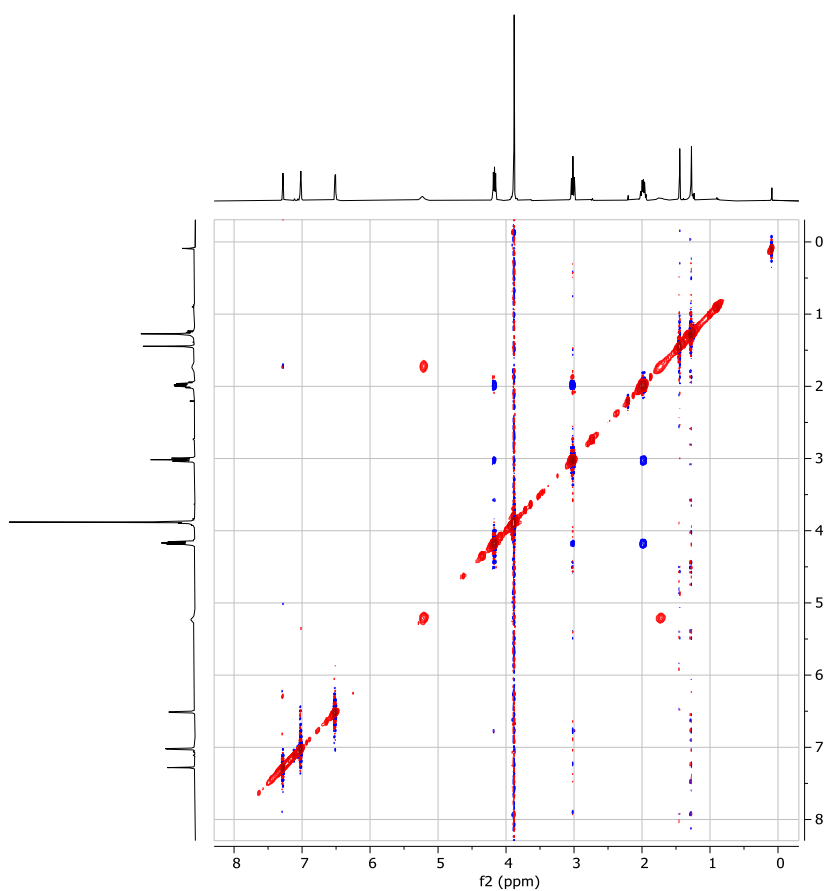
17. ^1H NMR spectrum of compound 4b



18. ^{13}C NMR spectrum of compound 4b

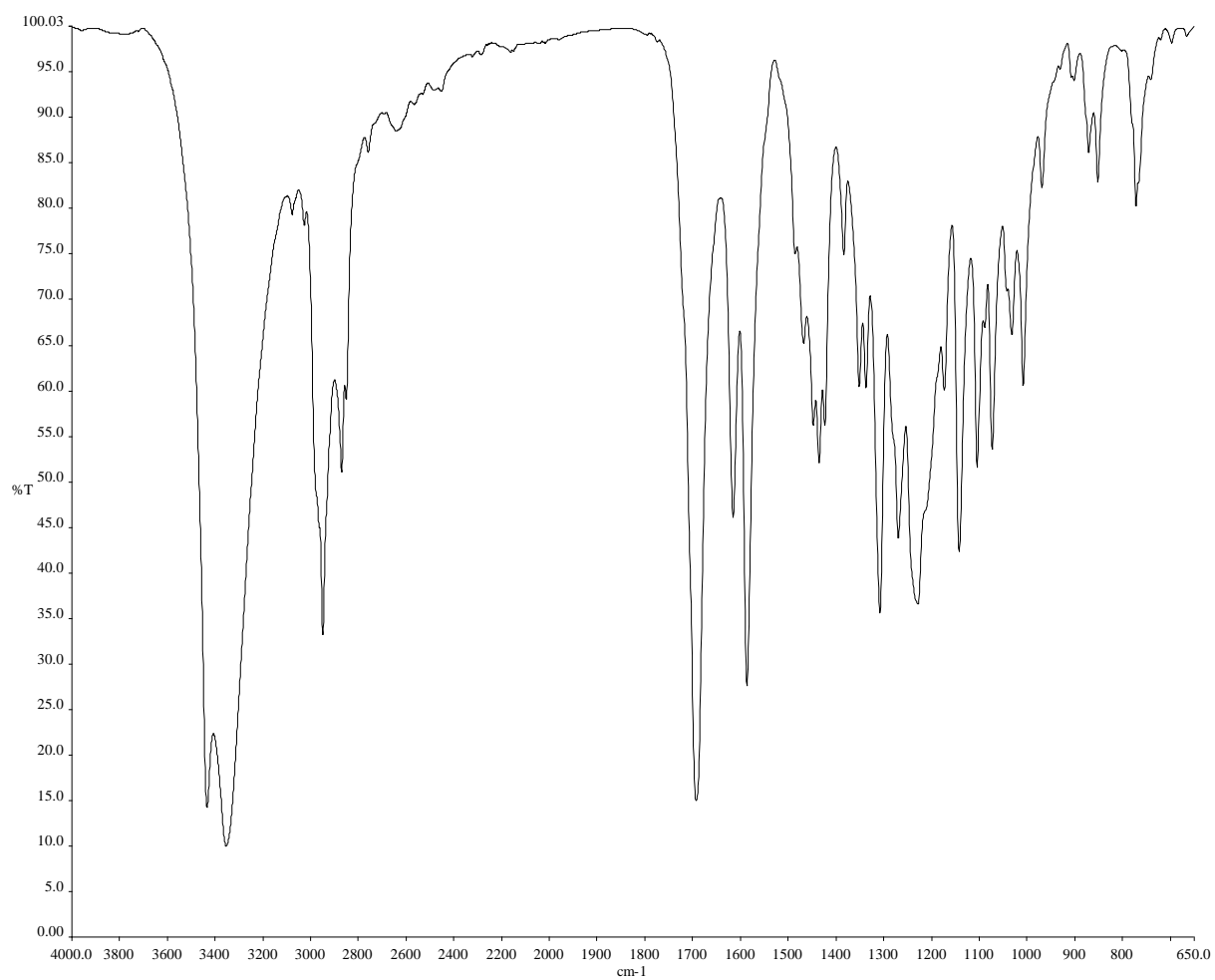


19. NOESY spectrum of compound 4



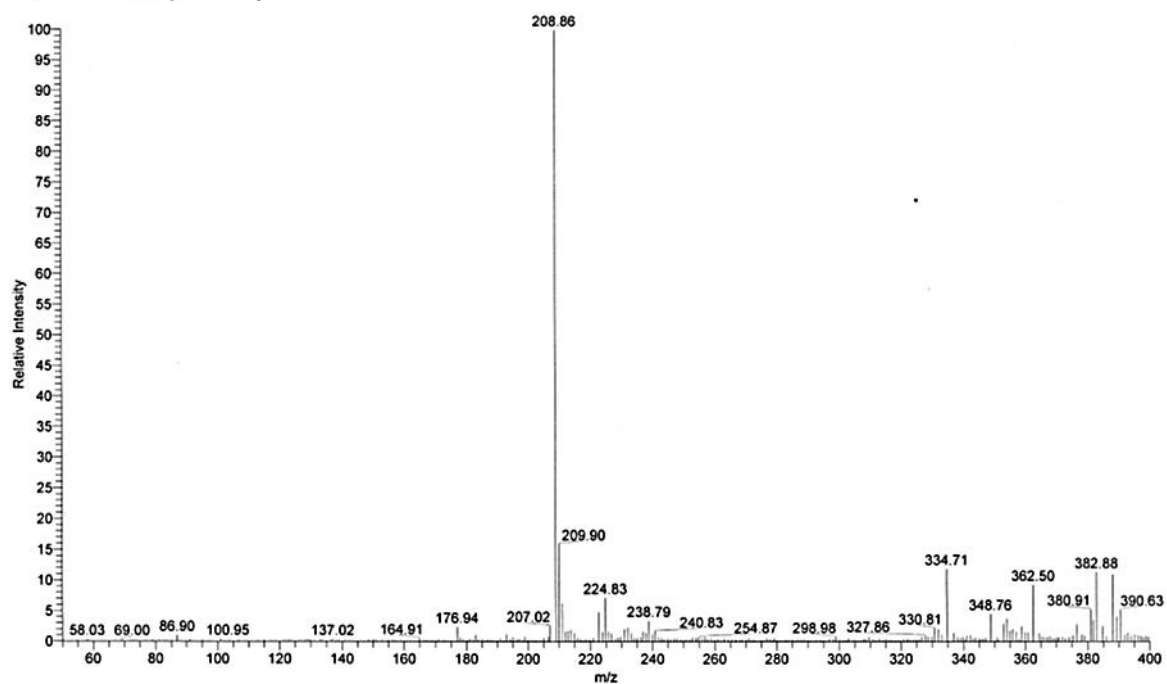
Parameter	Value (f2, f1)
Data File Name	C:/ Desktop/ NMR/ NMR 300MHz _ Am
Title	Compound 4b
Comment	4b NOESYph in CDCl3 a T=amb., tmix=1.2s
Origin	Bruker BioSpin GmbH
Owner	nmr
Site	
Spectrometer	spect
Author	
Solvent	CDCl3
Temperature	300.0
Pulse Sequence	noesyph
Experiment	NOESY
Probe	5 mm QNP 1H/ 13C/ 31P/ 19F Z- grad Z8352/ 0036
Number of Scans	8
Receiver Gain	1820
Relaxation Delay	2.5000
Pulse Width	11.5000
Acquisition Time	0.3965
Acquisition Date	2019-02-18T14:24:34
Modification Date	2019-02-18T16:17:00
Class	
Spectrometer Frequency	(300.13, 300.13)
Spectral Width	(2582.6, 2582.7)
Lowest Frequency	(-93.5, -93.5)
Nucleus	(1H, 1H)
Acquired Size	(1024, 202)
Spectral Size	(2048, 2048)

20. FT-IR spectrum of compound 4b

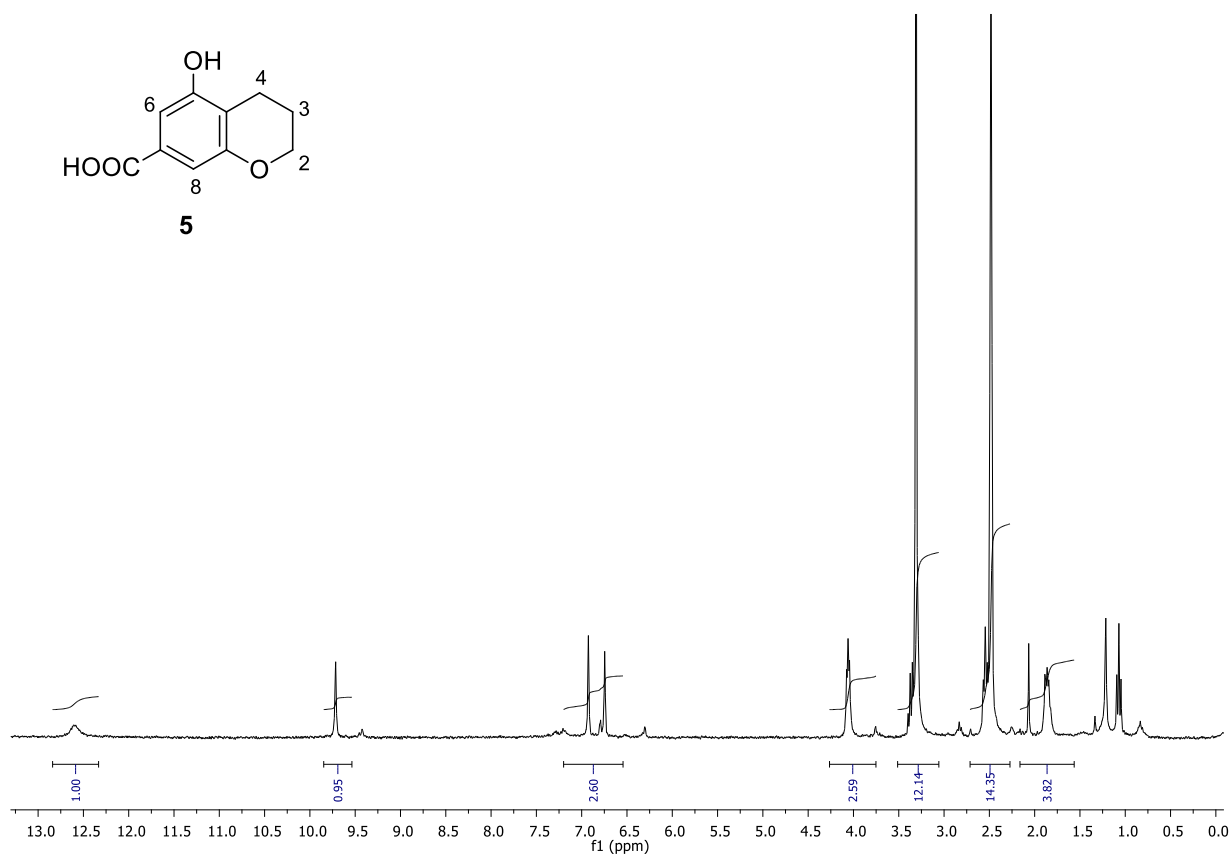


21. ESI MS spectrum of compound 4b

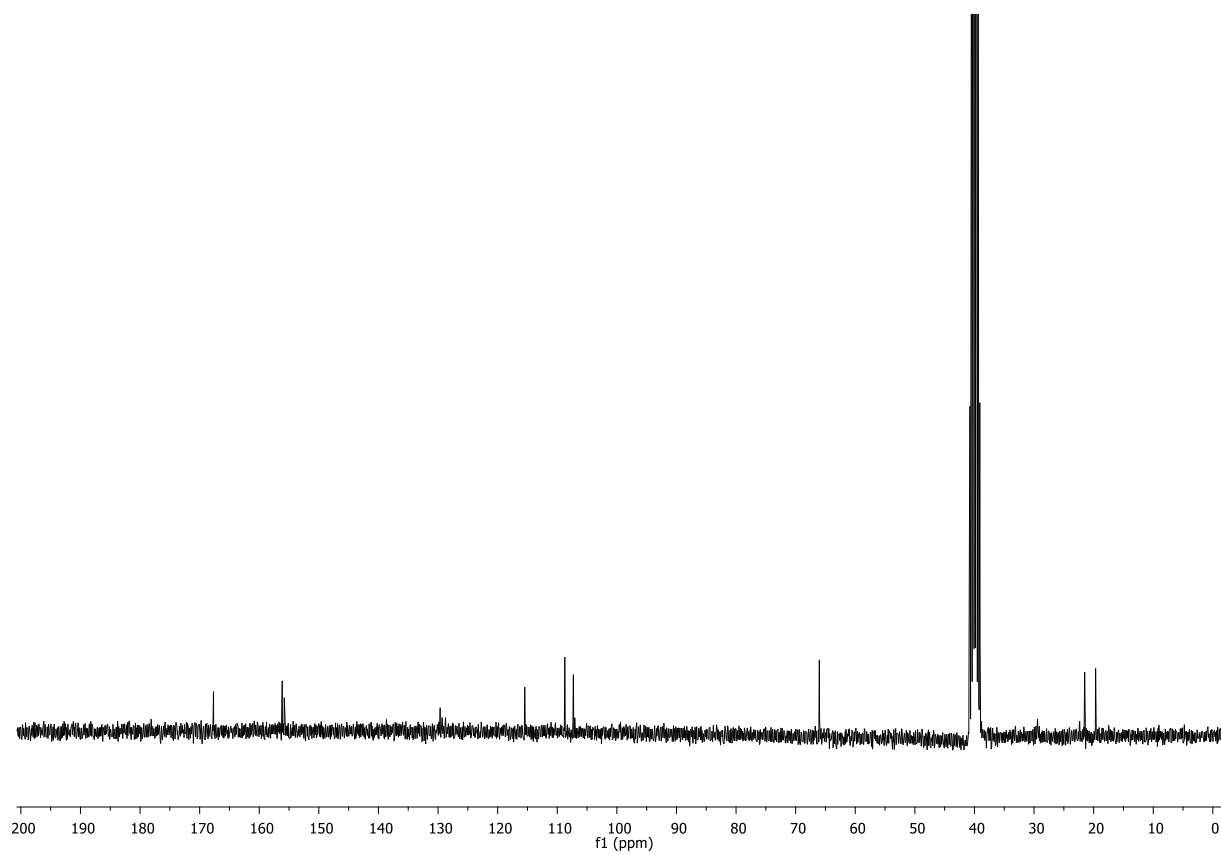
#13375 AV: 10 IT: 7.071 ST: 0.34 uS: 3 NL: 4.02E4
F: ITMS + c HESI Full ms [50.00-400.00]



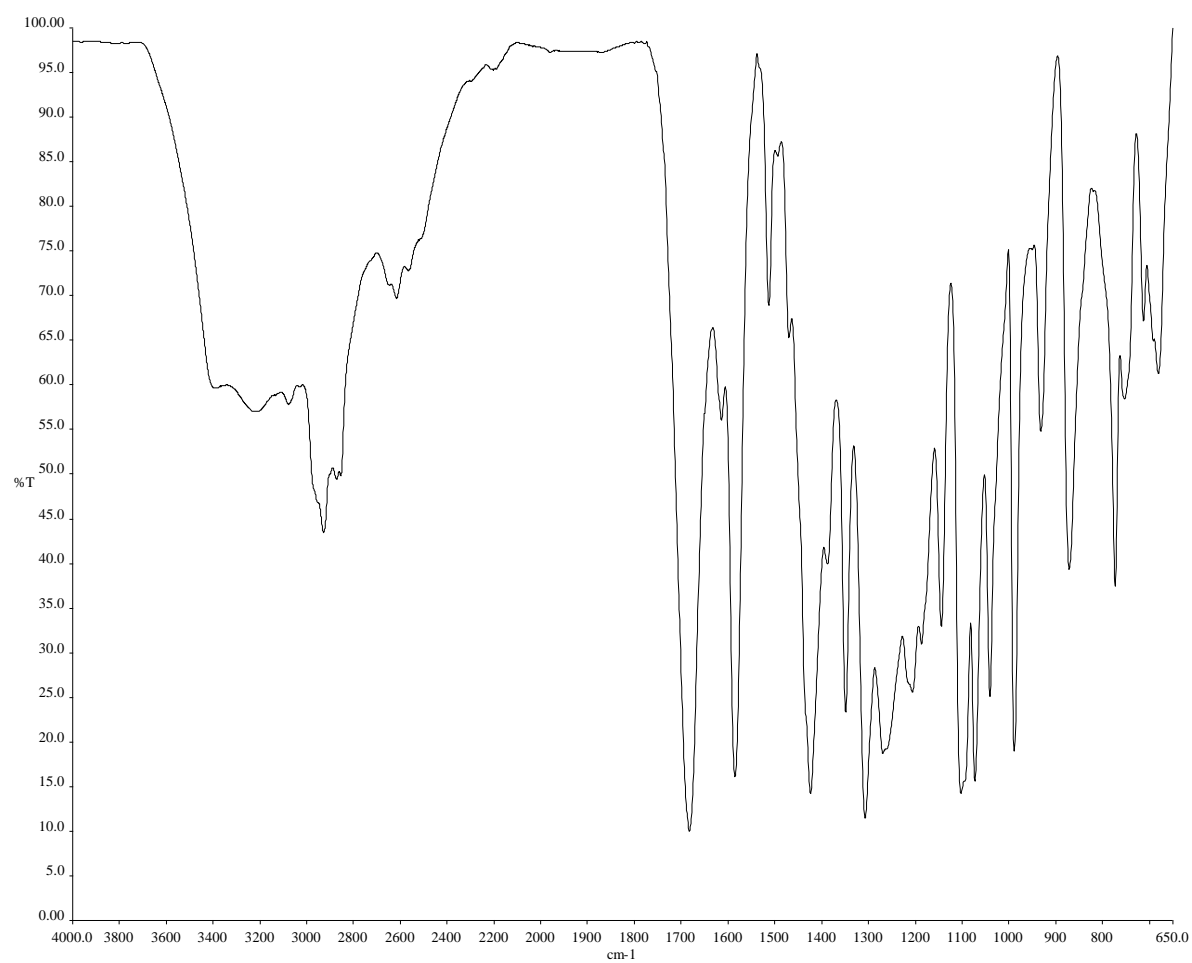
22. ^1H NMR spectrum of compound 5



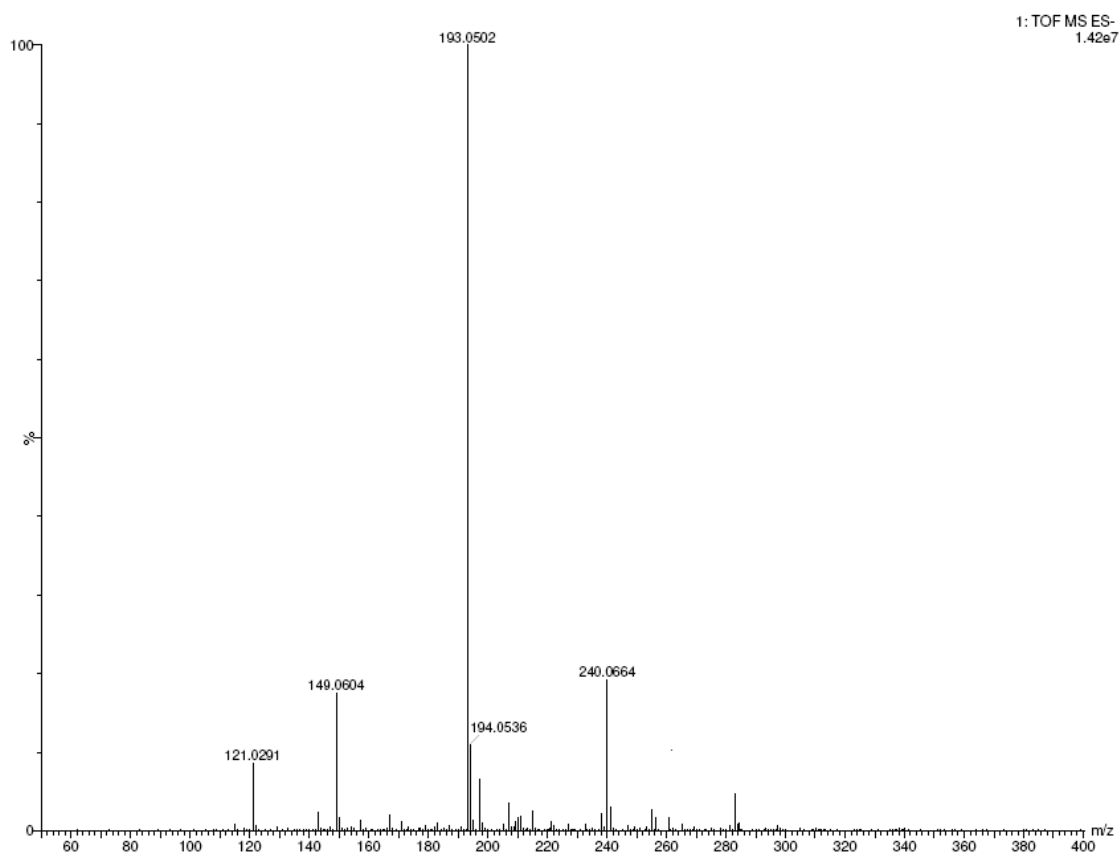
23. ^{13}C spectrum of compound 5



24. FT-IR spectrum of compound 5



25. HRMS spectrum of compound 5



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 PPM / DBE: min = -5.0, max = 300.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 5

Monoisotopic Mass, Even Electron Ions

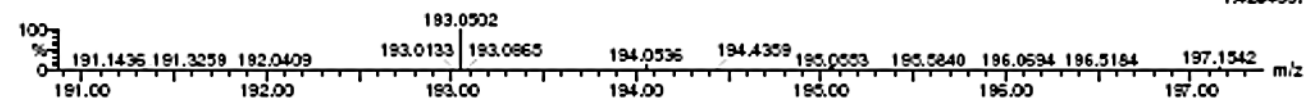
3 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 10-10 H: 9-11 O: 4-4 Na: 0-2

AD32b 40 (0.752) AM2 (Ar,40000.0,0.00,0.00); Cm (20-50)

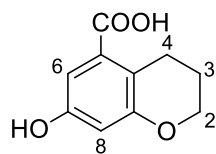
1: TOF MS ES-
1.42e+007



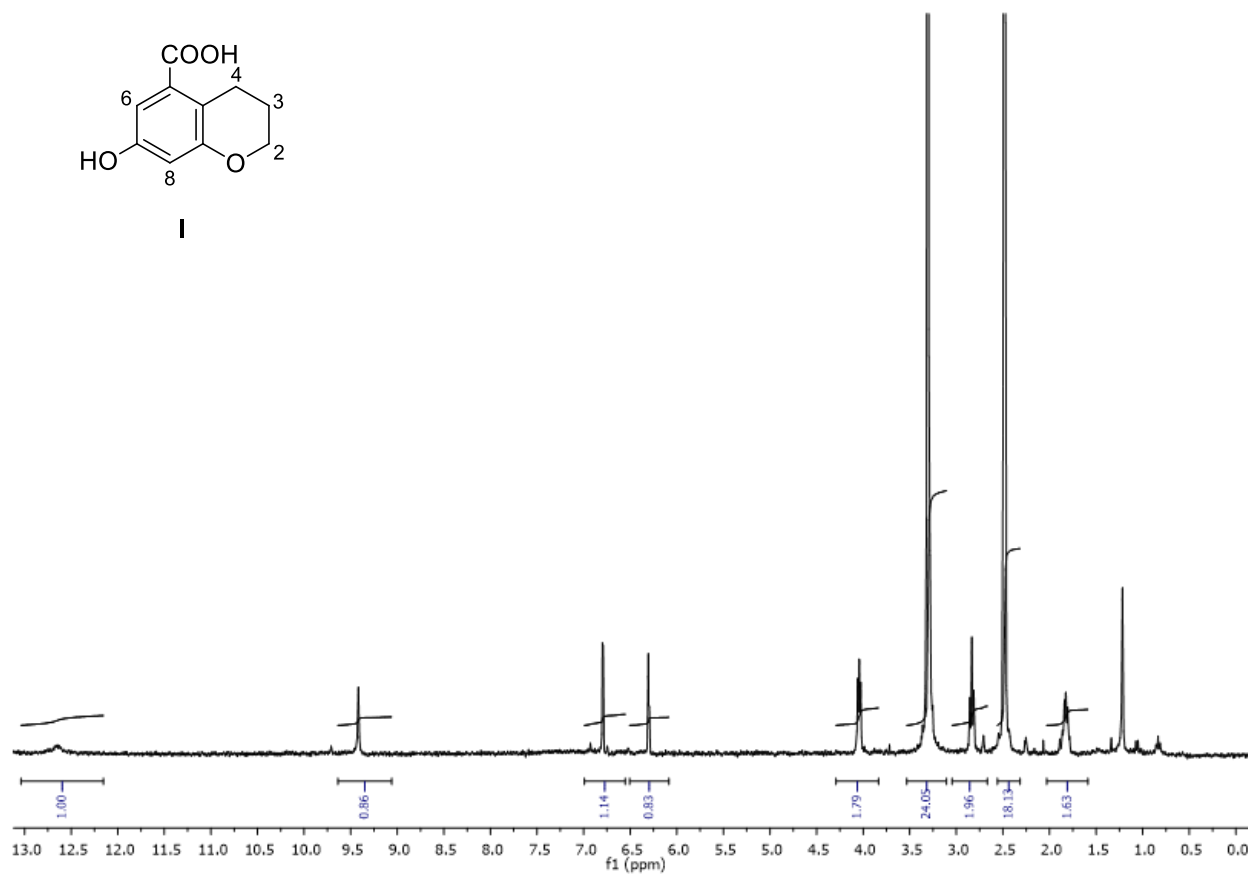
Minimum: -5.0
Maximum: 5.0 5.0 300.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
193.0502	193.0501	0.1	0.5	6.5	3489.2	n/a	n/a	C10 H9 O4

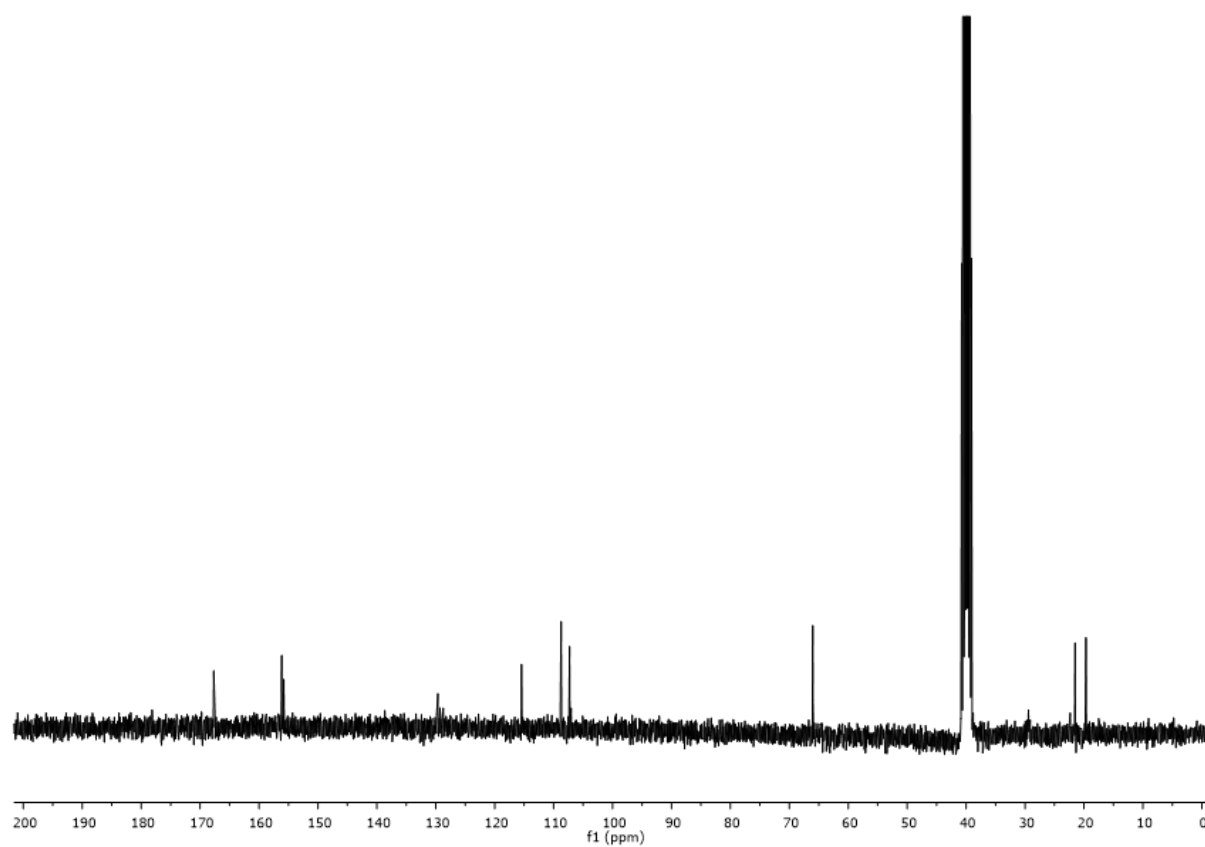
26. ^1H NMR spectrum of compound I



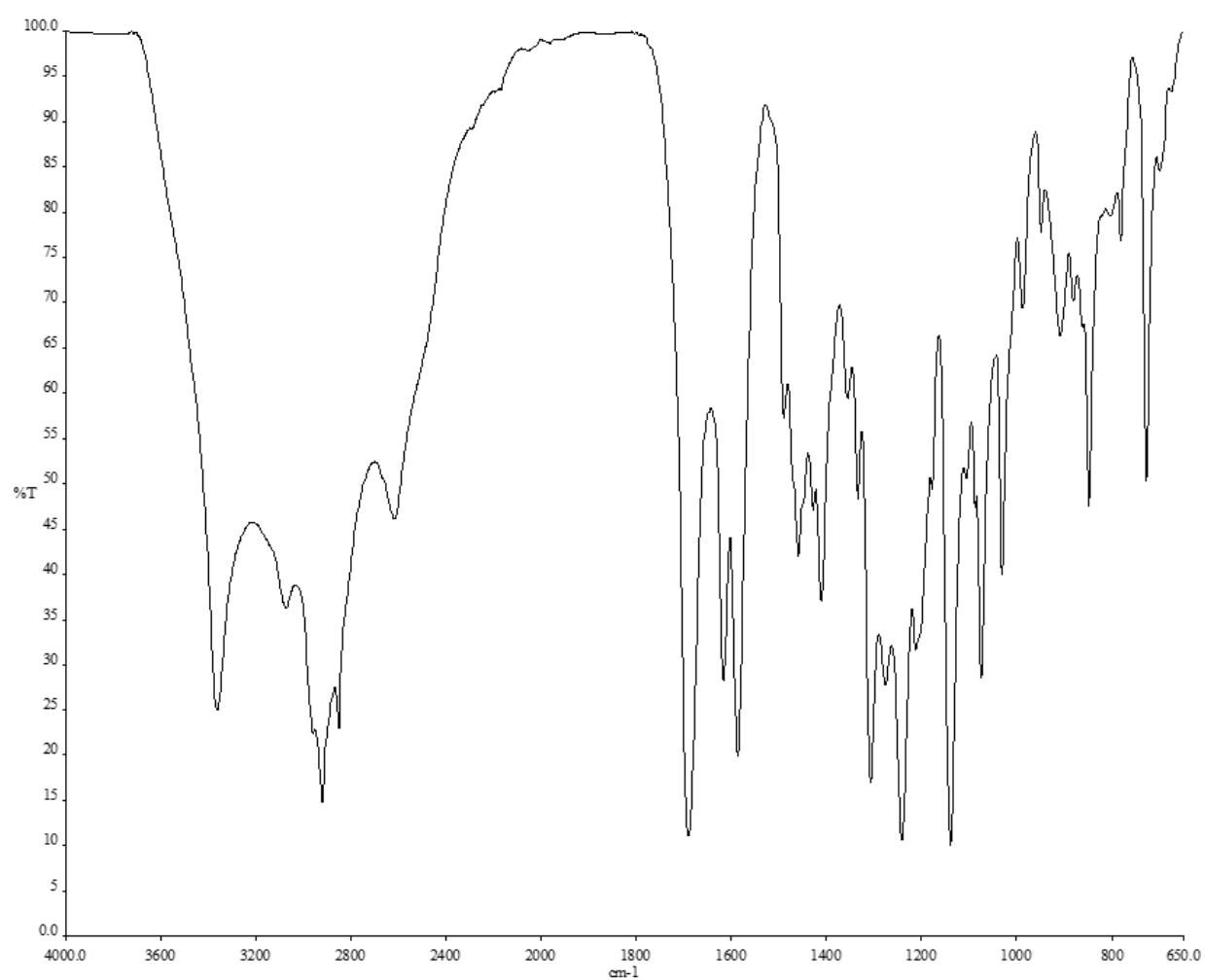
I



27. ^{13}C spectrum of compound I



28. FT-IR spectrum of compound I



29. ESI MS spectrum of compound I

