

Supporting Information for:

New aryloxy-quinone derivatives as potential Anti-Chagasic agents: Synthesis, trypanosomicidal activity, electrochemical properties, pharmacophore elucidation and 3D-QSAR analysis.

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^e Área de Radiofarmacia, Centro de Investigaciones Nucleares, Facultad de Ciencias, Universidad de la República, Mataojo 2055, Montevideo, Uruguay.

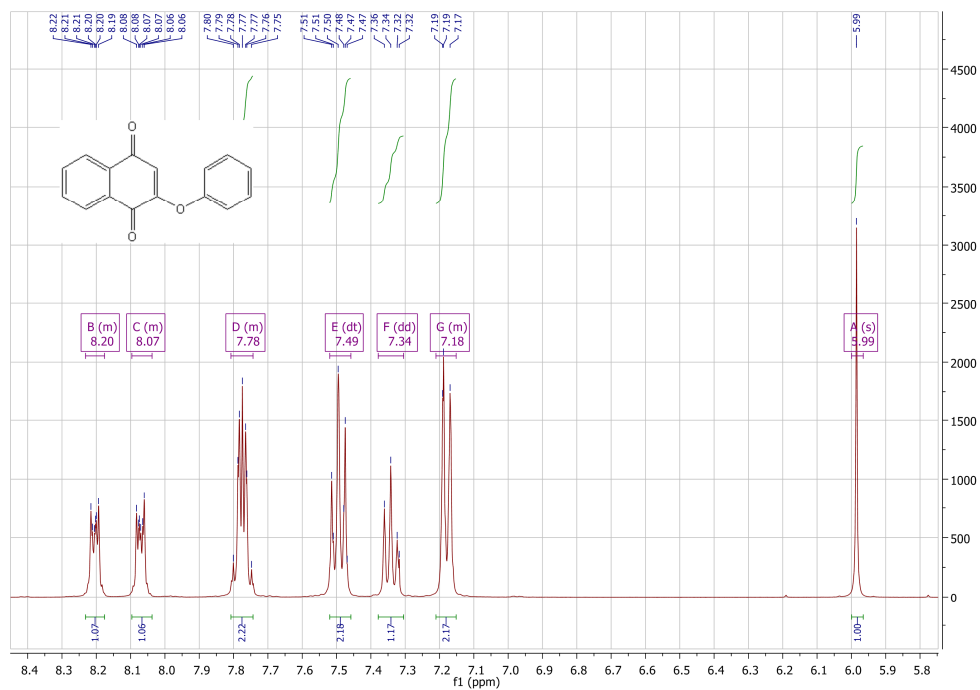
^f Centro de Bioinformática Estructural-DETEMA, Facultad de Química, Universidad de la República, C.C. 1157, Montevideo, Uruguay.

*Corresponding authors. E-mail address: margot@fq.edu.uy (M. Paulino) and cosalas@uc.cl (C.O. Salas).

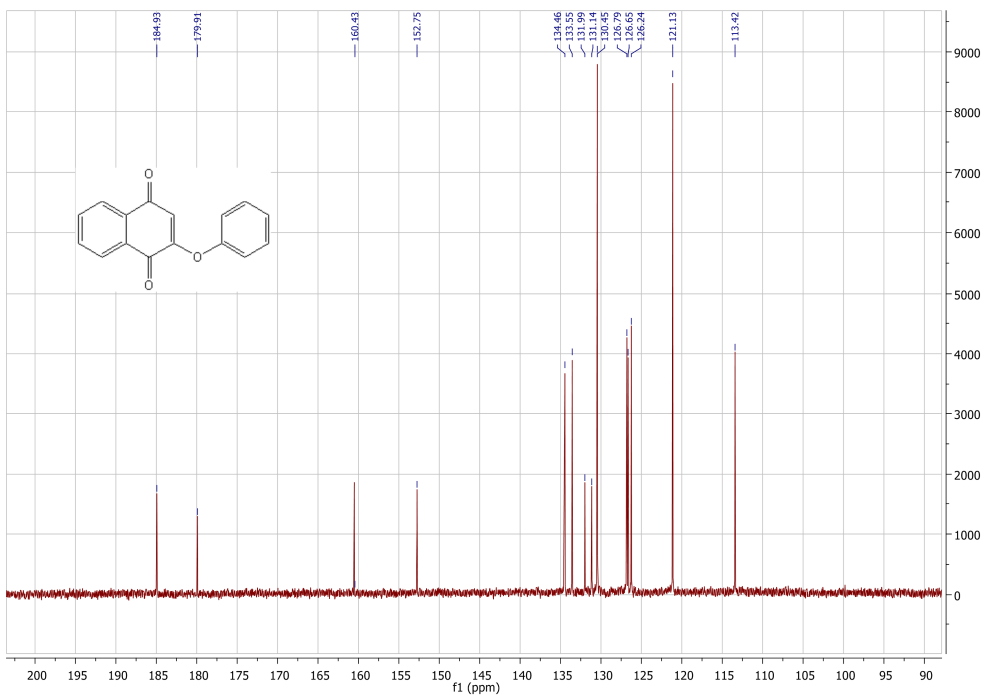
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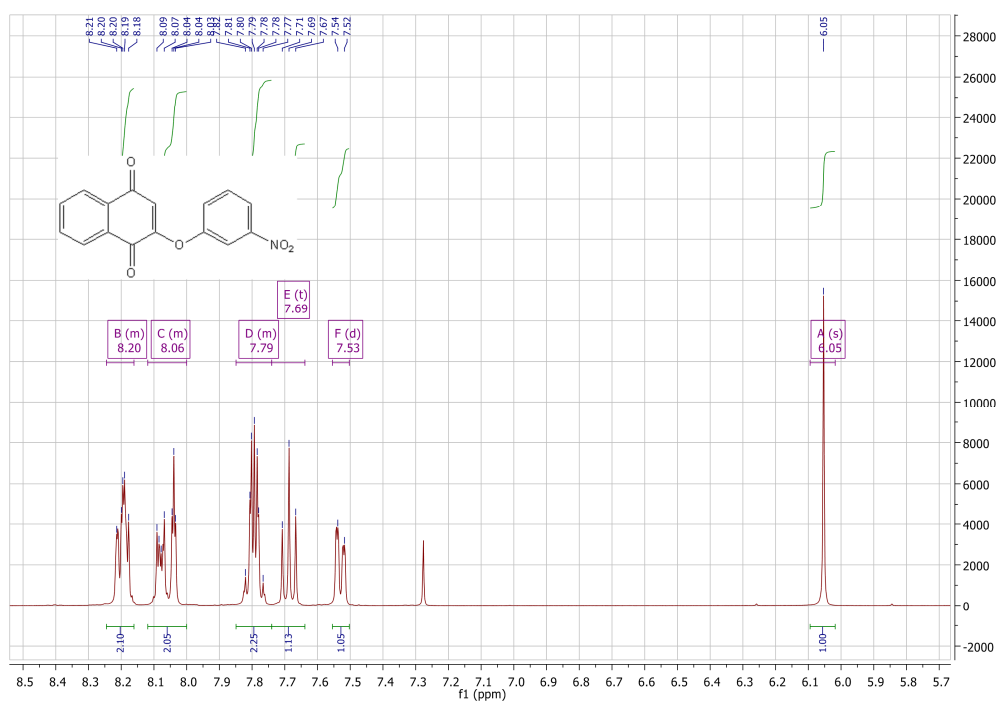
^1H NMR spectra of compound **3a**



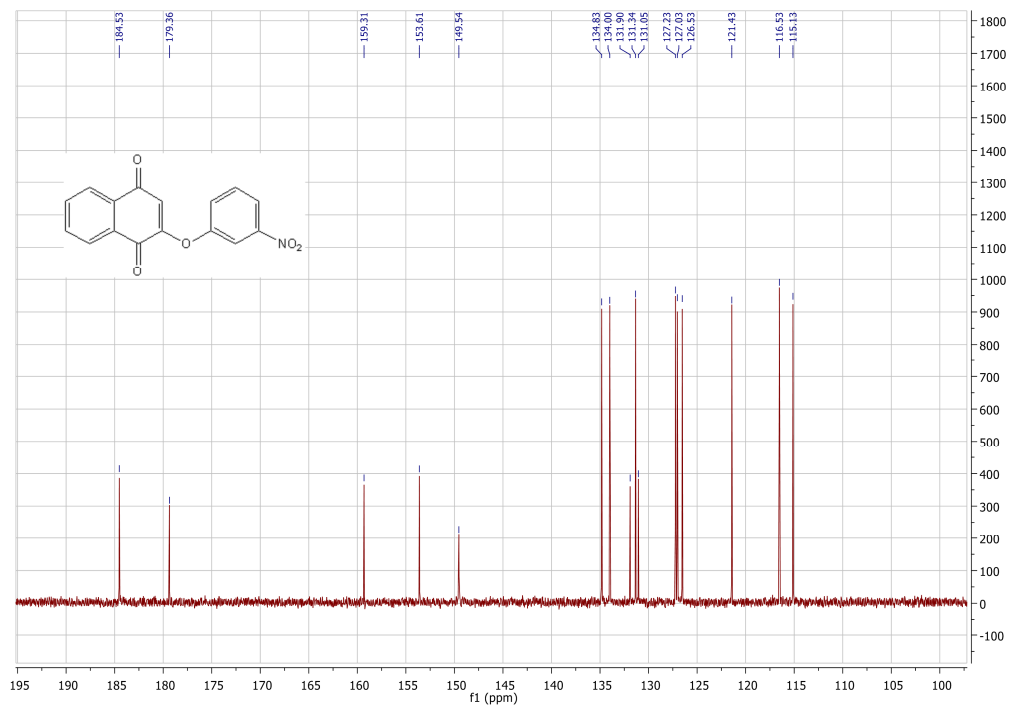
^{13}C NMR spectra of compound **3a**



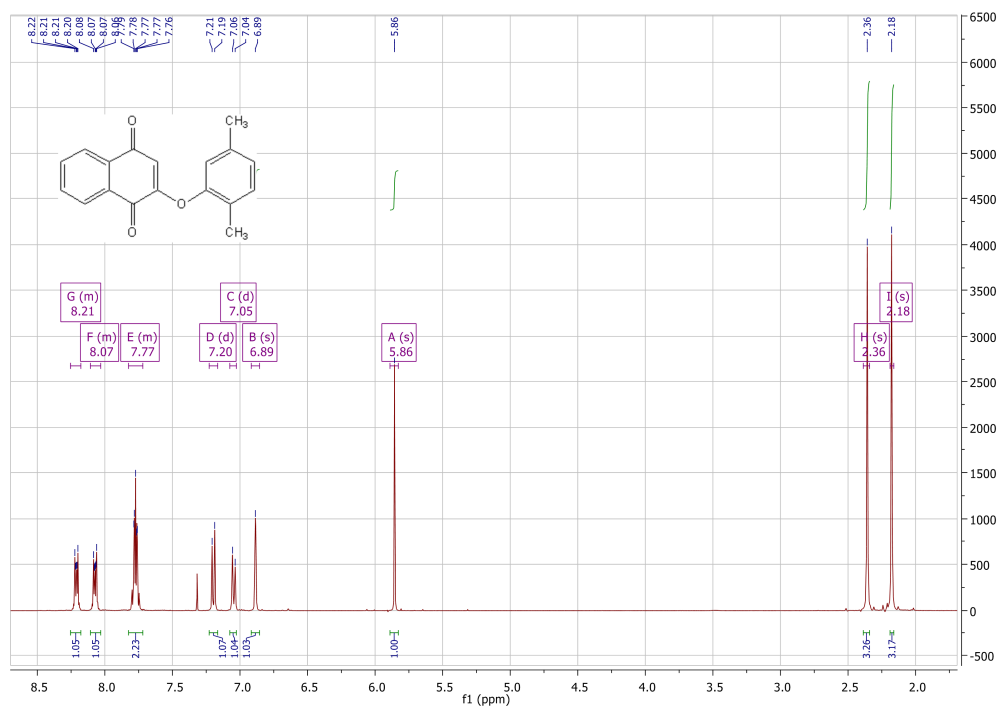
¹H NMR spectra of compound **3b**



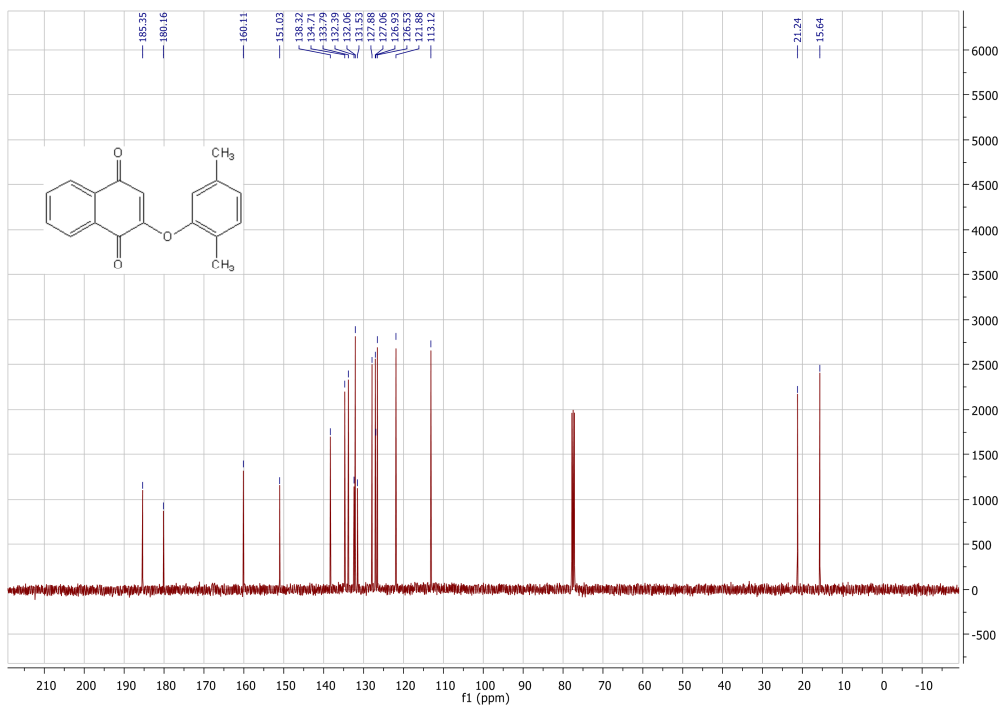
¹³C NMR spectra of compound **3b**



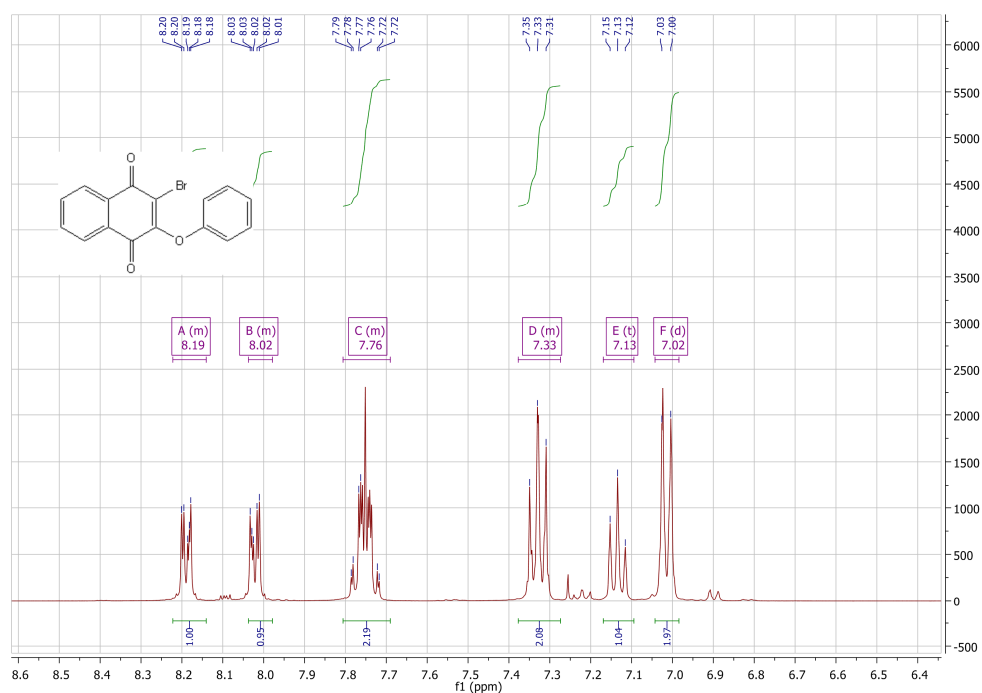
¹H NMR spectra of compound **3c**



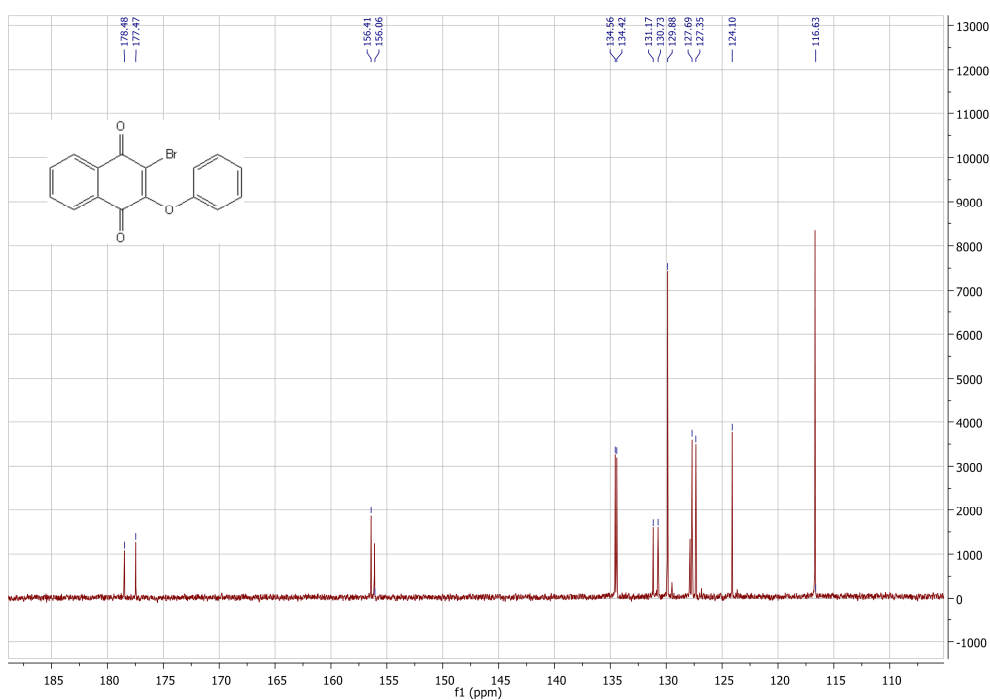
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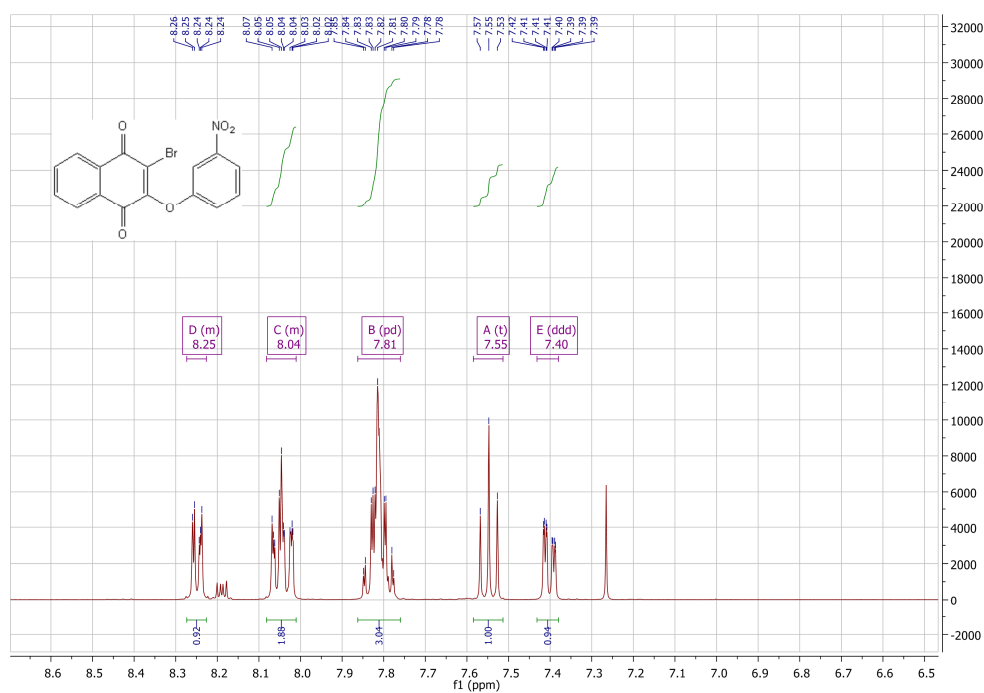
¹H NMR spectra of compound **3d**



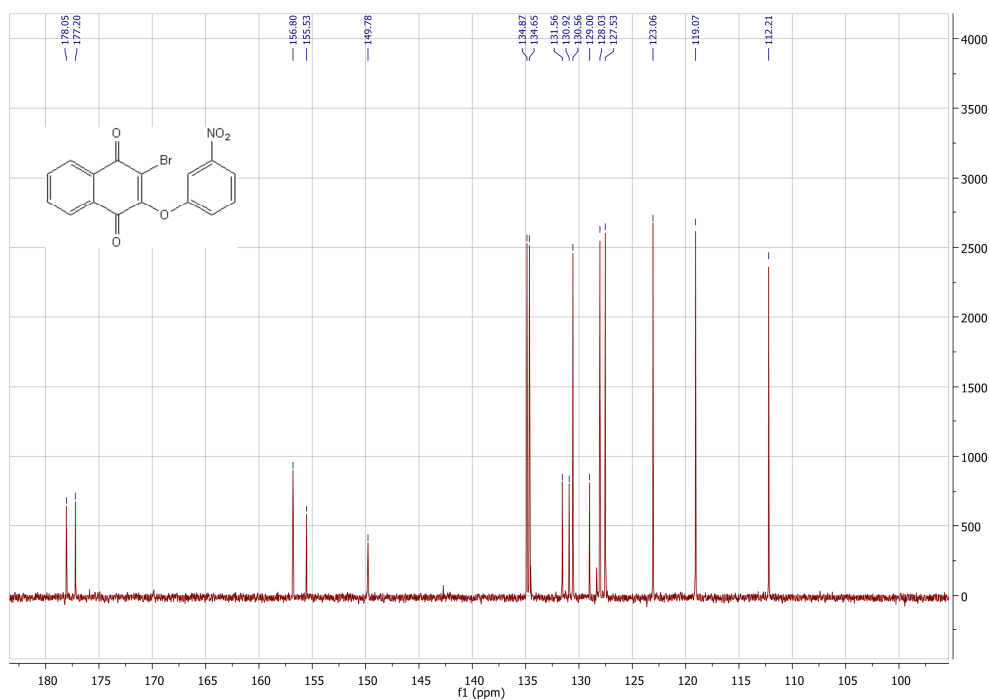
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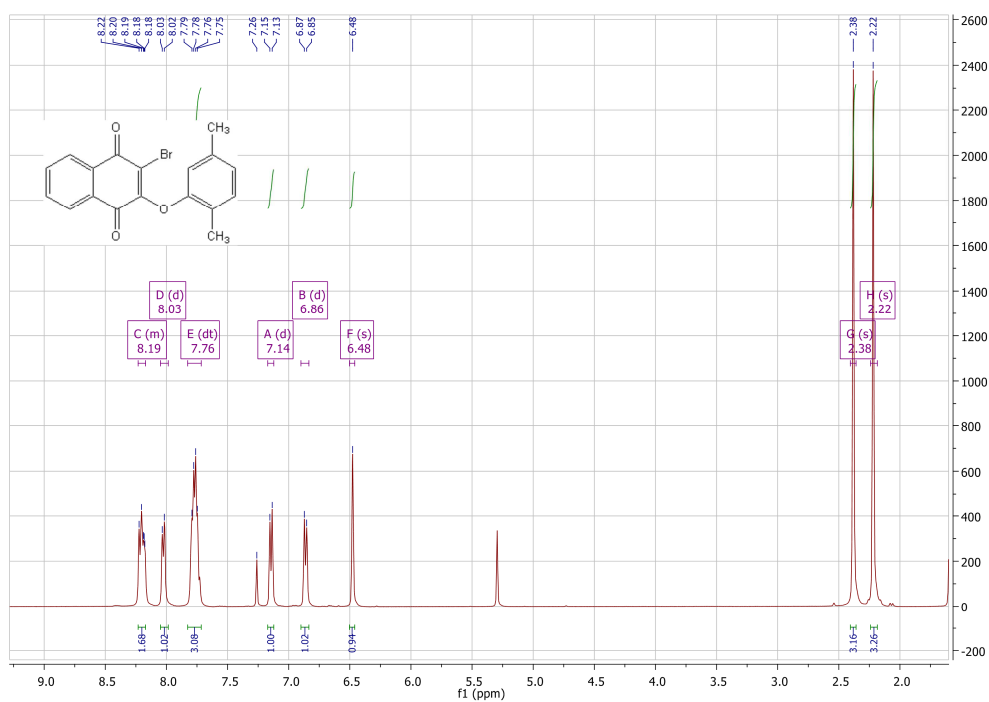
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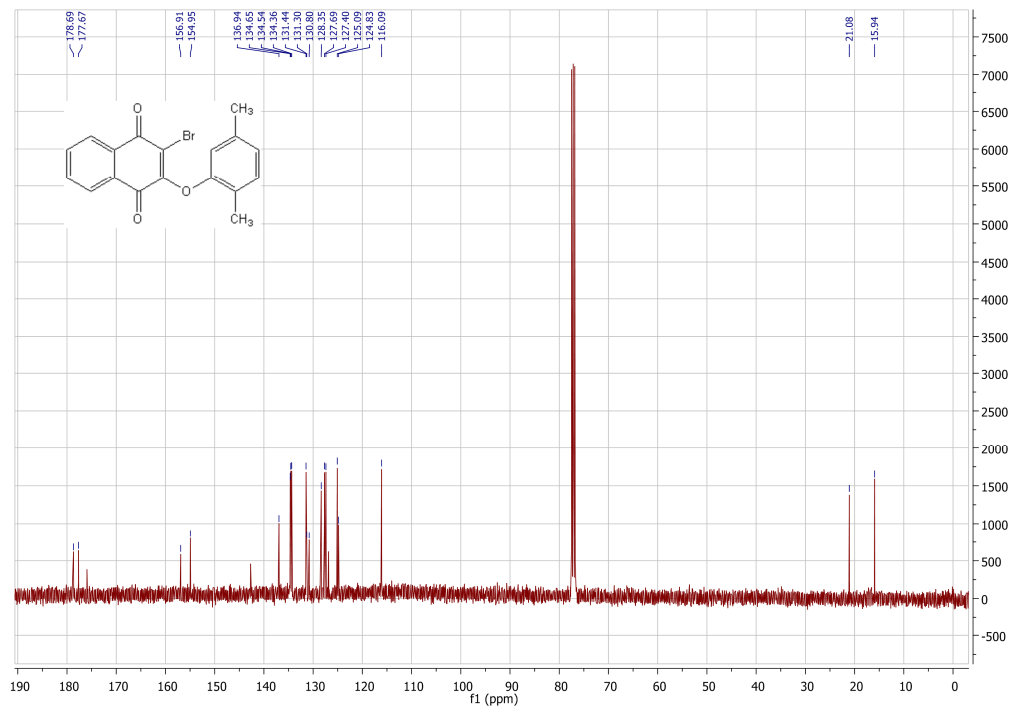
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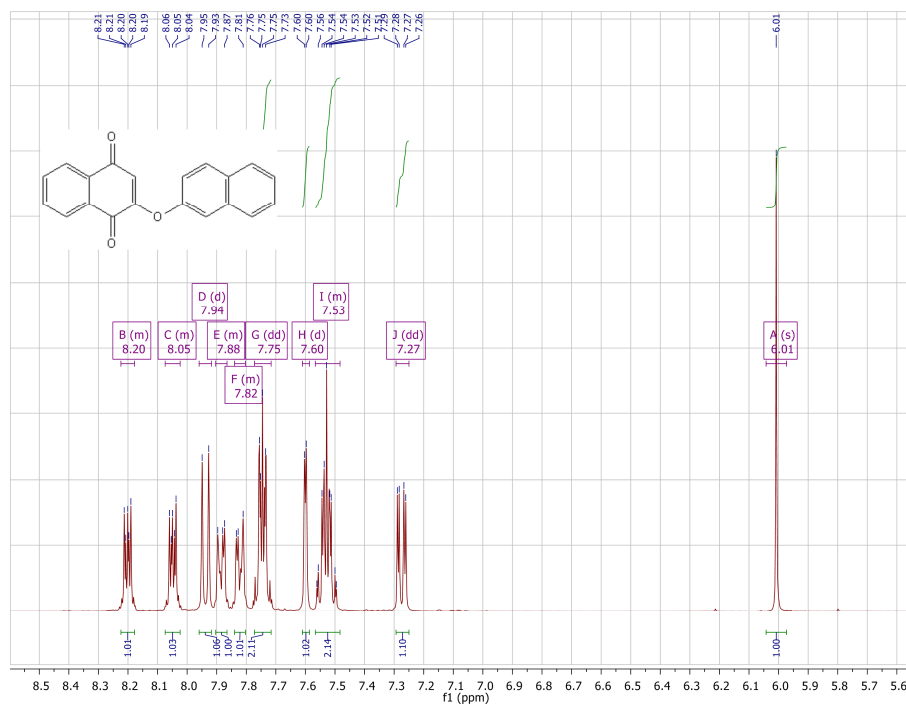
¹H NMR spectra of compound **3f**



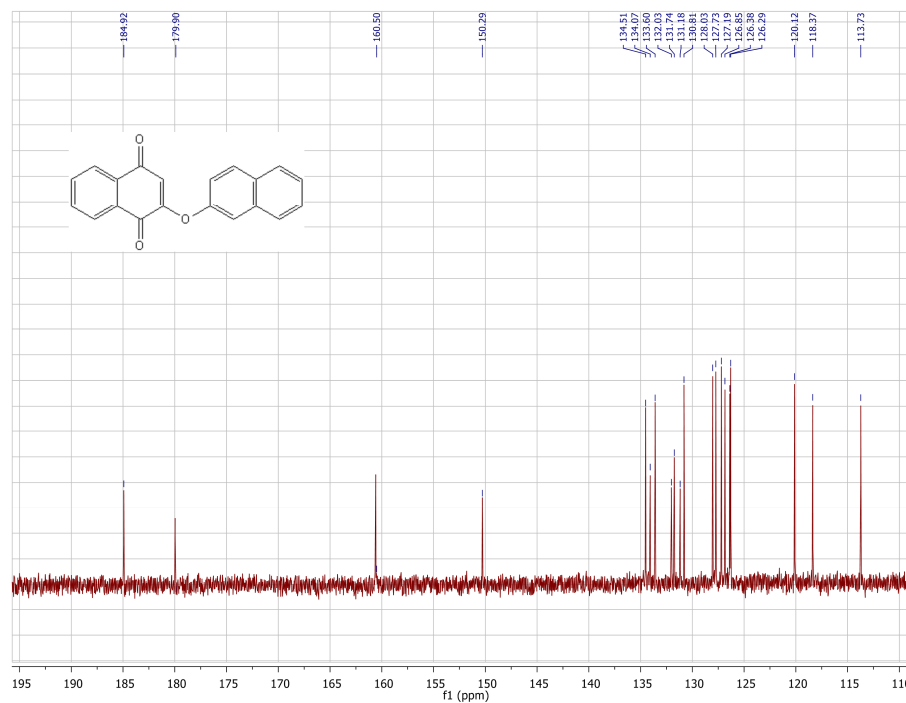
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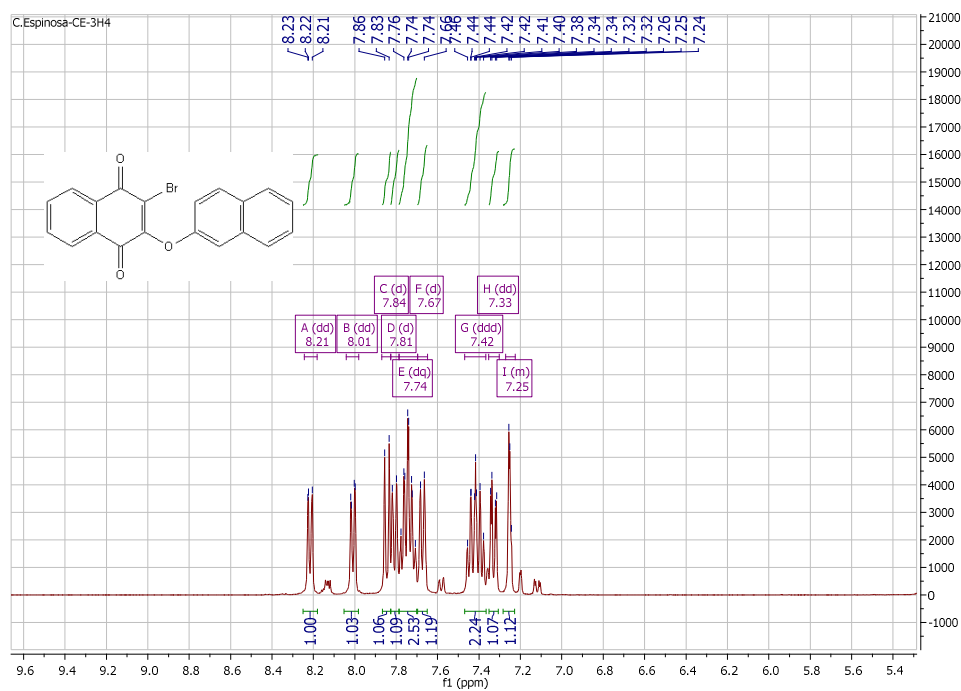
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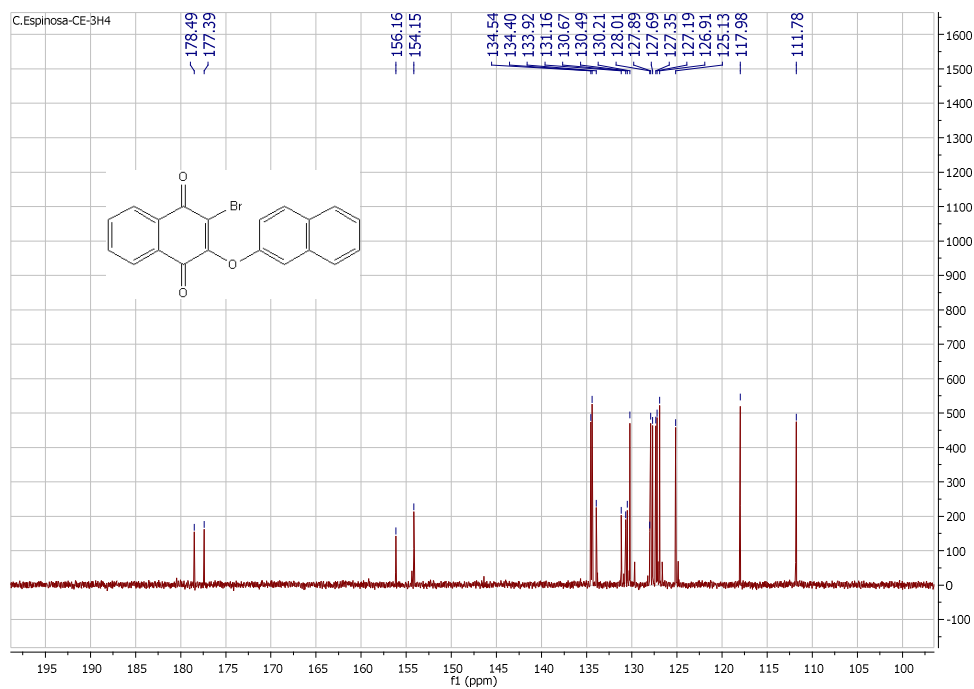
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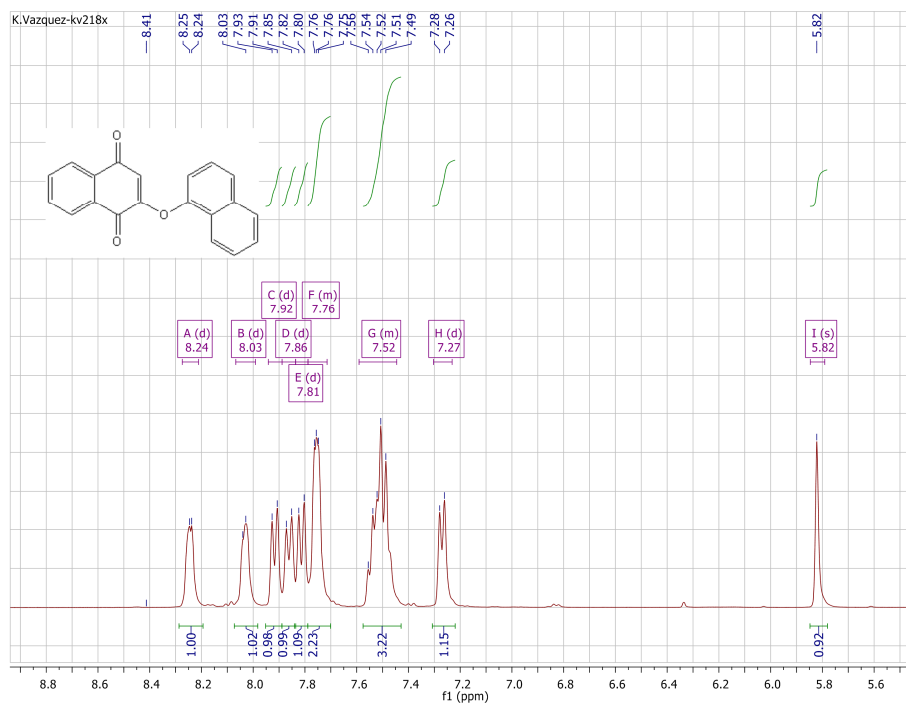
^1H NMR spectra of compound **3h**



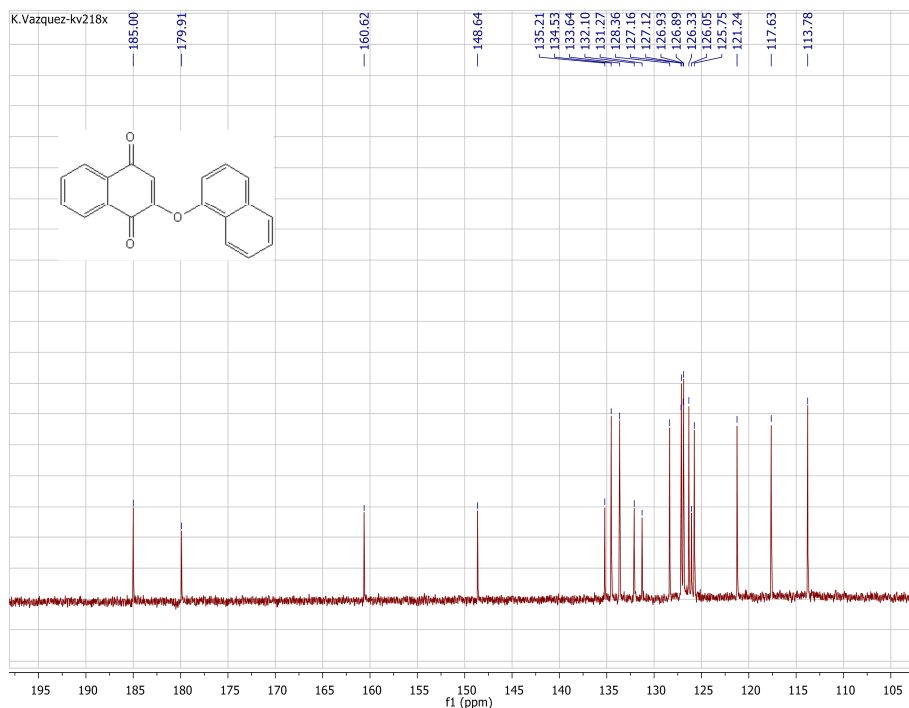
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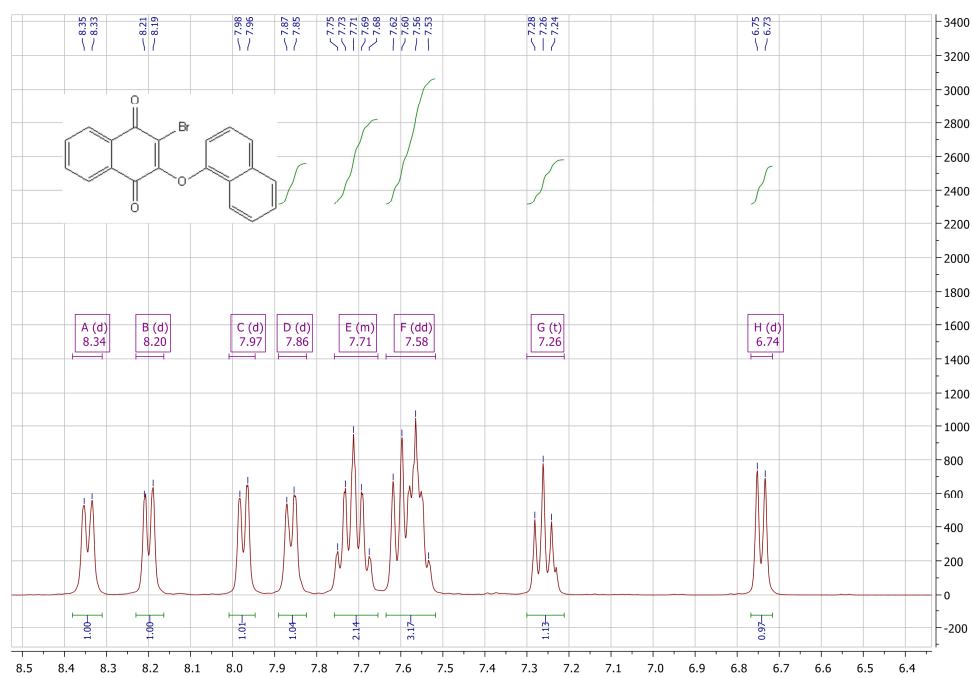
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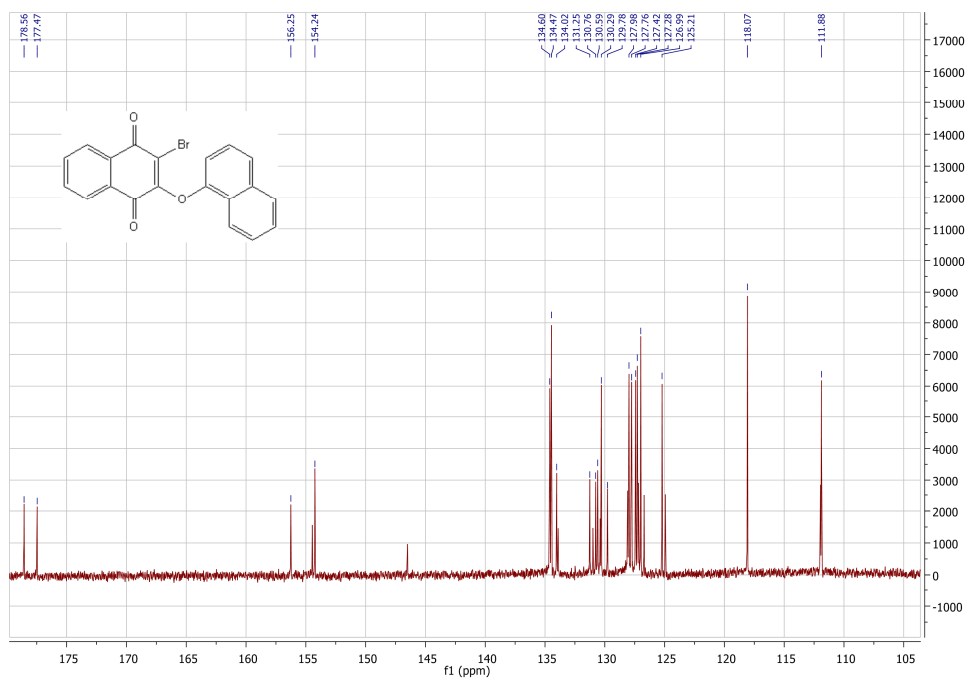
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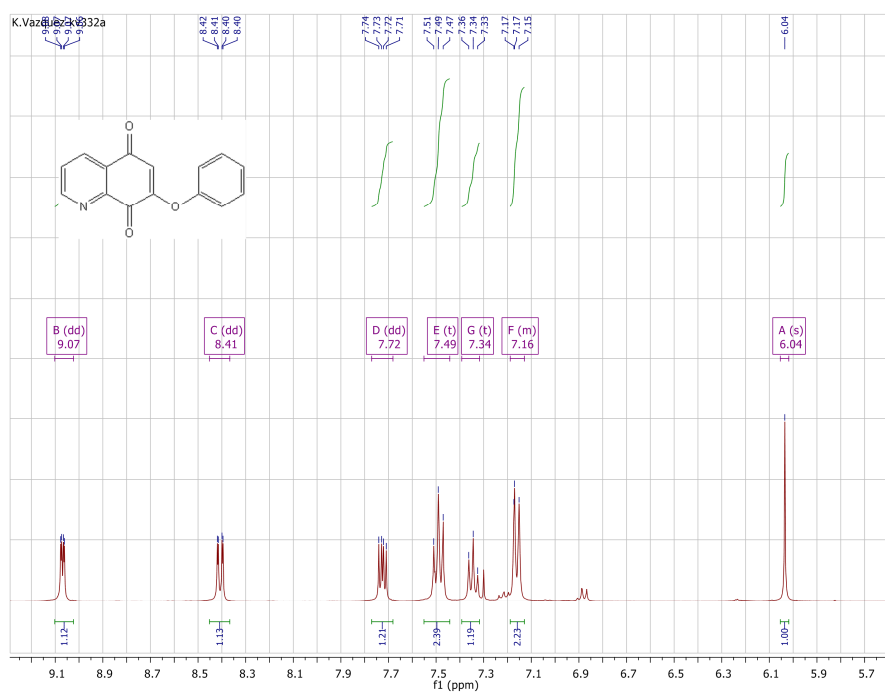
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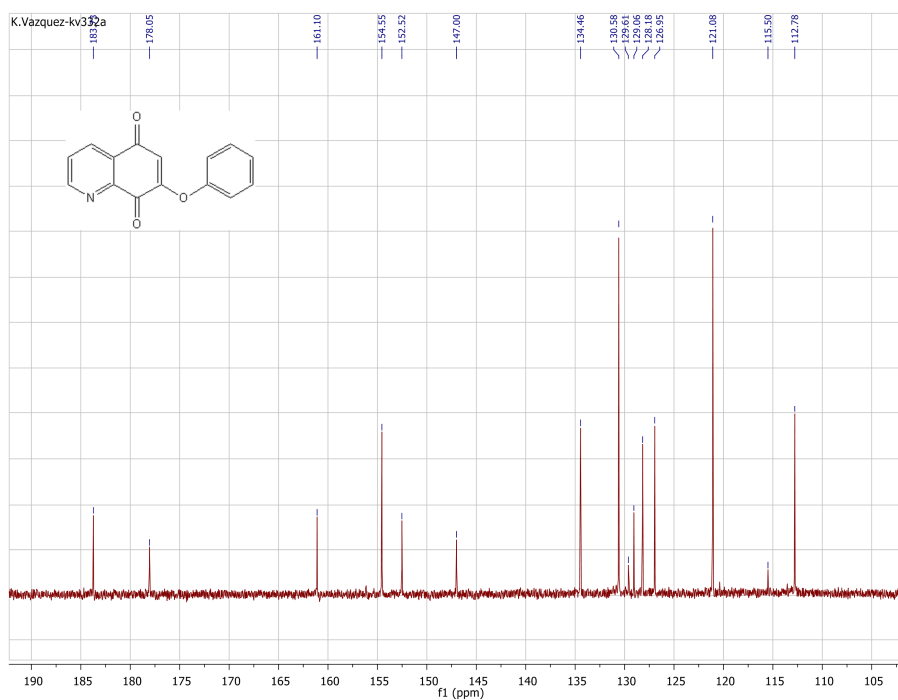
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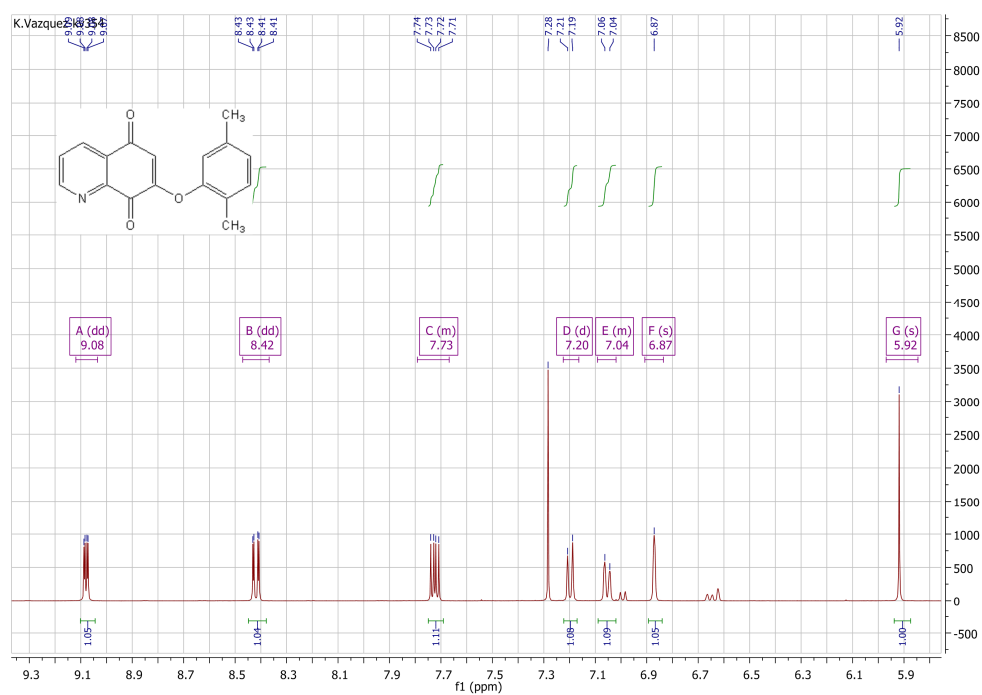
¹H NMR spectra of compound **7a**



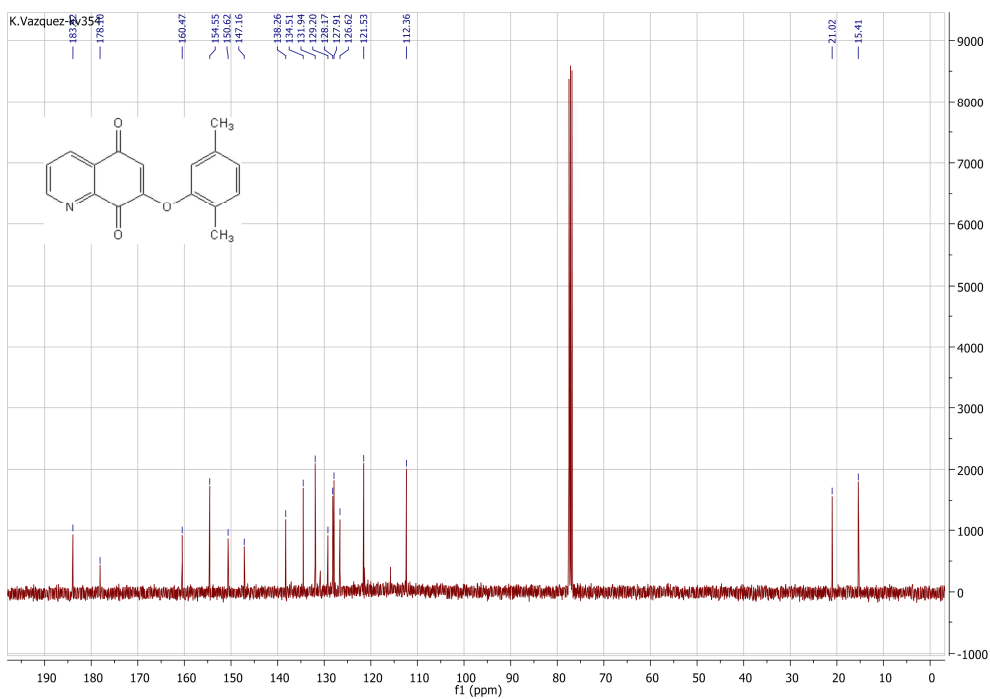
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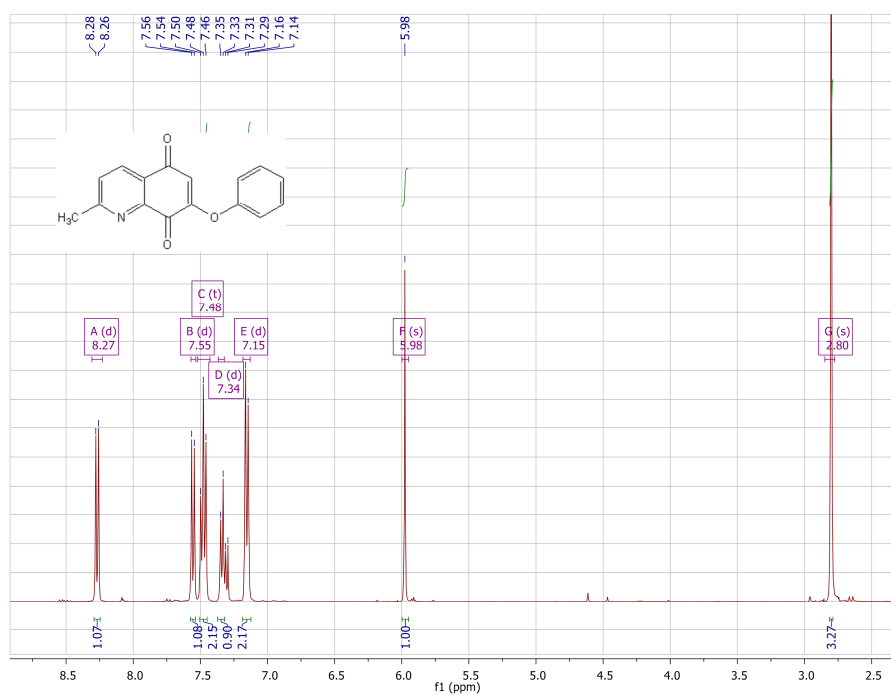
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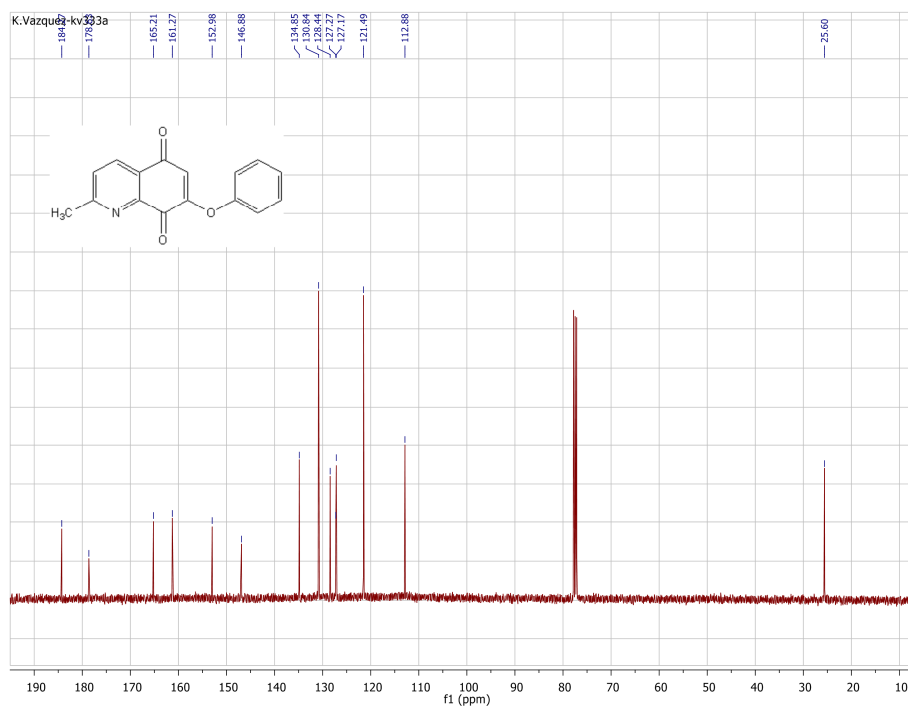
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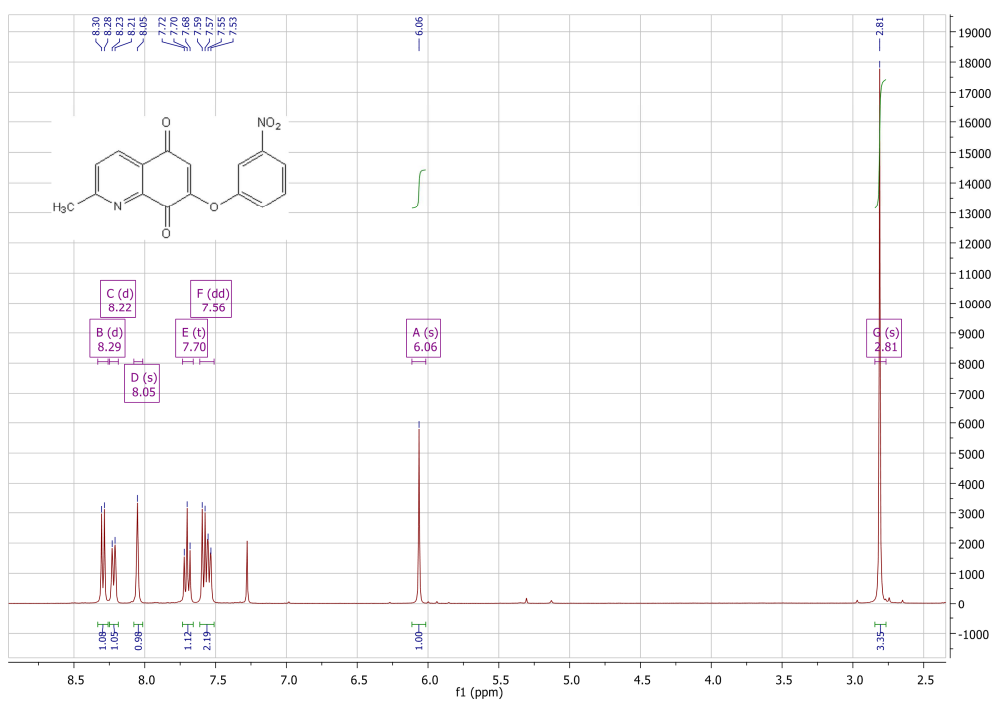
¹H NMR spectra of compound **7c**



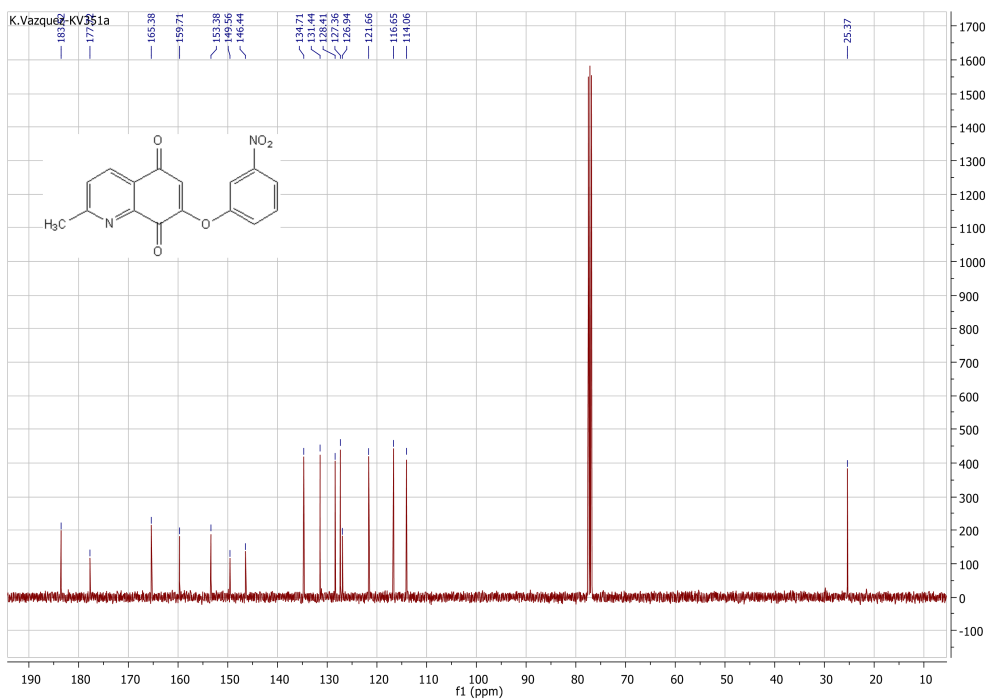
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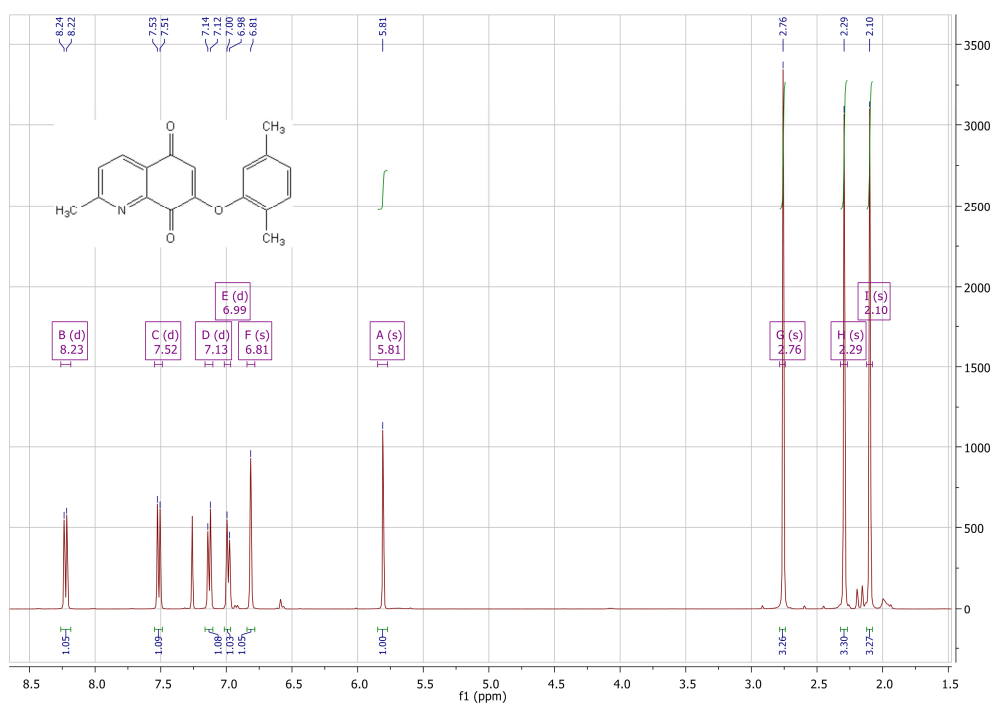
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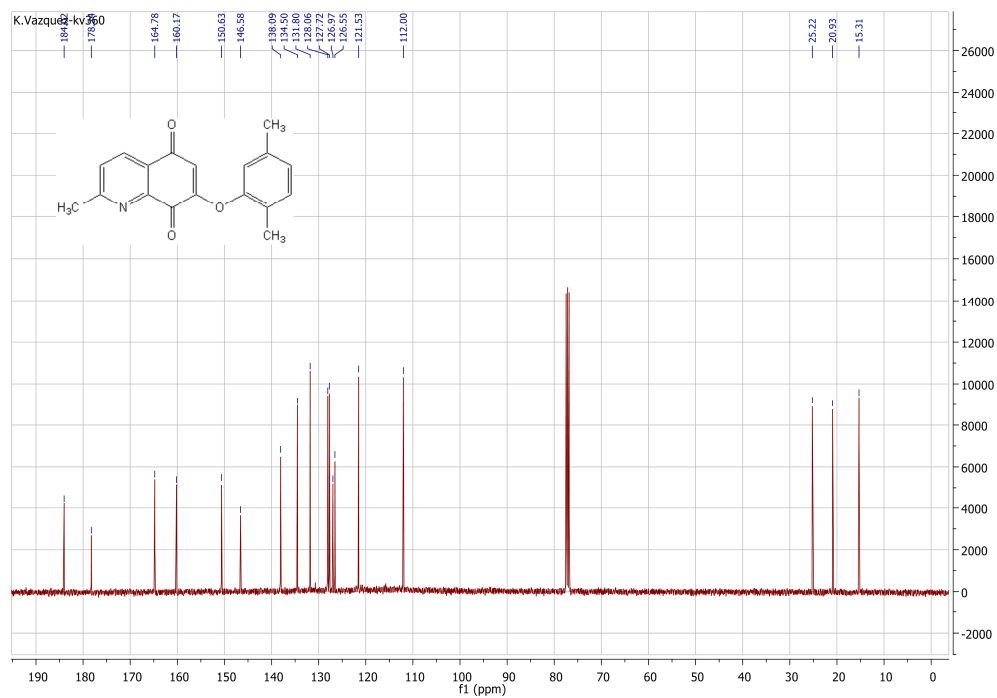
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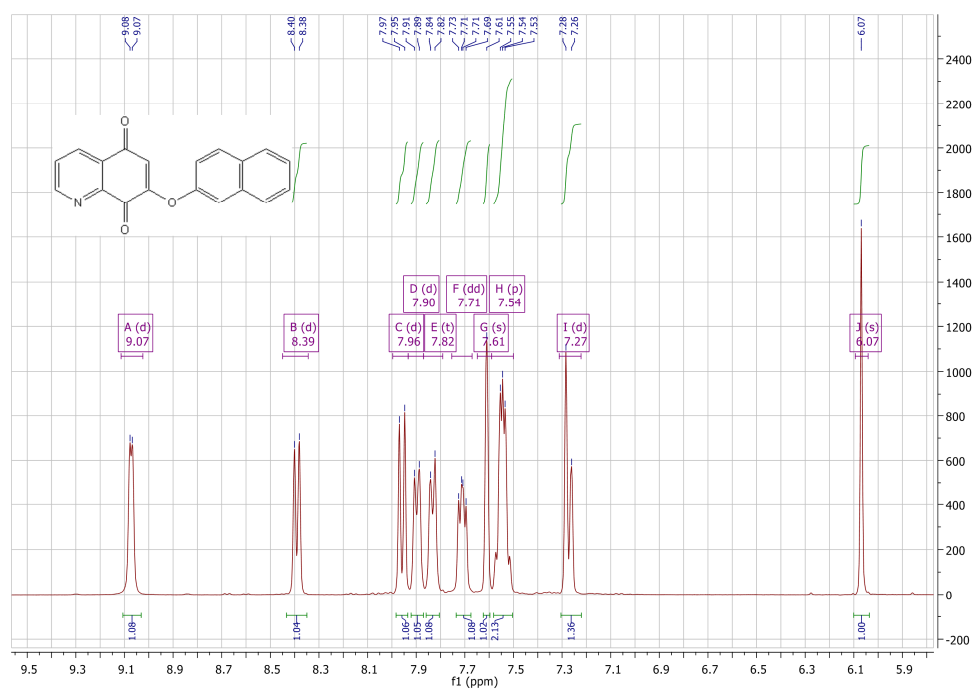
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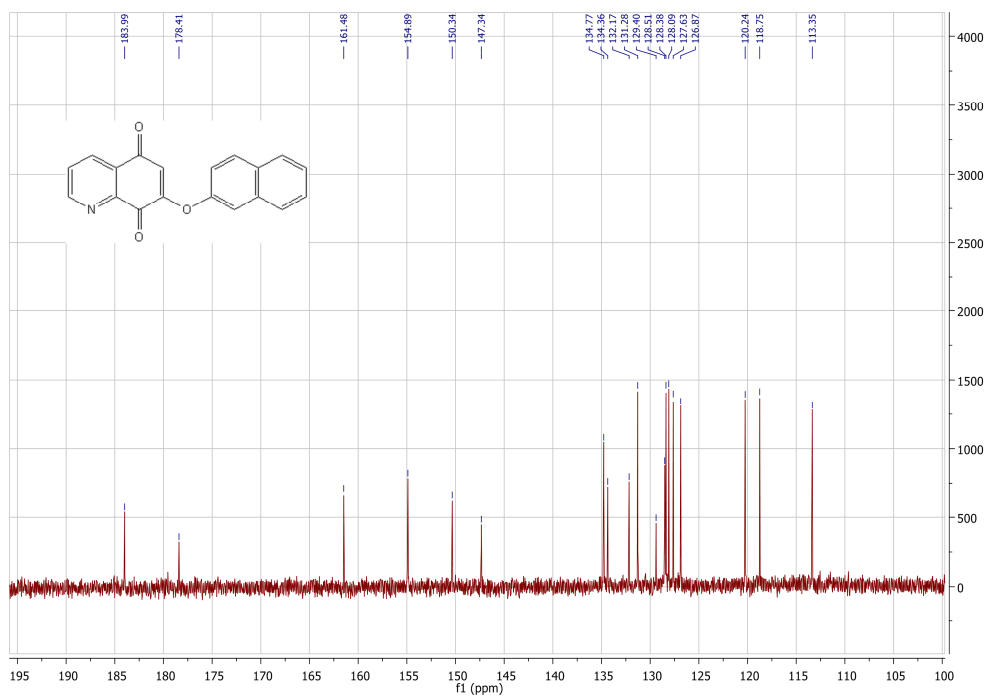
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¹H NMR spectra of compound **7f**



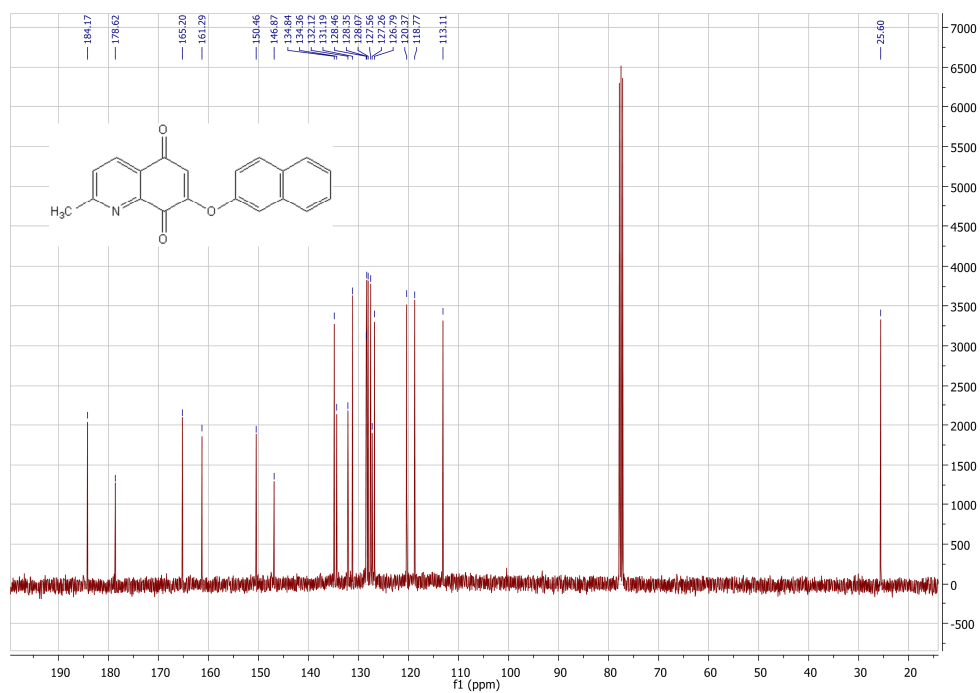
¹³C NMR spectra of compound **7f**



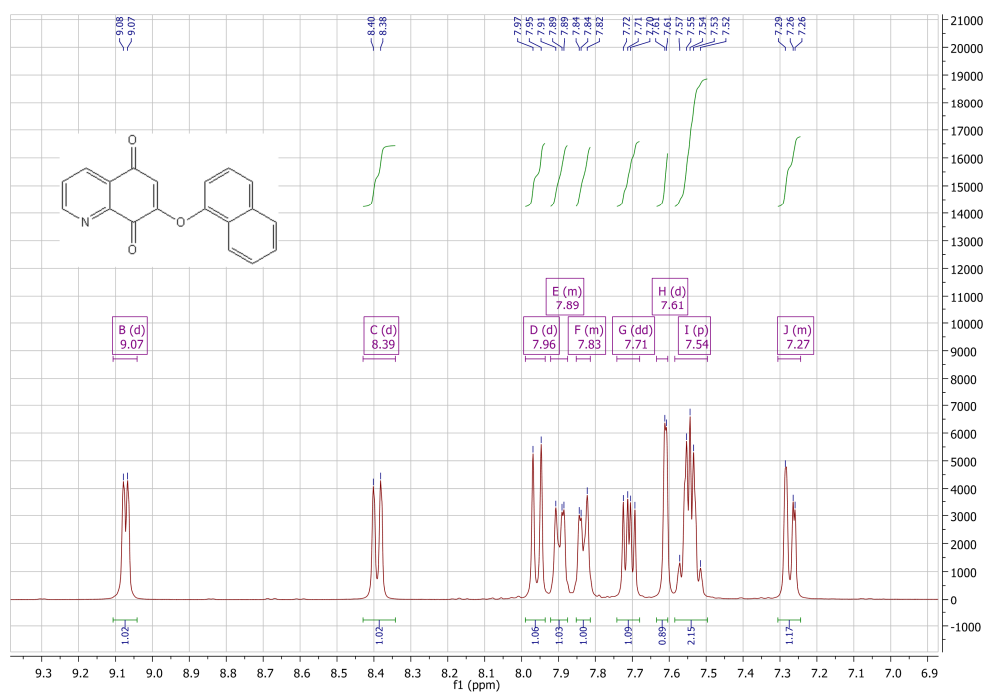
¹H NMR spectra of compound **7g**



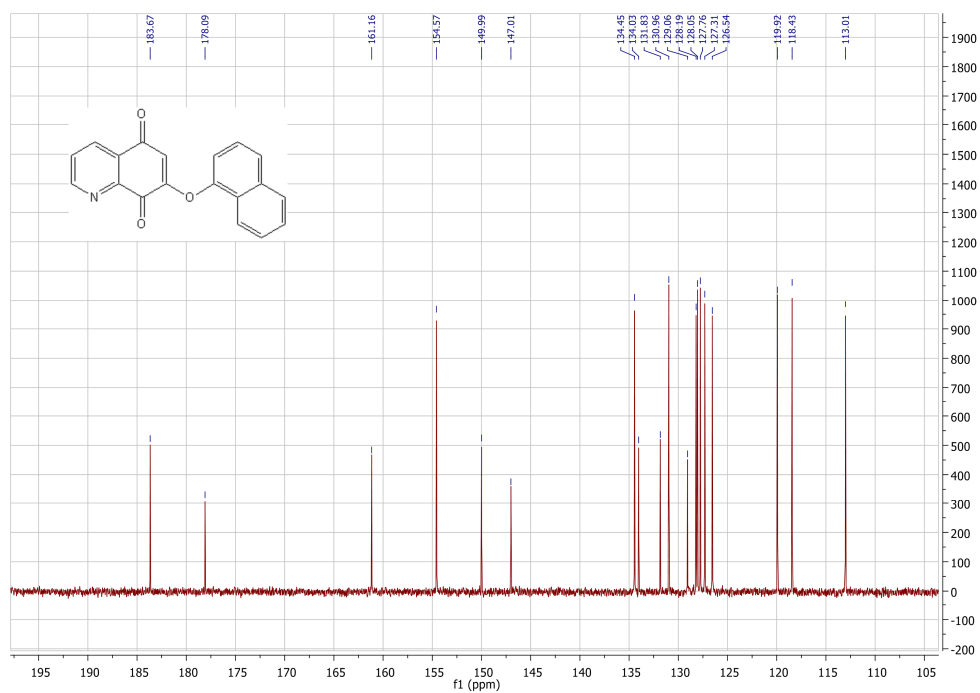
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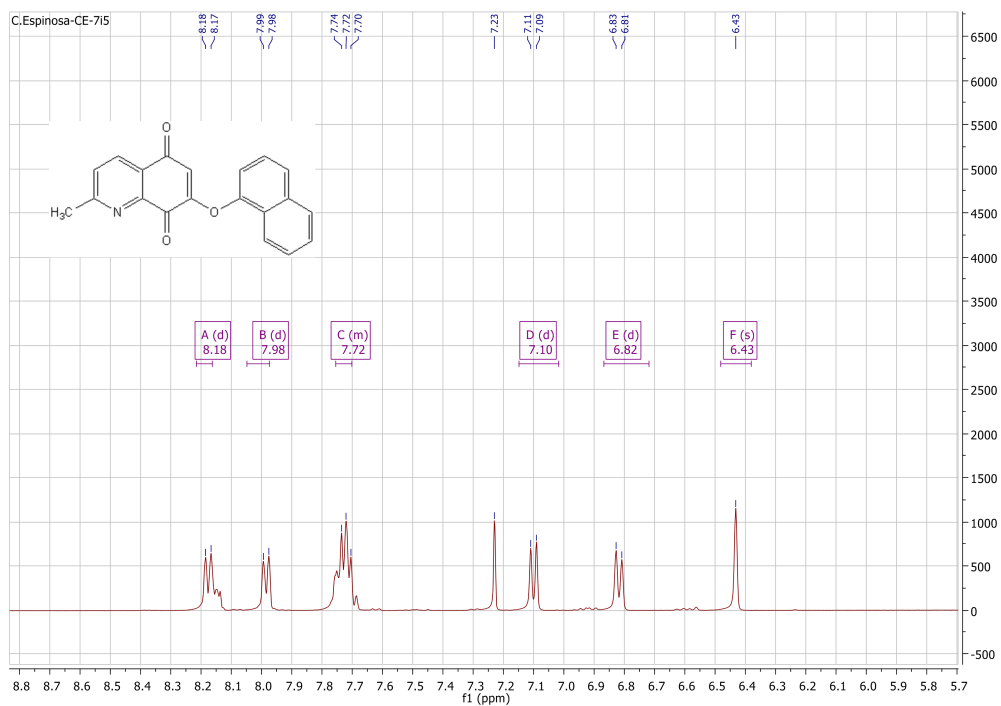
¹H NMR spectra of compound **7h**



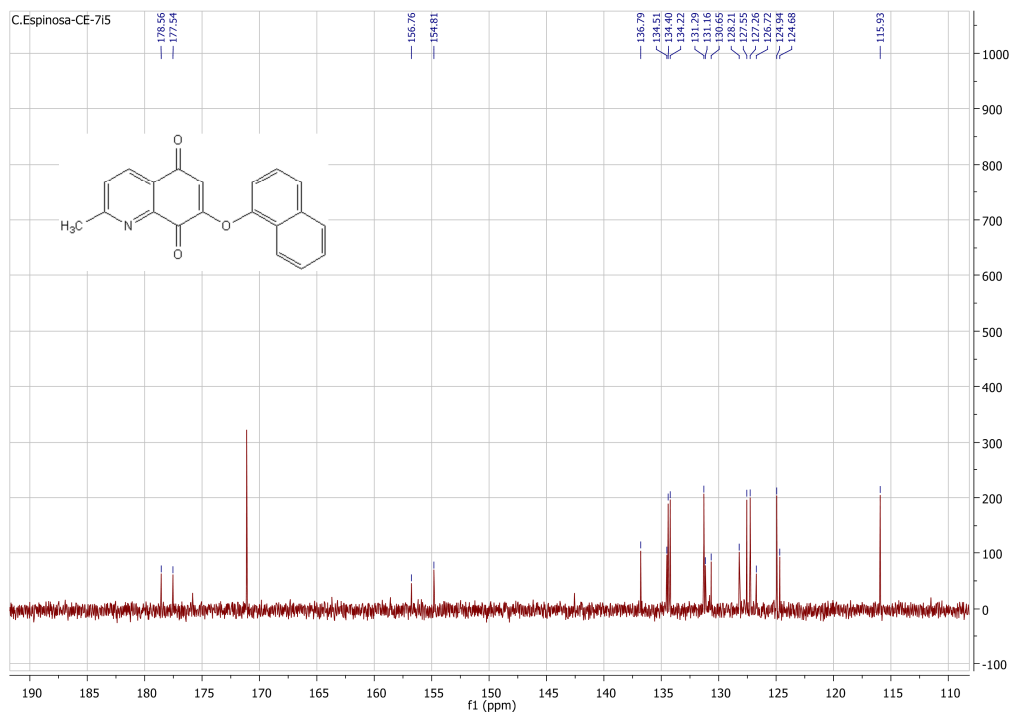
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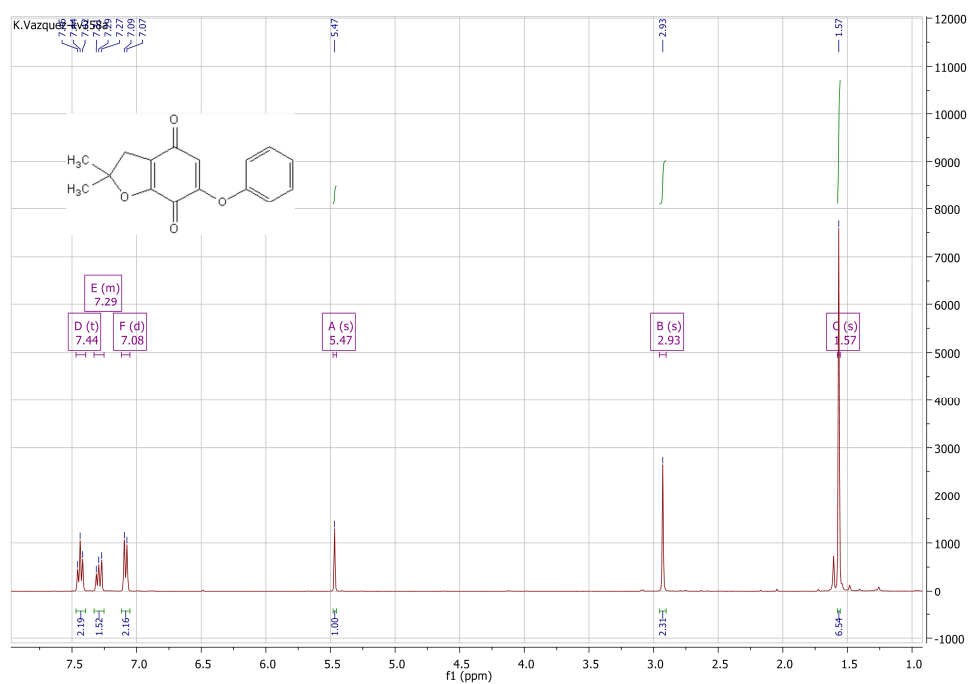
^1H NMR spectra of compound **7i**



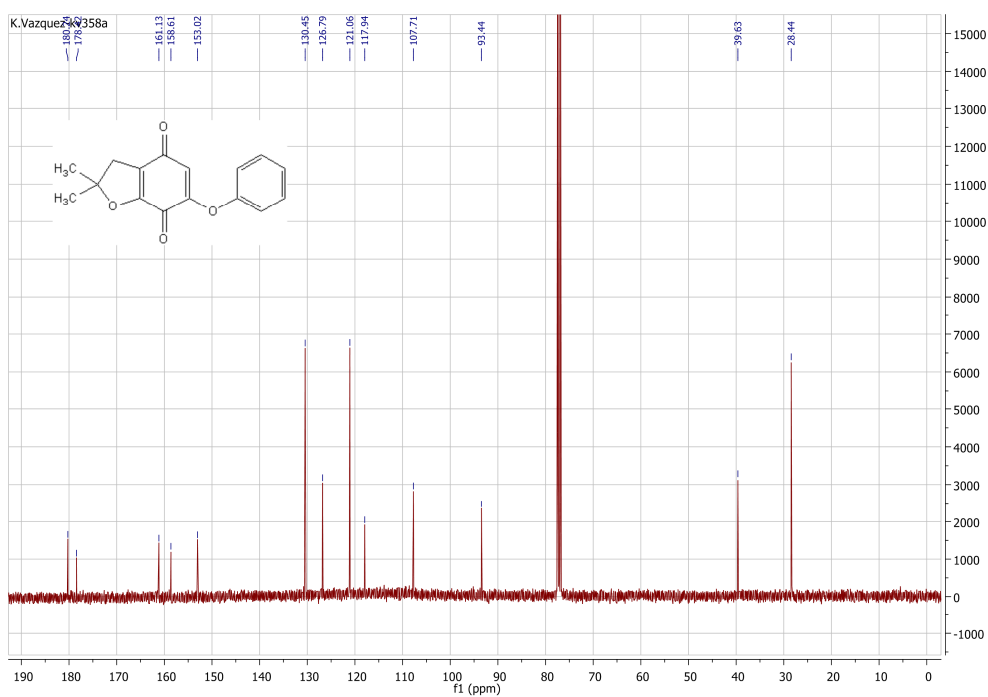
^{13}C NMR spectra of compound **7i**



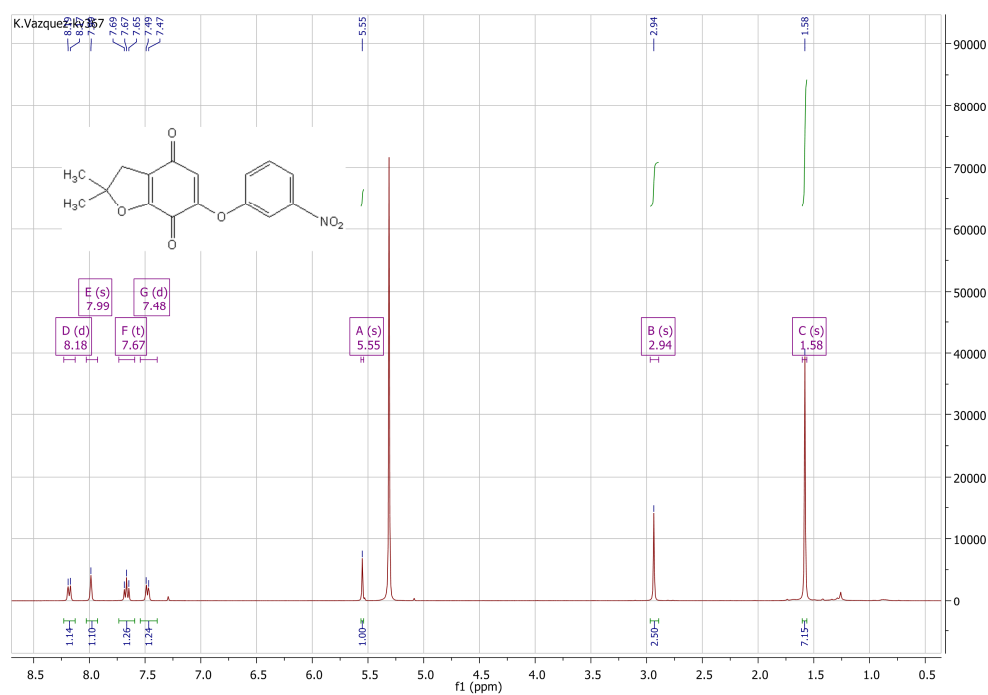
¹H NMR spectra of compound **11a**



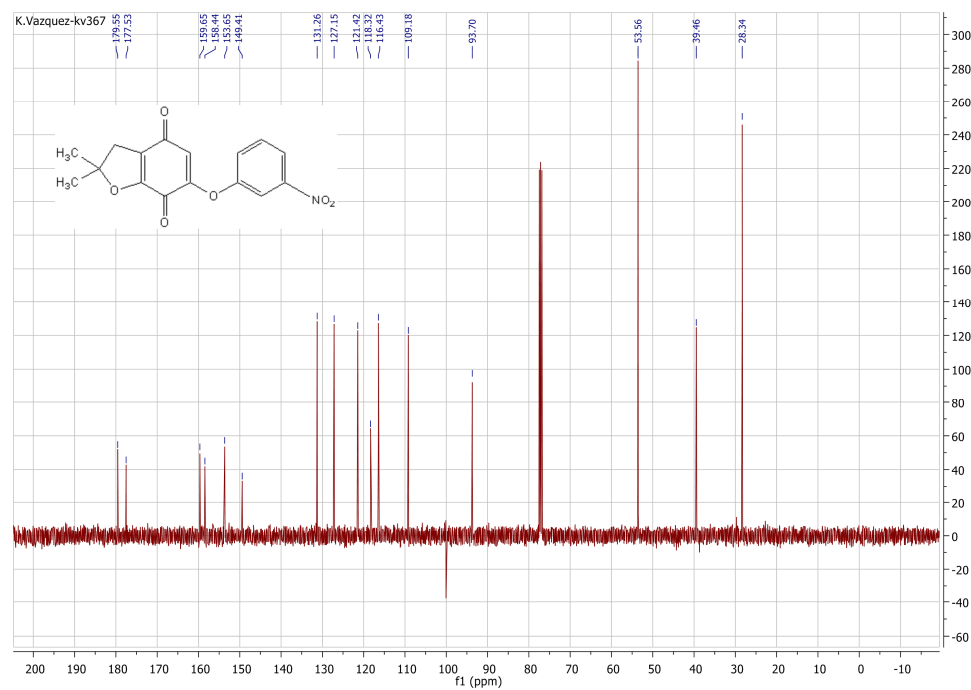
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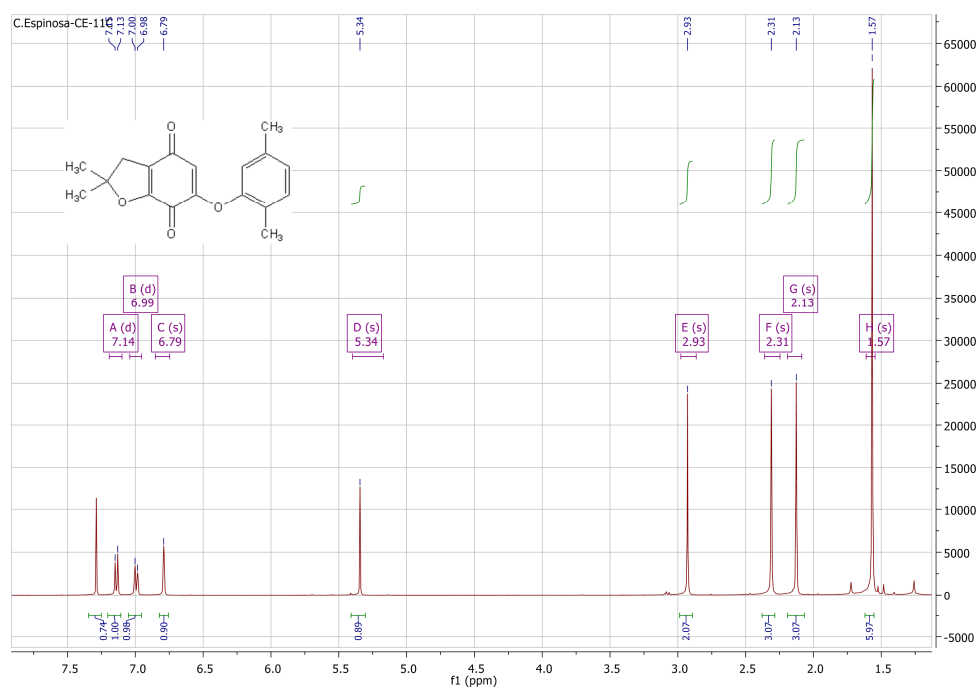
¹H NMR spectra of compound **11b**



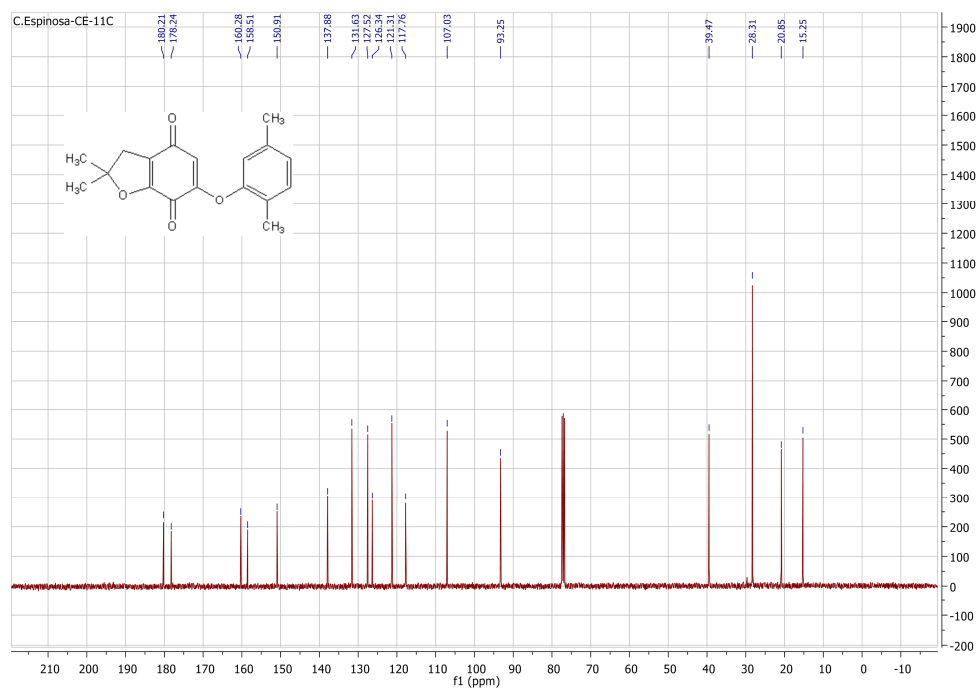
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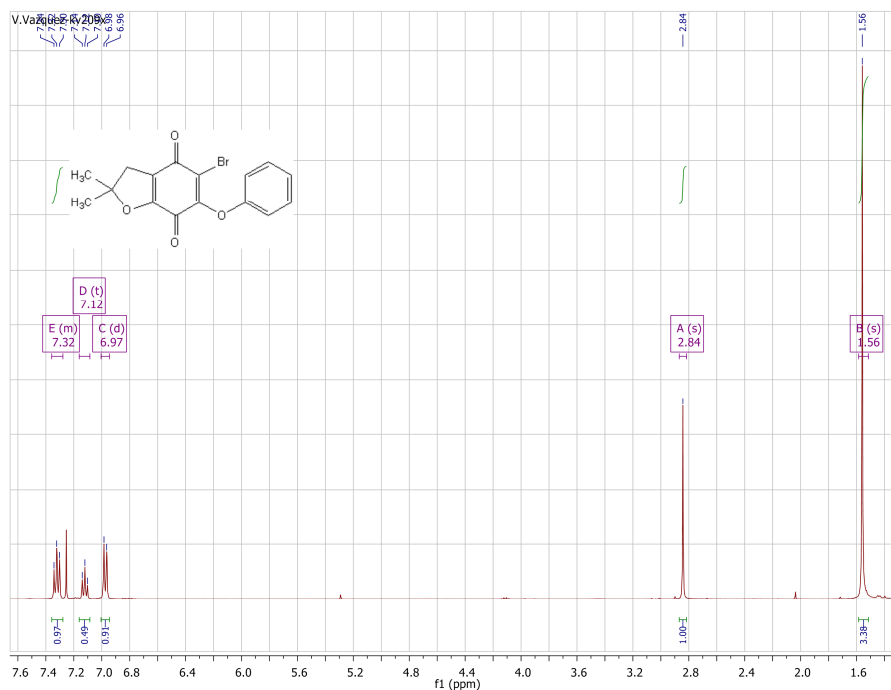
¹H NMR spectra of compound **11c**



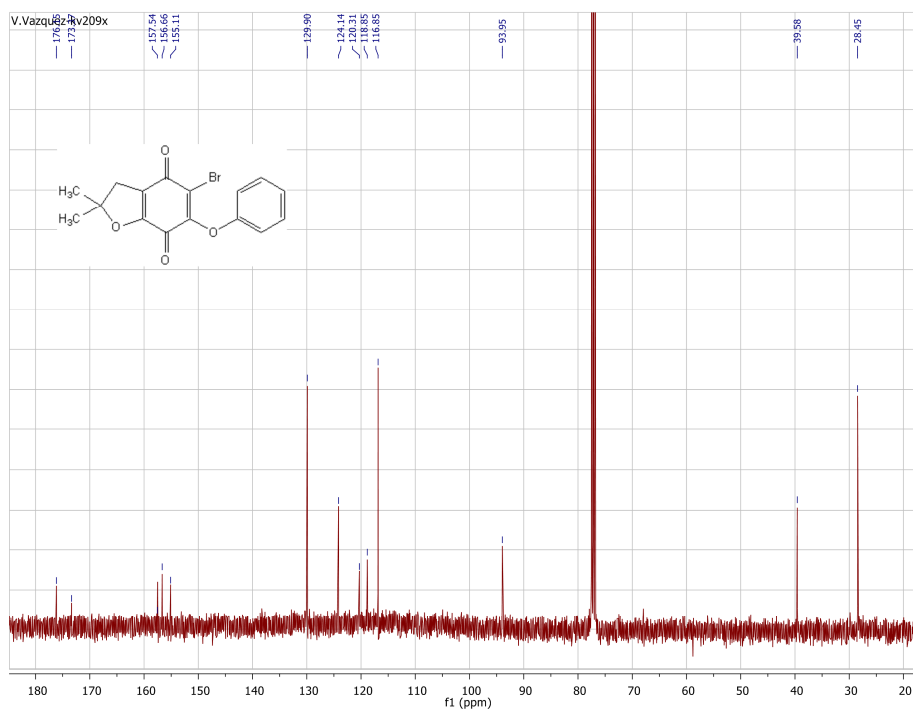
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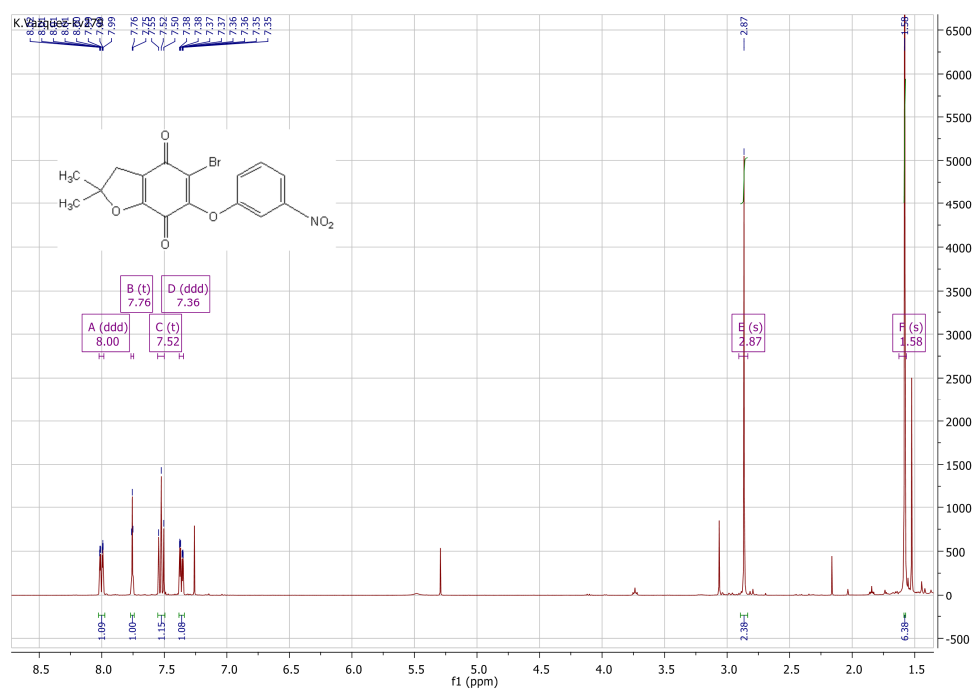
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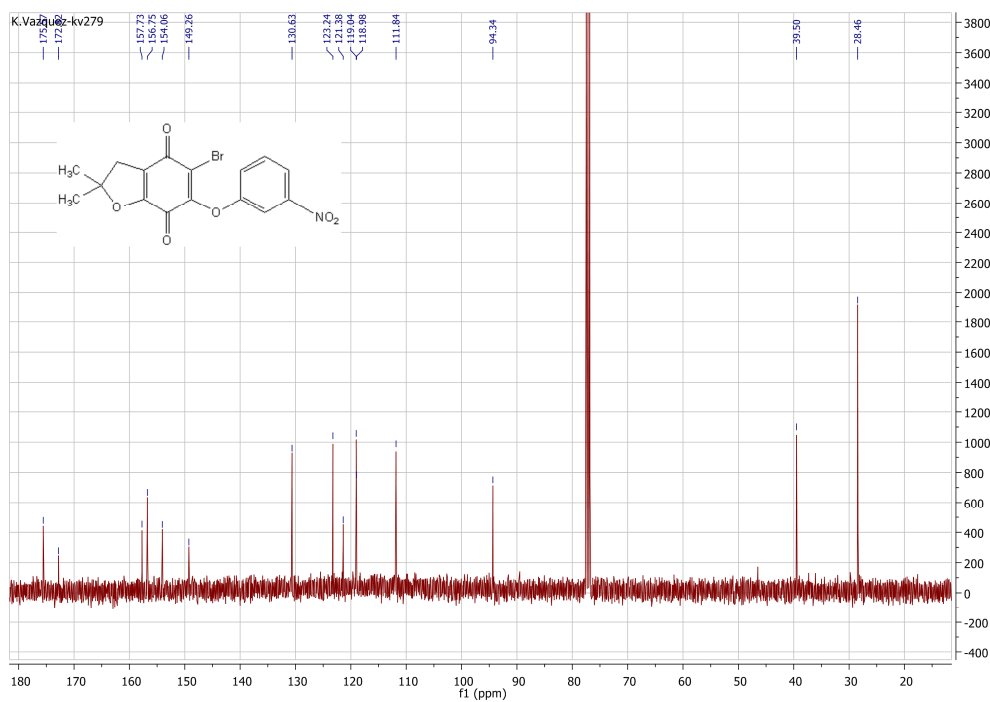
¹³C NMR spectra of compound **11d**



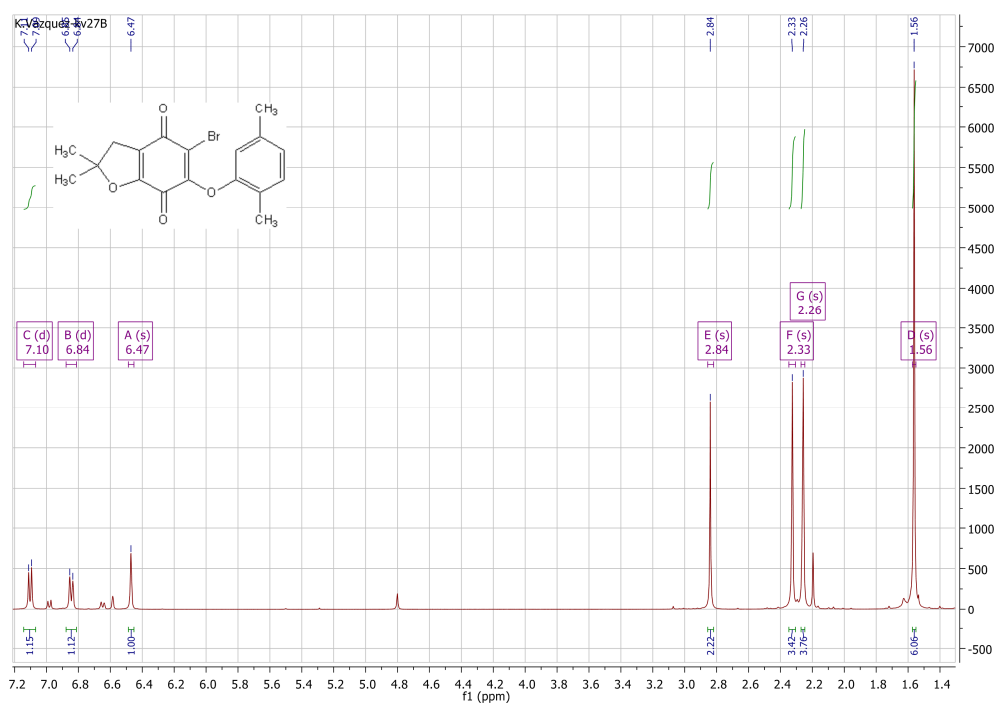
¹H NMR spectra of compound **11e**



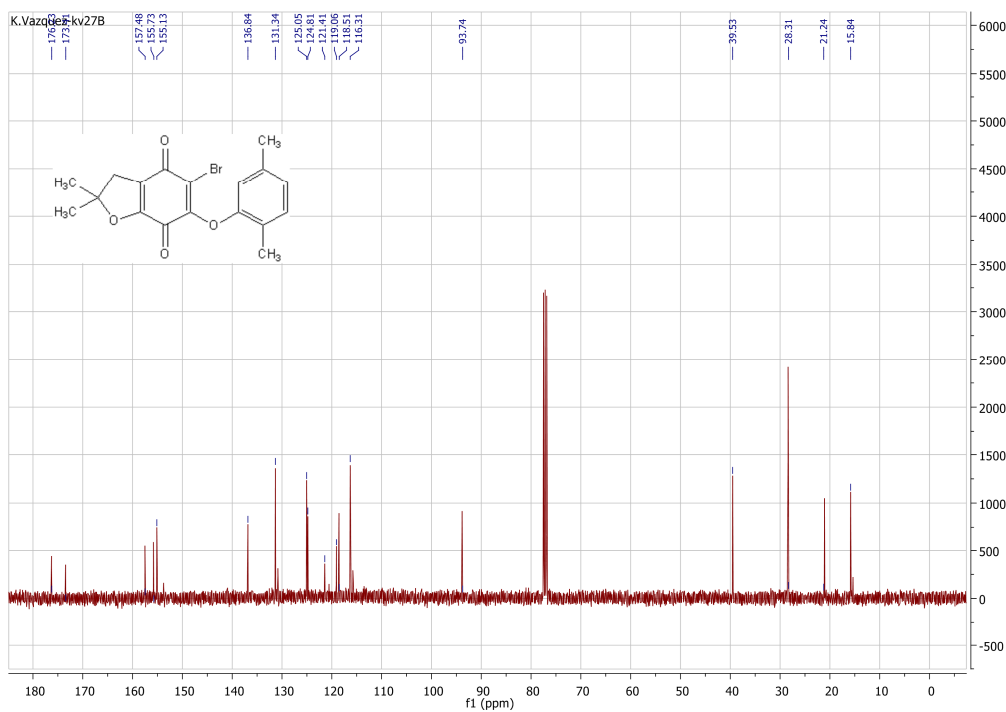
¹³C NMR spectra of compound **11e**



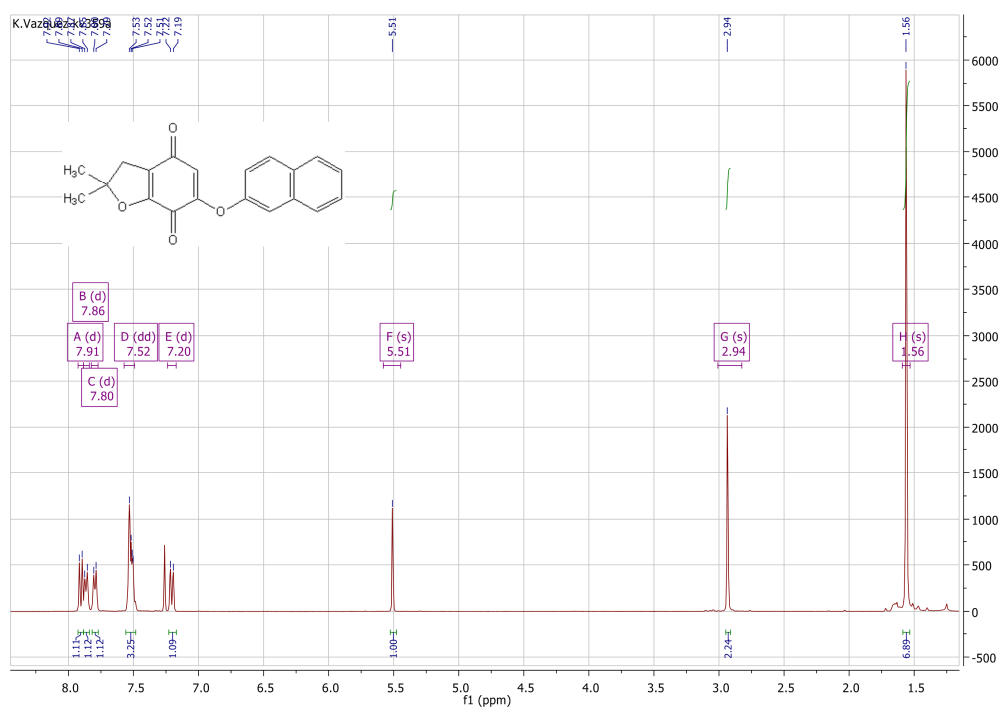
¹H NMR spectra of compound **11f**



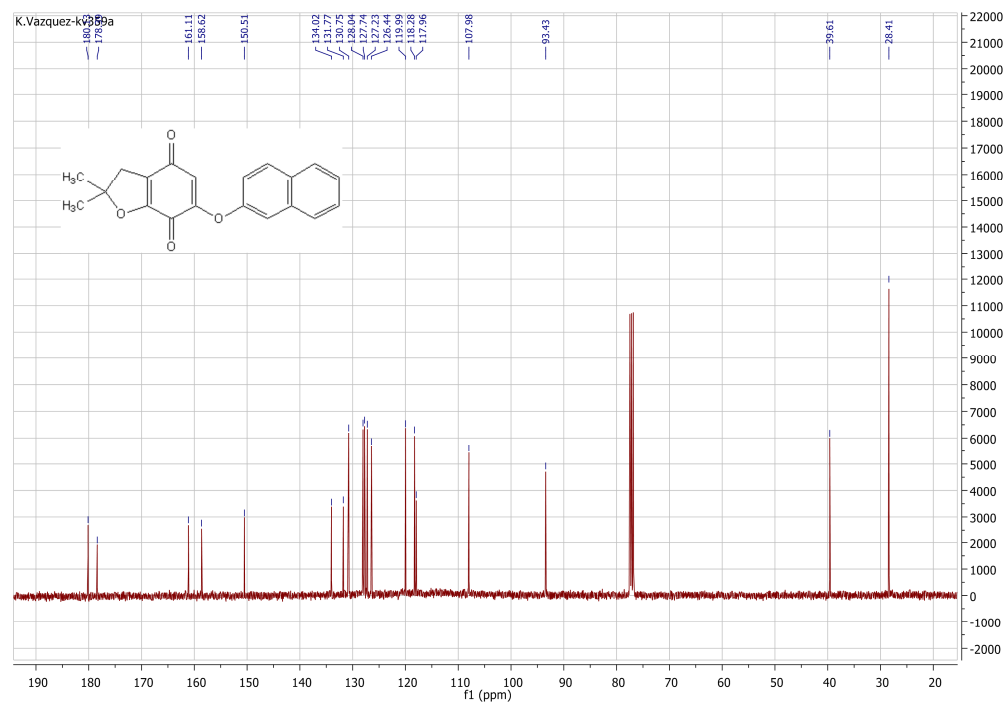
¹³C NMR spectra of compound **11f**



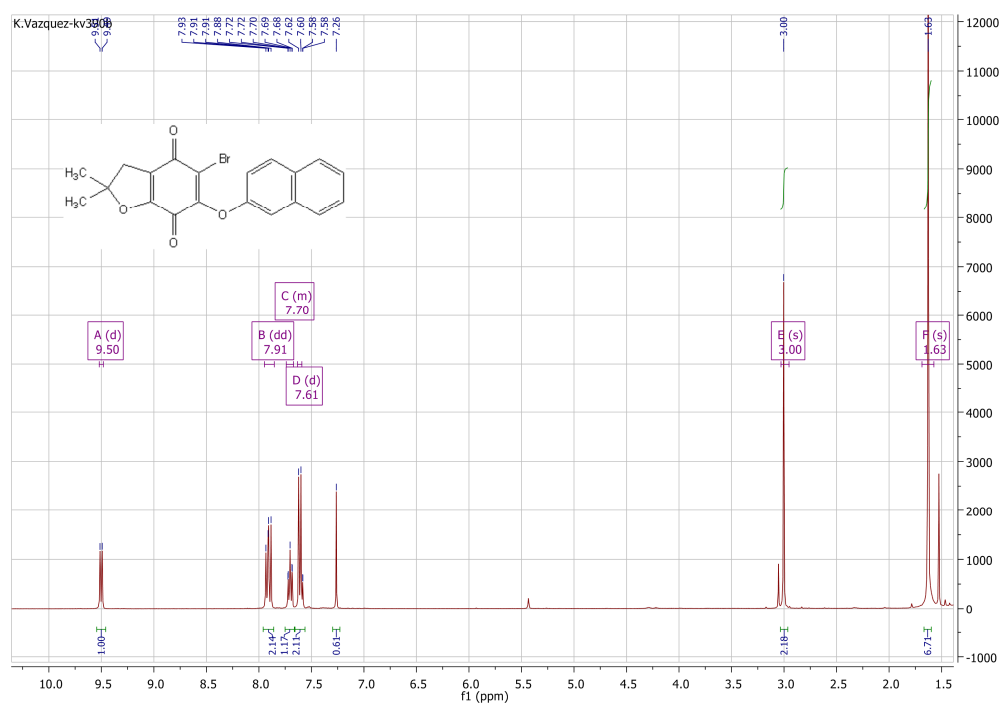
¹H NMR spectra of compound **11g**



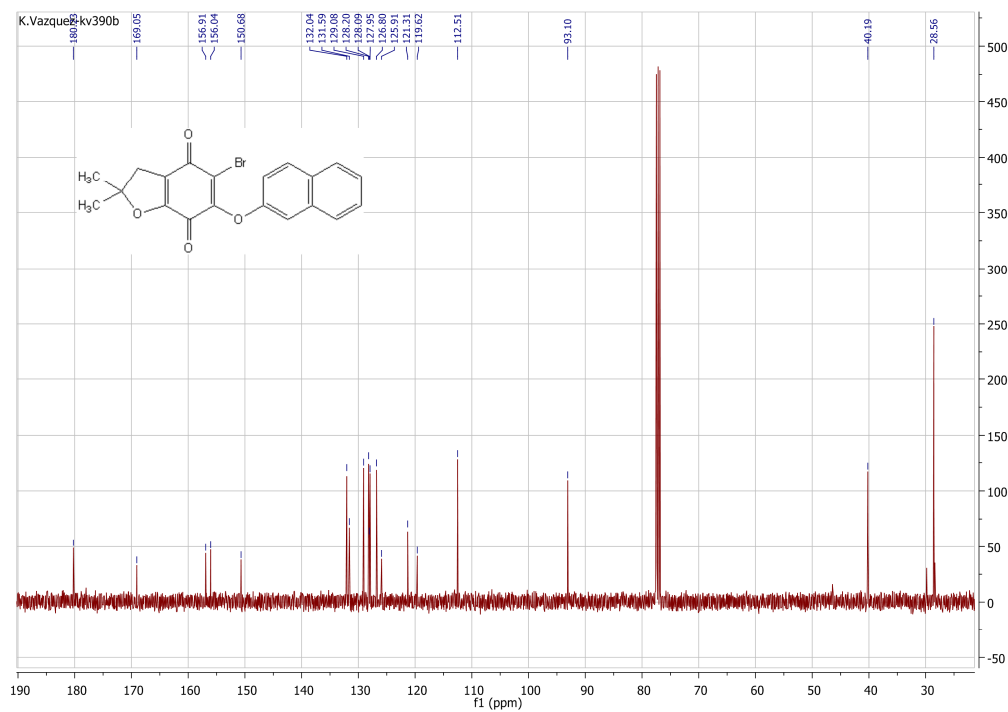
¹³C NMR spectra of compound **11g**



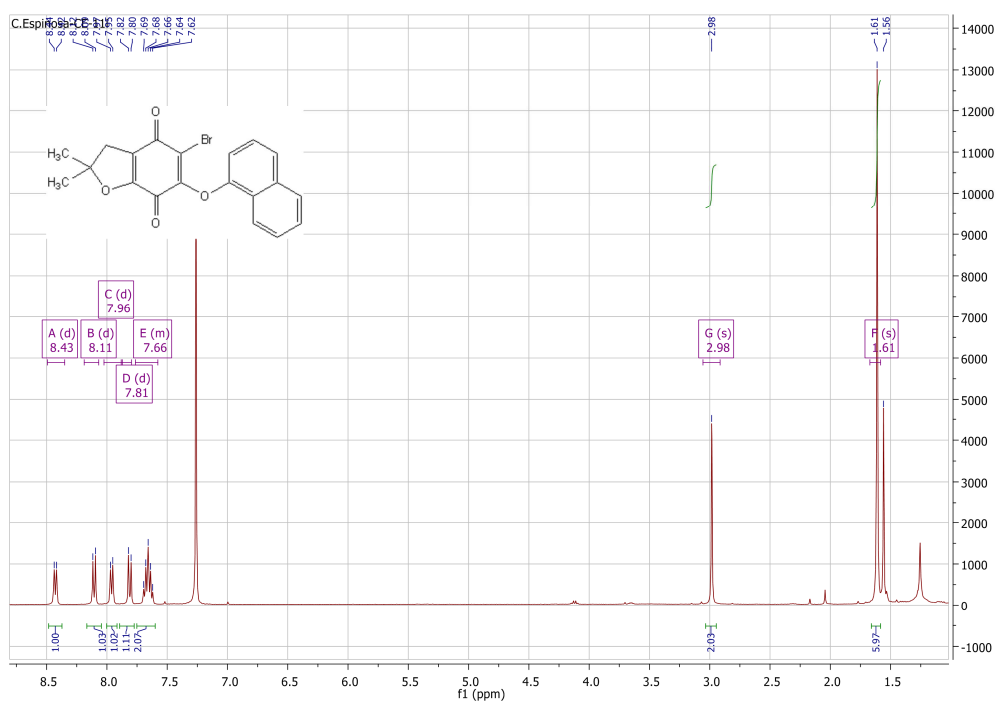
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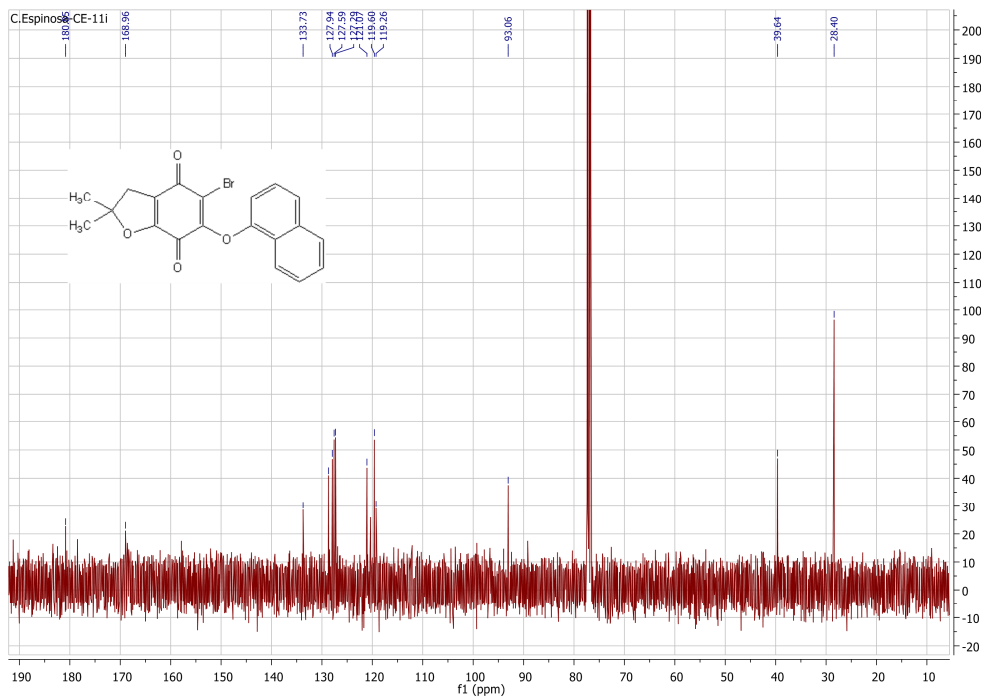
¹³C NMR spectra of compound **11h**



¹H NMR spectra of compound **11i**



¹³C NMR spectra of compound **11i**



Mass spectra of compound **3a**

Elemental Composition Report

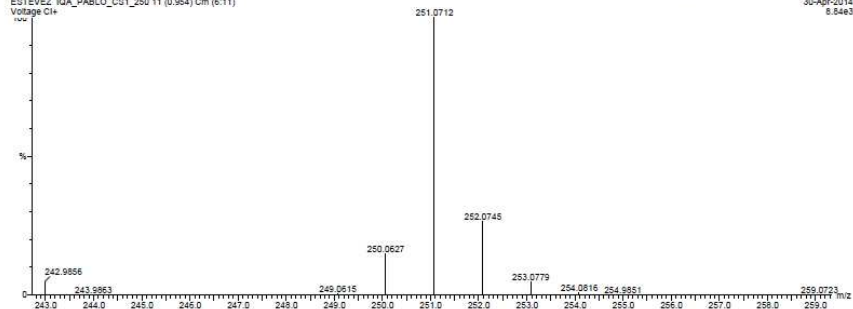
Page 1

Multiple Mass Analysis: 14 mass(es) processed - displaying only valid results
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Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
4 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:

C: 16-16 H: 11-11 O: 3-3
ESTEVEZ IQA_PABLO_CS1_250
ESTEVEZ IQA_PABLO_CS1_250 11 (0.954) Cm (E:11)

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30-Apr-2014
8.84e3



Minimum:	0.01					-1.5	
Maximum:	100.00		5.0	5.0	100.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
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Mass spectra of compound **3b**

Elemental Composition Report

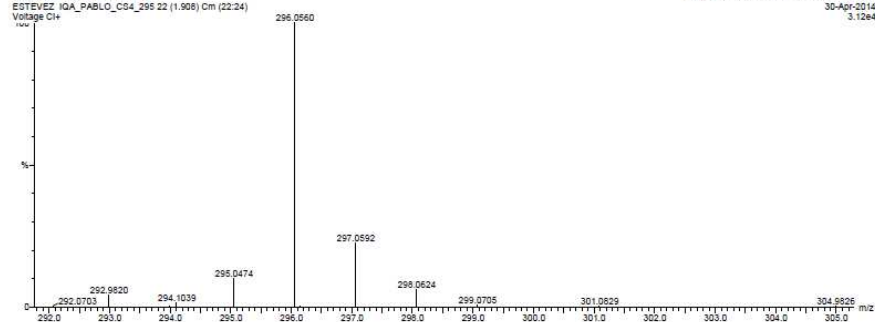
Page 1

Multiple Mass Analysis: 13 mass(es) processed - displaying only valid results
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Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
2 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:

C: 16-16 H: 10-10 N: 1-1 O: 5-5
ESTEVEZ IQA_PABLO_CS4_295
ESTEVEZ IQA_PABLO_CS4_295 22 (1.908) Cm (22:24)

UNIDADE DE MASAS E PROTEOMICA USC
30-Apr-2014
3.12e4



Minimum:	0.01				-1.5		
Maximum:	100.00		5.0	5.0	100.0		
Mass	RA	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
296.0560	100.00	296.0559	0.1	0.2	12.5	38.0	C16 H10 N O5

Mass spectra of compound **3c**

Elemental Composition Report

Page 1

Multiple Mass Analysis: 14 mass(es) processed - displaying only valid results
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
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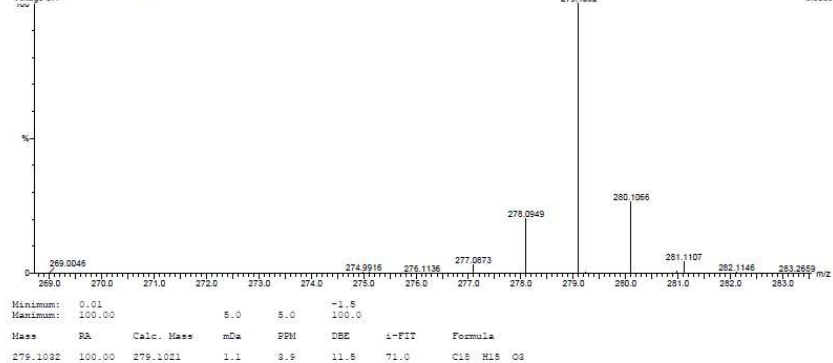
Elements Used:

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Voltage C1+

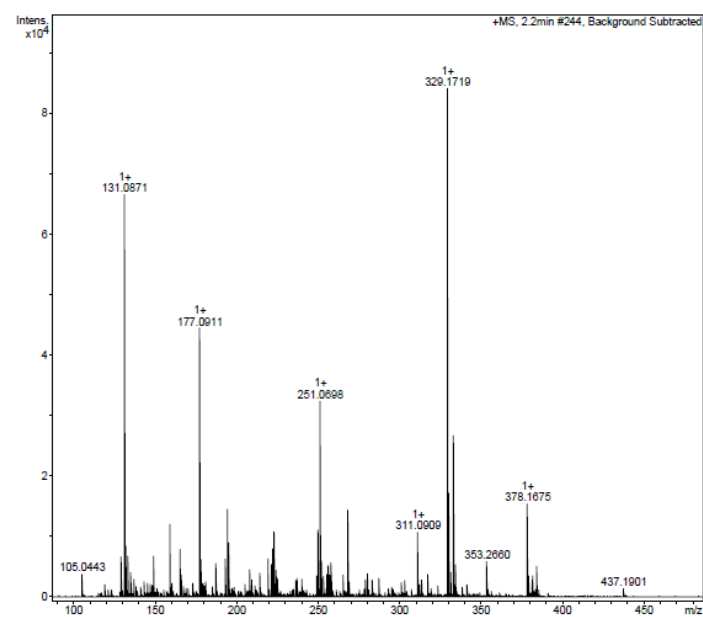


Mass spectra of compound **3d**

Analysis Info

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Method fia_pos_bajo_50-450_egf.m

Acquisition Date 6/8/2014 4:42:20 PM
Instrument micrOTOF

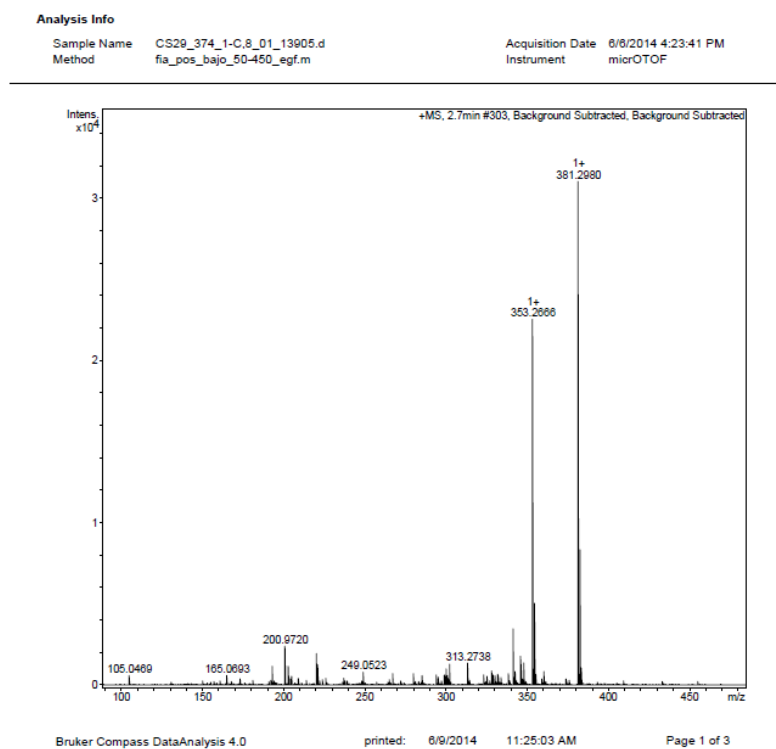


Bruker Compass DataAnalysis 4.0

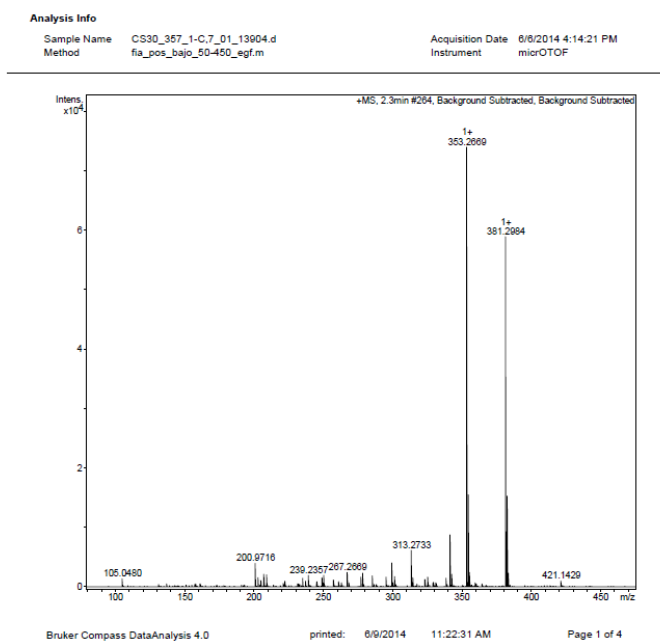
printed: 6/9/2014 1:14:22 PM

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Mass spectra of compound **3e**



Mass spectra of compound **3f**



Mass spectra of compound **3g**

Elemental Composition Report

Page 1

Multiple Mass Analysis: 18 mass(es) processed - displaying only valid results

Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

2 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

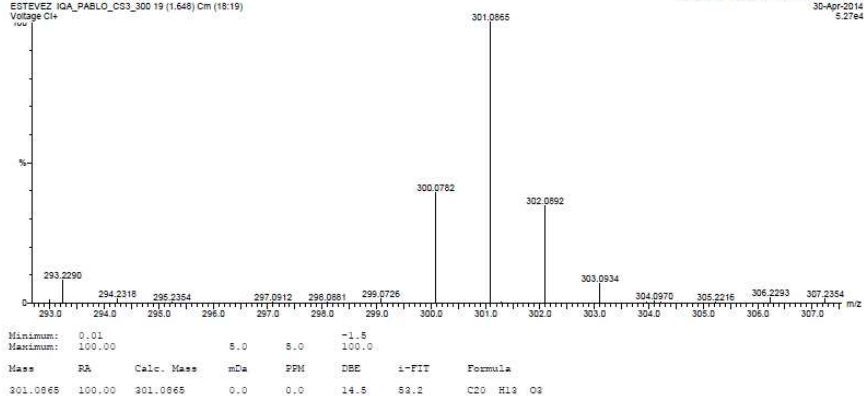
C: 20-20 H: 13-13 O: 3-3

ESTEVEZ IQA_PABLO_CS3_300

ESTEVEZ IQA_PABLO_CS3_300 19 (1.648) Cm (18:19)

Voltage C1+

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30-Apr-2014
5.2764

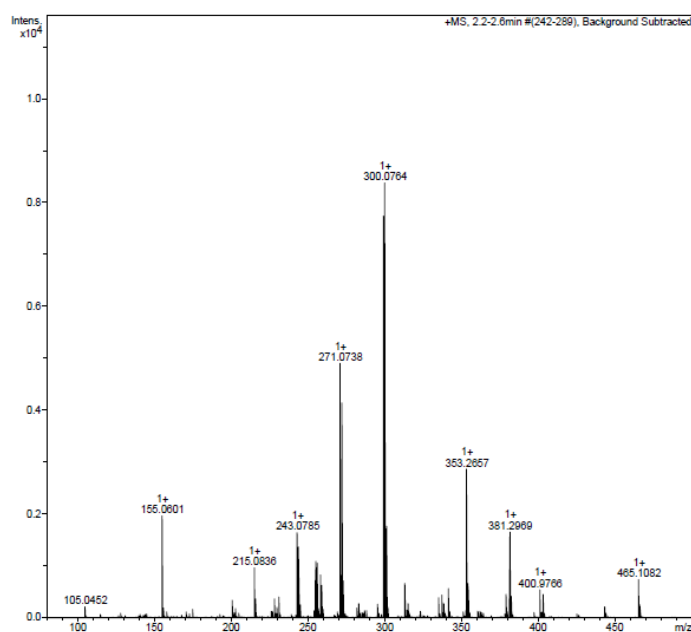


Mass spectra of compound **3h**

Analysis Info

Sample Name CS28_379_1-B_5_01_13880.d
Method fia_pos_bajo_50-450_egf.m

Acquisition Date 6/6/2014 12:01:24 PM
Instrument micrOTOF



Mass spectra of compound **3i**

Elemental Composition Report

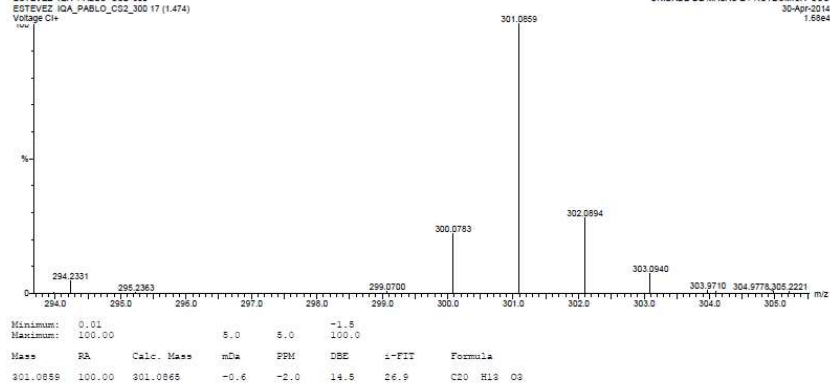
Page 1

Multiple Mass Analysis: 12 mass(es) processed - displaying only valid results
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Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
1 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:
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ESTEVEZ IQA PABLO CS2 300 17 (1.474)
Voltage CH

UNIDADE DE MASAS E PROTEOMICA USC
30-Apr-2014
1.6564

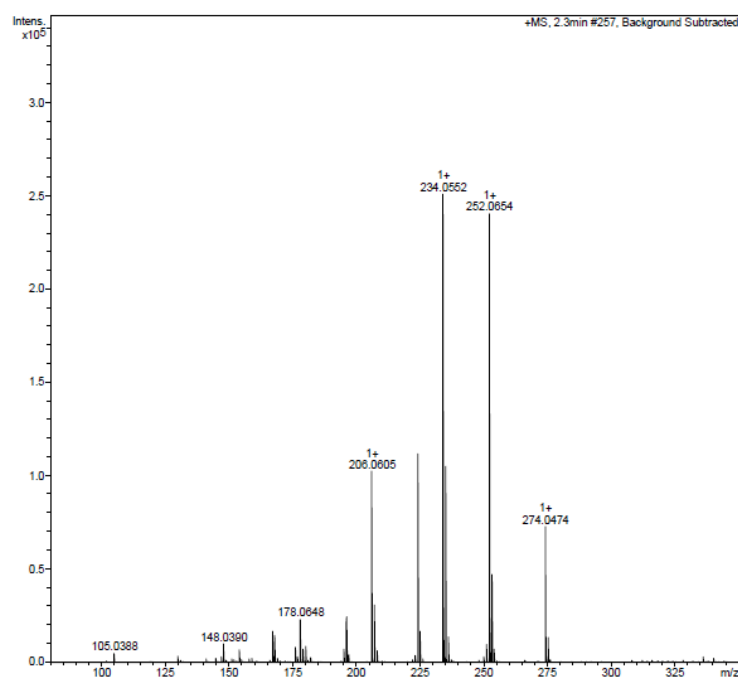


Mass spectra of compound **3j**

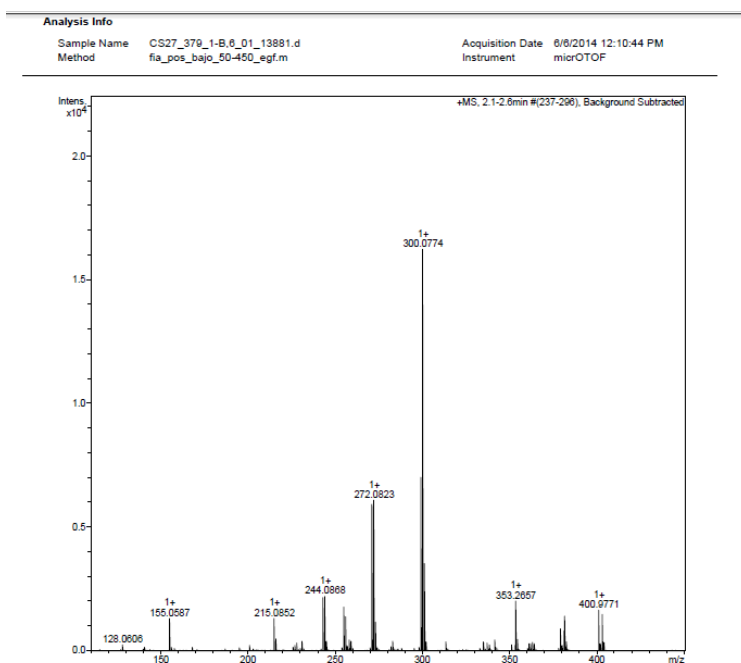
Analysis Info

Sample Name CS16_251_1-B_2_01_13517.d
Method fia_pos_bajo_50-450_egf.m

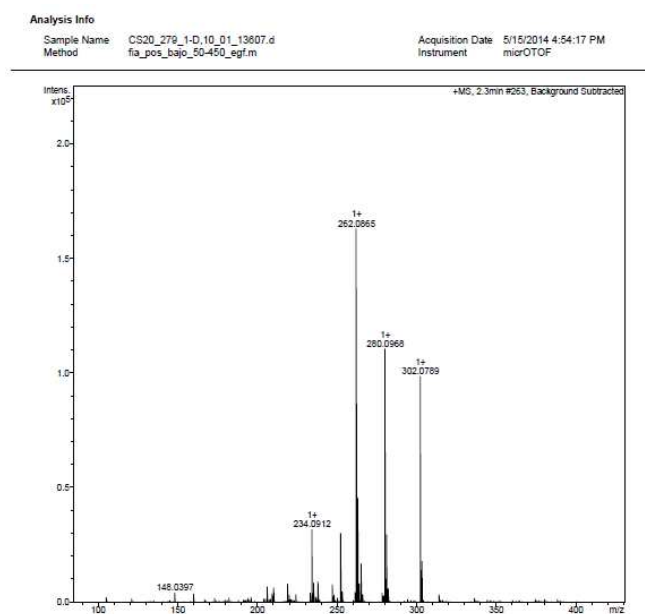
Acquisition Date 4/29/2014 5:23:11 PM
Instrument micrOTOF



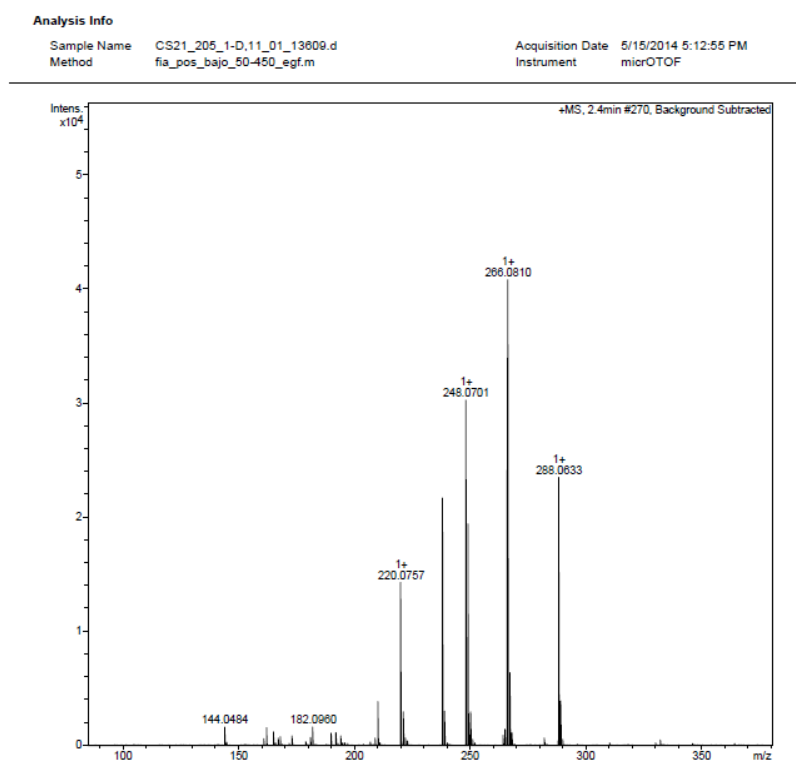
Mass spectra of compound **7a**



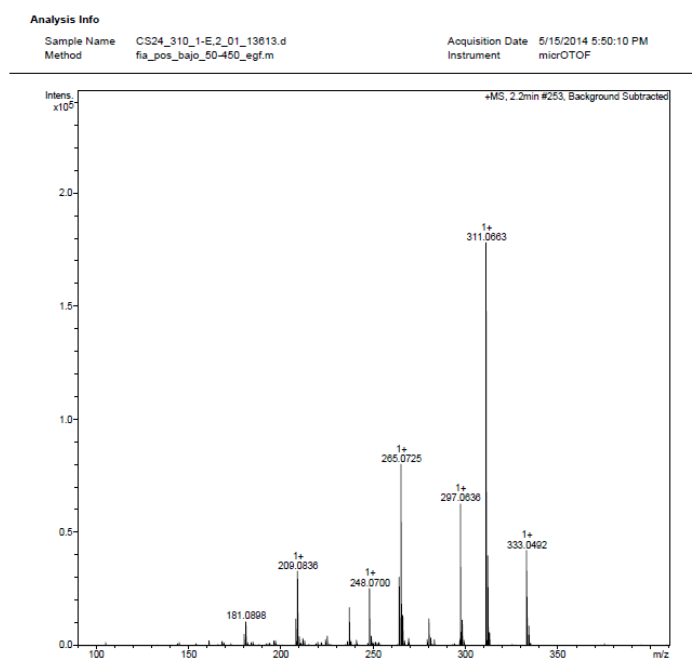
Mass spectra of compound **7b**



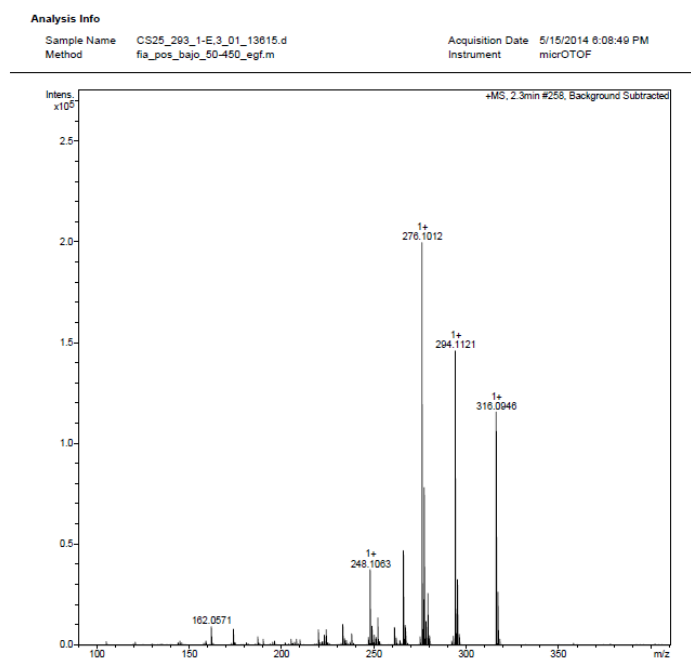
Mass spectra of compound **7c**



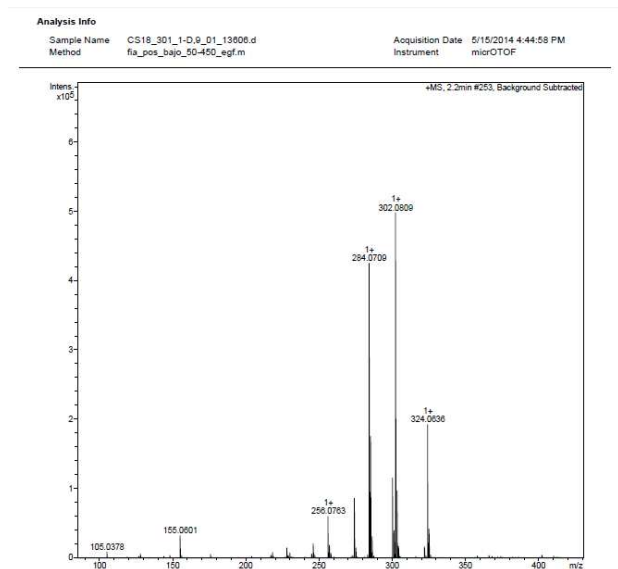
Mass spectra of compound **7d**



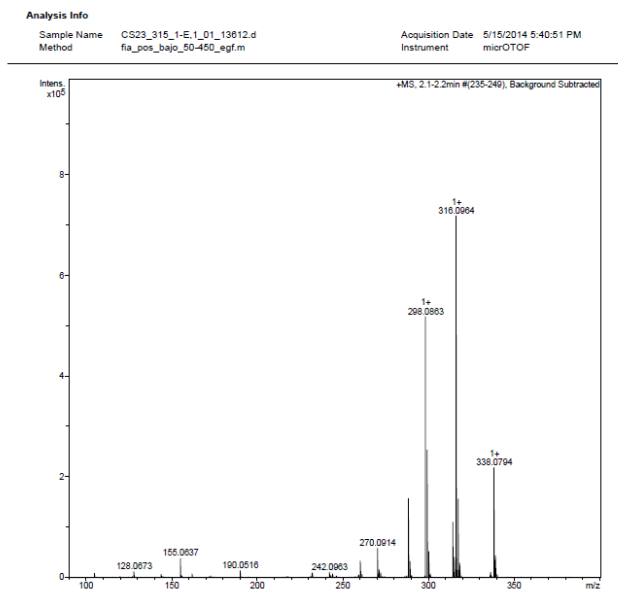
Mass spectra of compound **7e**



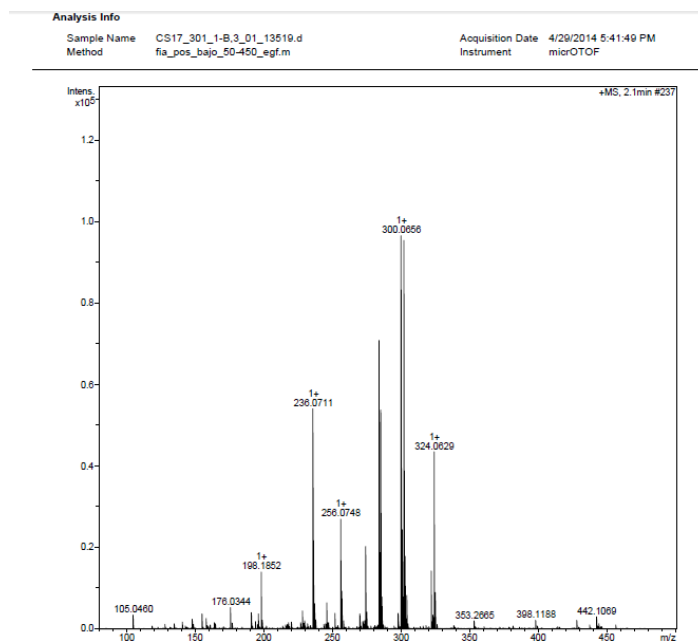
Mass spectra of compound **7f**



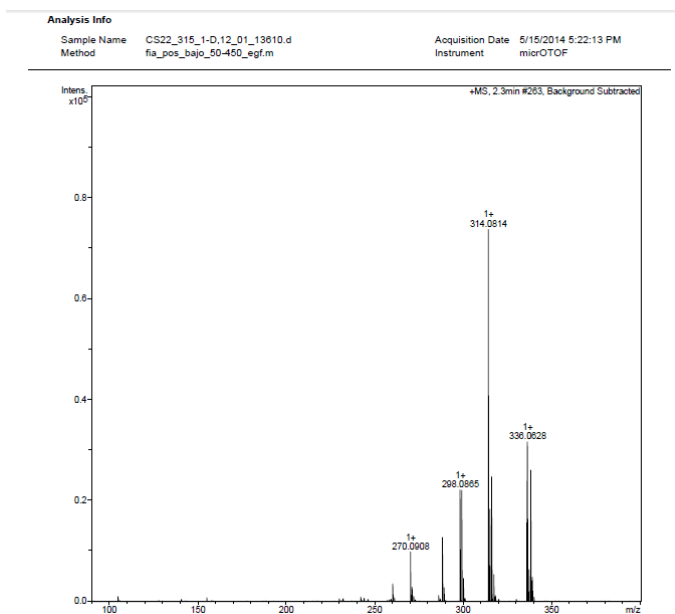
Mass spectra of compound **7g**



Mass spectra of compound **7h**



Mass spectra of compound **7i**



Mass spectra of compound **11a**

Elemental Composition Report

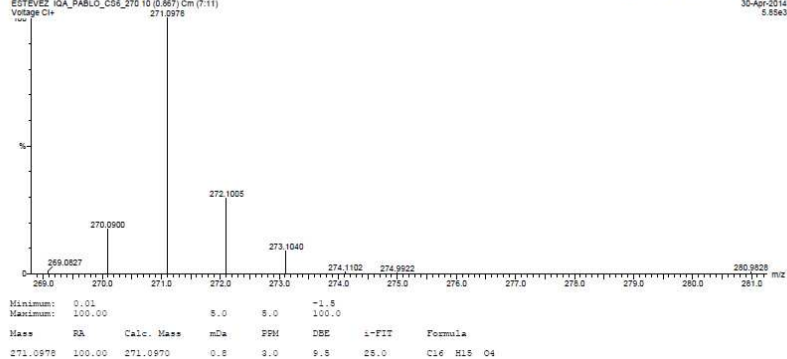
Page 1

Multiple Mass Analysis: 8 mass(es) processed - displaying only valid results
Tolerance = 5.0 PPM / DBE: min = -1.5, max = 100.0
Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions
1 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:

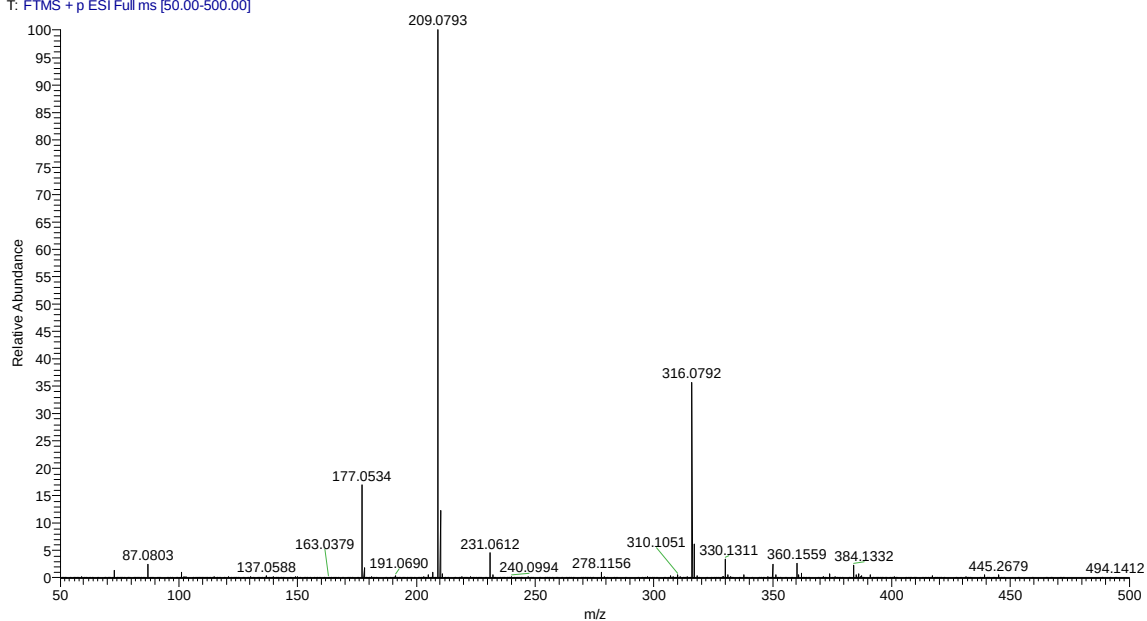
C: 15-16 H: 15-15 O: 4-4
ESTEVEZ IGA PABLO CG6 270
ESTEVEZ IGA PABLO CG6 270 10 (0.867) Cm (7:11)
Voltage CH

UNIDADE DE MASSAS E PROTEOMICA USC
30-Apr-2014
6:55:43



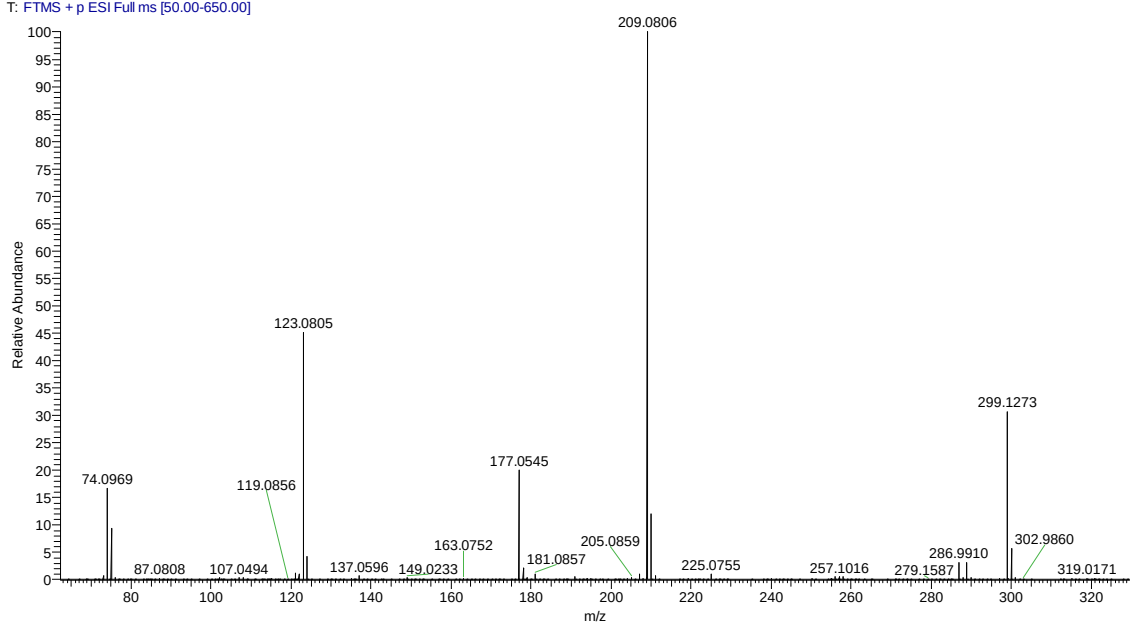
Mass spectra of compound **11b**

CS9 #29 RT: 0.31 AV: 1 NL: 5.27E6
T: FTMS + p ESI Full ms [50.00-500.00]

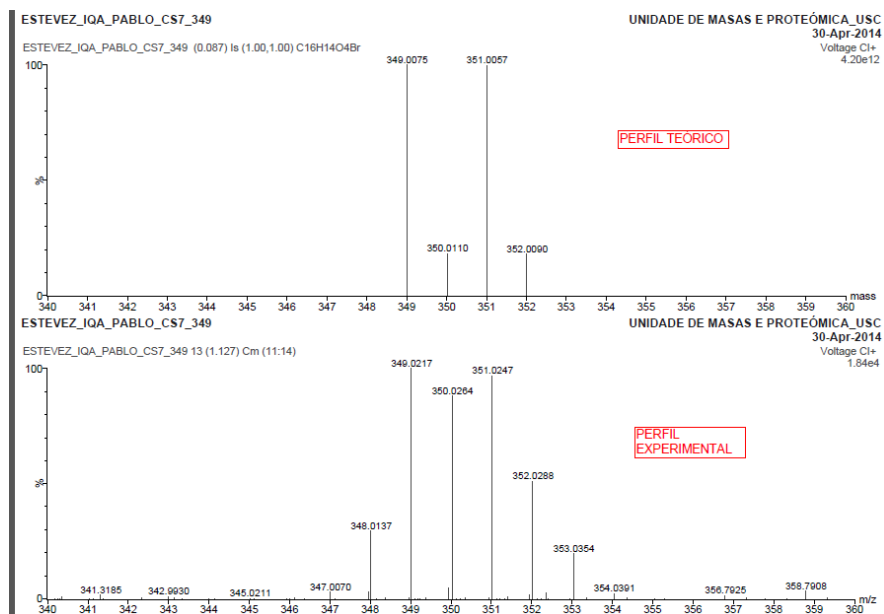


Mass spectra of compound **11c**

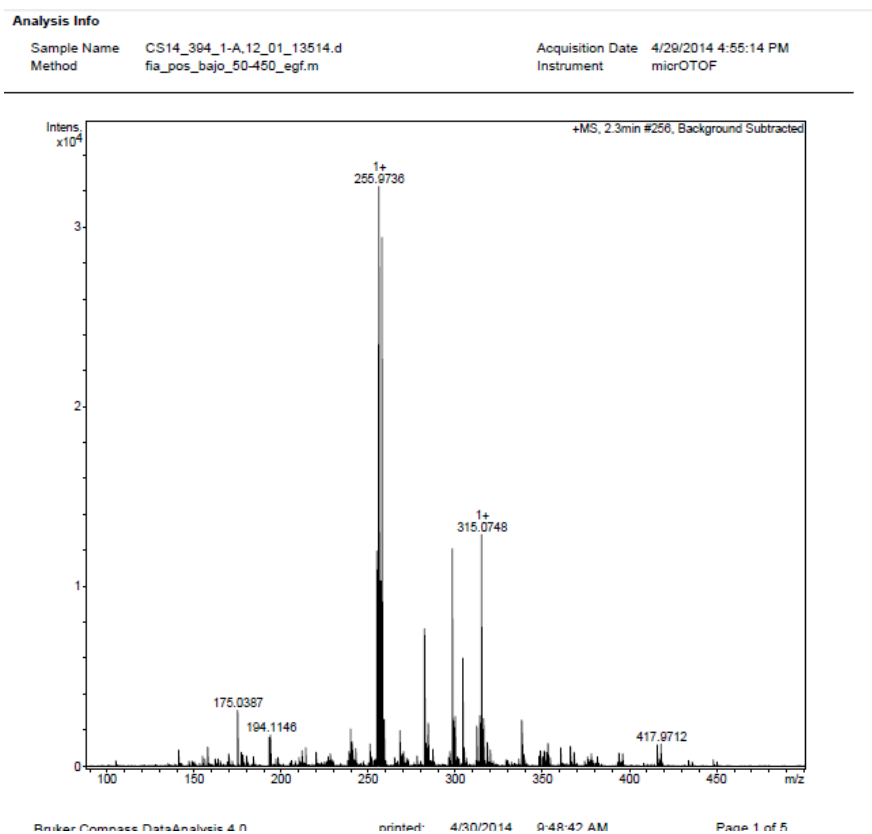
Muestra CS10 #68 RT: 0.73 AV: 1 NL: 1.65E9
T: FTMS + p ESI Full ms [50.00-650.00]



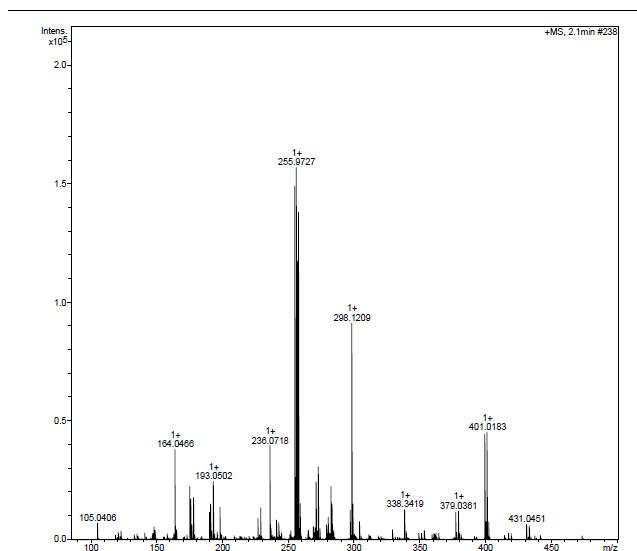
Mass spectra of compound **11d**



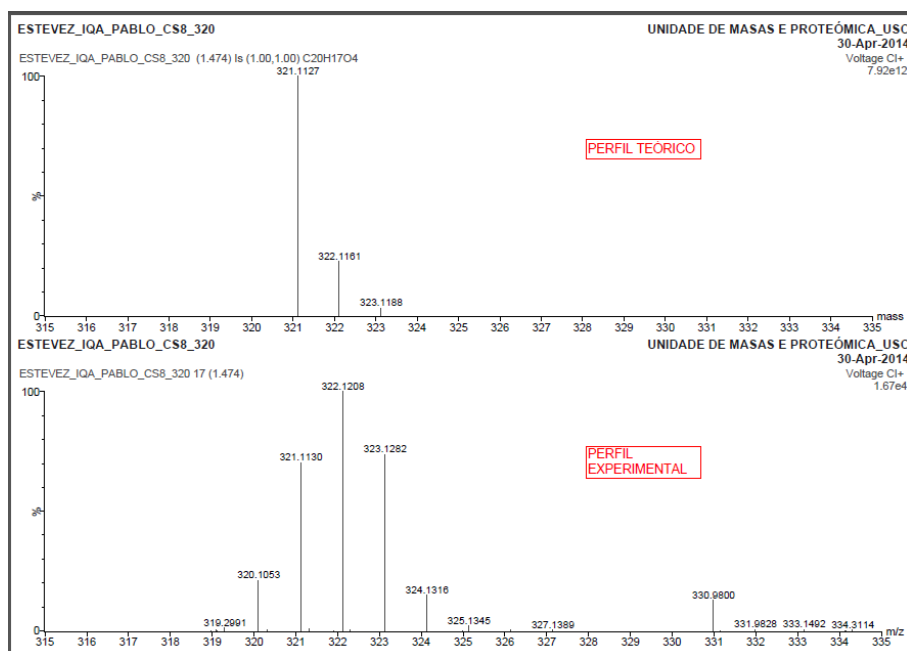
Mass spectra of compound **11e**



Mass spectra of compound **11f**

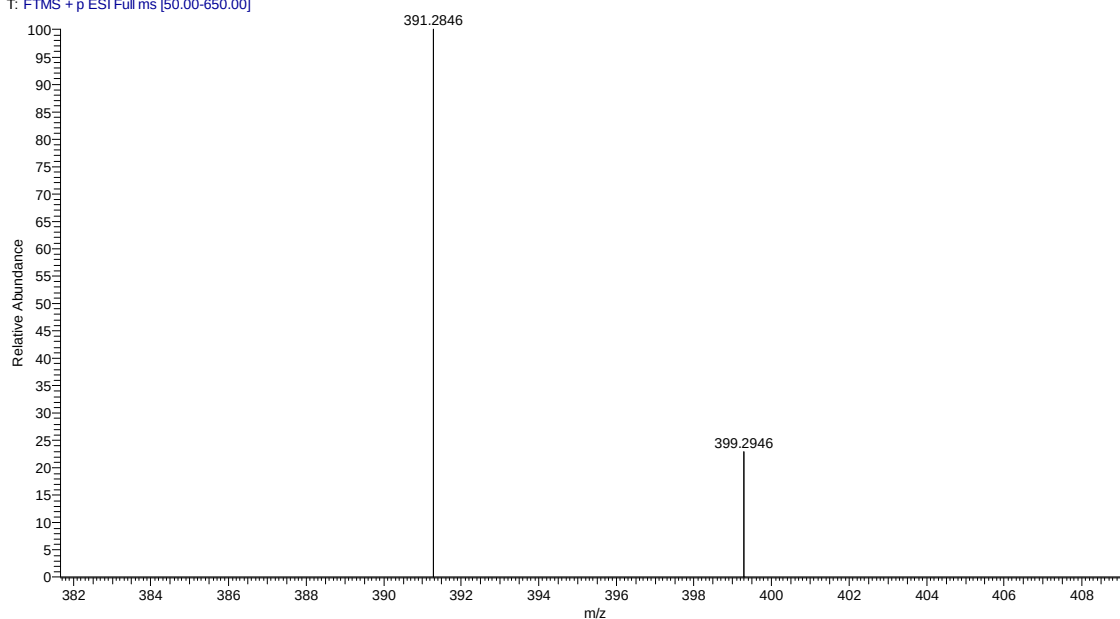


Mass spectra of compound **11g**



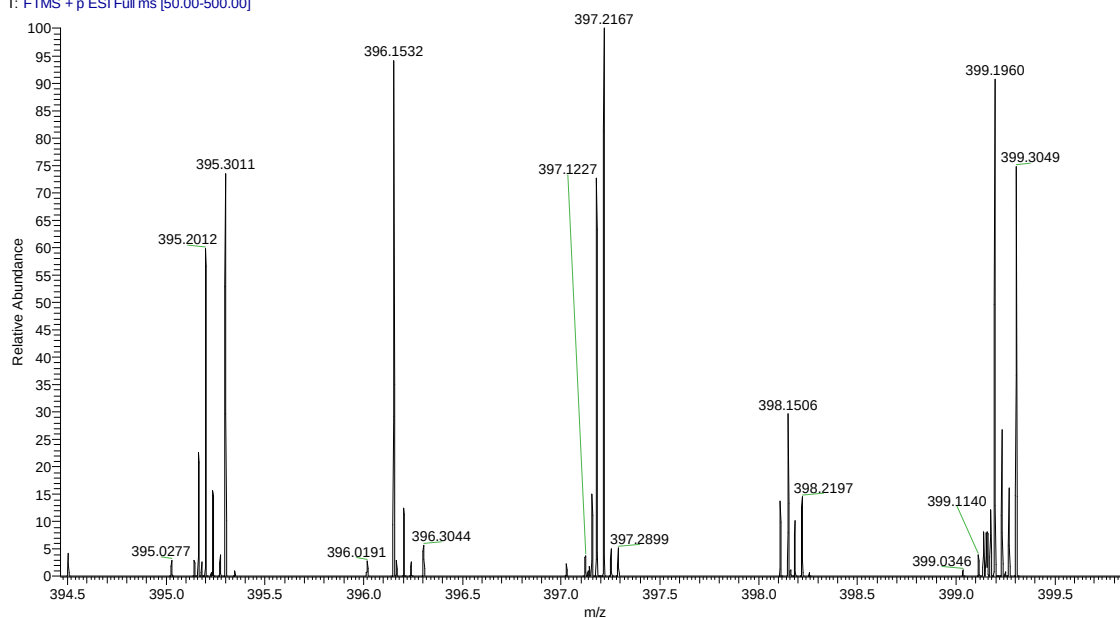
Mass spectra of compound **11h**

Muestra CS13 #56 RT: 0.71 AV: 1 NL: 1.02E3
T: FTMS + p ESI Full ms [50.00-650.00]



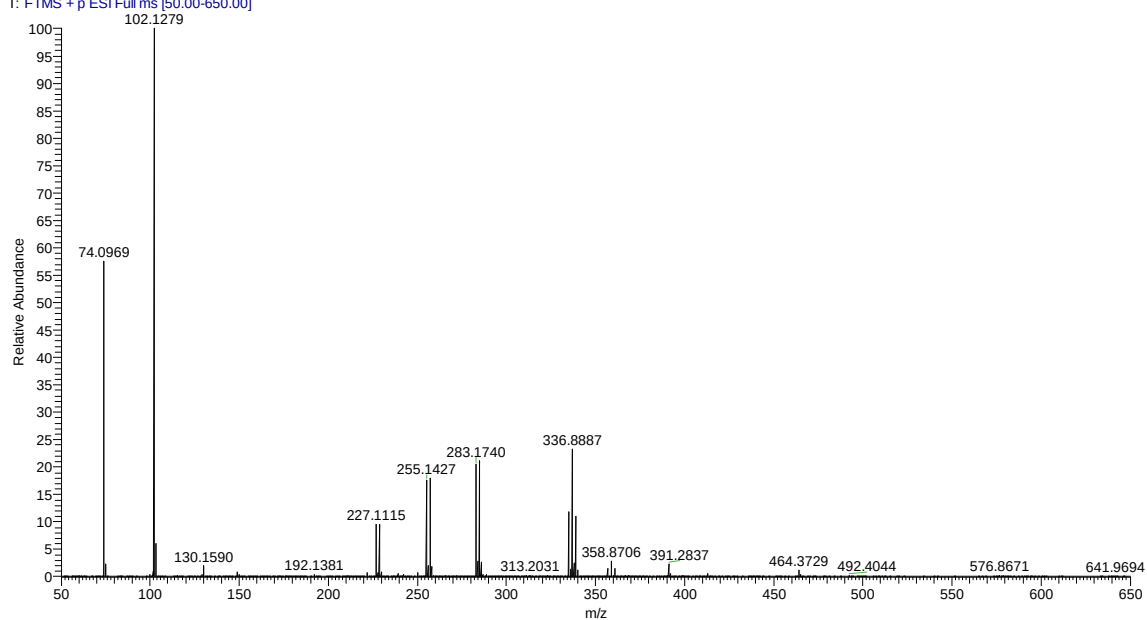
Mass spectra of compound **11i**

CS12 #14 RT: 0.14 AV: 1 NL: 7.45E5
T: FTMS + p ESI Full ms [50.00-500.00]

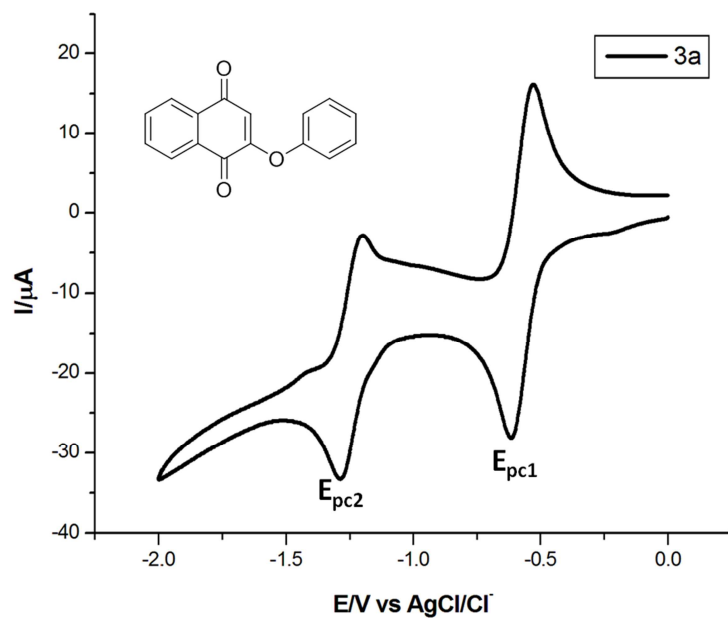


Mass spectra of compound **10b**

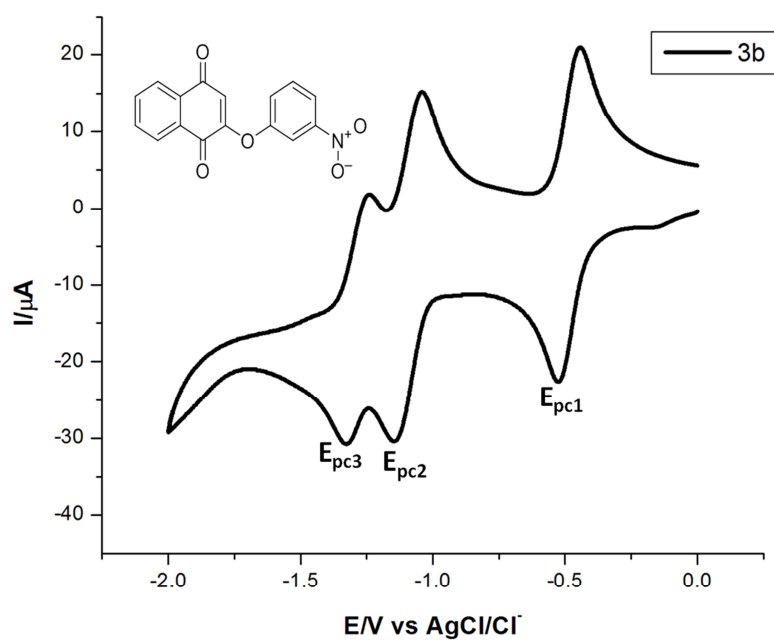
Muestra KV1 #11 RT: 0.13 AV: 1 NL: 2.01E9
T: FTMS + p ESI Full ms [50.00-650.00]



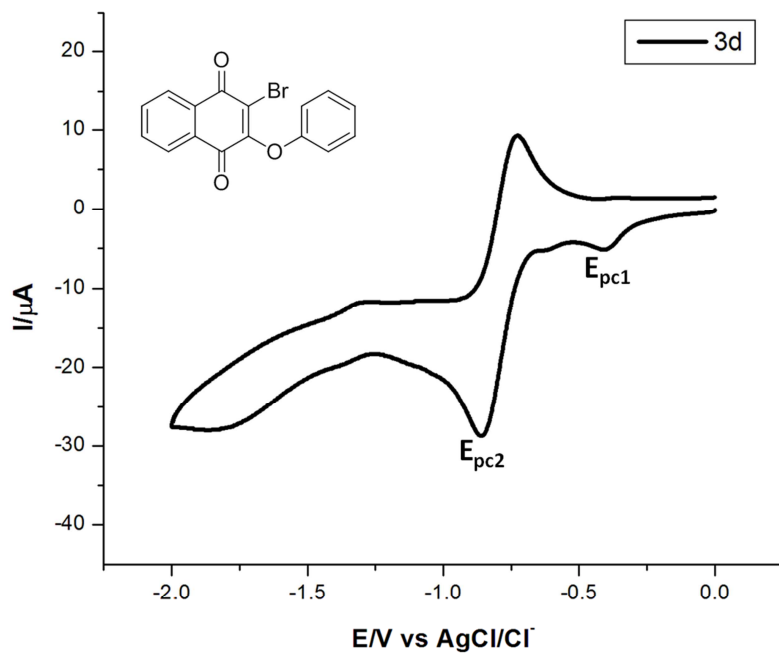
Voltammogram of Compound **3a**



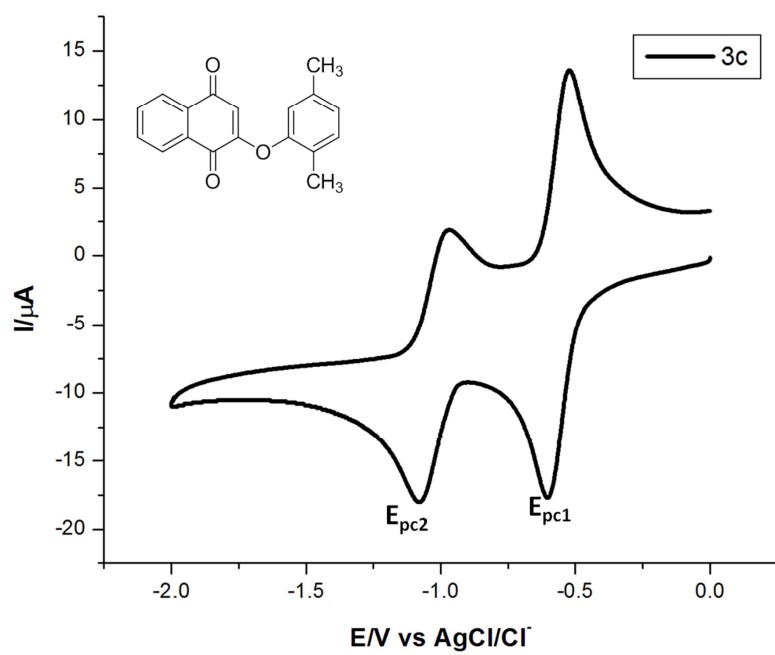
Voltammogram of Compound **3b**



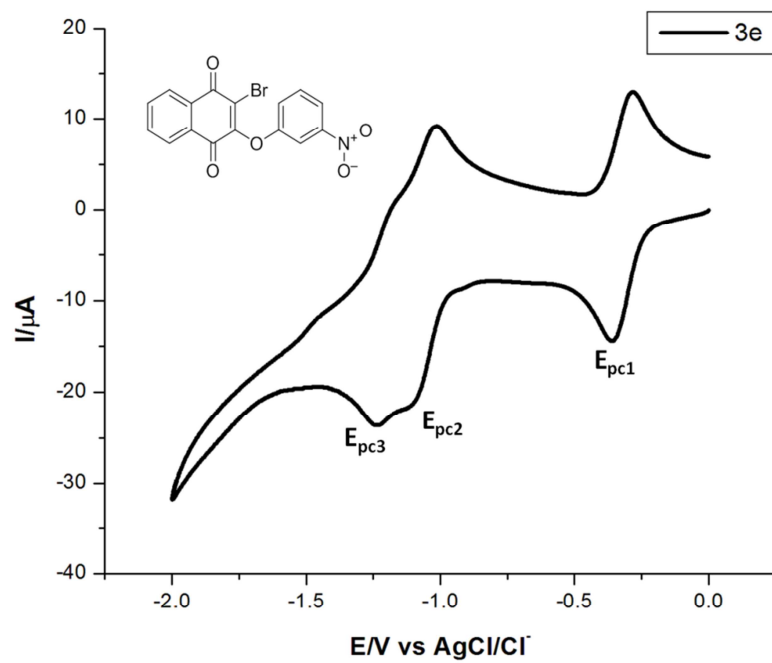
Voltammogram of Compound **3c**



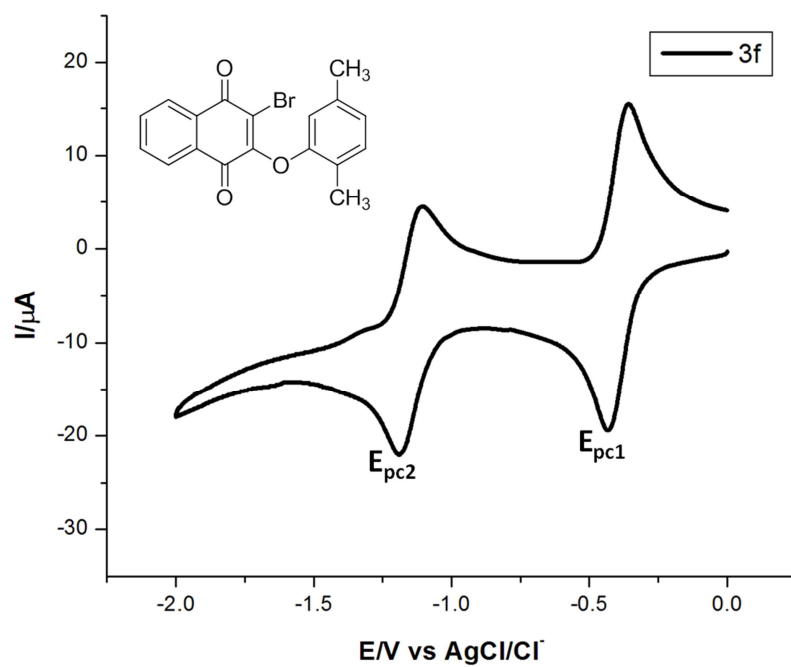
Voltammogram of Compound **3d**



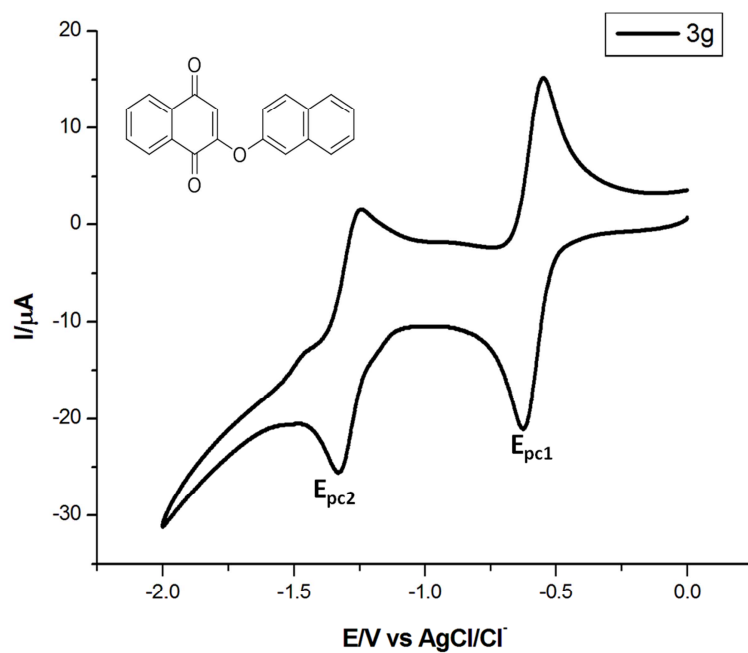
Voltammogram of Compound **3e**



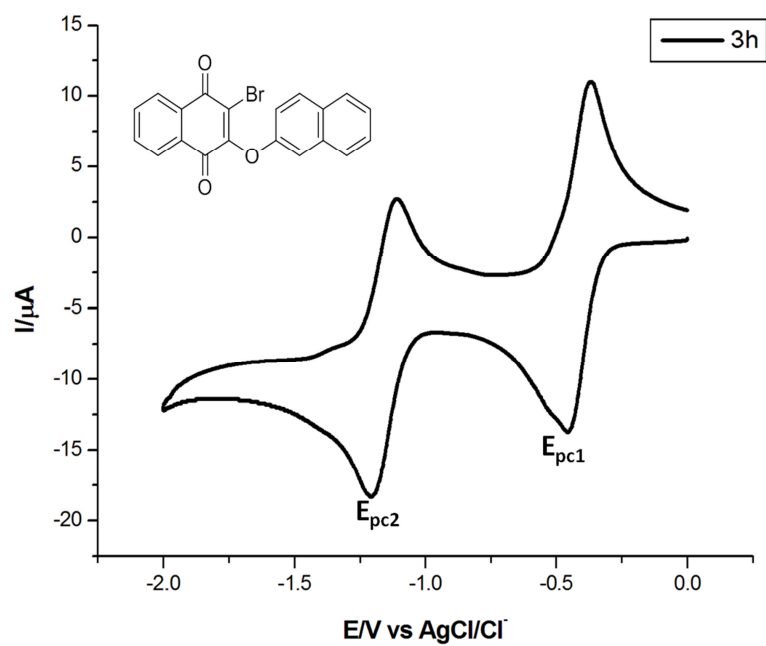
Voltammogram of Compound **3f**



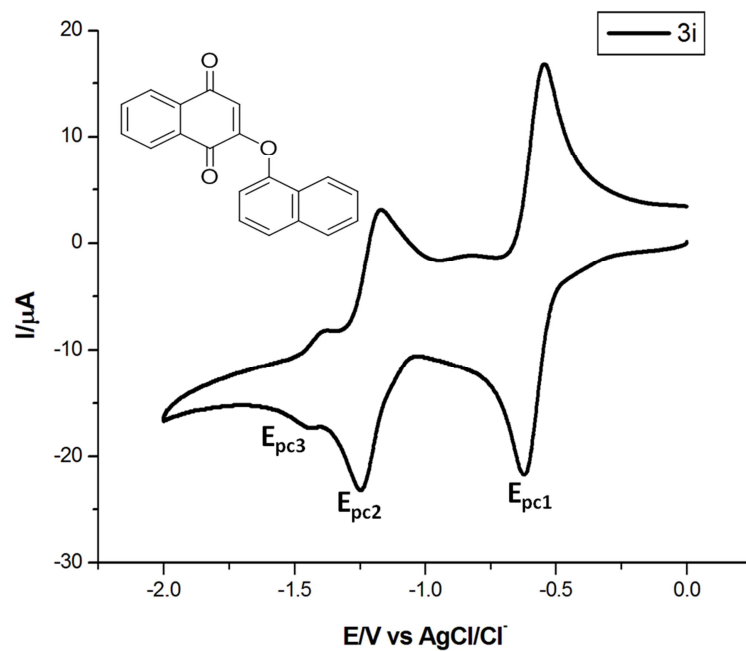
Voltammogram of Compound **3g**



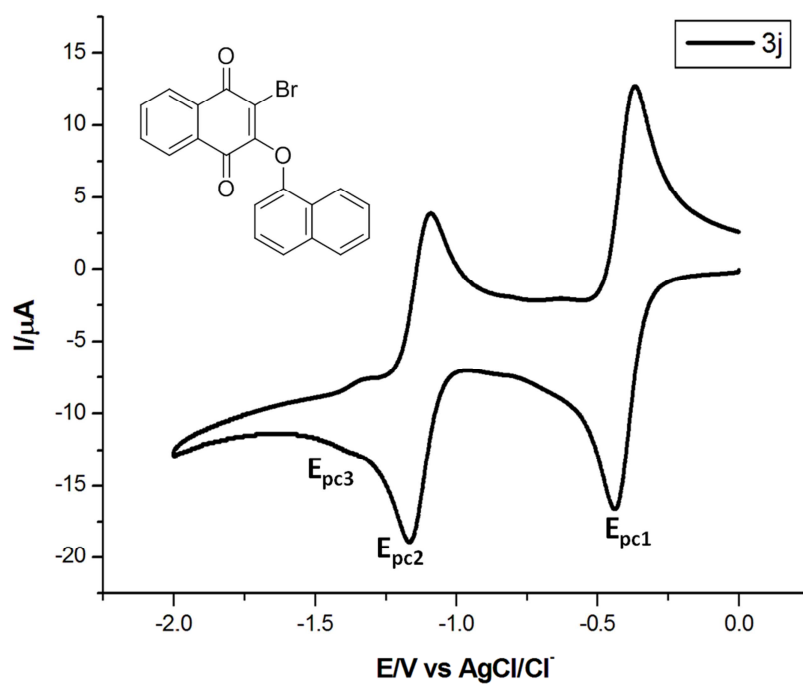
Voltammogram of Compound **3h**



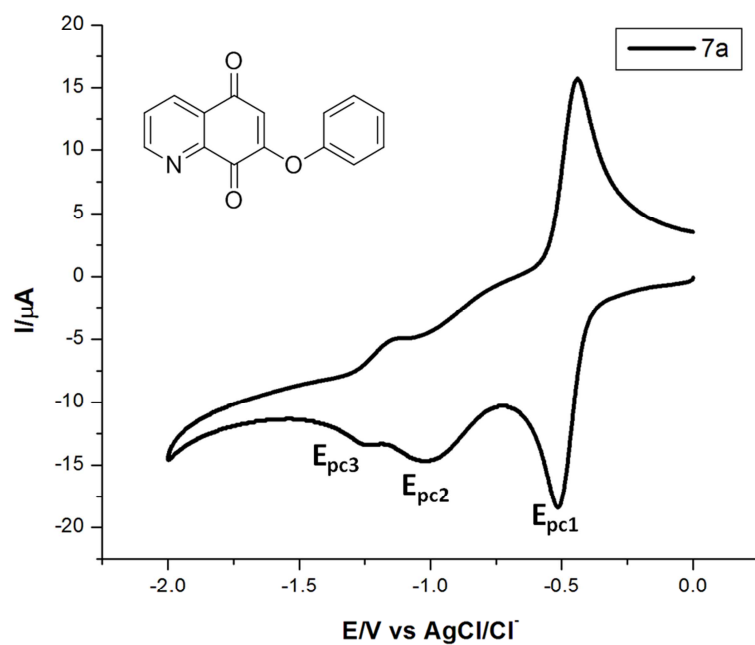
Voltammogram of Compound **3i**



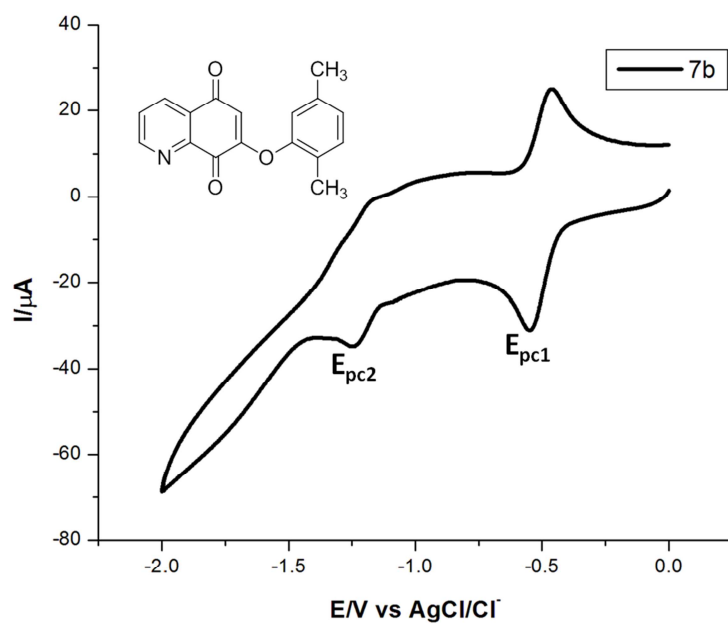
Voltammogram of Compound **3j**



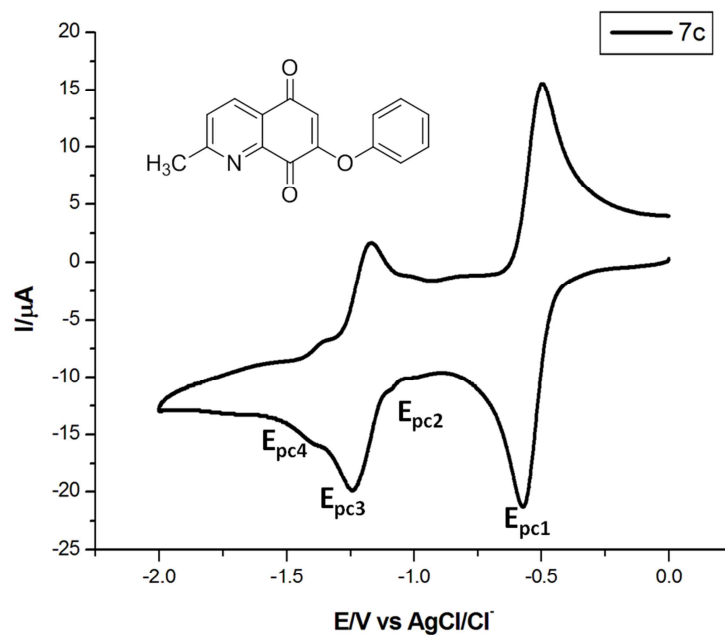
Voltammogram of Compound **7a**



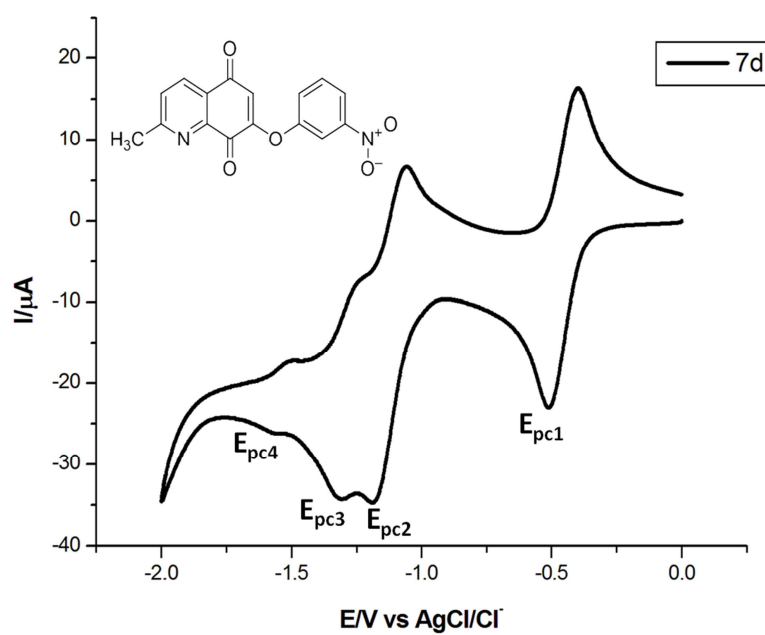
Voltammogram of Compound **7b**



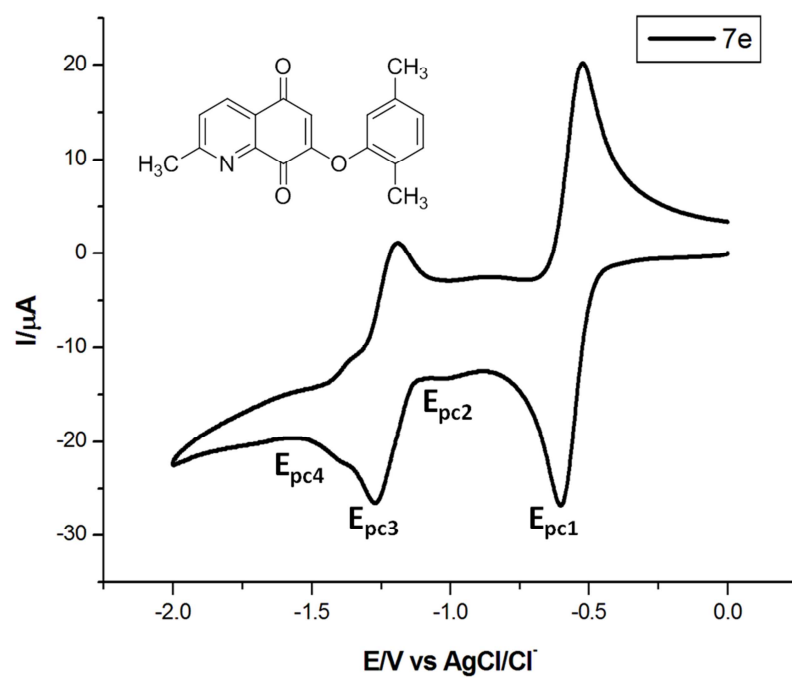
Voltammogram of Compound **7c**



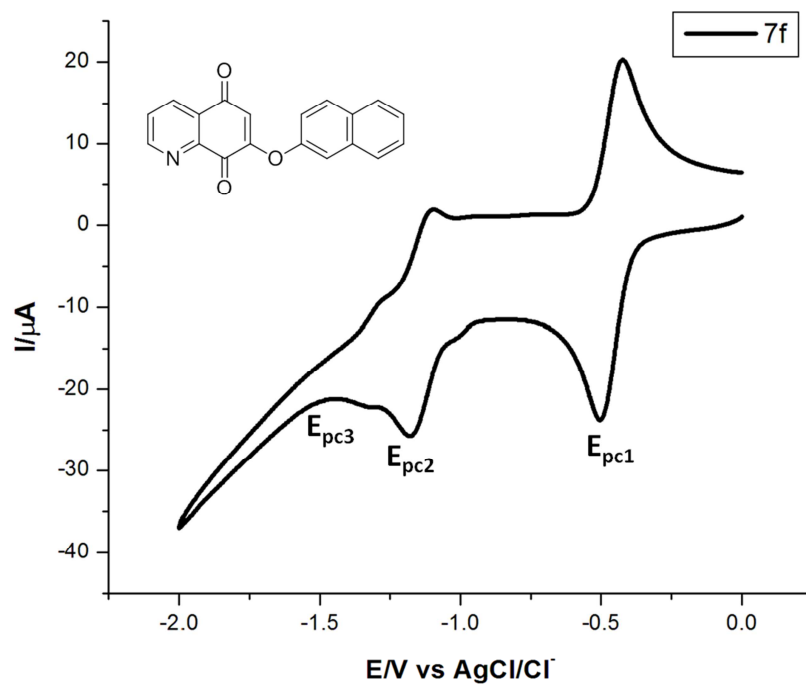
Voltammogram of Compound **7d**



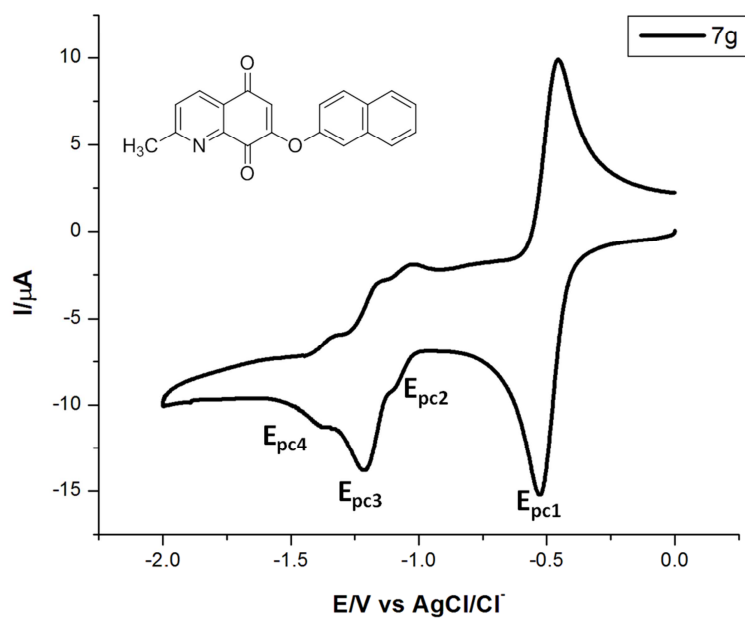
Voltammogram of Compound **7e**



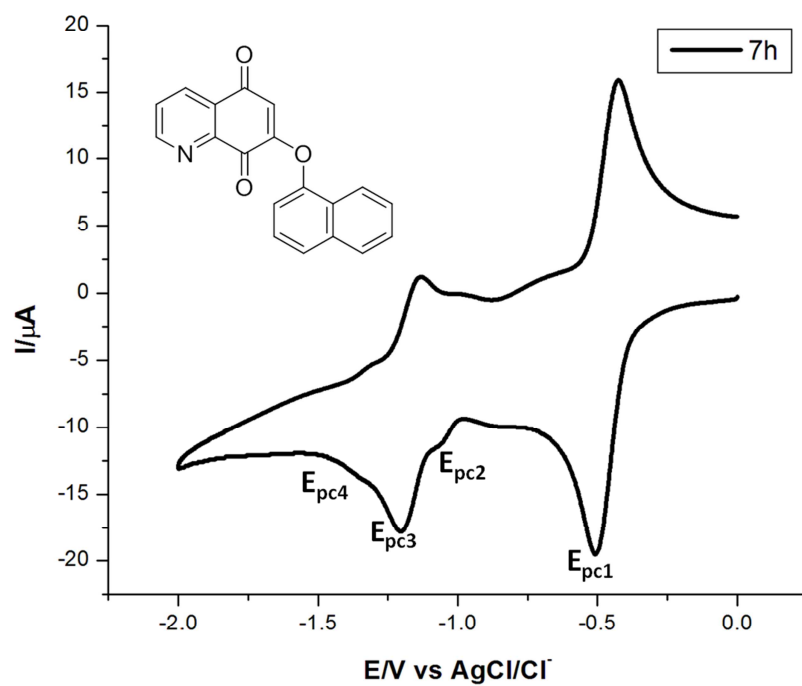
Voltammogram of Compound **7f**



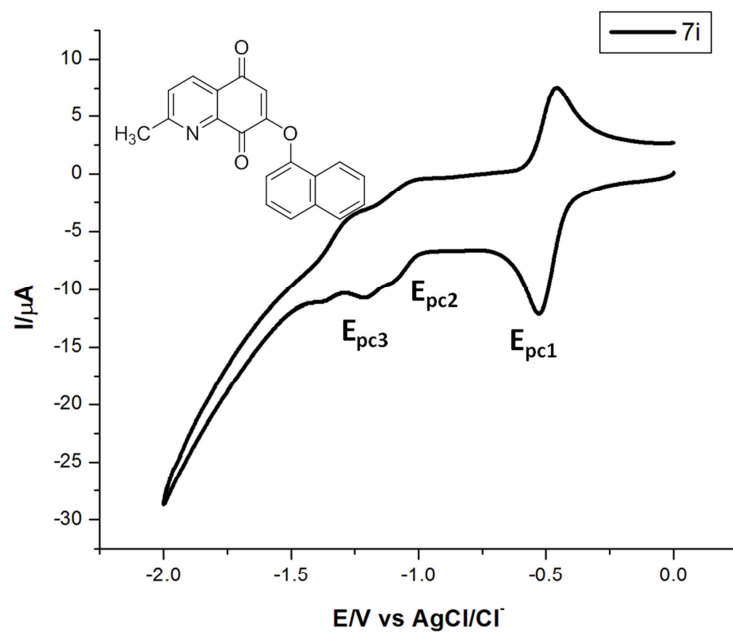
Voltammogram of Compound **7g**



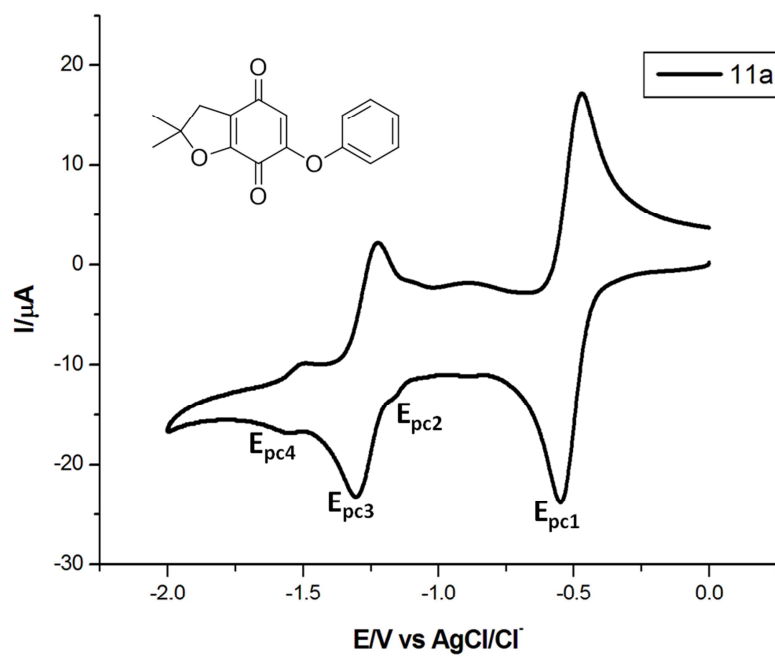
Voltammogram of Compound **7h**



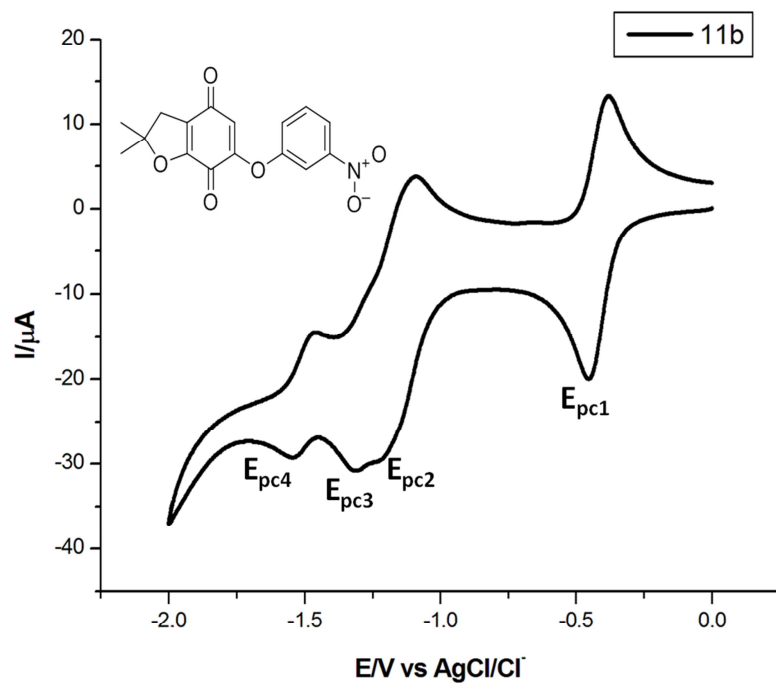
Voltammogram of Compound **7i**



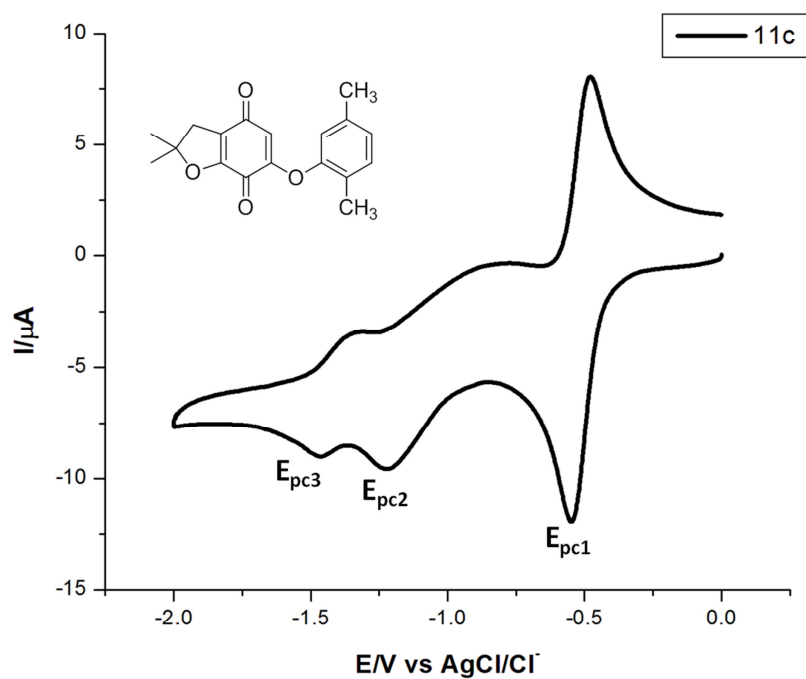
Voltammogram of Compound **11a**



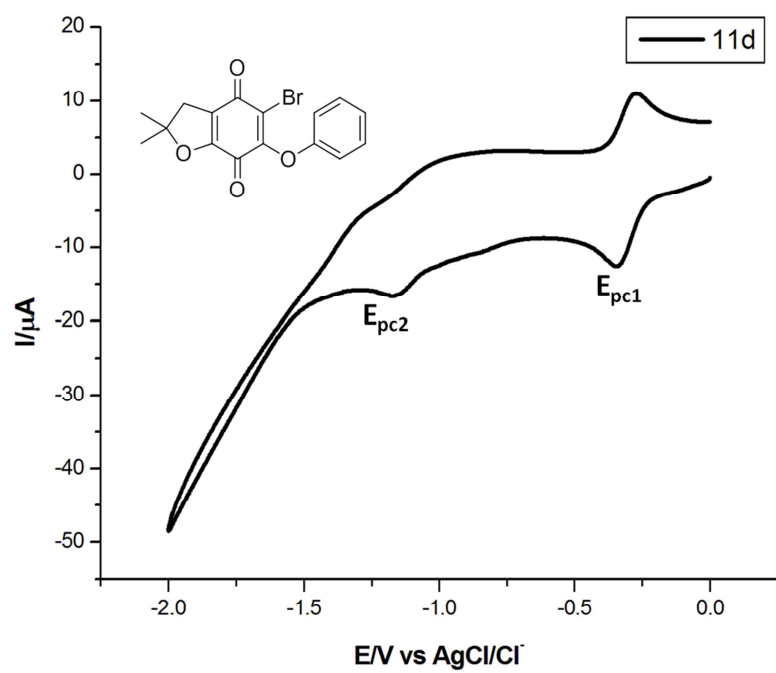
Voltammogram of Compound **11b**



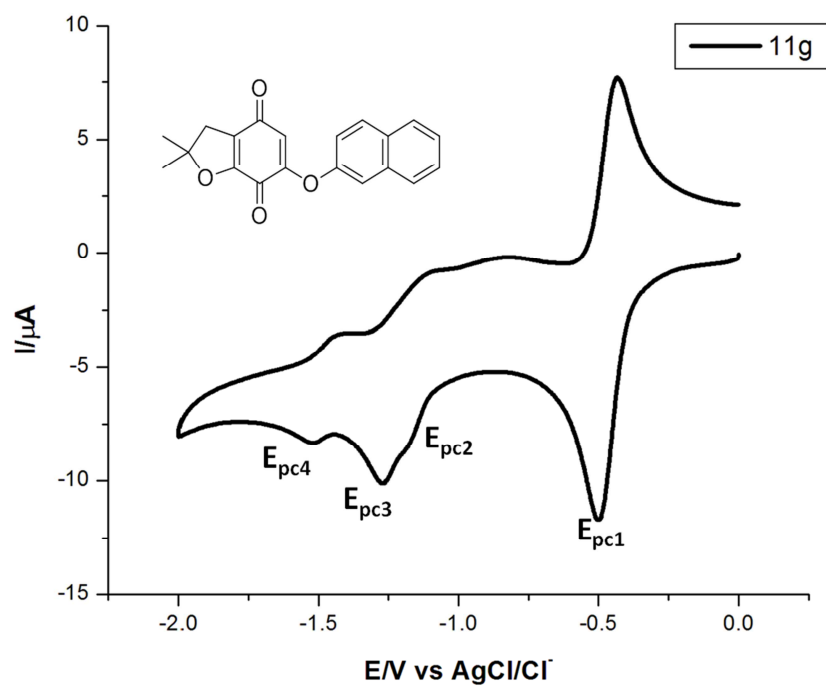
Voltammogram of Compound **11c**



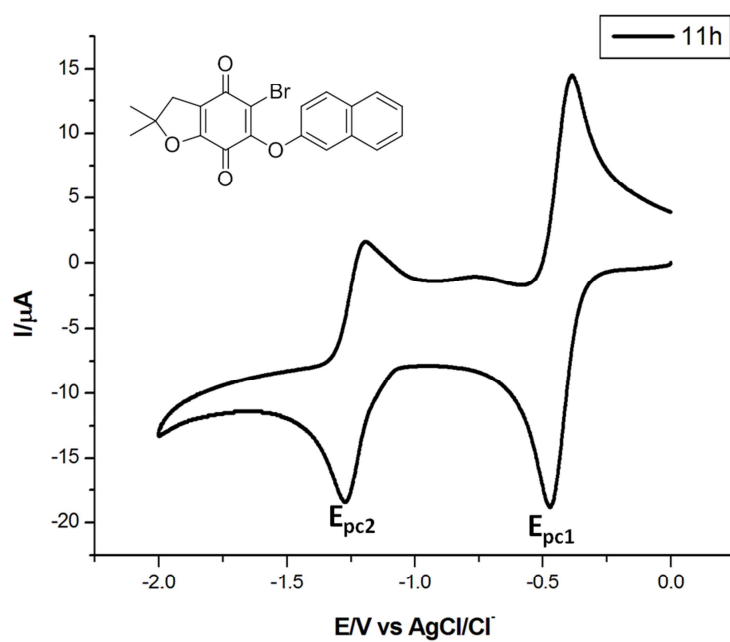
Voltammogram of Compound **11d**



Voltammogram of Compound **11g**



Voltammogram of Compound **11h**



Voltammogram of Compound **11i**

