

Supplementary data

Synthesis of amino acid-naphthoquinones and *in vitro* studies on cervical and breast cell lines

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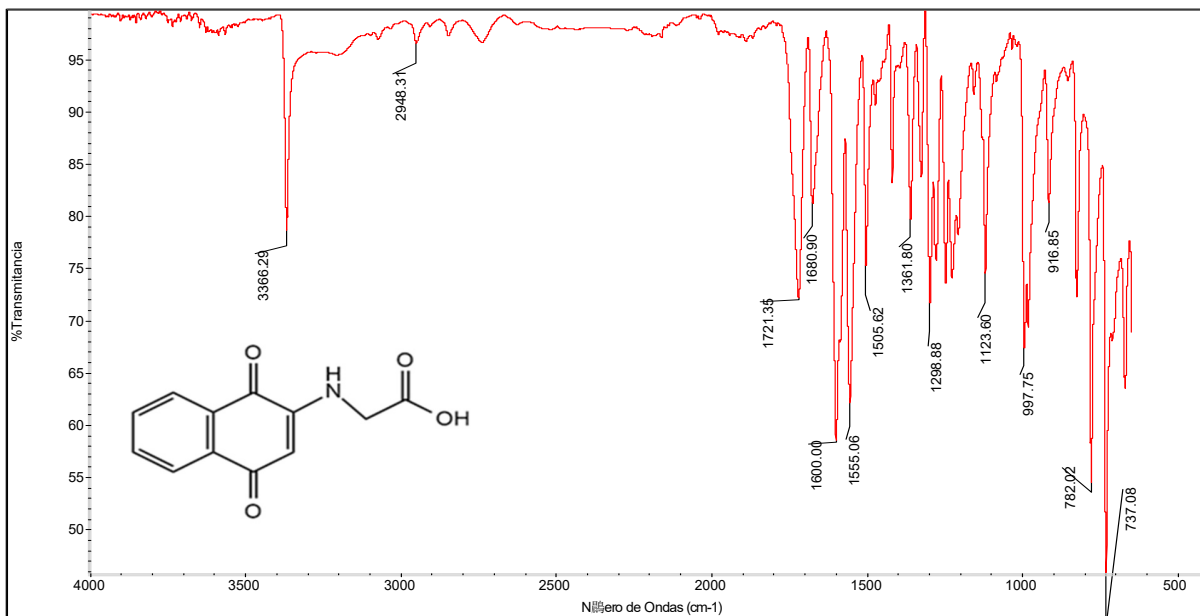
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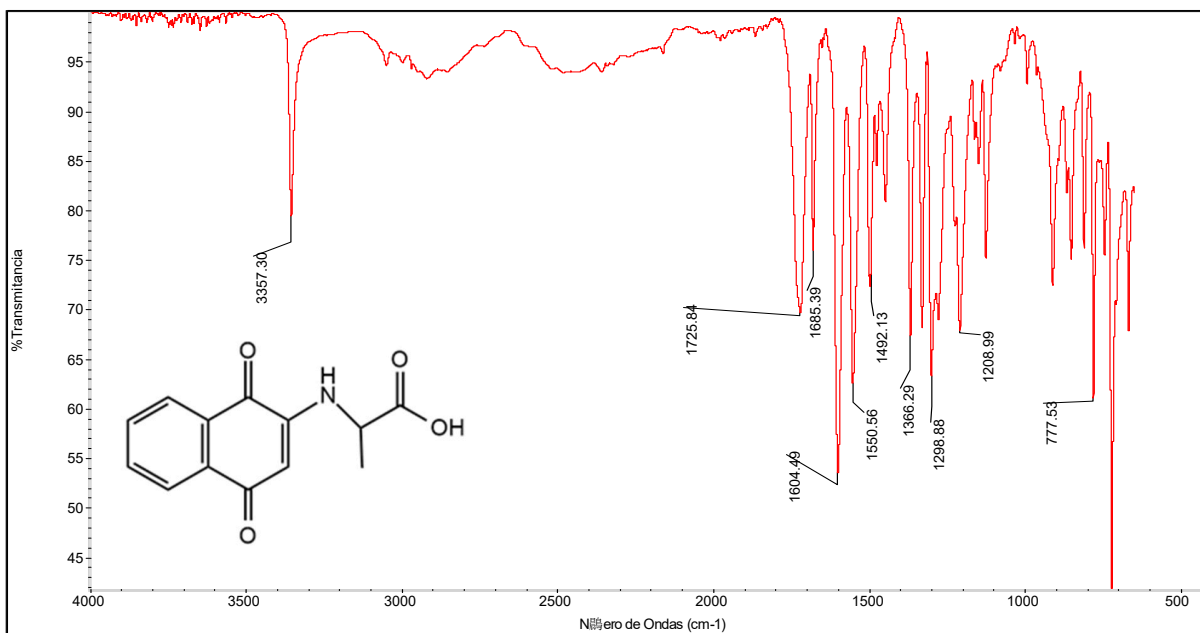
1. Infrared characterization

Amino acids-1,4-naphthoquinone derivatives:

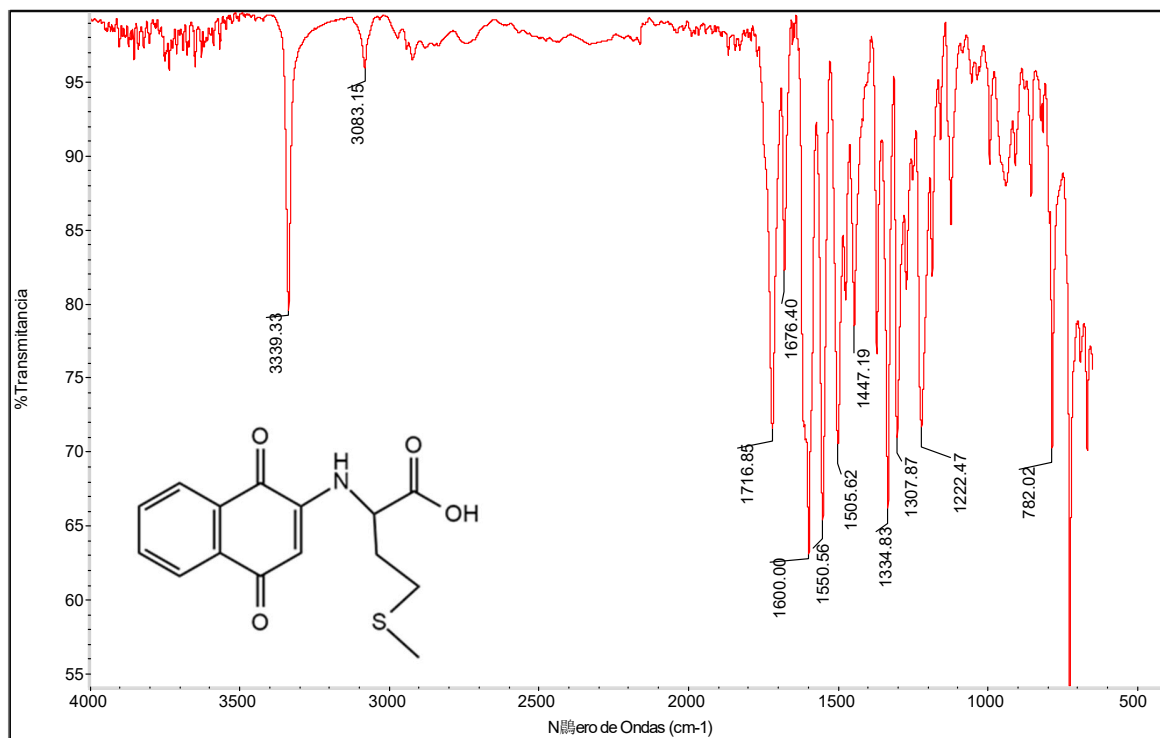
(3a)



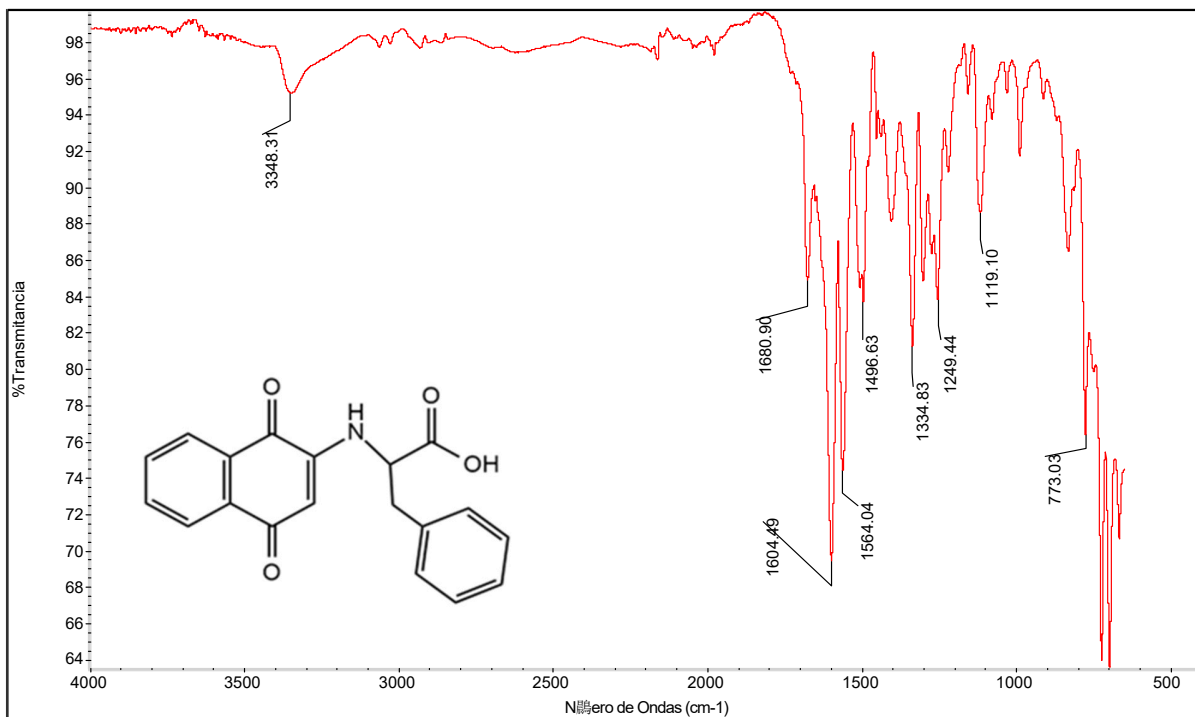
(3b)



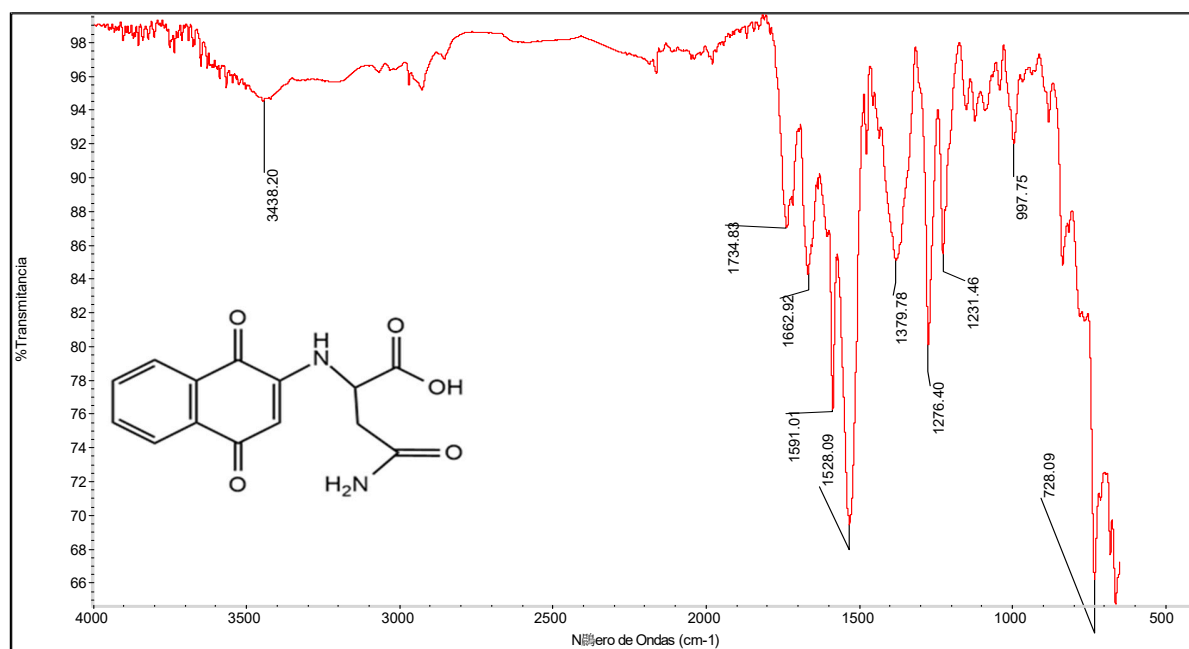
(3c)



(3d)

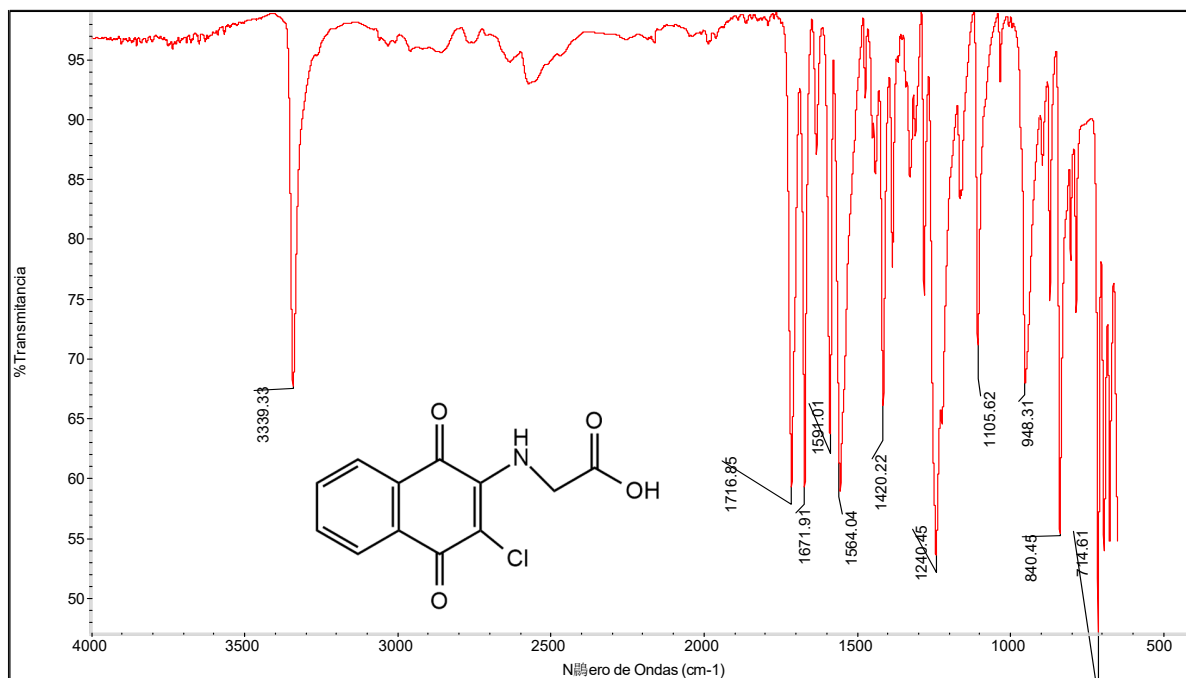


(3e)

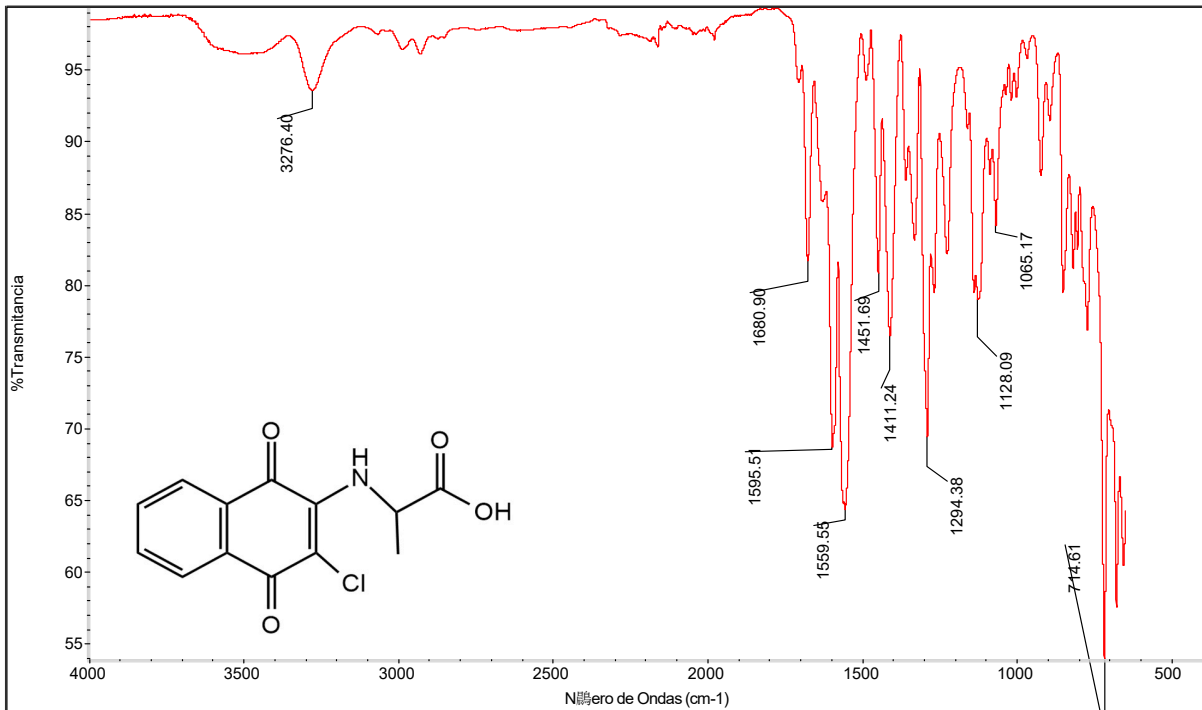


Amino acids-2,3-dichloronaphthoquinone derivatives:

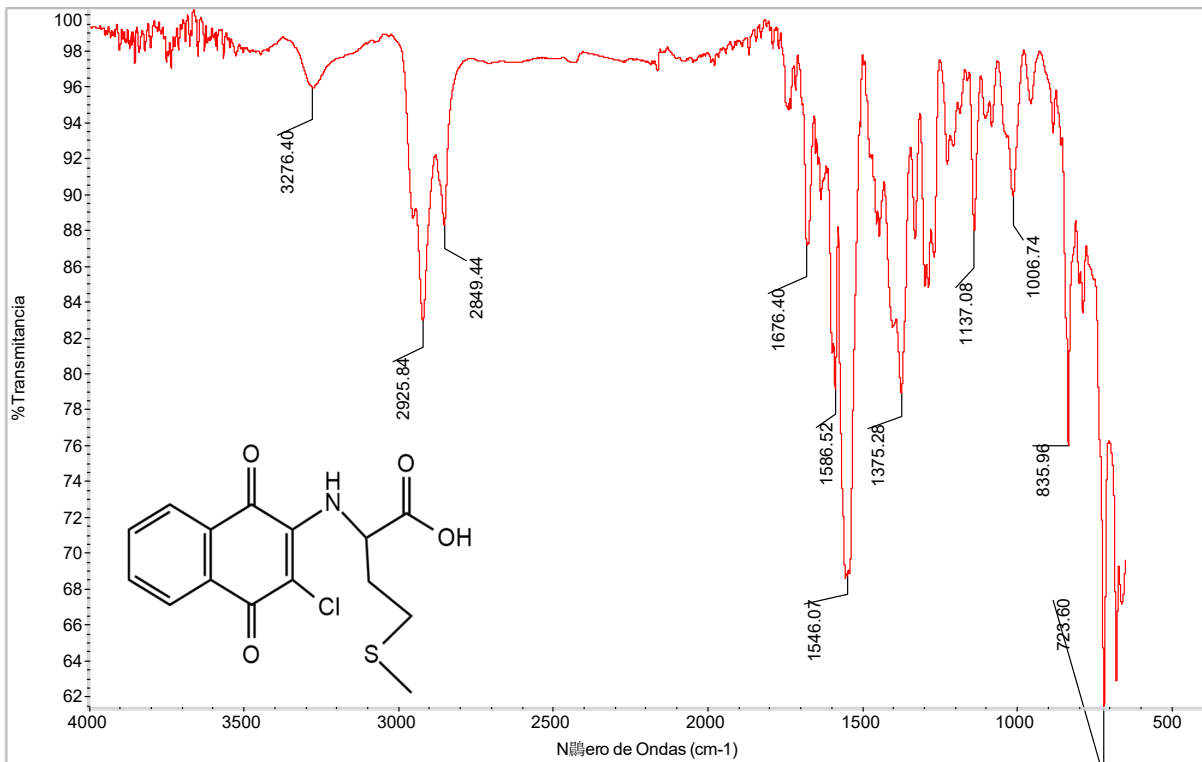
(4a)



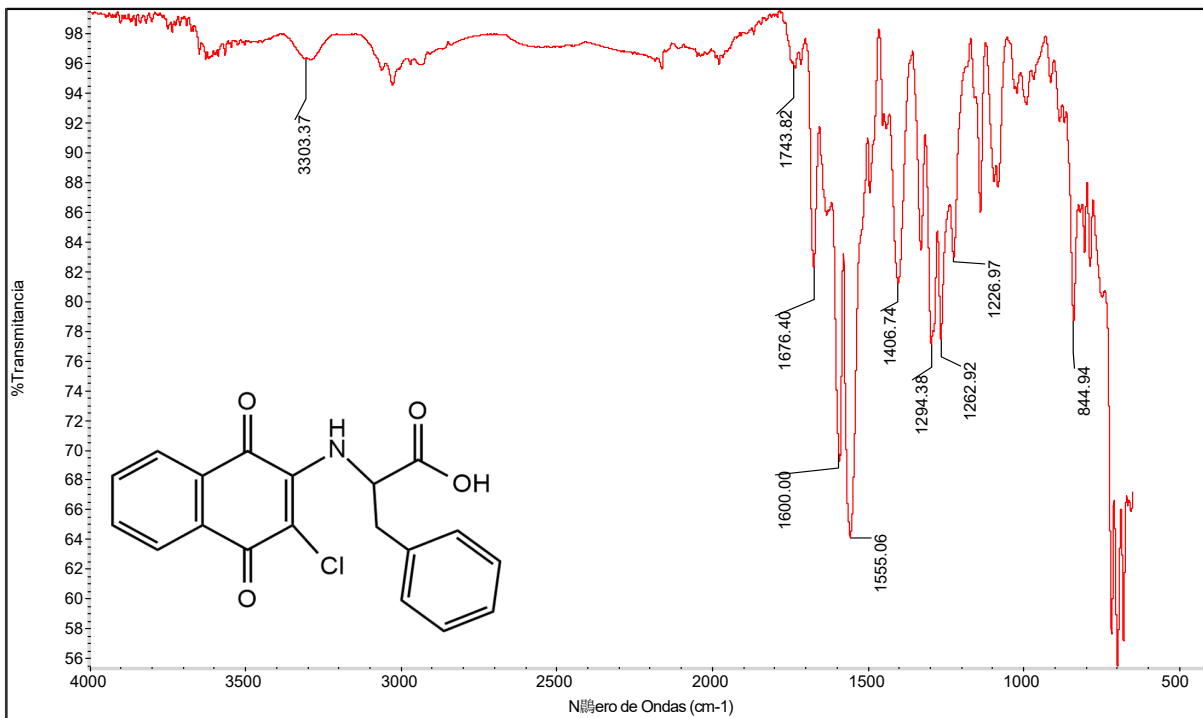
(4b)



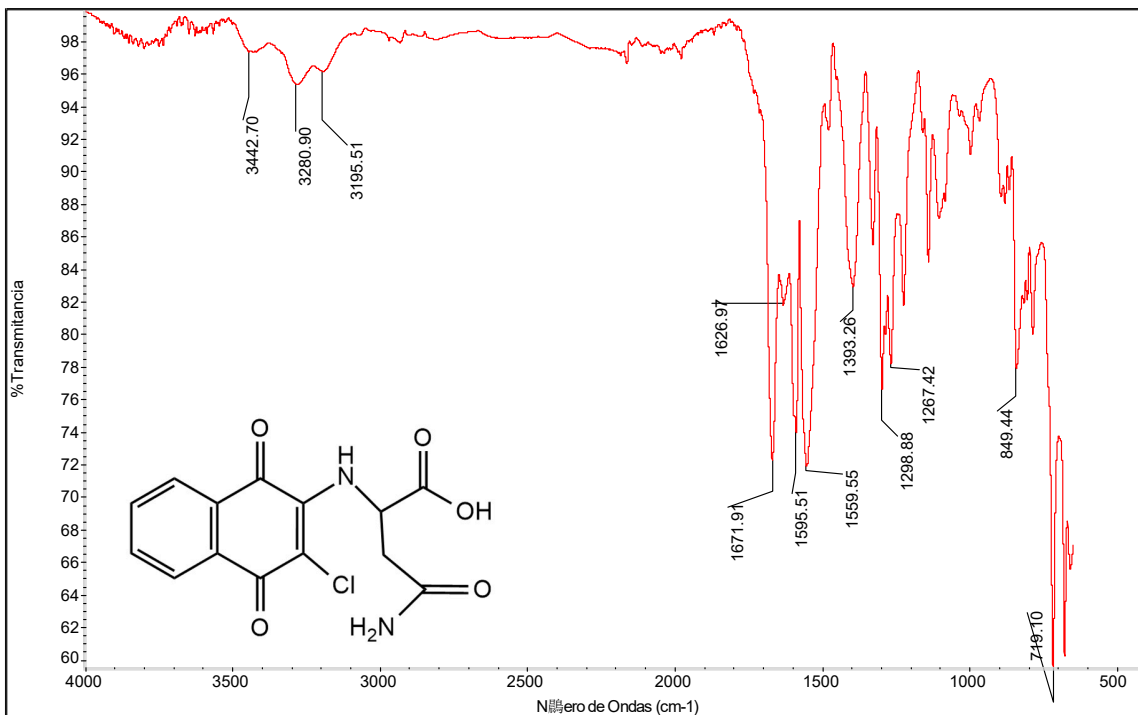
(4c)



(4d)



(4e)



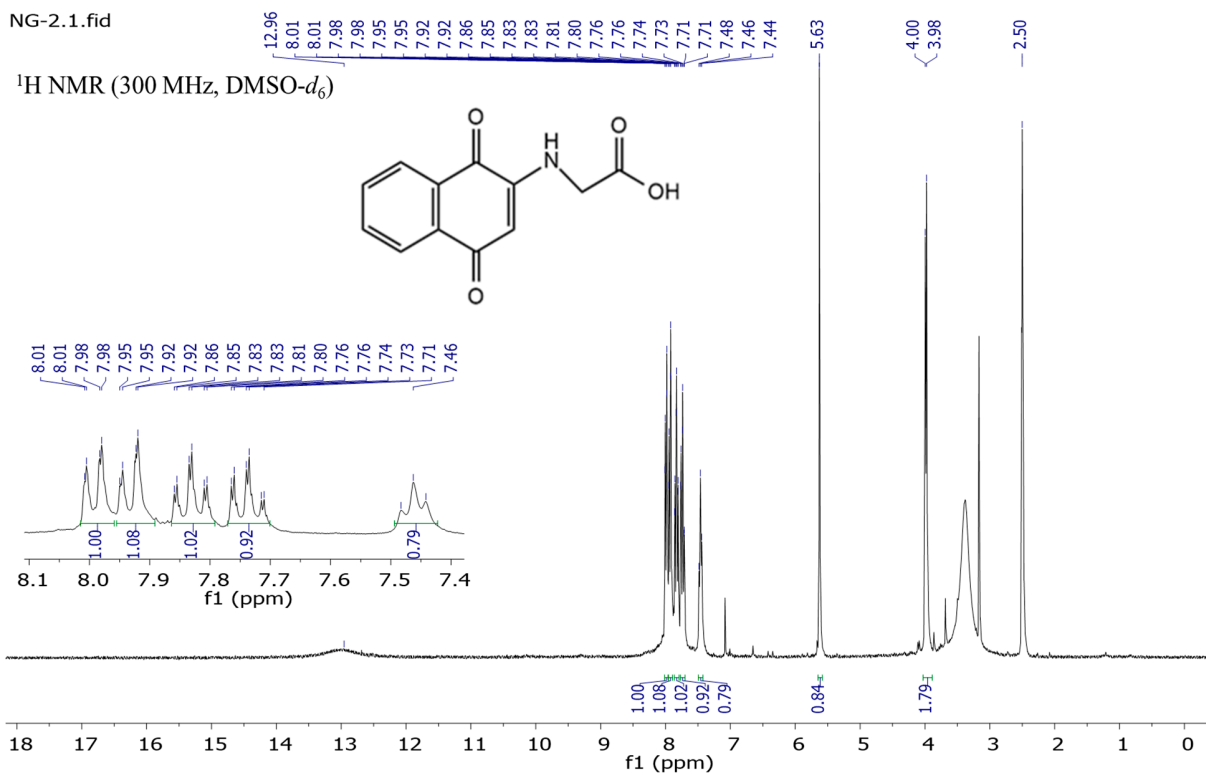
2. NMR characterization.

Amino acids-1,4-naphthoquinone derivatives:

(3a)

NG-2.1.fid

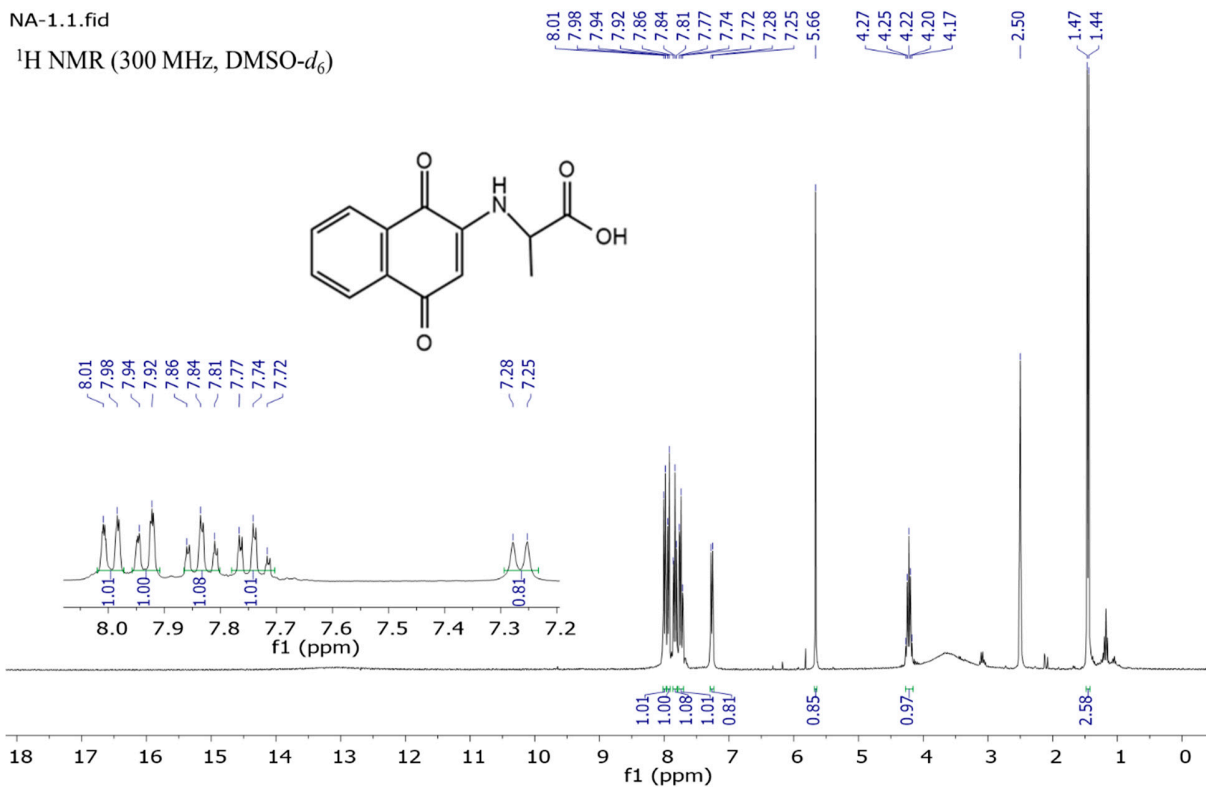
^1H NMR (300 MHz, $\text{DMSO}-d_6$)



(3b)

NA-1.1.fid

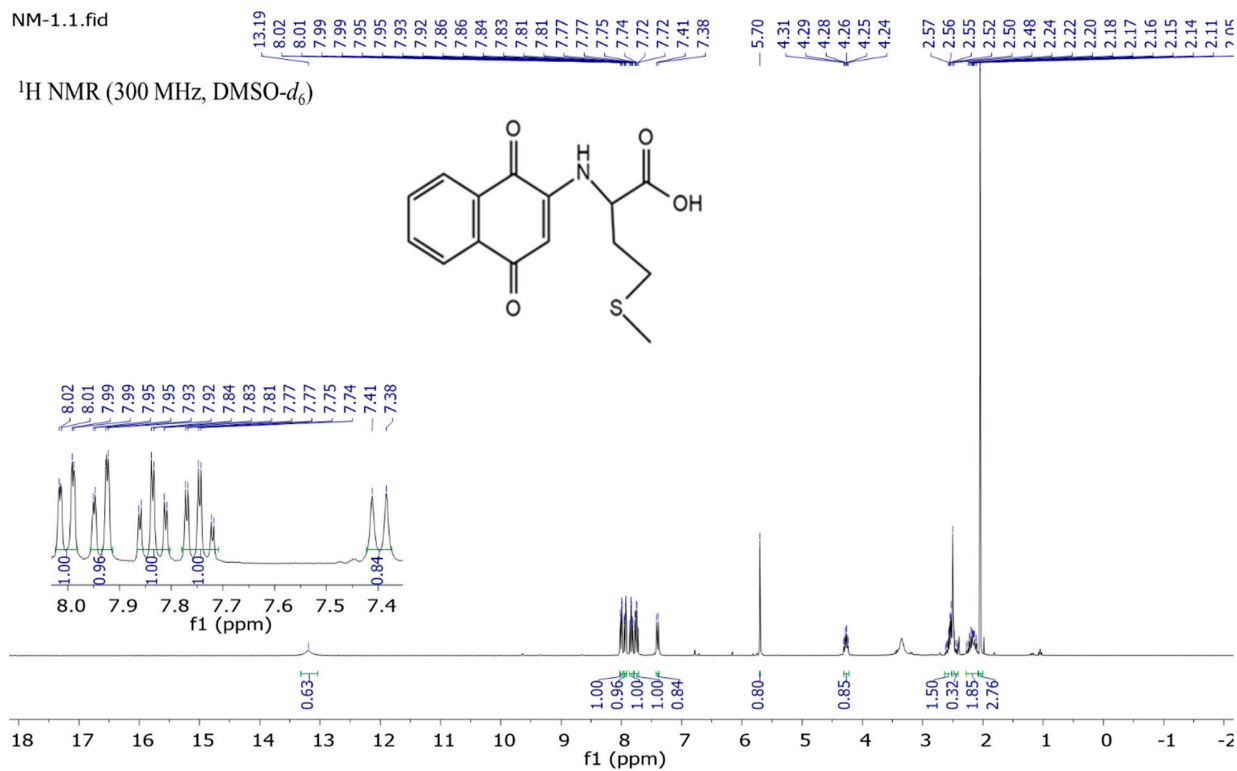
^1H NMR (300 MHz, $\text{DMSO}-d_6$)



(3c)

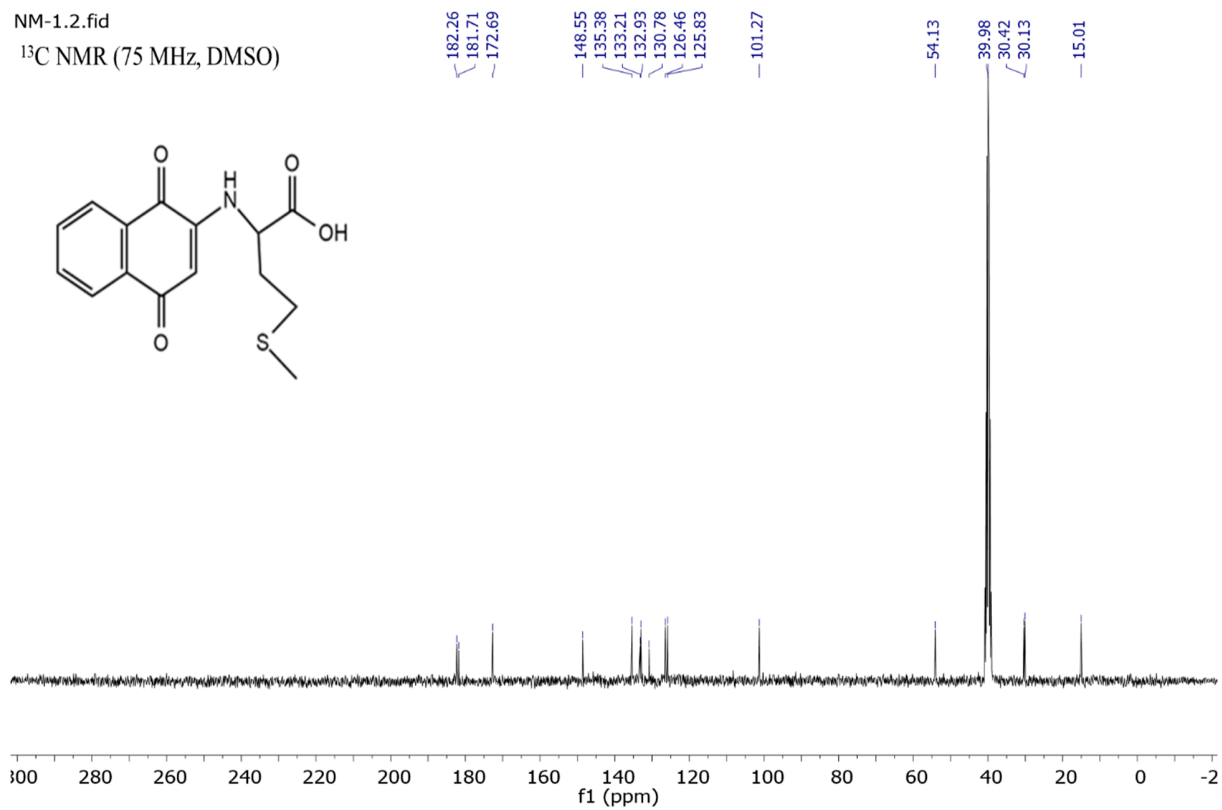
NM-1.1.fid

¹H NMR (300 MHz, DMSO-d₆)



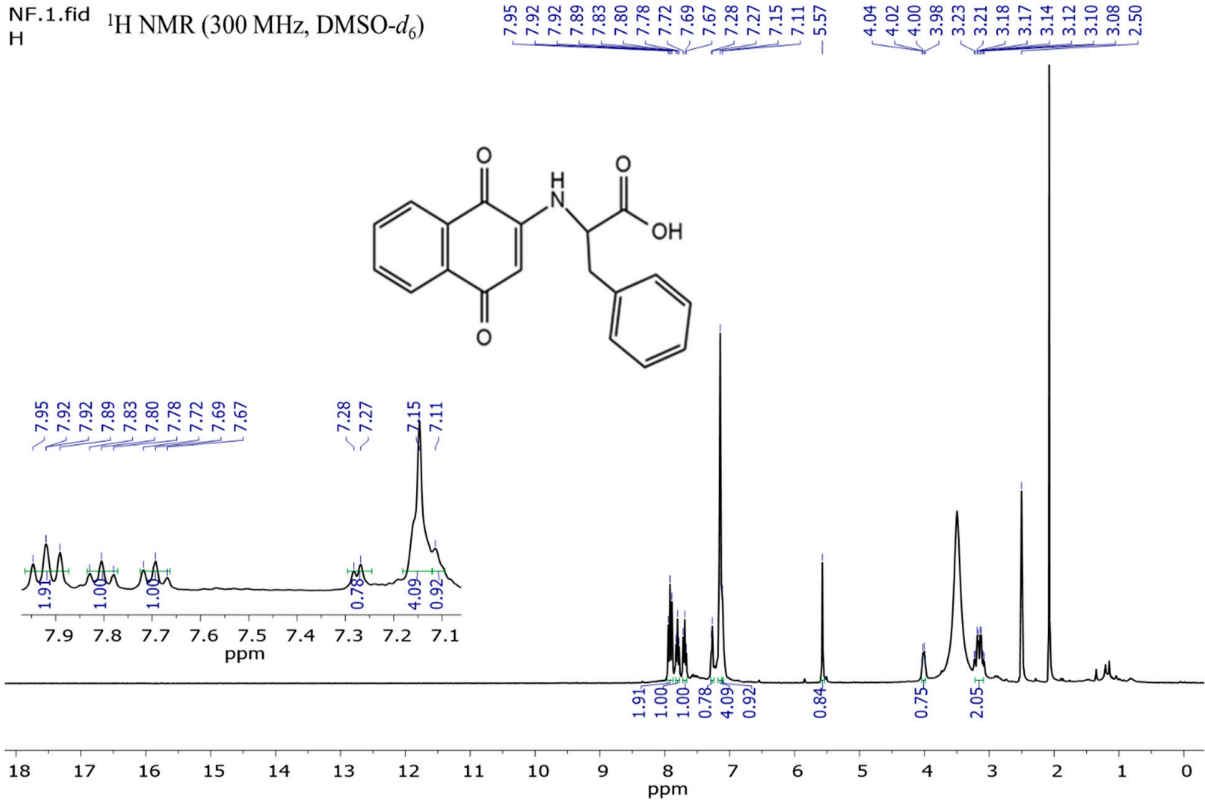
NM-1.2.fid

¹³C NMR (75 MHz, DMSO)



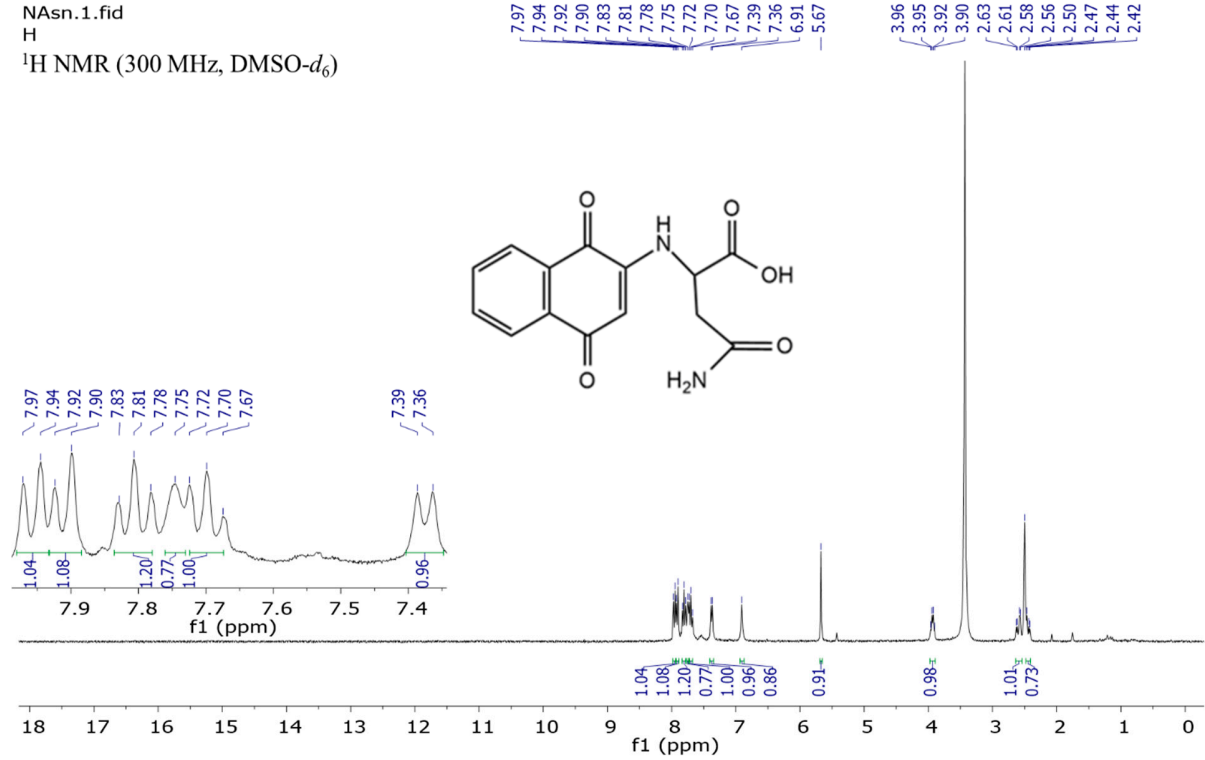
(3d)

NF.1.fid ¹H NMR (300 MHz, DMSO-d₆)
H



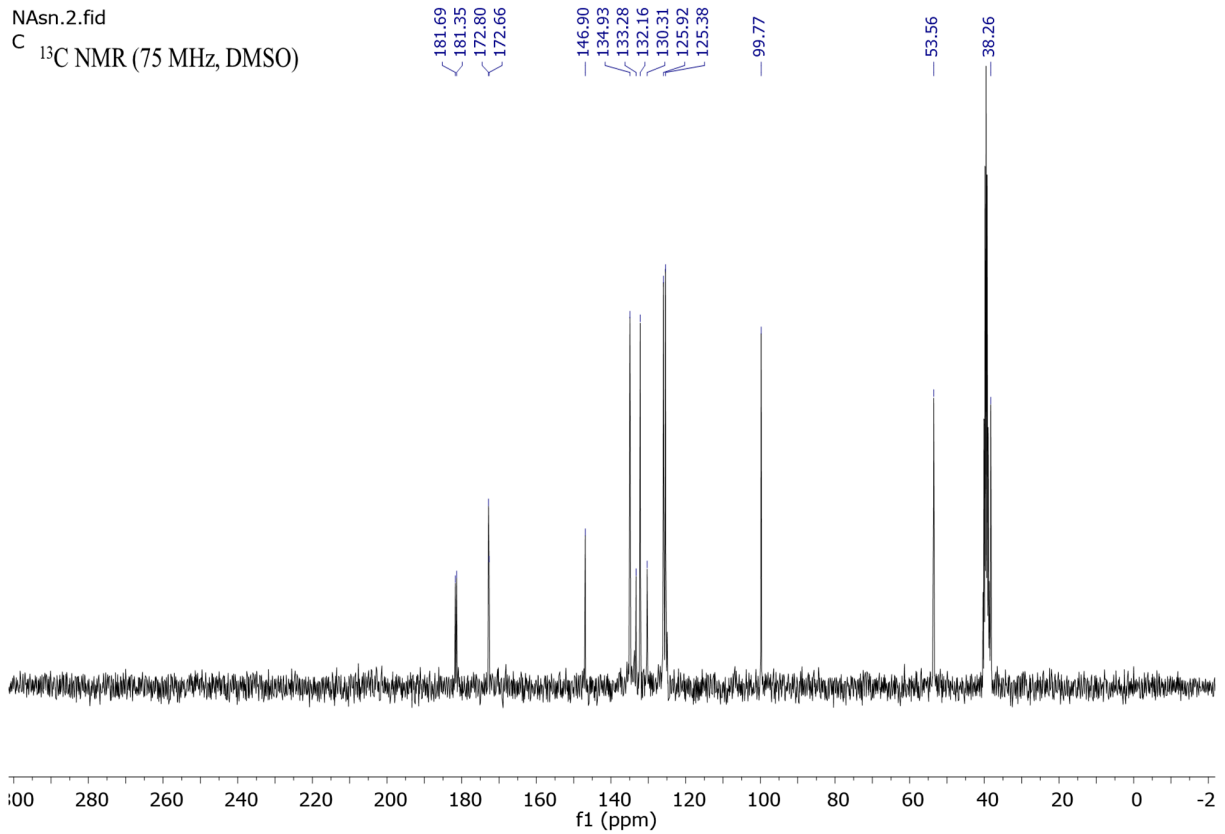
(3e)

NA.sn.1.fid
H
¹H NMR (300 MHz, DMSO-d₆)



NAsn.2.fid

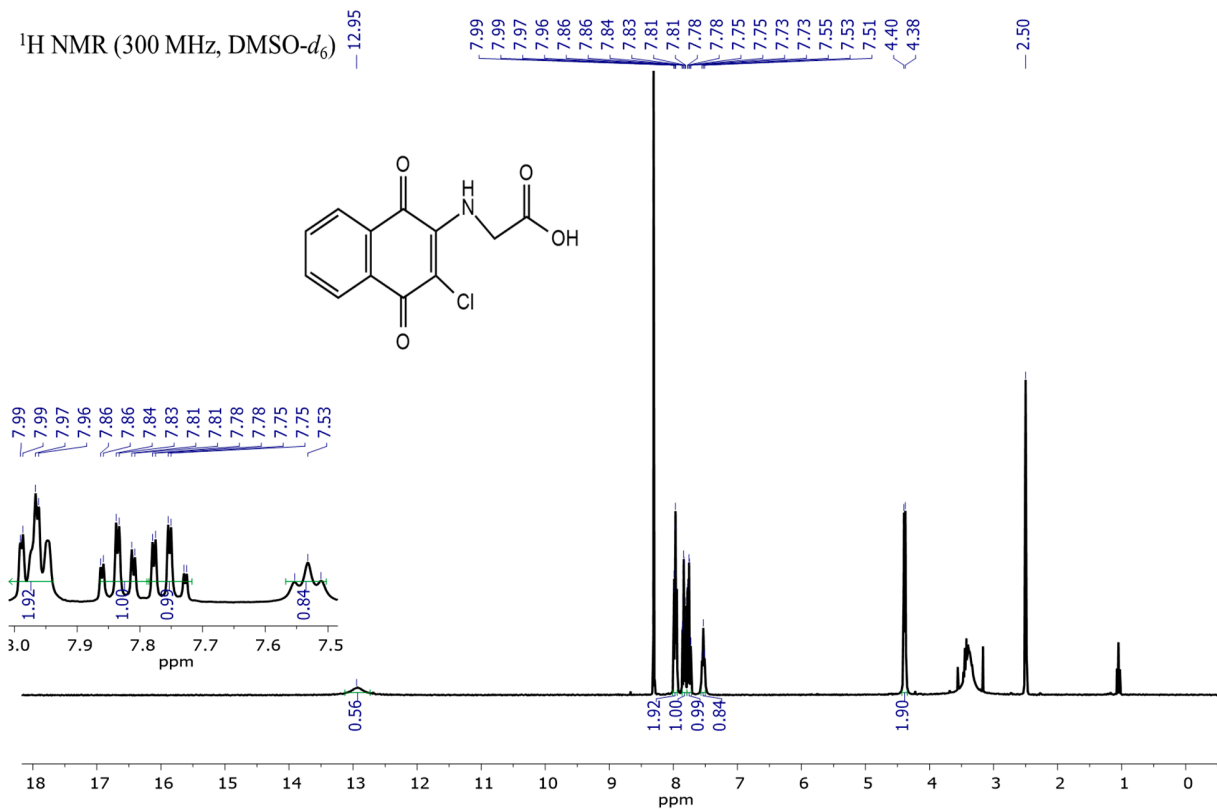
¹³C NMR (75 MHz, DMSO)



Amino acids-2,3-dichloronaphthoquinone derivatives:

(4a)

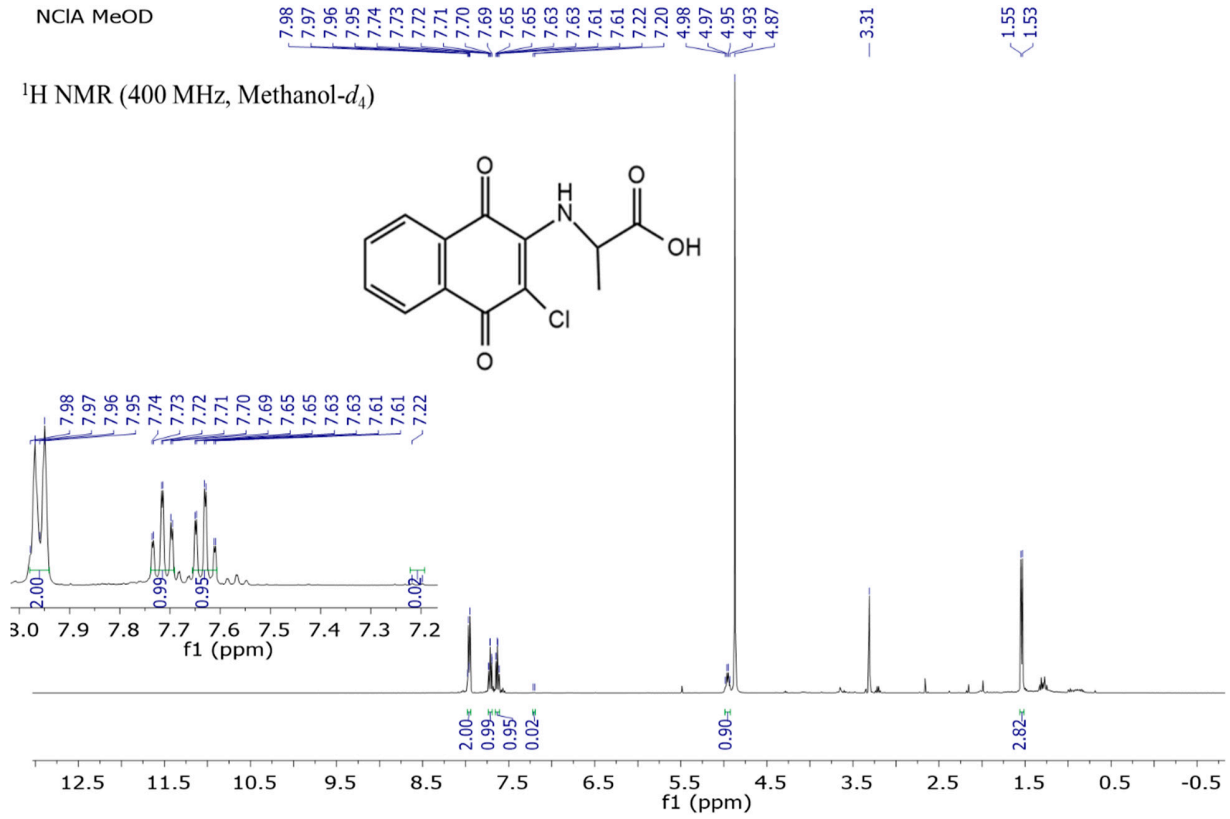
¹H NMR (300 MHz, DMSO-d₆)



(4b)

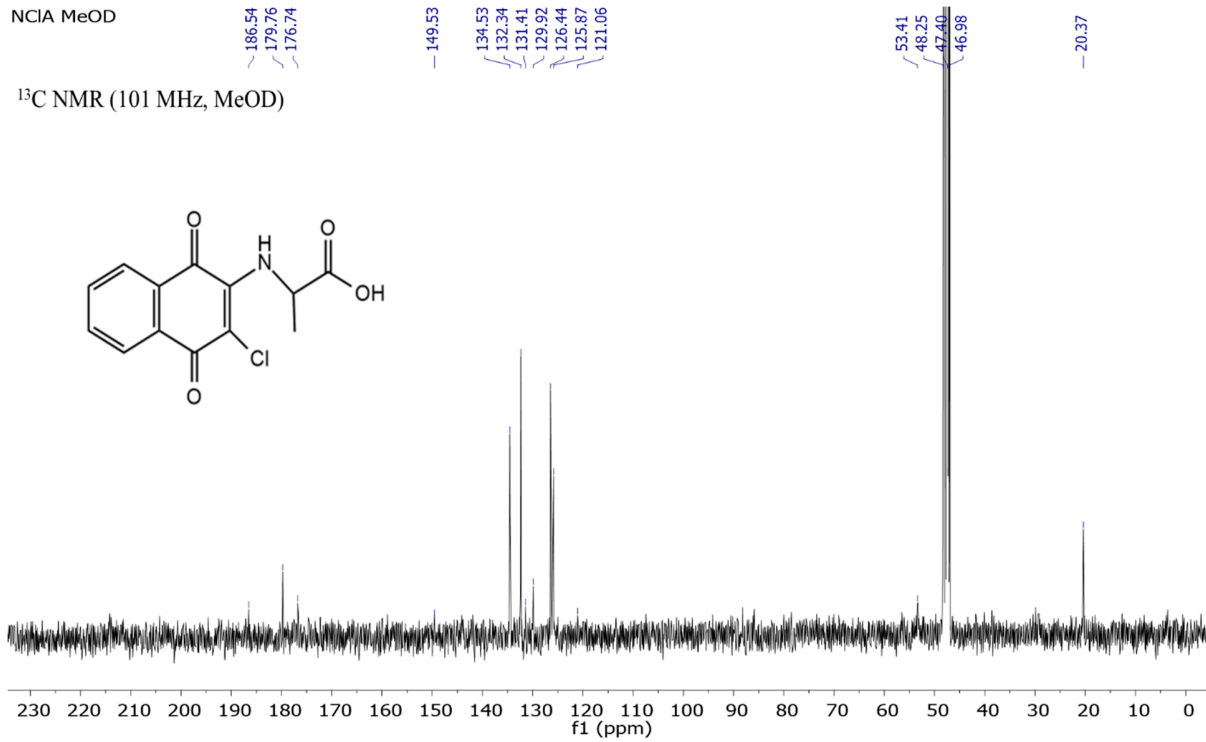
NCIA MeOD

^1H NMR (400 MHz, Methanol- d_4)

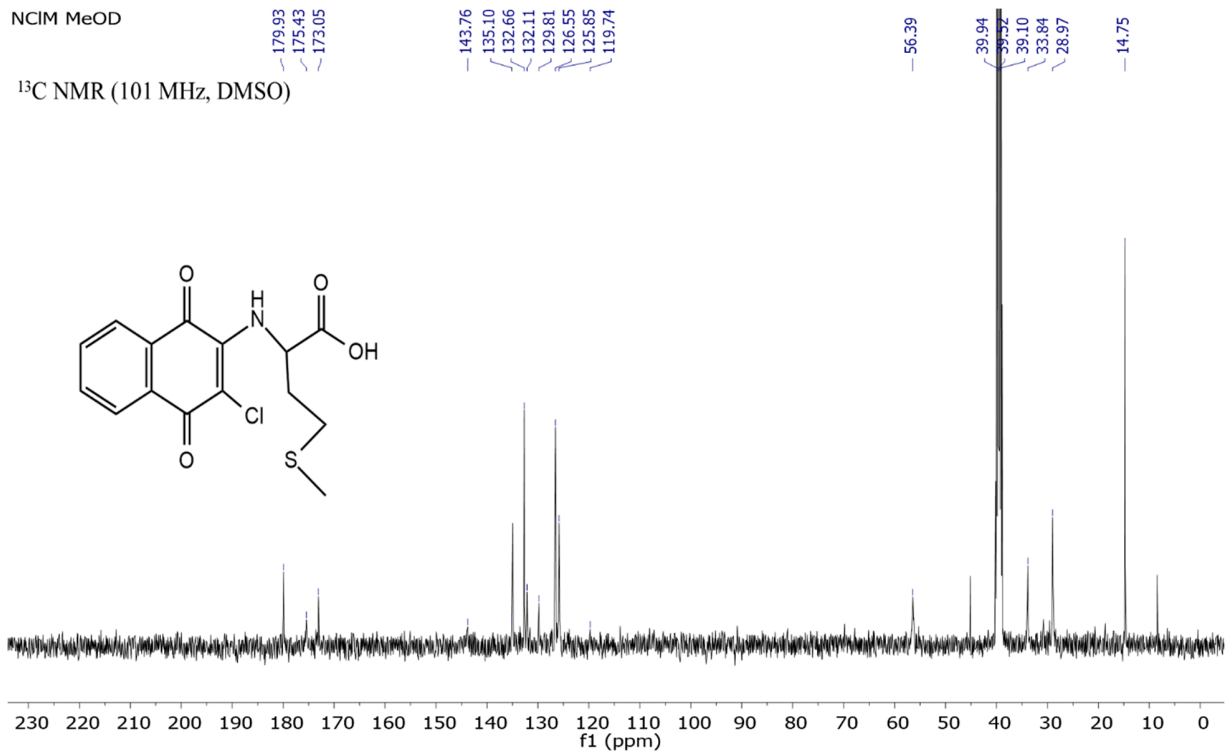
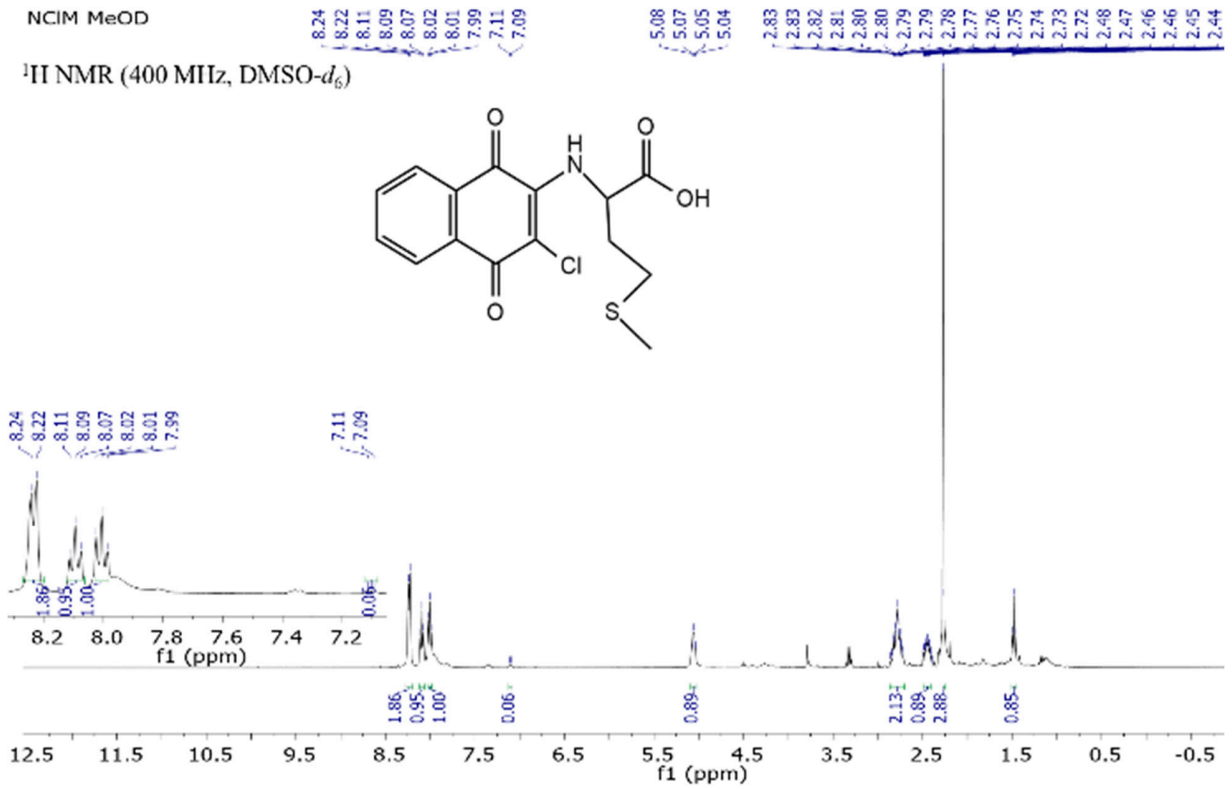


NCIA MeOD

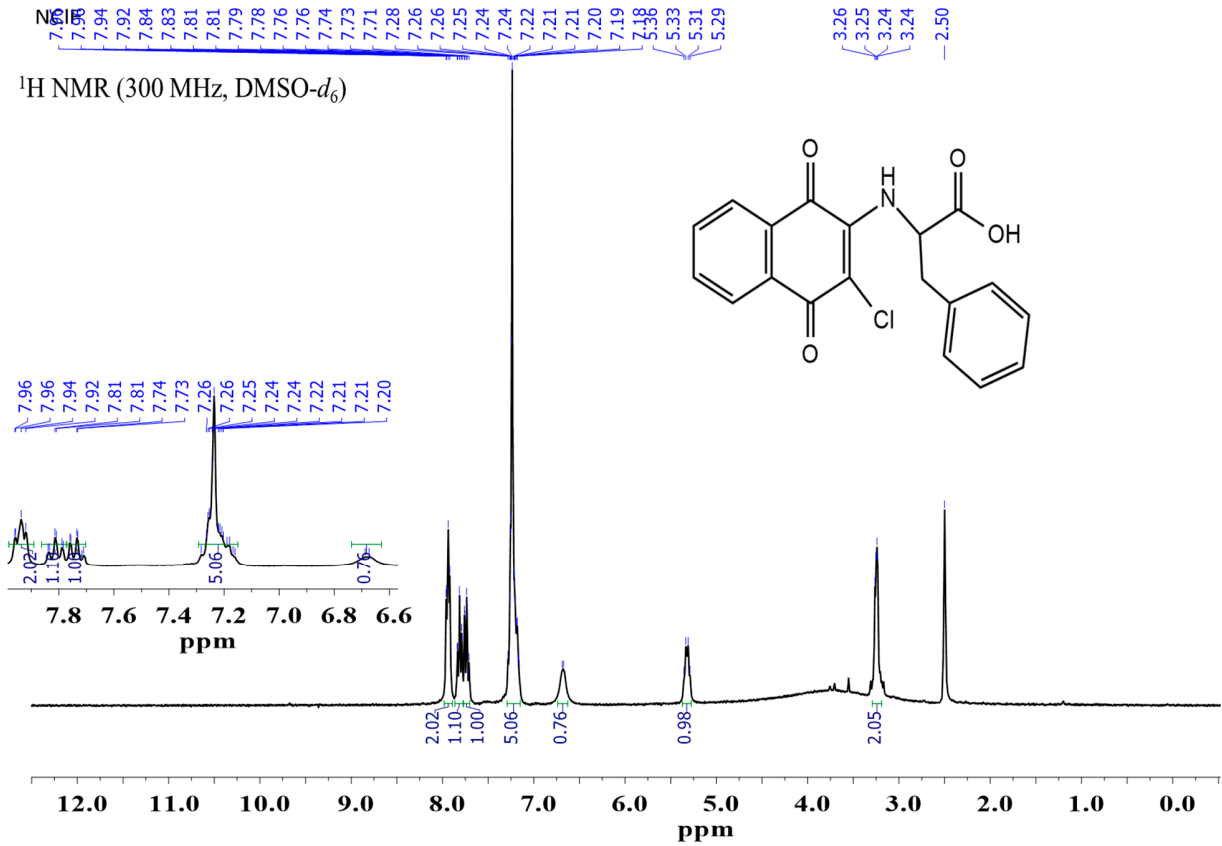
^{13}C NMR (101 MHz, MeOD)



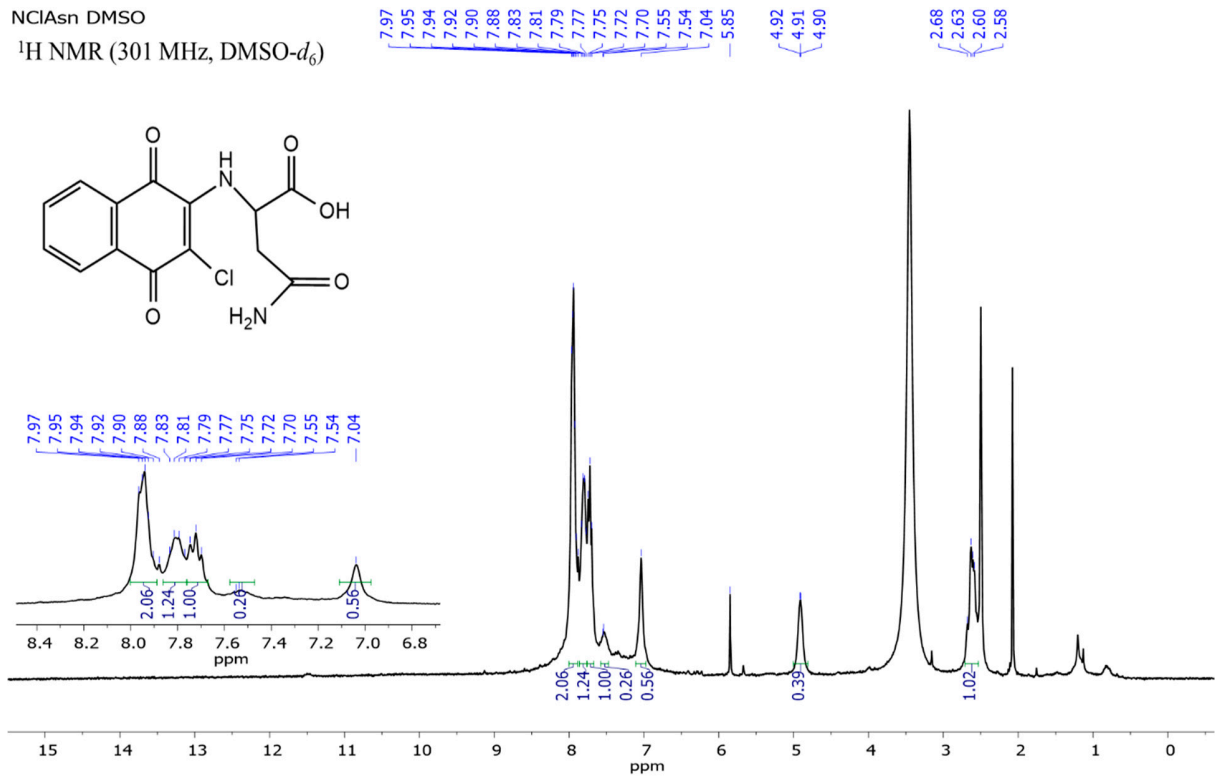
(4c)



(4d)



(4e)



NCIAsn DMSO

^{13}C NMR (75 MHz, DMSO)

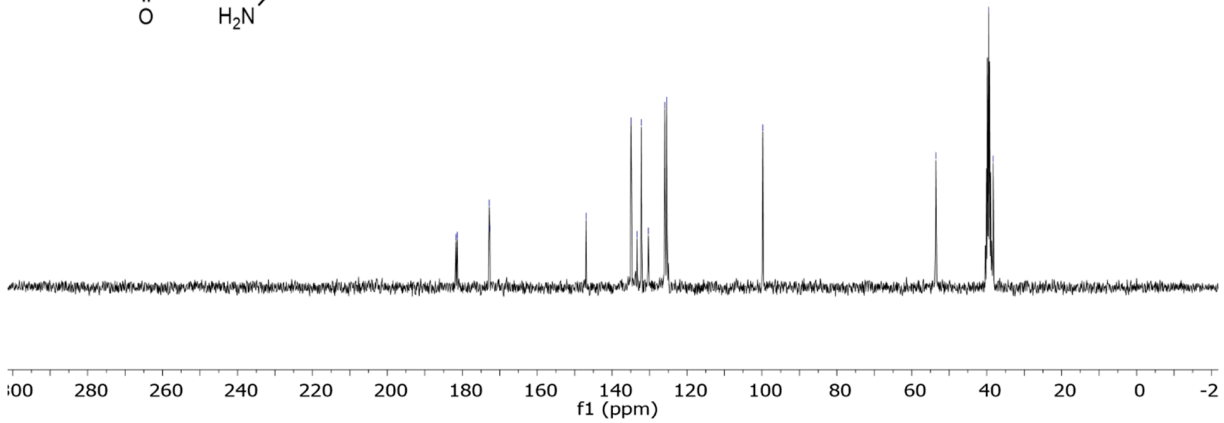
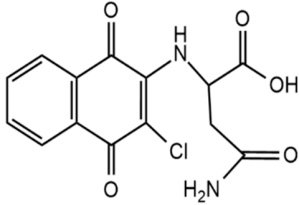
181.69
181.35
172.80
172.66

146.90
134.93
133.28
132.16
130.31
125.92
125.38

99.77

53.56

39.52
38.26



3. Mass spectrometry characterization of compounds 3c, 3e, 4b, 4c and 4e. (3c)

Data:U-278 NM1-MS-GC

Sample Name:Lizbeth Rodriguez

Description:

Ionization Mode:ESI+

History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[1.0%]];Correct Base[5.0%];Average[MS[1] 0..1)

Acquired:2/28/2018 10:26:25 AM

Operator:AccuTOF

Mass Calibration data:Cal Peg 600

Created:3/7/2018 9:26:00 AM

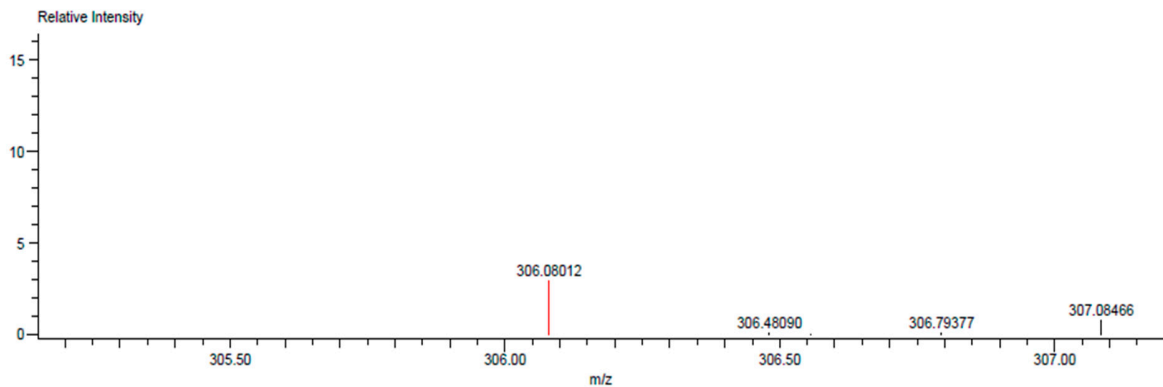
Created by:

Charge number:1

Tolerance:2.00(mmu)

Unsaturation Number:0.0 .. 20.0 (Fraction:Both)

Element: ^{12}C :0 .. 22, ^1H :1 .. 50, ^{14}N :0 .. 3, ^{16}O :3 .. 5, ^{32}S :1 .. 1

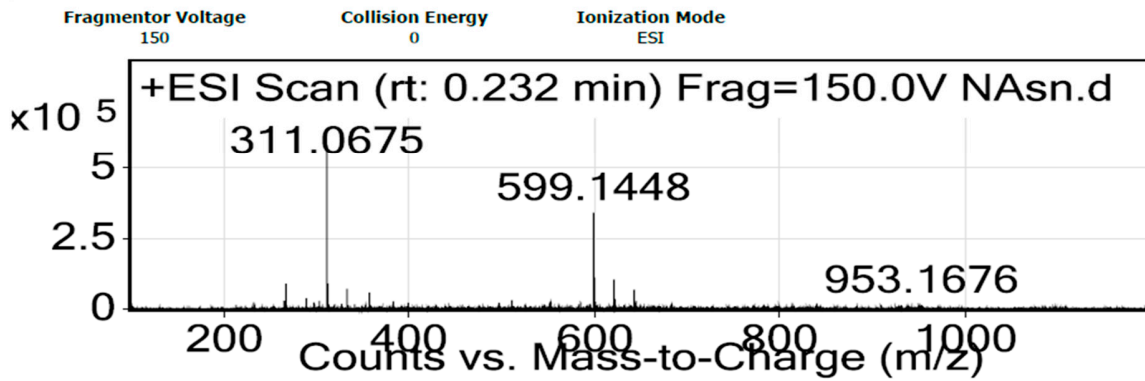


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
306.08012	7591.35	306.08000	0.12	0.38	$^{12}\text{C}_{15}\text{H}_{16}\text{N}_1\text{O}_4\text{S}_1$	9.5

(3e)

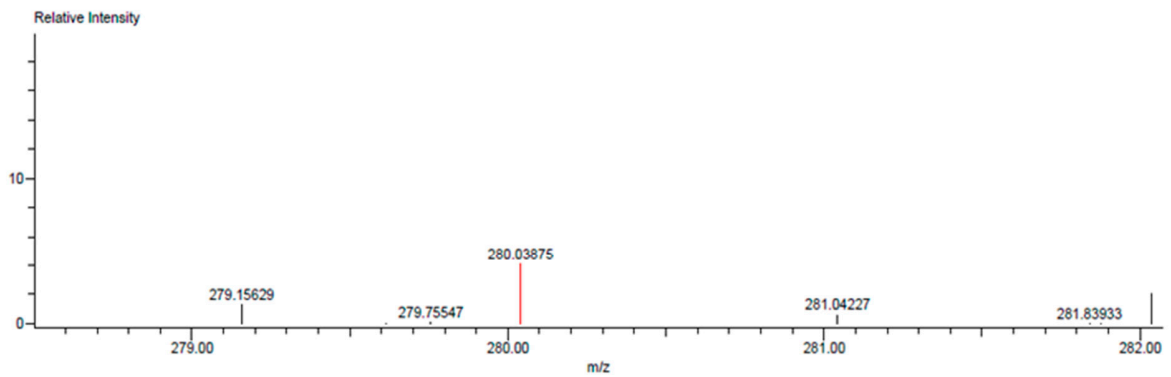
Data Filename	NAsn.d	Sample Name	NAsn
Sample Type	Sample	Position	P1-B3
Instrument Name	LC QTOF-LANCIC	User Name	
Acq Method	Ine directa pos.m	Acquired Time	8/2/2018 2:19:53 PM
IRM Calibration Status	Success	DA Method	Default.m
Comment			
Sample Group		Info.	
Stream Name	LC 1	Acquisition SW	6200 series TOF/6500 series
		Version	Q-TOF B.06.01 (B6172 SP1)

User Spectra



(4b)

Data: U-279 NCLA-MS	Acquired: 2/28/2018 10:29:53 AM
Sample Name: Lizbeth Rodriguez	Operator: AccuTOF
Description:	Mass Calibration data: Cal Peg 600
Ionization Mode: ESI+	Created: 3/7/2018 9:35:13 AM
History: Determine m/z [Peak Detect [Centroid, 30, Area]; Correct Base [1.0%]; Correct Base [5.0%]; Average (MS [1] 1..1)	Created by:
Charge number: 1 Tolerance: 2.00 (mmu)	Unsaturation Number: 5.0 .. 20.0 (Fraction: Both)
Element: ¹² C: 0 .. 22, ¹ H: 1 .. 50, ³⁵ Cl: 1 .. 1, ³⁷ Cl: 0 .. 1, ¹⁴ N: 0 .. 3, ¹⁶ O: 3 .. 5	



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
280.03875	6898.75	280.03766	1.09	3.88	¹² C ₁₃ ¹ H ₁₁ ³⁵ Cl ₁ ¹⁴ N ₁ ¹⁶ O ₄	8.5

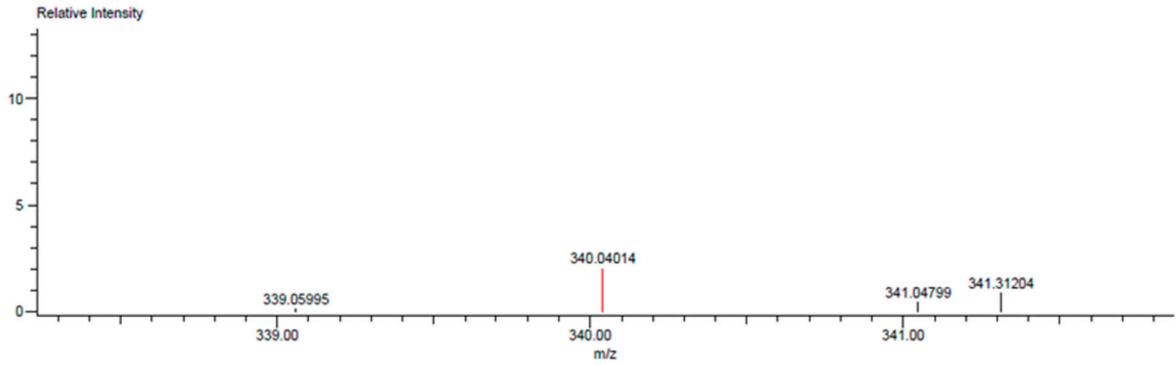
(4c)

Data:U-280 NCLM-MS
Sample Name:Lizbeth Rodriguez
Description:
Ionization Mode:ESI+
History:Determine m/z[Peak Detect[Centroid,30,Area];Correct Base[1.0%]];Correct Base[5.0%];Average[MS[1] 1..1]

Acquired:2/28/2018 10:32:39 AM
Operator:AccuTOF
Mass Calibration data:Cal Peg 600
Created:3/7/2018 9:48:45 AM
Created by:

Charge number:1
Tolerance:2.00(mmu)
Element:¹²C:0 .. 22, ¹H:1 .. 50, ³⁵Cl:1 .. 1, ³⁷Cl:0 .. 1, ¹⁴N:0 .. 3, ¹⁶O:3 .. 5, ³²S:1 .. 1

Unsaturation Number:5.0 .. 20.0 (Fraction:Both)



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
340.04014	41284.85	340.04103	-0.89	-2.61	¹² C ₁₅ ¹ H ₁₅ ³² S ₁ ¹⁴ N ₁ ¹⁶ O ₄ ³² S ₁	9.5

(4e)

Data Filename	NCL2Asn.d	Sample Name	NCL2Asn
Sample Type	Sample	Position	P1-B5
Instrument Name	LC QTOF-LANCIC	User Name	
Acq Method	Ine directa pos.m	Acquired Time	8/2/2018 2:34:02 PM
IRM Calibration Status	Success	DA Method	Default.m
Comment			

Sample Group		Info.	
Stream Name	LC 1	Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.06.01 (B6172 SP1)

User Spectra

