

Supplementary Materials

Unexpected formation of 4-[(1-carbamoyl-3-oxo-1,3-dihydro-2-benzofuran-1-yl)amino]benzoic acid from 4-[(3-amino-1-oxo-1*H*-2-benzopyran-4-yl)amino]benzoic acid

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¹H-NMR Spectrum of compound 10a	S1
¹³C-NMR Spectrum of compound 10a	S2
APT Spectrum of compound 10a	S3
¹H-¹³C -HSQC Spectrum of compound 10a	S4
¹H-¹³C -HMBC Spectrum of compound 10a	S5
FT-IR Spectrum of compound 10a	S6
HR-MS Spectrum of compound 10a	S7
¹H-NMR Spectrum of compound 11a	S8
¹³C-NMR Spectrum of compound 11a	S9
APT Spectrum of compound 11a	S10
¹H-¹H-COSY Spectrum of compound 11a	S11
¹H-¹³C -HSQC Spectrum of compound 11a	S12
¹H-¹³C -HMBC Spectrum of compound 11a	S13
FT-IR Spectrum of compound 11a	S14
HR-MS Spectrum of compound 11a	S15

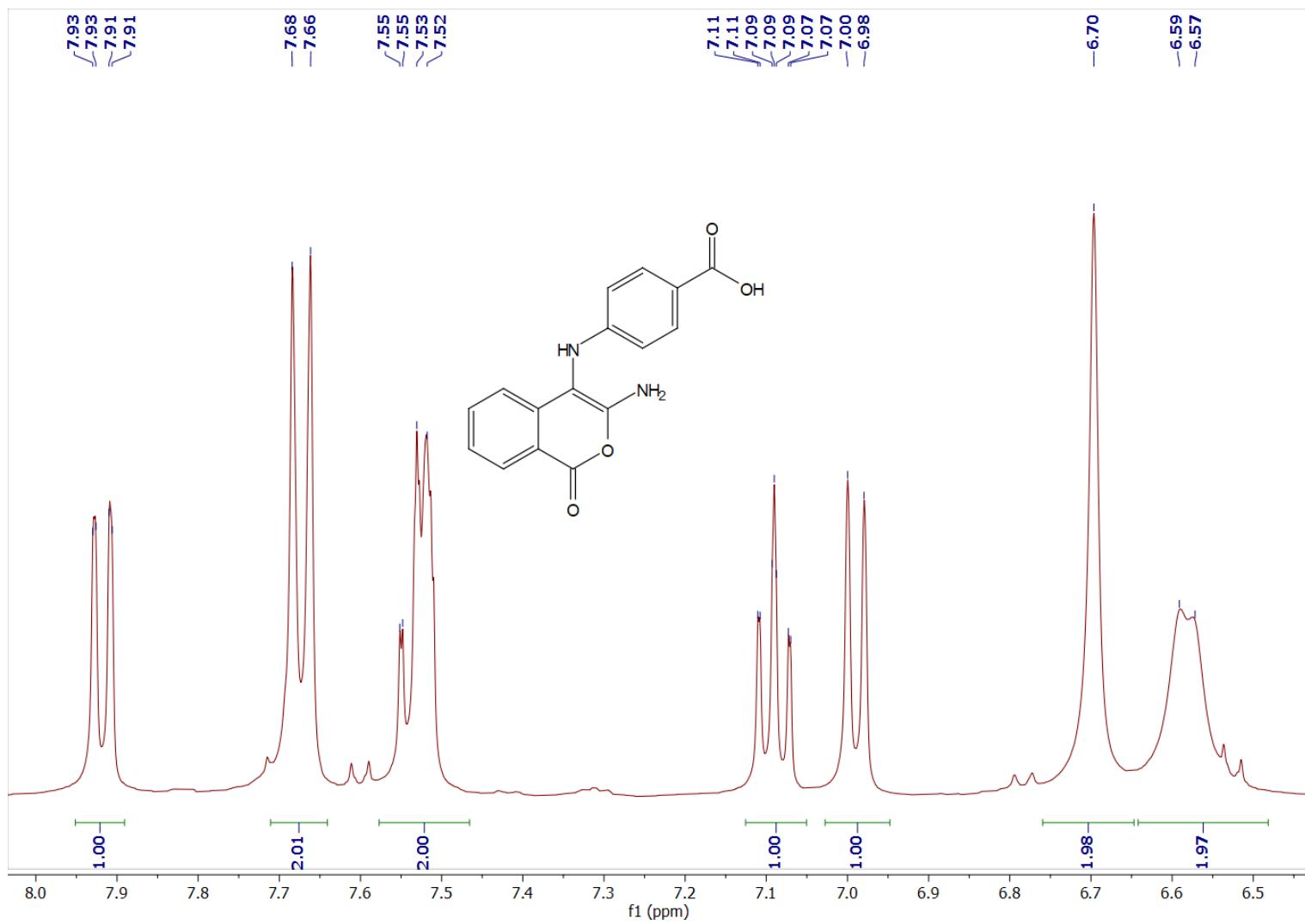


Figure S1. ¹H-NMR spectrum for compound 10a.

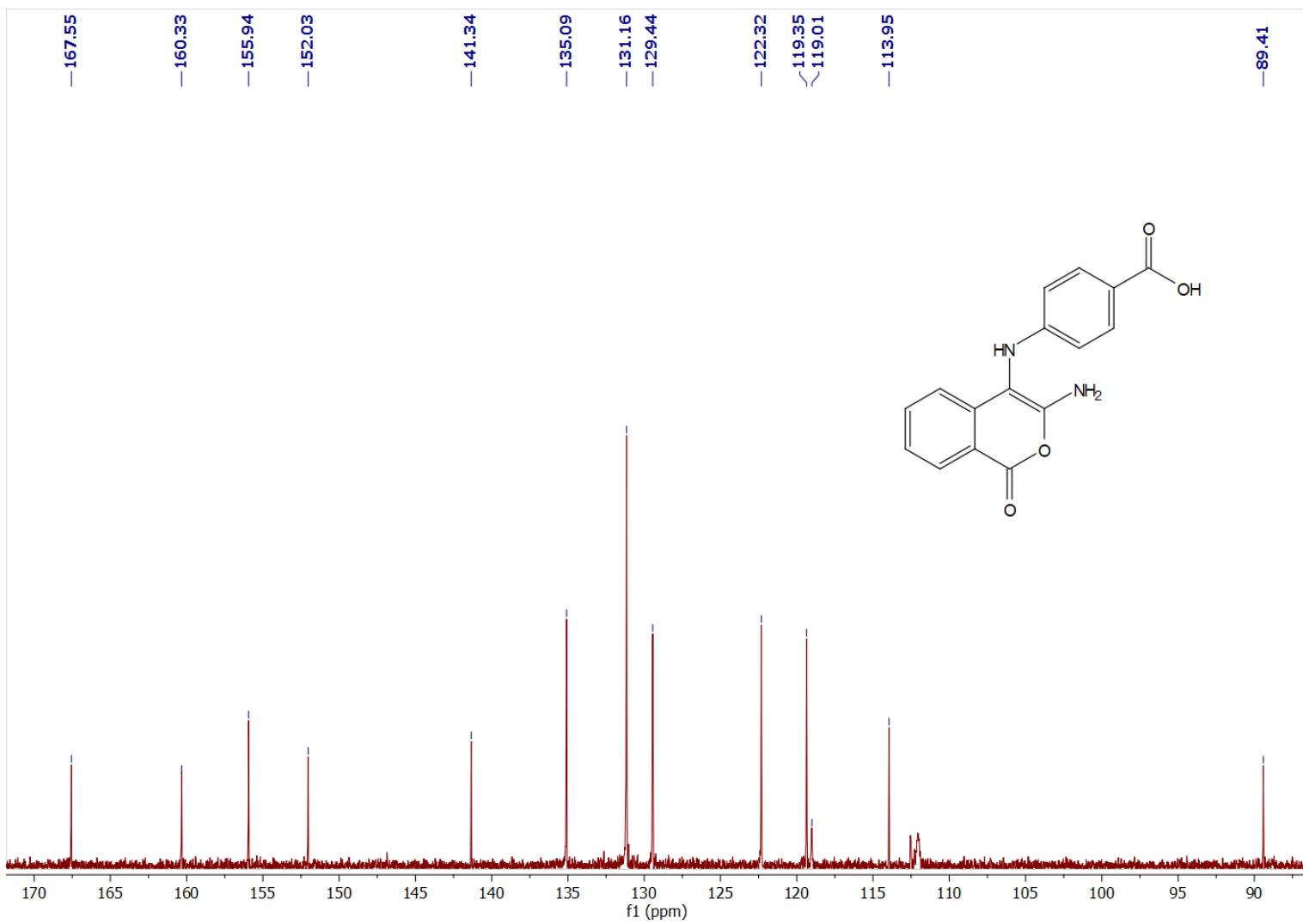


Figure S2. ^{13}C -NMR spectrum for compound 10a.

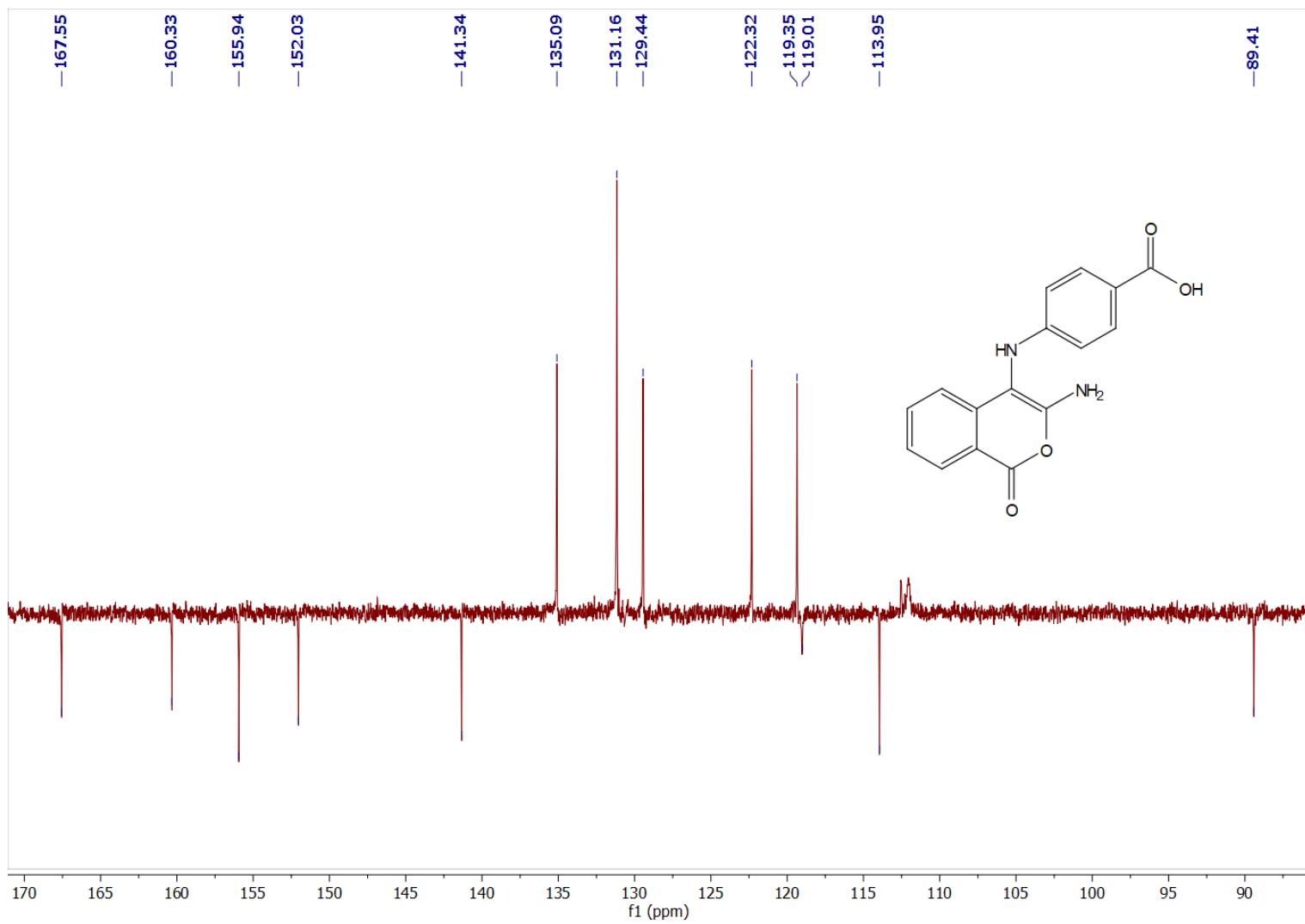


Figure S3. APT spectrum for compound **10a**.

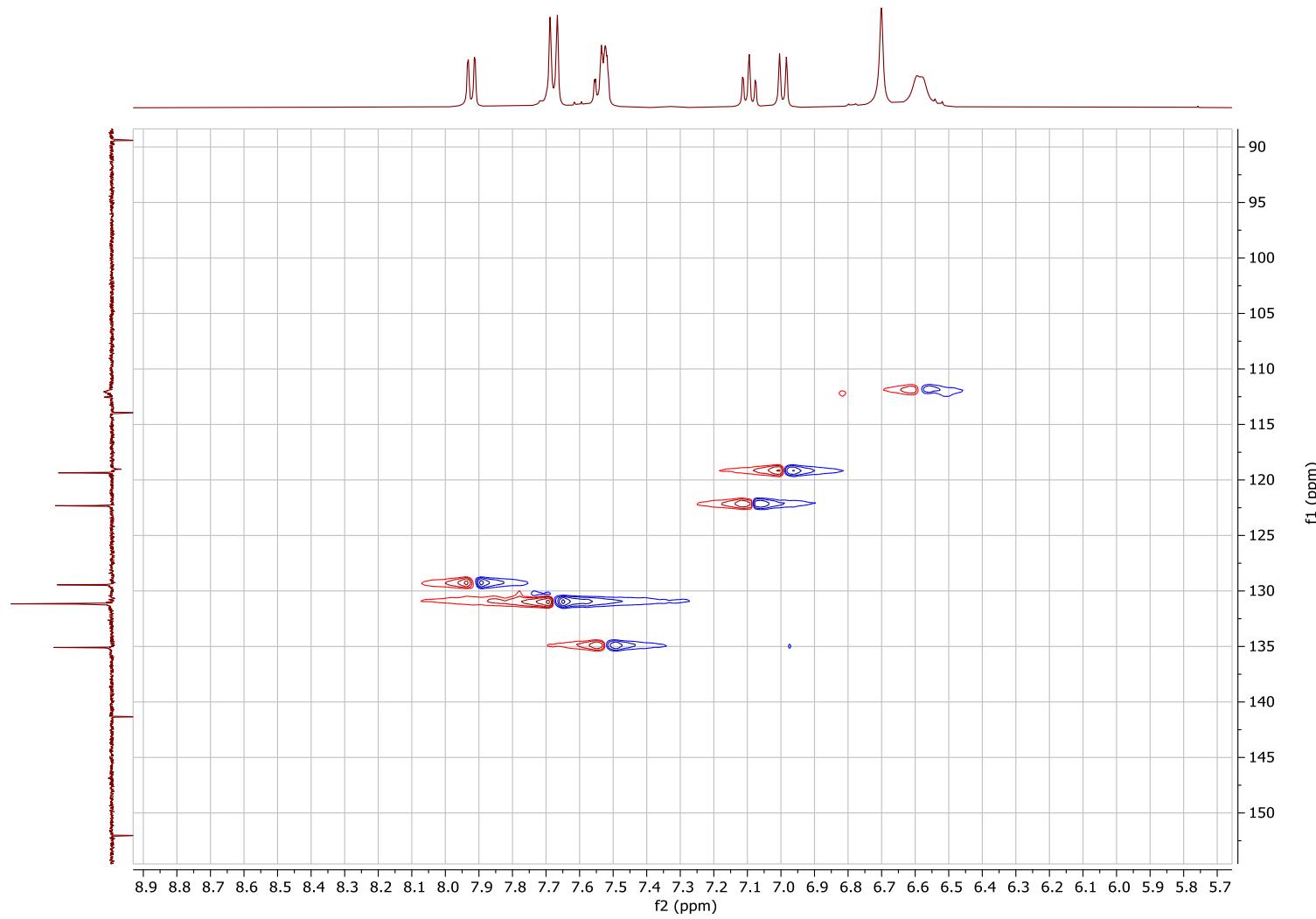


Figure S4. ^1H - ^{13}C -HSQC spectrum of compound 10a.

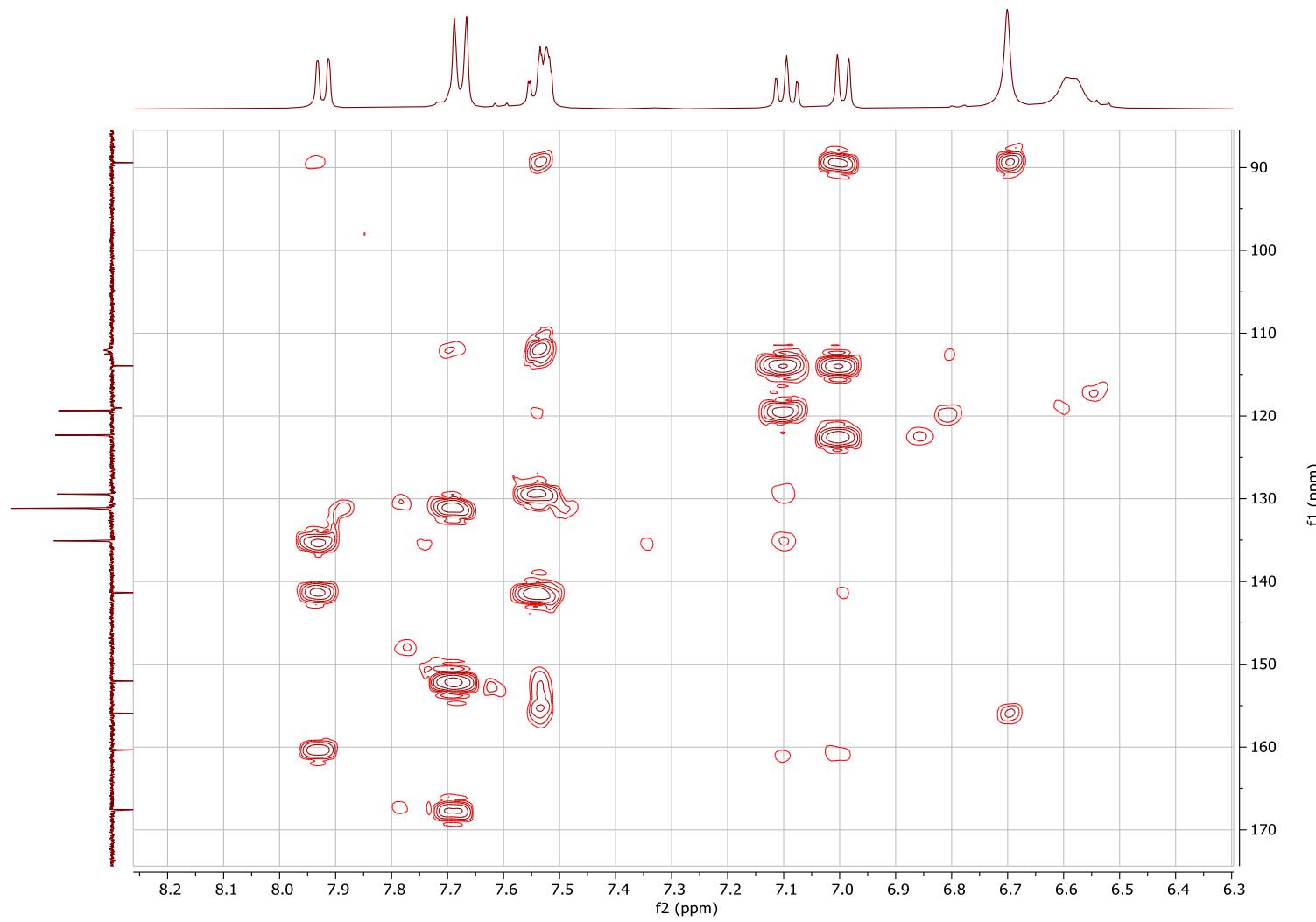
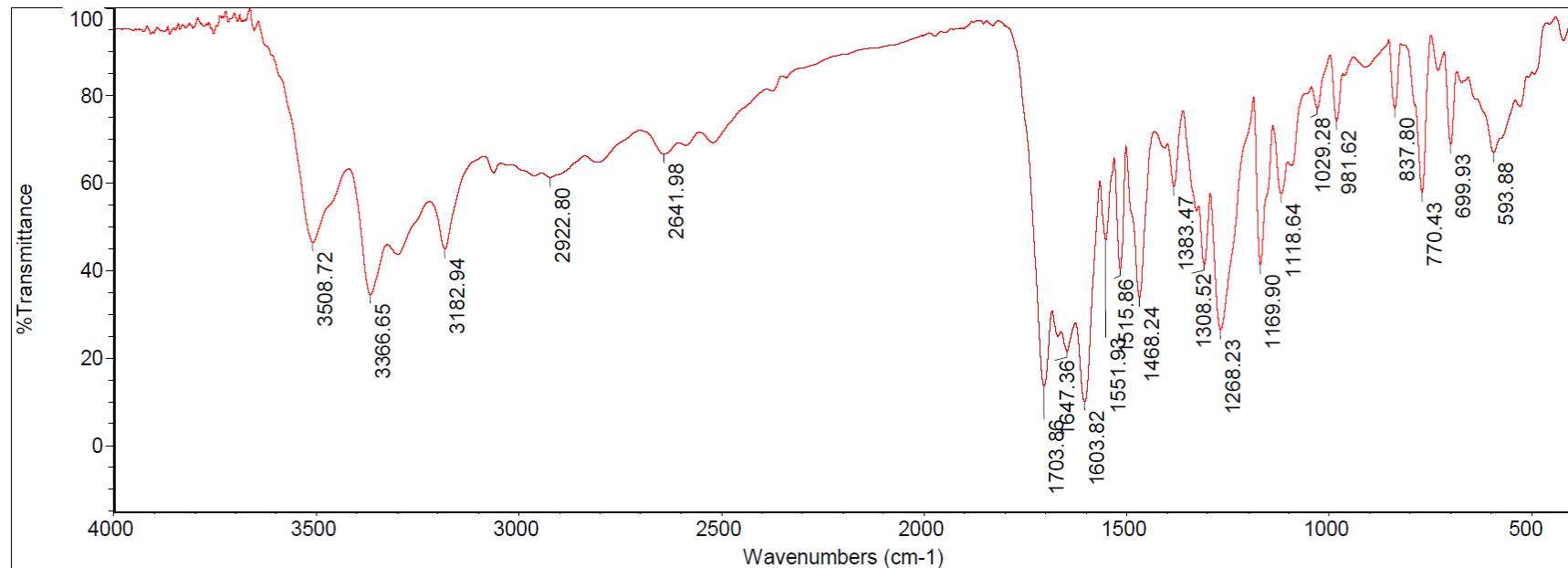


Figure S5. ^1H - ^{13}C -HMBC spectrum of compound 10a.



Condiciones
Instrumentales

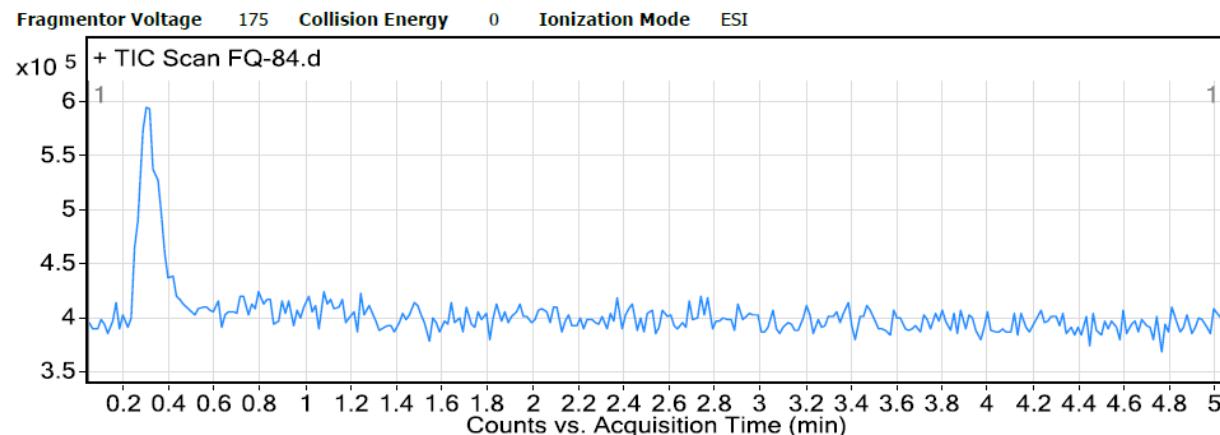
Number of sample scans: 16
Number of background scans: 16
Resolution: 4.000
Sample gain: 1.0
Optical velocity: 0.4747
Aperture: 100.00

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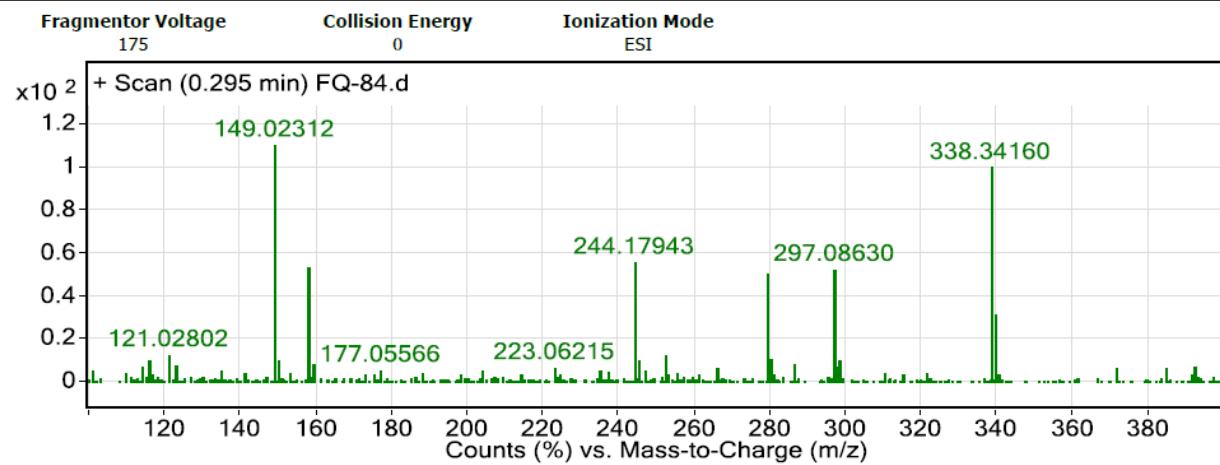
Método de análisis: Pastilla de KBr
Nicolet iS5 Espectrometer
Thermo Scientific

Figure S6. FT-IR spectrum for compound 10a.

User Chromatograms



User Spectra



Peak List

m/z	z	Abund
88.93253		8814.8
149.02312	1	30626.5
149.05215		4045.3
158.15315	1	14831.4
244.17943	1	15484.7
279.07702	1	13987
297.0863	1	14578.8
338.3416	1	27721.3
339.34492	1	8802.5
922.011	1	7409.3

Figure S7. HR-MS spectrum of compound 10a.

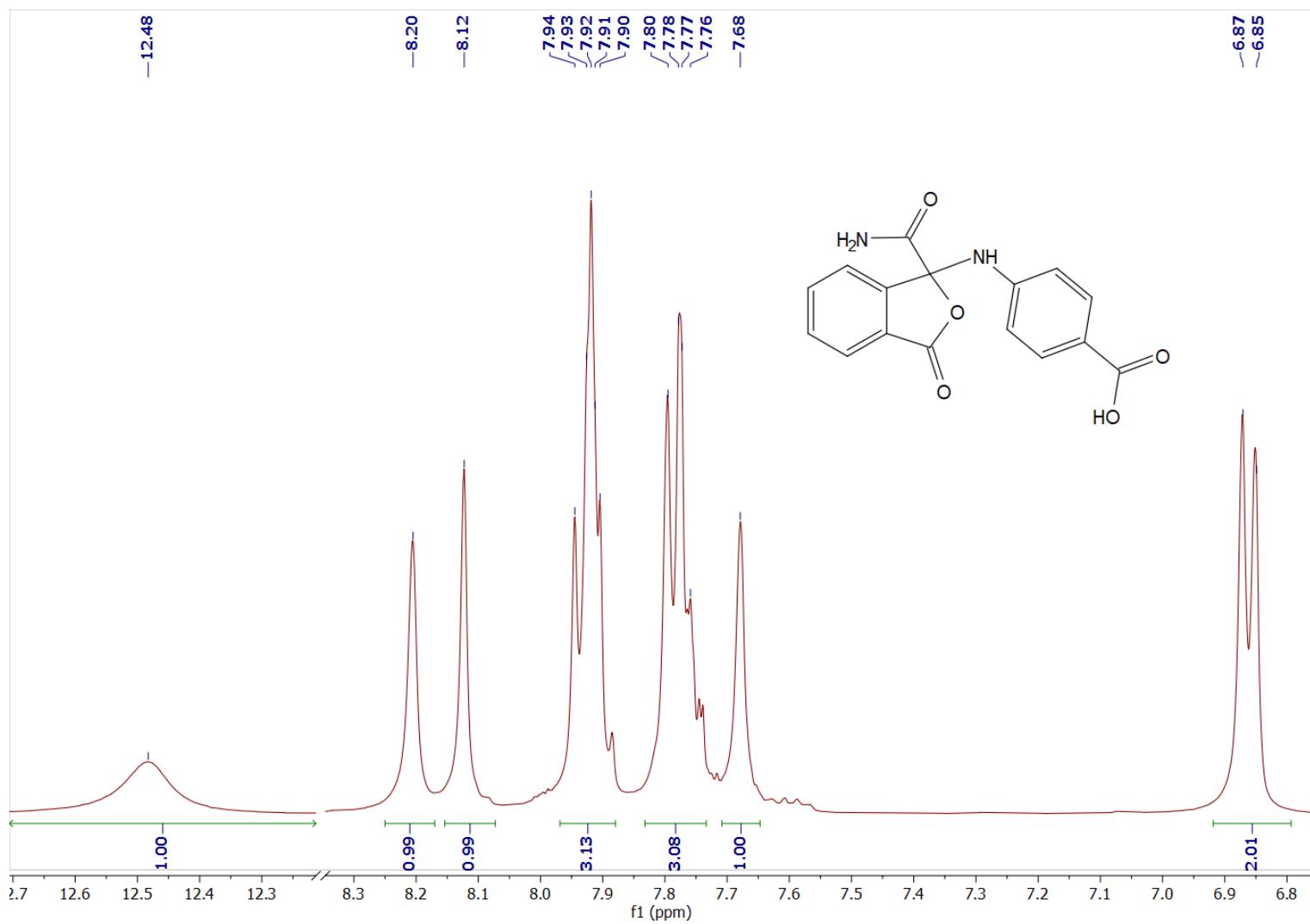


Figure S8. ¹H-NMR spectrum for compound 11a.

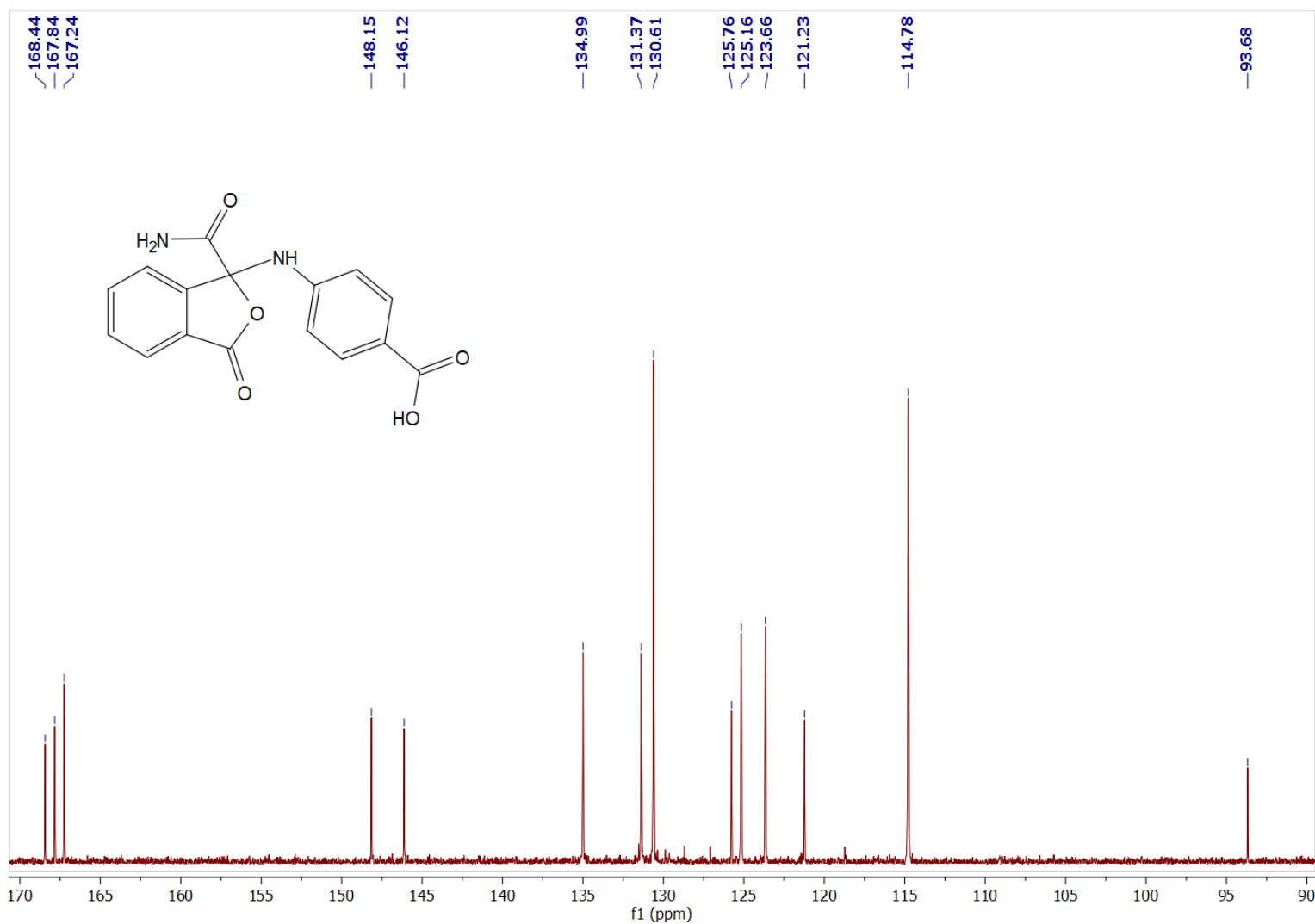


Figure S9. ¹³C-NMR spectrum for compound 11a.

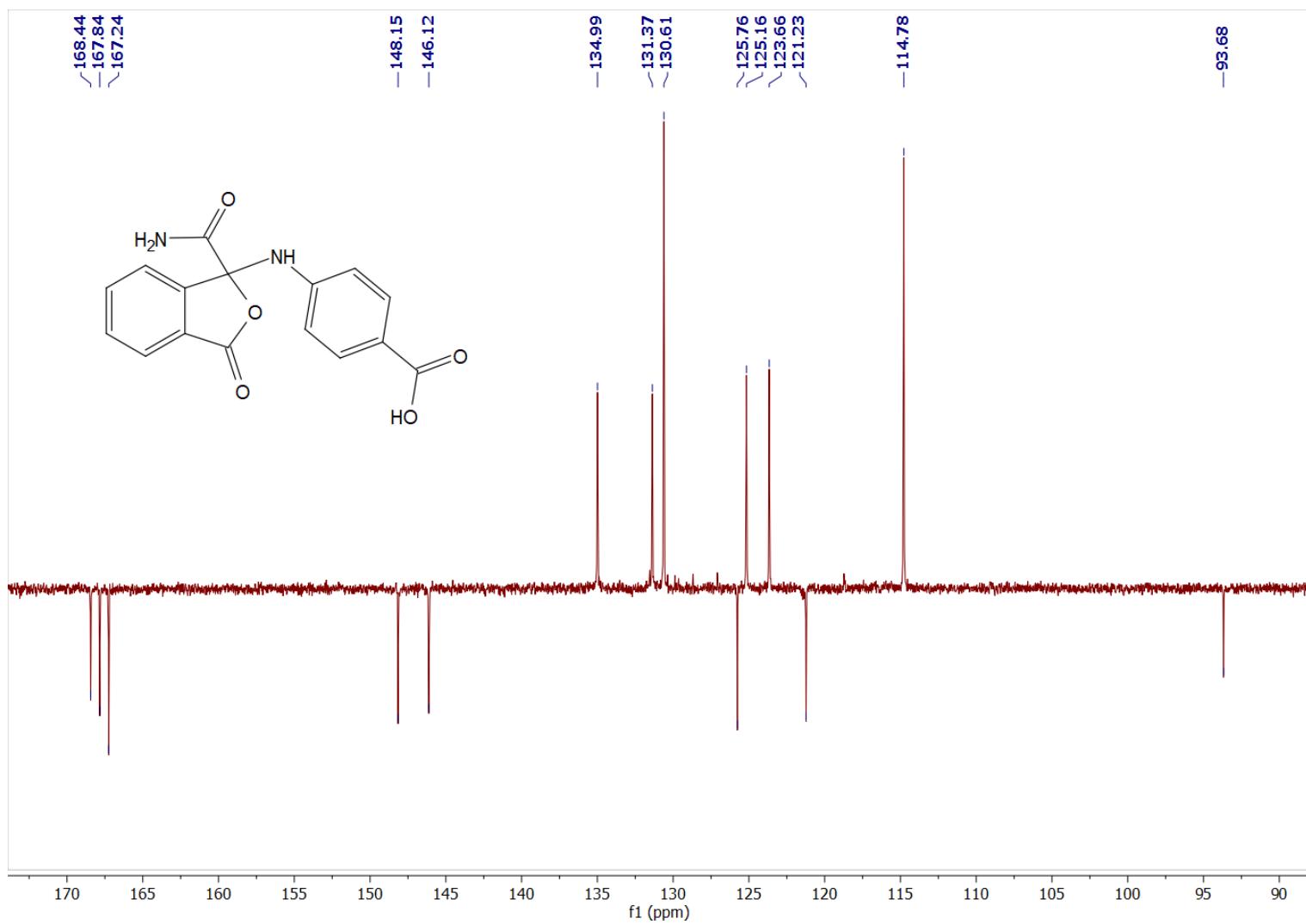


Figure S10. APT spectrum for compound 11a.

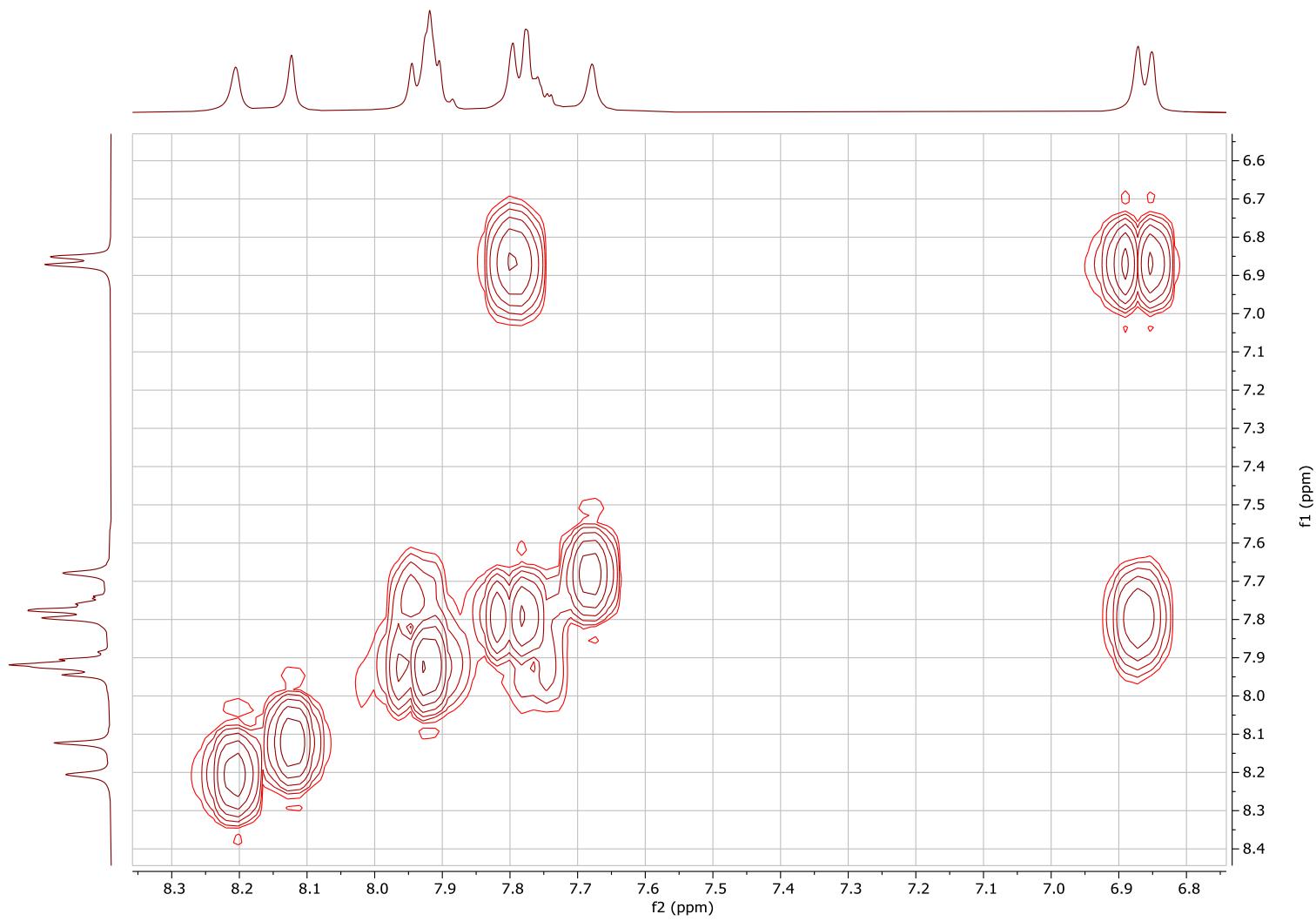


Figure S11. ^1H - ^1H -COSY spectrum for compound 11a.

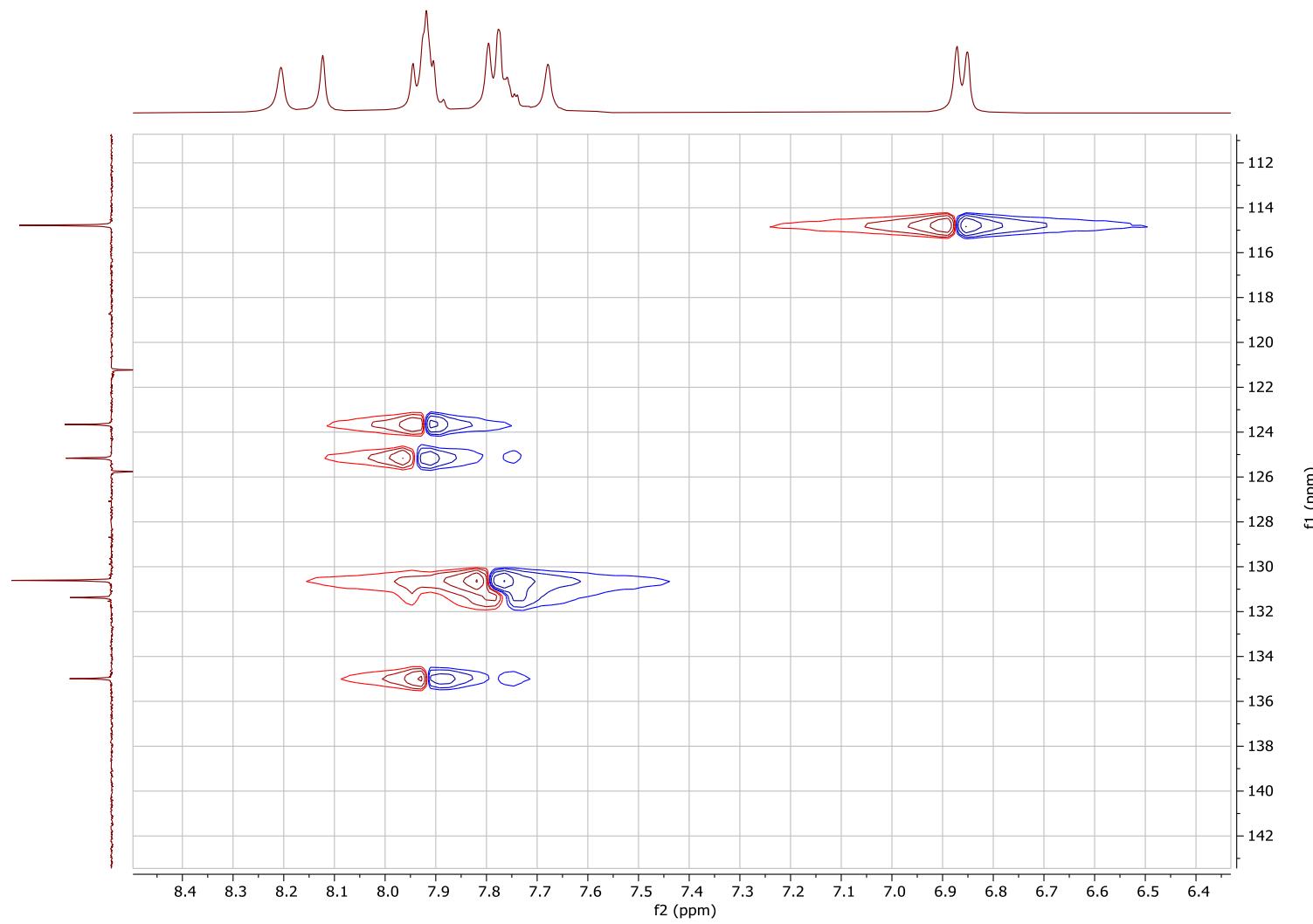


Figure S12. ^1H - ^{13}C -HSQC spectrum for compound 11a.

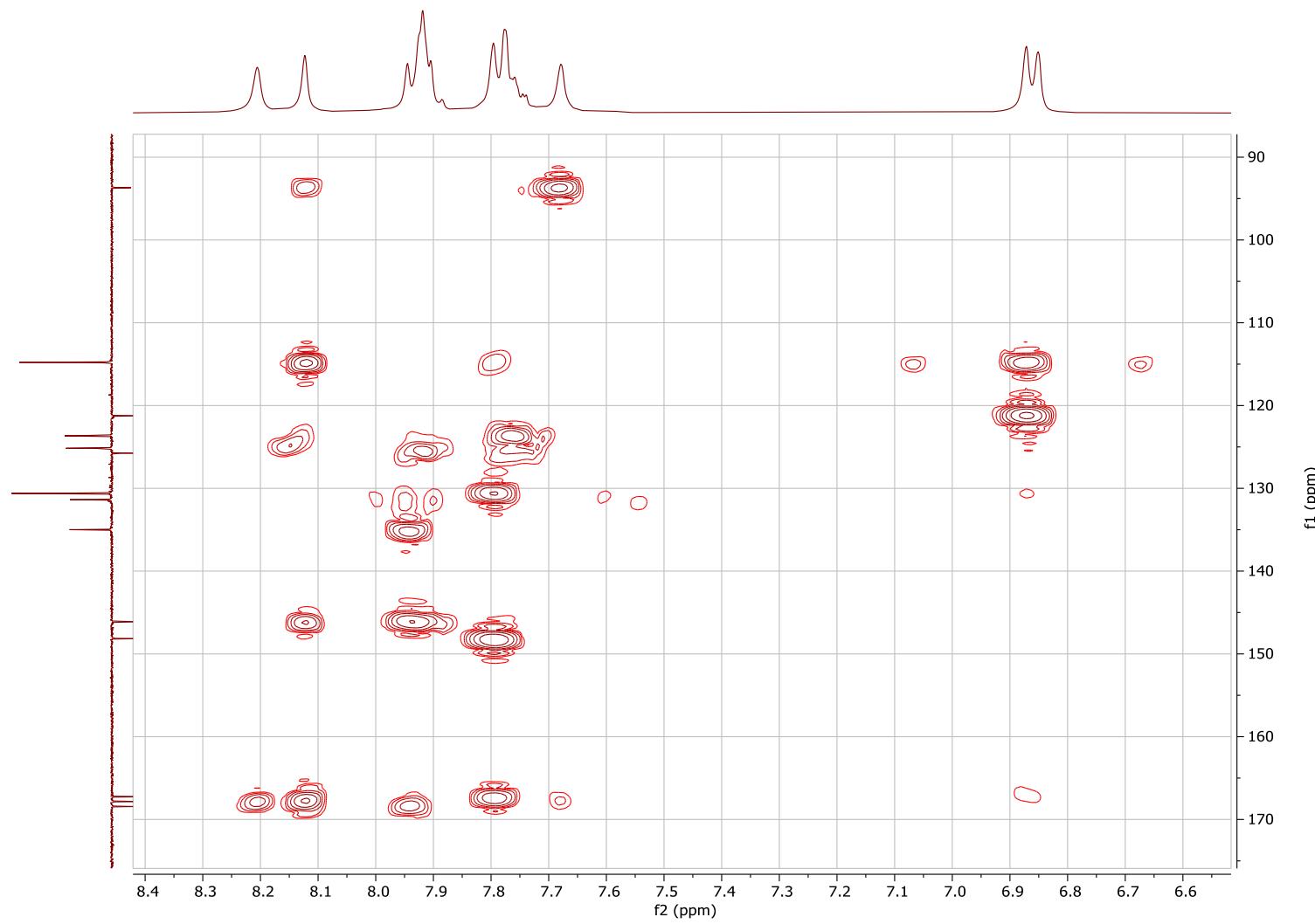
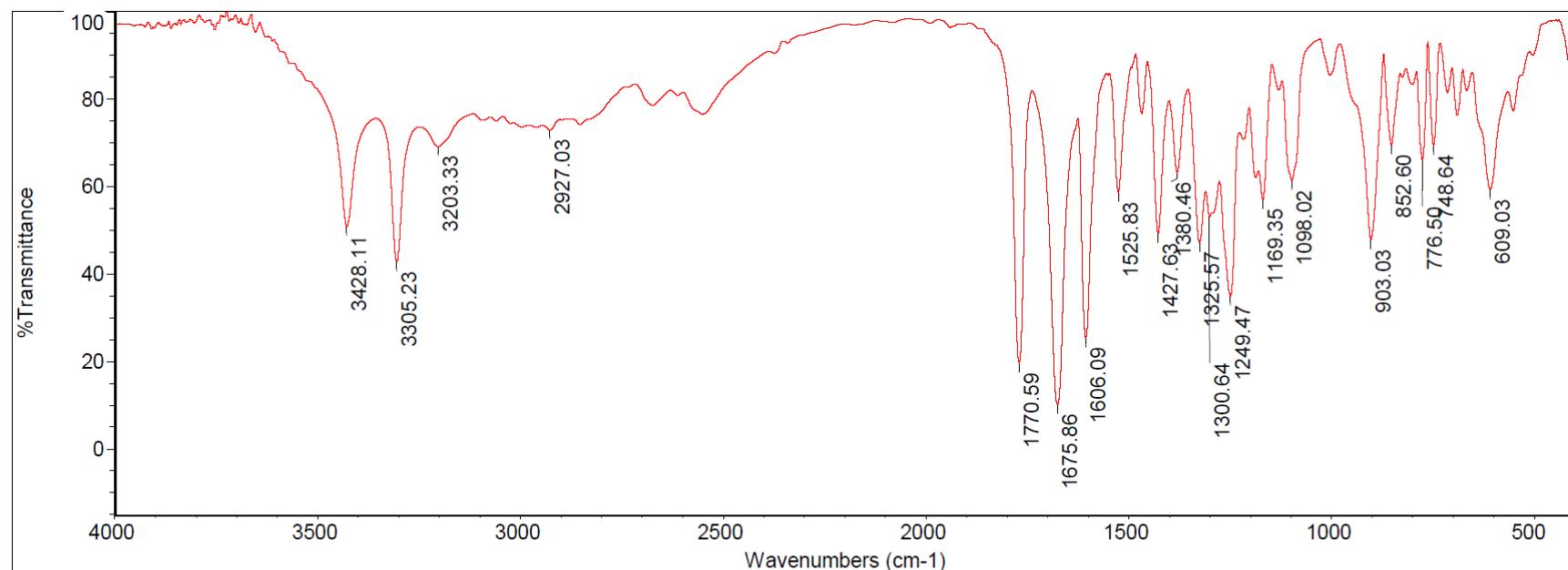


Figure S13. ^1H - ^{13}C -HMBC spectrum for compound 11a.



Condiciones
Instrumentales

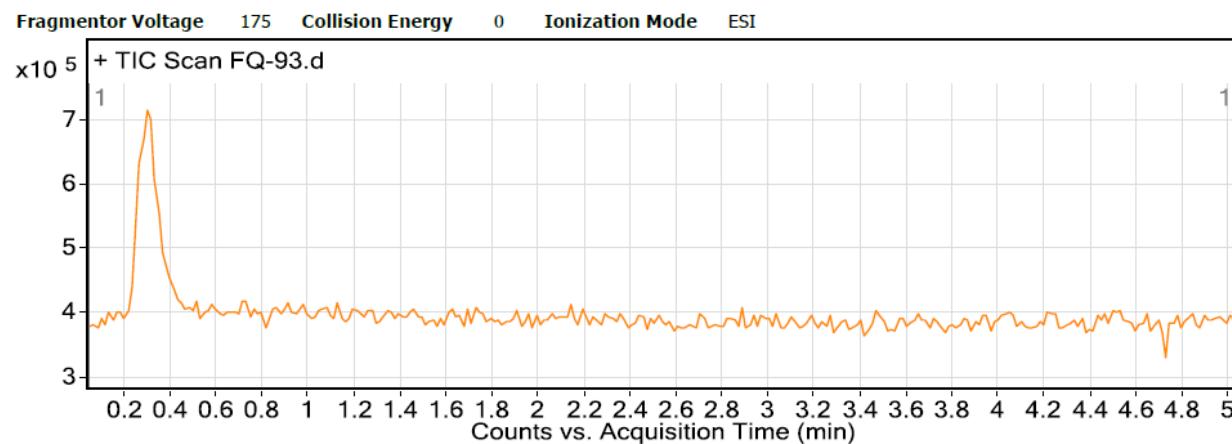
Number of sample scans: 16
Number of background scans: 16
Resolution: 4.000
Sample gain: 1.0
Optical velocity: 0.4747
Aperture: 100.00

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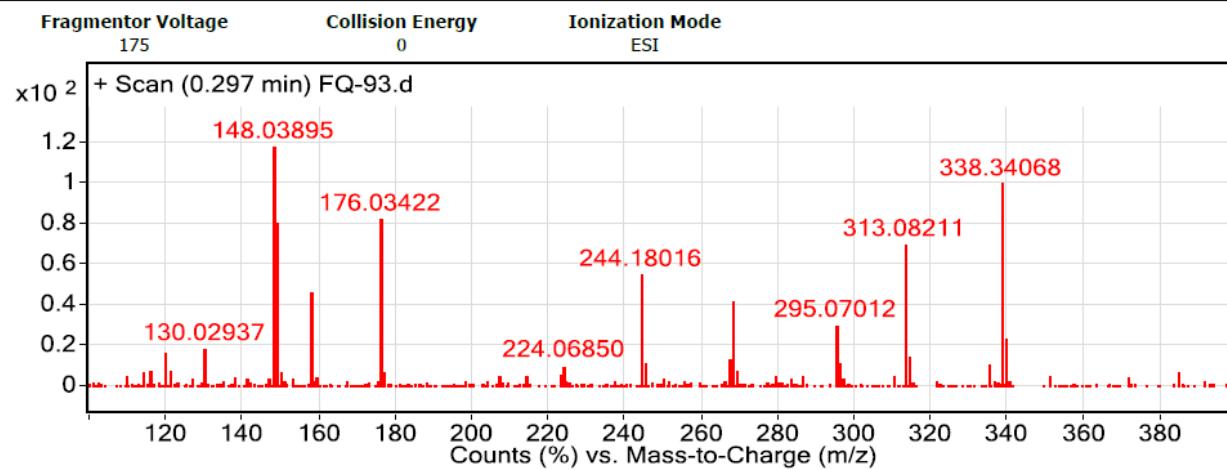
Método de análisis: Pastilla de KBr
Nicolet iS5 Espectrometer
Thermo Scientific

Figure S14. FT-IR spectrum for compound 11a.

User Chromatograms



User Spectra



Peak List

m/z	z	Abund
148.03895	1	36270.9
149.02427	1	24918.4
158.15402		14099.8
176.03422	1	25329.6
244.18016	1	16903.8
268.06094	1	13025.4
295.07012	1	9237.3
313.08211	1	21480.3
338.34068	1	30638.9
339.34492	1	7241.4

Figure S15. HR-MS spectrum of compound 11a.