

Supplementary Information

Thiazolidin-4-ones from 3-(Aminomethyl)pyridine, Arenealdehydes and Mercaptoacetic Acid: Synthesis and Radical Scavenger Activity

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The ¹H and ¹³C NMR spectra recorded on a Varian Oxford AS-400 spectrometer, the files were proceeding in the ACD/Lab 6.00 - ACD/SpecManager software.

The ¹H and ¹³C NMR spectra recorded on a Bruker Ac-200F spectrometer, the files were proceeding in the MestReC 4.7.0.0. software.

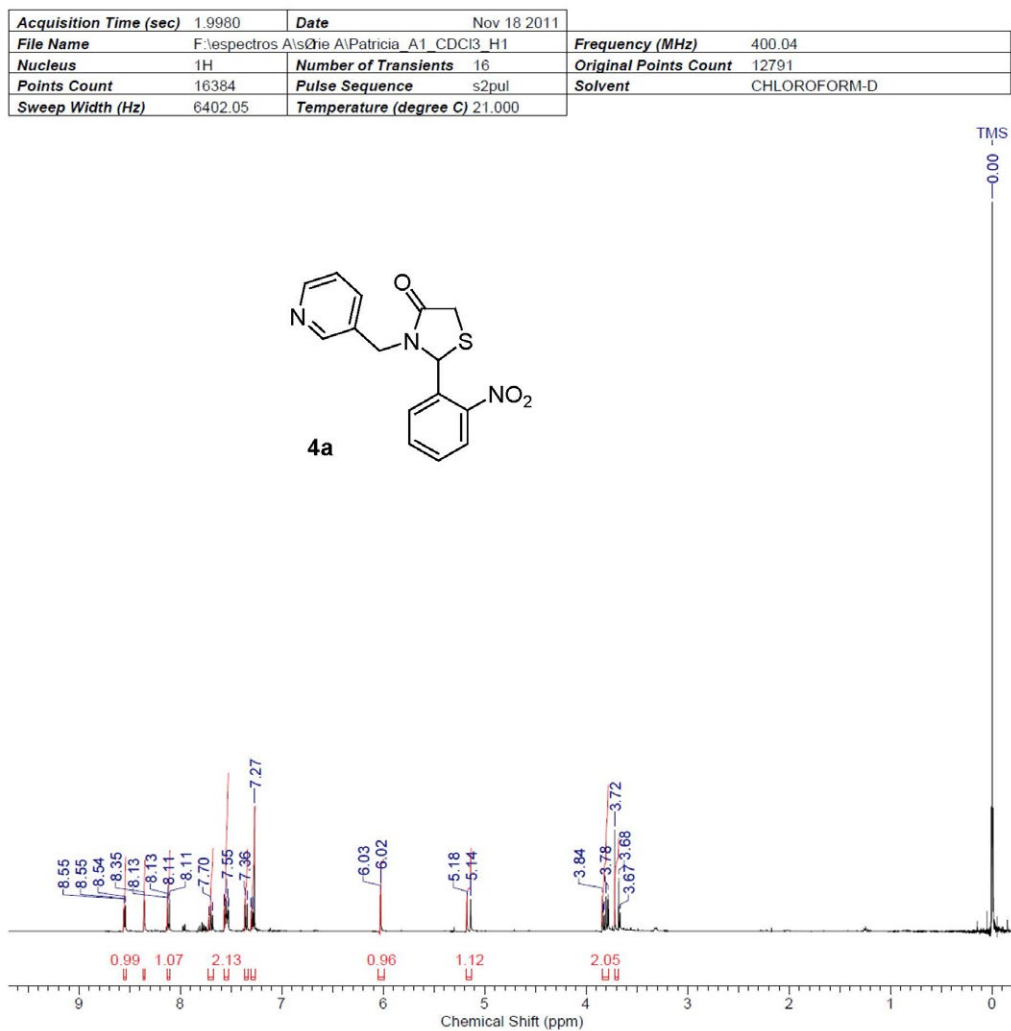


Figure S1. ¹H NMR spectrum (400 MHz, CDCl₃) of compound 4a.

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Acquisition Time (sec)	1.3005	Date	Nov 21 2011
File Name	Filespectros A1s01e A1Patricia A1	CDCl3	C13
Nucleus	13C	Number of Transients	12000
Points Count	32768	Pulse Sequence	s2pul
Sweep Width (Hz)	24154.59	Temperature (degree C)	22.000
Frequency (MHz)	100.60	Original Points Count	31413
Solvent	CHLOROFORM-D		

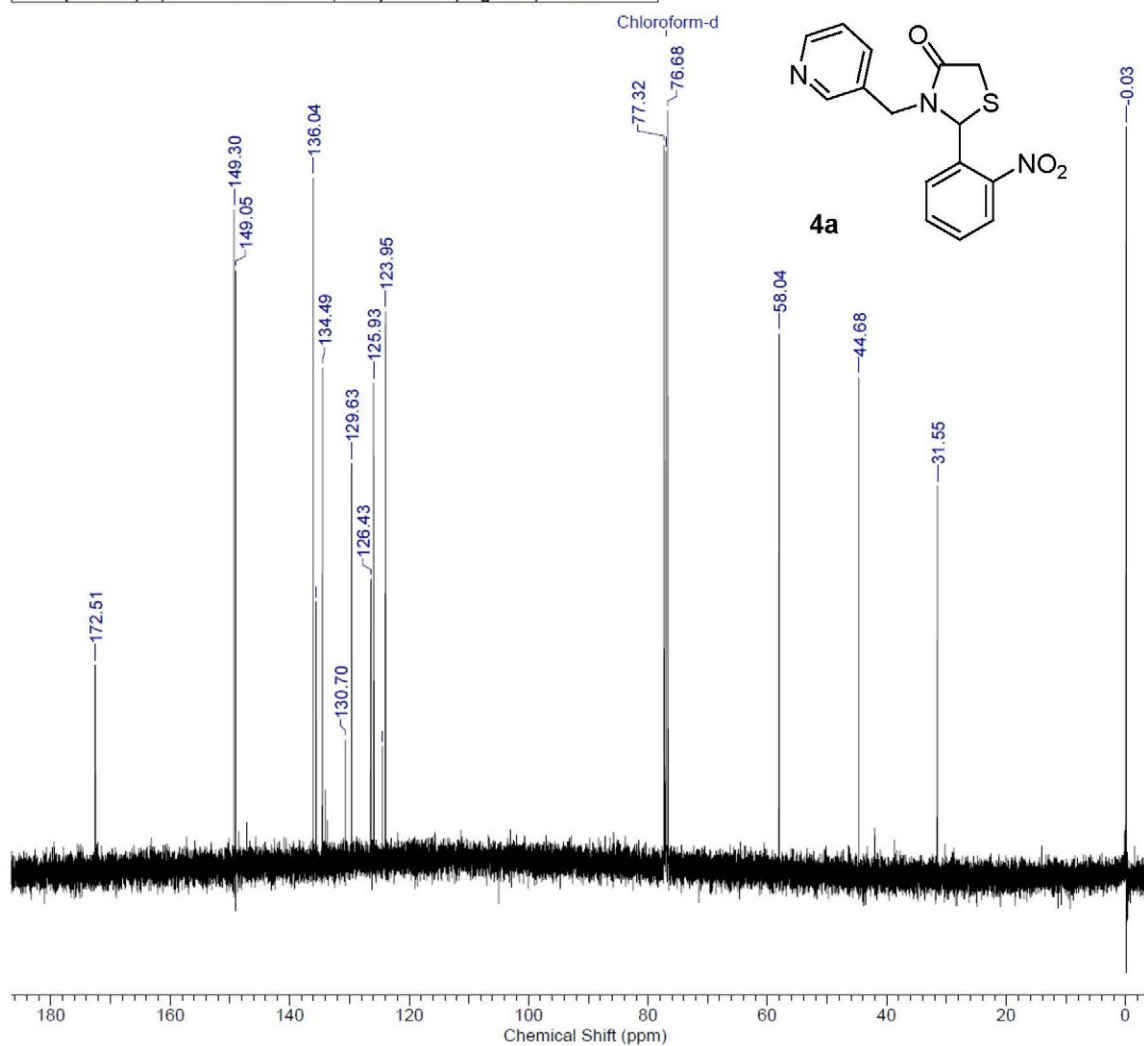


Figure S2. ^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **4a**.

Acquisition Time (sec)	1.9980	Date	Nov 18 2011
File Name	C:\Users\Andre\Desktop\Die A\Patricia A2_CDCl3_H1	Frequency (MHz)	400.04
Nucleus	1H	Number of Transients	16
Points Count	16384	Pulse Sequence	s2pul
Sweep Width (Hz)	6402.05	Temperature (degree C)	21.000
		Original Points Count	12791
		Solvent	CHLOROFORM-D

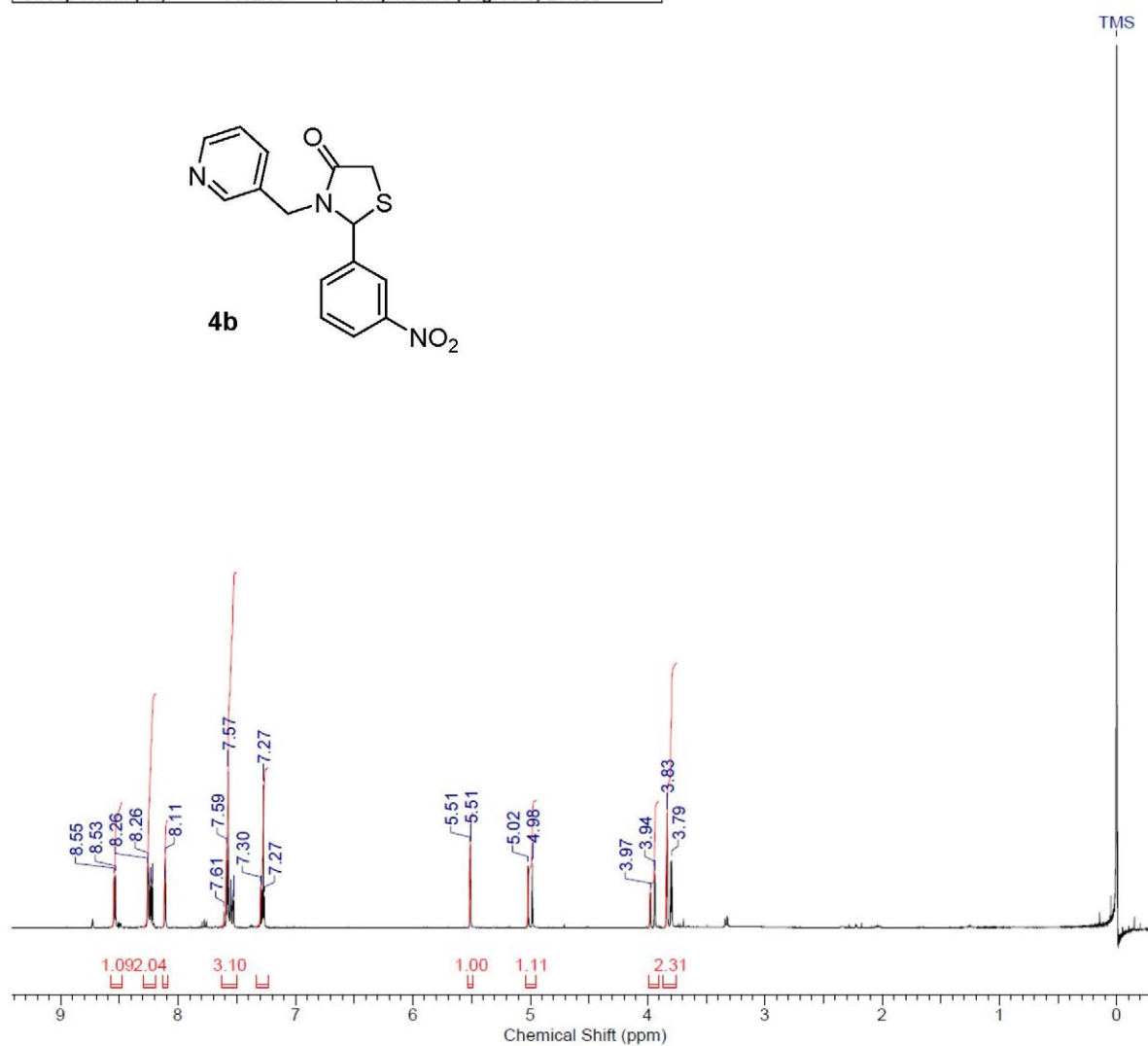


Figure S3. ¹H NMR spectrum (400 MHz, CDCl₃) of compound **4b**.

Acquisition Time (sec)	1.3005	Date	Apr 2 2013	File Name	F:\spectros AVA2 R 3-NO2\C13\fid.txt
Frequency (MHz)	100.60	Nucleus	13C	Number of Transients	2000
Original Points Count	31413	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24154.59		
Temperature (degree C)	19.000				

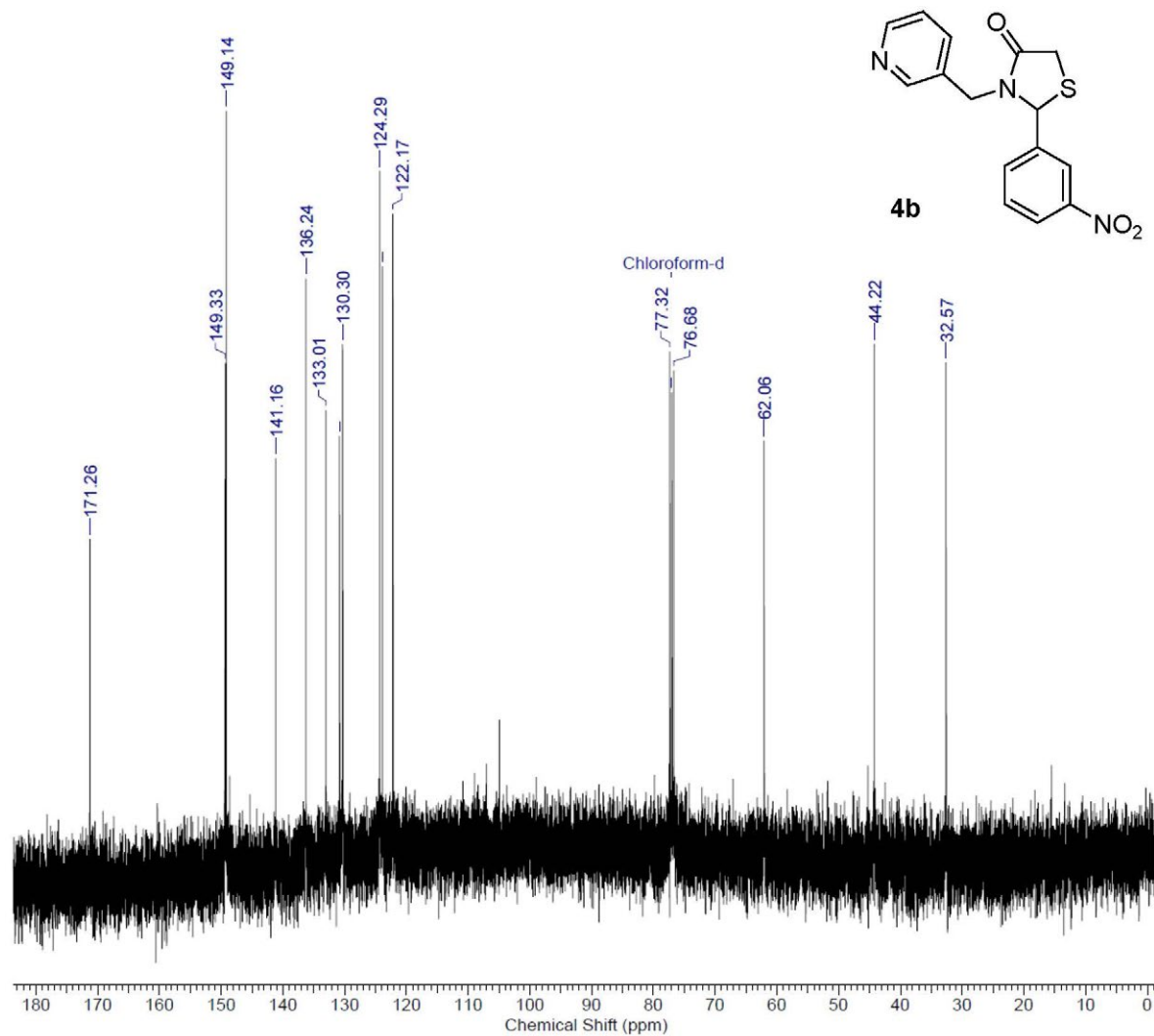


Figure S4. ^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **4b**.

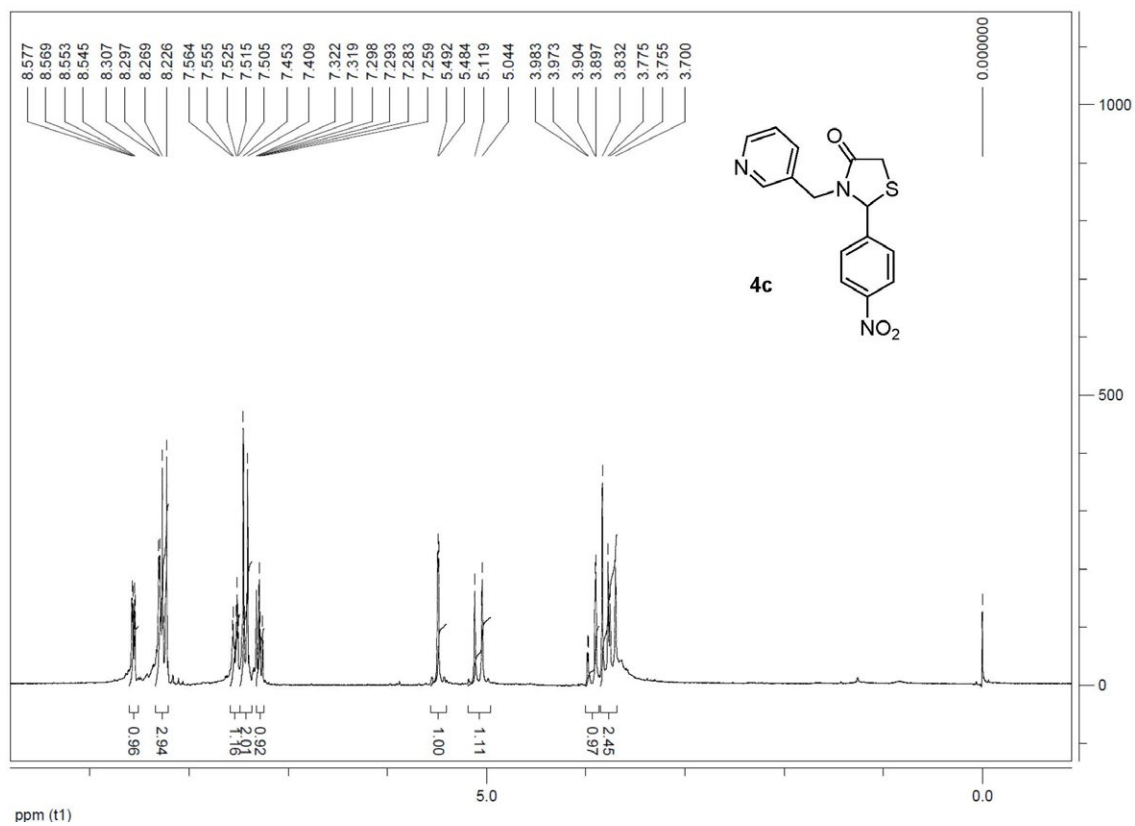


Figure S5. ¹H NMR spectrum (200 MHz, CDCl₃) of compound 4c.

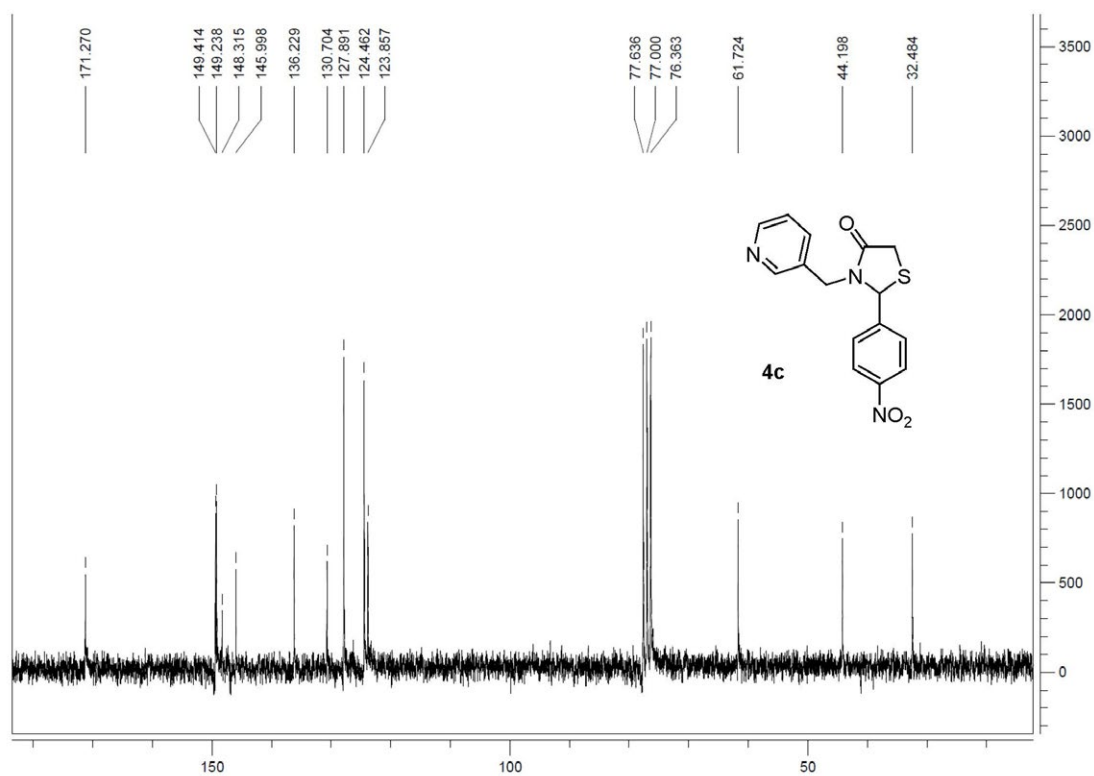


Figure S6. ¹³C NMR spectrum (50 MHz, CDCl₃) of compound 4c.

Acquisition Time (sec)	1.9980	Date	Apr. 2 2013	Frequency (MHz)	400.04
File Name	F:\espectros\AVA4 R 2-F\H1\fid.txt	Number of Transients	16	Original Points Count	12791
Nucleus	¹ H	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D
Points Count	16384	Temperature (degree C)	19.000		
Sweep Width (Hz)	6402.05				

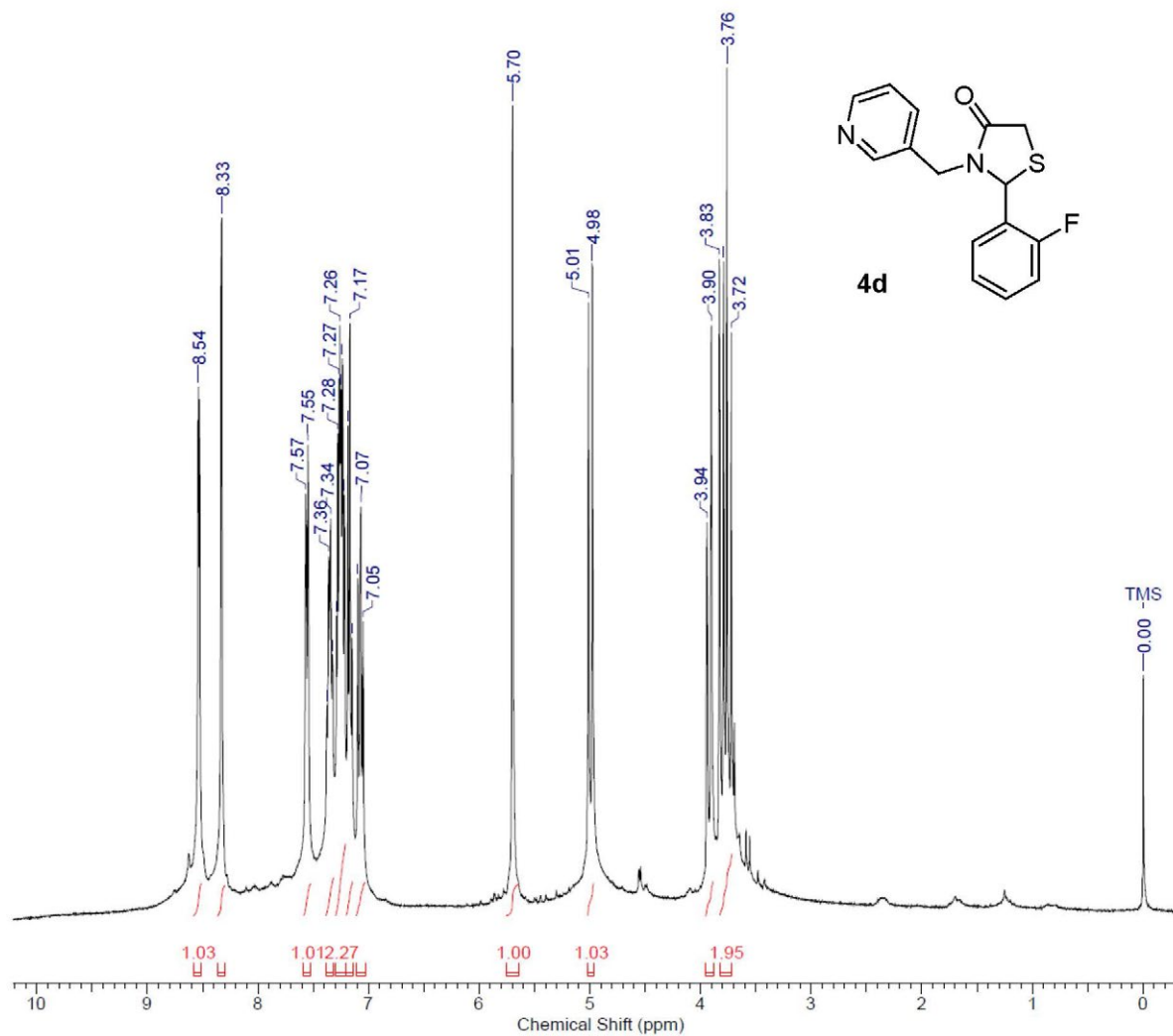


Figure S7. ¹H NMR spectrum (400 MHz, CDCl₃) of compound **4d**.

Acquisition Time (sec)	1.3005	Date	Apr 2 2013	File Name	F:\espectros AIA4 R 2-F1C13\fid.txt
Frequency (MHz)	100.60	Nucleus	13C	Number of Transients	2000
Original Points Count	31413	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24154.59		
Temperature (degree C)	19.000				

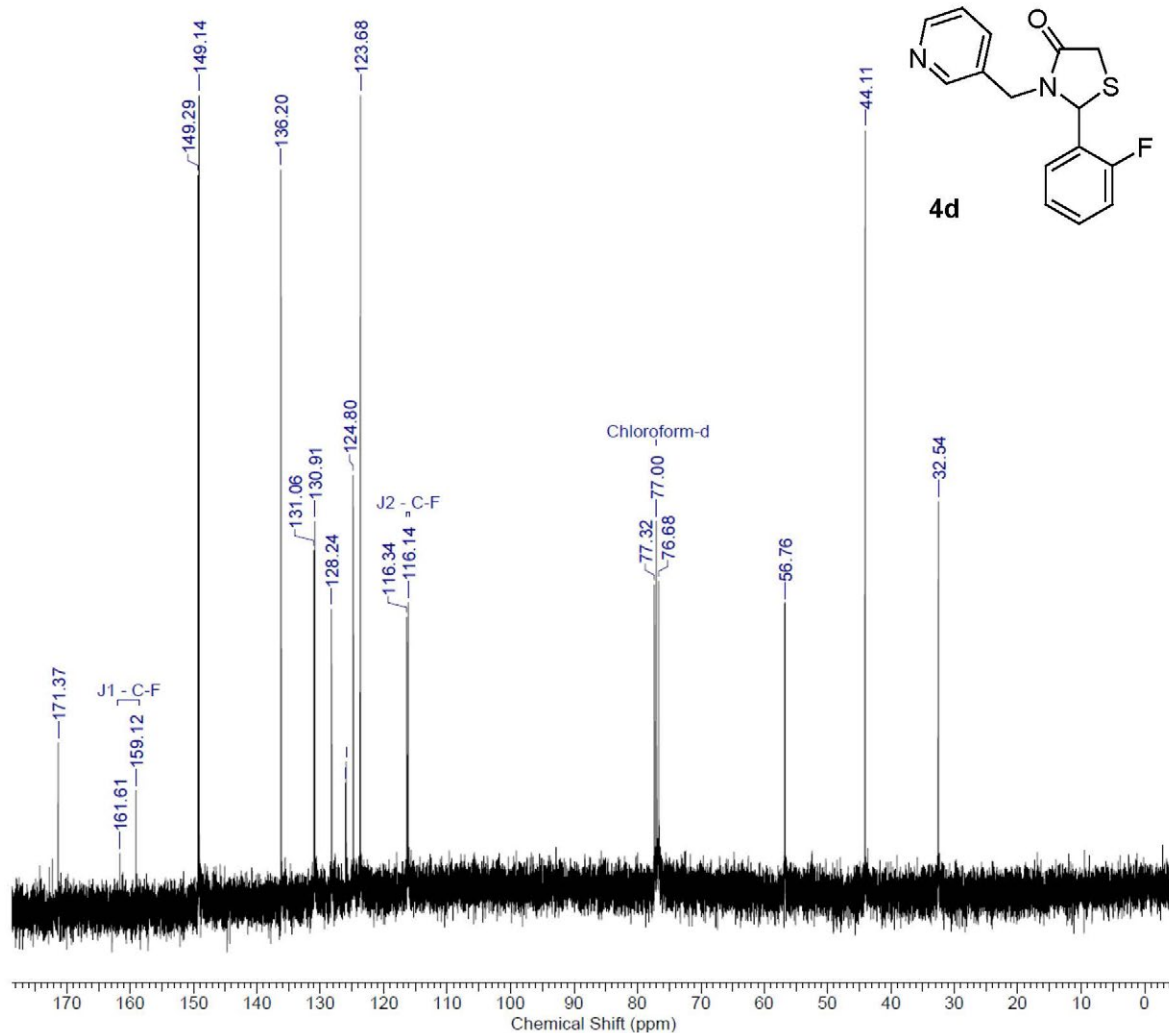


Figure S8. ^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **4d**.

Acquisition Time (sec)	1.9980	Date	Apr 1 2013
File Name	F:\espectros\A\A5 R 3-F\H1\fid.txt	Frequency (MHz)	400.04
Nucleus	¹ H	Number of Transients	16
Points Count	16384	Original Points Count	12791
Sweep Width (Hz)	6402.05	Pulse Sequence	s2pul
		Solvent	CHLOROFORM-D
		Temperature (degree C)	19.000

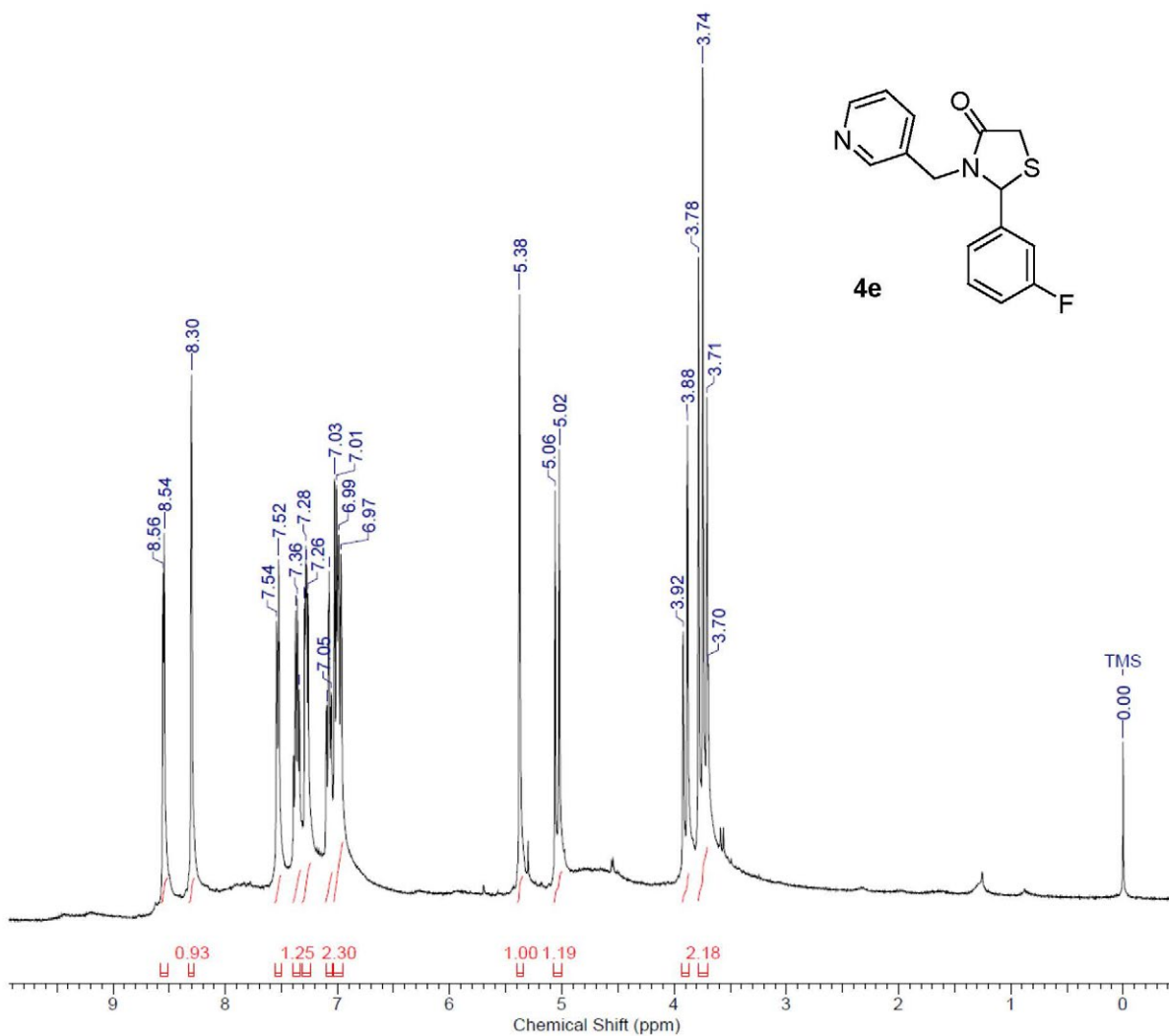


Figure S9. ¹H NMR spectrum (400 MHz, CDCl₃) of compound **4e**.

Acquisition Time (sec)	1.3005	Date	Apr 1 2013	File Name	F:\spectros\A\A5 R 3-FIC13\fid.txt
Frequency (MHz)	100.60	Nucleus	13C	Number of Transients	2200
Original Points Count	31413	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24154.59		
Temperature (degree C)	19.000				

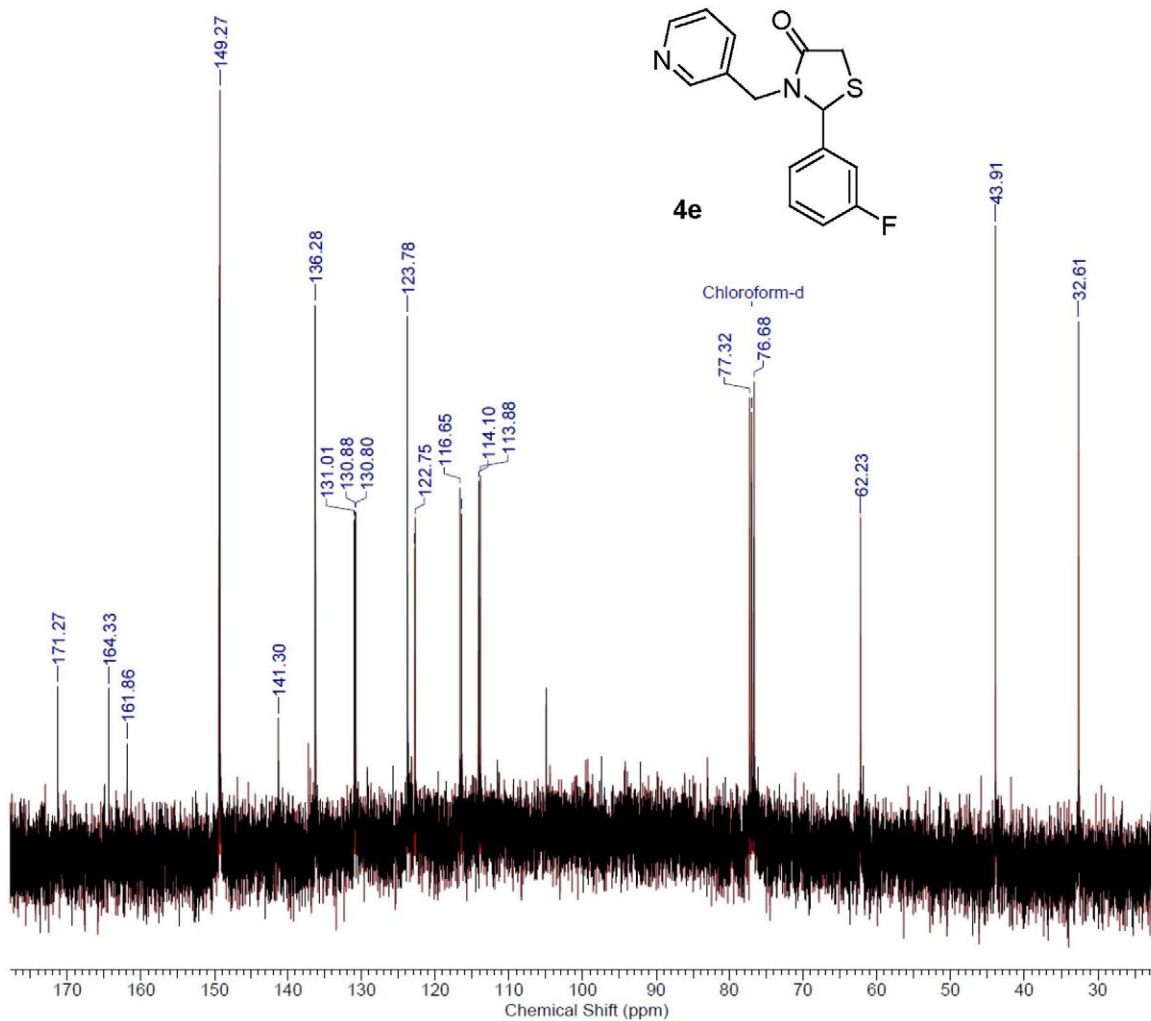


Figure S10. ^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **4e**.

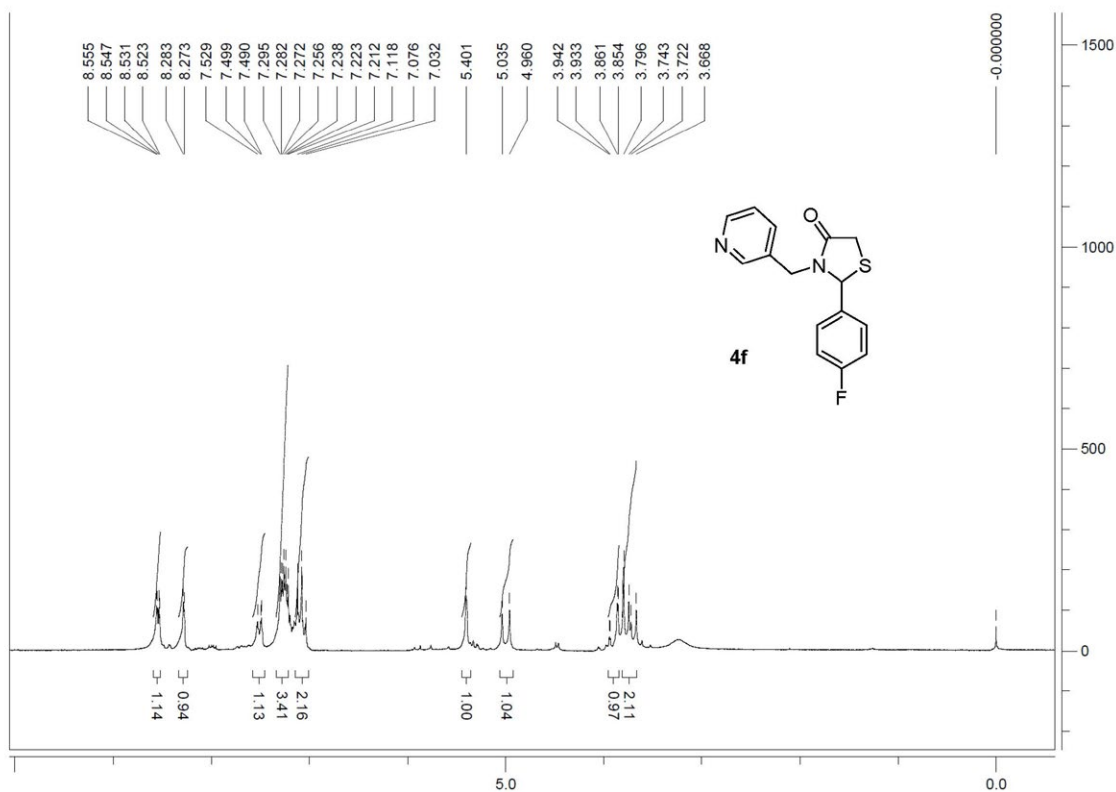


Figure S11. ¹H NMR spectrum (200 MHz, CDCl₃) of compound 4f.

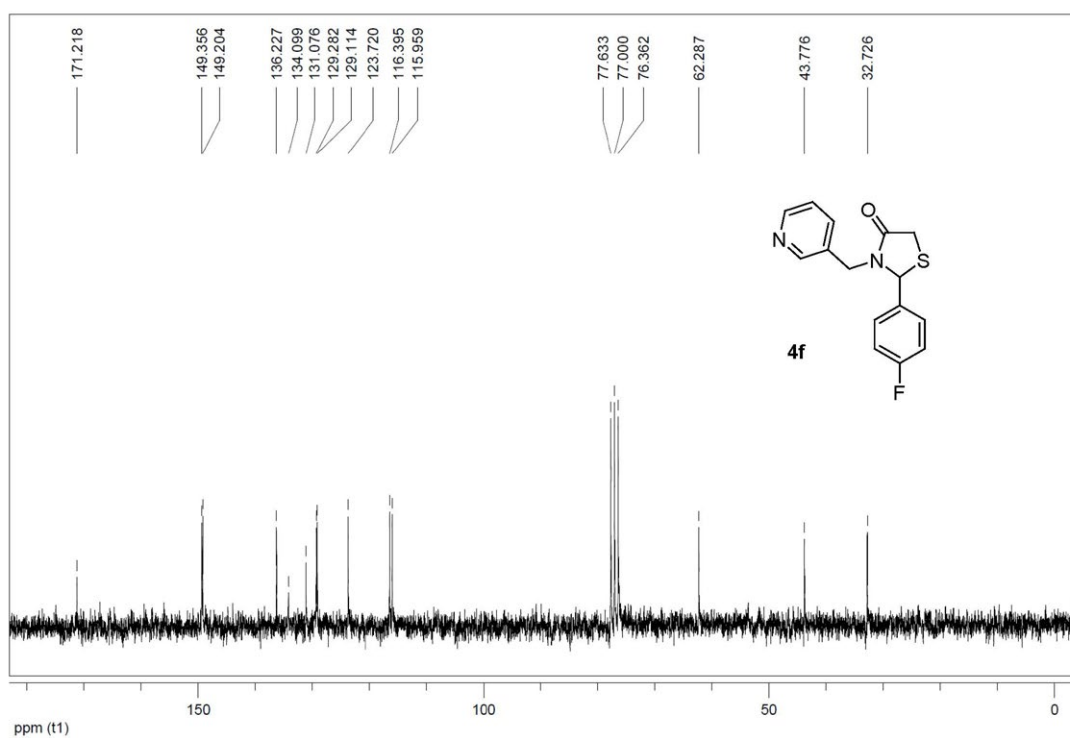


Figure S12. ¹³C NMR spectrum (50 MHz, CDCl₃) of compound 4f.

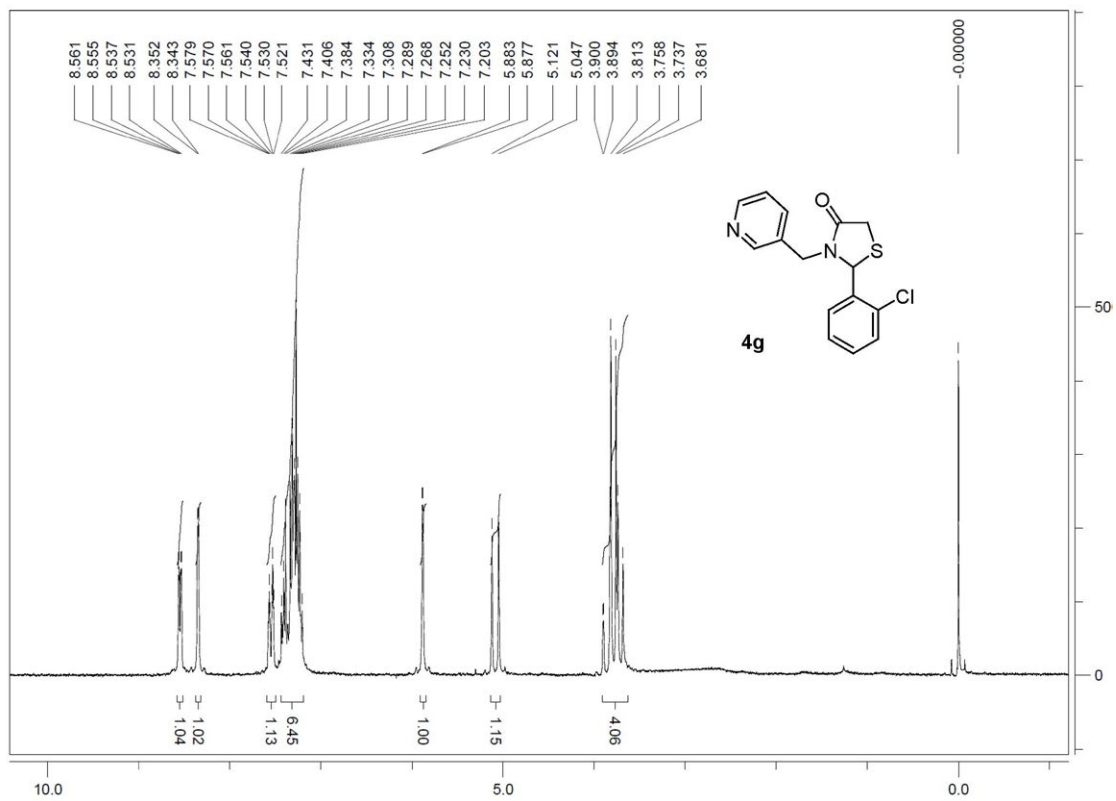


Figure S13. ¹H NMR spectrum (200 MHz, CDCl₃) of compound **4g**.

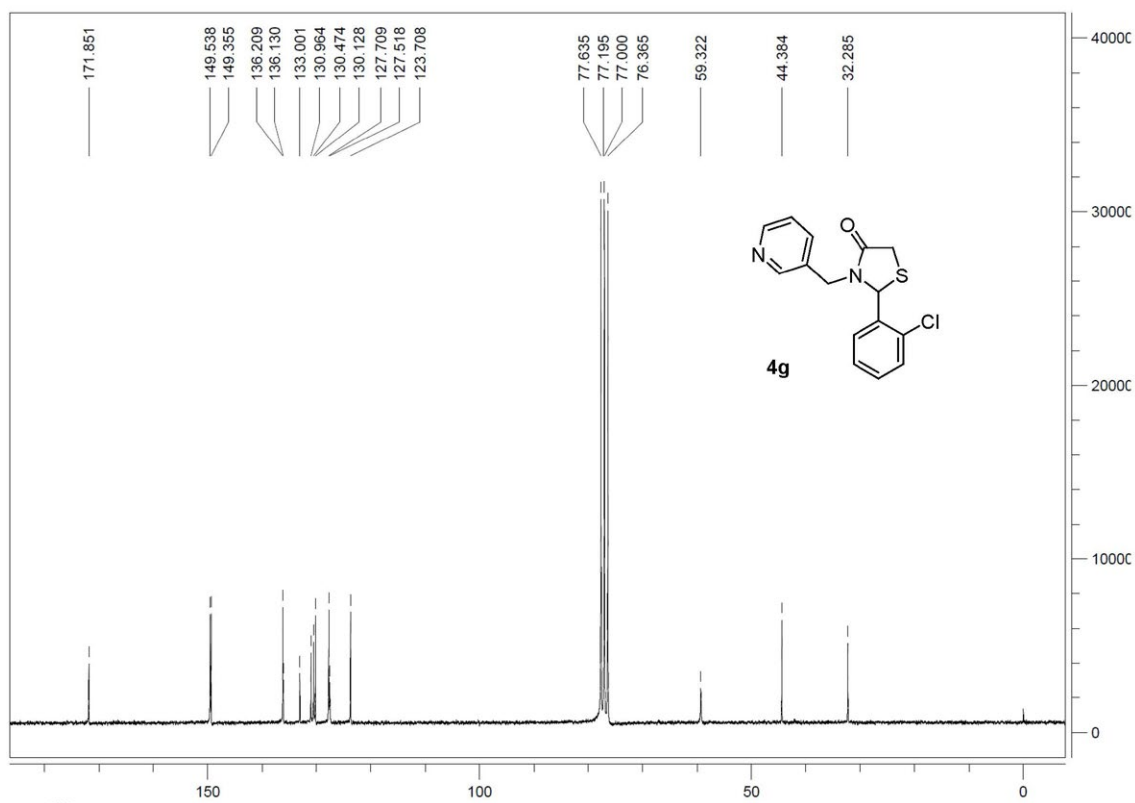


Figure S14. ¹³C NMR spectrum (50 MHz, CDCl₃) of compound **4g**.

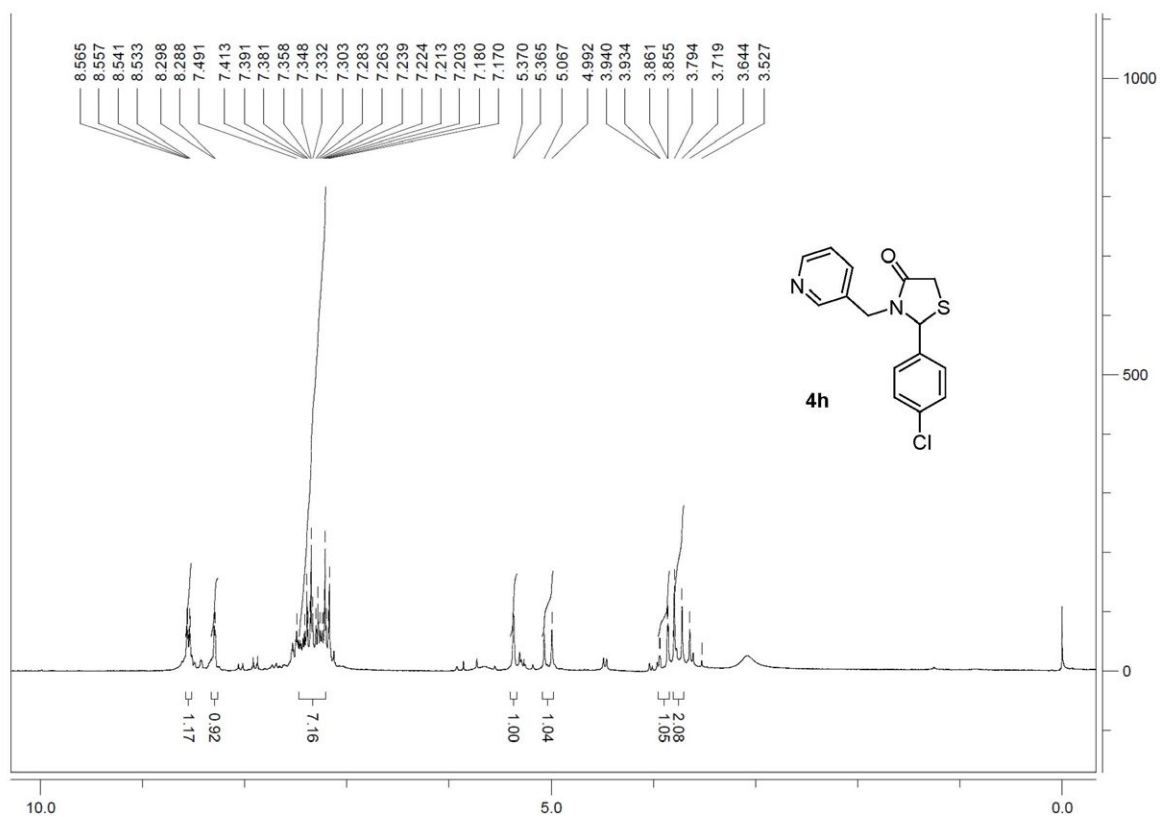


Figure S15. ¹H NMR spectrum (200 MHz, CDCl₃) of compound 4h.

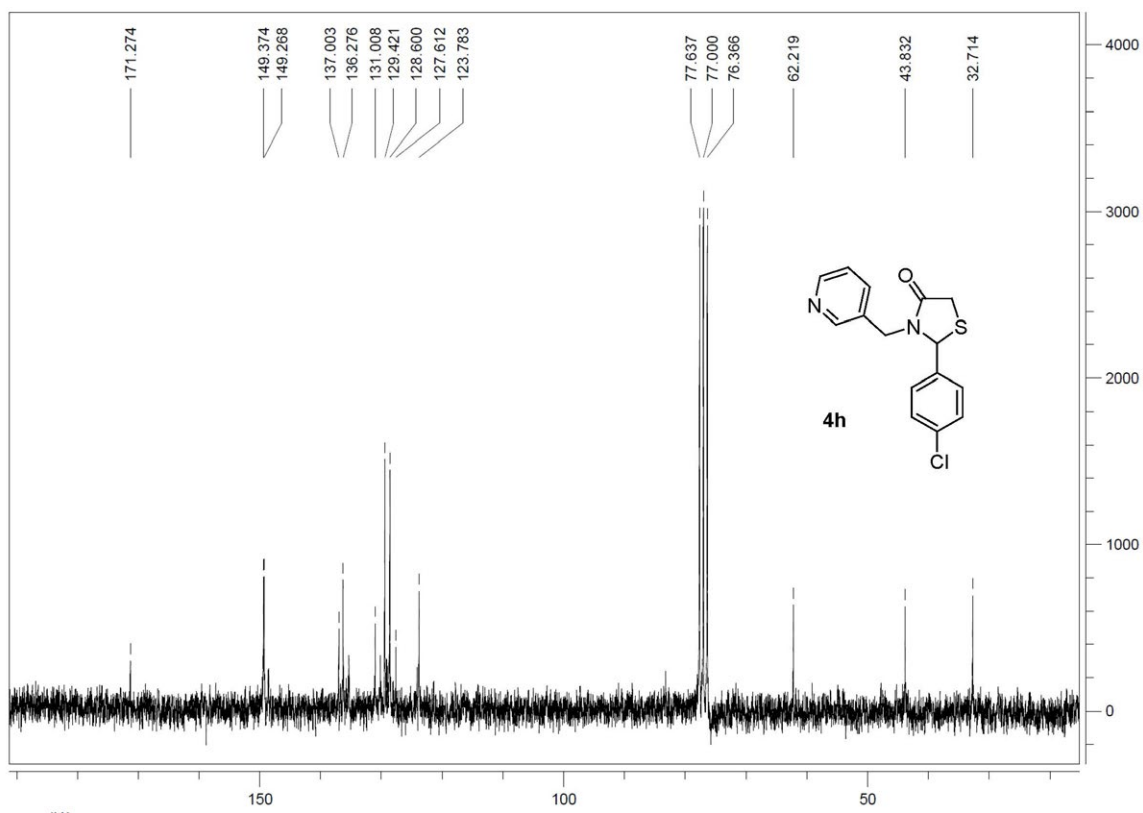


Figure S16. ¹³C NMR spectrum (50 MHz, CDCl₃) of compound 4h.

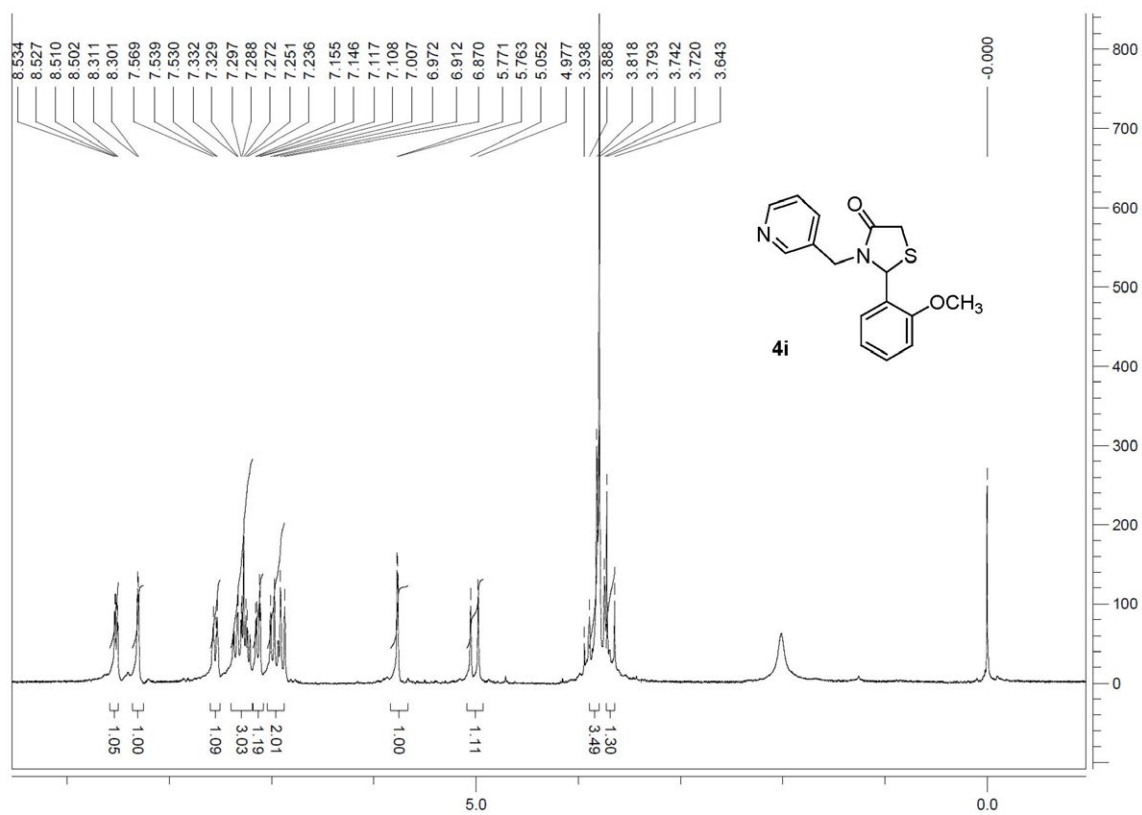


Figure S17. ¹H NMR spectrum (200 MHz, CDCl₃) of compound **4i**.

Acquisition Time (sec)	1.3005	Date	Apr 8 2013	Frequency (MHz)	100.60
File Name	F:\espectros\AA9 R 2-OCH3\C13\fid.txt	Number of Transients	2800	Original Points Count	31413
Nucleus	13C	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D
Points Count	32768	Temperature (degree C)	19.000		
Sweep Width (Hz)	24154.59				

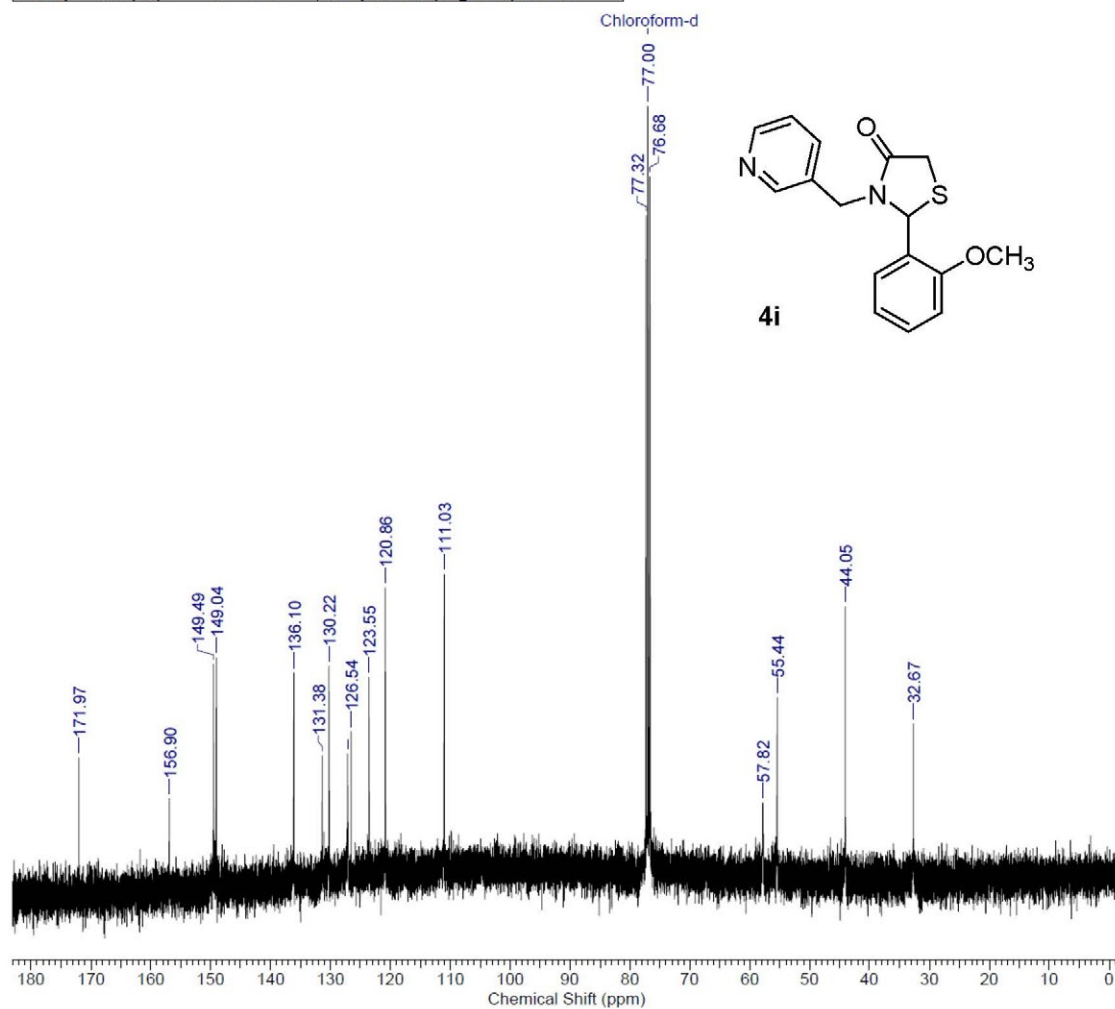


Figure S18. ^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **4i**.

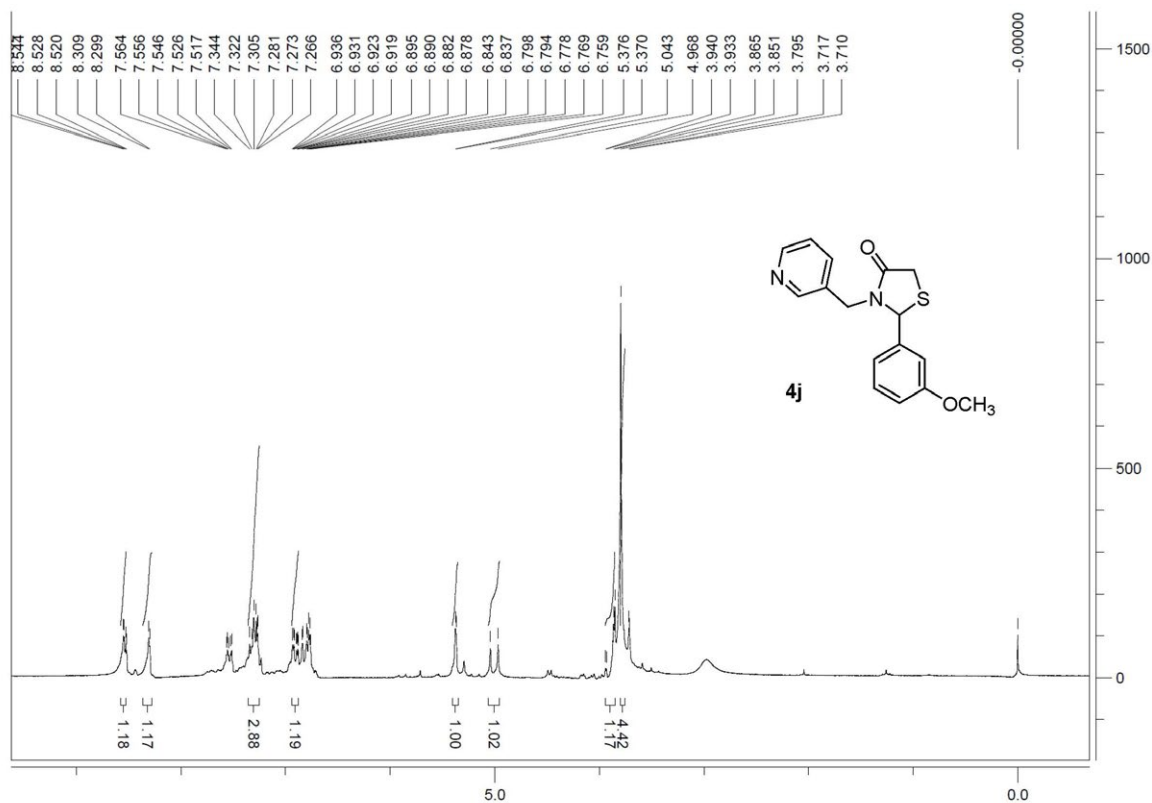


Figure S19. ¹H NMR spectrum (200 MHz, CDCl₃) of compound **4j**.

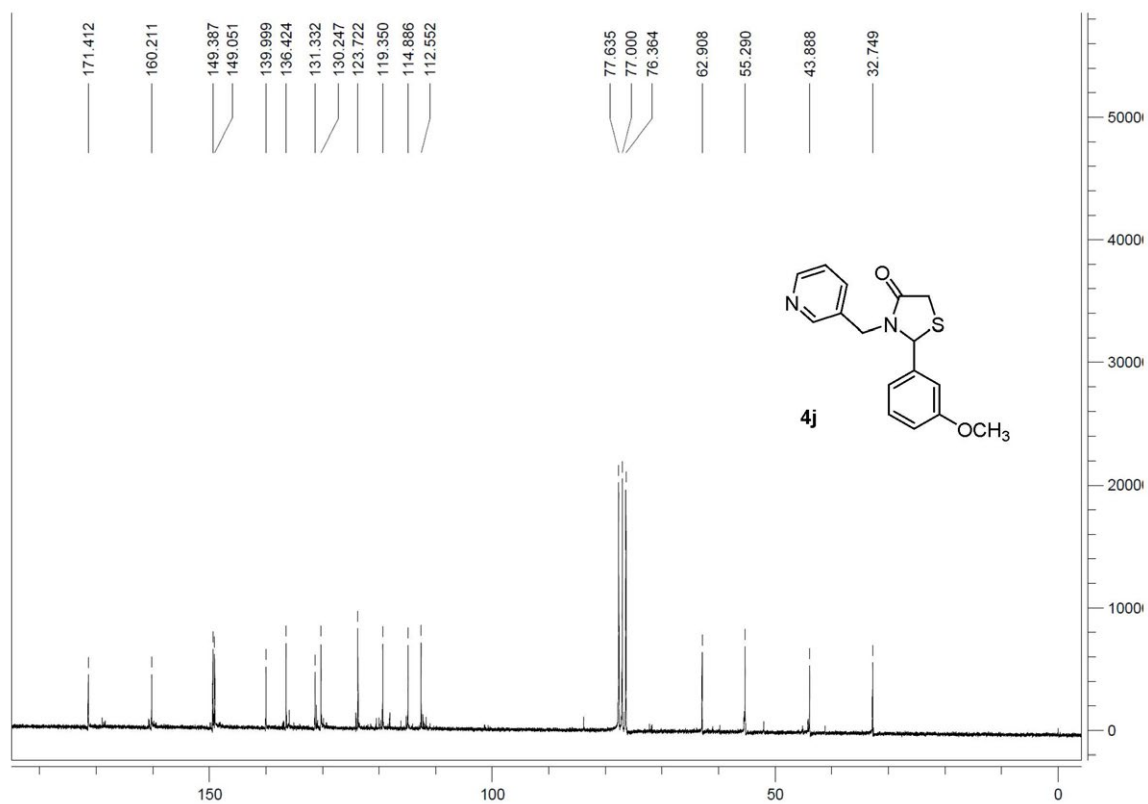


Figure S20. ¹³C NMR spectrum (50 MHz, CDCl₃) of compound **4j**.

Acquisition Time (sec)	1.9980	Date	Apr 4 2013	Frequency (MHz)	400.04
File Name	F:\espectros AA11 R 4-OCH3\H1 melhorfid.txt	Number of Transients	16	Original Points Count	12791
Nucleus	¹ H	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D
Points Count	16384	Temperature (degree C)	19.000		
Sweep Width (Hz)	6402.05				

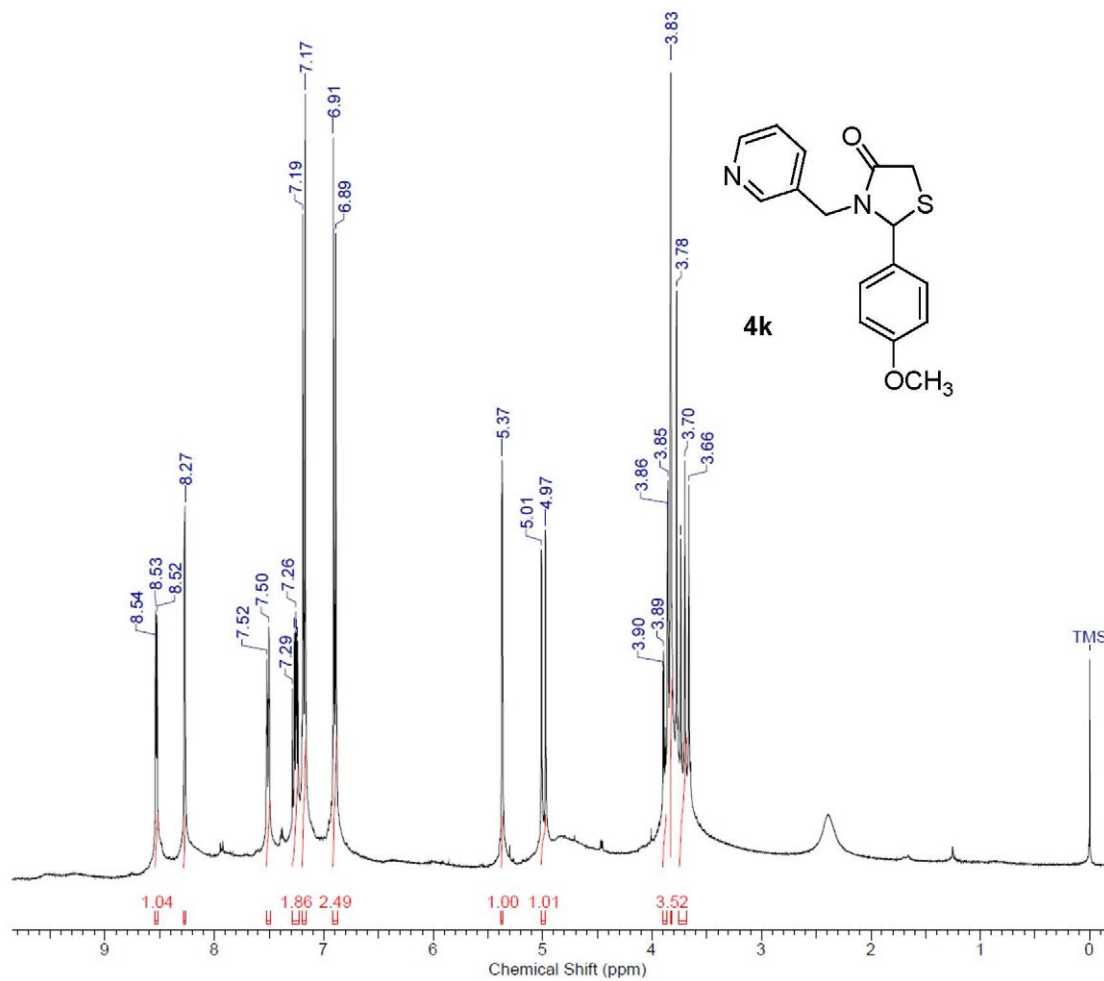


Figure S21. ¹H NMR spectrum (400 MHz, CDCl₃) of compound **4k**.

Acquisition Time (sec)	1.3005	Date	Apr 4 2013
File Name	F:\espectros A\A11 R 4-OCH3\13\fid.txt	Frequency (MHz)	100.60
Nucleus	13C	Number of Transients	2000
Points Count	32768	Pulse Sequence	s2pul
Sweep Width (Hz)	24154.59	Temperature (degree C)	19.000
		Original Points Count	31413
		Solvent	CHLOROFORM-D

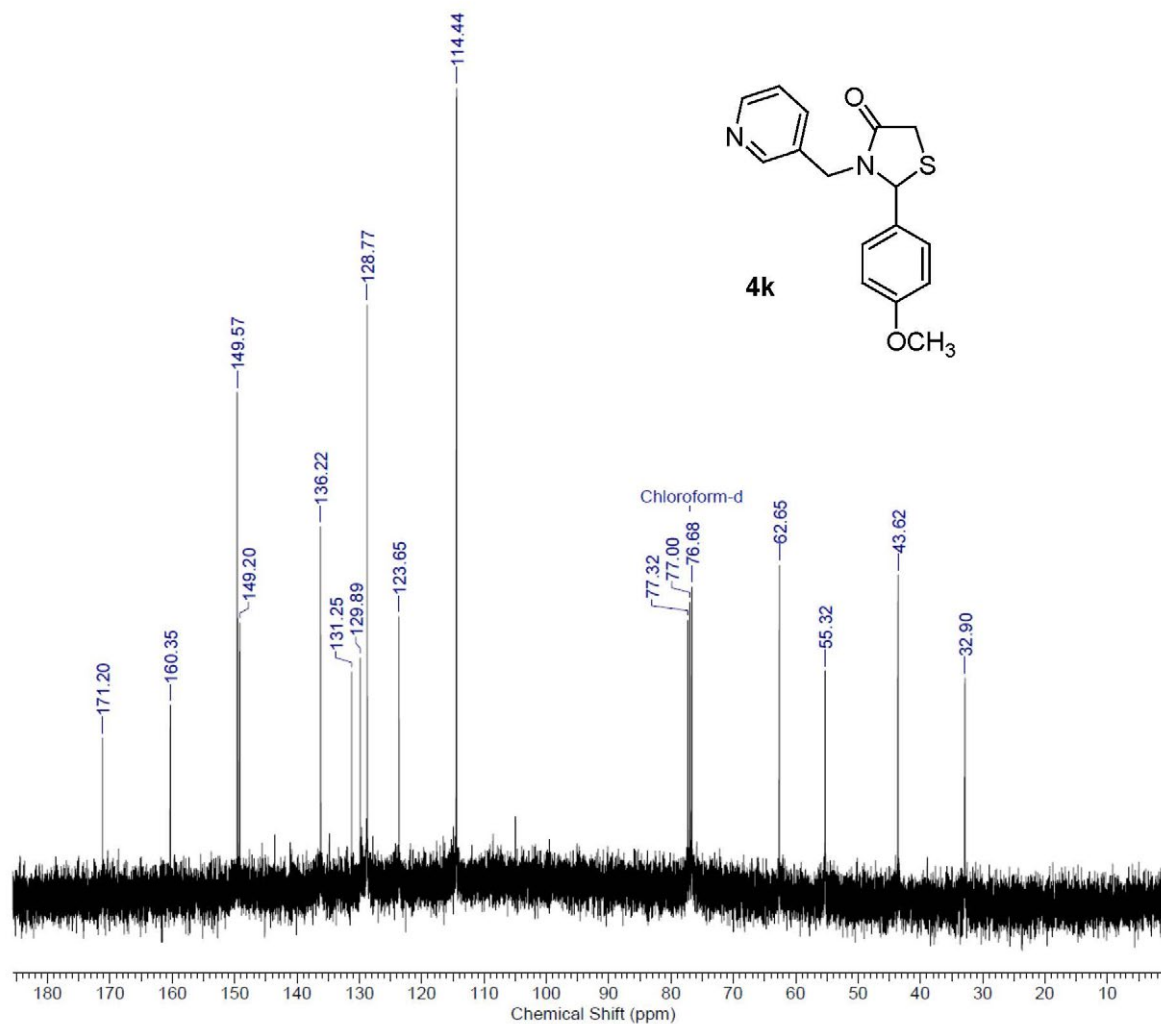


Figure S22. ^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **4k**.

Acquisition Time (sec)	1.9980	Date	Jun 21 2012		
File Name	E:\artigo\antioxidant\adriana\A17 2-OH FAZER\2\fid.txt		Frequency (MHz)	400.04	
Nucleus	1H	Number of Transients	8	Original Points Count	12791
Points Count	16384	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D
Sweep Width (Hz)	6402.05	Temperature (degree C)	20.000		

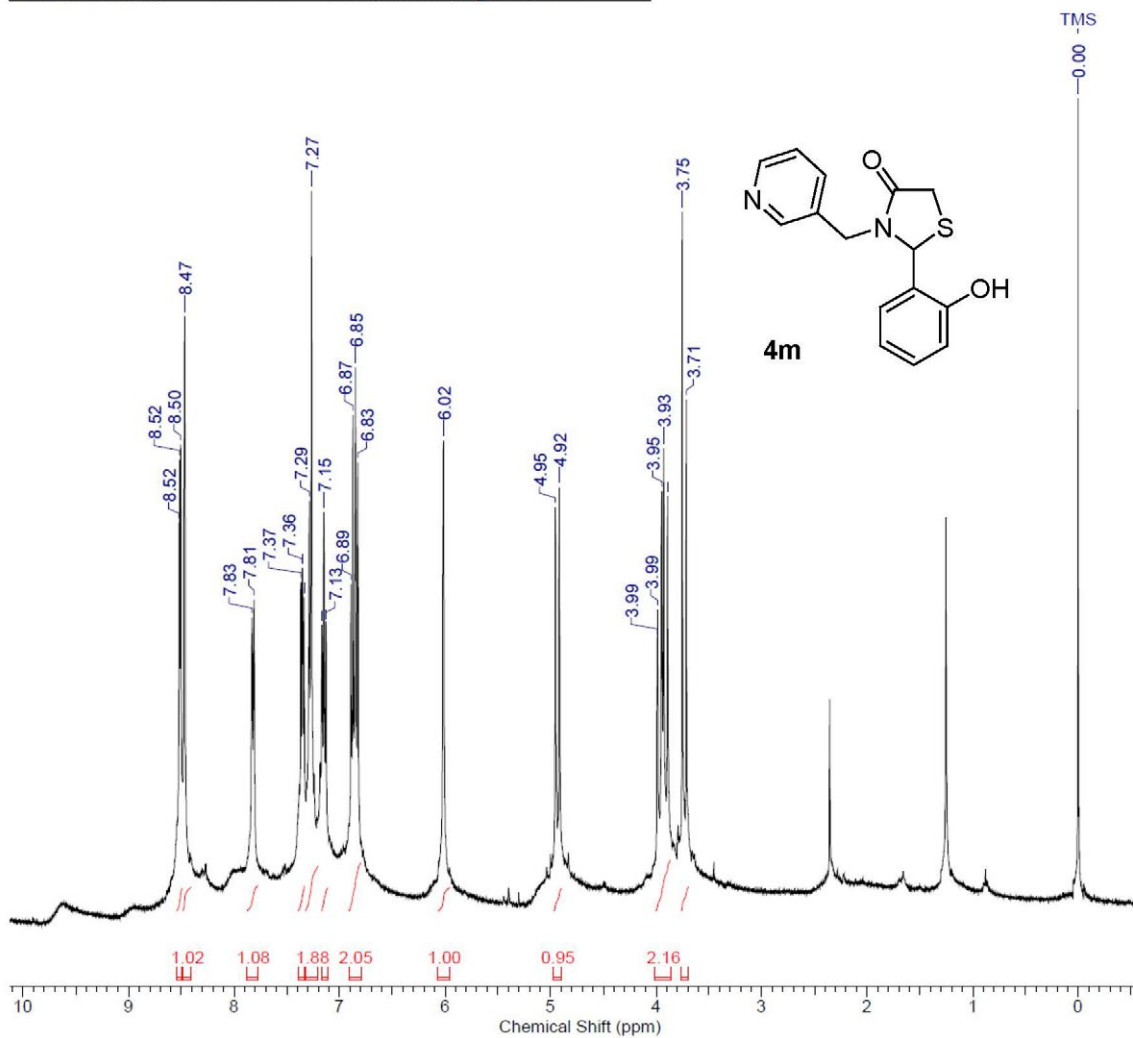


Figure S23. ¹H NMR spectrum (400 MHz, CDCl₃) of compound **4m**.

Acquisition Time (sec)	1.3005	Date	Sep 26 2012		
File Name	E:\artigo\antioxidant\adriana\A17 2-OH FAZERA\A17 C\fid.txt				
Frequency (MHz)	100.60	Nucleus	¹³ C	Number of Transients	28000
Original Points Count	31413	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D	Sweep Width (Hz)	24154.59		
Temperature (degree C)	22.000				

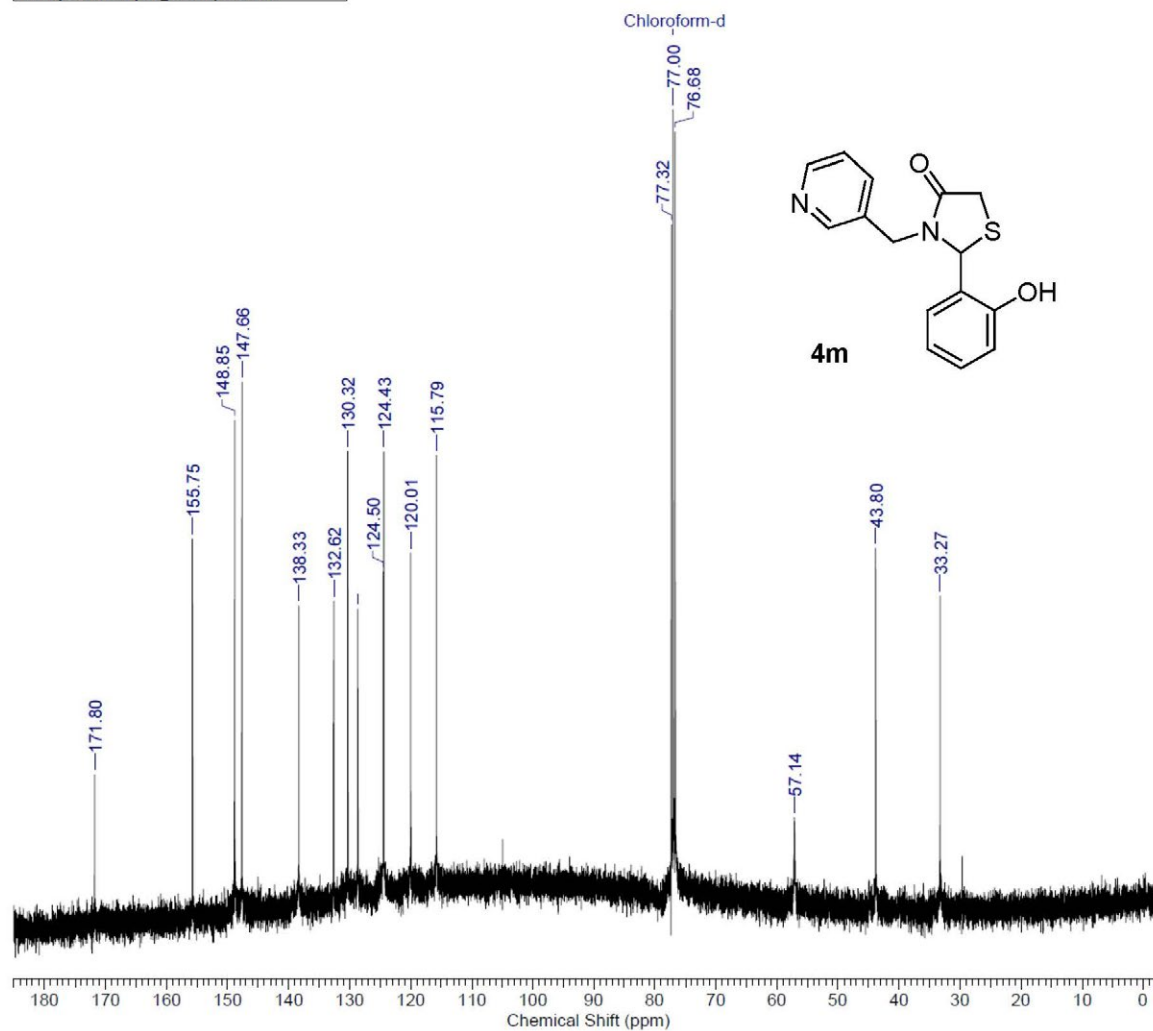


Figure S24. ¹³C NMR spectrum (100 MHz, CDCl₃) of compound **4m**.

Acquisition Time (sec)	1.9980	Date	Apr 4 2013			
File Name	E:\artigo\antioxidant\adriana\A15 R 3-OH FAZER\H1\fid.txt					
Frequency (MHz)	400.04	Nucleus	1H	Number of Transients	16	
Original Points Count	12791	Points Count	16384	Pulse Sequence	s2pul	
Solvent	CHLOROFORM-D		Sweep Width (Hz)			6402.05
Temperature (degree C)	19.000					

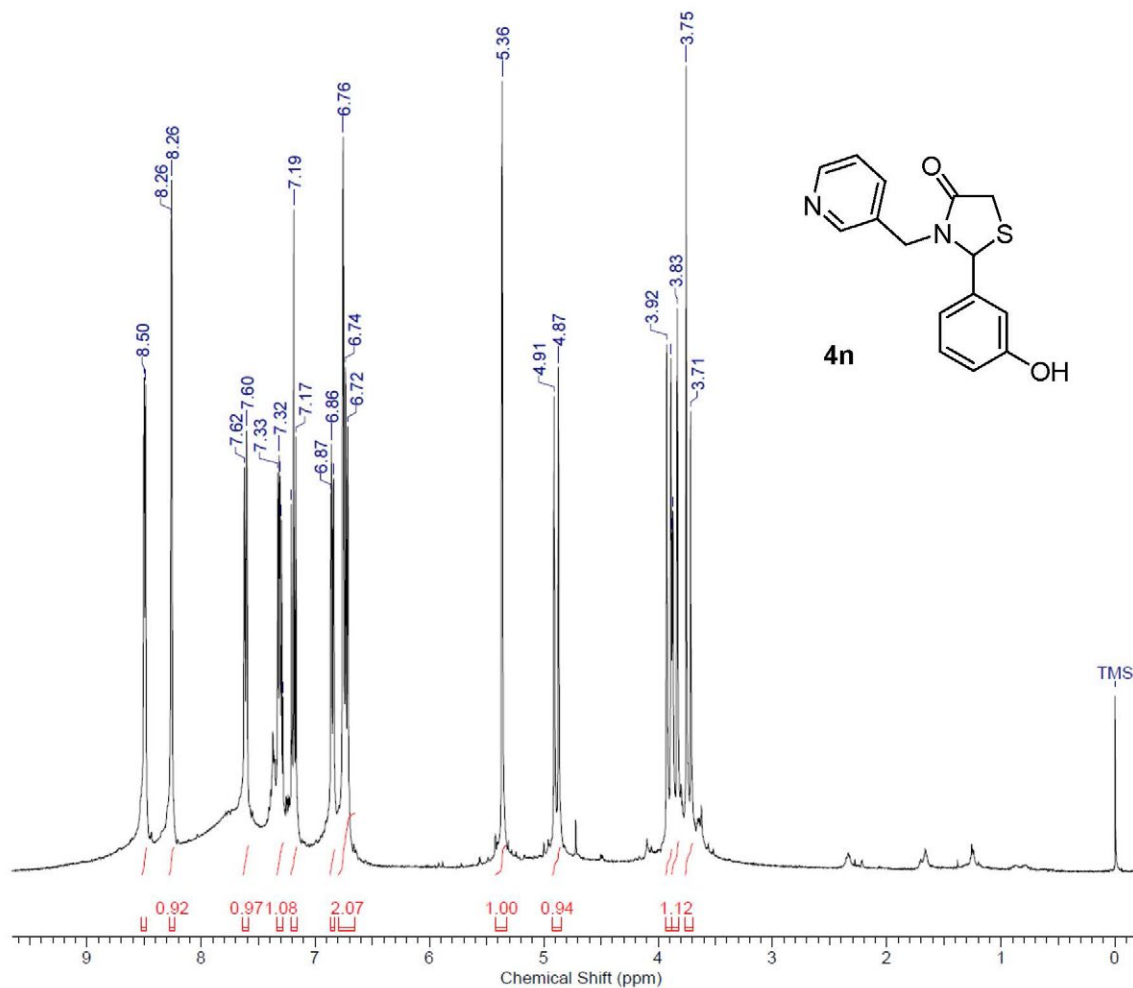


Figure S25. ¹H NMR spectrum (400 MHz, CDCl₃) of compound **4n**.

Acquisition Time (sec)	1.3005	Date	Apr 4 2013		
File Name	E:\artigo\antioxidant\adriana\A15 R 3-OH FAZER\C13\fid.txt				
Frequency (MHz)	100.60	Nucleus	¹³ C	Number of Transients	2000
Original Points Count	31413	Points Count	32768	Pulse Sequence	s2pul
Solvent	CHLOROFORM-D		Sweep Width (Hz)	24154.59	
Temperature (degree C)	19.000				

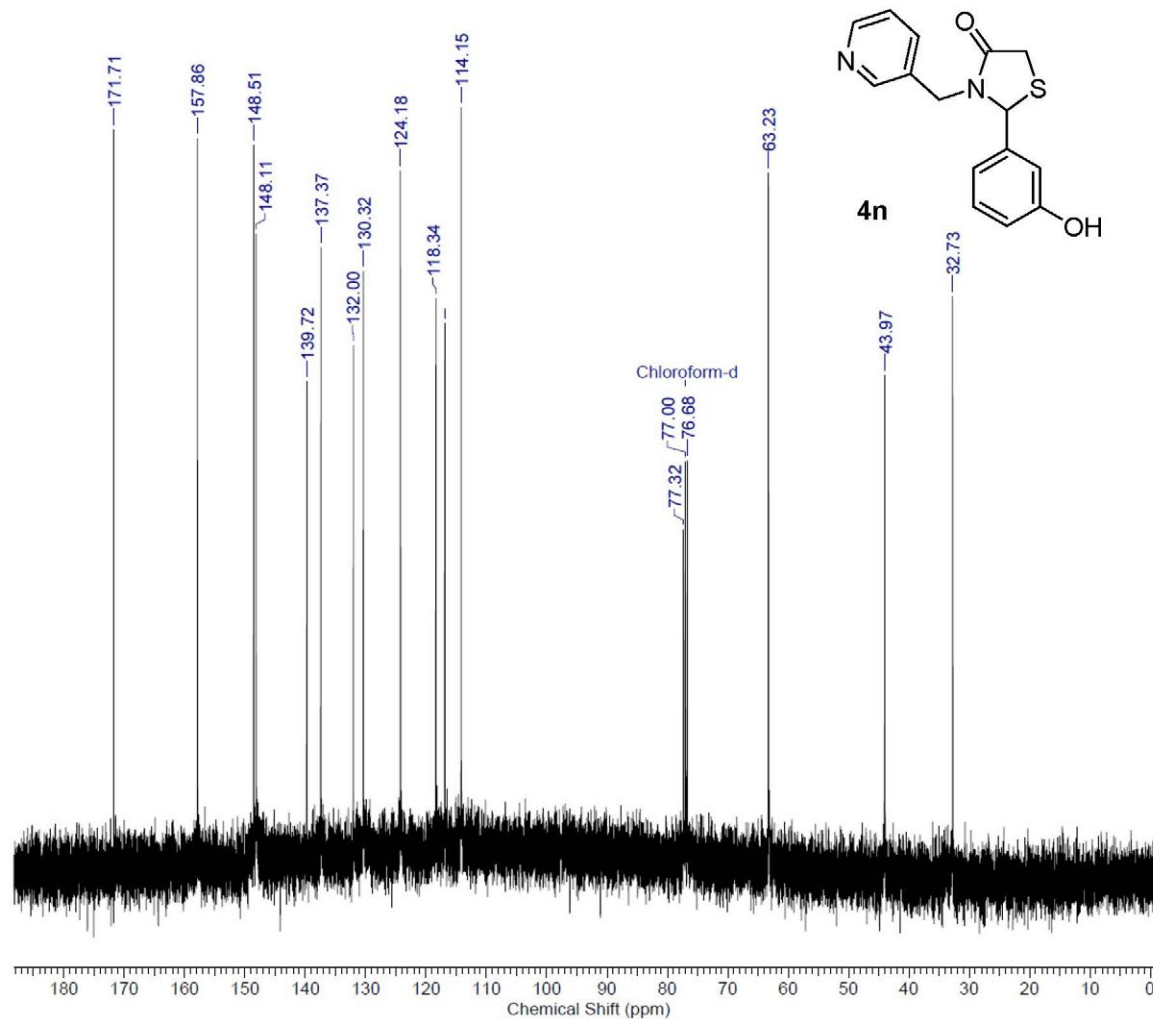


Figure S26. ¹³C NMR spectrum (100 MHz, CDCl₃) of compound **4n**.

Acquisition Time (sec)	1.9980	Date	Apr 4 2013	Frequency (MHz)	400.04
File Name	G:\artigo\antioxidant\adriana\A16 4-OH\H1	Number of Transients	16	Original Points Count	12791
Nucleus	¹ H	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D
Points Count	16384	Temperature (degree C)	19.000		
Sweep Width (Hz)	6402.05				

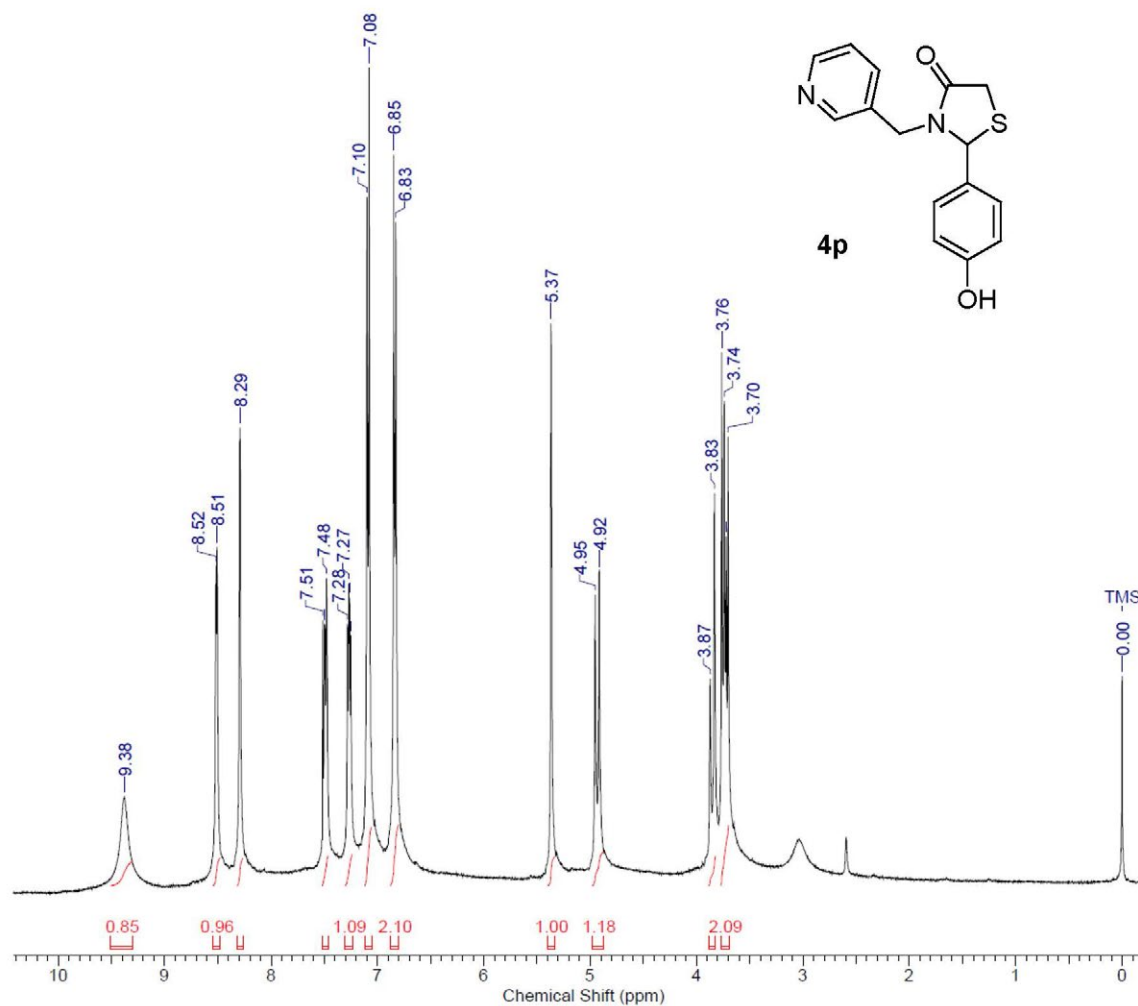


Figure S27. ¹H NMR spectrum (400 MHz, CDCl₃) of compound **4o**.

Acquisition Time (sec)	1.9980	Date	Apr 4 2013	Frequency (MHz)	400.04
File Name	G:\artigol\antioxidant\adriana\A16 4-OH\H1	Number of Transients	16	Original Points Count	12791
Nucleus	¹ H	Pulse Sequence	s2pul	Solvent	CHLOROFORM-D
Points Count	16384	Temperature (degree C)	19.000		
Sweep Width (Hz)	6402.05				

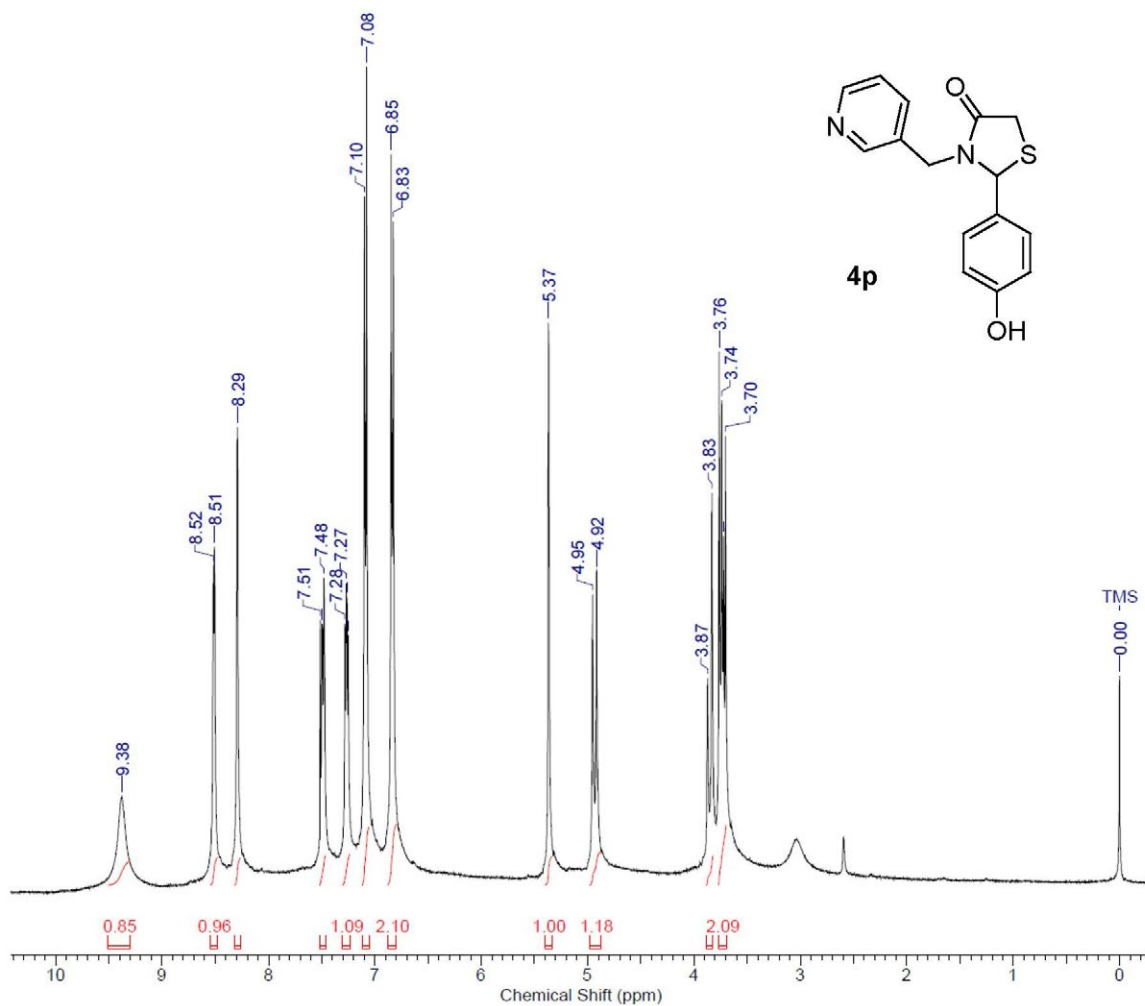
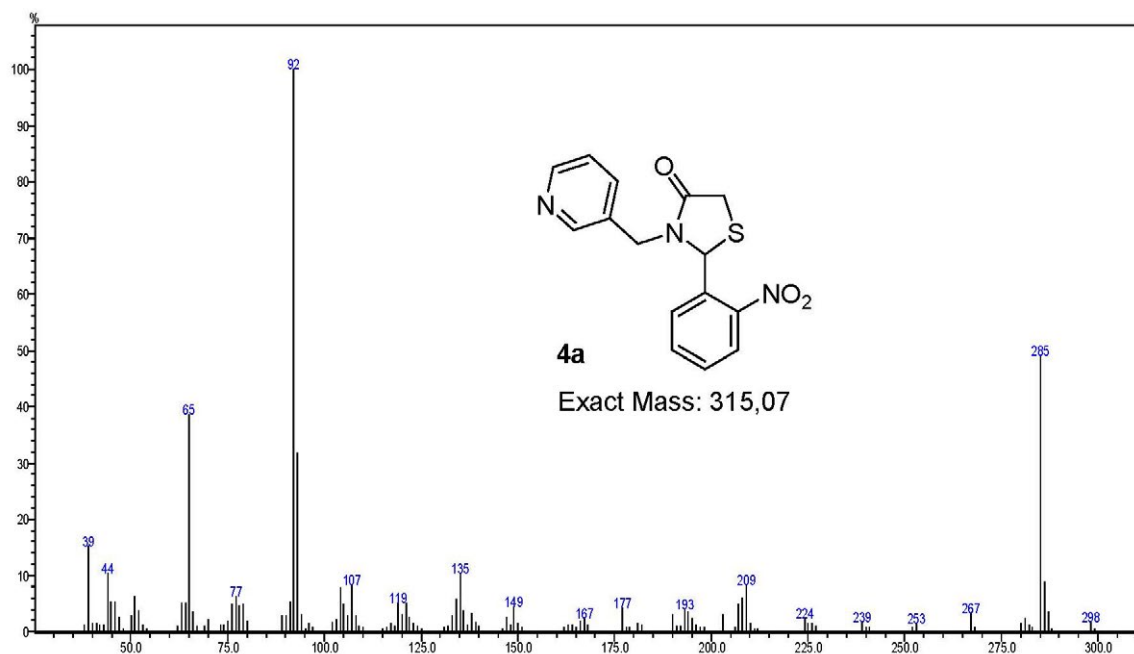
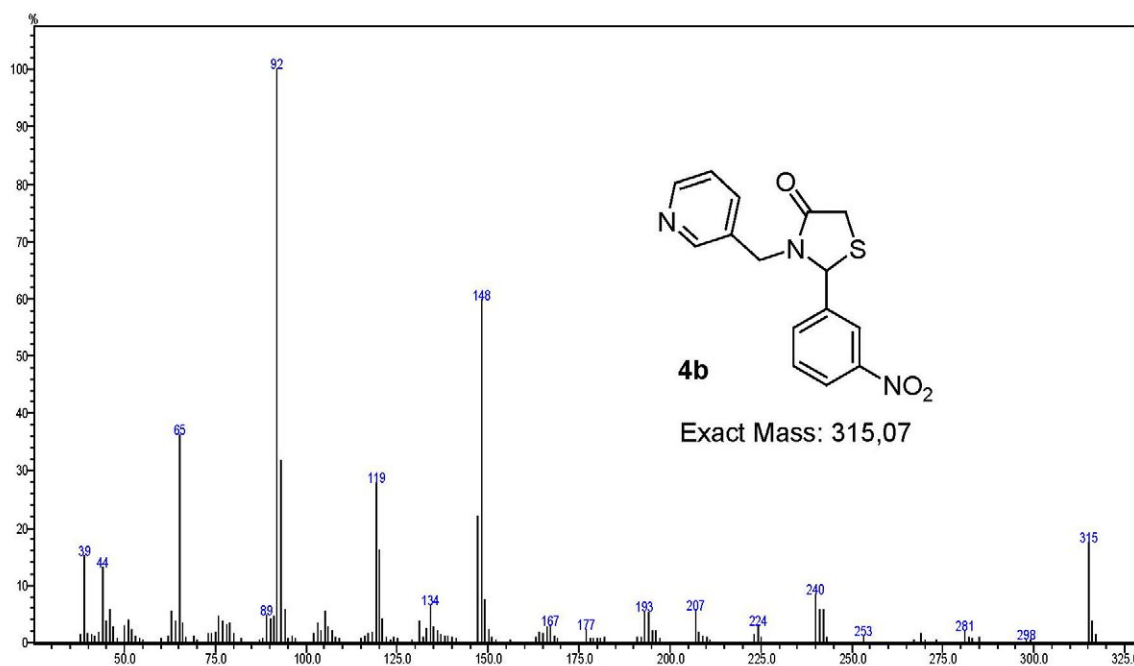


Figure S28. ¹³C NMR spectrum (100 MHz, CDCl₃) of compound **4o**.

Figure S29. Mass spectrum of compound **4a**.Figure S30. Mass spectrum of compound **4b**.

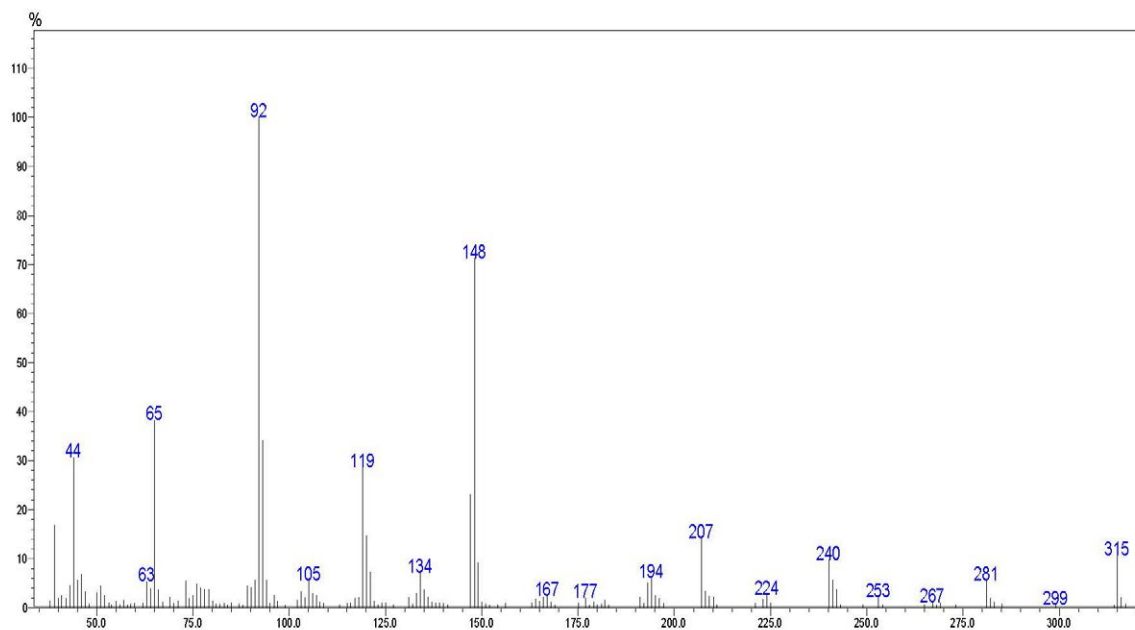


Figure S31. Mass spectrum of compound 4c.

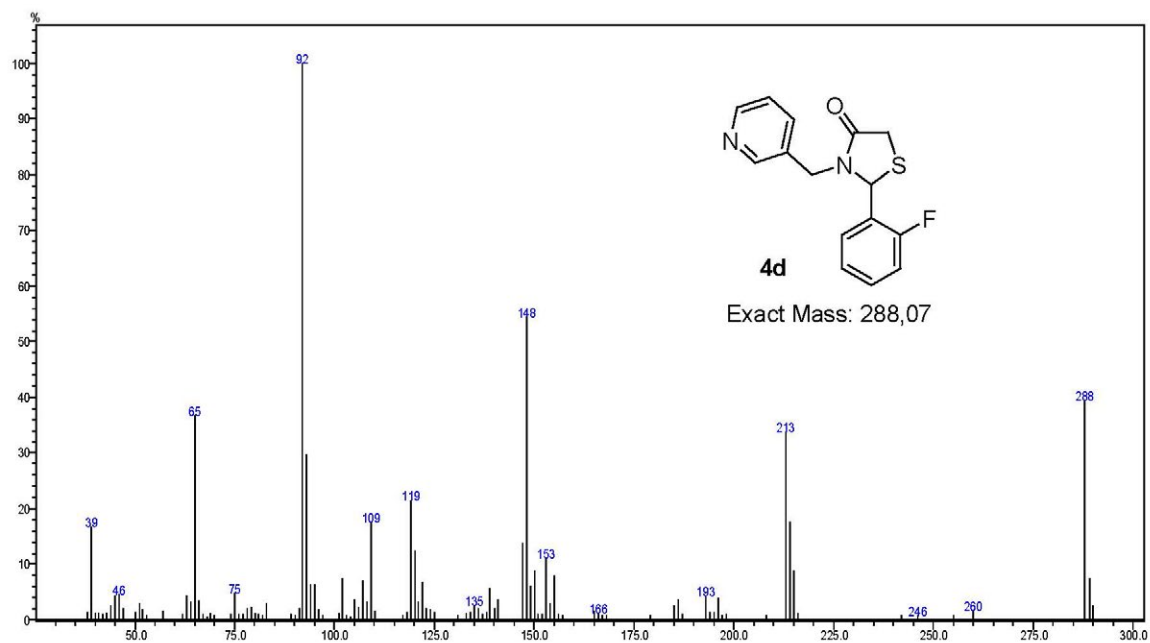
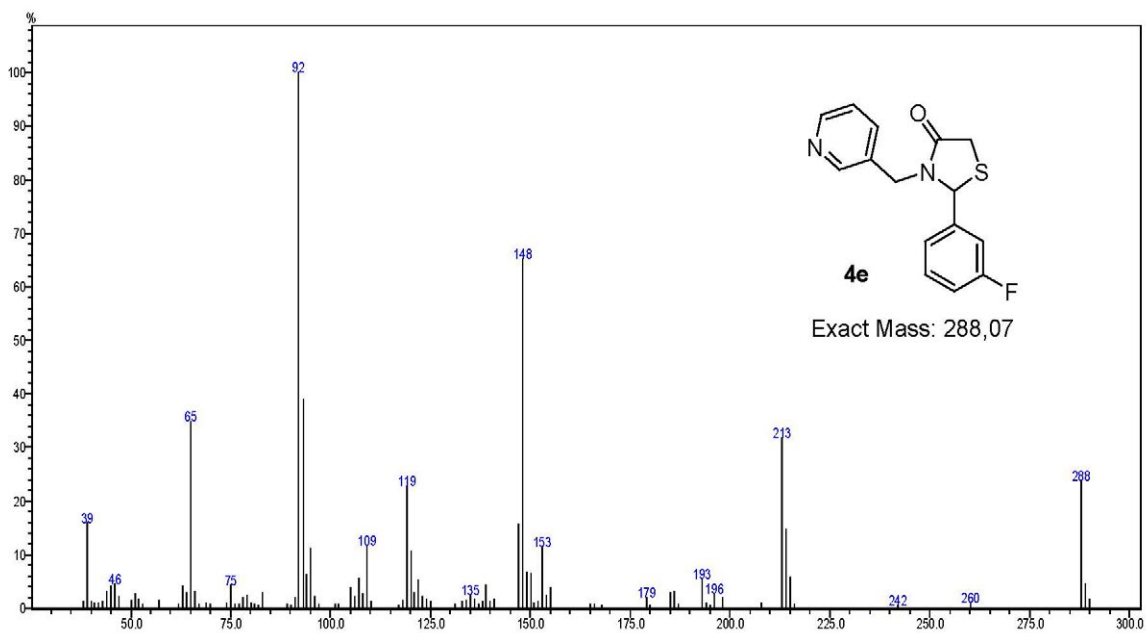
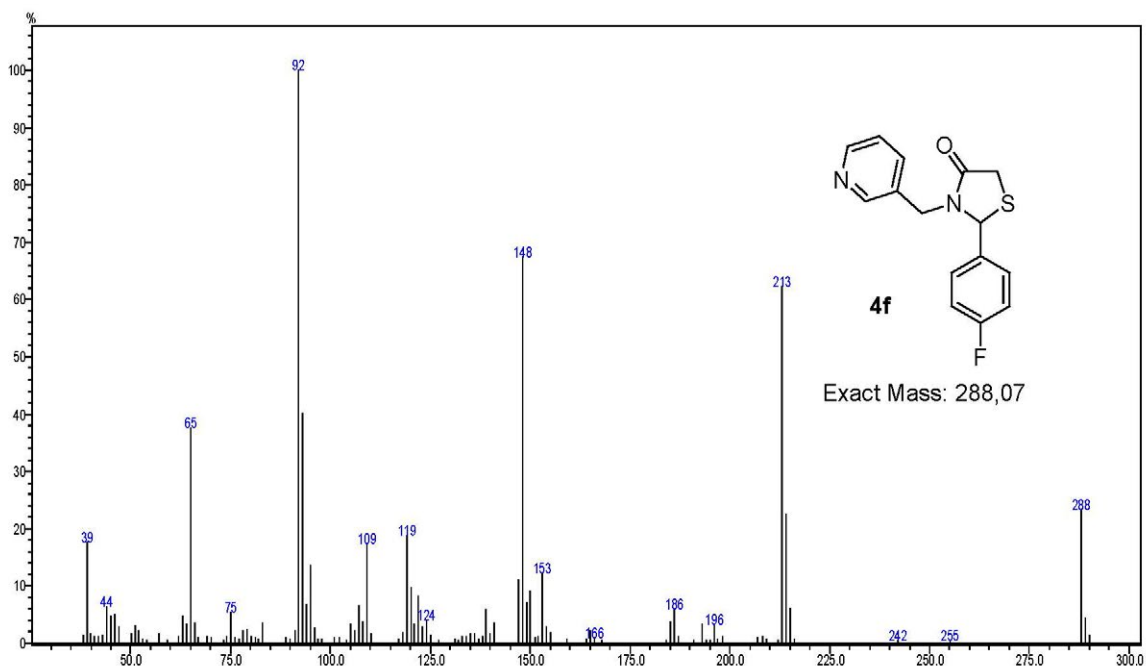


Figure S32. Mass spectrum of compound 4d.

Figure S33. Mass spectrum of compound **4e**.Figure S34. Mass spectrum of compound **4f**.

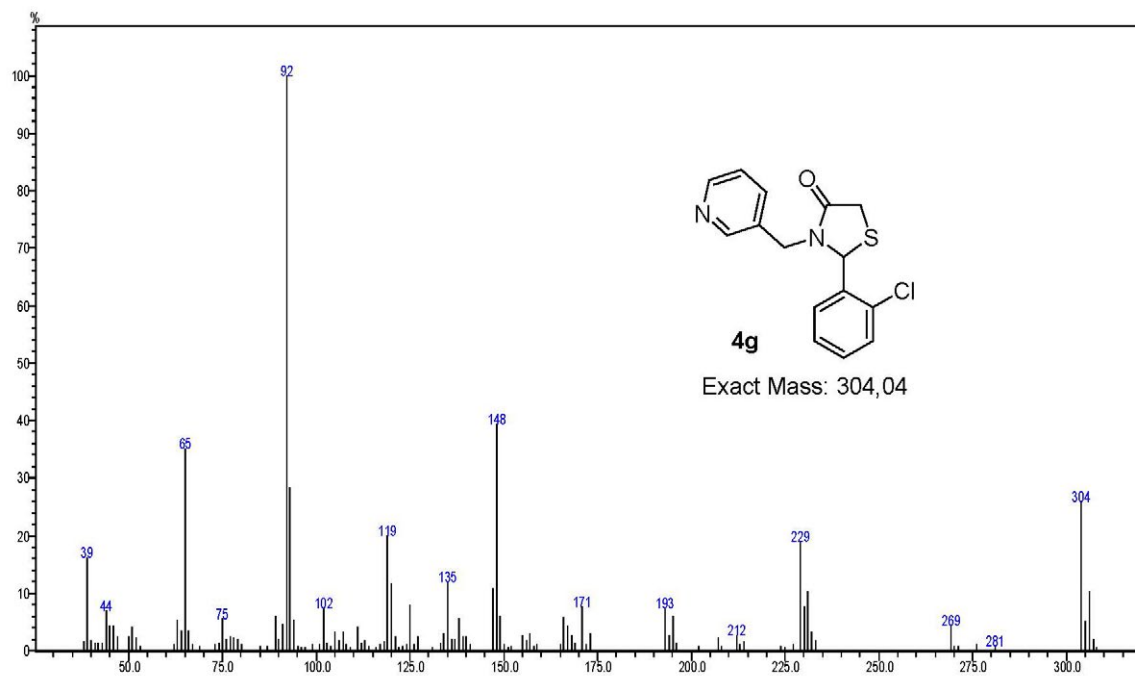


Figure S35. Mass spectrum of compound **4g**.

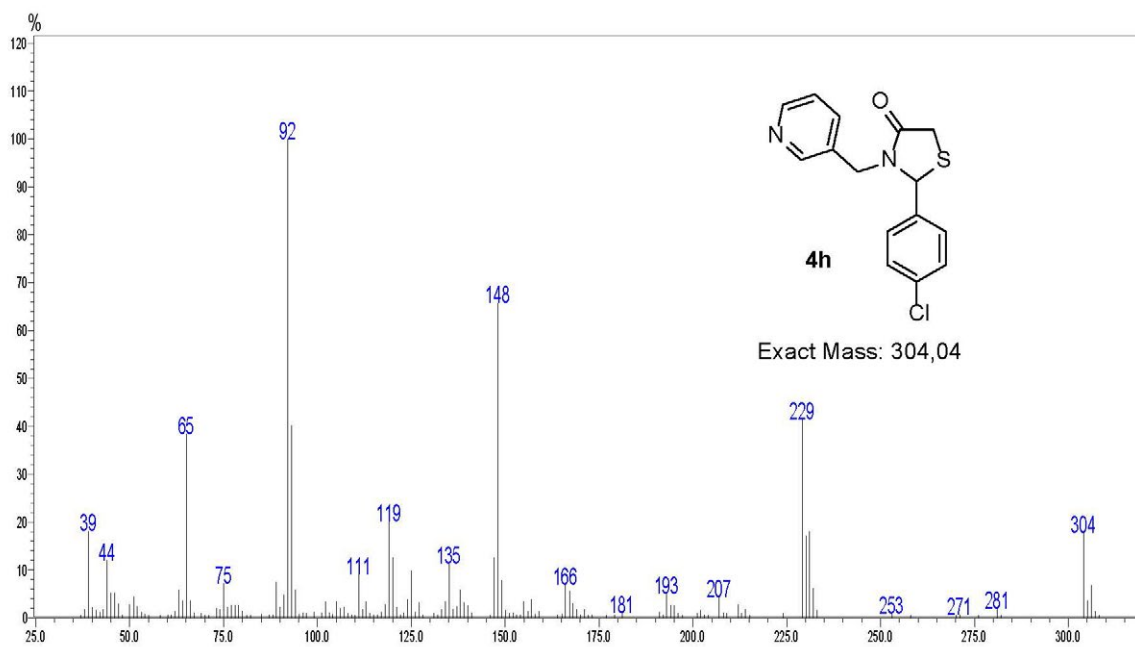
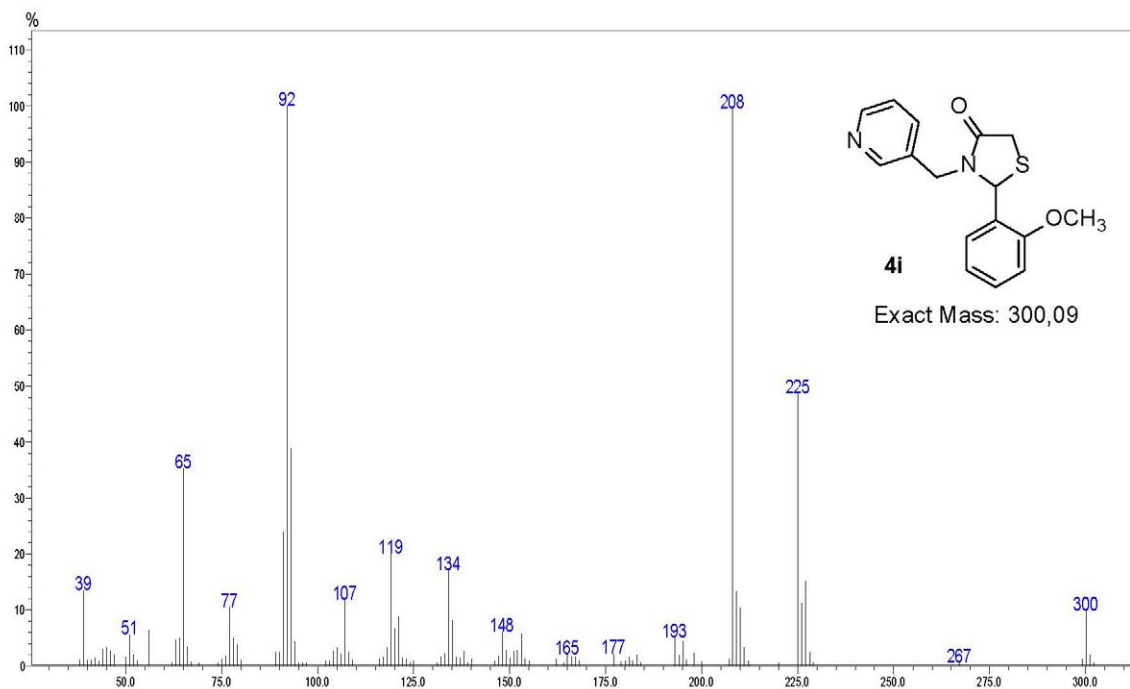
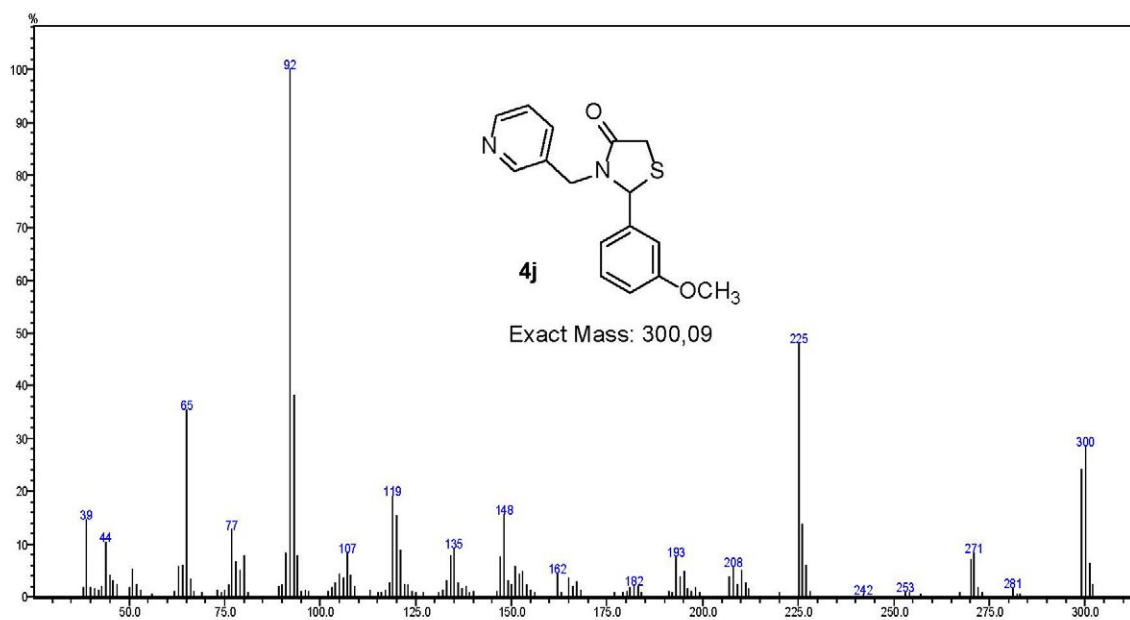
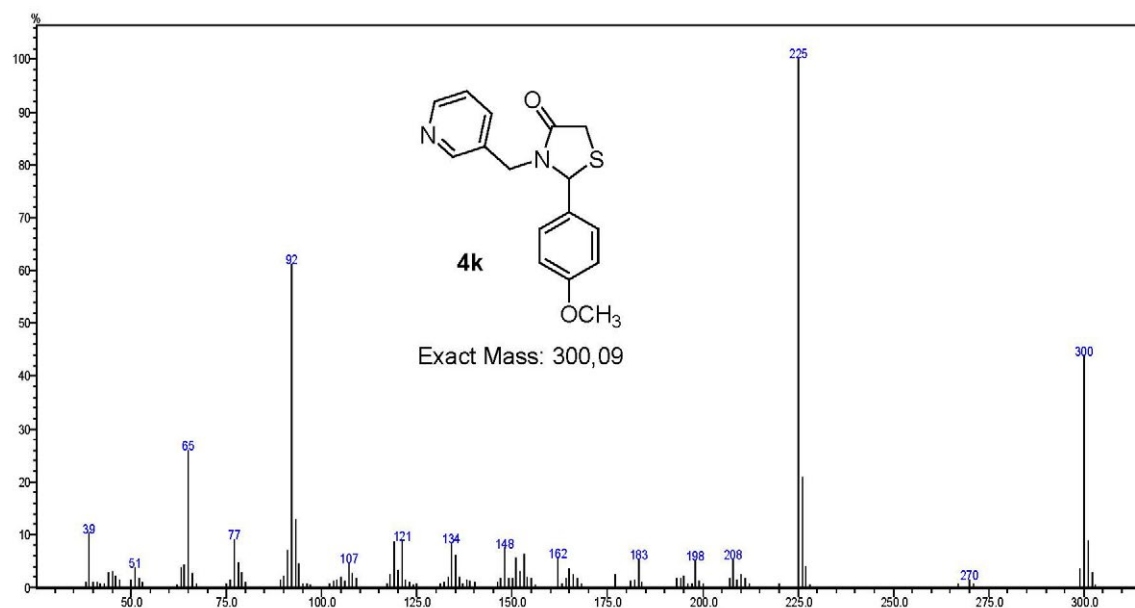
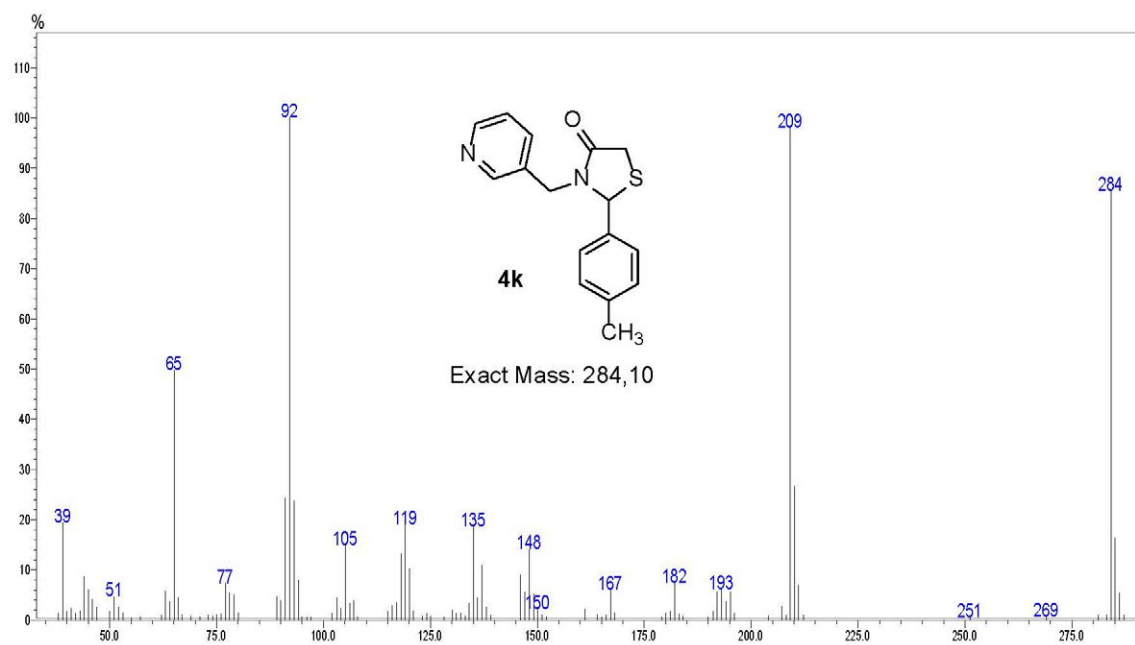
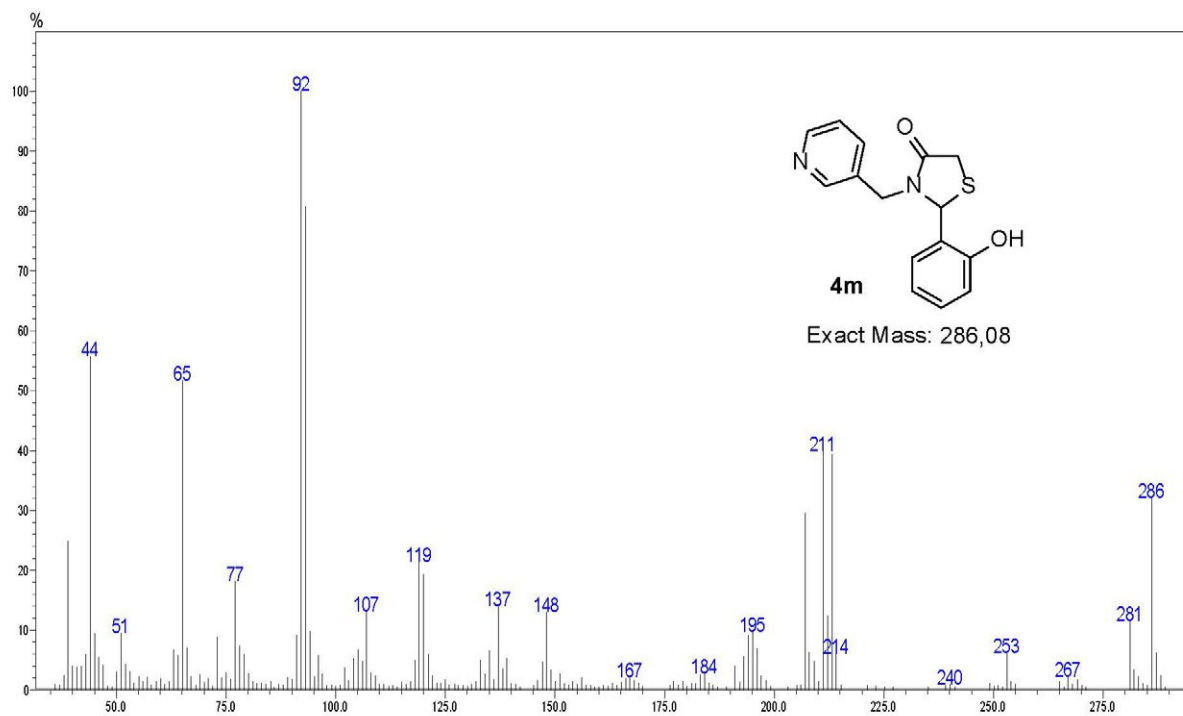
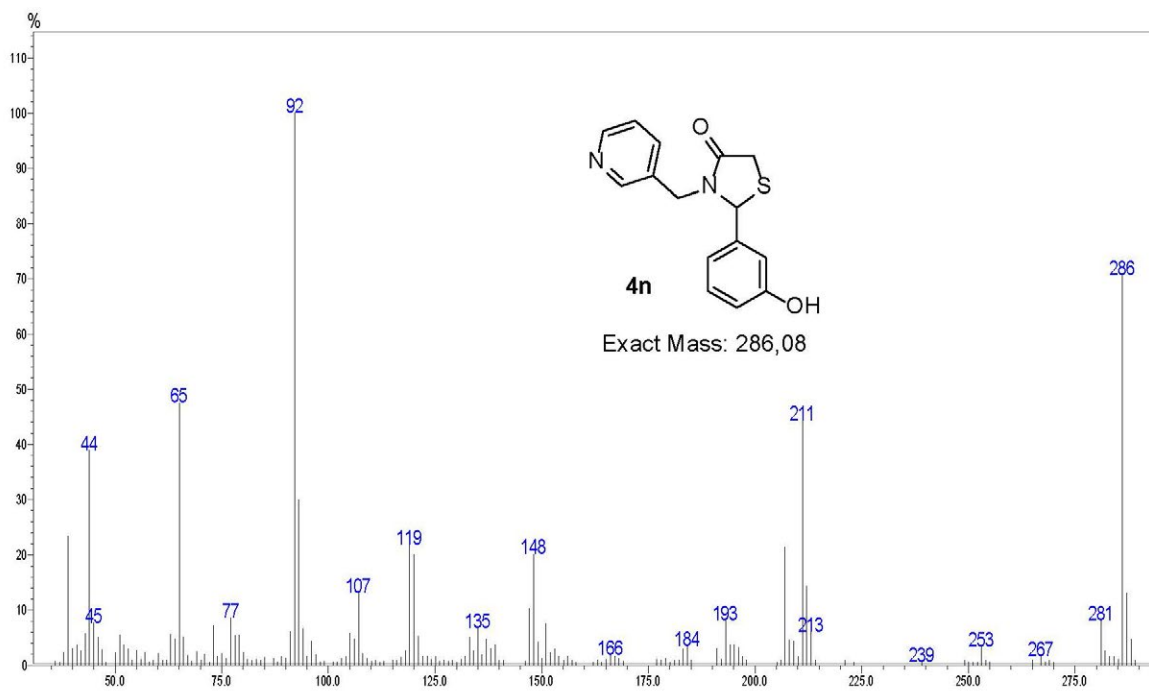
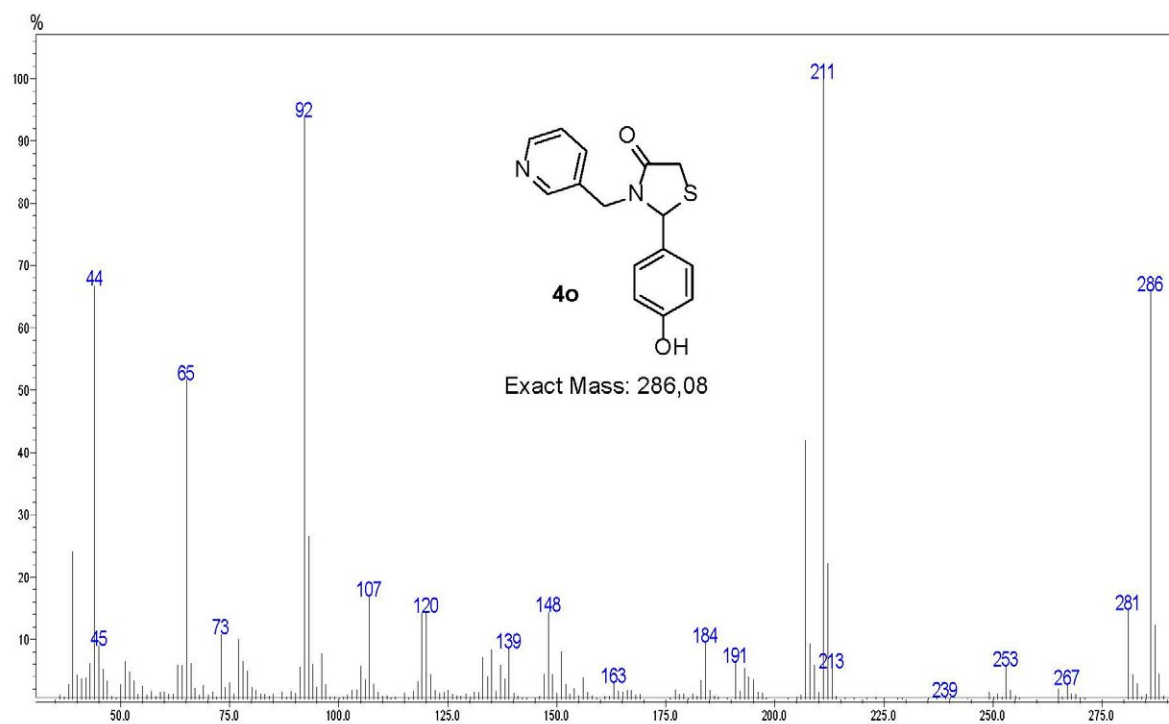


Figure S36. Mass spectrum of compound **4h**.

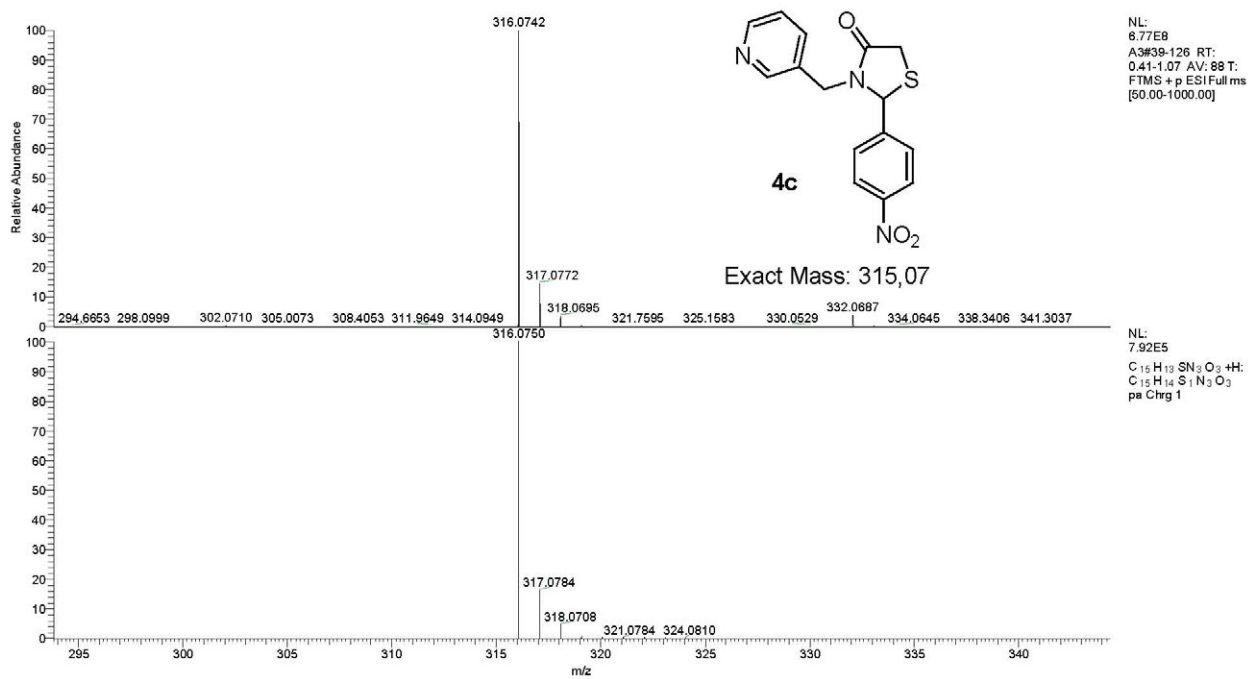
Figure S37. Mass spectrum of compound **4i**.Figure S38. Mass spectrum of compound **4j**.

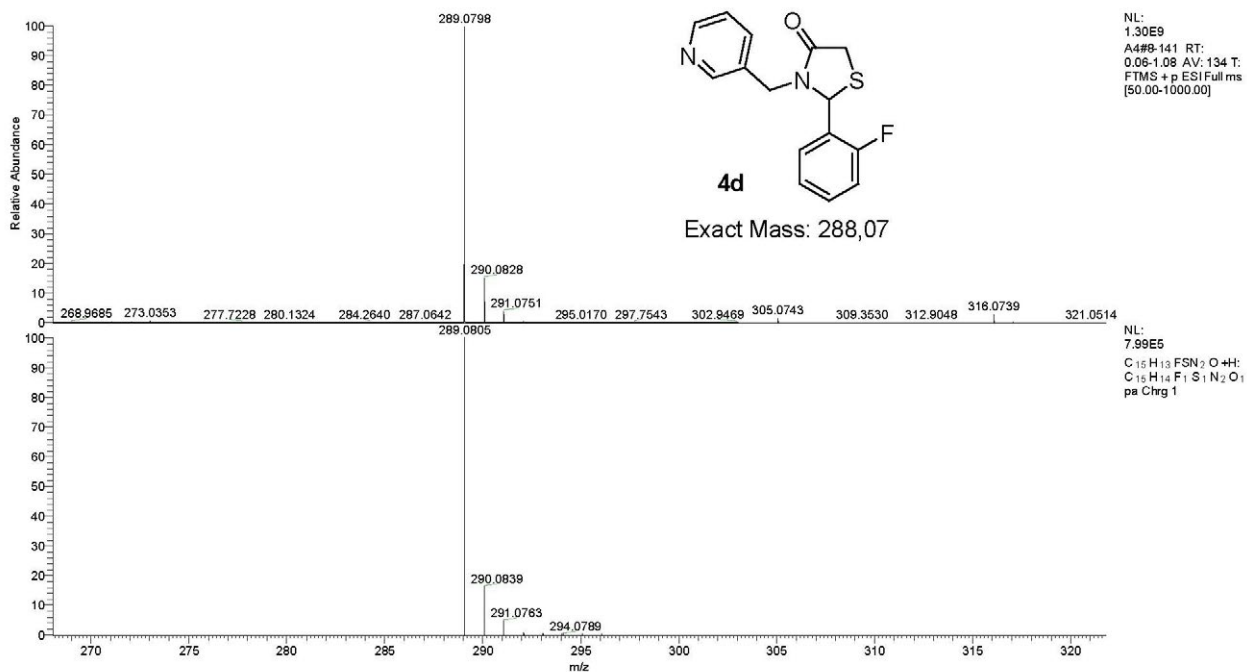
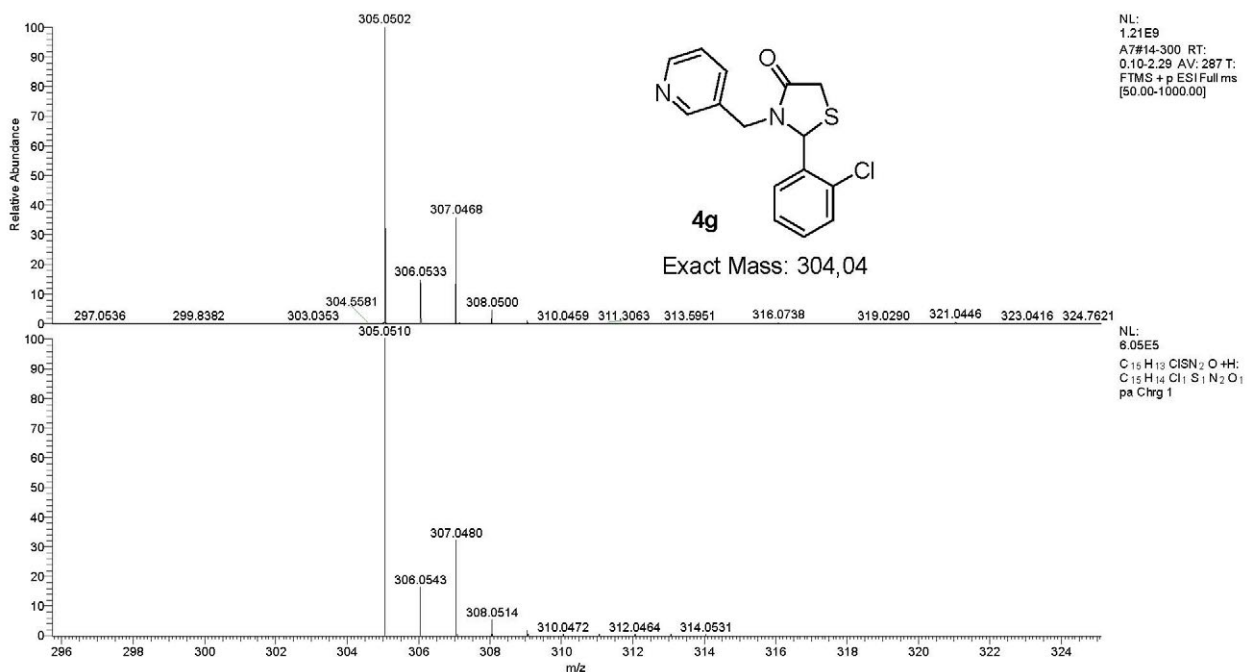
Figure S39. Mass spectrum of compound **4k**.Figure S40. Mass spectrum of compound **4l**.

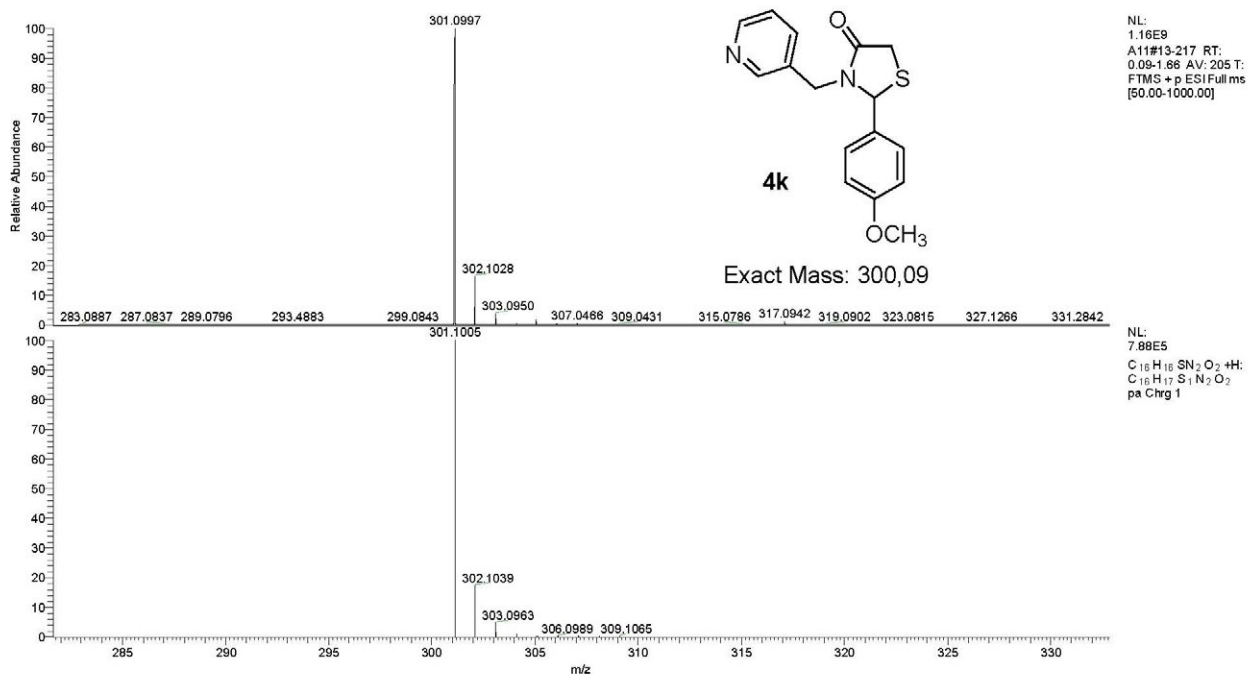
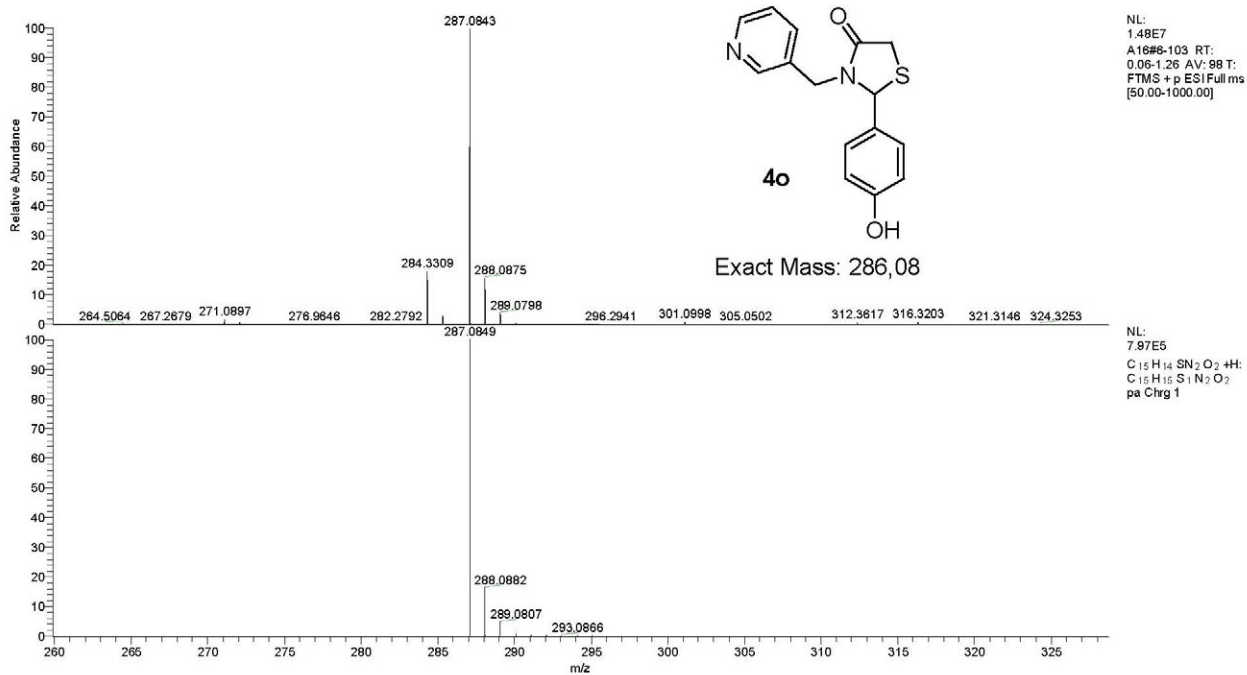
Figure S41. Mass spectrum of compound **4m**.Figure S42. Mass spectrum of compound **4n**.

Figure S43. Mass spectrum of compound **4o**.

High Resolution Mass Spectra (ESI)

Figure S44. HRMS of compound **4c** (found and calculated).

Figure S45. HRMS of compound **4d** (found and calculated).Figure S46. HRMS of compound **4g** (found and calculated).

Figure S47. HRMS of compound **4k** (found and calculated).Figure S48. HRMS of compound **4o** (found and calculated).