

Supplementary Information

On the Search for Potential Antimycobacterial Drugs: Synthesis of Naphthoquinoidal, Phenazinic and 1,2,3-Triazolic Compounds and Evaluation Against *Mycobacterium tuberculosis*

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Compound 4

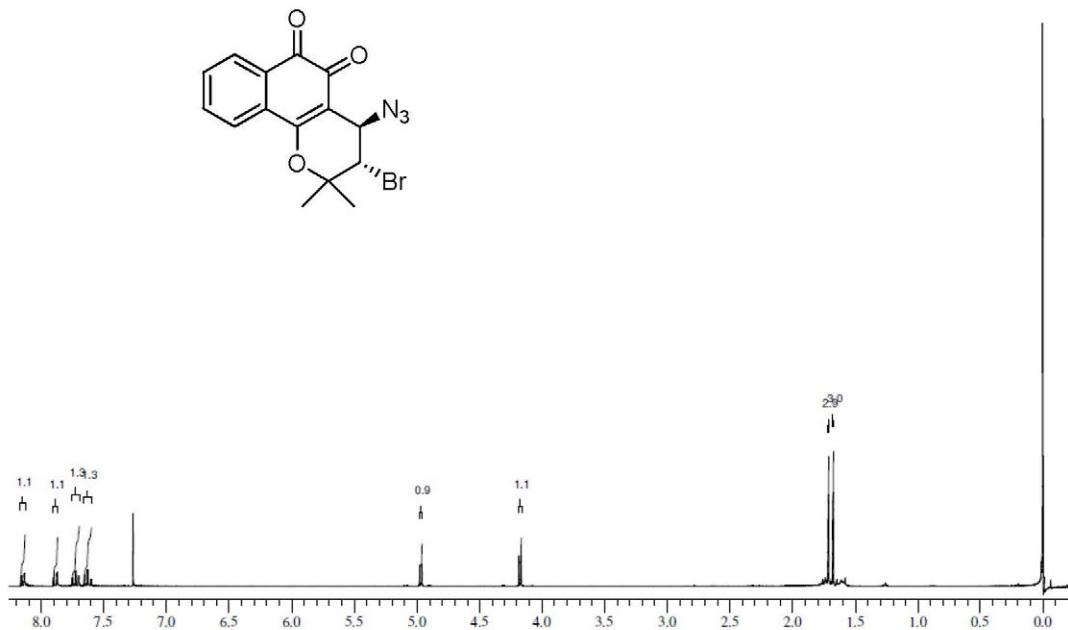


Figure S1. ¹H NMR spectrum (300 MHz, CDCl₃) of compound 4.

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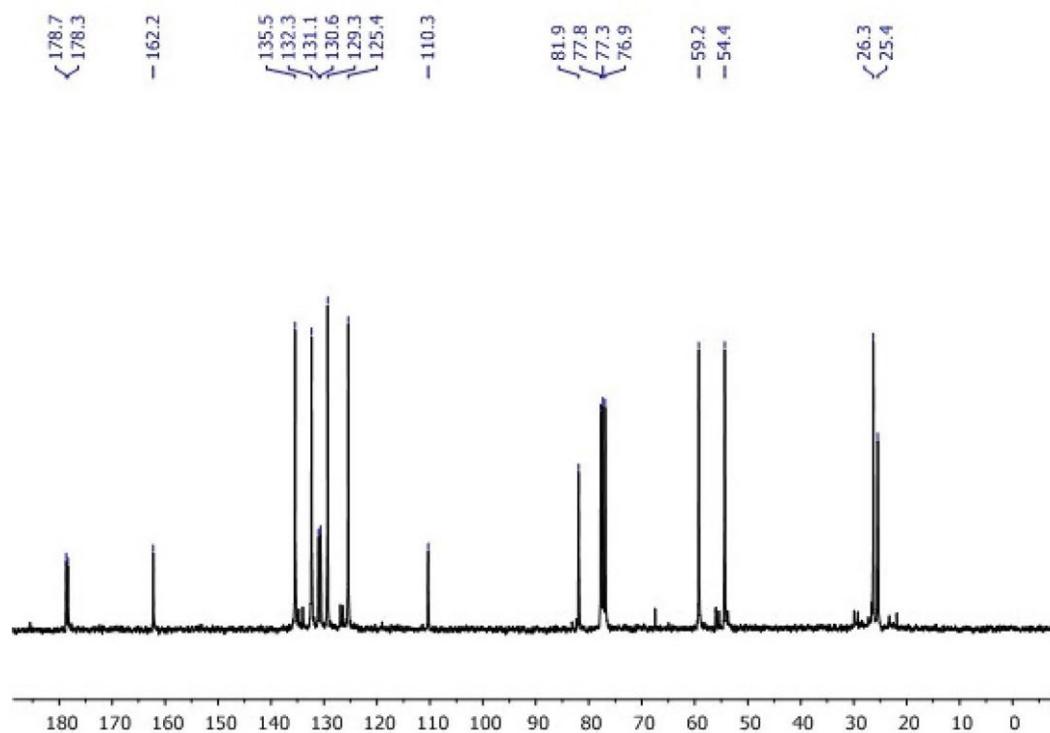


Figure S2. ¹³C NMR spectrum (75 MHz, CDCl₃) of compound 4.

Compound 5

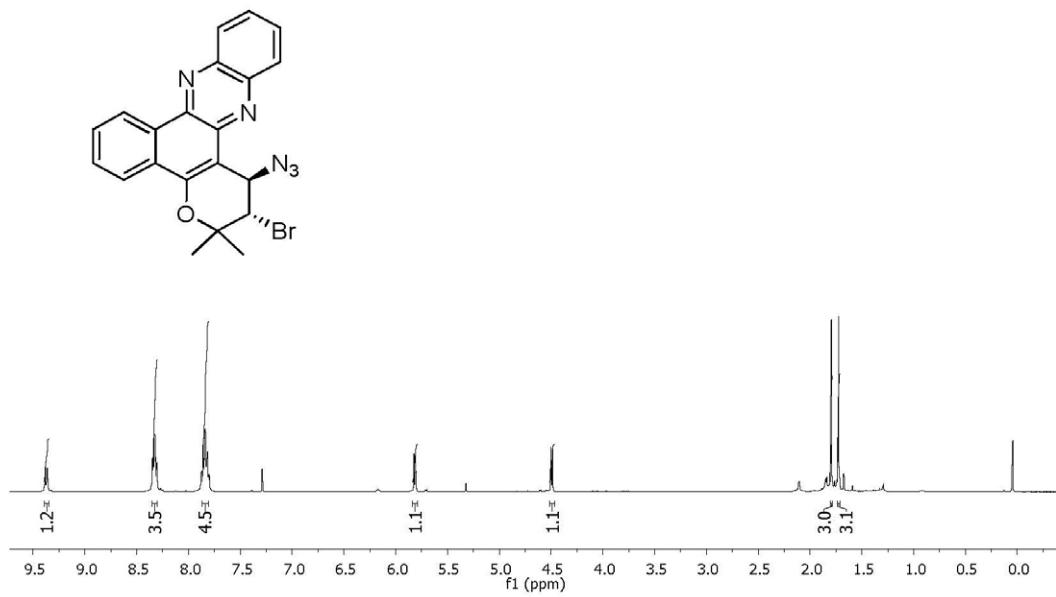


Figure S3. ¹H NMR spectrum (400 MHz, CDCl₃) of compound 5.

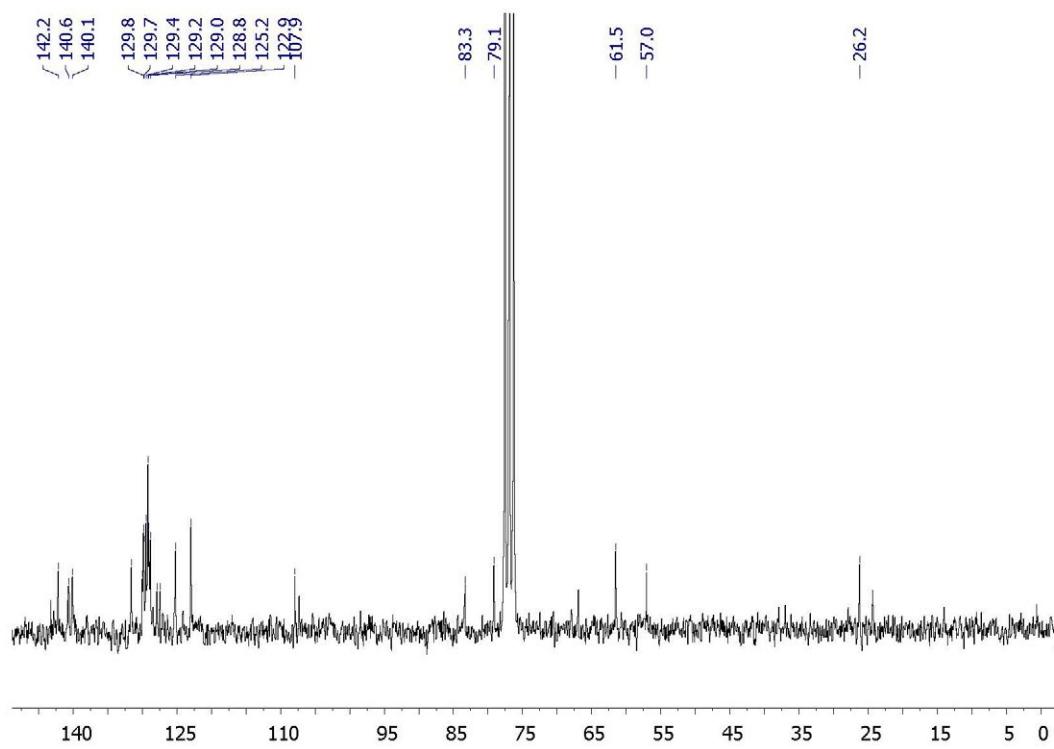


Figure S4. ^{13}C NMR spectrum (50 MHz, CDCl_3) of compound 5.

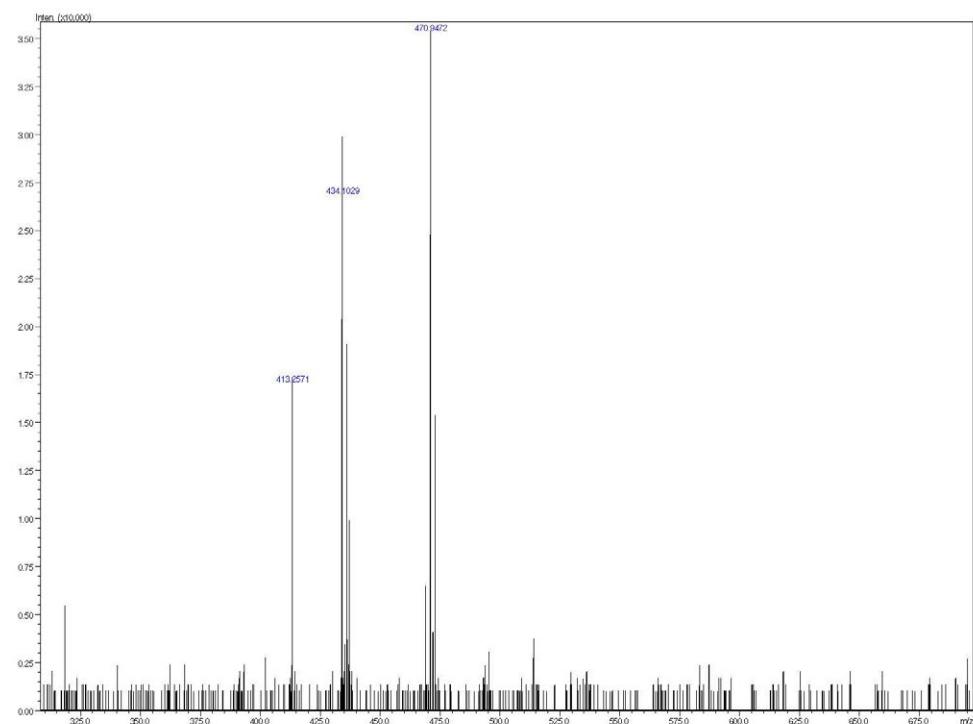


Figure S5. ESI-MS of compound 5.

Compound 6

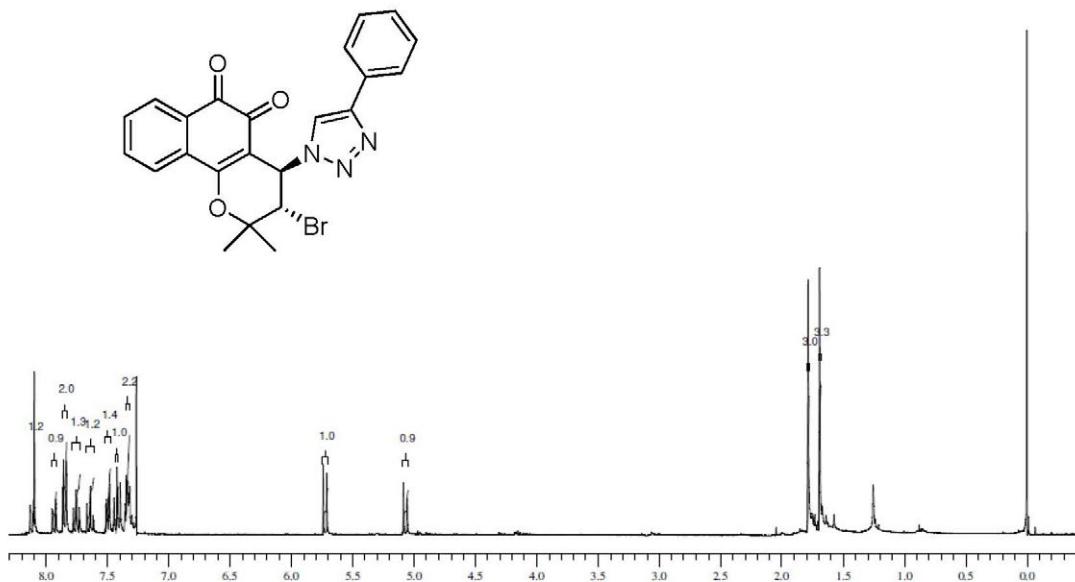


Figure S6. ¹H NMR spectrum (300 MHz, CDCl₃) of compound 6.

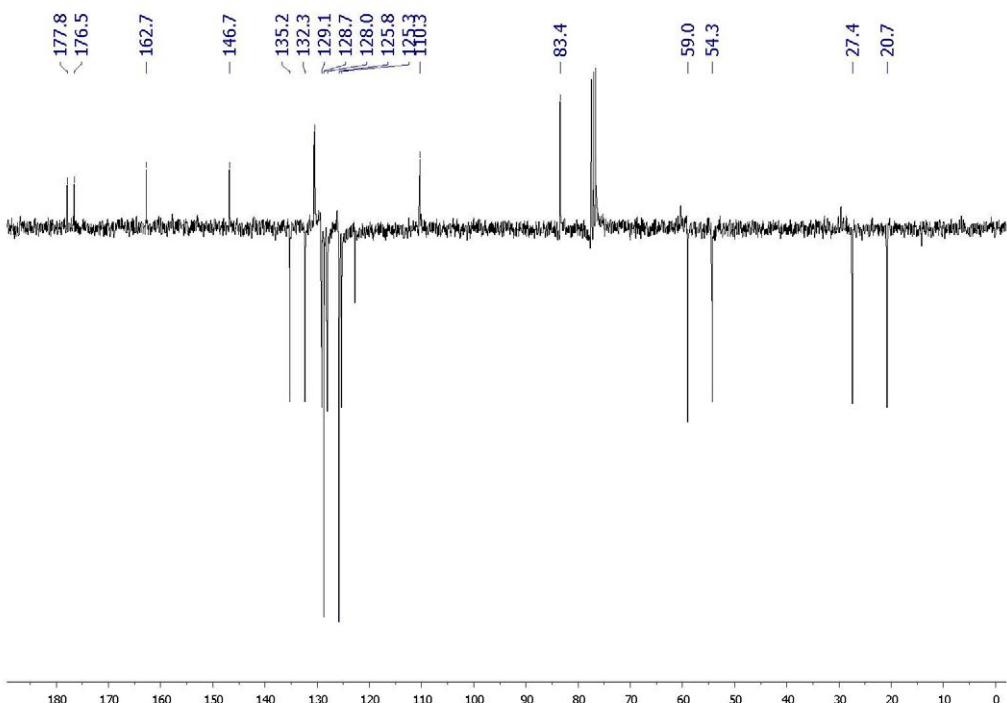


Figure S7. ¹³C-APT NMR spectrum (75 MHz, CDCl₃) of compound 6.

Compound 7

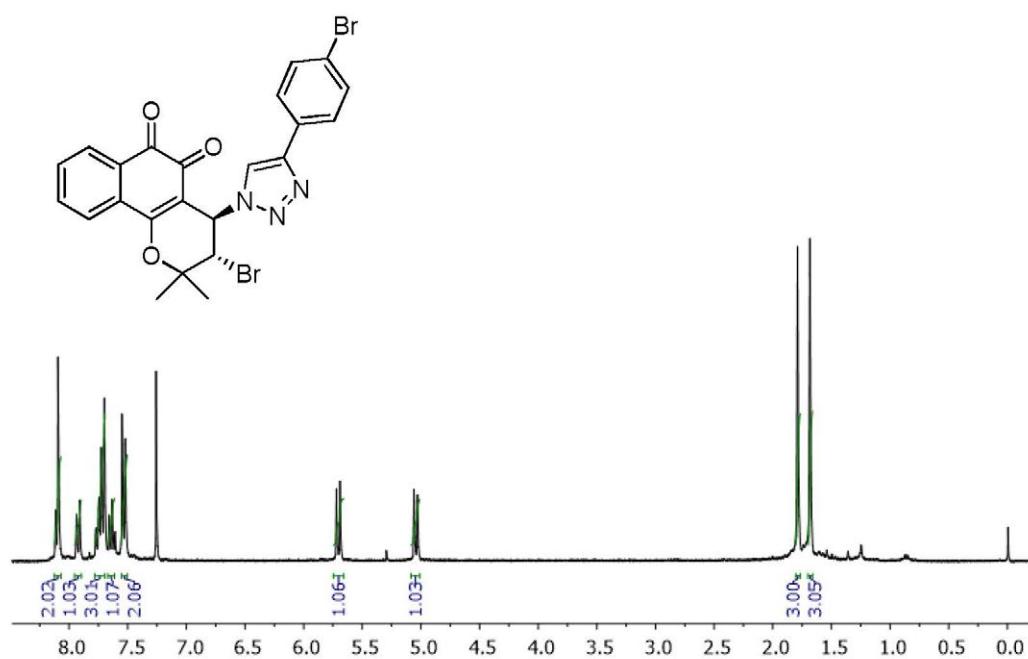


Figure S8. ¹H NMR spectrum (300 MHz, CDCl₃) of compound 7.

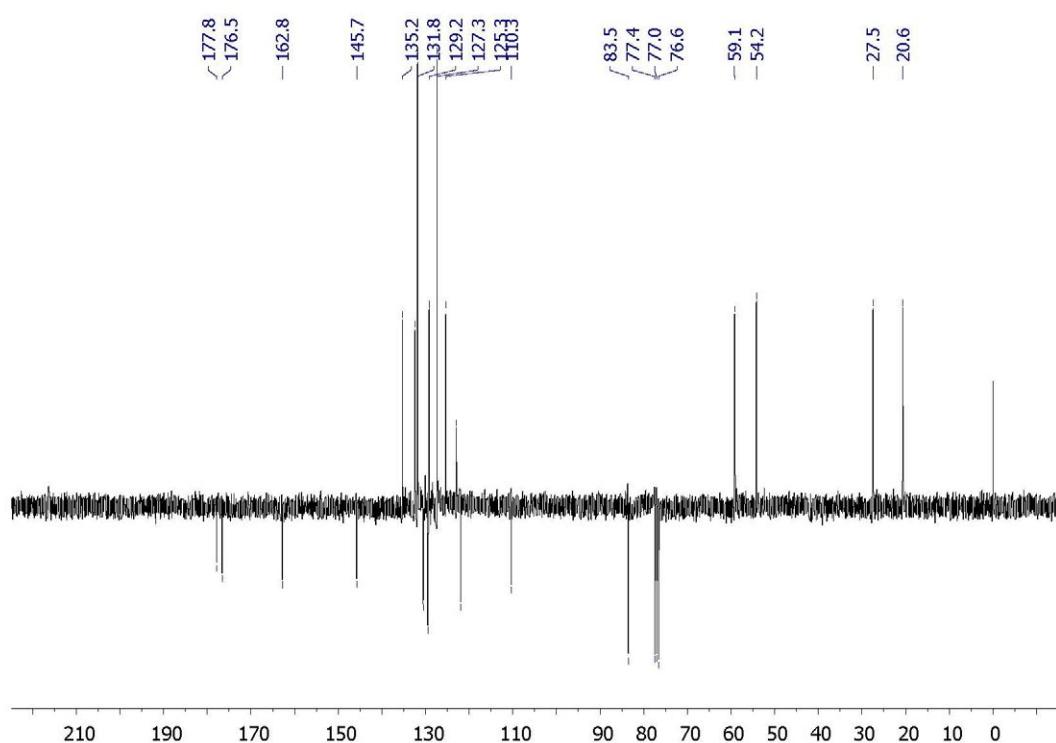


Figure S9. ¹³C-APT NMR spectrum (75 MHz, CDCl₃) of compound 7.

Compound 8

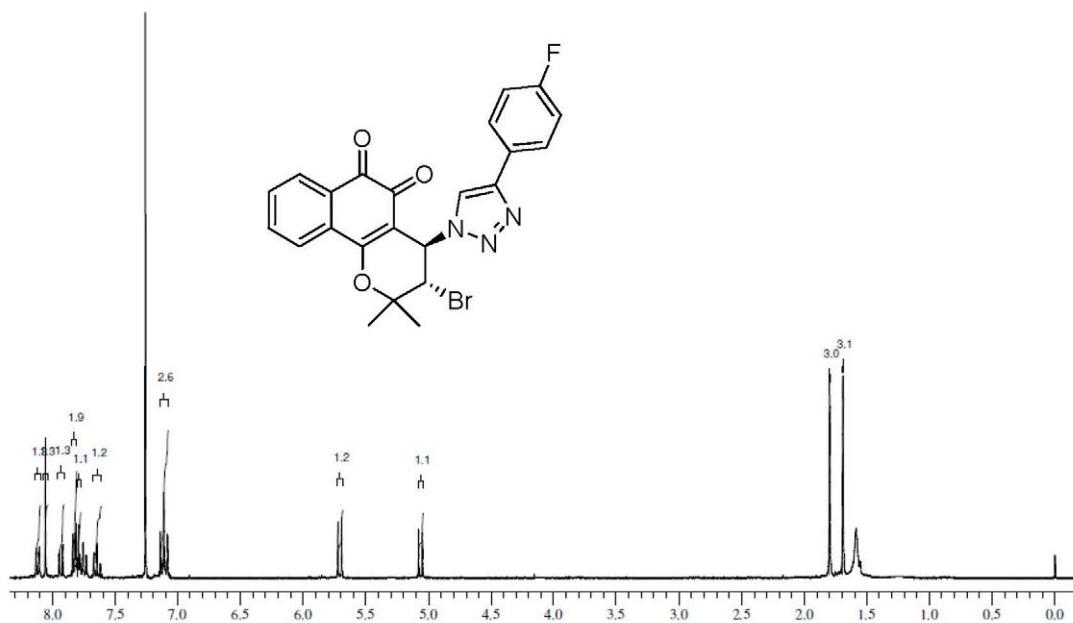


Figure S10. ¹H NMR spectrum (300 MHz, CDCl₃) of compound 8.

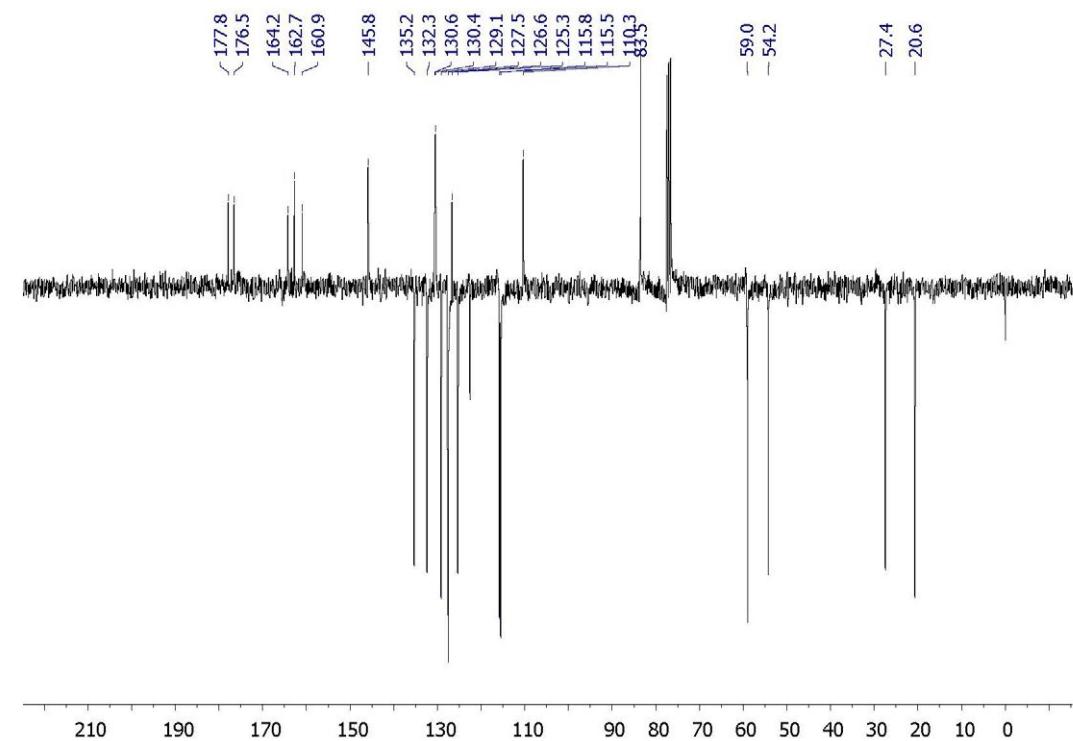
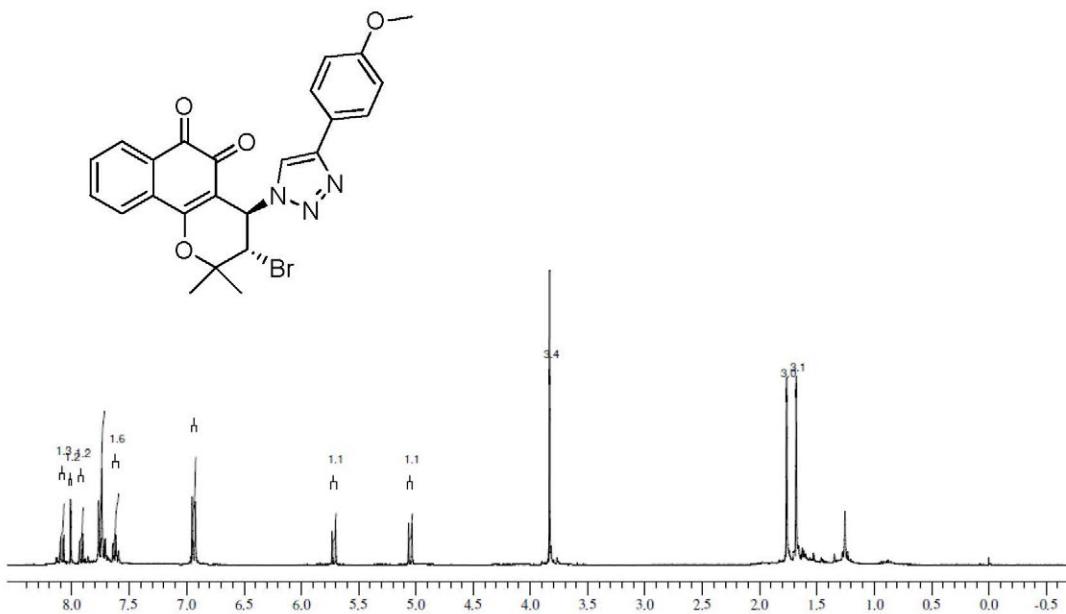
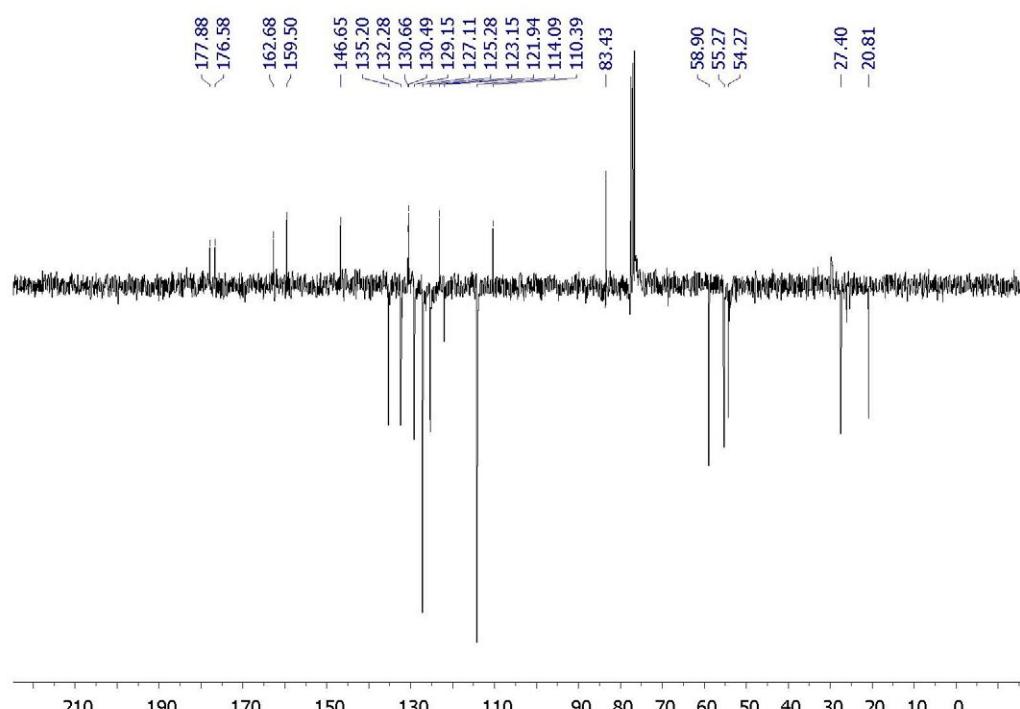
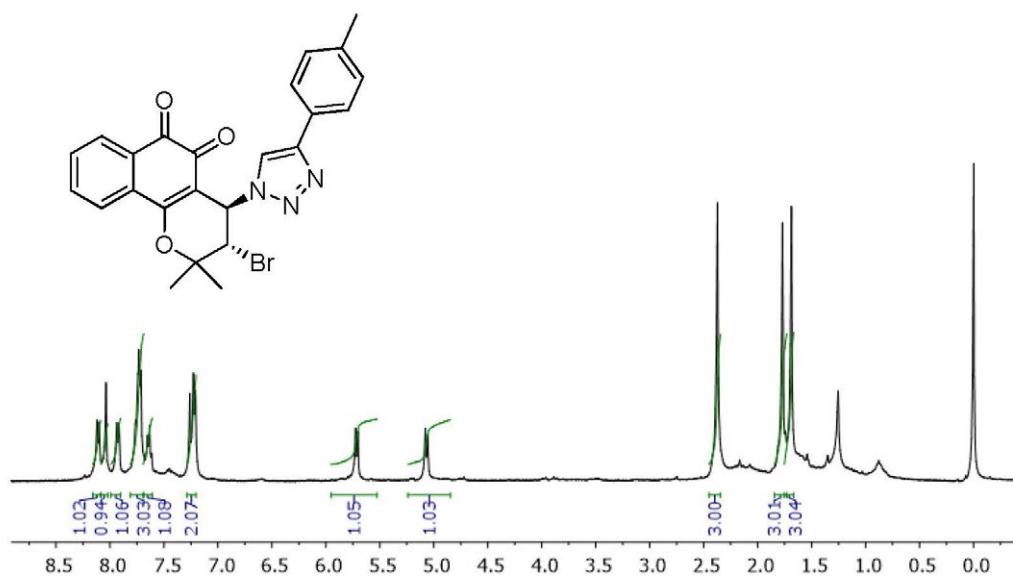
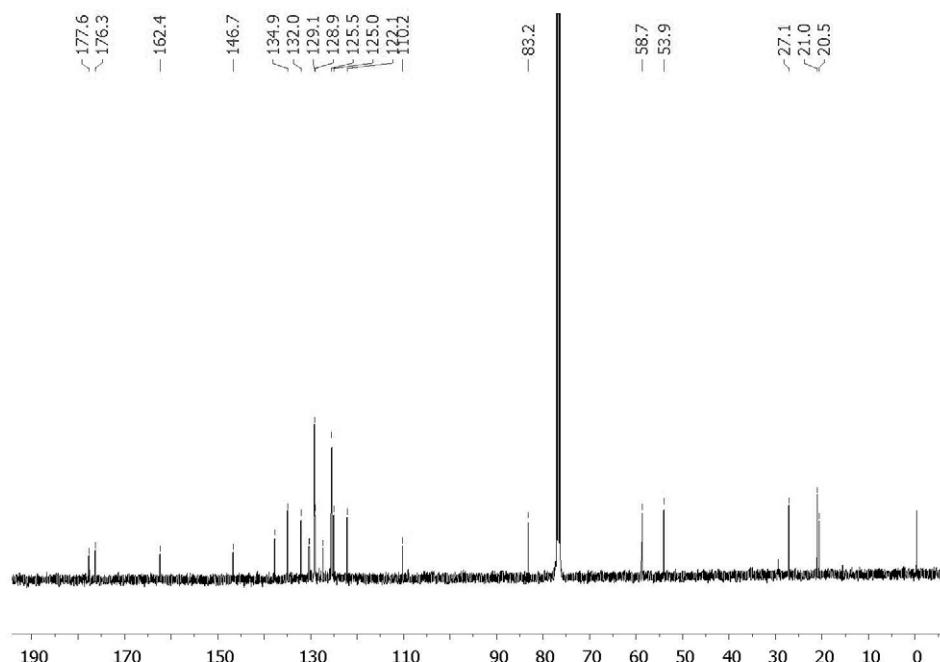
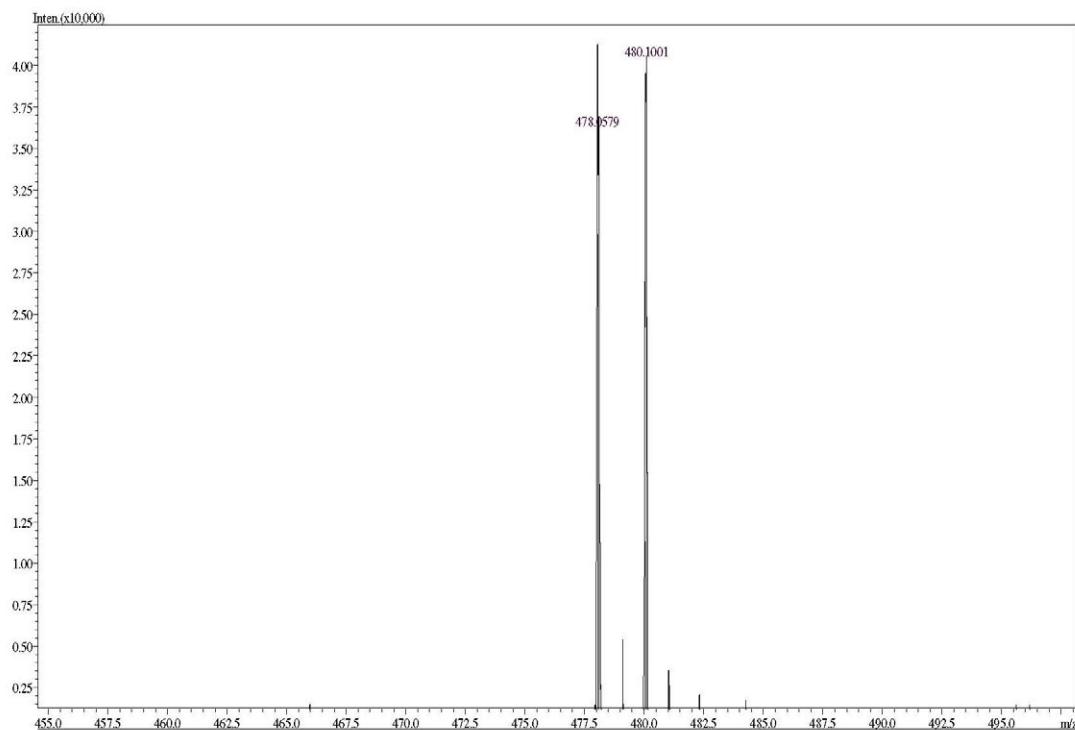
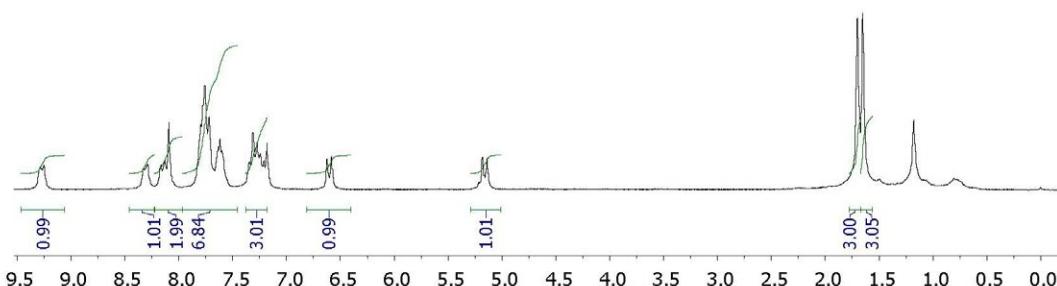


Figure S11. ¹³C-APT NMR spectrum (75 MHz, CDCl₃) of compound 8.

Compound **9****Figure S12.** ¹H NMR spectrum (300 MHz, CDCl₃) of compound **9**.**Figure S13.** ¹³C-APT NMR spectrum (75 MHz, CDCl₃) of compound **9**.

Compound **10****Figure S14.** ¹H NMR spectrum (200 MHz, CDCl₃) of compound **10**.**Figure S15.** ¹³C NMR spectrum (50 MHz, CDCl₃) of compound **10**.

**Figure S16.** ESI-MS of compound **10**.**Compound 11****Figure S17.** ^1H NMR spectrum (200 MHz, CDCl_3) of compound **11**.

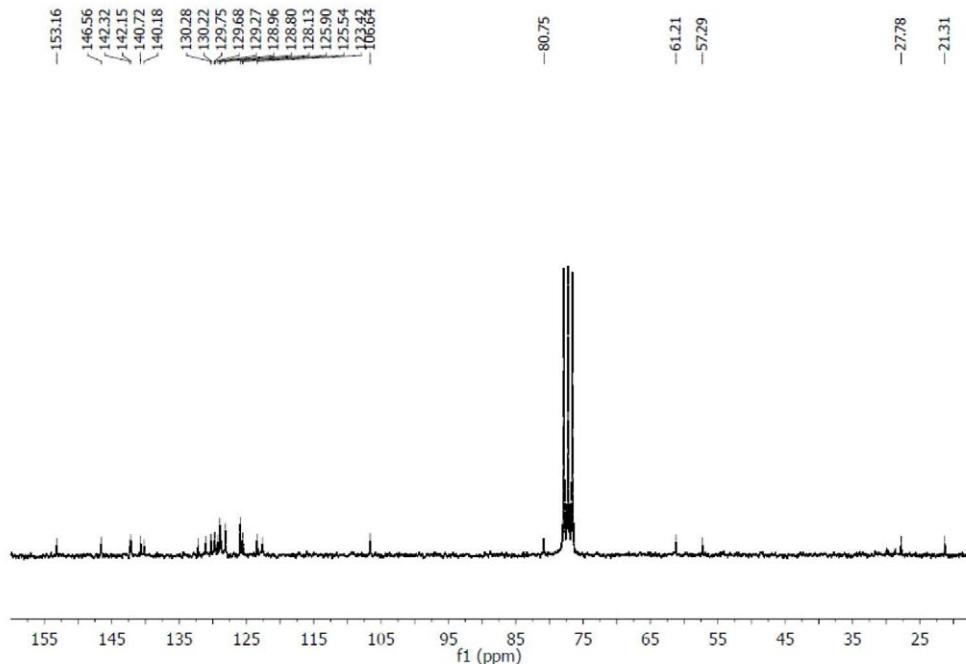


Figure S18. ¹³C NMR spectrum (50 MHz, CDCl₃) of compound 11.

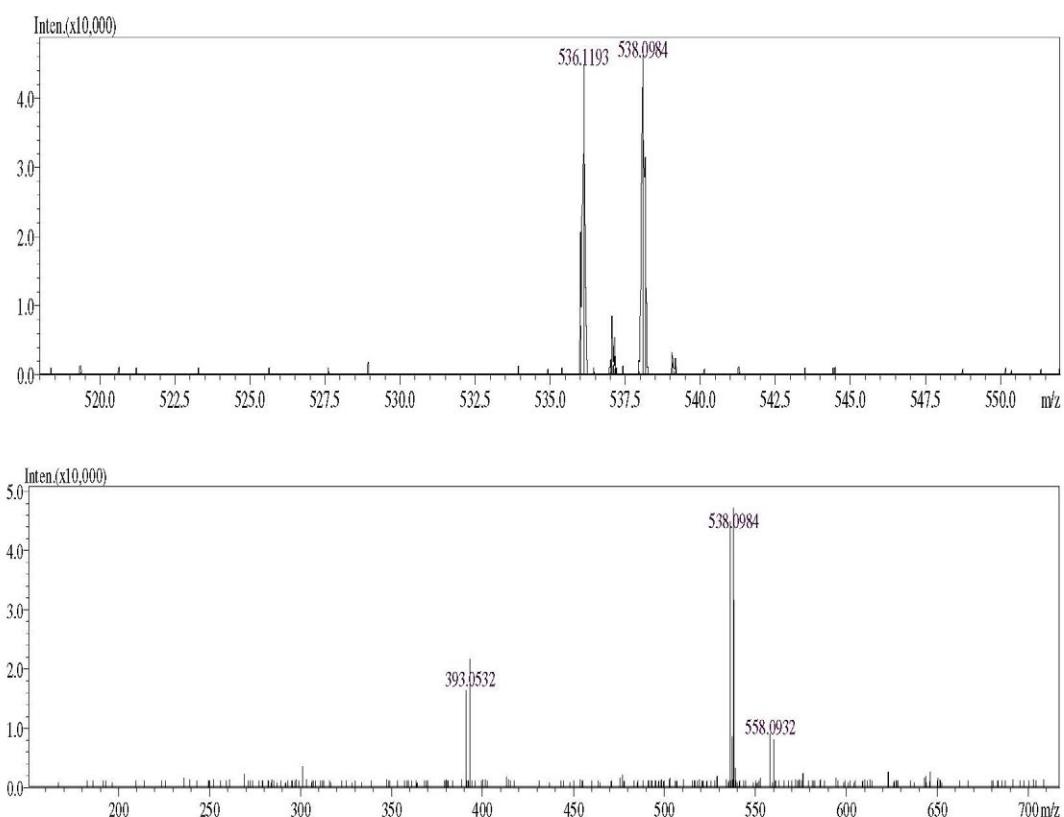
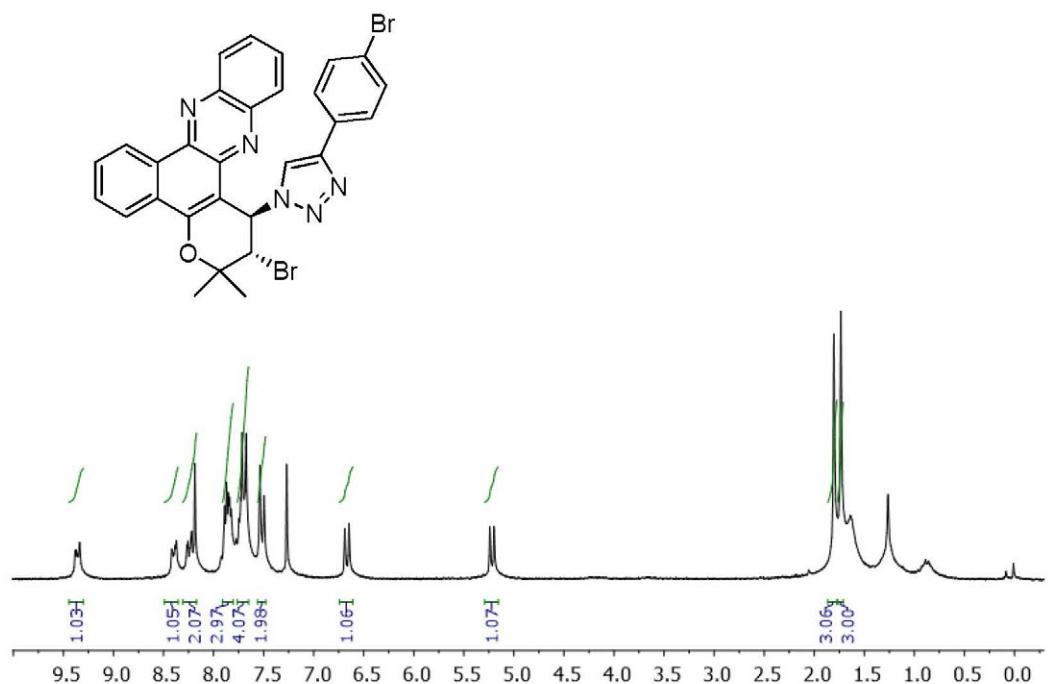
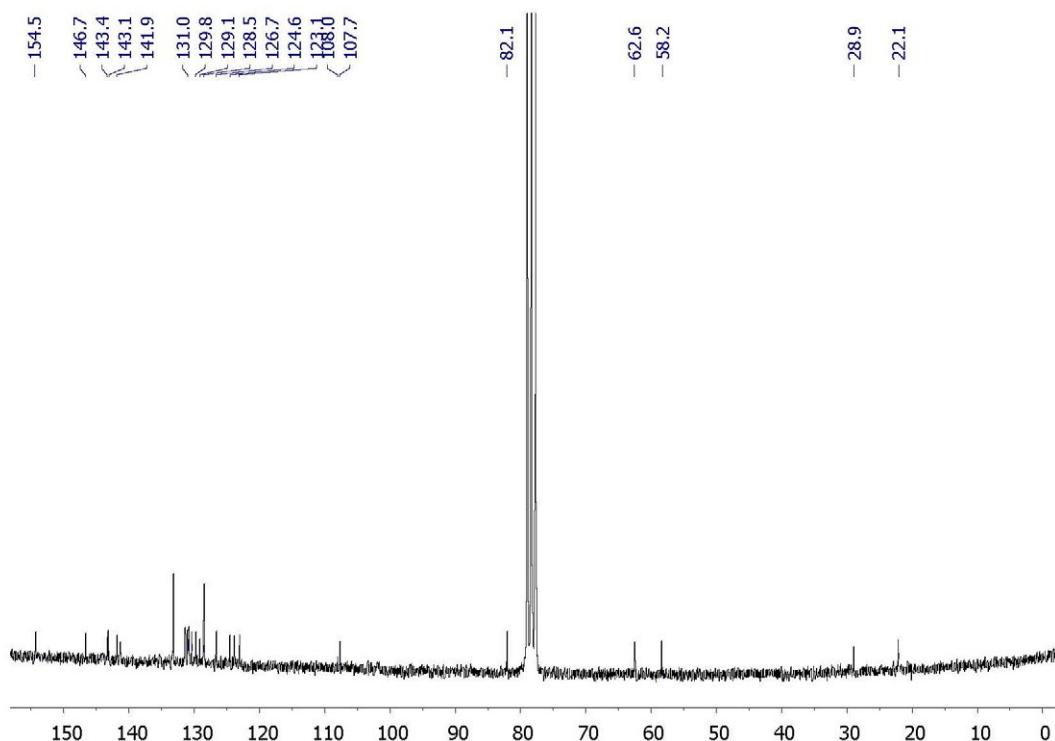
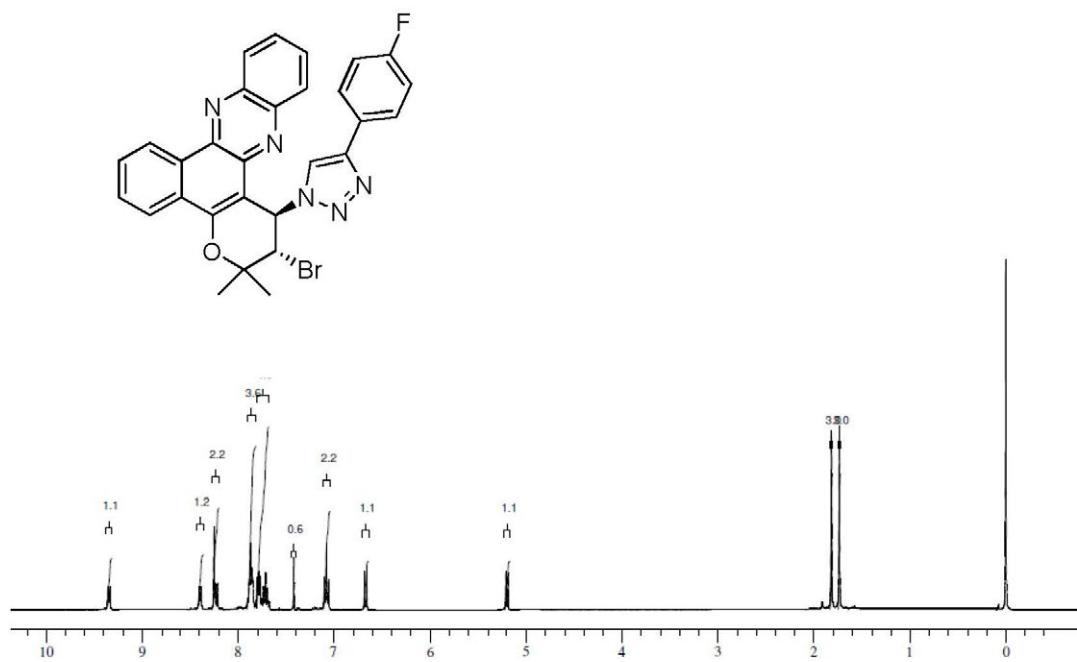
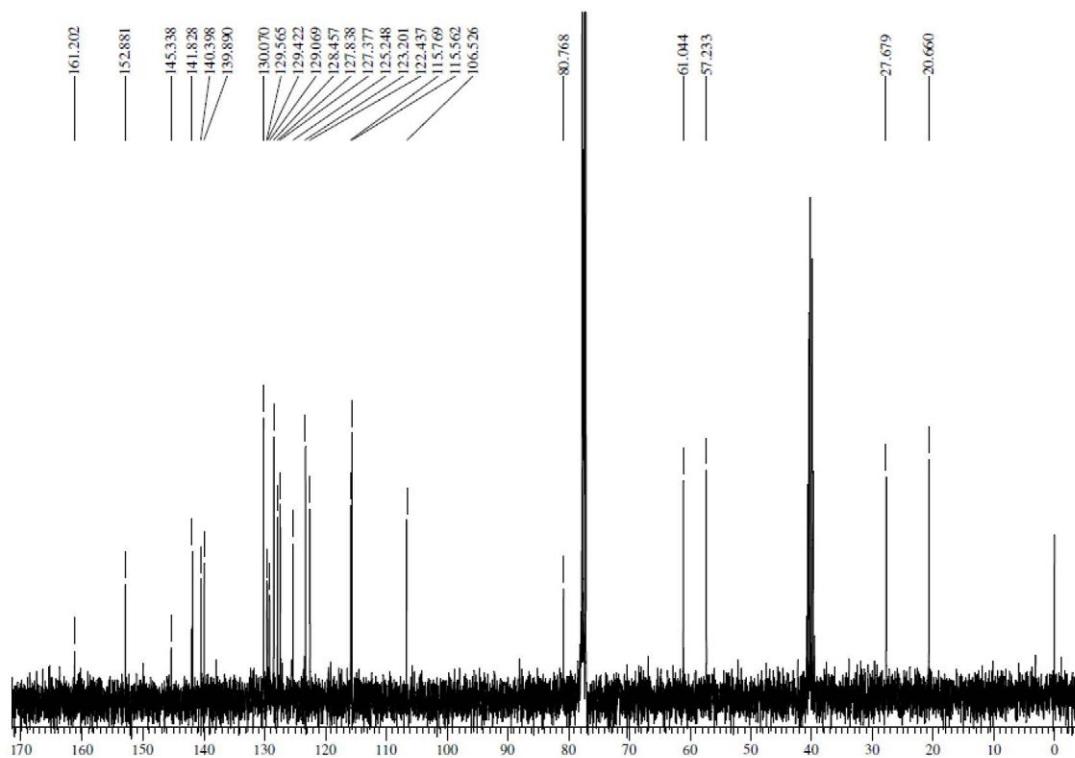


Figure S19. ESI-MS of compound 11.

Compound **12****Figure S20.** ¹H NMR spectrum (200 MHz, CDCl₃) of compound **12**.**Figure S21.** ¹³C NMR spectrum (50 MHz, CDCl₃) of compound **12**.

Compound **13****Figure S22.** ¹H NMR spectrum (400 MHz, CDCl₃) of compound **13**.**Figure S23.** ¹³C NMR spectrum (100 MHz, CDCl₃:DMSO-d₆) of compound **13**.

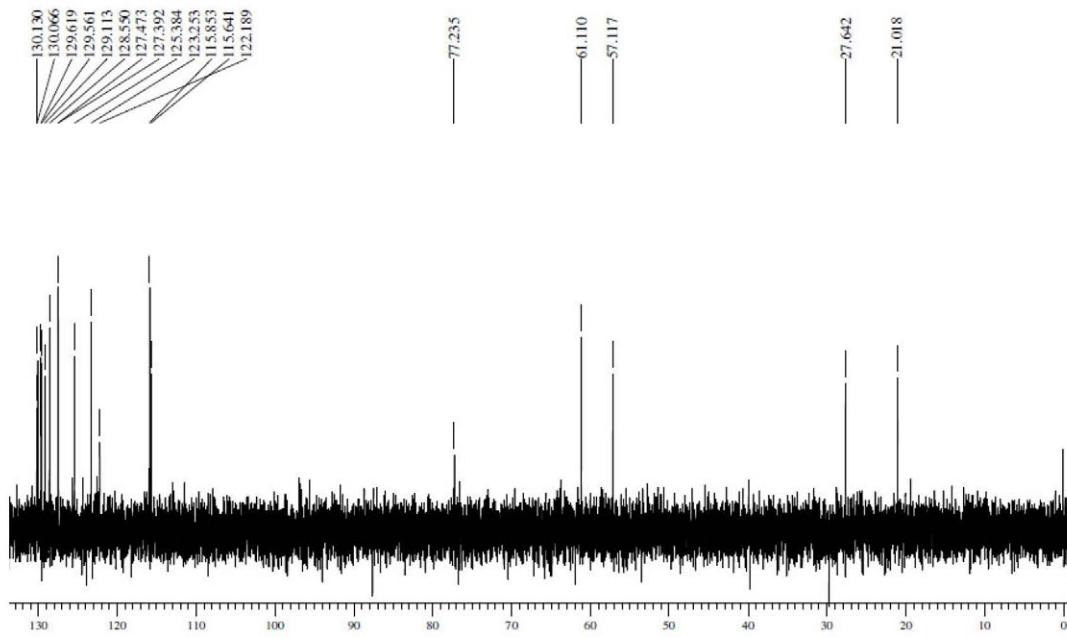


Figure S24. ^{13}C -DEPT NMR spectrum (100 MHz, CDCl_3) of compound 13.

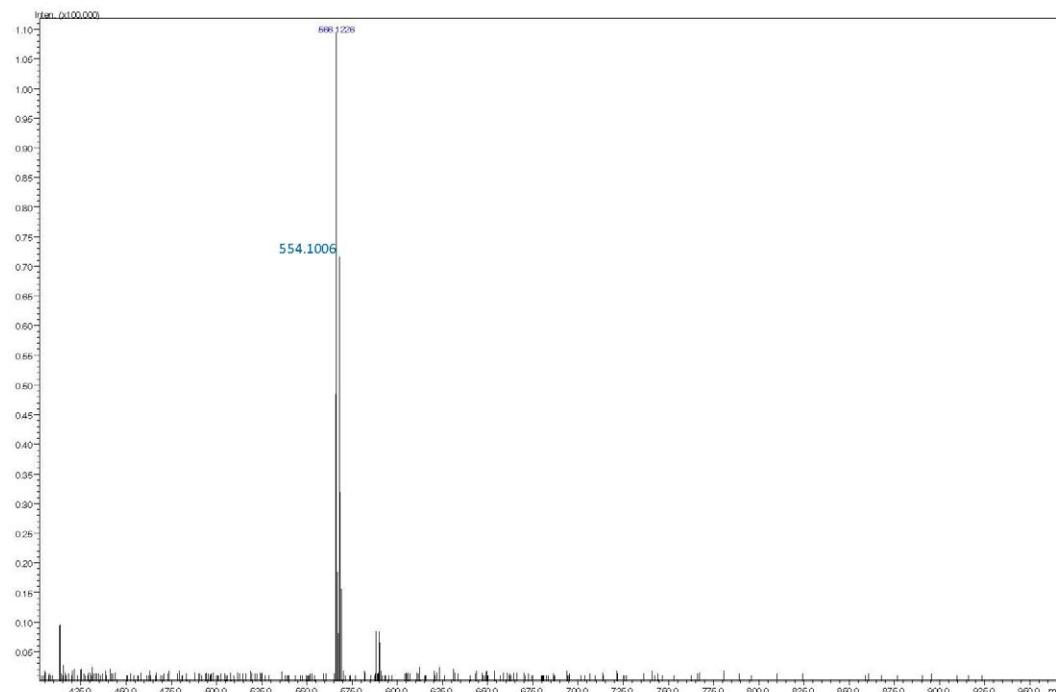


Figure S25. ESI-MS of compound 13.

Compound 14

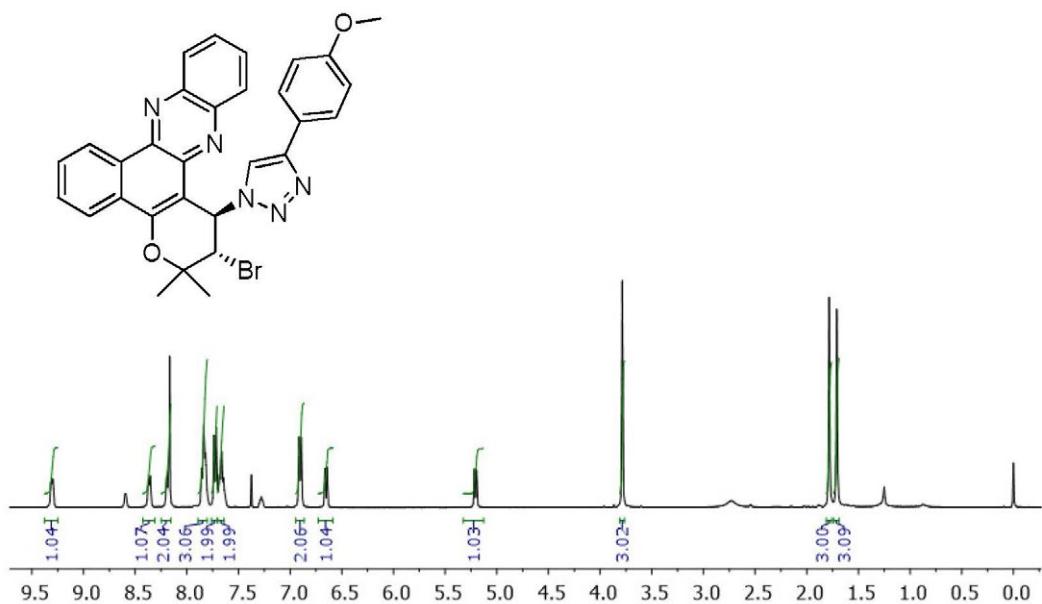


Figure S26. ^1H NMR spectrum (400 MHz, CDCl_3) of compound 14.

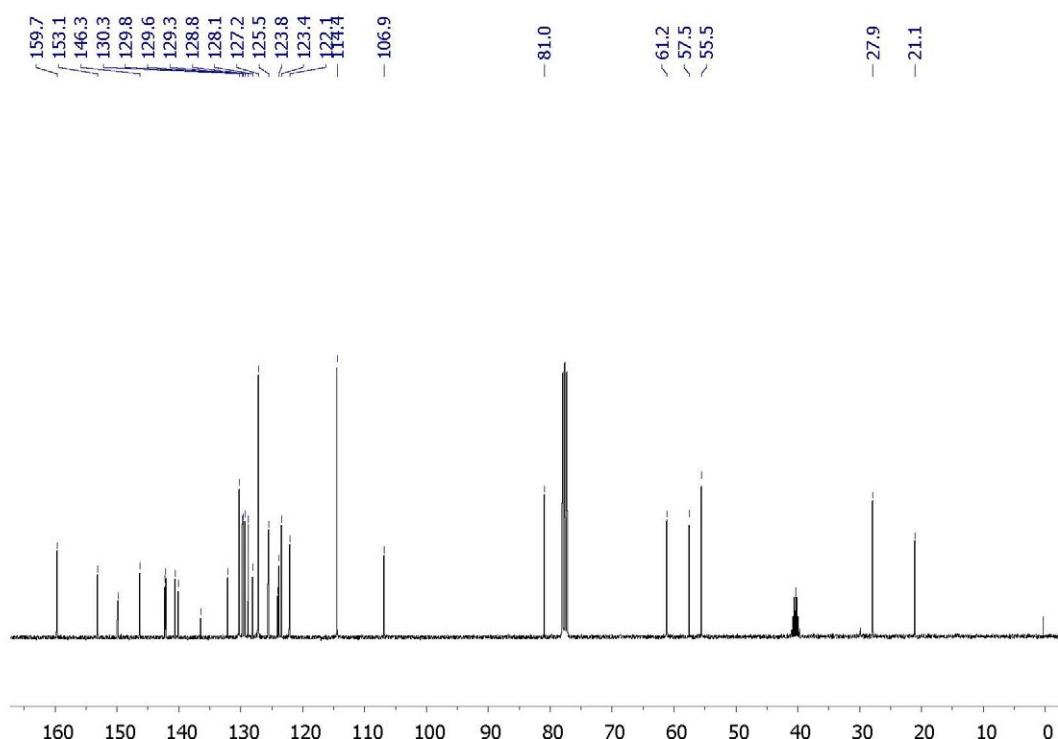
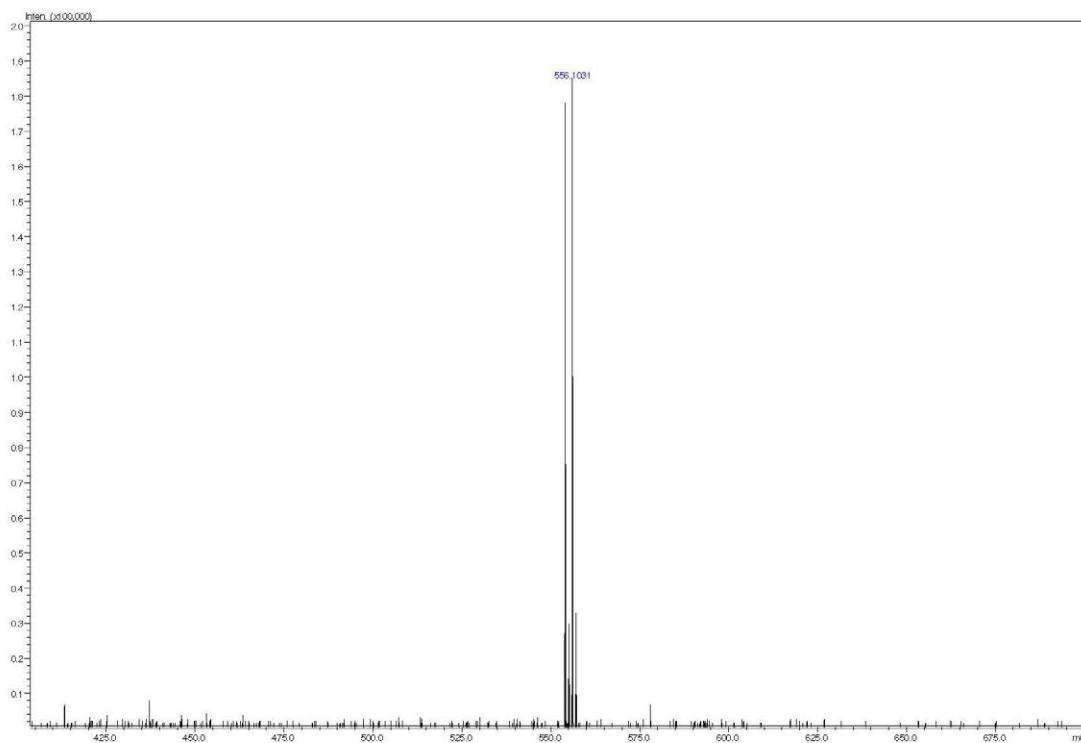
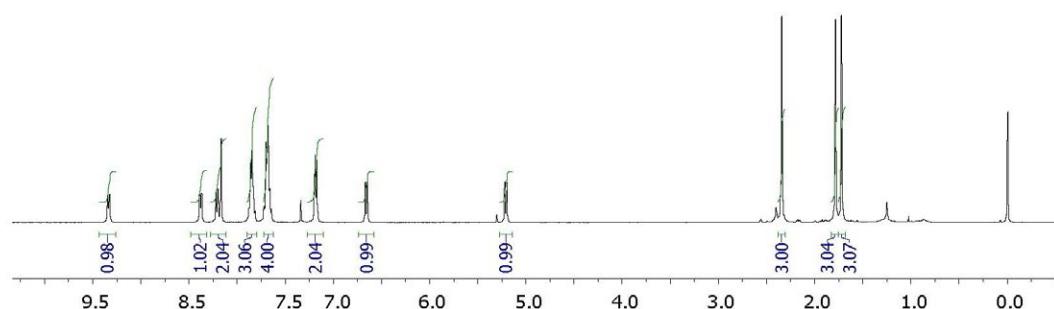
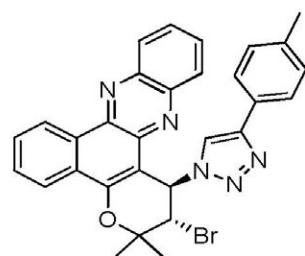


Figure S27. ^{13}C NMR spectrum (100 MHz, CDCl_3 , DMSO- d_6) of compound 14.

**Figure S28.** ESI-MS of compound **14**.**Compound 15****Figure S29.** ¹H NMR spectrum (400 MHz, CDCl₃) of compound **15**.

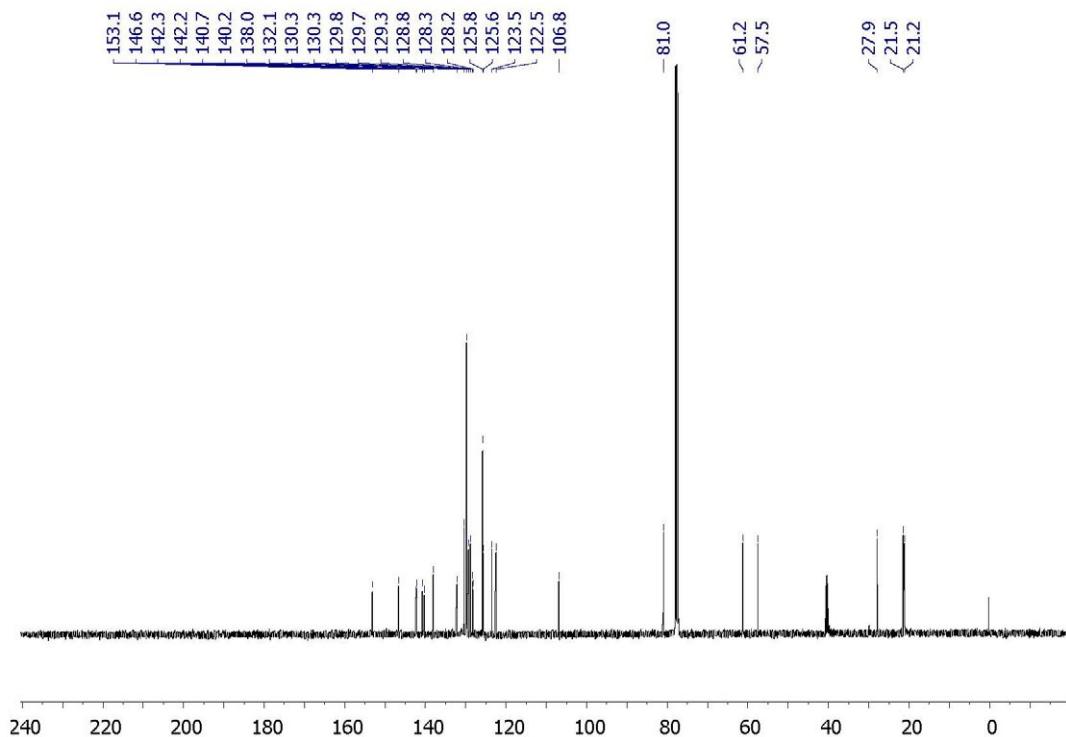


Figure S30. ^{13}C NMR spectrum (100 MHz, CDCl_3 , $\text{DMSO}-d_6$) of compound **15**.

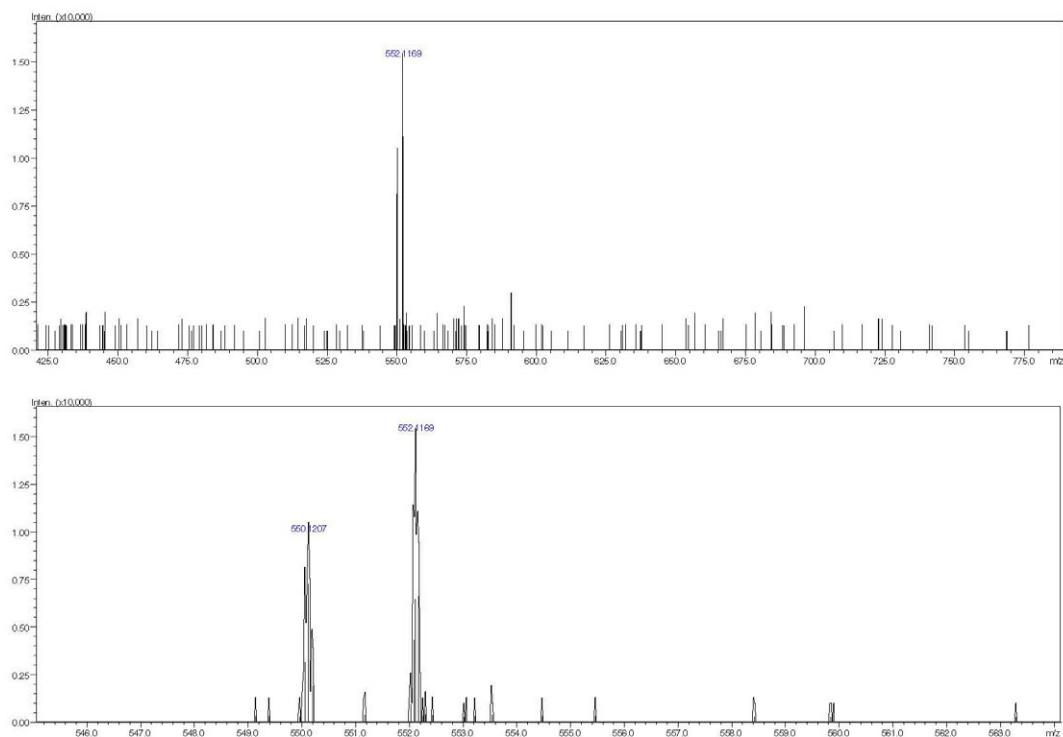


Figure S31. ESI-MS of compound **15**.

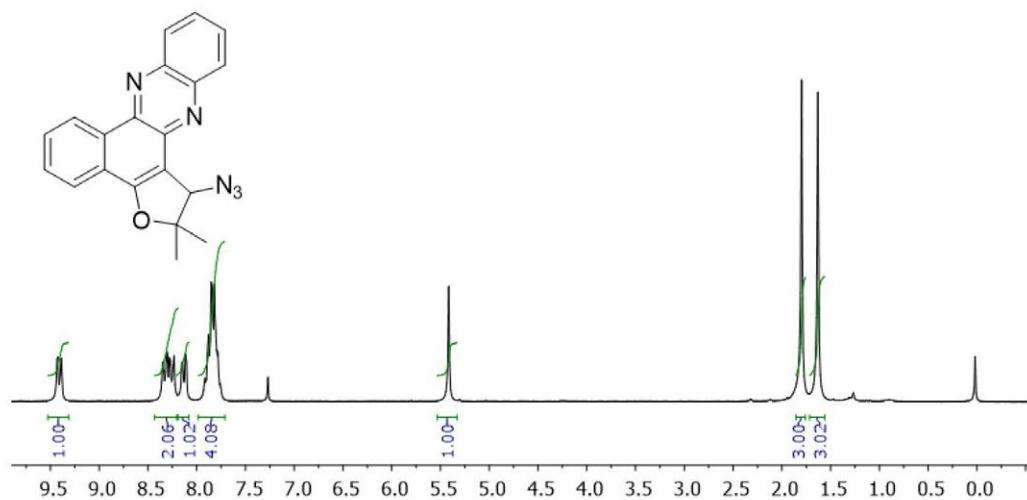
Compound **18**

Figure S32. ¹H NMR spectrum (200 MHz, CDCl₃) of compound **18**.

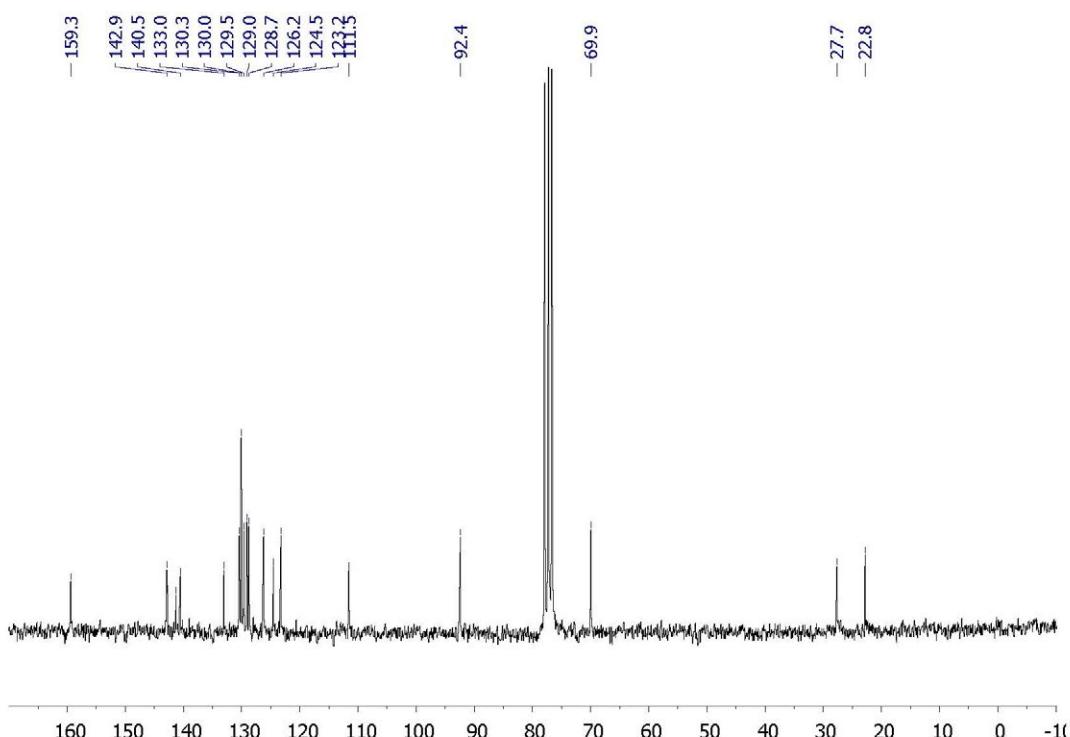


Figure S33. ¹³C NMR spectrum (50 MHz, CDCl₃) of compound **18**.

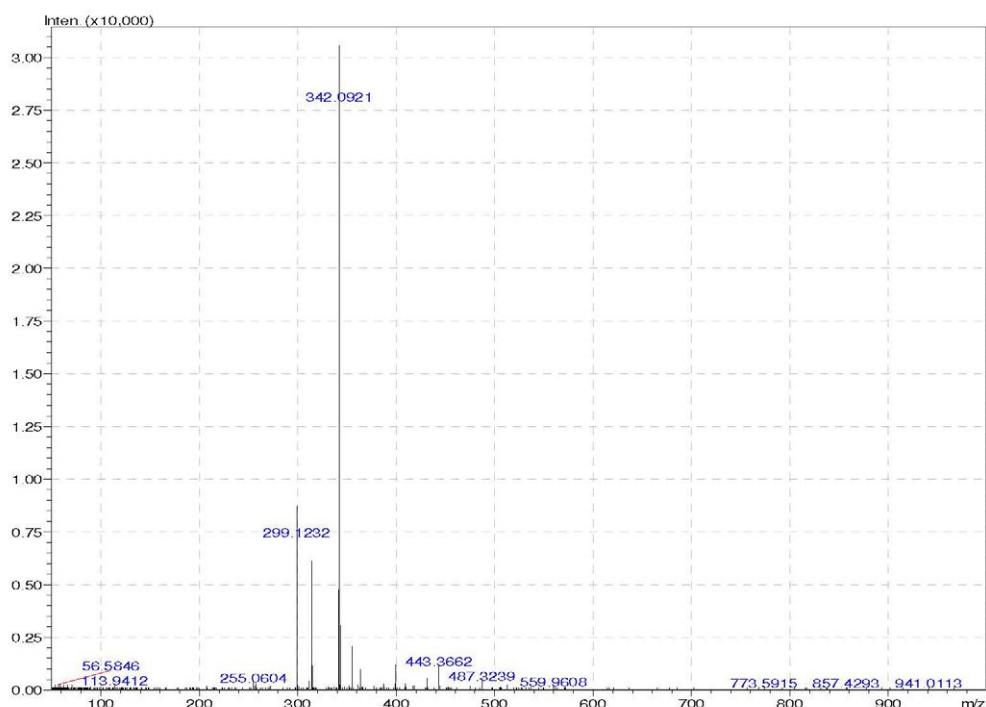


Figure S34. ESI-MS of compound **18**.

Compound **19**

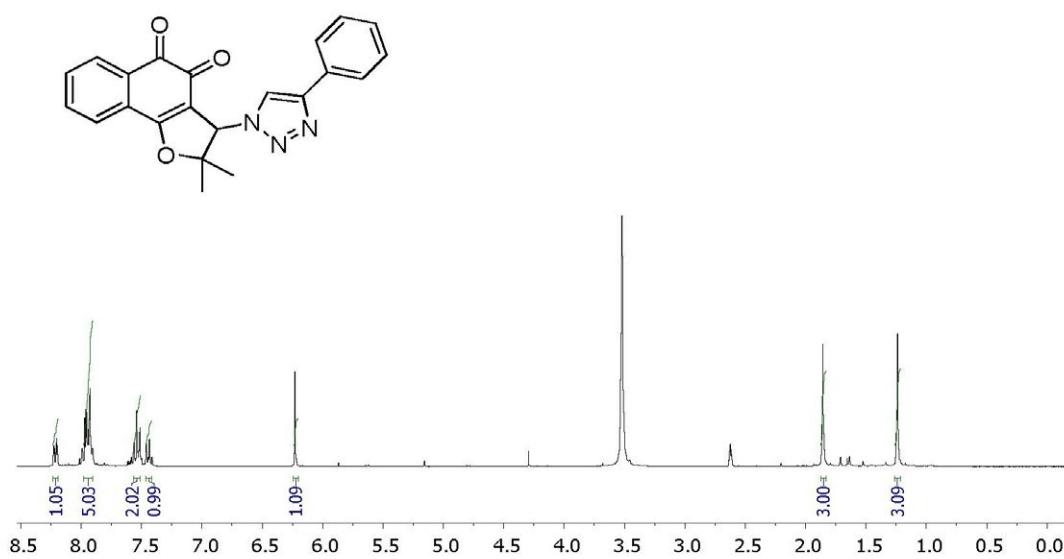


Figure S35. ¹H NMR spectrum (300 MHz, DMSO-d₆) of compound **19**.

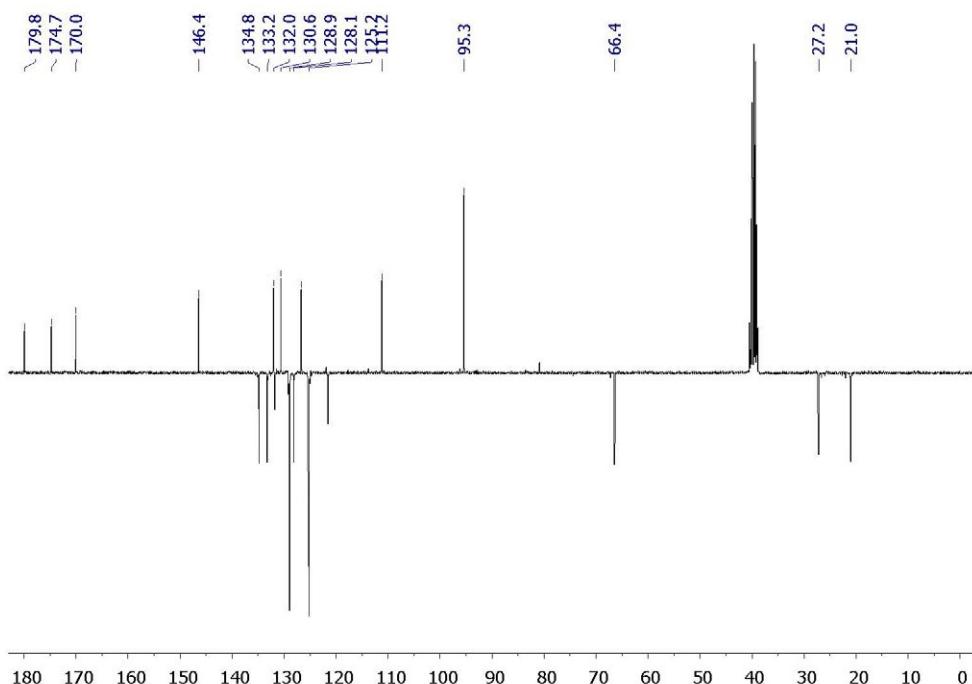


Figure S36. ^{13}C -APT NMR spectrum (75 MHz, $\text{DMSO}-d_6$) of compound **19**.

Compound **20**

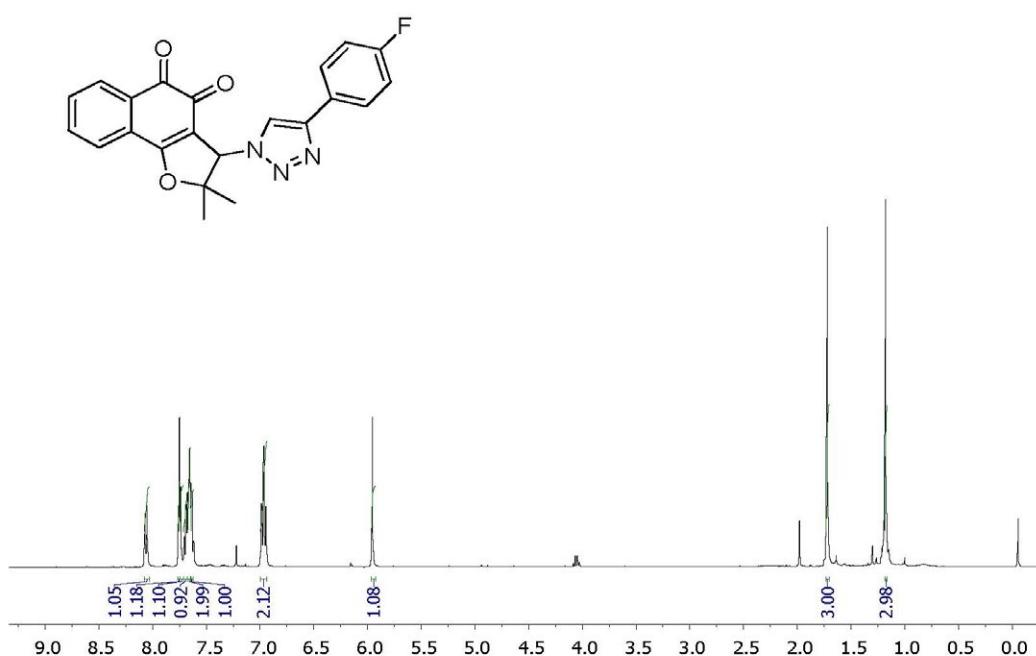


Figure S37. ^1H NMR spectrum (400 MHz, CDCl_3) of compound **20**.

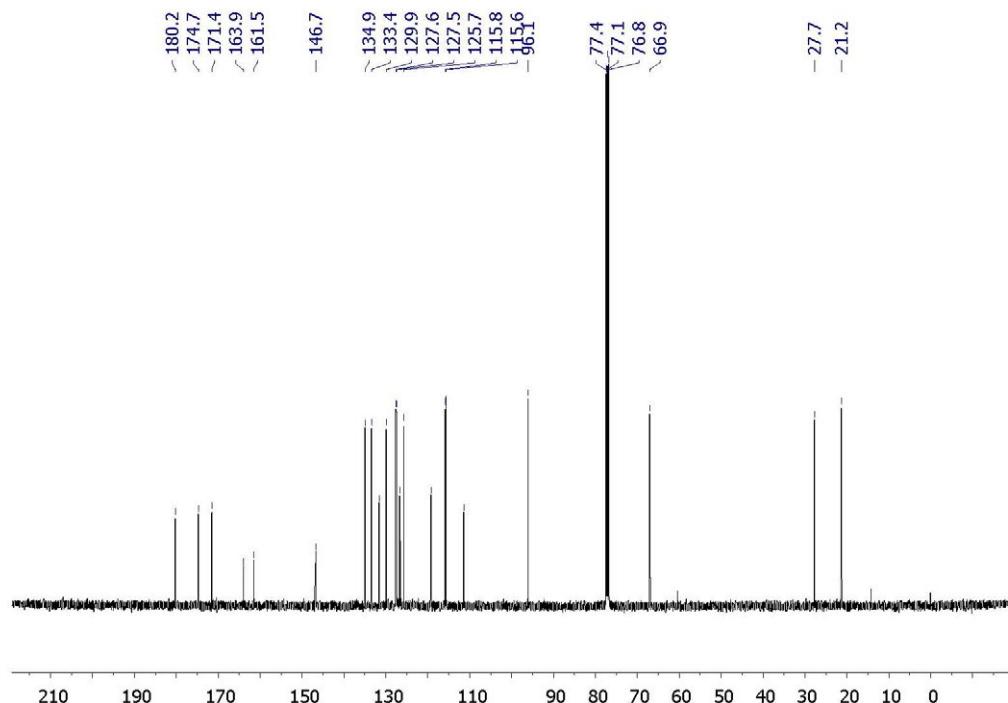


Figure S38. ^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **20**.

Compound **21**

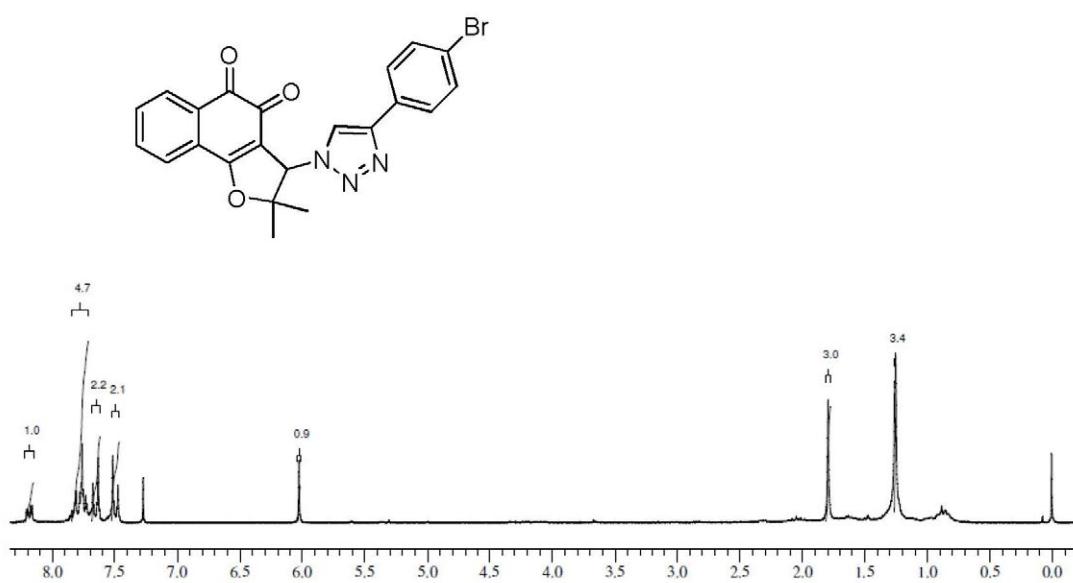


Figure S39. ^1H NMR spectrum (400 MHz, CDCl_3) of compound **21**.

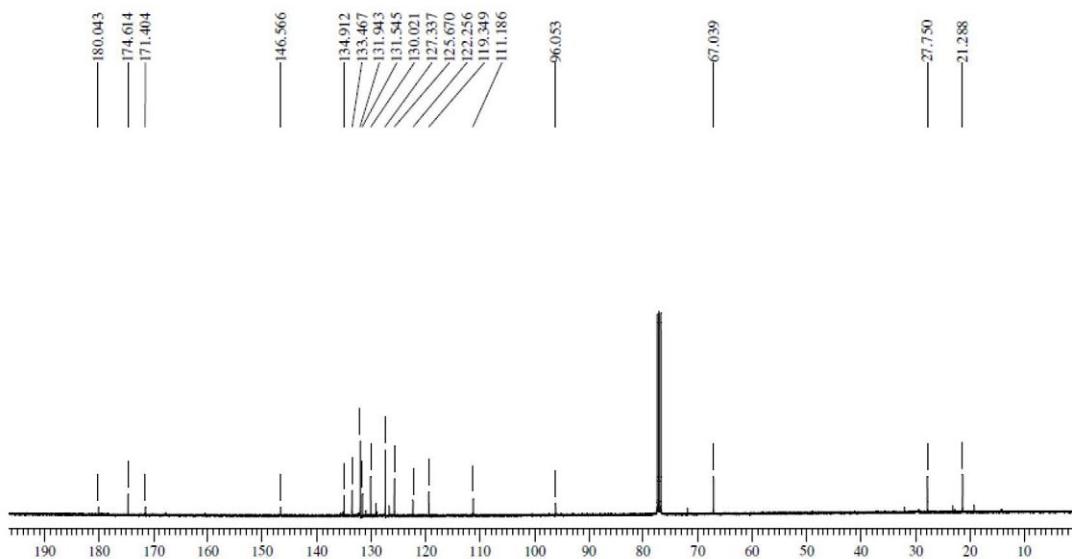


Figure S40. ^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **21**.

Compound 22

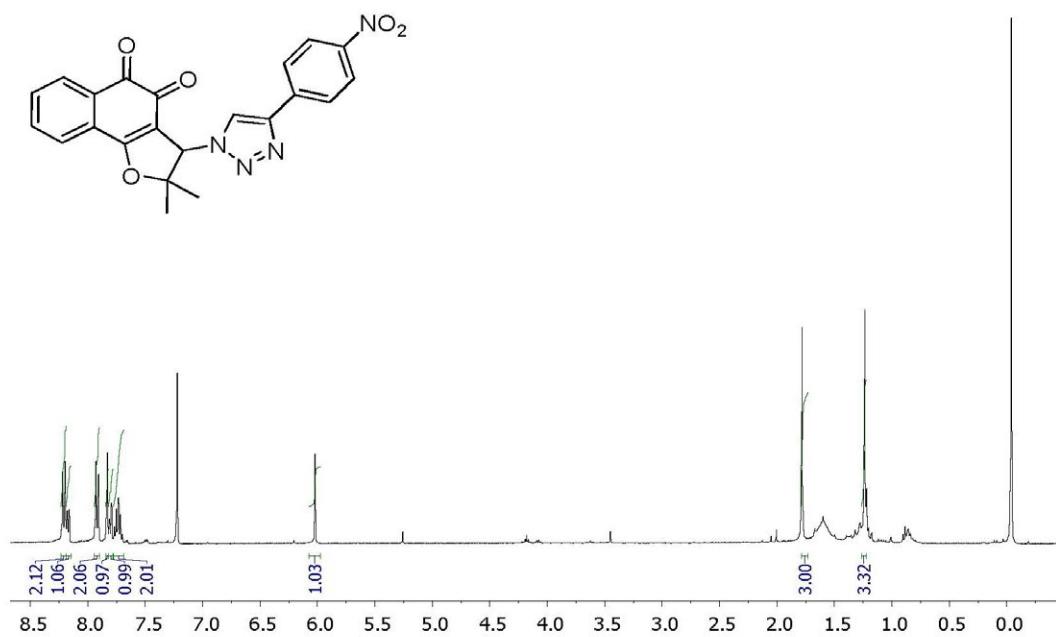


Figure S41. ^1H NMR spectrum (400 MHz, CDCl_3) of compound **22**.

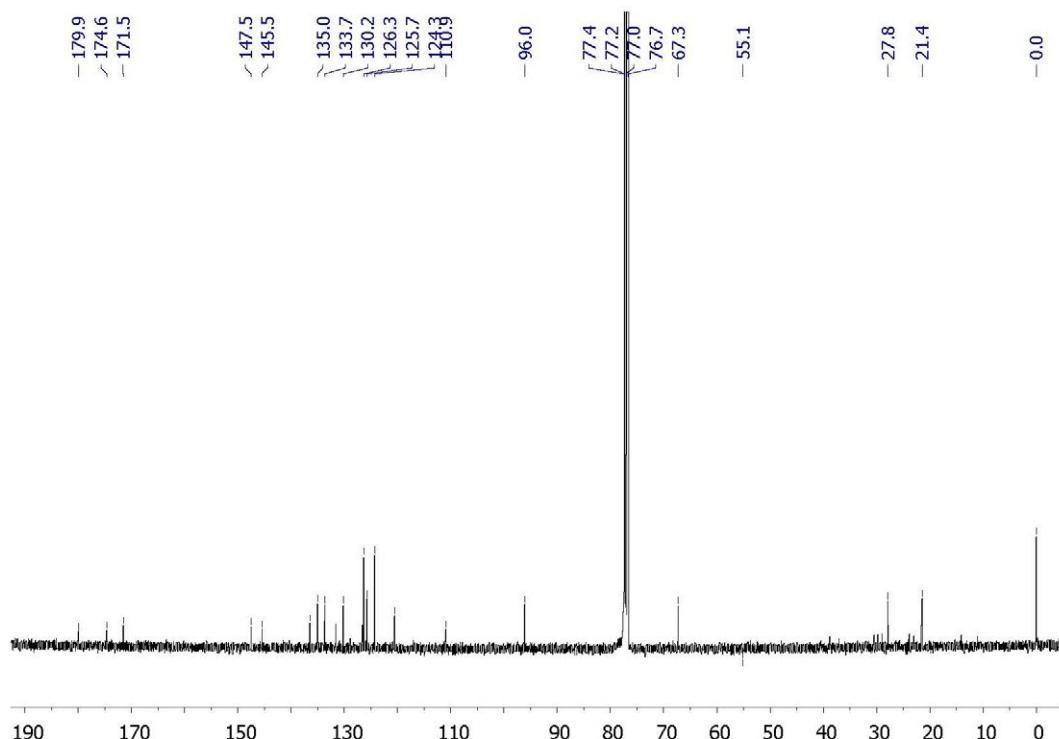


Figure S42. ^{13}C NMR spectrum (100 MHz, CDCl_3) of compound 22.

Compound 23

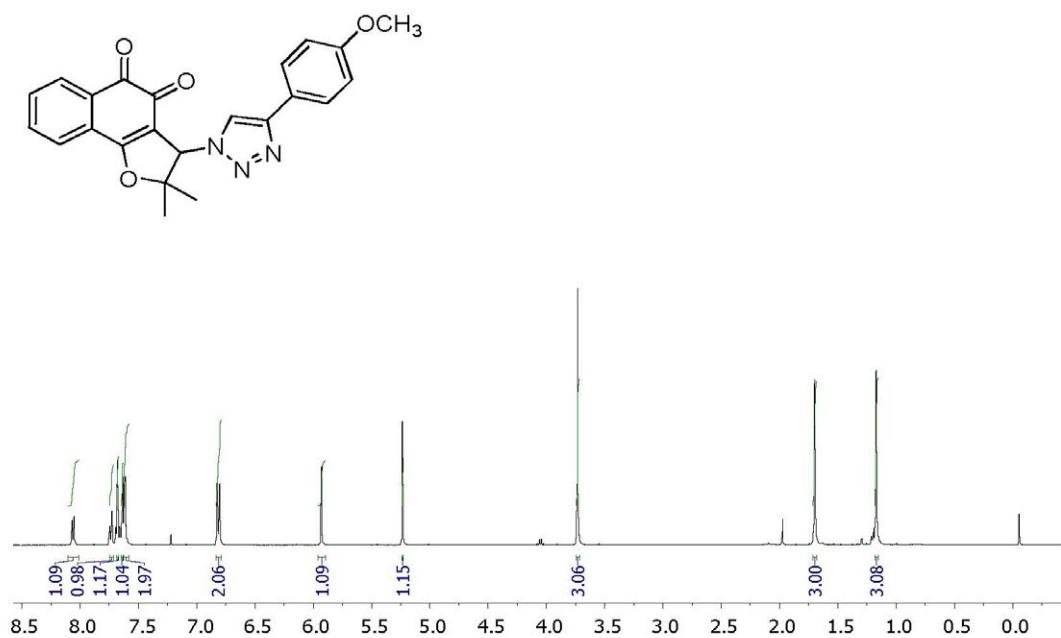


Figure S43. ^1H NMR spectrum (400 MHz, CDCl_3) of compound 23.

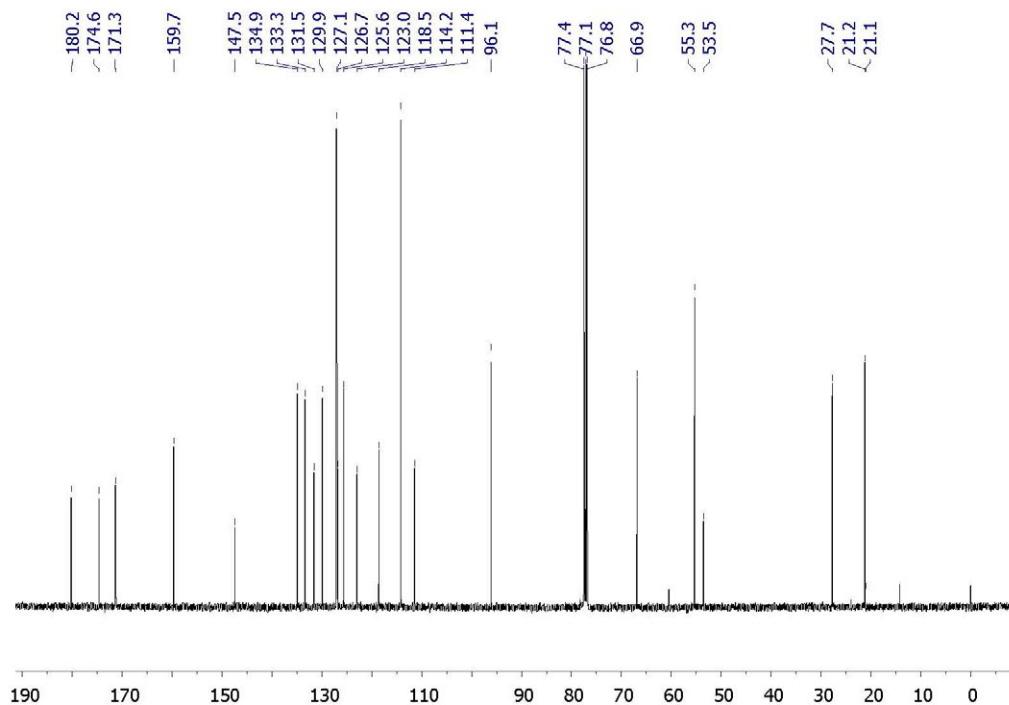


Figure S44. ^{13}C NMR spectrum (100 MHz, CDCl_3) of compound 23.

Compound 24

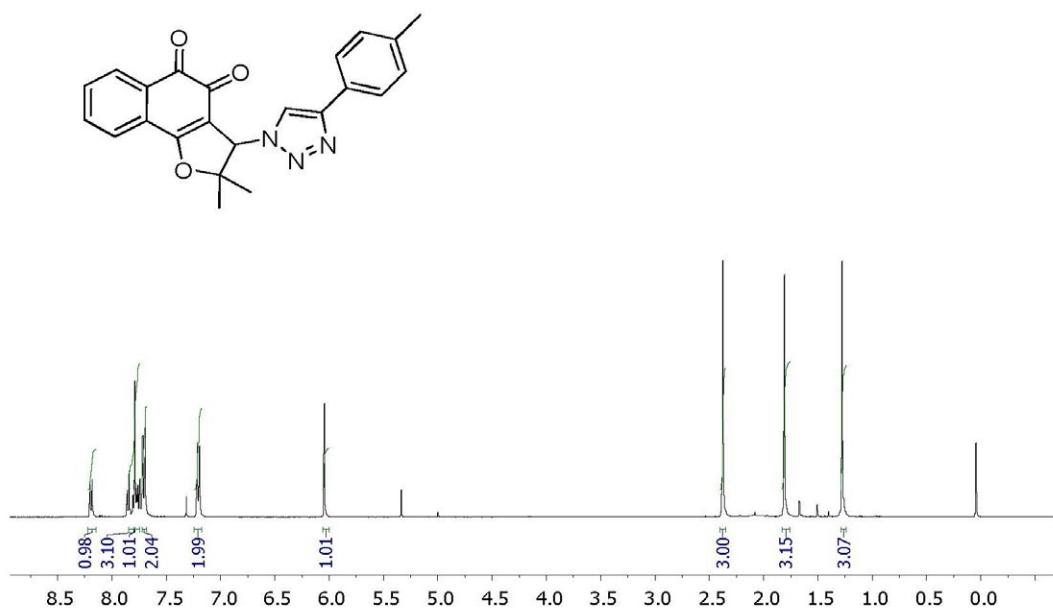


Figure S45. ^1H NMR spectrum (200 MHz, CDCl_3) of compound 24.

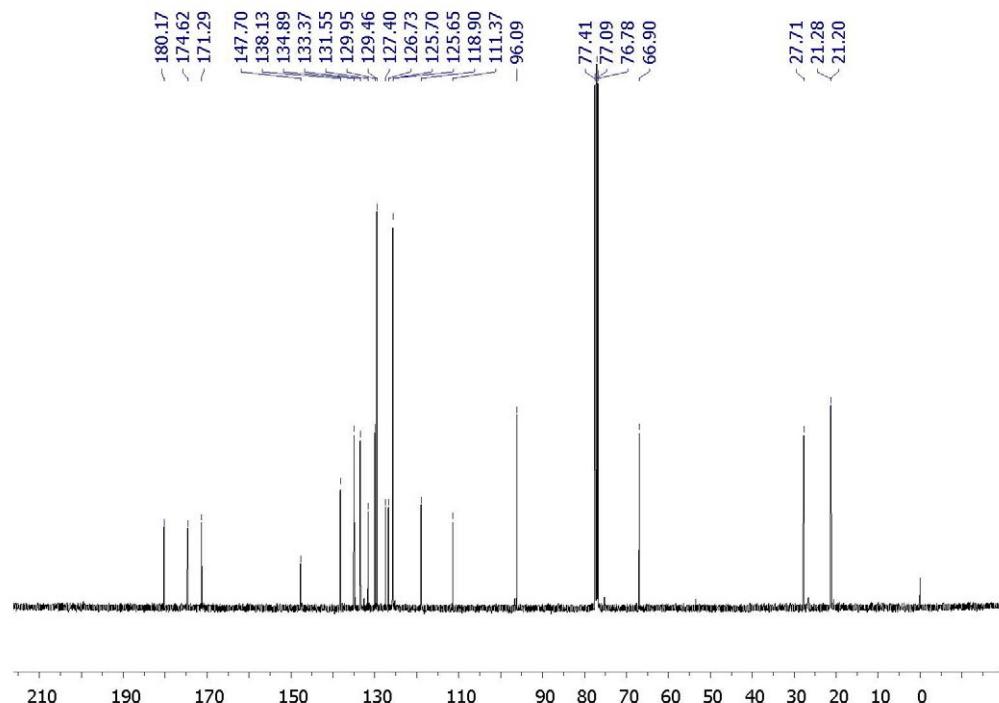


Figure S46. ^{13}C NMR spectrum (50 MHz, CDCl_3) of compound 24.

Compound 25

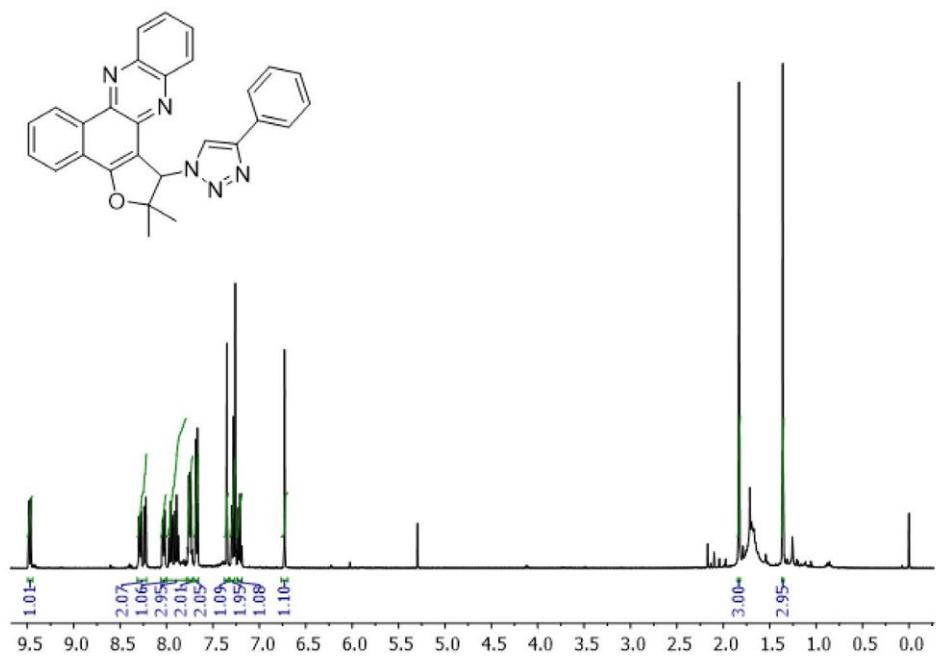


Figure S47. ^1H NMR spectrum (400 MHz, CDCl_3) of compound 25.

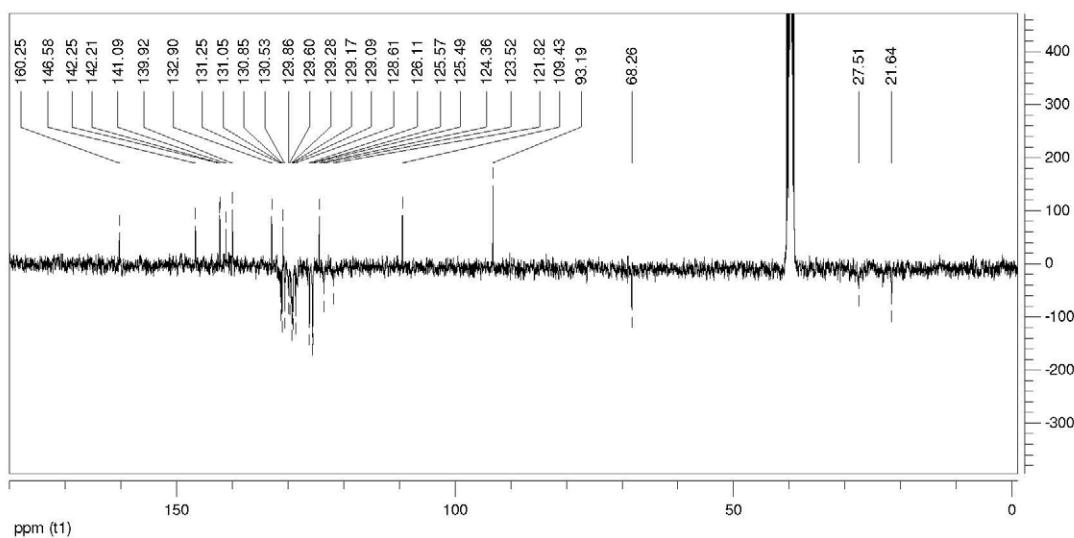


Figure S48. ^{13}C -APT NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound **25**.

Compound **26**

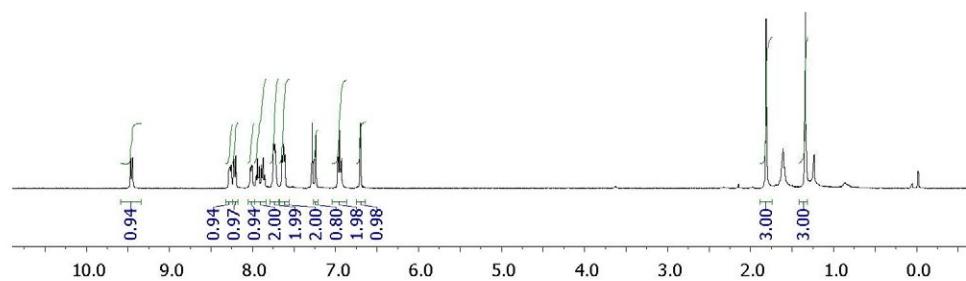
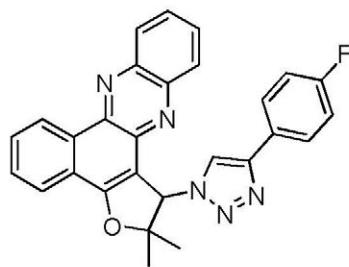


Figure S49. ^1H NMR spectrum (400 MHz, CDCl_3) of compound **26**.

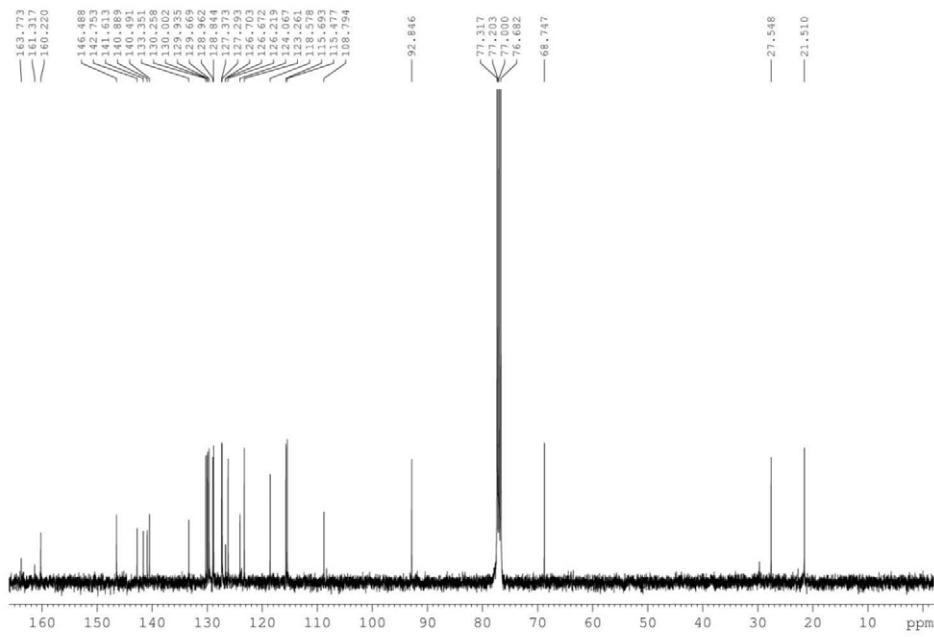


Figure S50. ^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **26**.

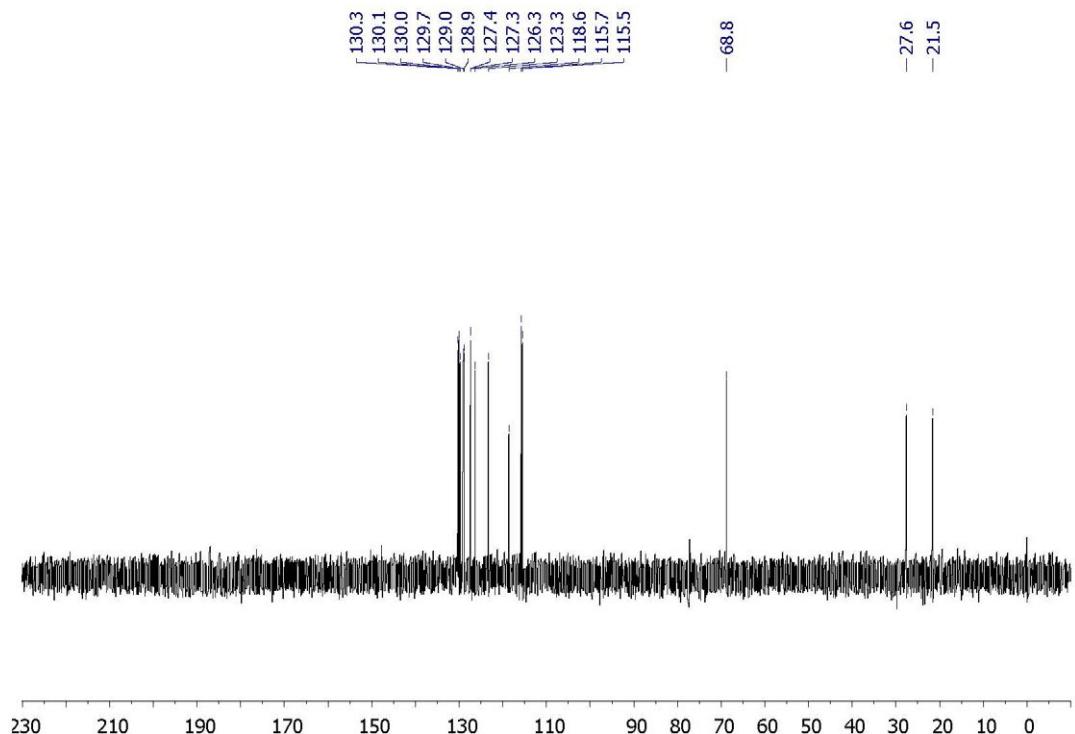


Figure S51. ^{13}C -DEPT NMR spectrum (100 MHz, CDCl_3) of compound **26**.

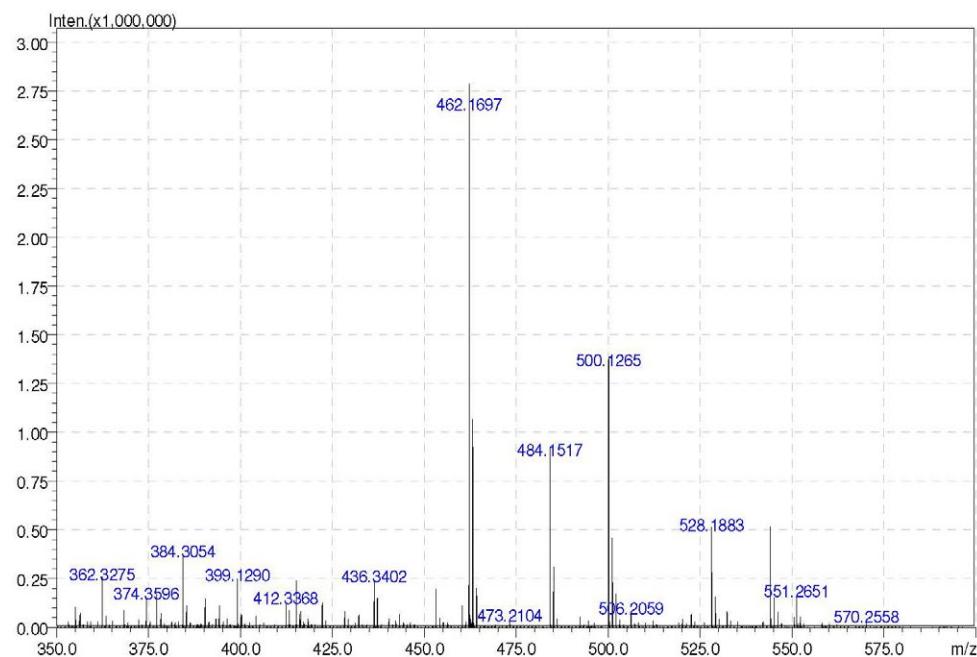


Figure 52. ESI-MS of compound 26.

Compound 27

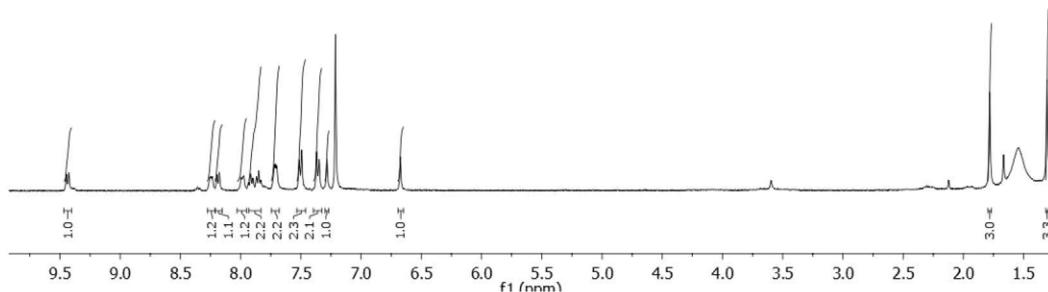
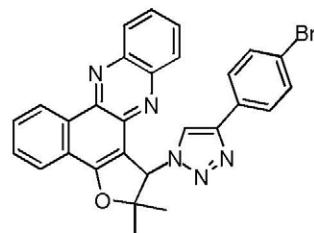


Figure S53. ¹H NMR spectrum (400 MHz, CDCl₃) of compound 27.

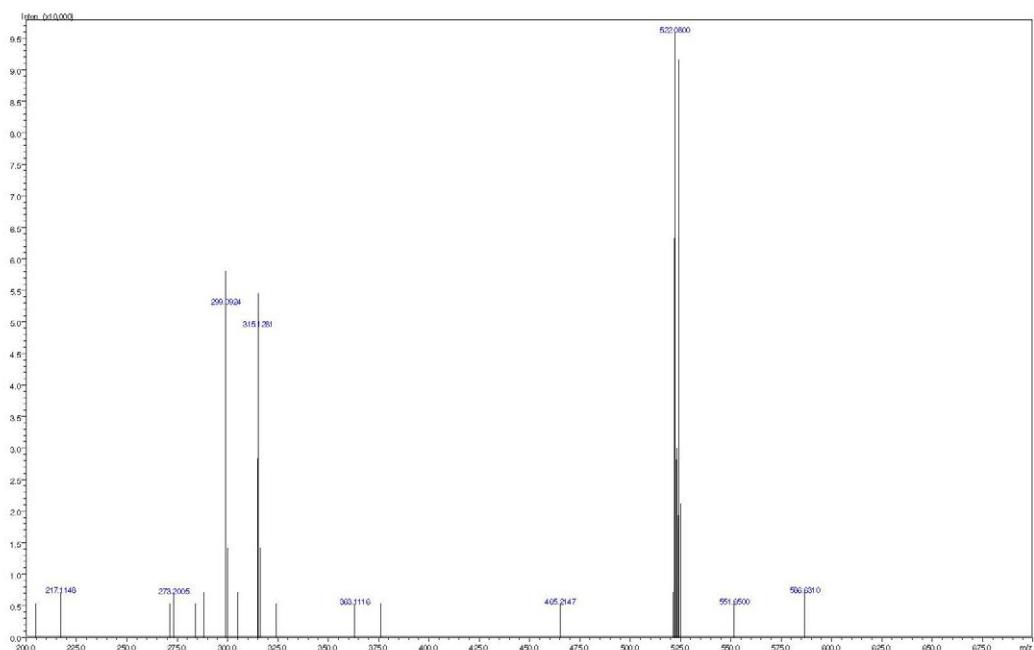


Figure S54. ESI-MS of compound 27.

Compound 28

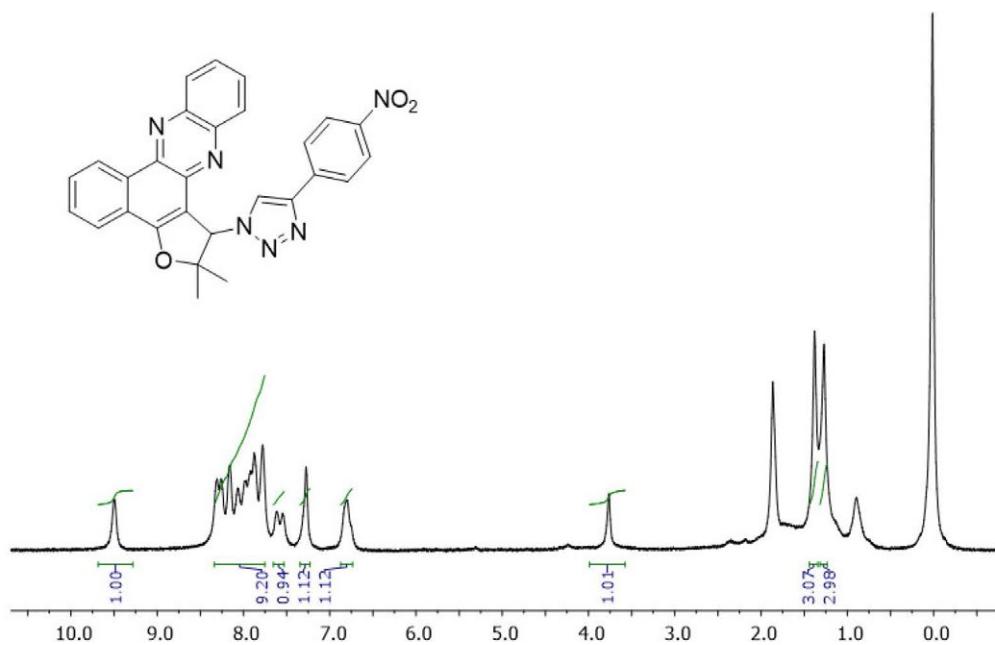


Figure S55. ¹H NMR spectrum (400 MHz, CDCl₃) of compound 28.

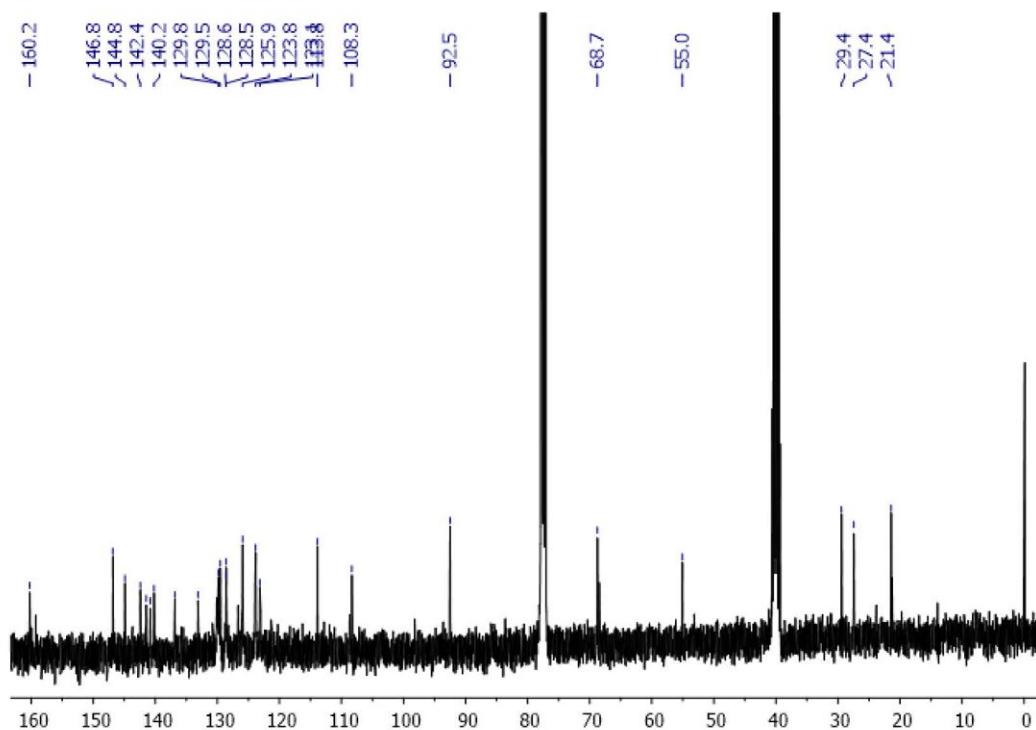


Figure S56. ^{13}C NMR spectrum (100 MHz, CDCl_3) of compound 28.

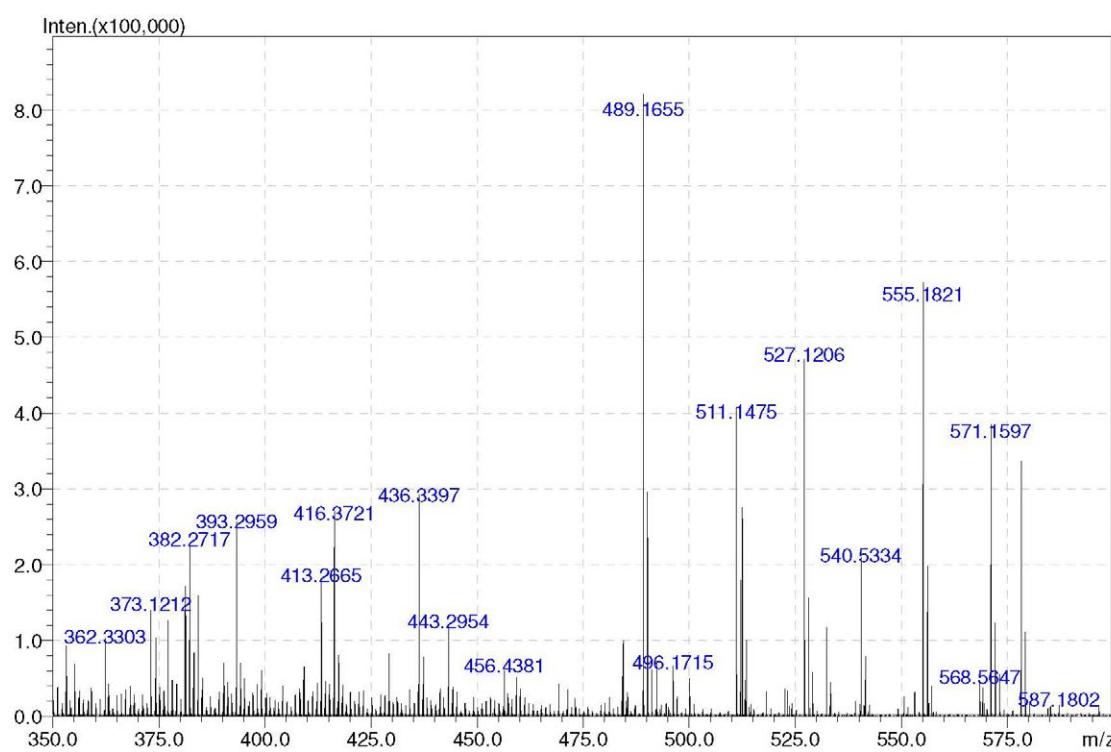


Figure S57. ESI-MS of compound 28.

Compound 29

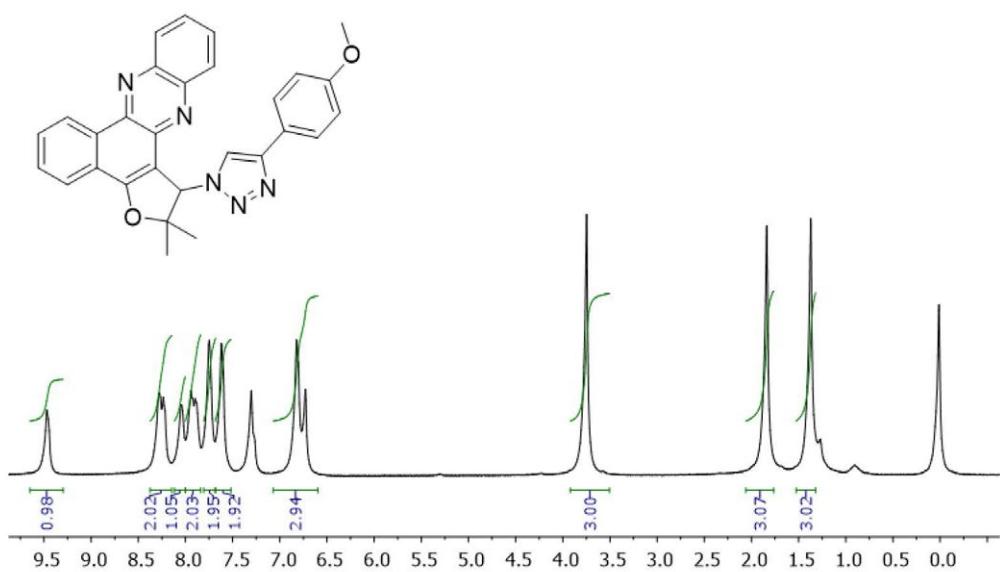


Figure S58. ¹H NMR spectrum (400 MHz, CDCl₃) of compound 29.

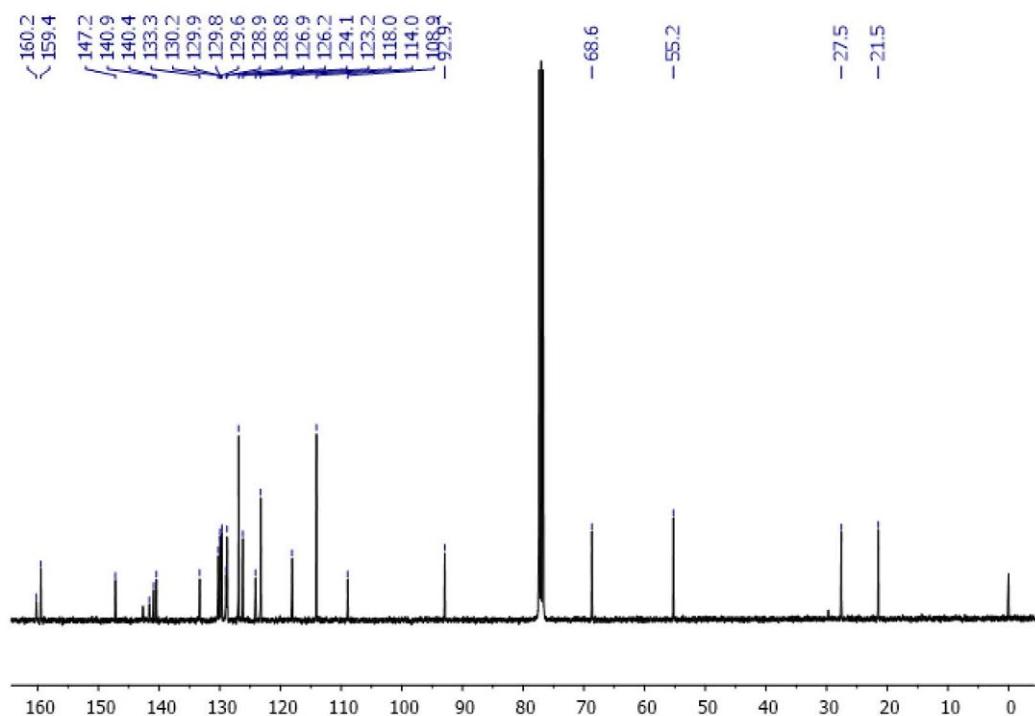


Figure S59. ¹³C NMR spectrum (100 MHz, CDCl₃) of compound 29.

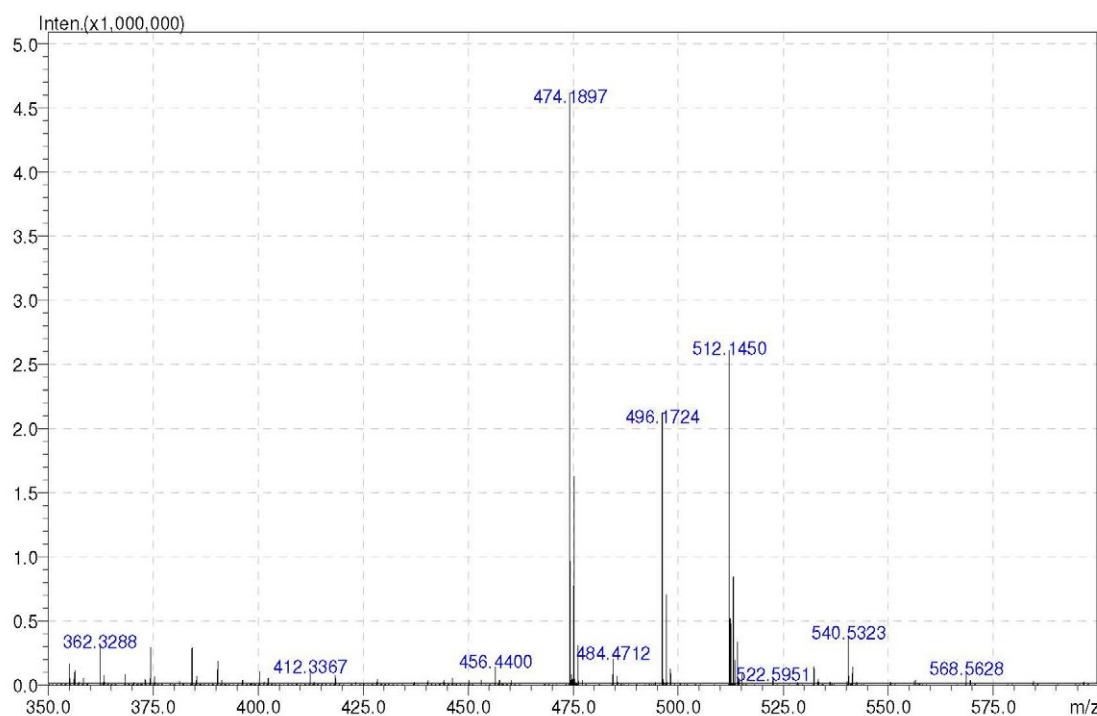


Figure S60. ESI-MS of compound **29**.

Compound **30**

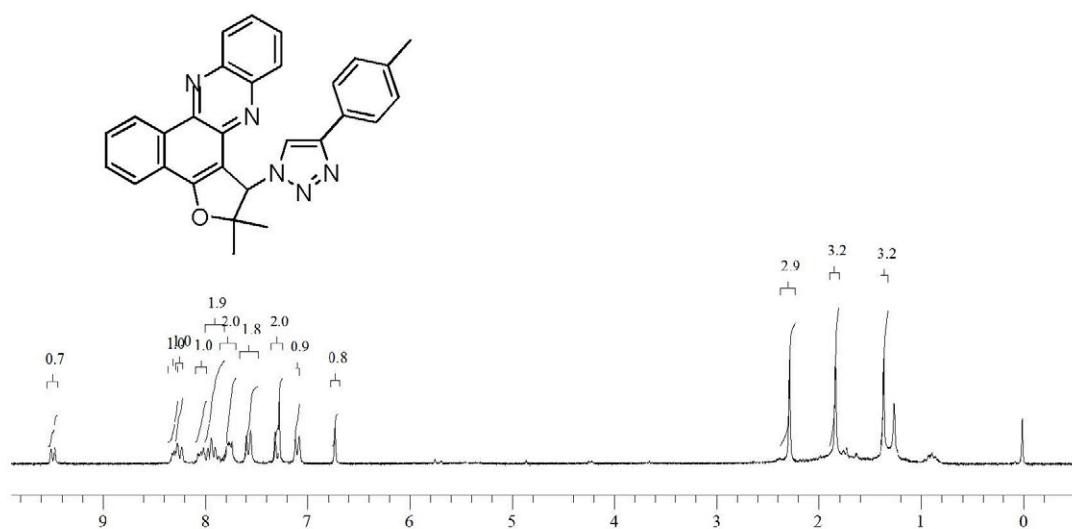


Figure S61. ¹H NMR spectrum (400 MHz, CDCl₃) of compound **30**.

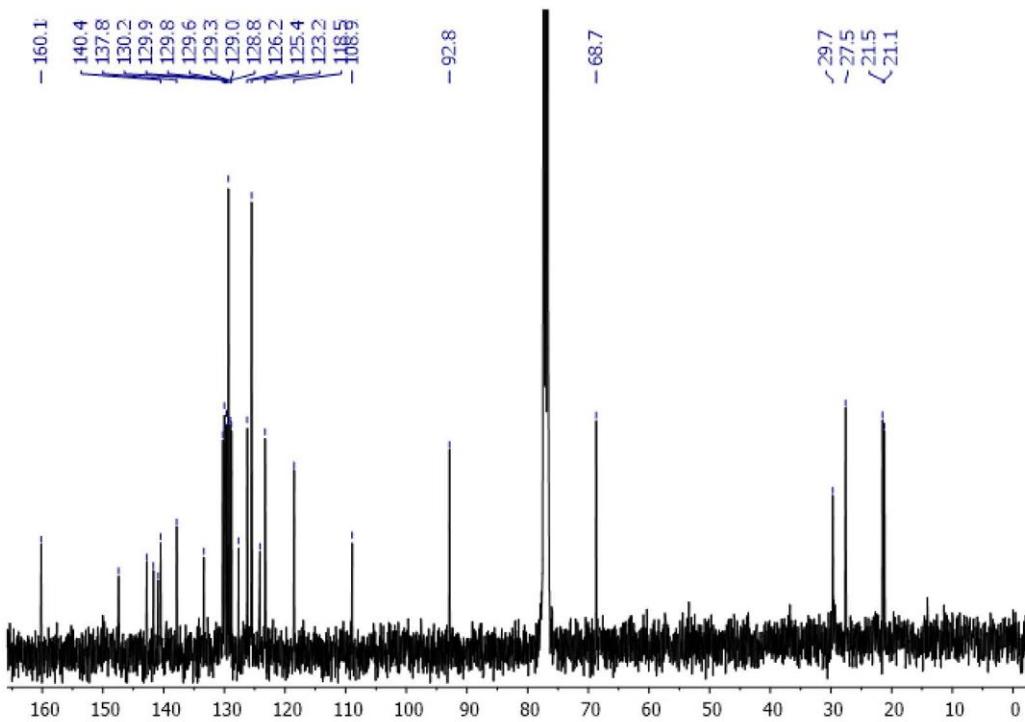


Figure S62. ^{13}C NMR spectrum (100 MHz, CDCl_3) of compound **30**.

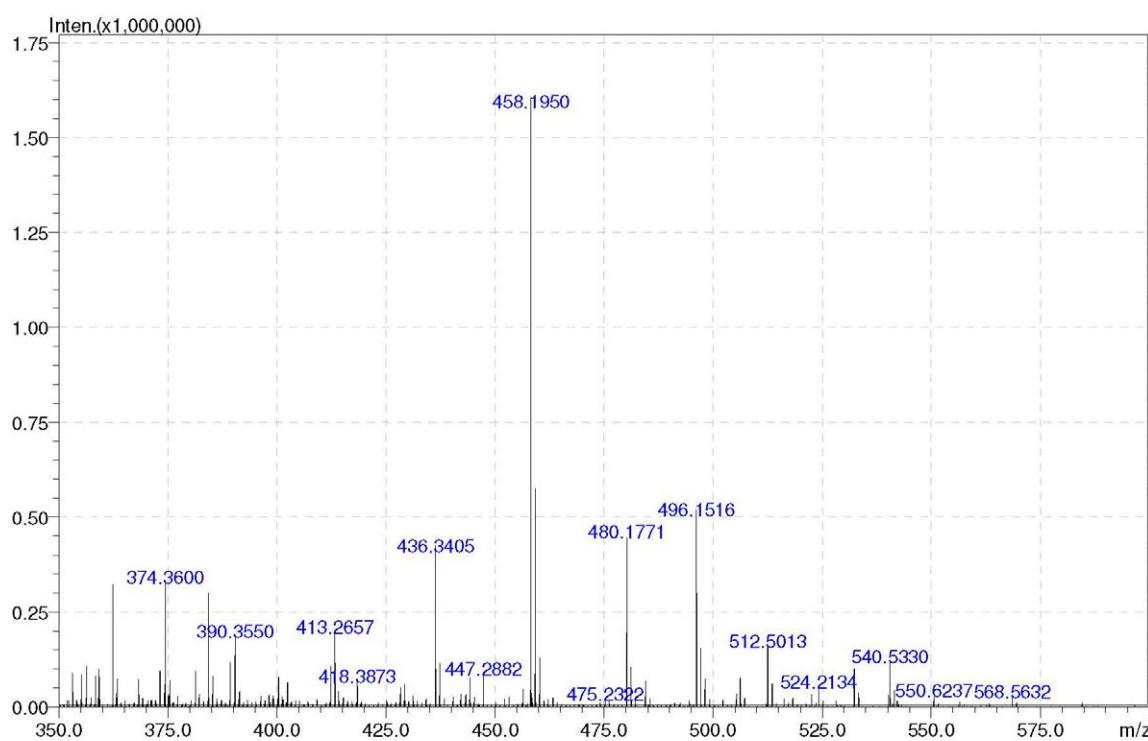
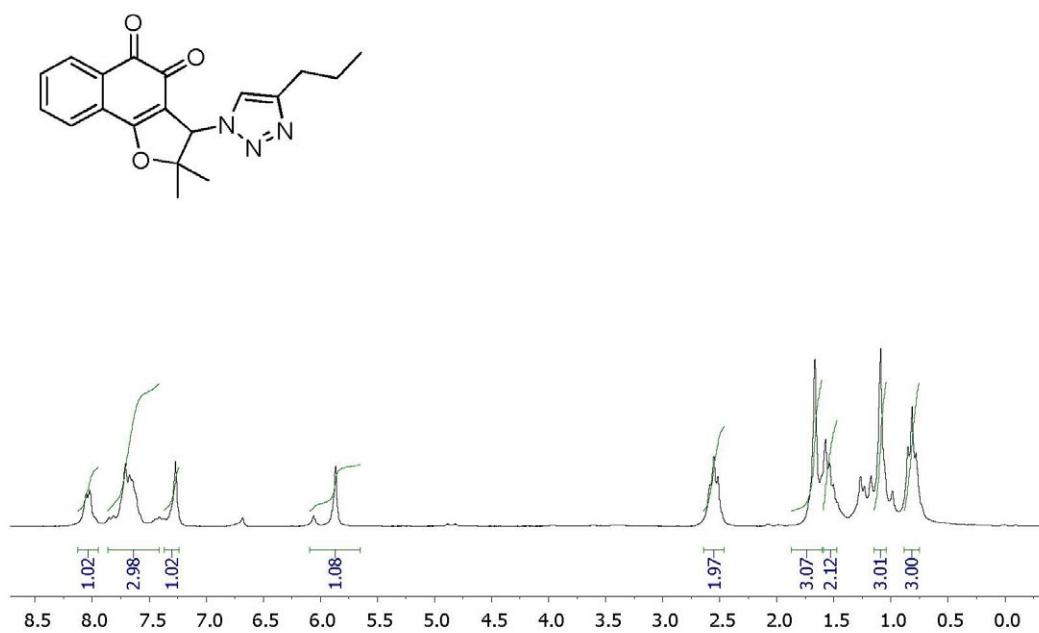
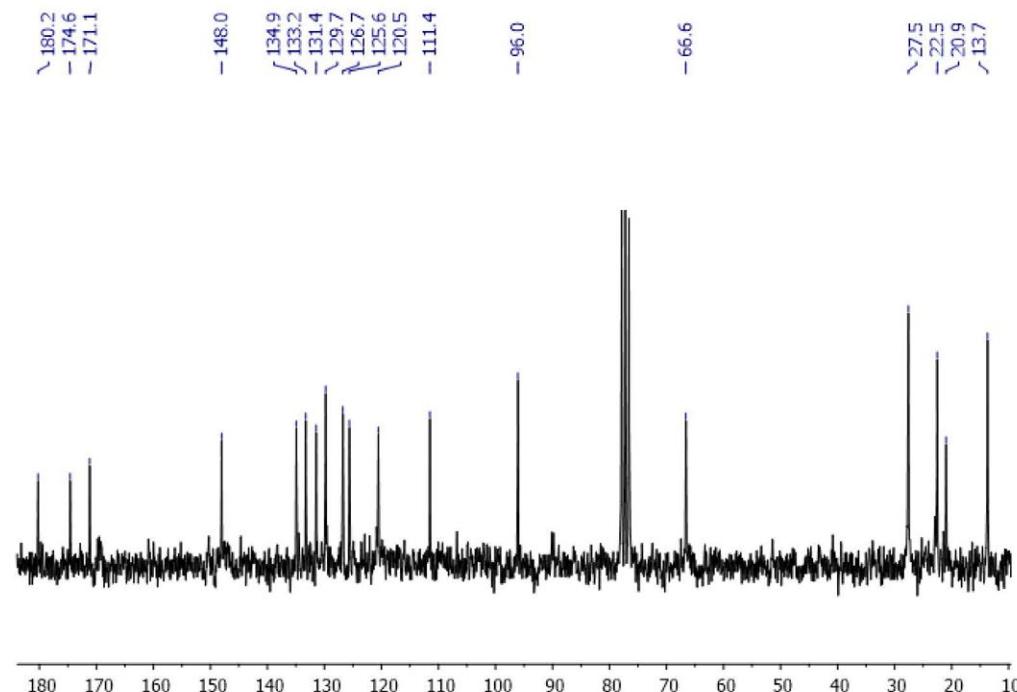


Figure S63. ESI-MS of compound **30**.

Compound **31****Figure S64.** ¹H NMR spectrum (200 MHz, CDCl₃) of compound **31**.**Figure S65.** ¹³C NMR spectrum (50 MHz, CDCl₃) of compound **31**.

Compound 32

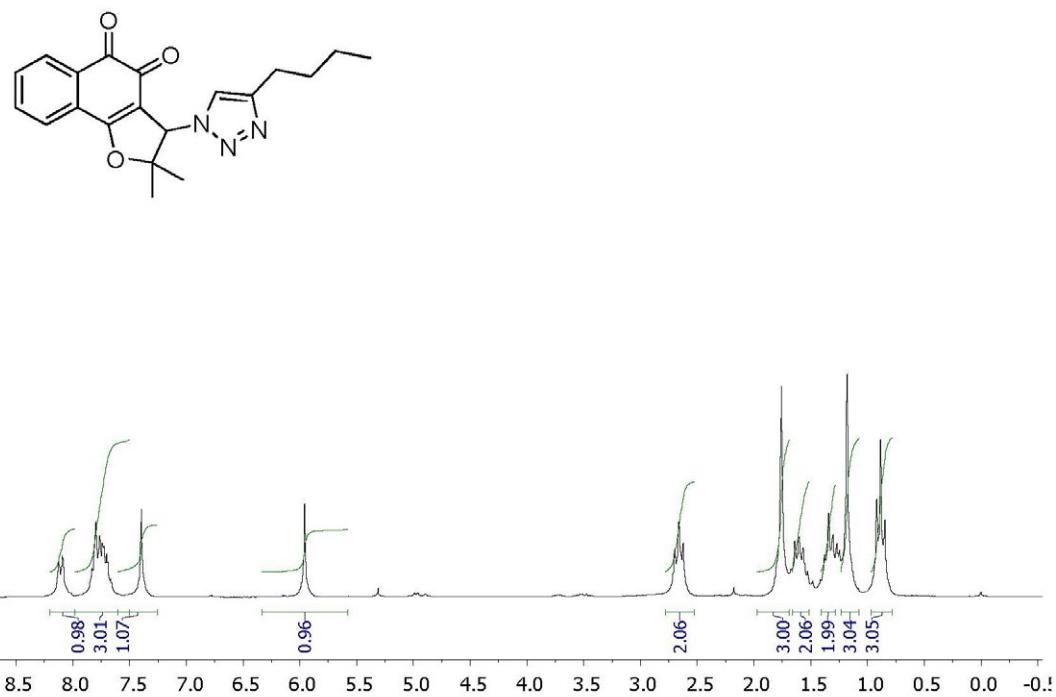


Figure S66. ¹H NMR spectrum (200 MHz, CDCl₃) of compound 32.

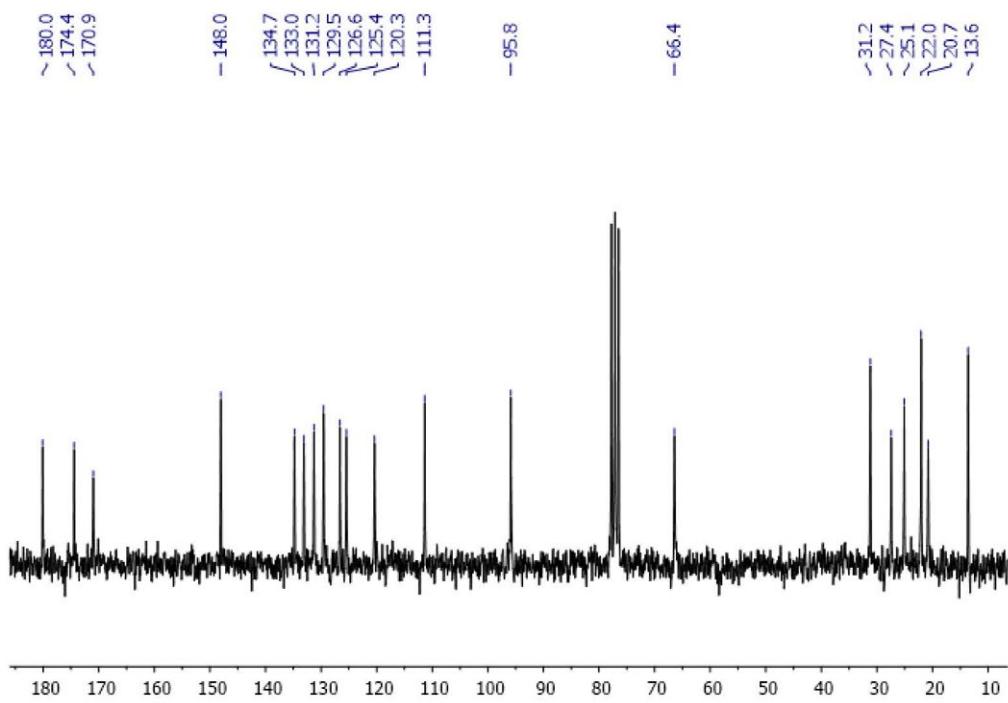
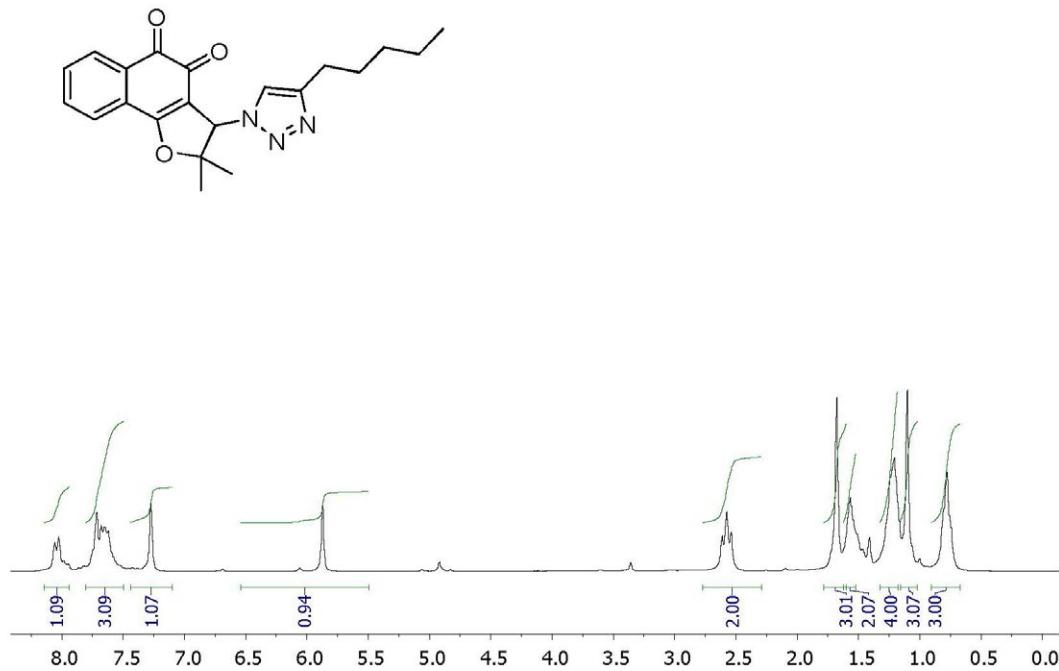
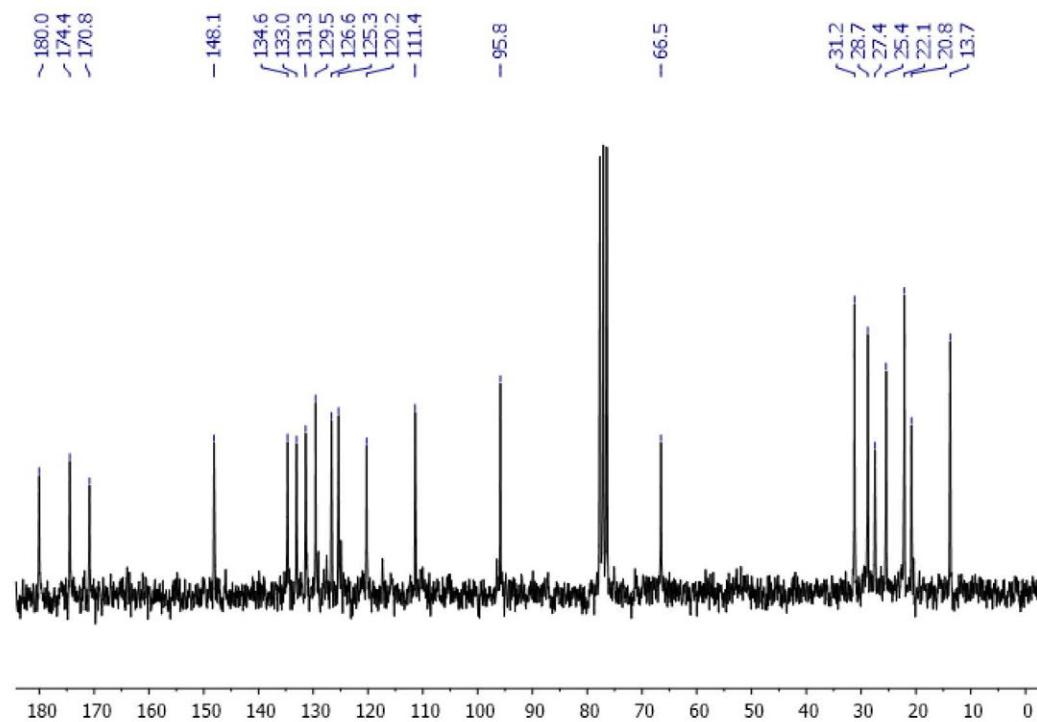


Figure S67. ¹³C NMR spectrum (50 MHz, CDCl₃) of compound 32.

Compound **33****Figure S68.** ¹H NMR spectrum (200 MHz, CDCl₃) of compound **33**.**Figure S69.** ¹³C NMR spectrum (50 MHz, CDCl₃) of compound **33**.

Compound 34

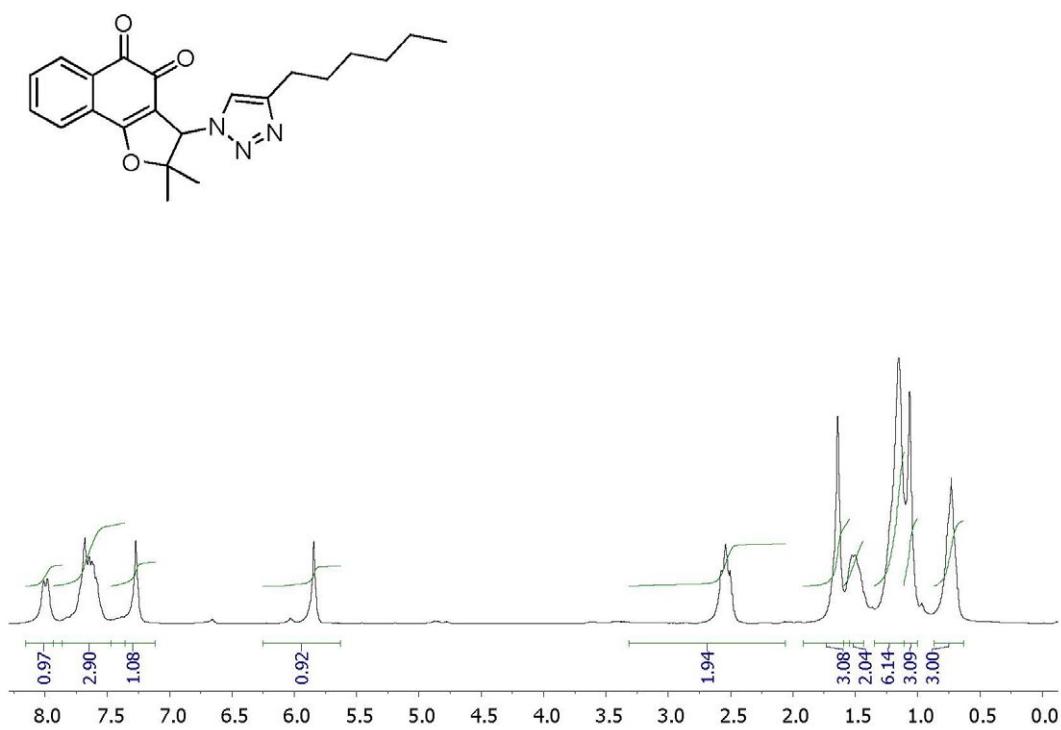


Figure S70. ¹H NMR spectrum (200 MHz, CDCl₃) of compound 34.

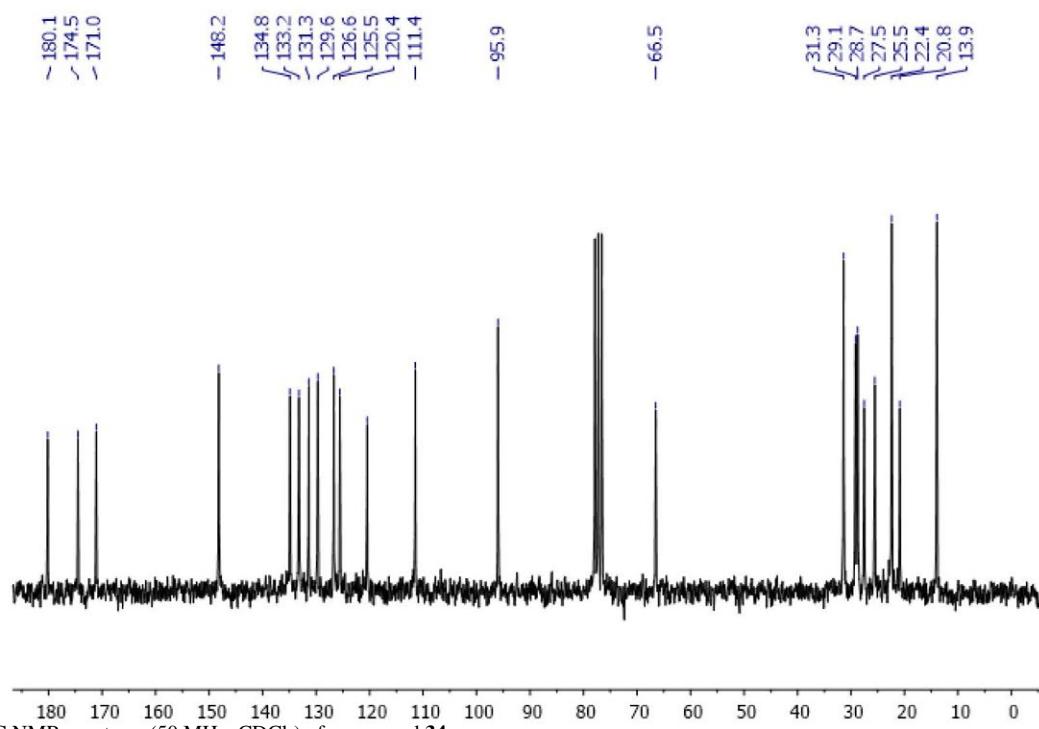


Figure S71. ¹³C NMR spectrum (50 MHz, CDCl₃) of compound 34.

Compound 35

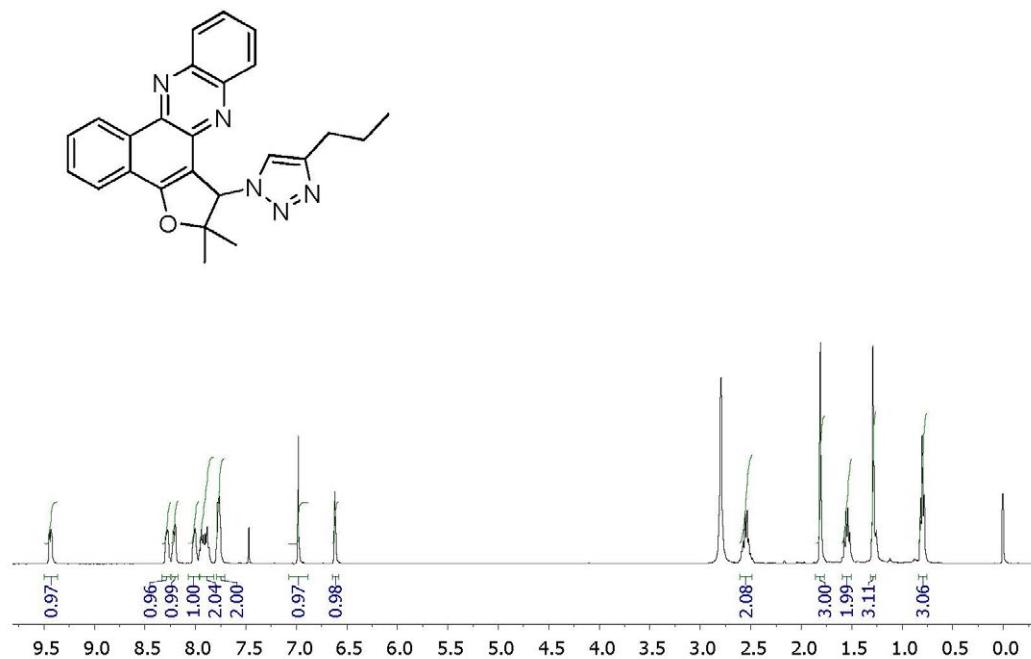


Figure S72. ¹H NMR spectrum (400 MHz, CDCl₃) of compound 35.

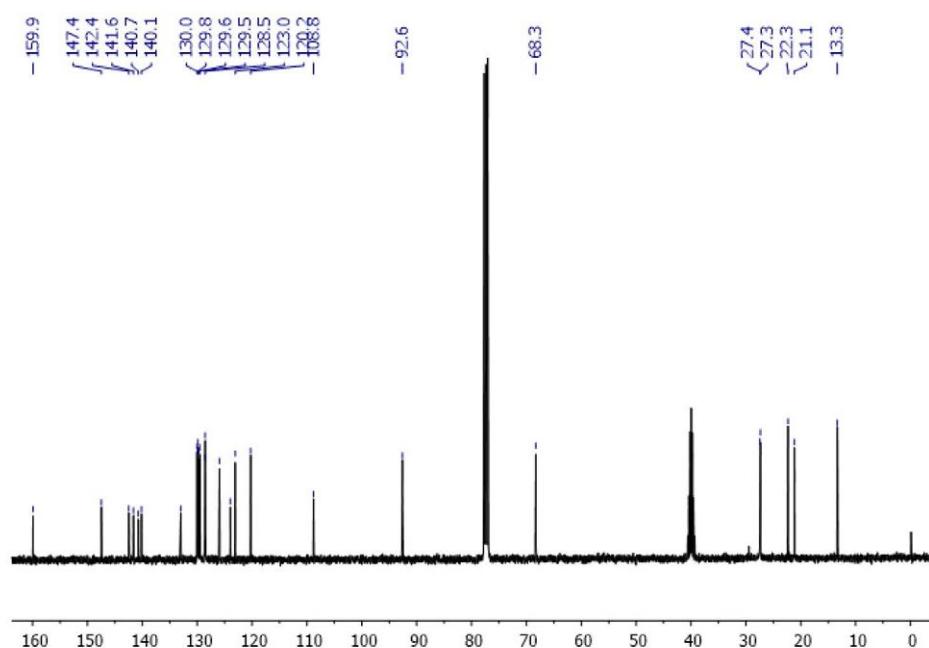


Figure S73. ¹³C NMR spectrum (100 MHz, CDCl₃) of compound 35.

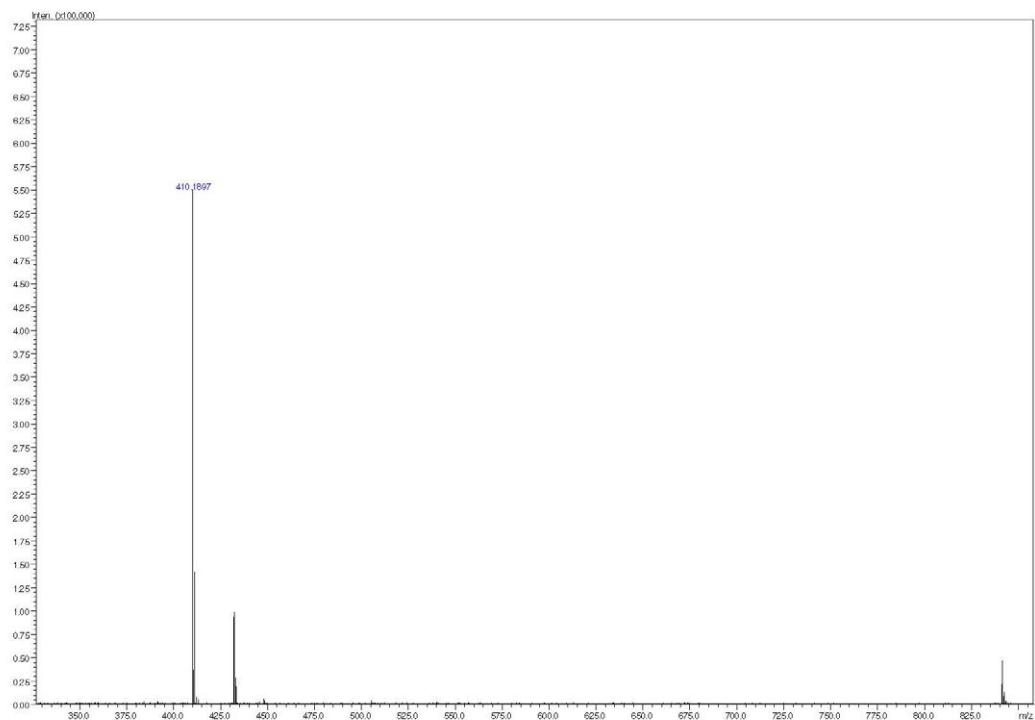


Figure S74. ESI-MS of compound 35.

Compound 36

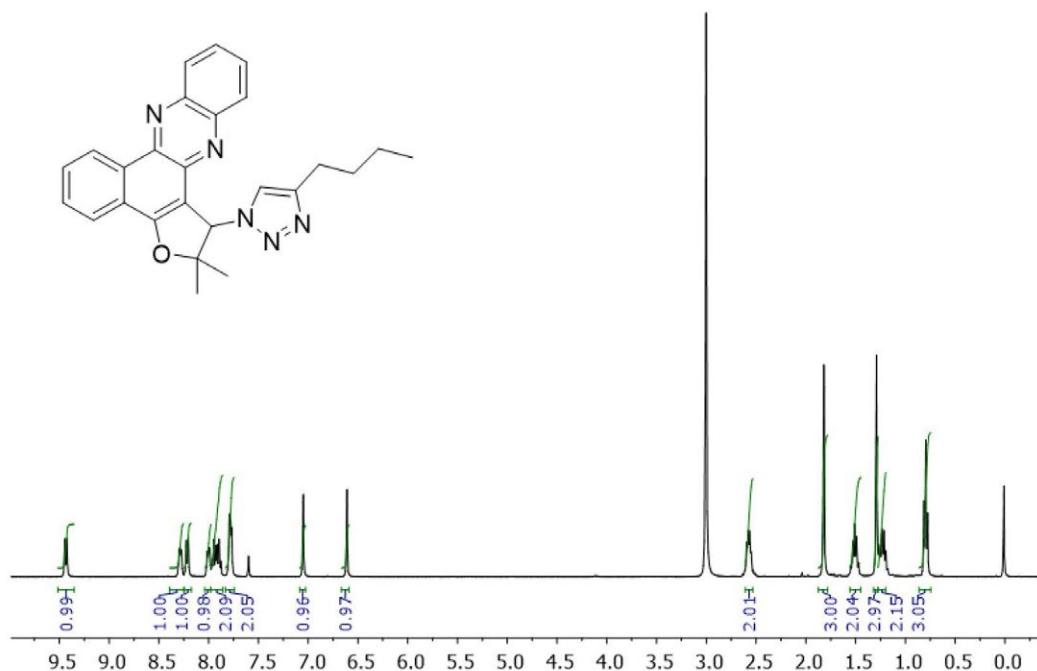


Figure S75. ¹H NMR spectrum (400 MHz, CDCl₃) of compound 36.

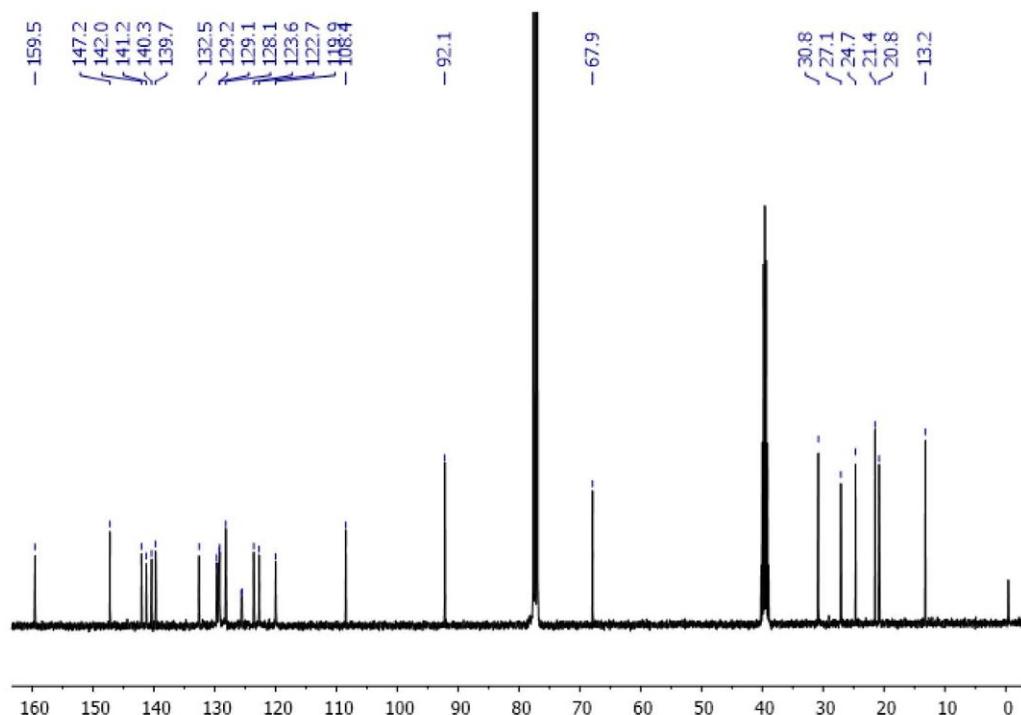


Figure S76. ^{13}C NMR spectrum (100 MHz, CDCl_3) of compound 36.

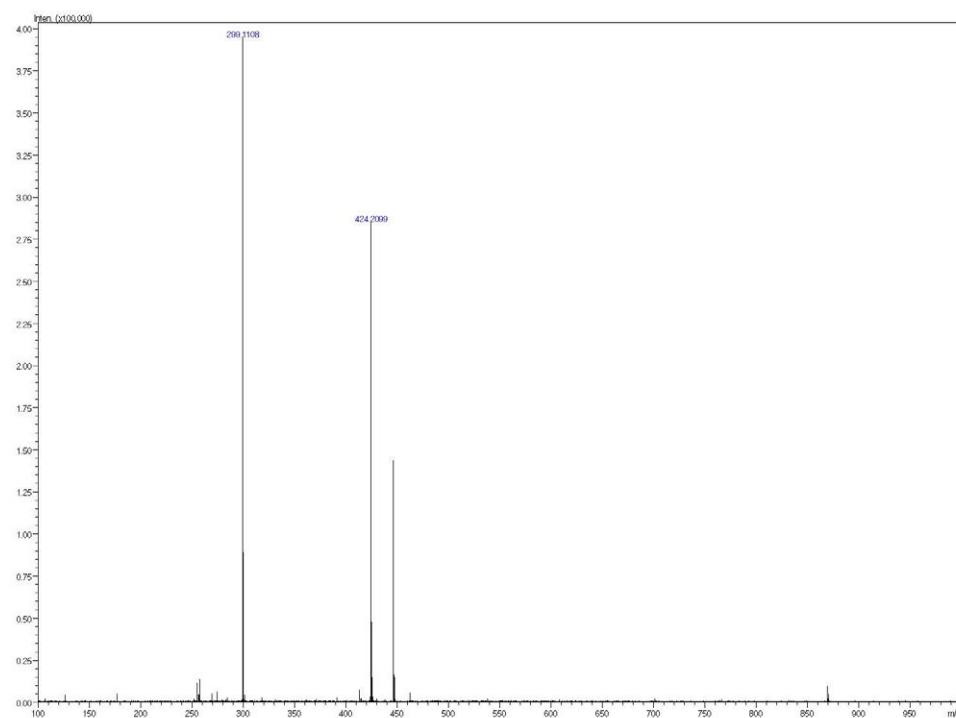


Figure S77. ESI-MS of compound 36.

Compound 37

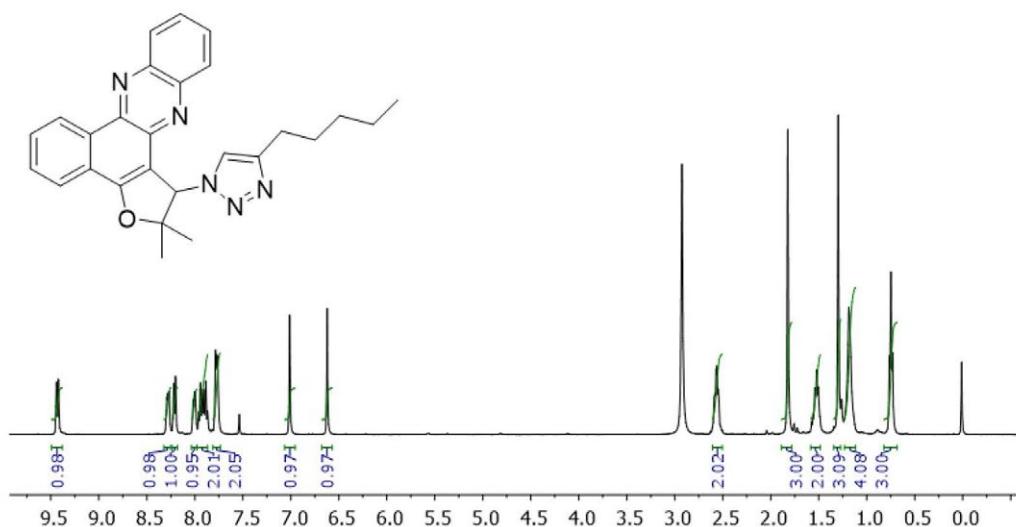


Figure S78. ¹H NMR spectrum (400 MHz, CDCl₃) of compound 37.

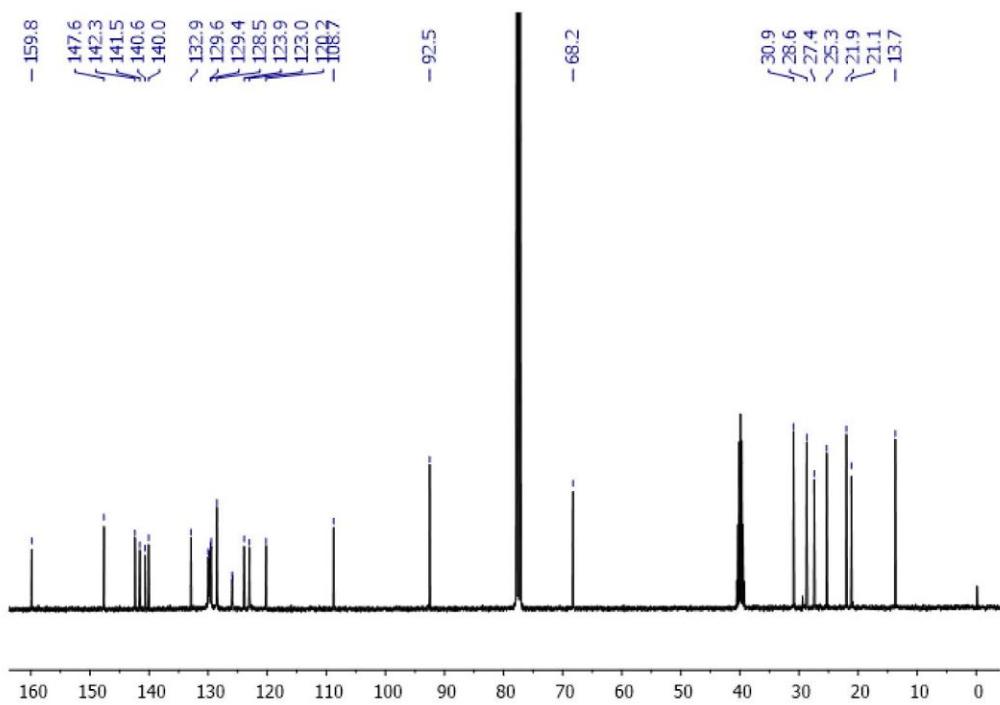


Figure S79. ¹³C NMR spectrum (100 MHz, CDCl₃) of compound 37

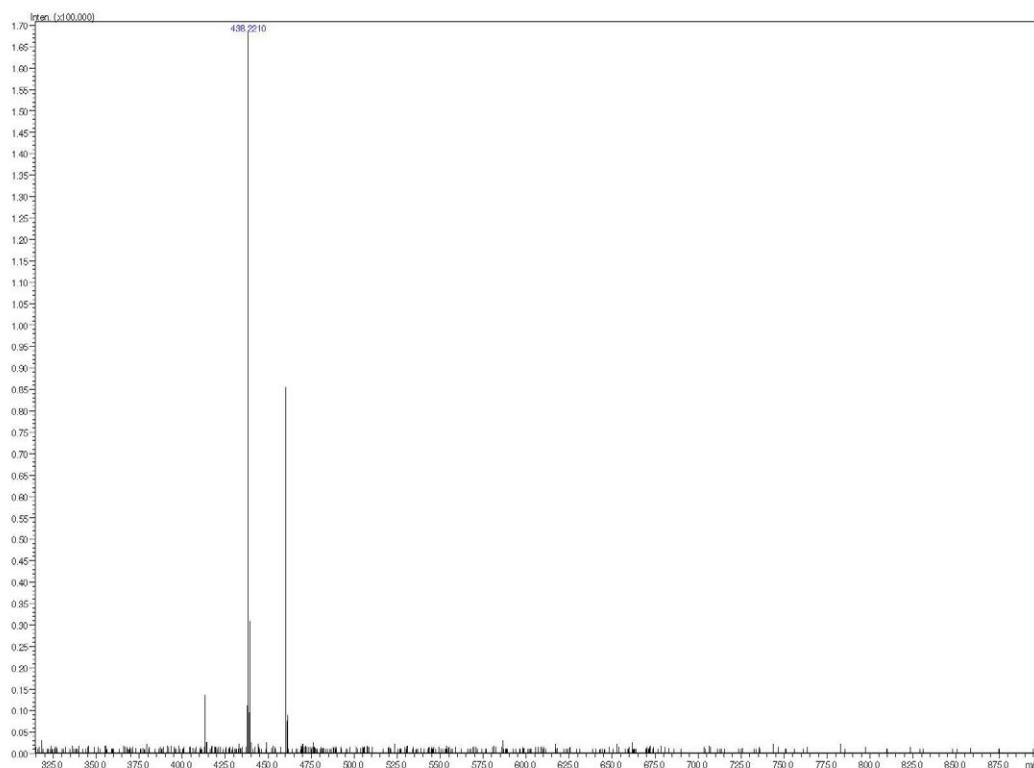


Figure S80. ESI-MS of compound 37.

Compound 38

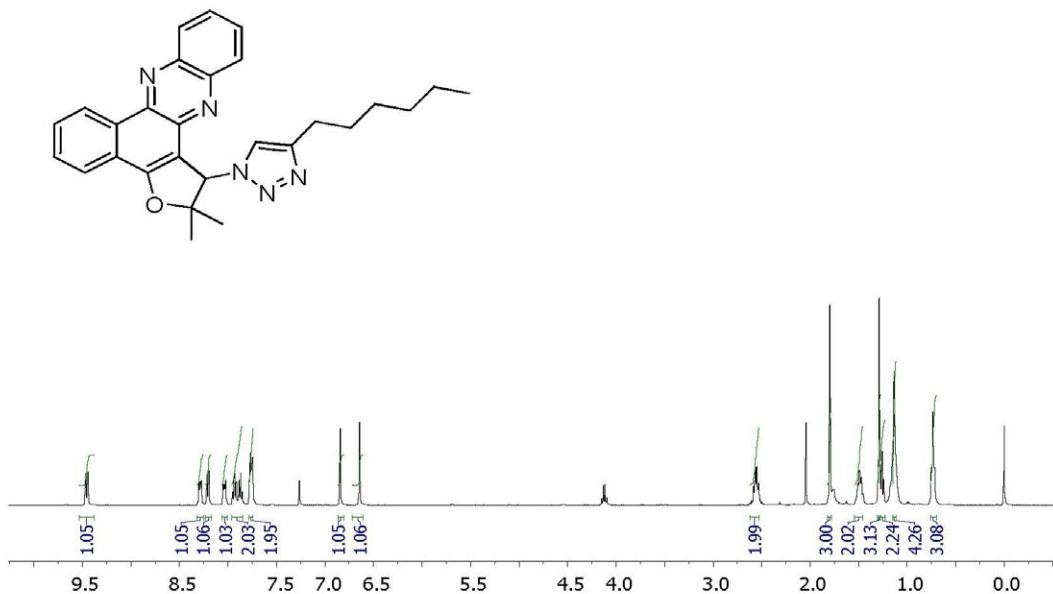


Figure S81. ¹H NMR spectrum (400 MHz, CDCl₃) of compound 38.

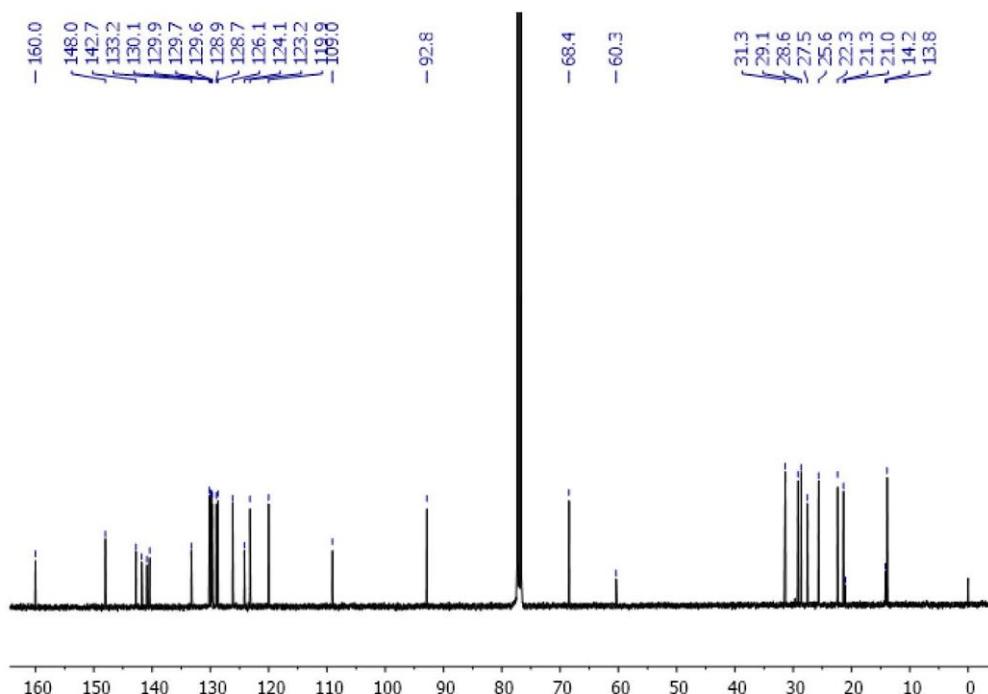


Figure S82. ¹³C NMR spectrum (100 MHz, CDCl₃) of compound 38.

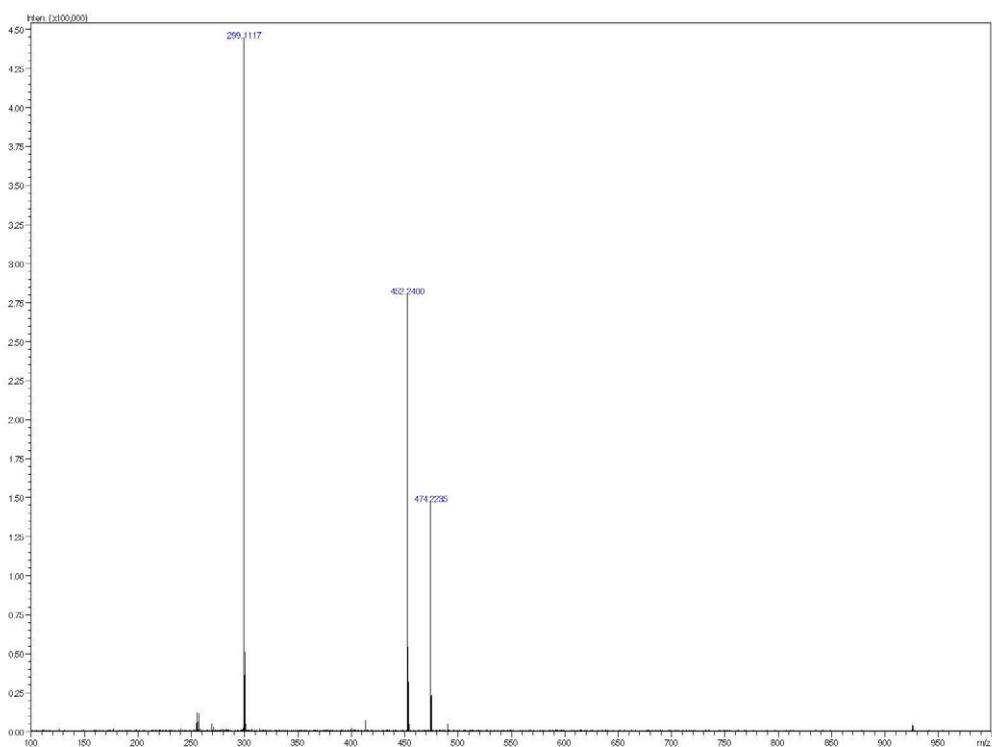


Figure S83. ESI-MS of compound 38.

Compound 41

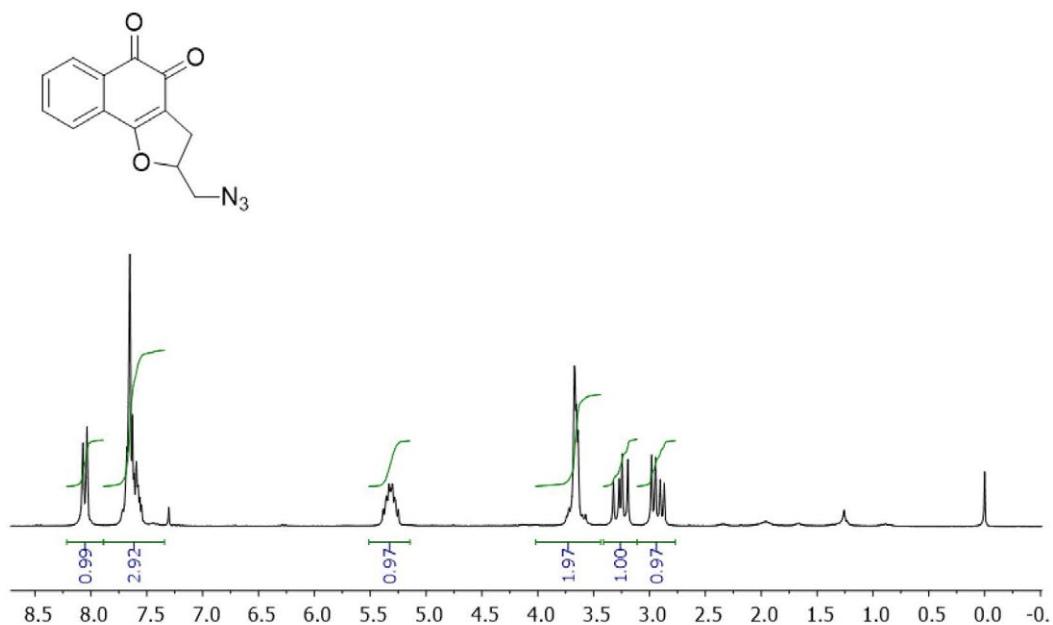


Figure S84. ¹H NMR spectrum (200 MHz, CDCl₃) of compound 41.

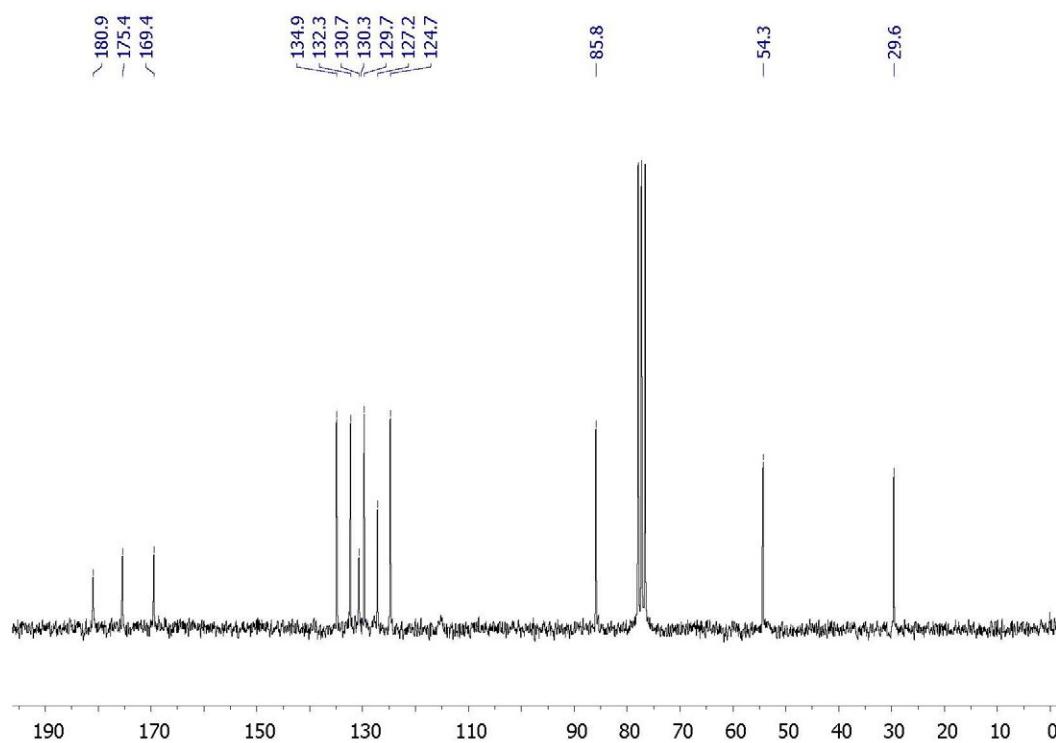


Figure S85. ¹³C NMR spectrum (50 MHz, CDCl₃) of compound 41.

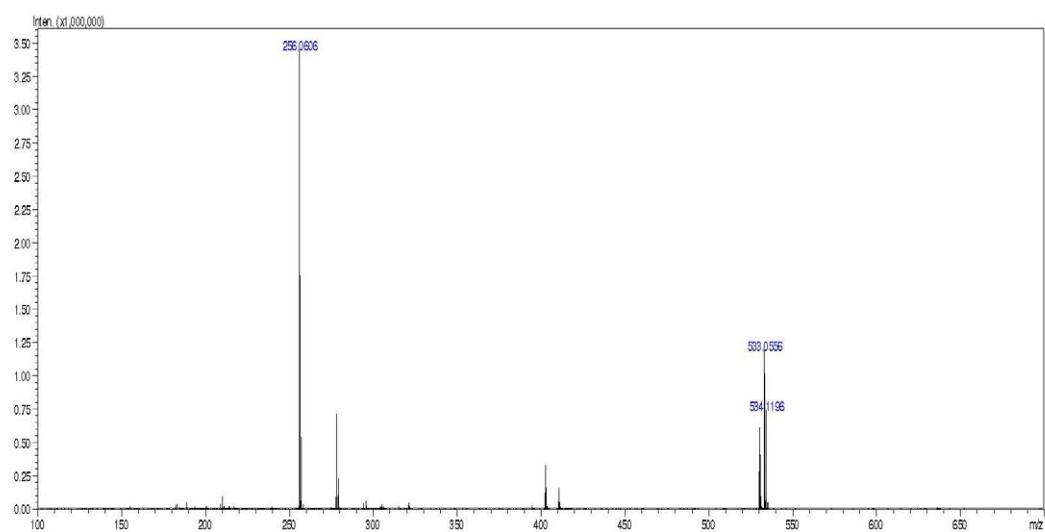


Figure S86. ESI-MS of compound 41.

Compound 42

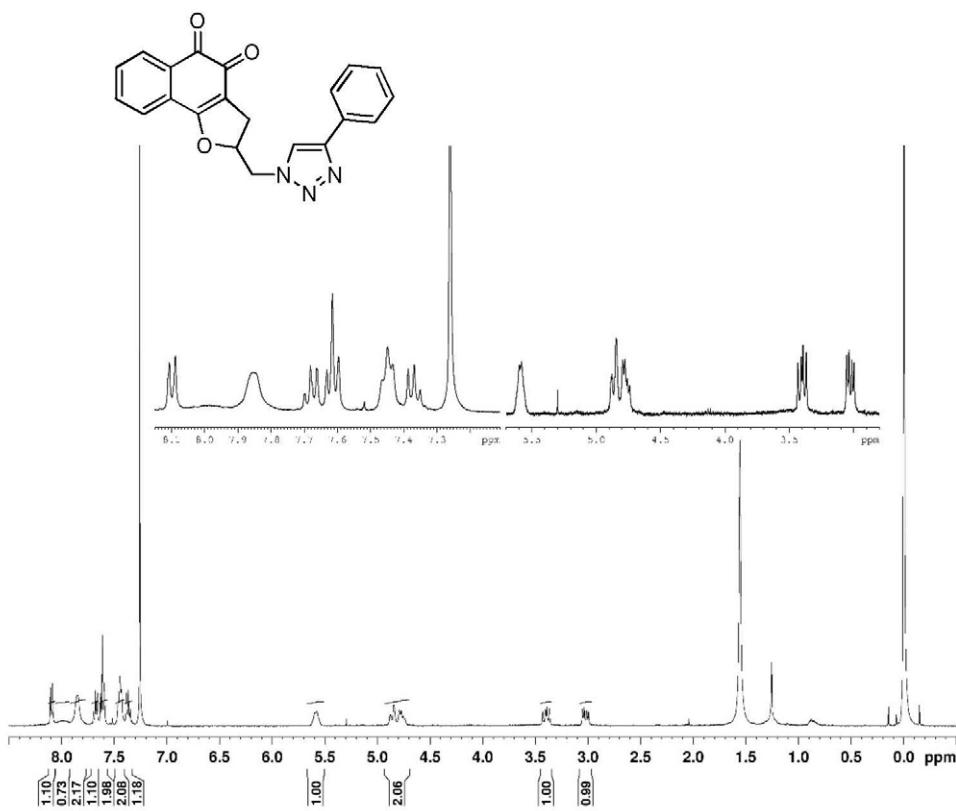


Figure S87. ^1H NMR spectrum (400 MHz, CDCl_3) of compound 42.

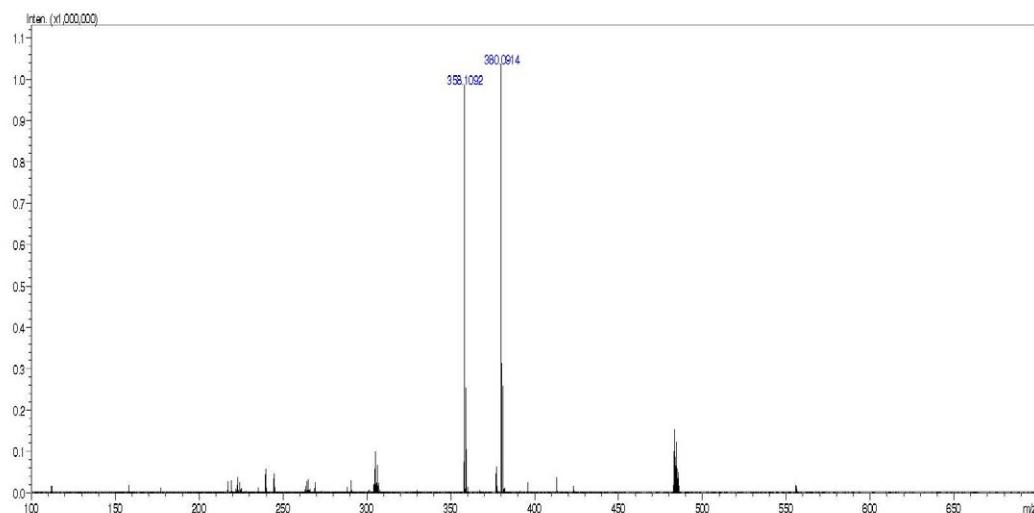


Figure S88. ESI-MS of compound **42**.

Compound 43

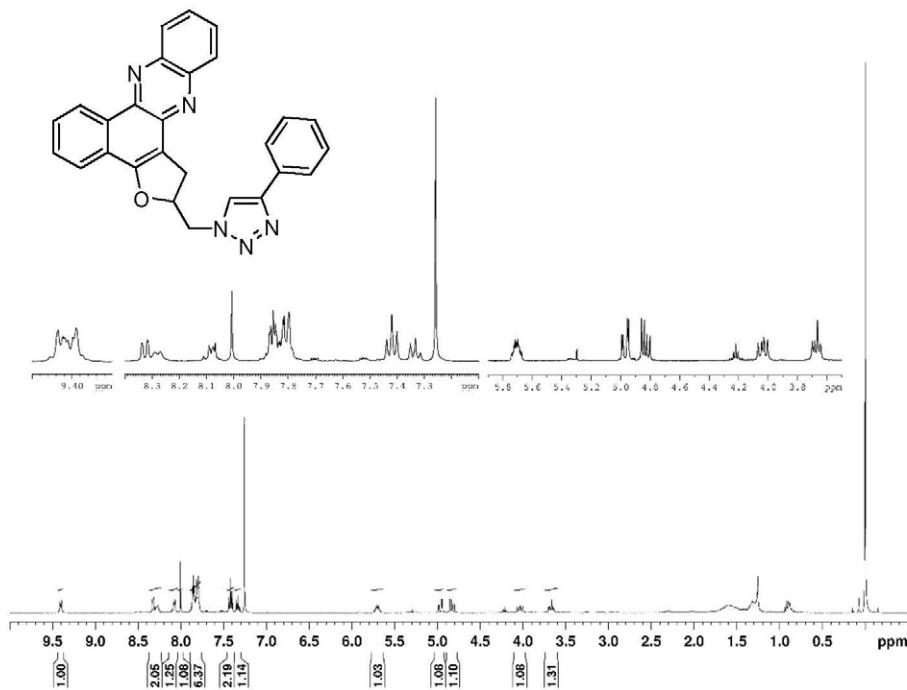


Figure S89. ^1H NMR spectrum (400 MHz, CDCl_3) of compound 43.

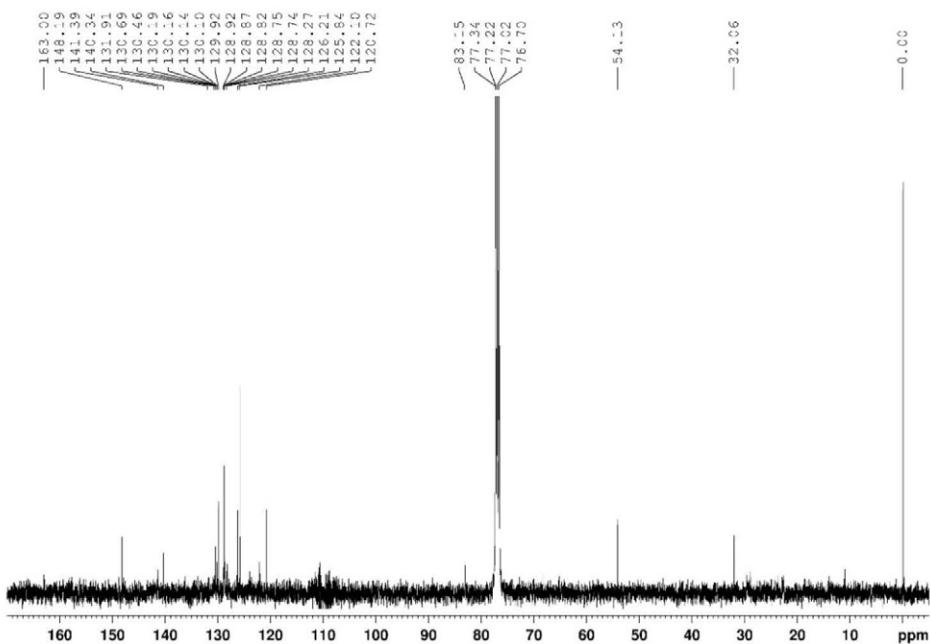


Figure S90. ^{13}C NMR spectrum (100 MHz, CDCl_3) of compound 43.

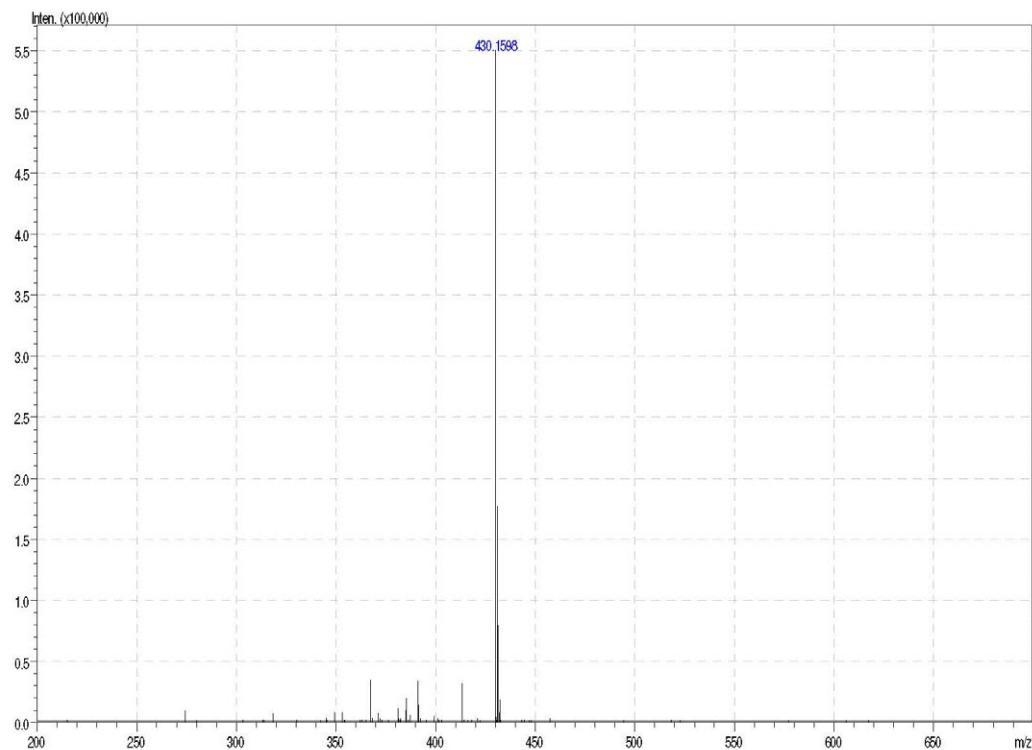


Figure S91. ESI-MS of compound 43.

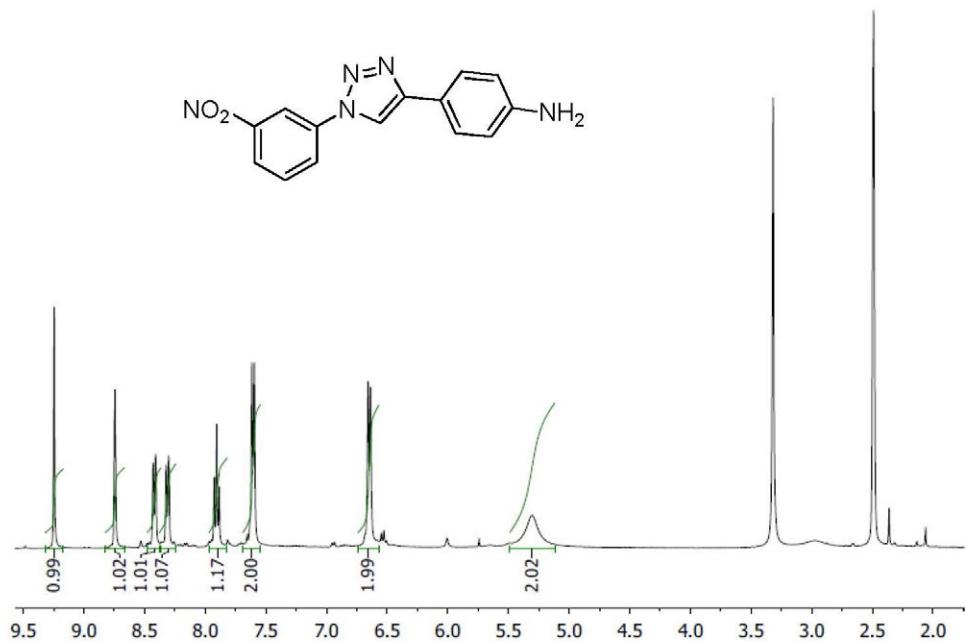
Compound **45**

Figure S92. ¹H NMR spectrum (400 MHz, DMSO-*d*₆) of compound **45**.

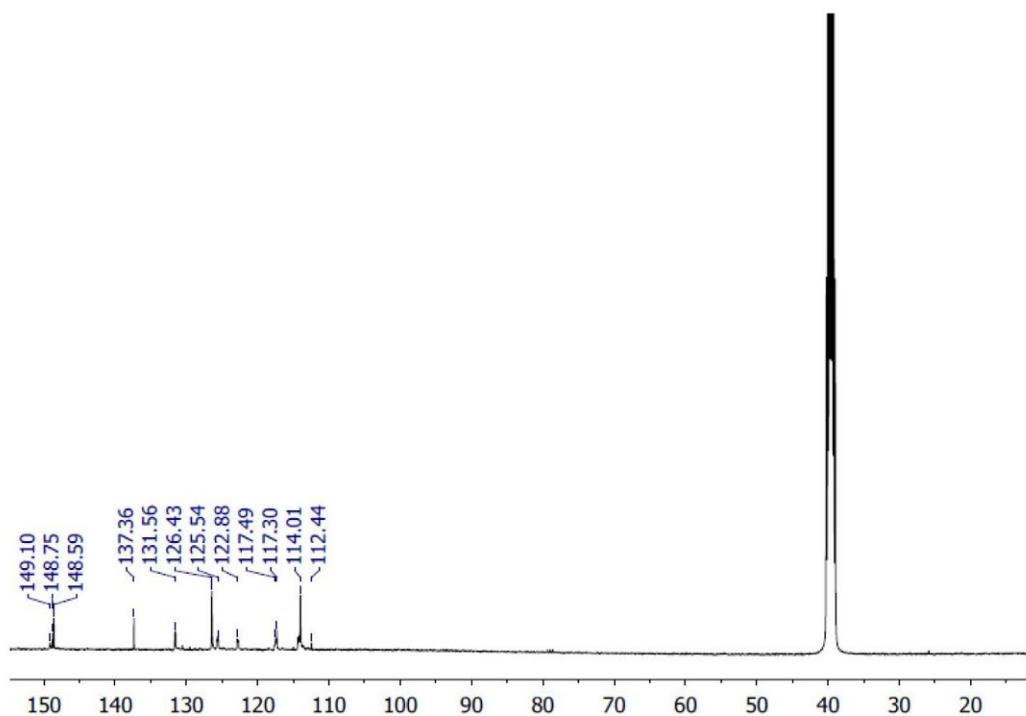


Figure S93. ¹³C NMR spectrum (100 MHz, DMSO-*d*₆) of compound **45**.

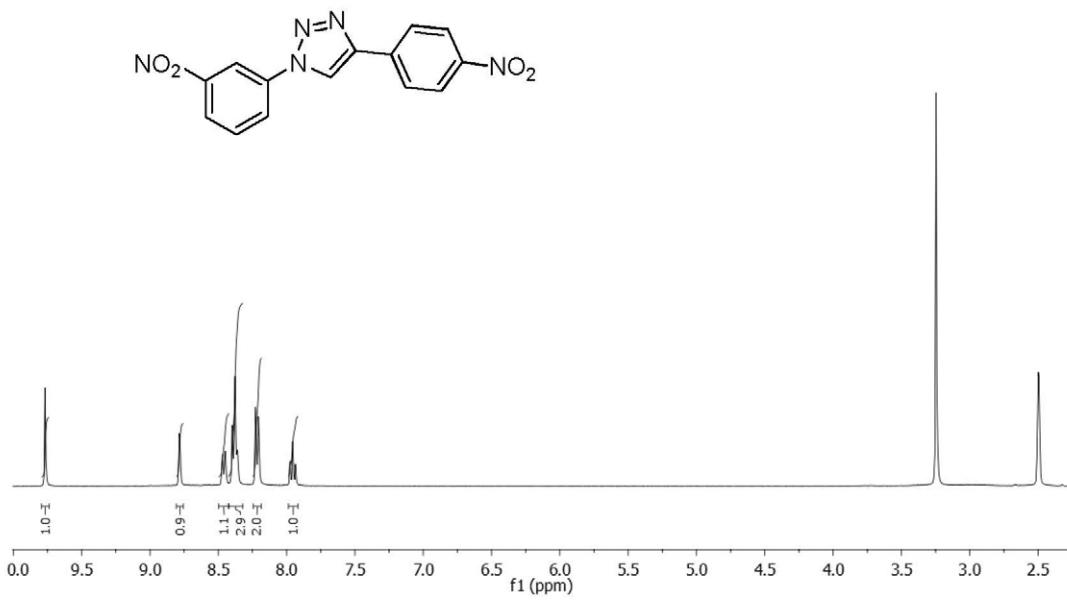
Compound **46**

Figure S94. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of compound **46**.

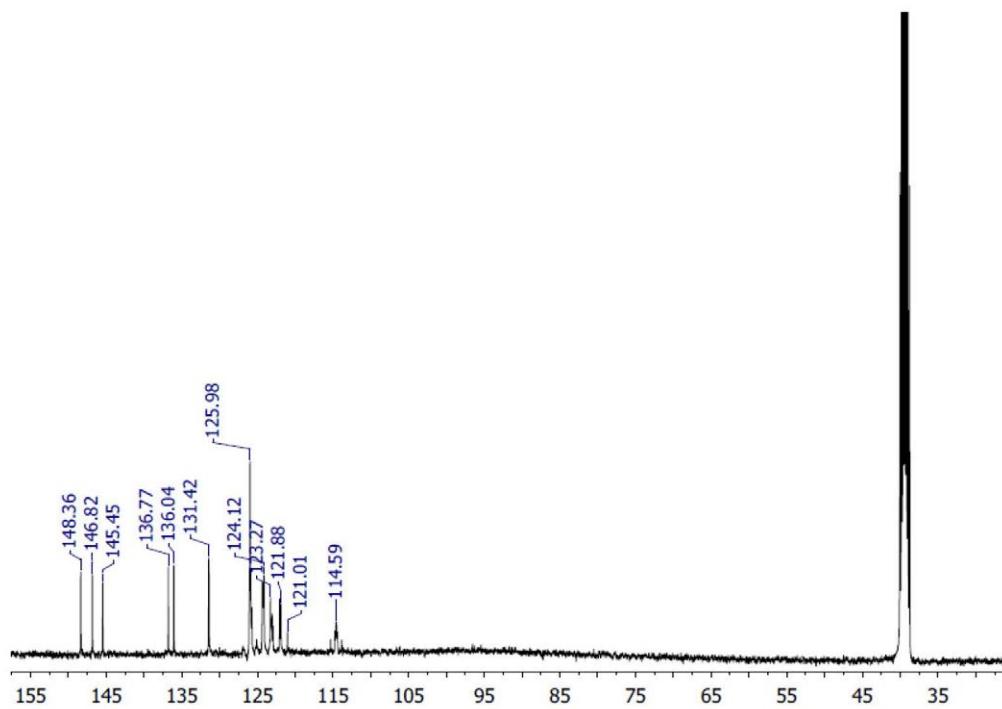


Figure S95. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound **46**.

Compound 47

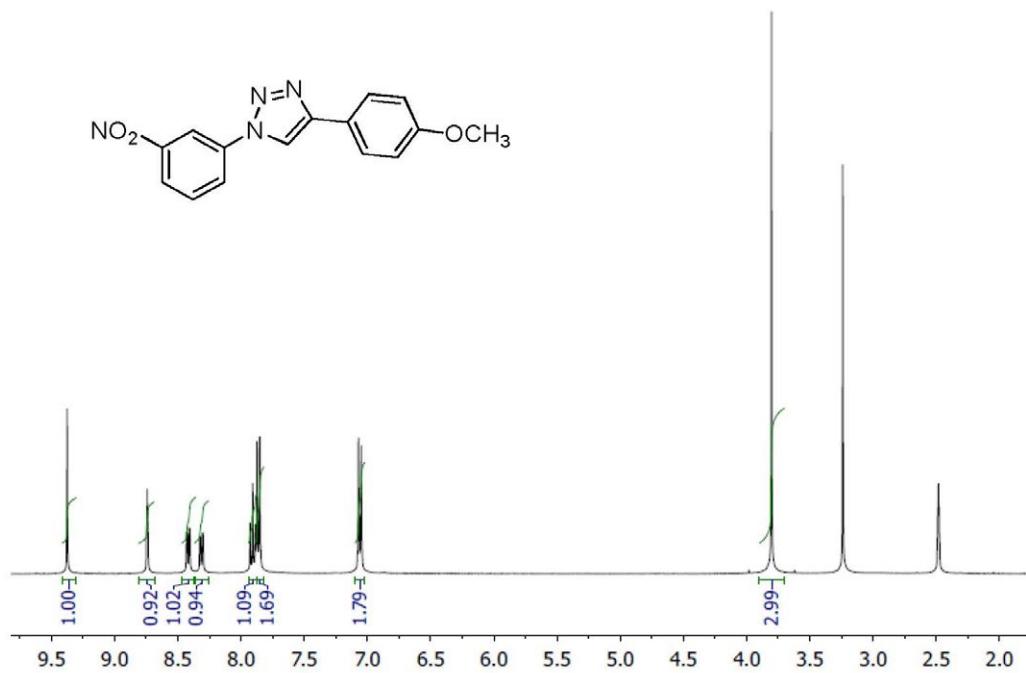


Figure S96. ¹H NMR spectrum (400 MHz, DMSO-*d*₆) of compound 47.

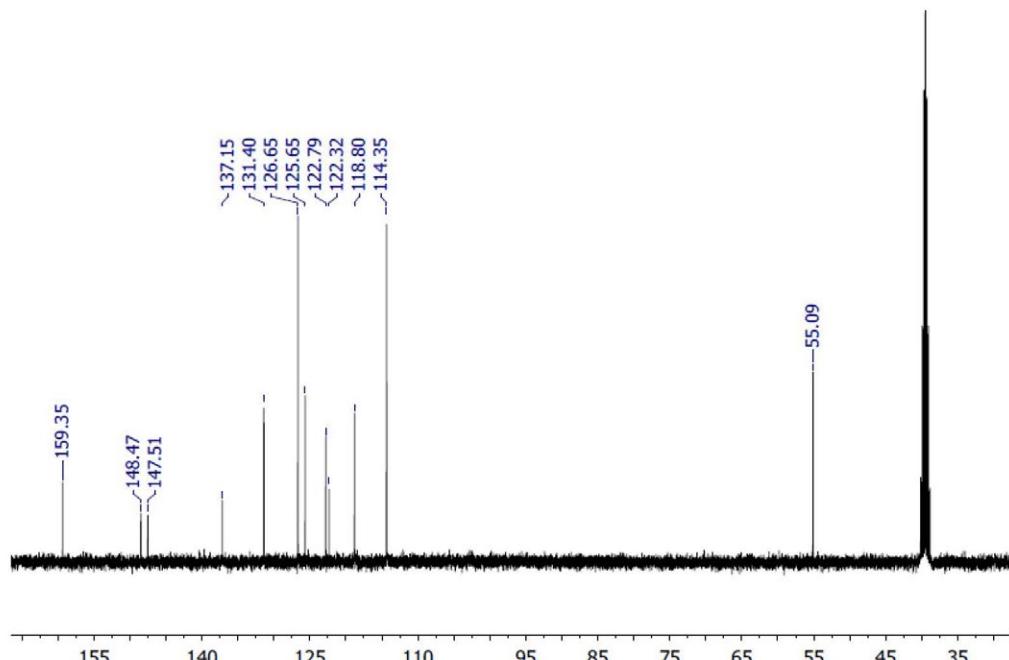


Figure S97. ¹³C NMR spectrum (100 MHz, DMSO-*d*₆) of compound 47.

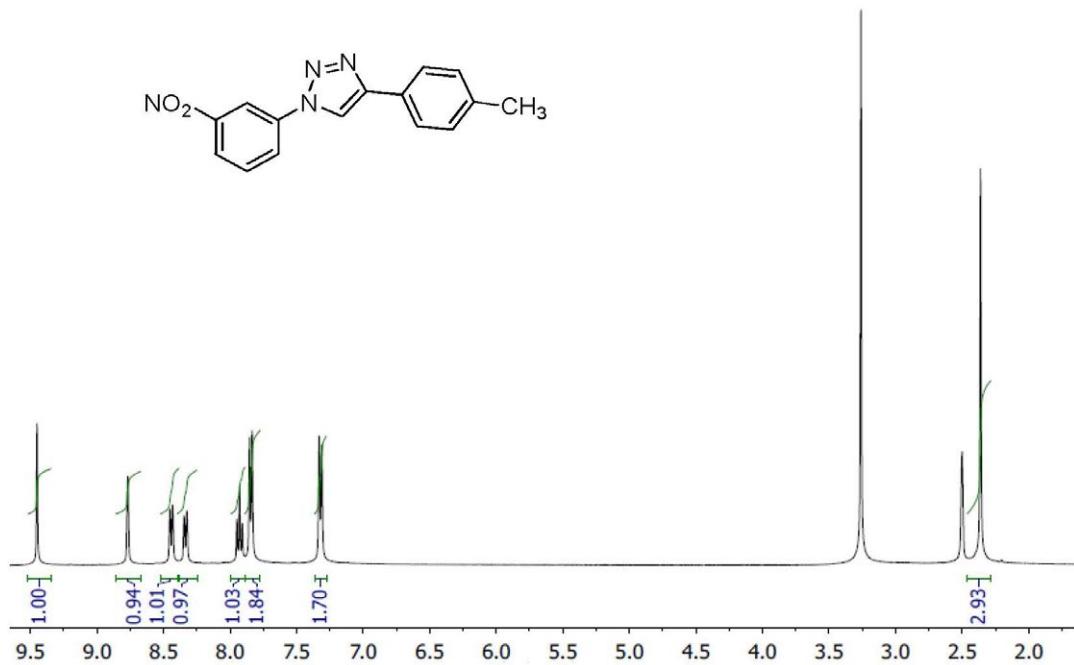
Compound **48**

Figure S98. ^1H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of compound **48**.

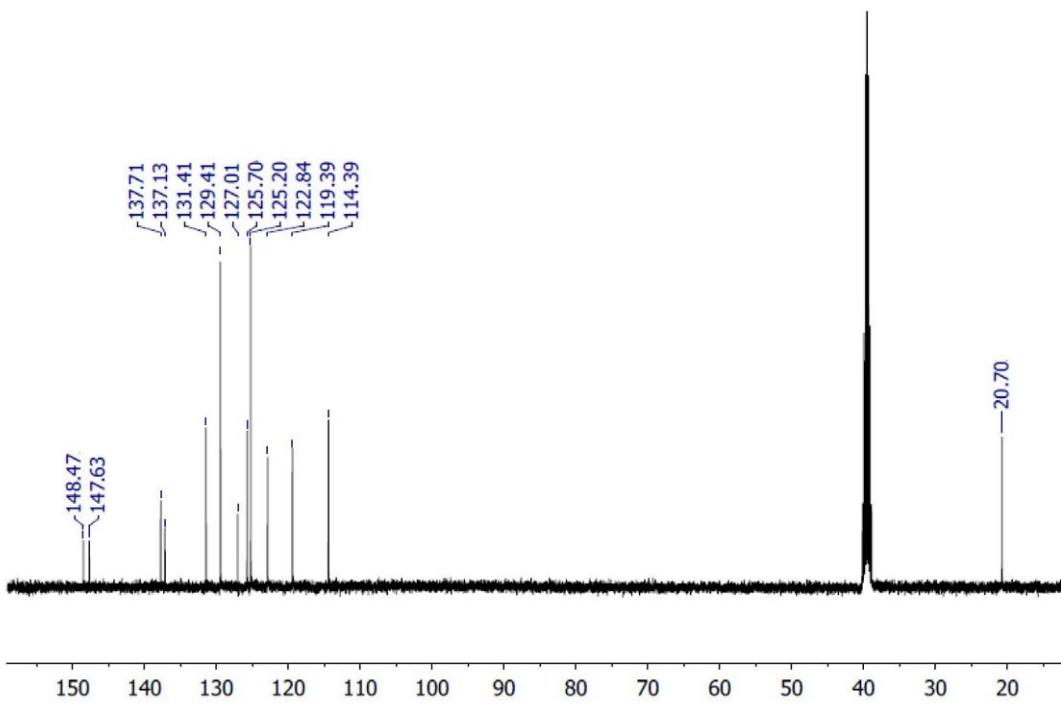


Figure S99. ^{13}C NMR spectrum (100 MHz, $\text{DMSO}-d_6$) of compound **48**.

Compound 49

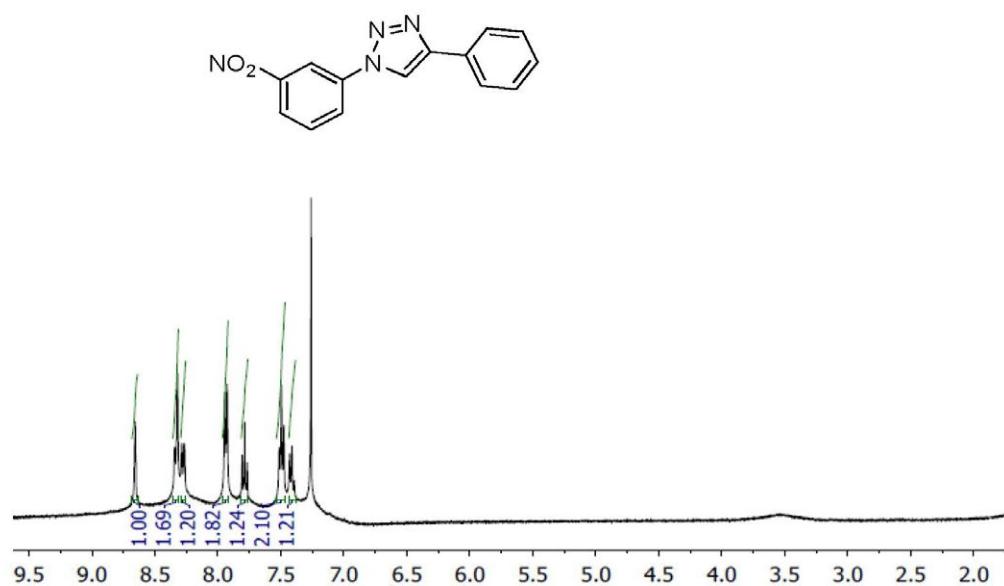


Figure S100. ¹H NMR spectrum (400 MHz, CDCl₃) of compound 49.

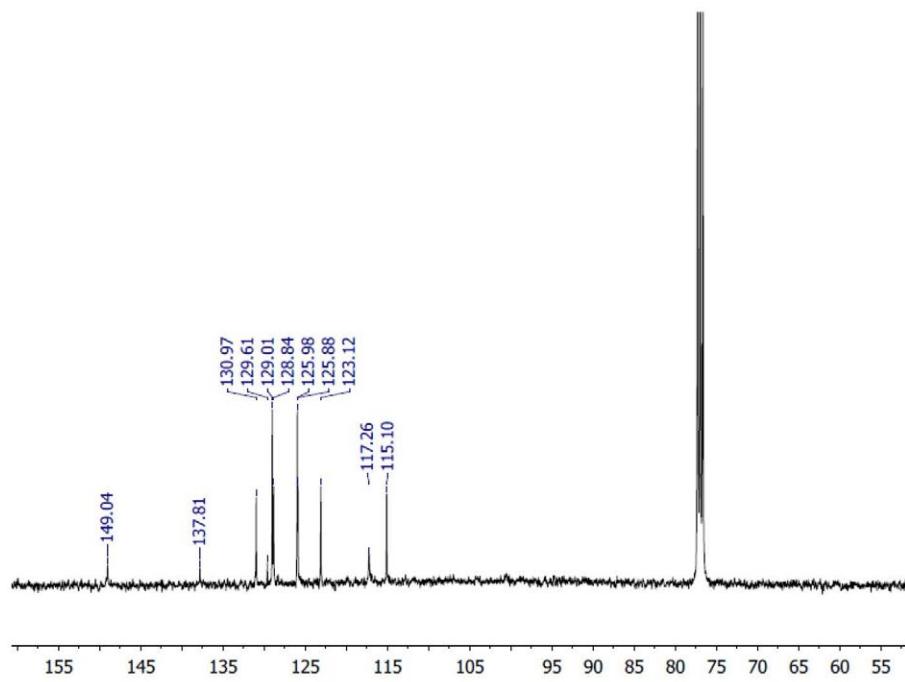


Figure S101. ¹³C NMR spectrum (100 MHz, CDCl₃) of compound 49.

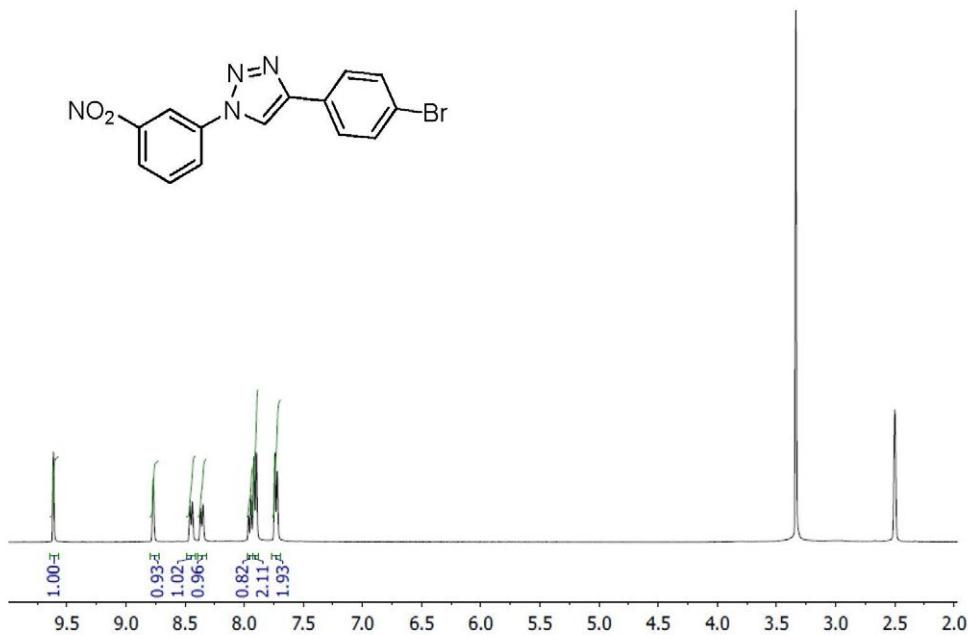
Compound **50**

Figure S102. ¹H NMR spectrum (400 MHz, DMSO-*d*₆) of compound **50**.

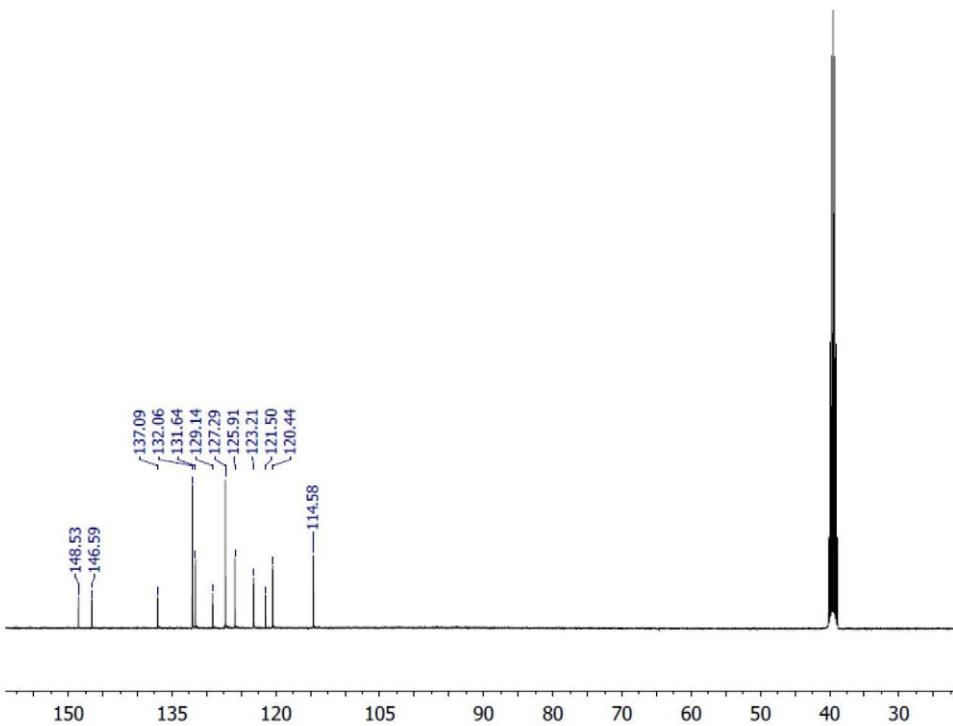


Figure S103. ¹³C NMR spectrum (100 MHz, DMSO-*d*₆) of compound **50**.

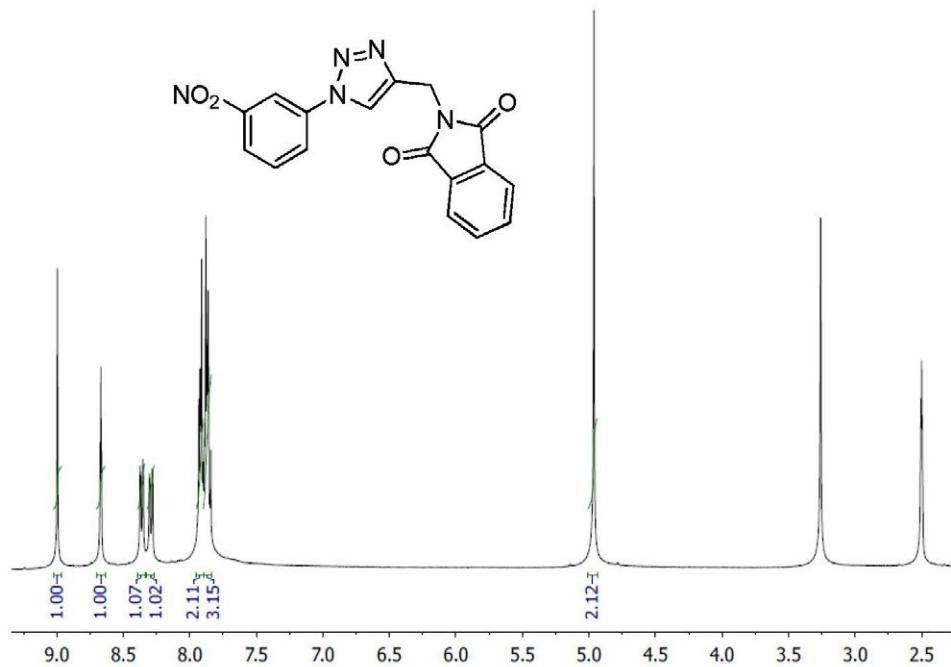
Compound **51**

Figure S104. ¹H NMR spectrum (400 MHz, DMSO-*d*₆) of compound **51**.

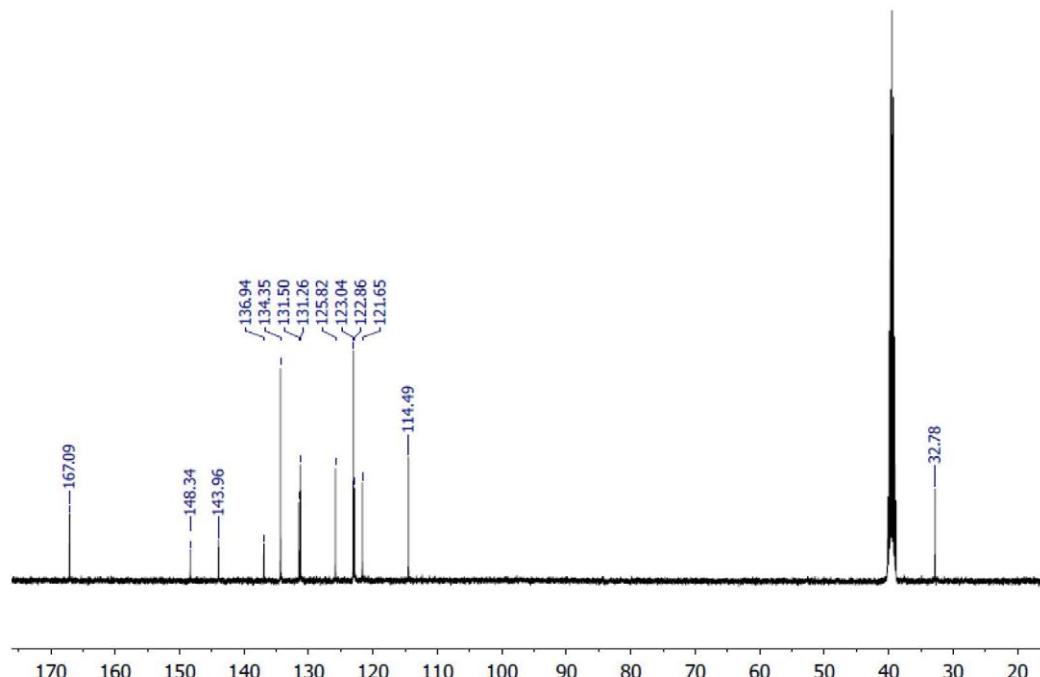


Figure S105. ¹³C NMR spectrum (100 MHz, DMSO-*d*₆) of compound **51**.

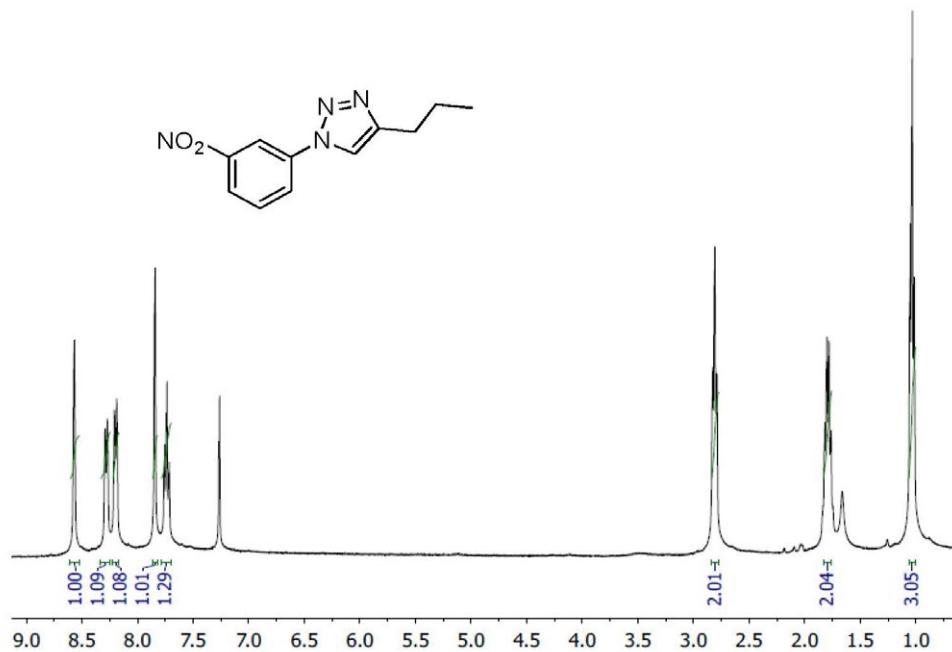
Compound **52**

Figure S106. ¹H NMR spectrum (400 MHz, CDCl₃) of compound **52**.

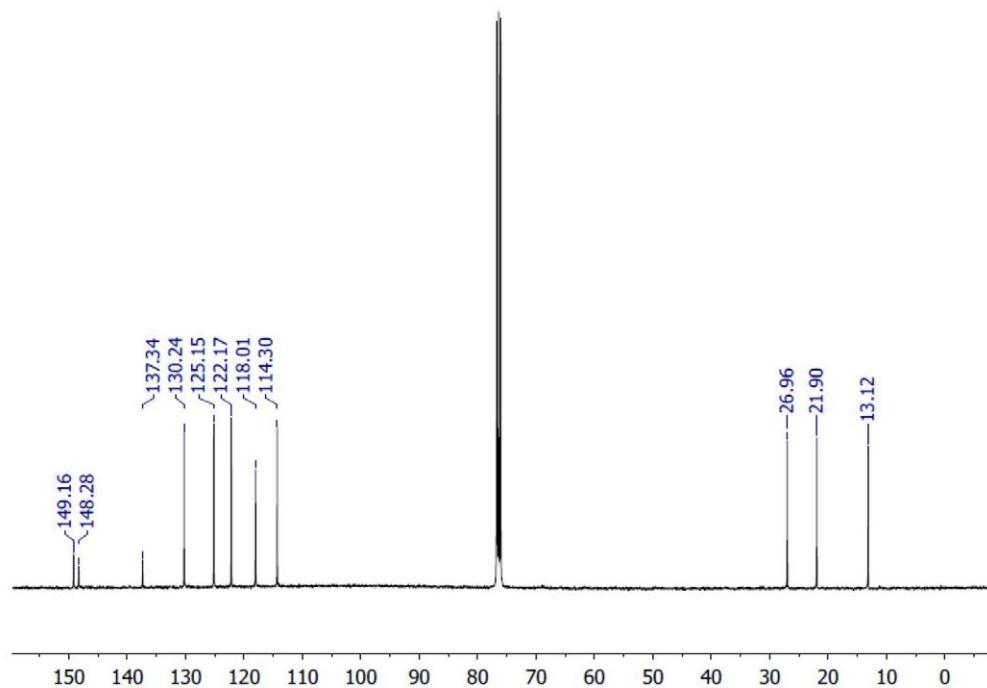


Figure S107. ¹³C NMR spectrum (100 MHz, CDCl₃) of compound **52**.

Compound 53

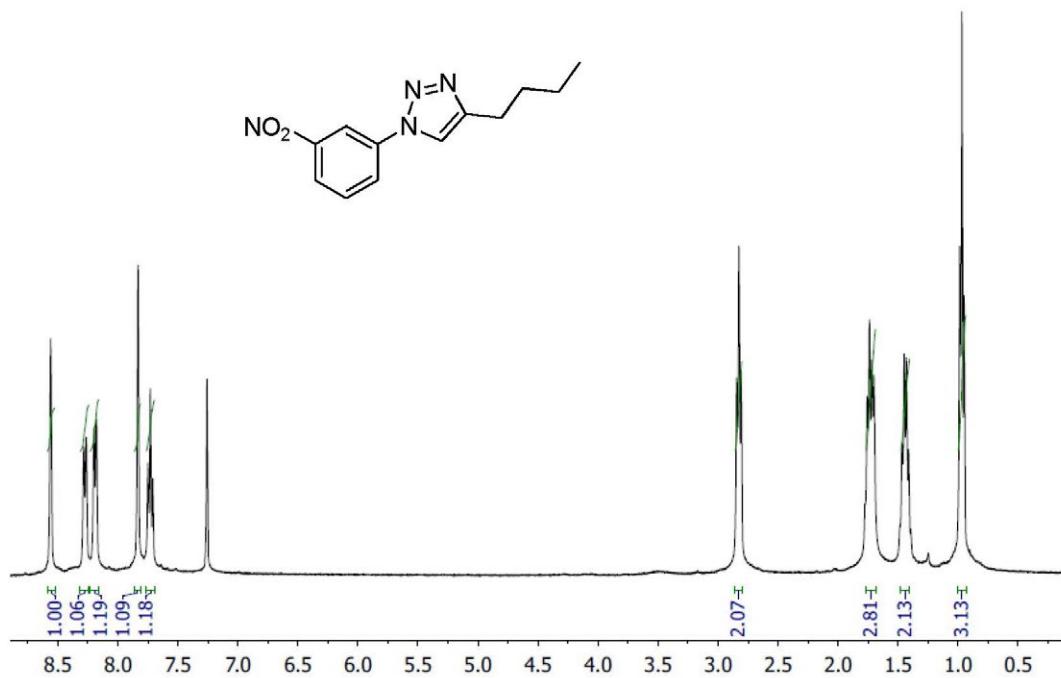


Figure S108. ¹H NMR spectrum (400 MHz, CDCl₃) of compound 53.

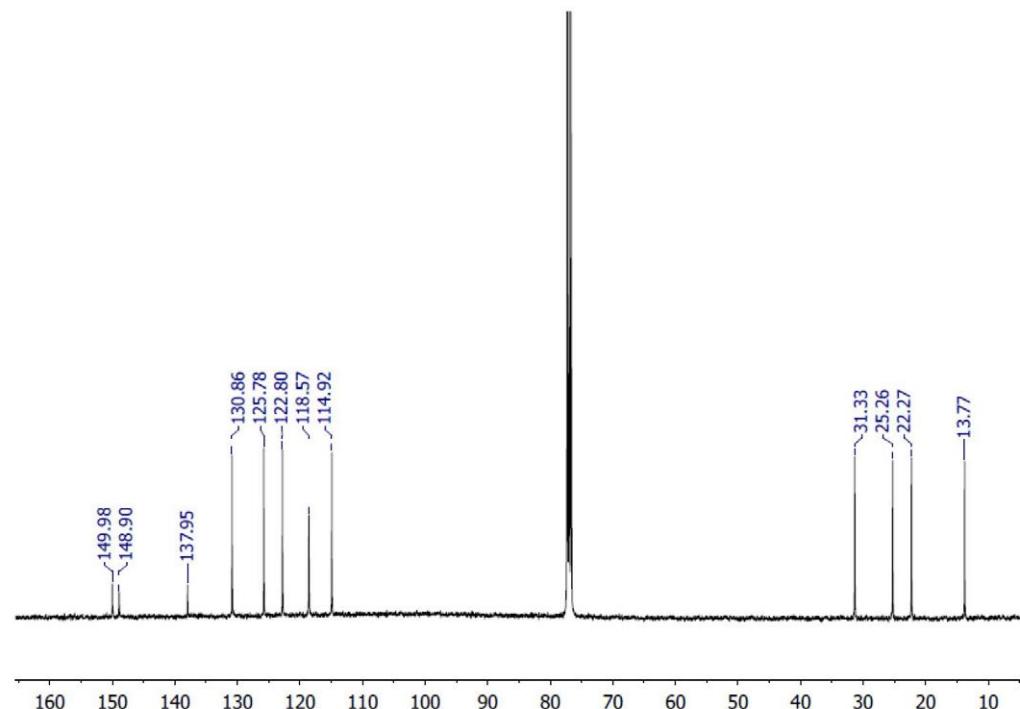


Figure S109. ¹³C NMR spectrum (100 MHz, CDCl₃) of compound 53.

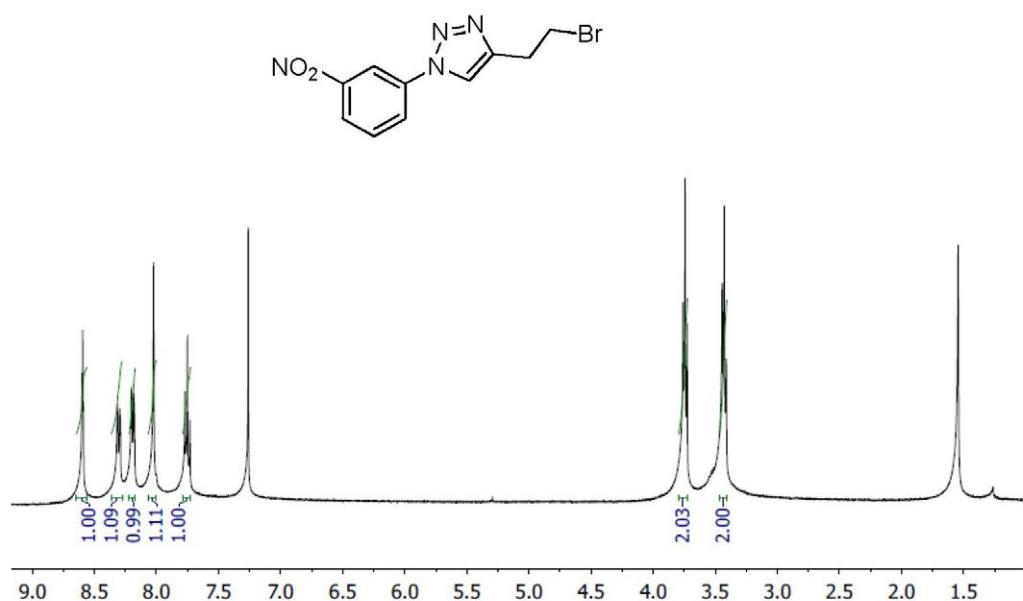
Compound **54**

Figure S110. ¹H NMR spectrum (400 MHz, CDCl₃) of compound **54**.

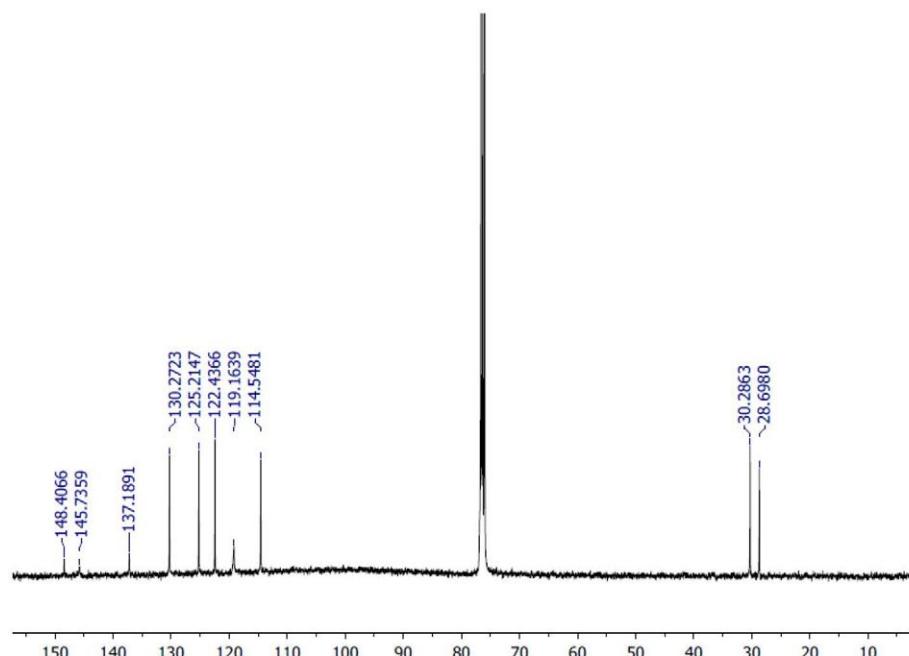


Figure S111. ¹³C NMR spectrum (100 MHz, CDCl₃) of compound **54**.

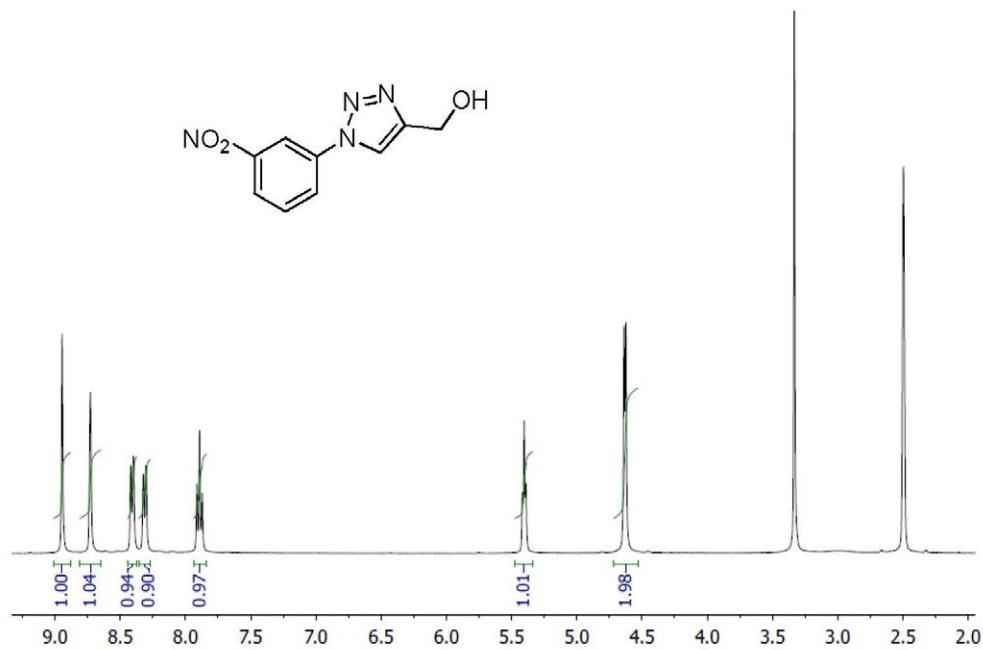
Compound **55**

Figure S112. ¹H NMR spectrum (400 MHz, $\text{DMSO}-d_6$) of compound **55**.

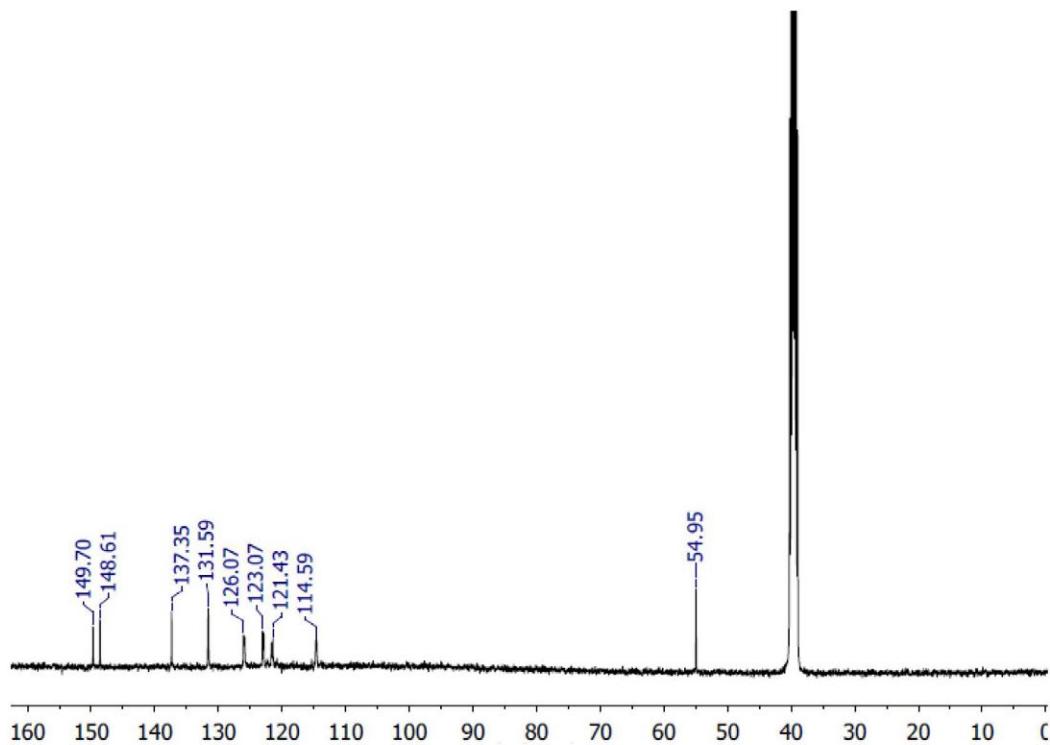


Figure S113. ¹³C NMR spectrum (100 MHz, CDCl_3) of compound **55**.

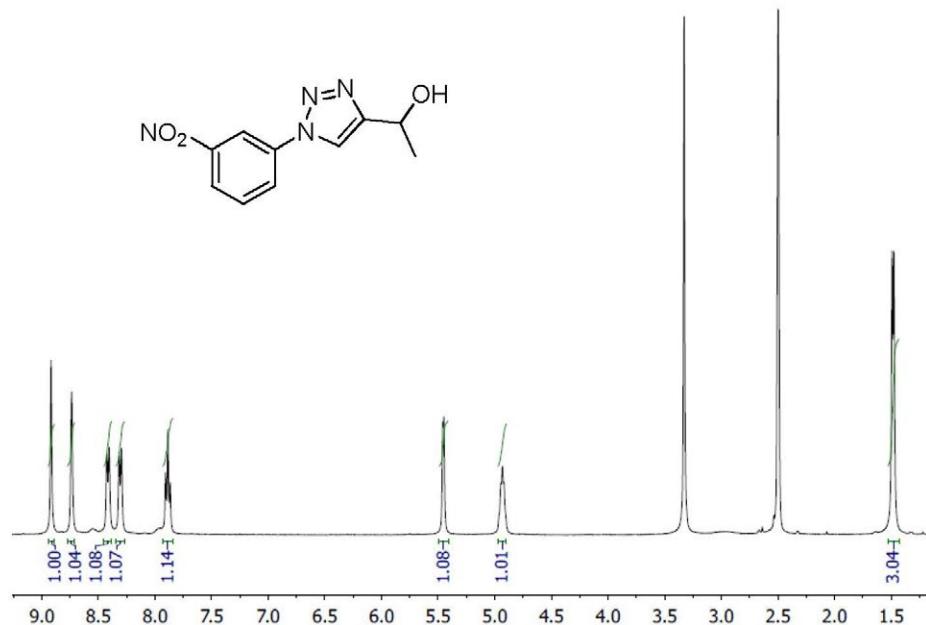
Compound **56**

Figure S114. ¹H NMR spectrum (400 MHz, DMSO-*d*₆) of compound **56**.

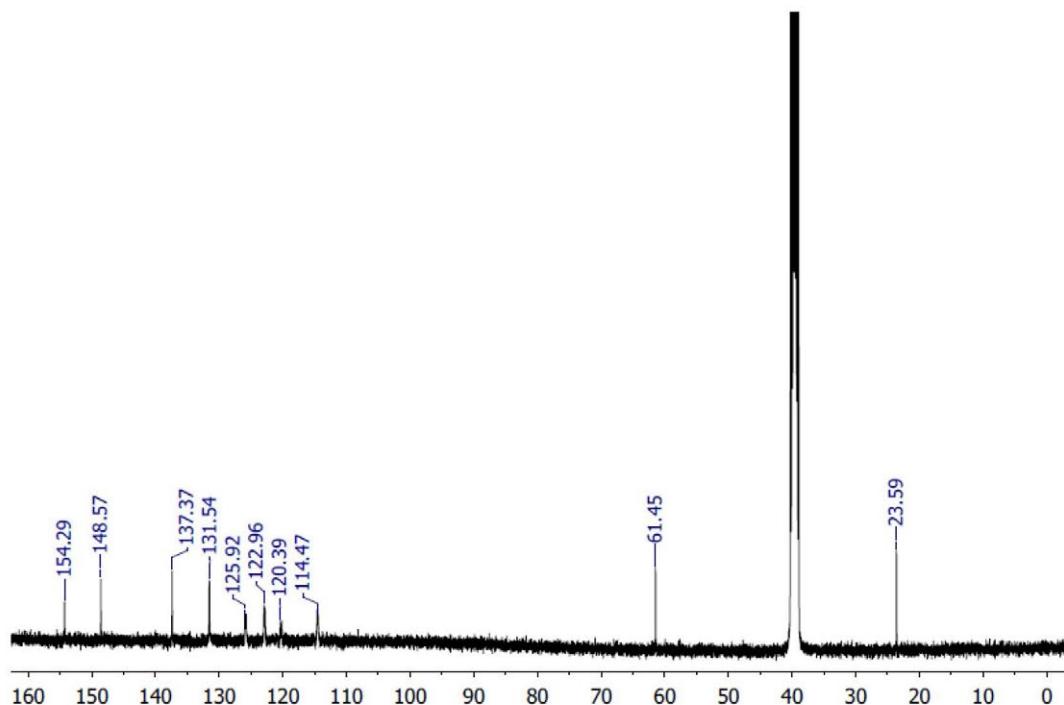


Figure S115. ¹³C NMR spectrum (100 MHz, DMSO-*d*₆) of compound **56**.

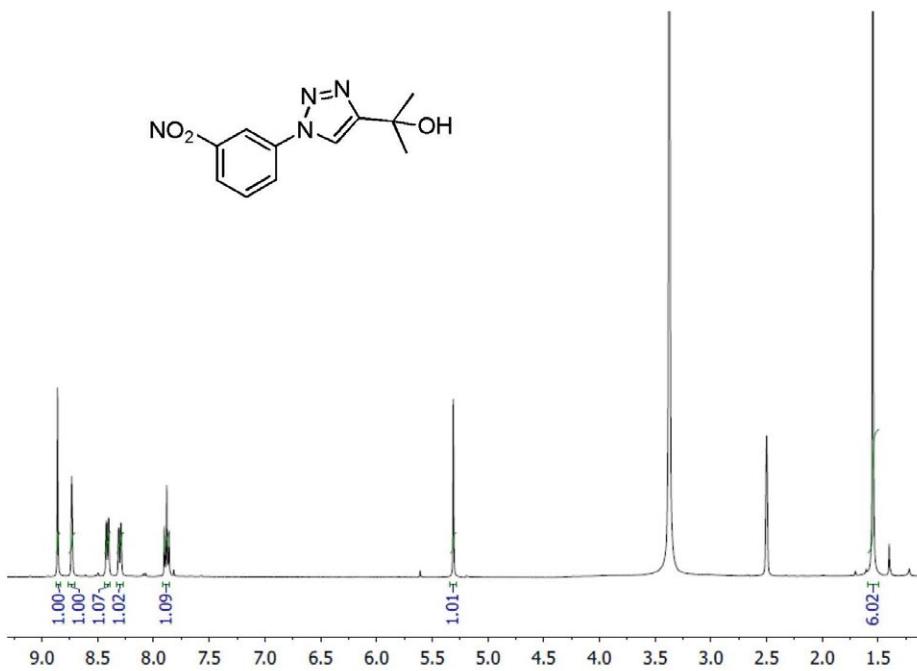
Compound **57**

Figure S116. ¹H NMR spectrum (400 MHz, DMSO-*d*₆) of compound **57**.

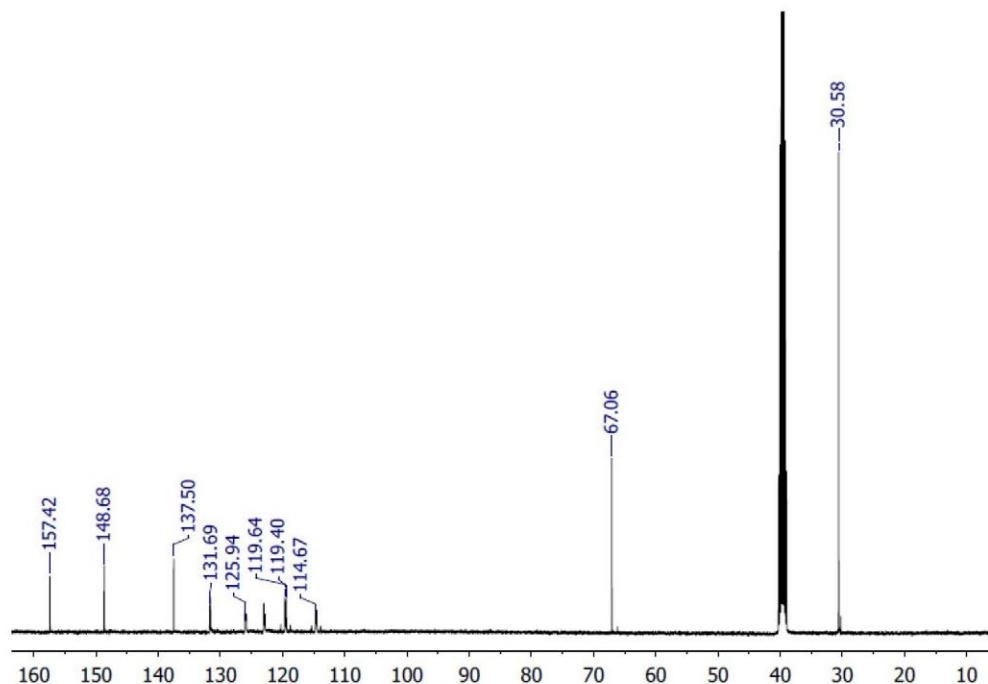


Figure S117. ¹³C NMR spectrum (100 MHz, DMSO-*d*₆) of compound **57**.

Compound 58

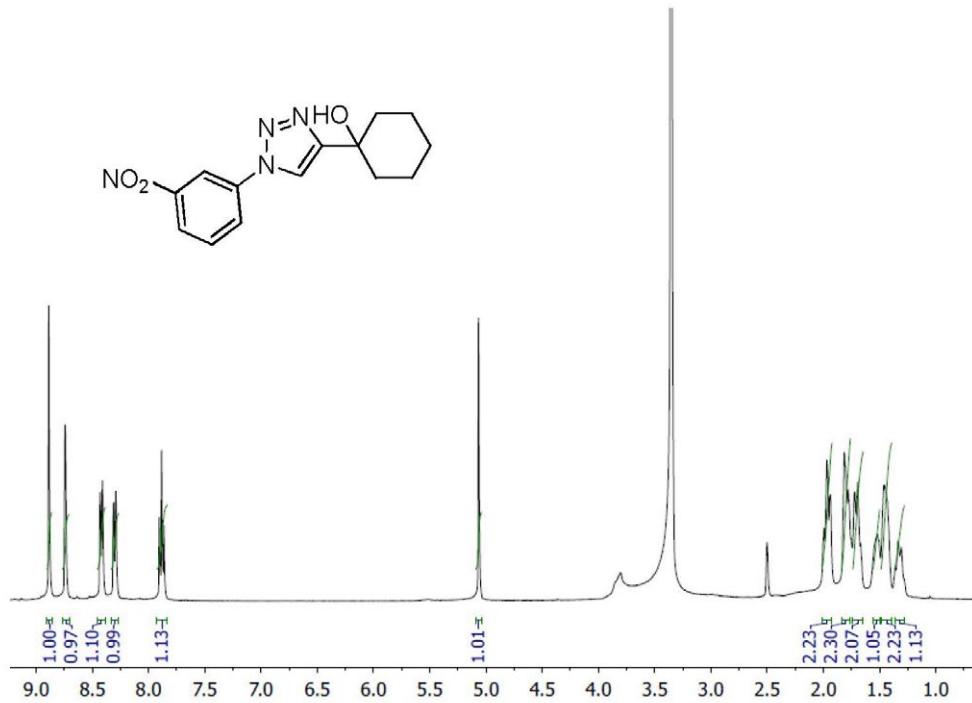


Figure S118. ¹H NMR spectrum (400 MHz, DMSO-*d*₆) of compound 58.

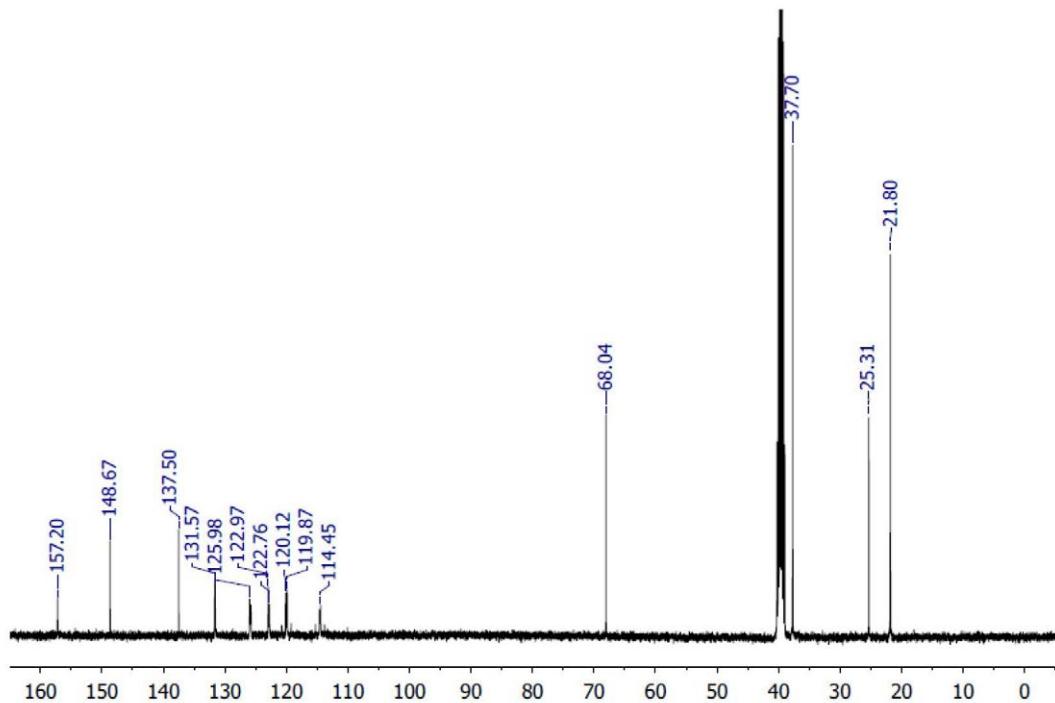


Figure S119. ¹³C NMR spectrum (100 MHz, DMSO-*d*₆) of compound 58.

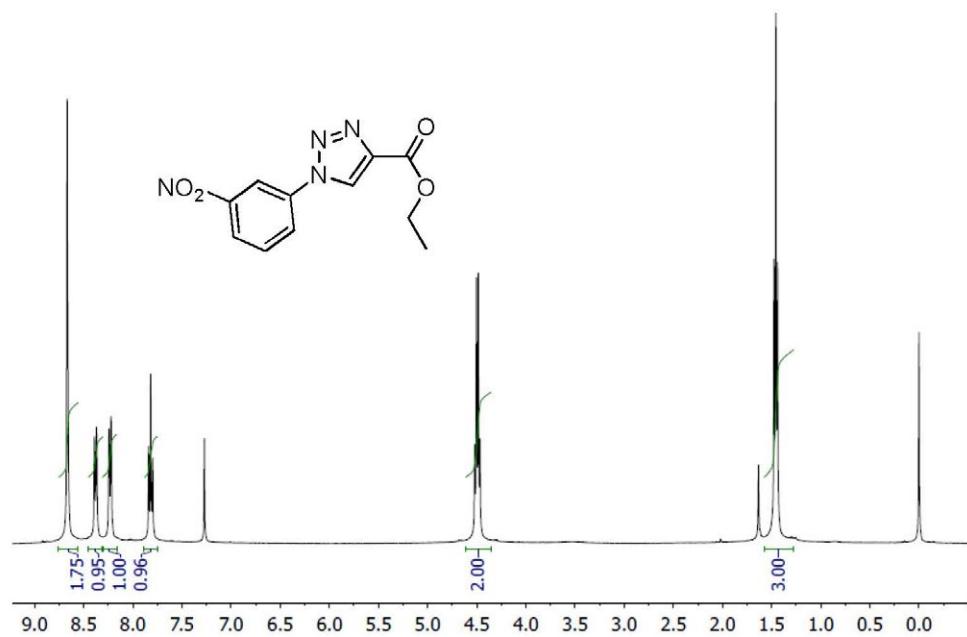
Compound **59**

Figure S120. ¹H NMR spectrum (400 MHz, CDCl₃) of compound **59**.

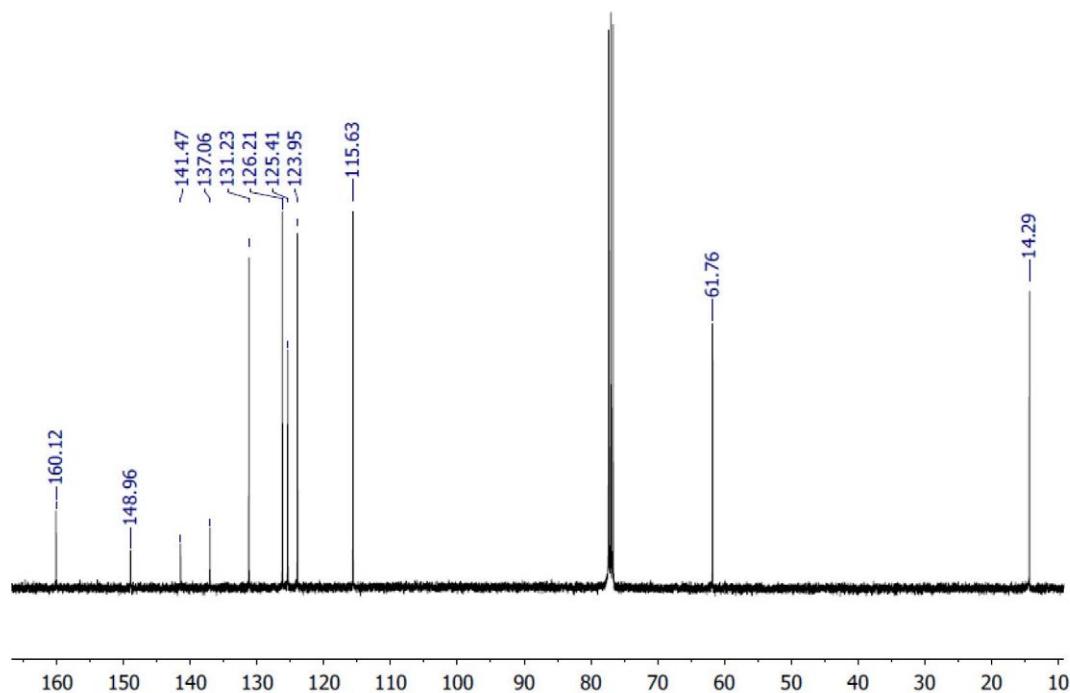


Figure S121. ¹³C NMR spectrum (100 MHz, CDCl₃) of compound **59**.

Table S1. Crystal data and structure refinement for the compounds **12**, **19** and **29**

Identification code	Compound 12	Compound 19	Compound 29			
Empirical formula	C ₂₉ H ₂₁ Br ₂ N ₅ O	C ₂₂ H ₁₇ N ₅ O ₃	C ₂₉ H ₂₃ N ₅ O ₂			
Formula weight	615.33	371.39	473.52			
Temperature / K	293(2)	293(2)	293(2)			
Wavelength / Å	0.71073	0.71073	1.5418			
Crystal system	orthorombic	orthorombic	monoclinic			
Space group	P2 ₁ 2 ₁ 2 ₁	P2 ₁ 2 ₁ 2 ₁	P2 ₁ /c			
Unit cell dimensions	a = 5.9458(3) Å b = 17.8994(8) Å c = 24.1333(17) Å	α = 90° β = 90° γ = 90°	a = 5.410 Å b = 12.669 Å c = 25.696 Å	α = 90° β = 90° γ = 90°	a = 5.0697 (10) Å b = 24.245 (5) Å c = 19.173 (4) Å	α = 90° β = 92.69 (3) γ = 90°
Volume / Å ³	2568.4(3)		1761.2			2354.0 (8)
Z	4		4			4
Density (calculated) / mg m ⁻³	1.591		1.401			1.336
Absorption coefficient / mm ⁻¹	3.189		0.095			0.70
F(000)	1232		776			992
Crystal size / mm ³	0.20 × 0.08 × 0.07		0.80 × 0.50 × 0.12			0.43 × 0.07 × 0.06
Theta range for data collection	2.04 to 29.54°		1.79 to 29.33°			2.9 to 66.0°
Index ranges	-7 ≤ h ≤ 7, -24 ≤ k ≤ 16, -31 ≤ l ≤ 20		-7 ≤ h ≤ 7, -17 ≤ k ≤ 15, -35 ≤ l ≤ 34			-5 ≤ h ≤ 4, -28 ≤ k ≤ 28, -22 ≤ l ≤ 22
Reflections collected	9550		13943			26157
Independent reflections	5668 [R(int) = 0.0259]		4356 [R(int) = 0.0324]			4078[R _{int} = 0.092]
Completeness to theta = 26.32°	99.9%		94.6%			—
Absorption correction	empirical		none			—
Refinement method	full-matrix least-squares on F2		full-matrix least-squares on F2			full-matrix least-squares on F2
Data / restraints / parameters	5668 / 0 / 336		4356 / 0 / 255			4078 / 0 / 326
Goodness-of-fit on F2	1.134		1.108			1.058
Final R indices [I > 2sigma(I)]	R1 = 0.0393, wR2 = 0.0768		R1 = 0.0410, wR2 = 0.0909			R1 = 0.0501, wR2 = 0.1222
R indices (all data)	R1 = 0.0623, wR2 = 0.1001		R1 = 0.0538, wR2 = 0.1060			R1 = 0.0774, wR2 = 0.1442
Absolute structure parameter	0.000(10)		1.2(11)			—
Largest diff. peak and hole / e.Å ⁻³	0.321 and -0.389		0.218 and -0.243			0.210 and -0.188