

SUPPORTING INFORMATION

Semisynthesis and biological evaluation of a focused library of unguinol derivatives as next-generation antibiotics

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Table of Contents

Figure S1. ¹ H NMR spectrum (600 MHz, DMSO- <i>d</i> ₆) of 1',2'-dihydrounguinol (2a).....	4
Figure S2. ¹³ C NMR spectrum (150 MHz, DMSO- <i>d</i> ₆) of 1',2'-dihydrounguinol (2a).....	5
Figure S3. ¹ H NMR spectrum (500 MHz, DMSO- <i>d</i> ₆) of <i>cis</i> -1',2'-epoxyunguinol (2b)	6
Figure S4. ¹³ C NMR spectrum (125 MHz, DMSO- <i>d</i> ₆) of <i>cis</i> -1',2'-epoxyunguinol (2b)	7
Figure S5. ¹ H NMR spectrum (600 MHz, DMSO- <i>d</i> ₆) of 1',2'-dihydroxyunguinol (2c)	8
Figure S6. ¹³ C NMR spectrum (150 MHz, DMSO- <i>d</i> ₆) of 1',2'-dihydroxyunguinol (2c).....	9
Figure S7. ¹ H NMR spectrum (500 MHz, DMSO- <i>d</i> ₆) of 2'-hydroxy-Δ ^{1',4'} -unguinol (2d)	10
Figure S8. ¹³ C NMR spectrum (125 MHz, DMSO- <i>d</i> ₆) of 2'-hydroxy-Δ ^{1',4'} -unguinol (2d)	11
Figure S9. ¹ H NMR spectrum (600 MHz, DMSO- <i>d</i> ₆) of 2'-oxo-Δ ^{1',4'} -unguinol (2e).....	12
Figure S10. ¹ H NMR spectrum (150 MHz, DMSO- <i>d</i> ₆) of 2'-oxo-Δ ^{1',4'} -unguinol (2e).....	13
Figure S11. ¹ H NMR spectrum (600 MHz, DMSO- <i>d</i> ₆) of 2'-hydroperoxy-Δ ^{1',4'} -unguinol (2f)	14
Figure S12. ¹³ C NMR spectrum (150 MHz, DMSO- <i>d</i> ₆) of 2'-hydroperoxy-Δ ^{1',4'} -unguinol (2f)	15
Figure S13. ¹ H NMR spectrum (600 MHz, DMSO- <i>d</i> ₆) of 2,7-dibromo-1',2'-dihydrounguinol (3a).....	16
Figure S14. ¹³ C NMR spectrum (150 MHz, DMSO- <i>d</i> ₆) of 2,7-dibromo-1',2'-dihydrounguinol (3a).....	17
Figure S15. ¹ H NMR spectrum (600 MHz, DMSO- <i>d</i> ₆) of 2,4,7-tribromo-1',2'-dihydrounguinol (3b)	18
Figure S16. ¹³ C NMR spectrum (150 MHz, DMSO- <i>d</i> ₆) of 2,4,7-tribromo-1',2'-dihydrounguinol (3b)	19
Figure S17. ¹ H NMR spectrum (600 MHz, DMSO- <i>d</i> ₆) of 2,4-diiodo-1',2'-dihydrounguinol (3c)	20
Figure S18. ¹³ C NMR spectrum (150 MHz, DMSO- <i>d</i> ₆) of 2,4-diiodo-1',2'-dihydrounguinol (3c)	21
Figure S19. ¹ H NMR spectrum (600 MHz, DMSO- <i>d</i> ₆) of methylunguinate (4a)	22
Figure S20. ¹³ C NMR spectrum (150 MHz, DMSO- <i>d</i> ₆) of methylunguinate (4a)	23
Figure S21. ¹ H NMR spectrum (600 MHz, DMSO- <i>d</i> ₆) of unguinolamide (4b)	24
Figure S22. ¹³ C NMR spectrum (150 MHz, DMSO- <i>d</i> ₆) of unguinolamide (4b)	25
Figure S23. ¹ H NMR spectrum (600 MHz, DMSO- <i>d</i> ₆) of 3- <i>O</i> -methylunguinol (5a).....	26
Figure S24. ¹³ C NMR spectrum (150 MHz, DMSO- <i>d</i> ₆) of 3- <i>O</i> -methylunguinol (5a).....	27
Figure S25. ¹ H NMR spectrum (600 MHz, DMSO- <i>d</i> ₆) of 3,8-di- <i>O</i> -methylunguinol (5b)	28
Figure S26. ¹³ C NMR spectrum (150 MHz, DMSO- <i>d</i> ₆) of 3,8-di- <i>O</i> -methylunguinol (5b)	29
Figure S27. ¹ H NMR spectrum (600 MHz, DMSO- <i>d</i> ₆) of 3- <i>O</i> -benzylunguinol (6a)	30
Figure S28. ¹³ C NMR spectrum (150 MHz, DMSO- <i>d</i> ₆) of 3- <i>O</i> -benzylunguinol (6a)	31
Figure S29. ¹ H NMR spectrum (600 MHz, DMSO- <i>d</i> ₆) of 3,8- <i>O</i> -dibenzylunguinol (6b).....	32
Figure S30. ¹³ C NMR spectrum (150 MHz, DMSO- <i>d</i> ₆) of 3,8- <i>O</i> -dibenzylunguinol (6b).....	33
Figure S31. ¹ H NMR spectrum (600 MHz, DMSO- <i>d</i> ₆) of 3- <i>O</i> -(2-chlorobenzyl)unguinol (7a).....	34
Figure S32. ¹³ C NMR spectrum (150 MHz, DMSO- <i>d</i> ₆) of 3- <i>O</i> -(2-chlorobenzyl)unguinol (7a).....	35
Figure S33. ¹ H NMR spectrum (600 MHz, DMSO- <i>d</i> ₆) of 3- <i>O</i> -(3-chlorobenzyl)unguinol (7b).....	36

Figure S34. ^{13}C NMR spectrum (150 MHz, $\text{DMSO}-d_6$) of 3-O-(3-chlorobenzyl)unguinol (7b).....	37
Figure S35. ^1H NMR spectrum (600 MHz, $\text{DMSO}-d_6$) of 3-O-(4-chlorobenzyl)unguinol (7c)	38
Figure S36. ^{13}C NMR spectrum (150 MHz, $\text{DMSO}-d_6$) of 3-O-(4-chlorobenzyl)unguinol (7c)	39
Figure S37. ^1H NMR spectrum (600 MHz, $\text{DMSO}-d_6$) of 3-O-(2-fluorobenzyl)unguinol (7d)	40
Figure S38. ^{13}C NMR spectrum (150 MHz, $\text{DMSO}-d_6$) of 3-O-(2-fluorobenzyl)unguinol (7d)	41
Figure S39. ^1H NMR spectrum (600 MHz, $\text{DMSO}-d_6$) of 3-O-(3-fluorobenzyl)unguinol (7e).....	42
Figure S40. ^{13}C NMR spectrum (150 MHz, $\text{DMSO}-d_6$) of 3-O-(3-fluorobenzyl)unguinol (7e).....	43
Figure S41. ^1H NMR spectrum (600 MHz, $\text{DMSO}-d_6$) of 3-O-(4-fluorobenzyl)unguinol (7f)	44
Figure S42. ^{13}C NMR spectrum (150 MHz, $\text{DMSO}-d_6$) of 3-O-(4-fluorobenzyl)unguinol (7f)	45
Figure S43. ^1H NMR spectrum (600 MHz, $\text{DMSO}-d_6$) of 3-O-(2,4-difluorobenzyl)unguinol (7g)	46
Figure S44. ^{13}C NMR spectrum (150 MHz, $\text{DMSO}-d_6$) of 3-O-(2,4-difluorobenzyl)unguinol (7g)	47
Figure S45. ^1H NMR spectrum (500 MHz, $\text{DMSO}-d_6$) of 3-O-(3-bromobenzyl)unguinol (7h)	48
Figure S46. ^{13}C NMR spectrum (125 MHz, $\text{DMSO}-d_6$) of 3-O-(3-bromobenzyl)unguinol (7h)	49
Figure S47. ^1H NMR spectrum (500 MHz, $\text{DMSO}-d_6$) of 3-O-(3-methylbenzyl)unguinol (7i)	50
Figure S48. ^{13}C NMR spectrum (125 MHz, $\text{DMSO}-d_6$) of 3-O-(3-methylbenzyl)unguinol (7i).....	51
Figure S49. ^1H NMR spectrum (500 MHz, $\text{DMSO}-d_6$) of 3-O-(3-methoxybenzyl)unguinol (7j).....	52
Figure S50. ^{13}C NMR spectrum (125 MHz, $\text{DMSO}-d_6$) of 3-O-(3-methoxybenzyl)unguinol (7j).....	53
Figure S51. ^1H NMR spectrum (600 MHz, $\text{DMSO}-d_6$) of 3-O-(2-picolyl)unguinol (7k)	54
Figure S52. ^{13}C NMR spectrum (150 MHz, $\text{DMSO}-d_6$) of 3-O-(2-picolyl)unguinol (7k)	55
Figure S53. ^1H NMR spectrum (600 MHz, $\text{DMSO}-d_6$) of 3-O-(3-picolyl)unguinol (7l).....	56
Figure S54. ^{13}C NMR spectrum (150 MHz, $\text{DMSO}-d_6$) of 3-O-(3-picolyl)unguinol (7l)	57
Figure S55. ^1H NMR spectrum (600 MHz, $\text{DMSO}-d_6$) of 3-O-(4-picolyl)unguinol (7m)	58
Figure S56. ^{13}C NMR spectrum (150 MHz, $\text{DMSO}-d_6$) of 3-O-(4-picolyl)unguinol (7m)	59
Figure S57. ^1H NMR spectrum (600 MHz, $\text{DMSO}-d_6$) of 3-O-(4-morpholinoethyl)unguinol (7n)	60
Figure S58. ^{13}C NMR spectrum (150 MHz, $\text{DMSO}-d_6$) of 3-O-(4-morpholinoethyl)unguinol (7n).....	61
Figure S59. ^1H NMR spectrum (600 MHz, $\text{DMSO}-d_6$) of 3-O-(1-piperidinyethyl)unguinol (7o)	62
Figure S60. ^{13}C NMR spectrum (150 MHz, $\text{DMSO}-d_6$) of 3-O-(1-piperidinyethyl)unguinol (7o)	63
Figure S61. ^1H NMR spectrum (600 MHz, $\text{DMSO}-d_6$) of 3-O-(1-pyrrolidinyethyl)unguinol (7p).....	64
Figure S62. ^{13}C NMR spectrum (150 MHz, $\text{DMSO}-d_6$) of 3-O-(1-pyrrolidinyethyl)unguinol (7p).....	65
Figure S63. ^1H NMR spectrum (600 MHz, $\text{DMSO}-d_6$) of 3-O-benzyl-1',2'-dihydrounguinol (8a)	66
Figure S64. ^{13}C NMR spectrum (150 MHz, $\text{DMSO}-d_6$) of 3-O-benzyl-1',2'-dihydrounguinol (8a)	67
Figure S65. ^1H NMR spectrum (600 MHz, $\text{DMSO}-d_6$) of 3-O-(2-fluorobenzyl)-1',2'-dihydrounguinol (8b)	68
Figure S66. ^{13}C NMR spectrum (150 MHz, $\text{DMSO}-d_6$) of 3-O-(2-fluorobenzyl)-1',2'-dihydrounguinol (8b)	69
Figure S67. ^1H NMR spectrum (600 MHz, $\text{DMSO}-d_6$) of 3-O-(4-fluorobenzyl)-1',2'-dihydrounguinol (8c).....	70
Figure S68. ^{13}C NMR spectrum (150 MHz, $\text{DMSO}-d_6$) of 3-O-(4-fluorobenzyl)-1',2'-dihydrounguinol (8c).....	71
Figure S69. UV-vis spectrum of 1',2'-dihydrounguinol (2a) in MeOH.....	72
Figure S70. UV-vis spectrum of <i>cis</i> -1',2'-epoxyunguinol (2b) in MeOH.....	72
Figure S71. UV-vis spectrum of 1',2'-dihydroxyunguinol (2c) in MeOH	73
Figure S72. UV-vis spectrum of 2'-hydroxy- $\Delta^{1',4'}$ -unguinol (2d) in MeOH	73
Figure S73. UV-vis spectrum of 2'-oxo- $\Delta^{1',4'}$ -unguinol (2e) in MeOH	74
Figure S74. UV-vis spectrum of 2'-hydroperoxy- $\Delta^{1',4'}$ -unguinol (2f) in MeOH	74
Figure S75. UV-vis spectrum of 2,7-dibromo-1',2'-dihydrounguinol (3a) in MeOH.....	75
Figure S76. UV-vis spectrum of 2,4,7-tribromo-1',2'-dihydrounguinol (3b) in MeOH	75
Figure S77. UV-vis spectrum of 2,4-diiodo-1',2'-dihydrounguinol (3c) in MeOH	76
Figure S78. UV-vis spectrum of methylunguinolate (4a) in MeOH.....	76
Figure S79. UV-vis spectrum of unguinolamide (4b) in MeOH	77
Figure S80. UV-vis spectrum of 3-O-methylunguinol (5a) in MeOH.....	77
Figure S81. UV-vis spectrum of 3,8-di-O-methylunguinol (5b) in MeOH	78
Figure S82. UV-vis spectrum of 3-O-benzylunguinol (6a) in MeOH	78
Figure S83. UV-vis spectrum of 3,8-di-O-benzylunguinol (6b) in MeOH.....	79
Figure S84. UV-vis spectrum of 3-O-(2-chlorobenzyl)unguinol (7a) in MeOH	79
Figure S85. UV-vis spectrum of 3-O-(3-chlorobenzyl)unguinol (7b) in MeOH.....	80
Figure S86. UV-vis spectrum of 3-O-(4-chlorobenzyl)unguinol (7c) in MeOH	80

Figure S87. UV-vis spectrum of 3- <i>O</i> -(2-fluorobenzyl)unguinol (7d) in MeOH	81
Figure S88. UV-vis spectrum of 3- <i>O</i> -(3-fluorobenzyl)unguinol (7e) in MeOH	81
Figure S89. UV-vis spectrum of 3- <i>O</i> -(4-fluorobenzyl)unguinol (7f) in MeOH	82
Figure S90. UV-vis spectrum of 3- <i>O</i> -(2,4-difluorobenzyl)unguinol (7g) in MeOH.....	82
Figure S91. UV-vis spectrum of 3- <i>O</i> -(3-bromobenzyl)unguinol (7h) in MeOH.....	83
Figure S92. UV-vis spectrum of 3- <i>O</i> -(3-methylbenzyl)unguinol (7i) in MeOH	83
Figure S93. UV-vis spectrum of 3- <i>O</i> -(3-methoxybenzyl)unguinol (7j) in MeOH	84
Figure S94. UV-vis spectrum of 3- <i>O</i> -(2-picolyl)unguinol (7k) in MeOH.....	84
Figure S95. UV-vis spectrum of 3- <i>O</i> -(3-picolyl)unguinol (7l) in MeOH.....	85
Figure S96. UV-vis spectrum of 3- <i>O</i> -(4-picolyl)unguinol (7m) in MeOH.....	85
Figure S97. UV-vis spectrum of 3- <i>O</i> -(4-morpholinoethyl)unguinol (7n) in MeOH	86
Figure S98. UV-vis spectrum of 3- <i>O</i> -(1-piperidinyethyl)unguinol (7o) in MeOH.....	86
Figure S99. UV-vis spectrum of 3- <i>O</i> -(1-pyrrolidinyethyl)unguinol (7p) in MeOH.....	87
Figure S100. UV-vis spectrum of 3- <i>O</i> -1',2'-dihydrobenzylunguinol (8a) in MeOH	87
Figure S101. UV-vis spectrum of 3- <i>O</i> -(2-fluorobenzyl)-1',2'-dihydrounguinol (8b) in MeOH.....	88
Figure S102. UV-vis spectrum of 3- <i>O</i> -(4-fluorobenzyl)-1',2'-dihydrounguinol (8c) in MeOH	88
Figure S103. HRESI(+)-MS spectrum of 1',2'-dihydrounguinol (2a)	89
Figure S104. HRESI(-)-MS spectrum of <i>cis</i> -1',2'-epoxyunguinol (2b)	90
Figure S105. HRESI(-)-MS spectrum of 1',2'-dihydroxyunguinol (2c).....	91
Figure S106. HR-ESI(-)-MS spectrum of 2'-hydroxy- $\Delta^{1',4'}$ -unguinol (2d)	92
Figure S107. HRESI(-)-MS spectrum of 2'-oxo- $\Delta^{1',4'}$ -unguinol (2e).....	93
Figure S108. HR-ESI(-)-MS spectrum of 2'-hydroperoxy- $\Delta^{1',4'}$ -unguinol (2f)	94
Figure S109. HRESI(-)-MS spectrum of 2,7-dibromo-1',2'-dihydrounguinol (3a).....	95
Figure S110. HRESI(-)-MS spectrum of 2,4,7-tribromo-1',2'-dihydrounguinol (3b)	96
Figure S111. HRESI(-)-MS spectrum of 2,4-diiodo-1',2'-dihydrounguinol (3c)	97
Figure S112. HRESI(-)-MS spectrum of methylunguinolate (4a)	98
Figure S113. HRESI(-)-MS spectrum of unguinolamide (4b)	99
Figure S114. HRESI(-)-MS spectrum of 3- <i>O</i> -methylunguinol (5a)	100
Figure S115. HRESI(+)-MS spectrum of 3,8-di- <i>O</i> -methylunguinol (5b).....	101
Figure S116. HRESI(+)-MS spectrum of 3- <i>O</i> -benzylunguinol (6a).....	102
Figure S117. HRESI(+)-MS spectrum of 3,8-di- <i>O</i> -benzylunguinol (6b)	103
Figure S118. HRESI(+)-MS spectrum of 3- <i>O</i> -(2-chlorobenzyl)unguinol (7a).....	104
Figure S119. HRESI(-)-MS spectrum of 3- <i>O</i> -(3-chlorobenzyl)unguinol (7b).....	105
Figure S120. HRESI(-)-MS spectrum of 3- <i>O</i> -(4-chlorobenzyl)unguinol (7c)	106
Figure S121. HRESI(+)-MS spectrum of 3- <i>O</i> -(2-fluorobenzyl)unguinol (7d).....	107
Figure S122. HRESI(-)-MS spectrum of 3- <i>O</i> -(3-fluorobenzyl)unguinol (7e)	108
Figure S123. HRESI(-)-MS spectrum of 3- <i>O</i> -(4-fluorobenzyl)unguinol (7f)	109
Figure S124. HRESI(-)-MS spectrum of 3- <i>O</i> -(2,4-difluorobenzyl)unguinol (7g)	110
Figure S125. HRESI(-)-MS spectrum of 3- <i>O</i> -(3-bromobenzyl)unguinol (7h)	111
Figure S126. HRESI(-)-MS spectrum of 3- <i>O</i> -(3-methylbenzyl)unguinol (7i).....	112
Figure S127. HRESI(-)-MS spectrum of 3- <i>O</i> -(3-methoxybenzyl)unguinol (7j).....	113
Figure S128. HRESI(+)-MS spectrum of 3- <i>O</i> -(2-picolyl)unguinol (7k)	114
Figure S129. HRESI(+)-MS spectrum of 3- <i>O</i> -(3-picolyl)unguinol (7l)	115
Figure S130. HRESI(+)-MS spectrum of 3- <i>O</i> -(4-picolyl)unguinol (7m)	116
Figure S131. HRESI(+)-MS spectrum of 3- <i>O</i> -(4-morpholinoethyl)unguinol (7n).....	117
Figure S132. HRESI(+)-MS spectrum of 3- <i>O</i> -(1-piperidinyethyl)unguinol (7o).....	118
Figure S133. HRESI(+)-MS spectrum of 3- <i>O</i> -(1-pyrrolidinyethyl)unguinol (7p)	119
Figure S134. HRESI(+)-MS spectrum of 3- <i>O</i> -1',2'-dihydrobenzylunguinol (8a)	120
Figure S135. HRESI(+)-MS spectrum of 3- <i>O</i> -(2-fluorobenzyl)-1',2'-dihydrounguinol (8b).....	121
Figure S136. HRESI(+)-MS spectrum of 3- <i>O</i> -(4-fluorobenzyl)-1',2'-dihydrounguinol (8c).....	122

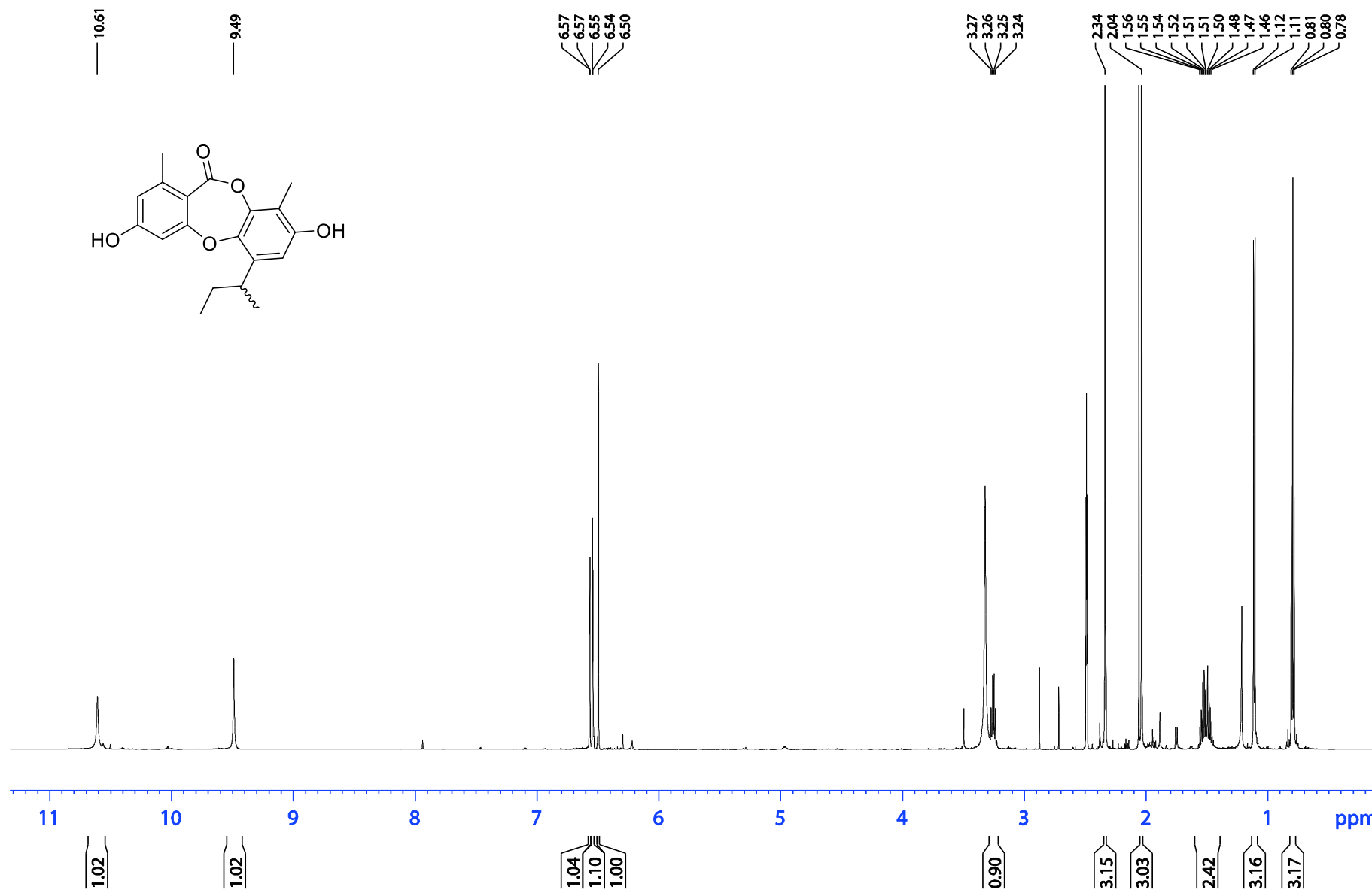


Figure S1. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of 1',2'-dihydroounginol (2a)

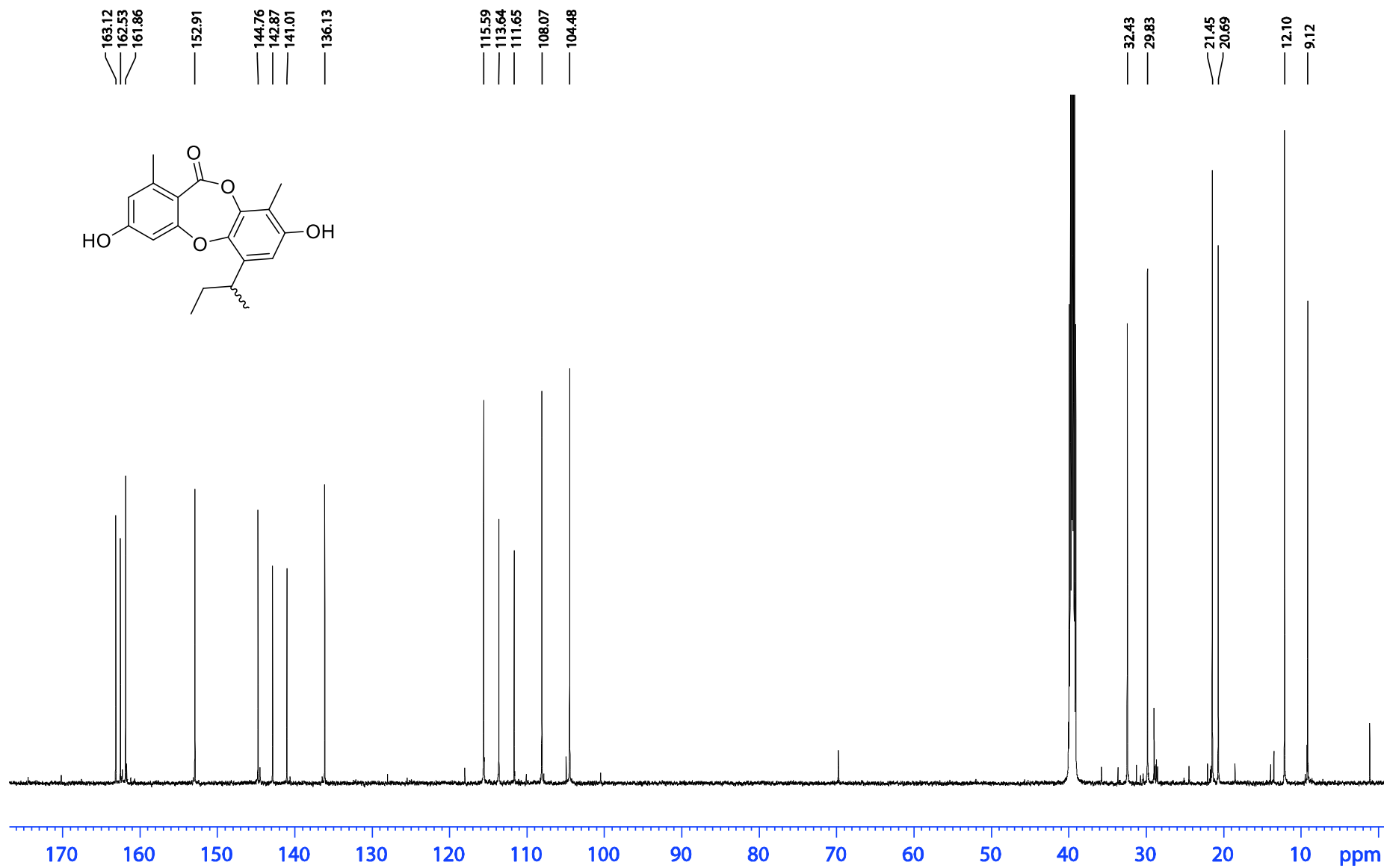


Figure S2. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) of 1',2'-dihydroanguinol (2a)

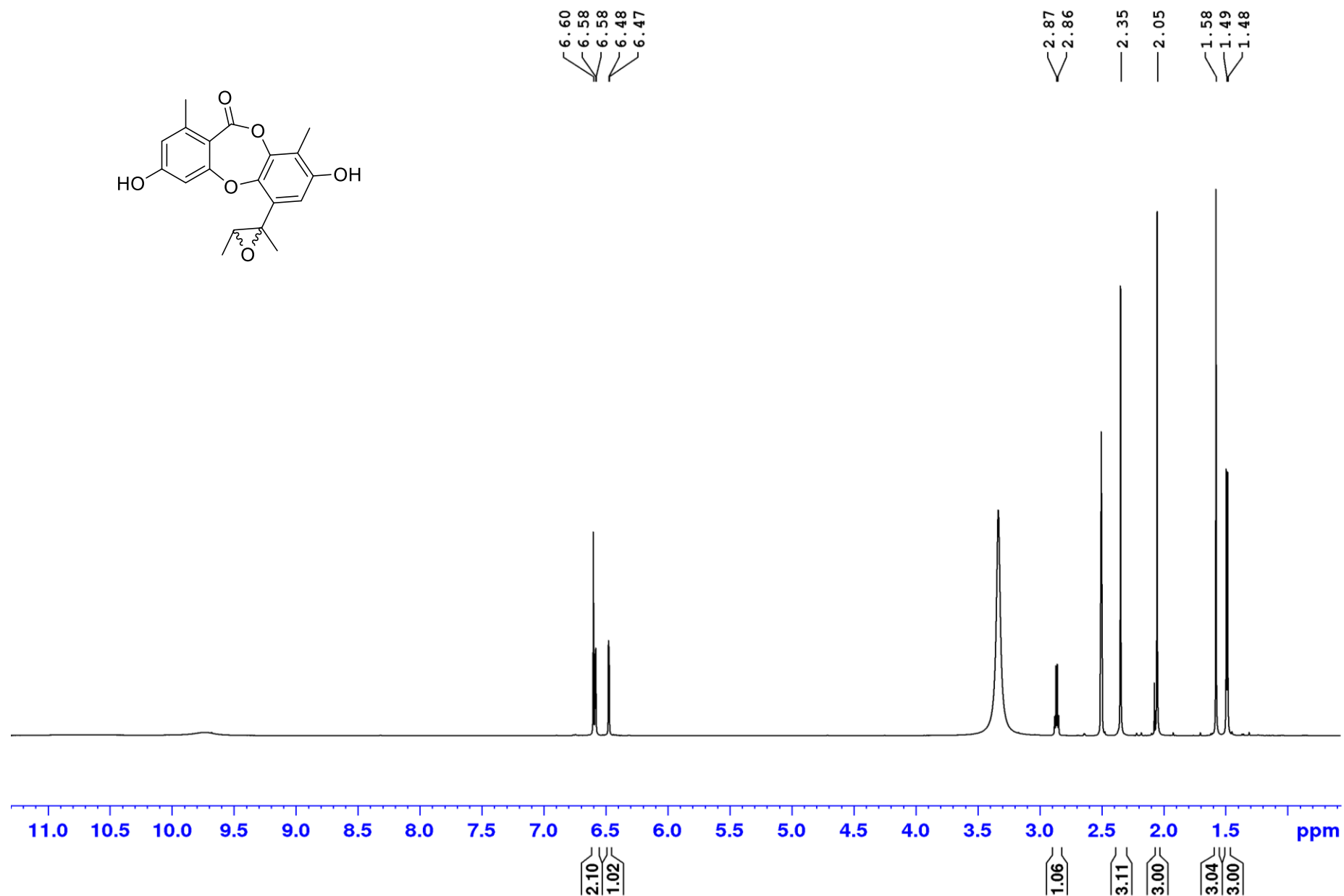


Figure S3. ¹H NMR spectrum (500 MHz, DMSO-*d*₆) of *cis*-1',2'-epoxyunguinol (2b)

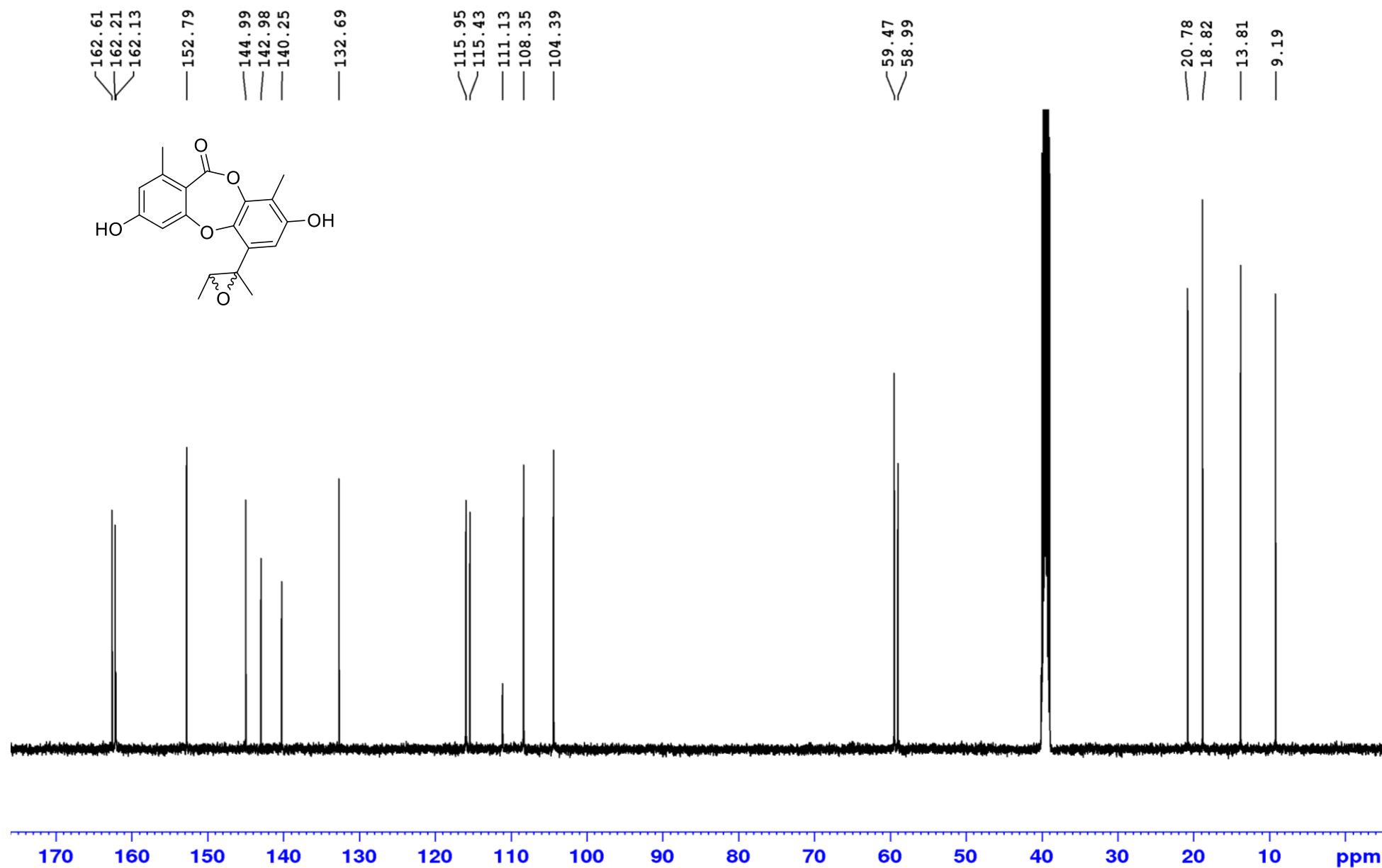


Figure S4. ¹³C NMR spectrum (125 MHz, DMSO-*d*₆) of *cis*-1',2'-epoxyunguinal (2b)

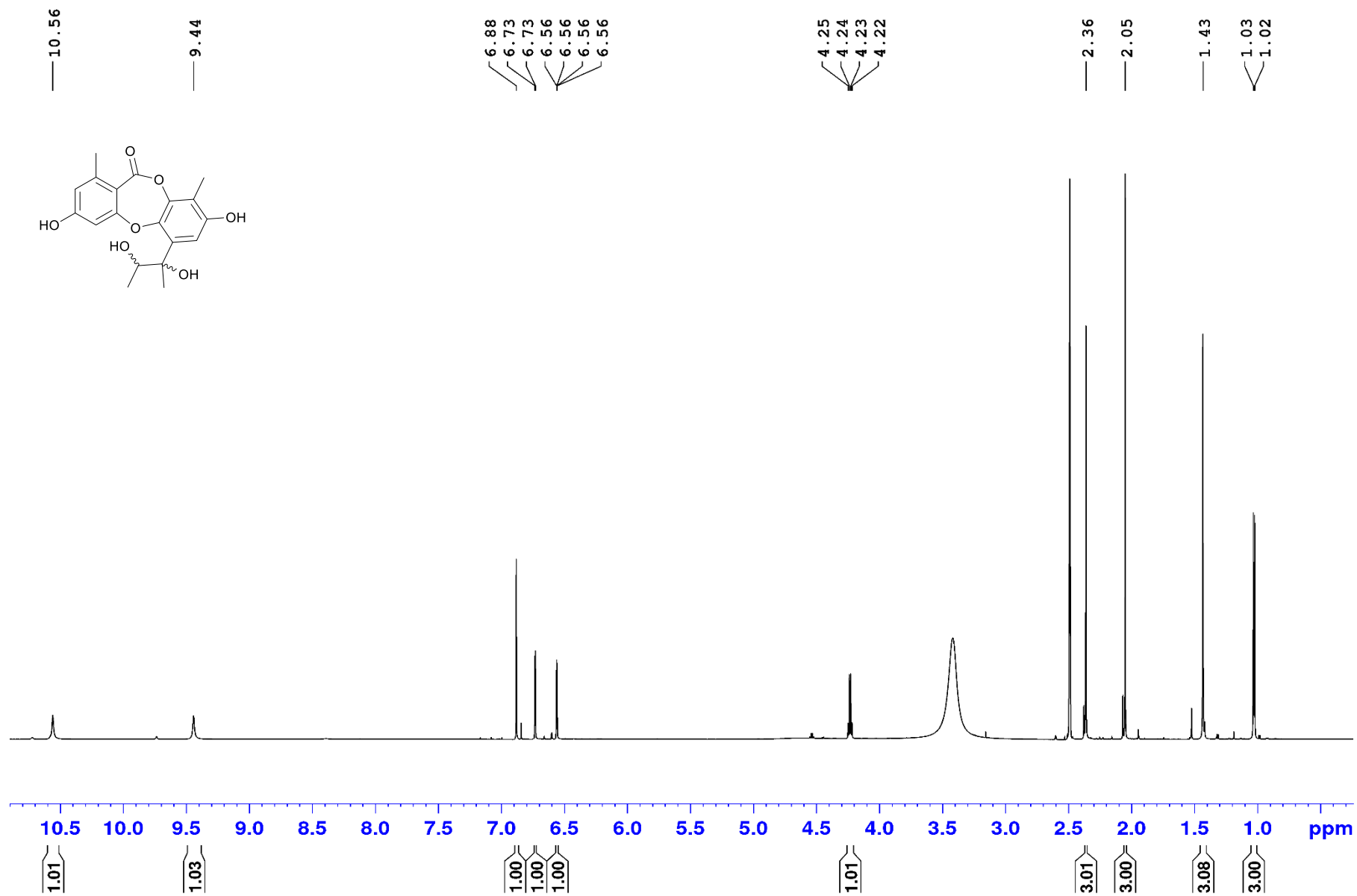


Figure S5. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of 1',2'-dihydroxyunguinal (2c)

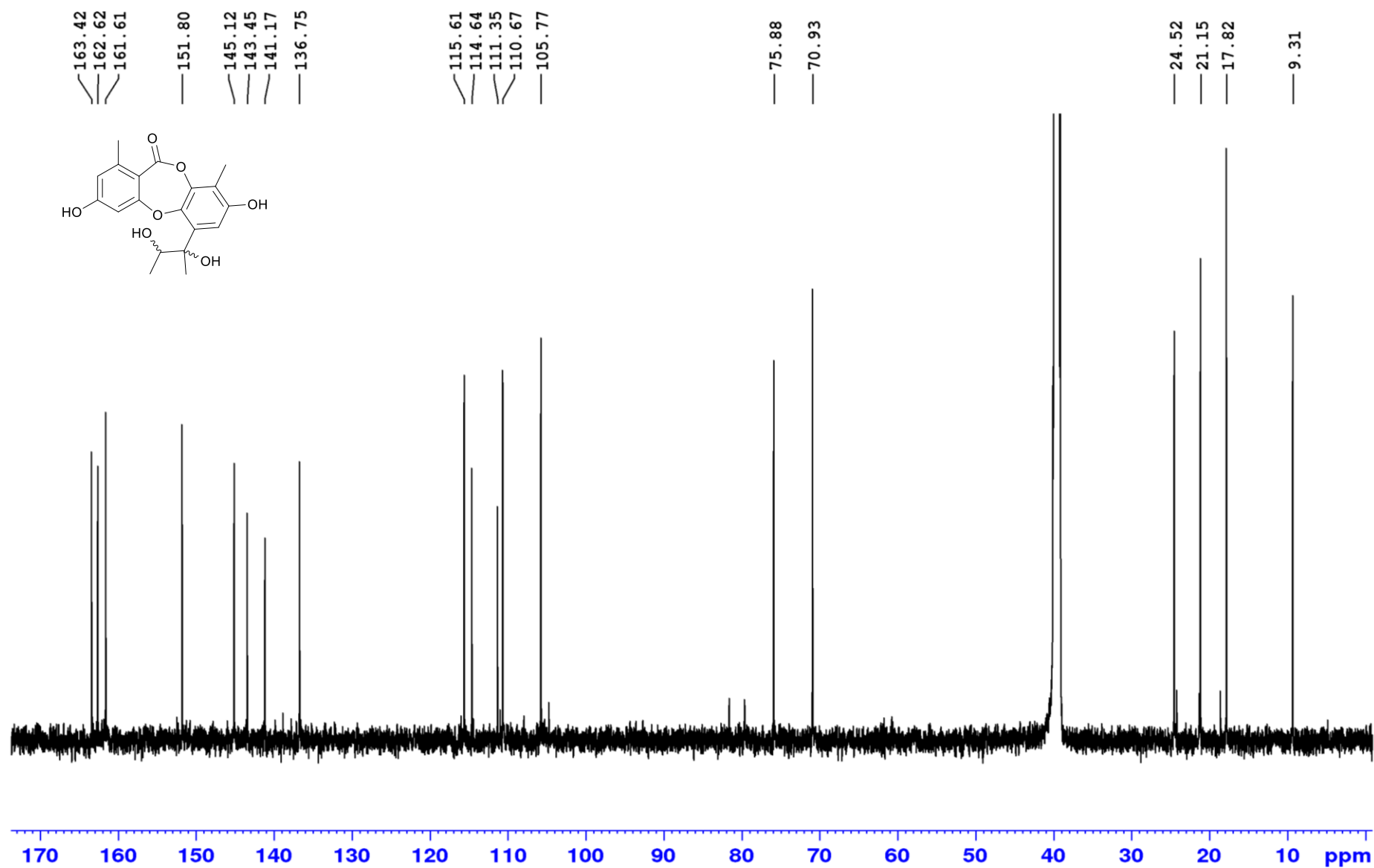


Figure S6. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) of 1',2'-dihydroxyunguinal (2c)

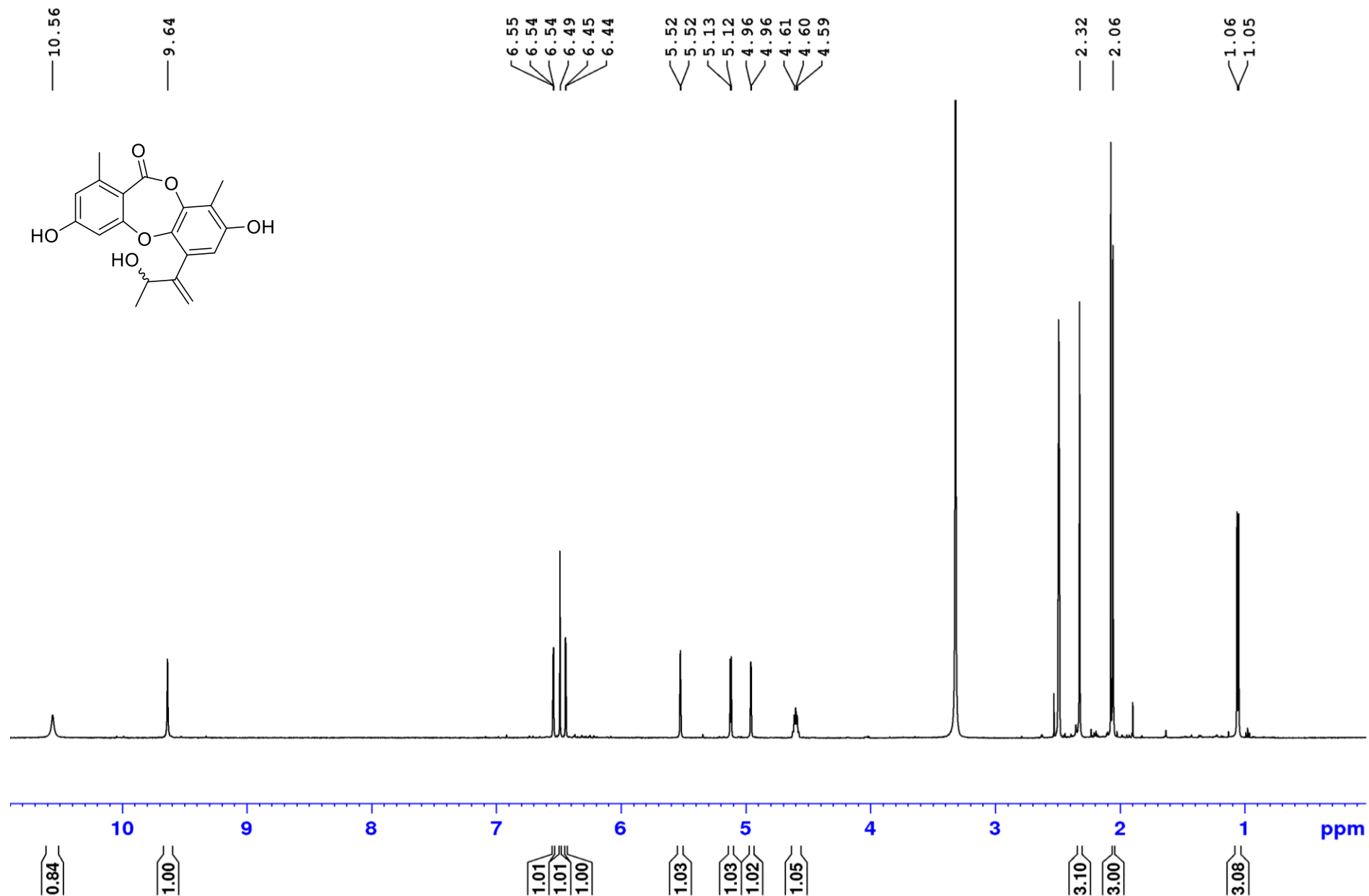


Figure S7. ¹H NMR spectrum (500 MHz, DMSO-*d*₆) of 2'-hydroxy- $\Delta^{1,4'}$ -unguol (2d)

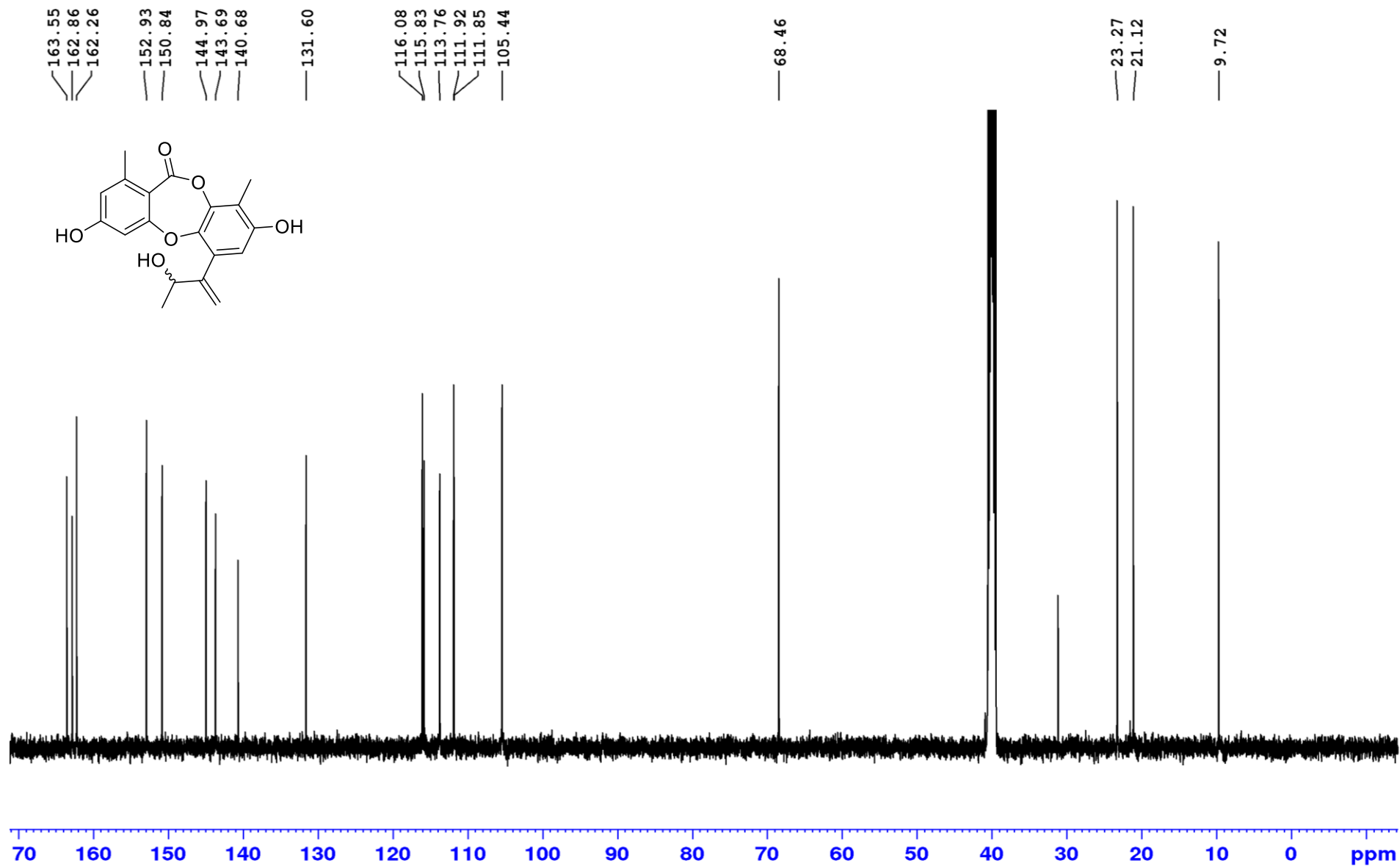


Figure S8. ¹³C NMR spectrum (125 MHz, DMSO-*d*₆) of 2'-hydroxy- $\Delta^{1,4'}$ -unguinol (2d)

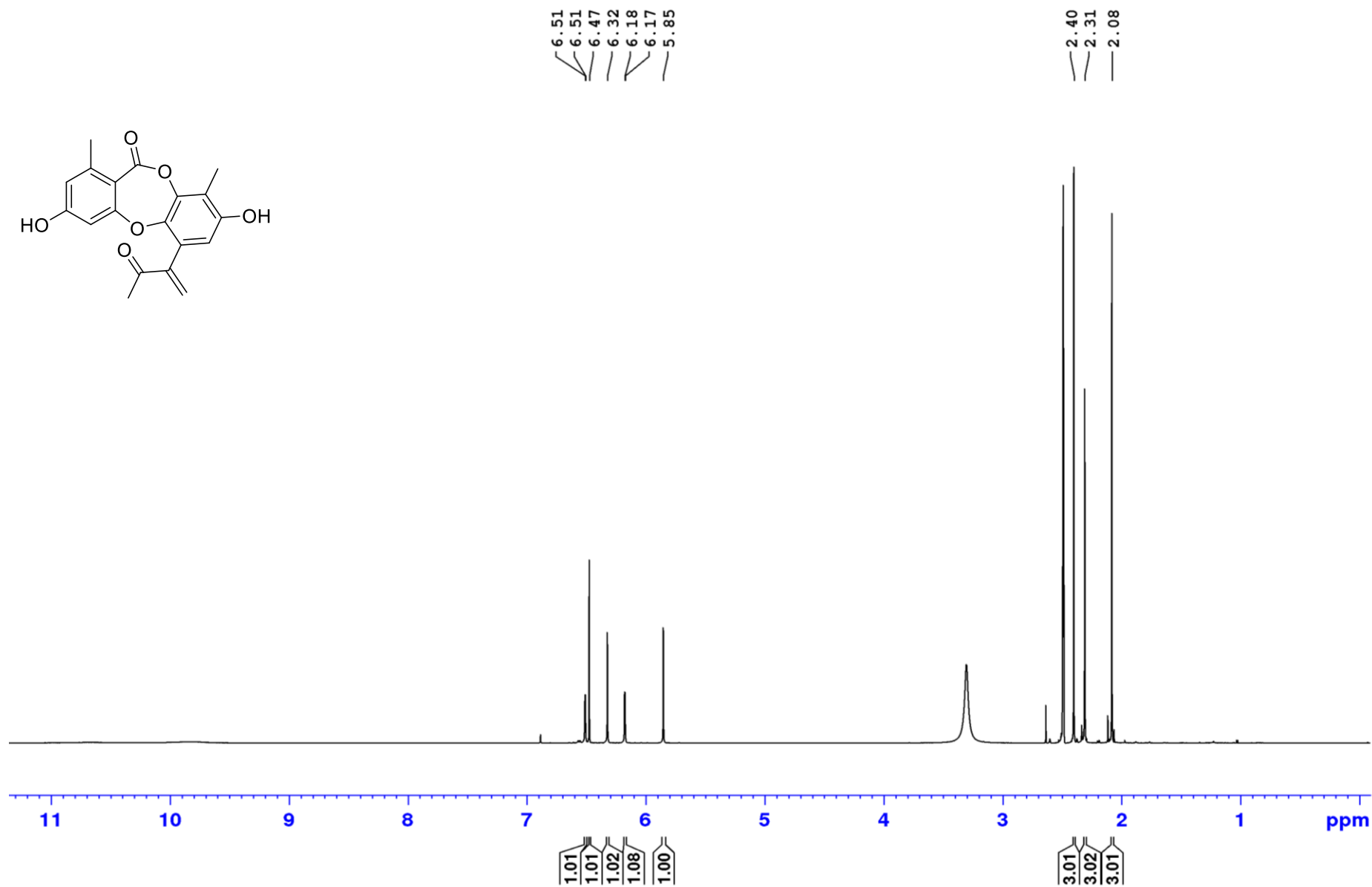


Figure S9. ^1H NMR spectrum (600 MHz, $\text{DMSO}-d_6$) of 2'-oxo- $\Delta^{1',4'}$ -unguinol (2e)

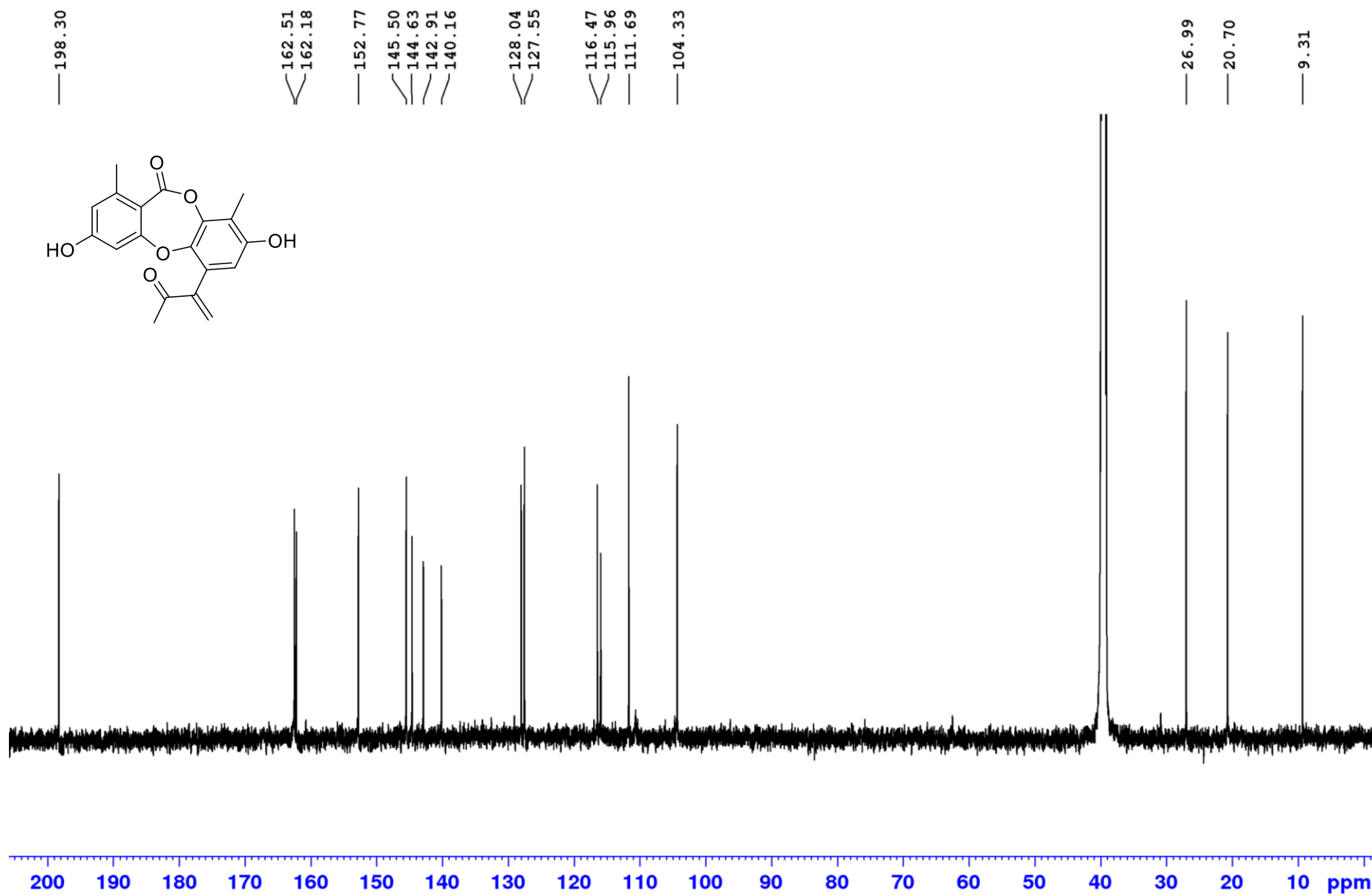


Figure S10. ¹H NMR spectrum (150 MHz, DMSO-*d*₆) of 2'-oxo- $\Delta^{1',4'}$ -unguinol (2e)

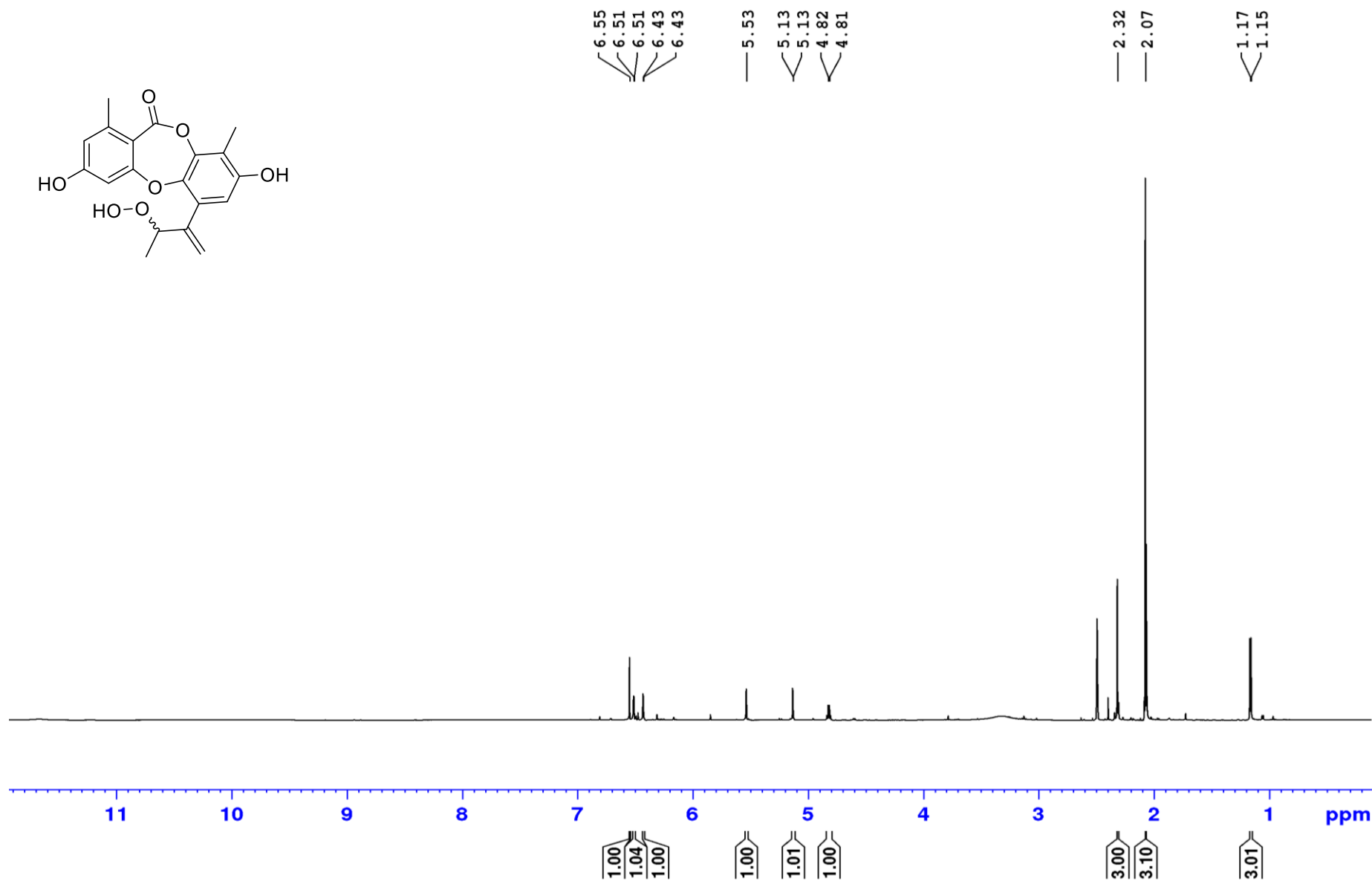


Figure S11. ^1H NMR spectrum (600 MHz, $\text{DMSO}-d_6$) of 2'-hydroperoxy- $\Delta^{1',4'}$ -unguinol (2f)

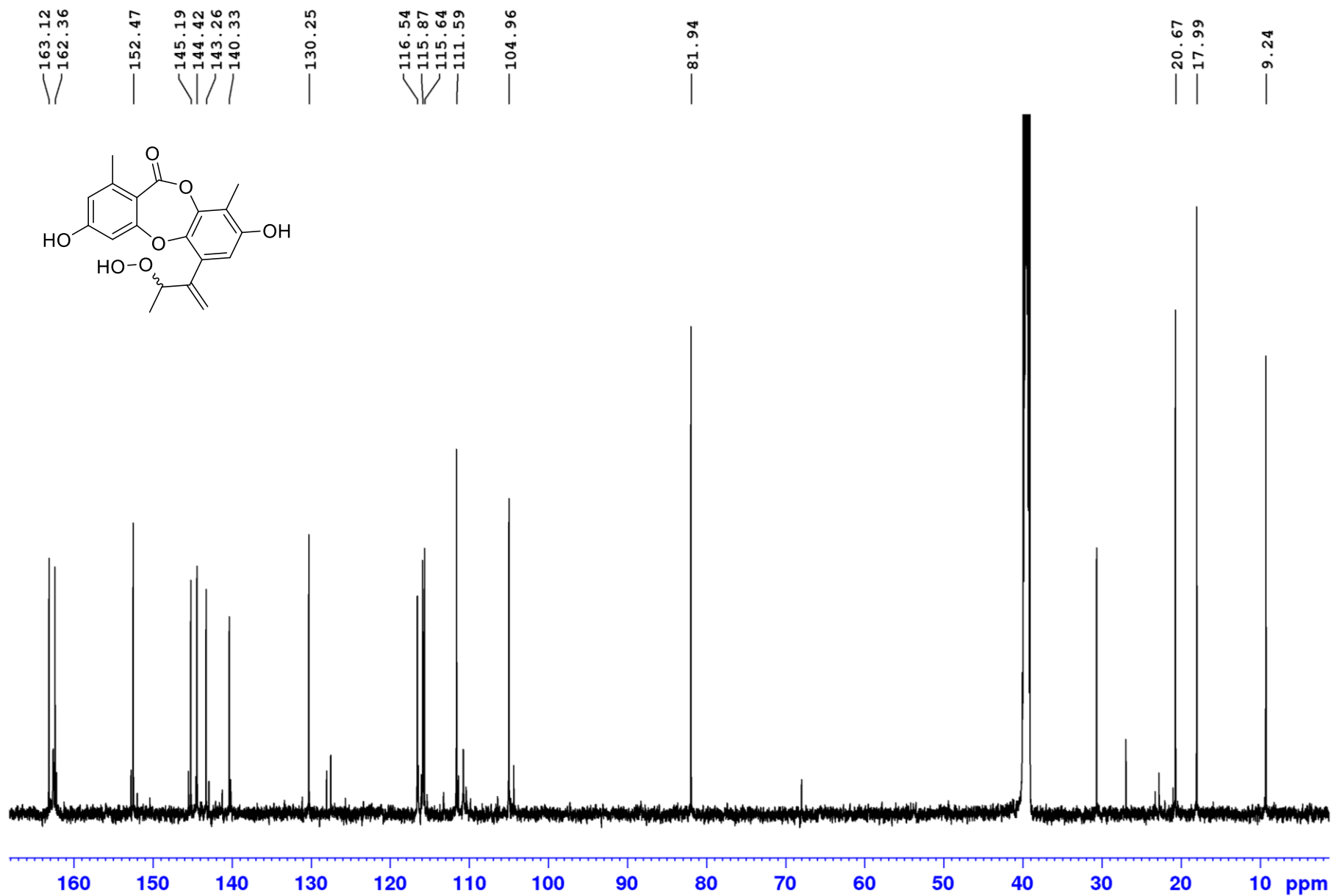


Figure S12. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) of 2'-hydroperoxy- $\Delta^{1,4'}$ -unguinol (2f)

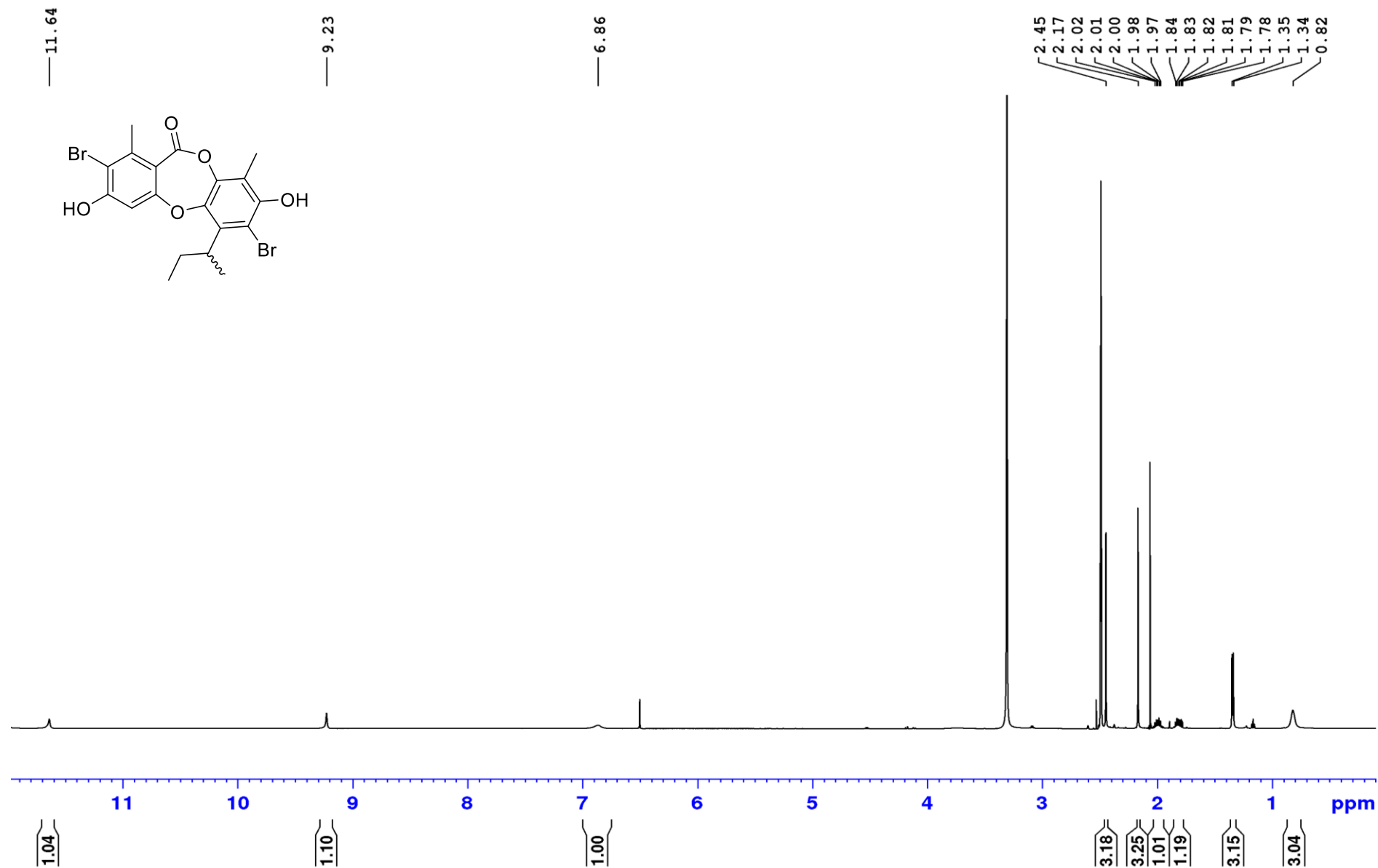


Figure S13. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of 2,7-dibromo-1',2'-dihydroquingol (3a)

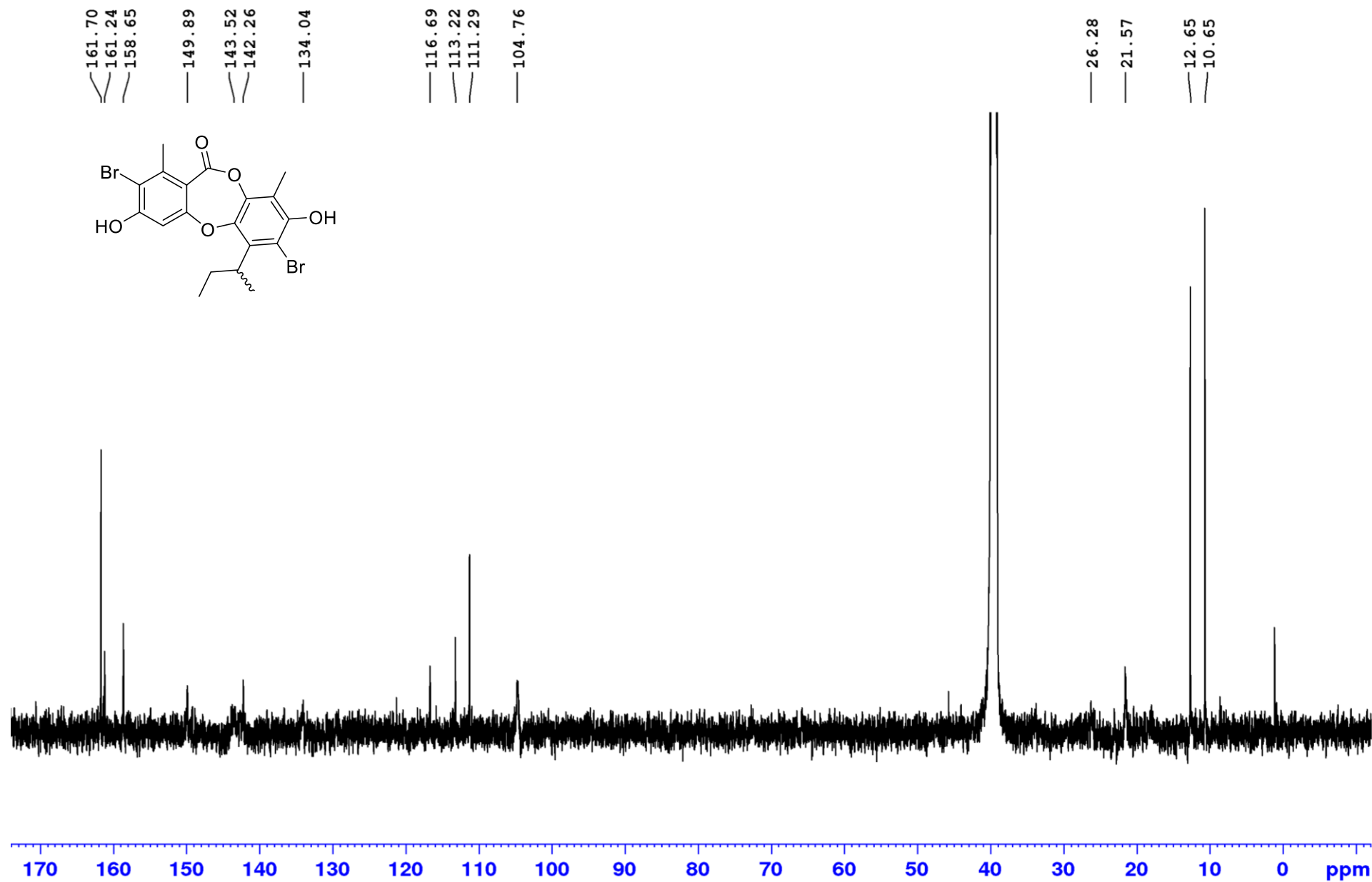


Figure S14. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) of 2,7-dibromo-1',2'-dihydroanguinol (3a)

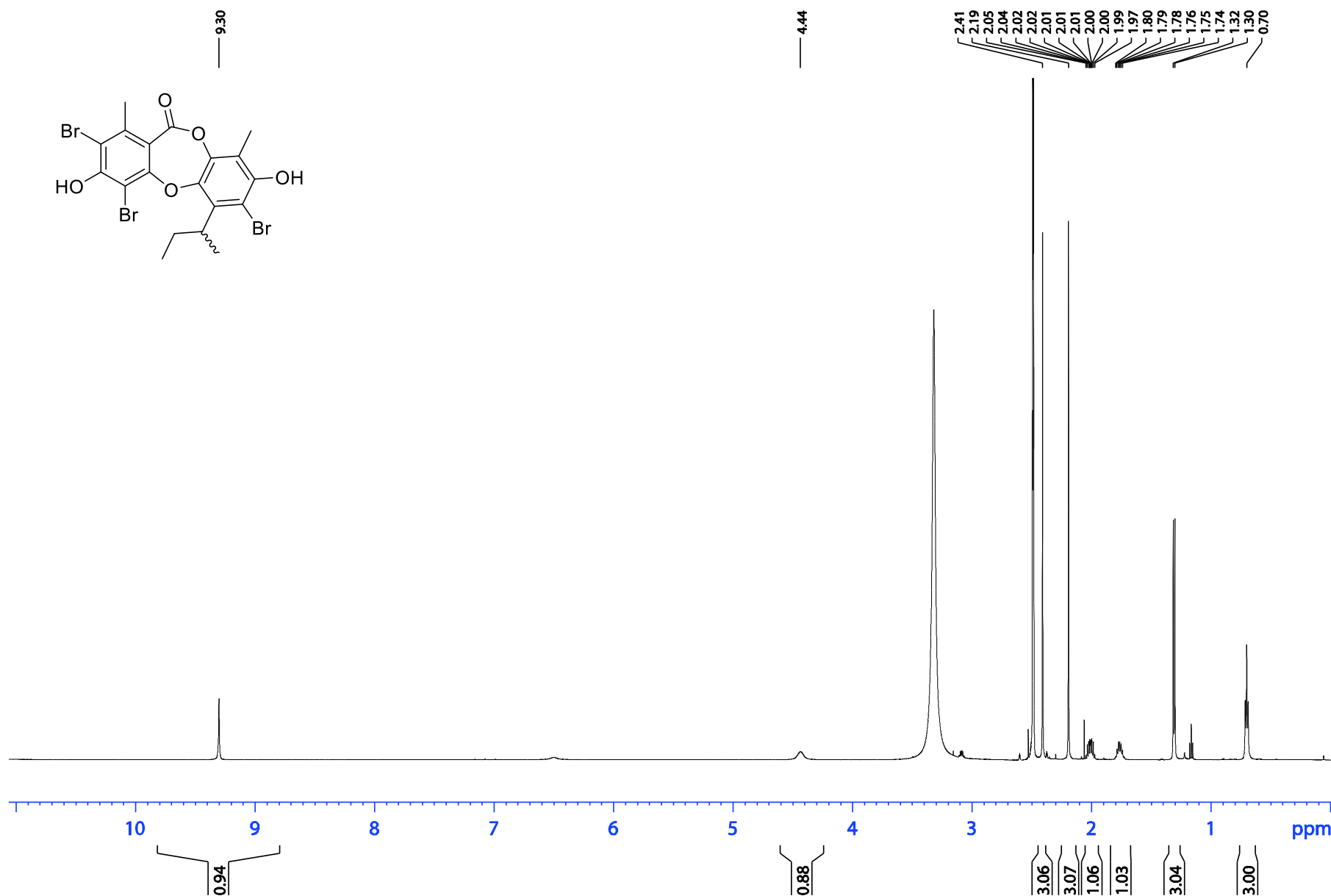


Figure S15. ^1H NMR spectrum (600 MHz, $\text{DMSO}-d_6$) of 2,4,7-tribromo-1',2'-dihydroquinol (3b)

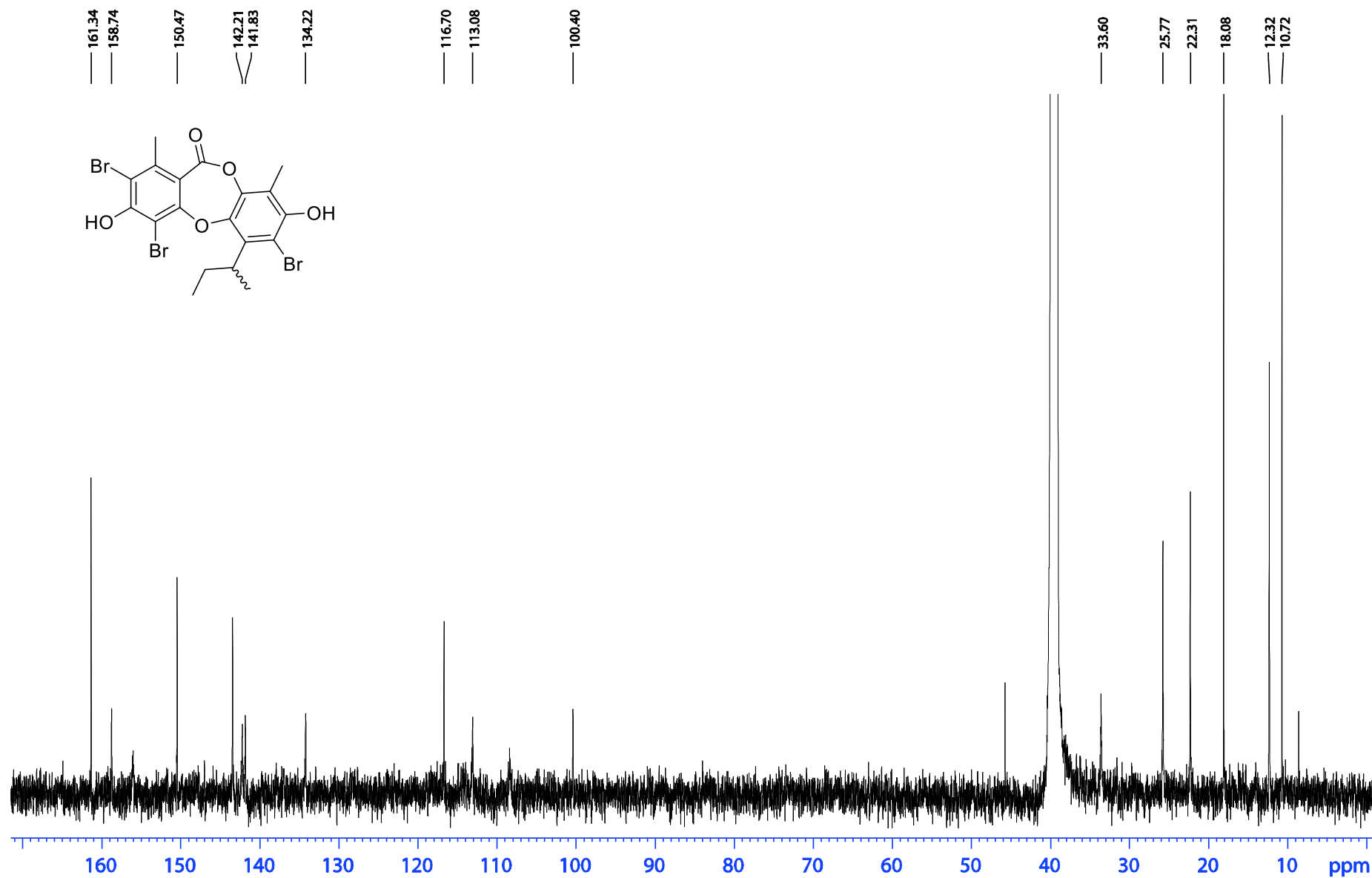


Figure S16. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) of 2,4,7-tribromo-1',2'-dihydroquinoxaline (3b)

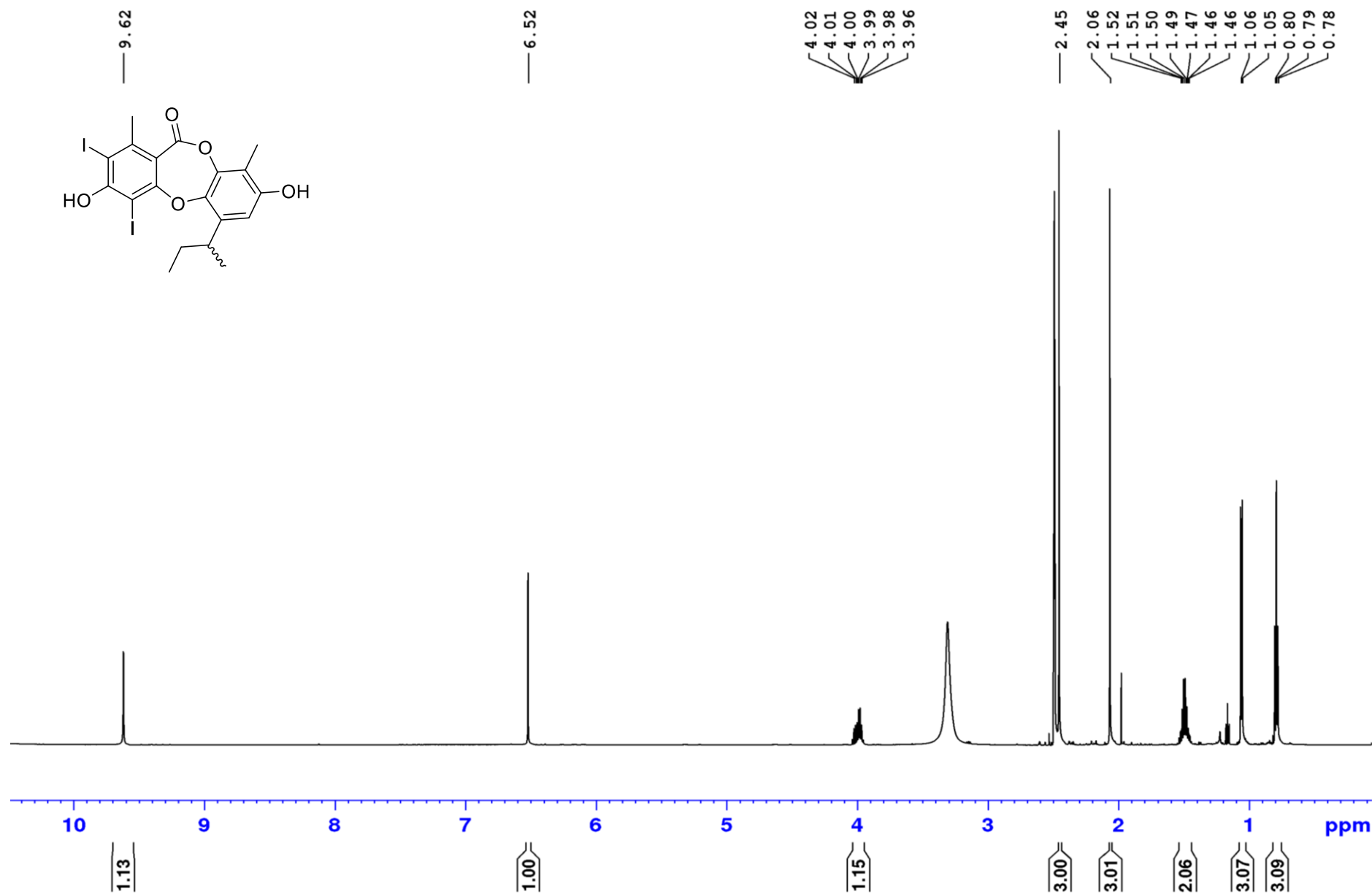


Figure S17. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of 2,4-diiodo-1',2'-dihydroanguinol (3c)

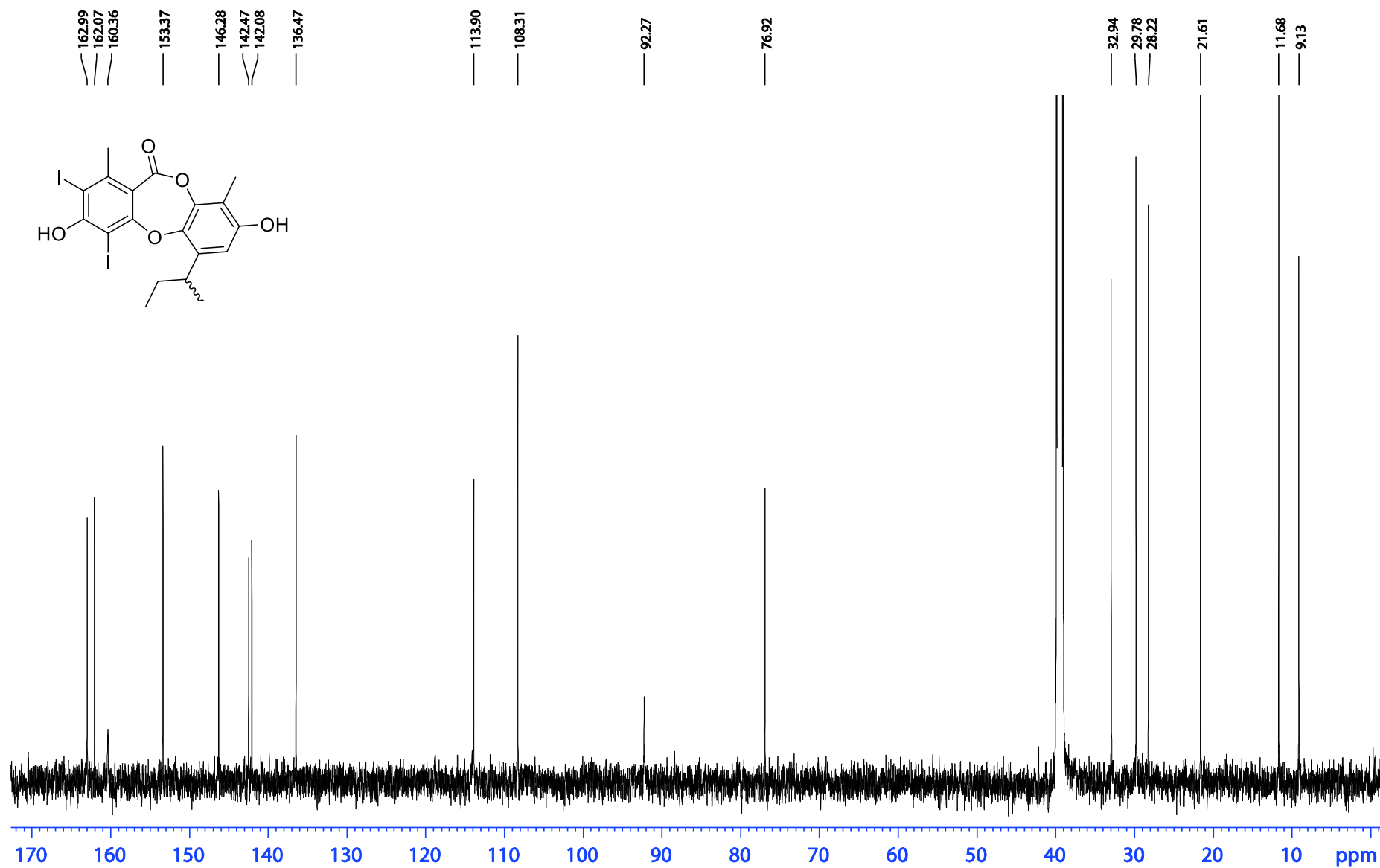


Figure S18. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) of 2,4-diiodo-1',2'-dihydroanguinol (3c)

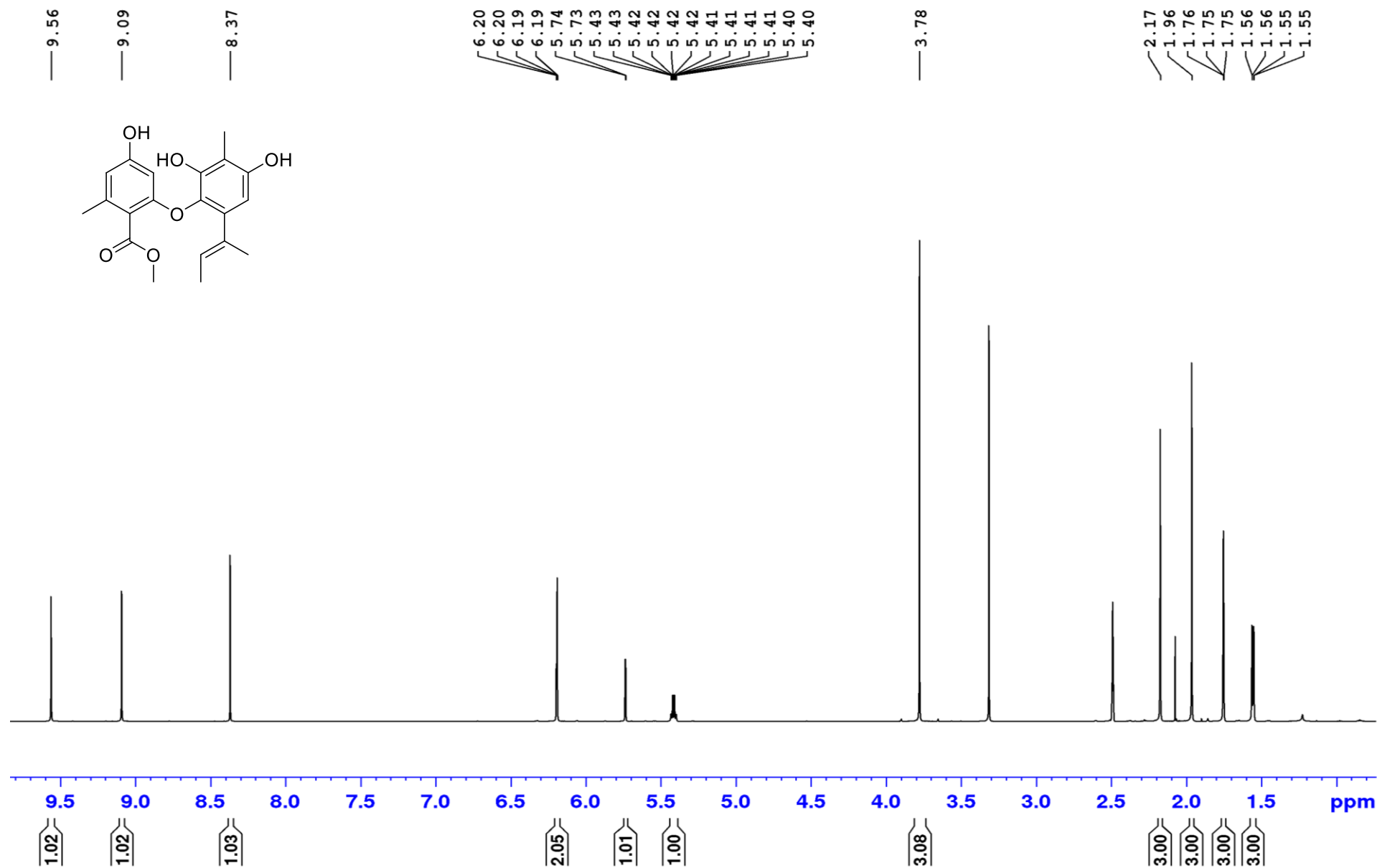


Figure S19. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of methylunguinolate (4a)

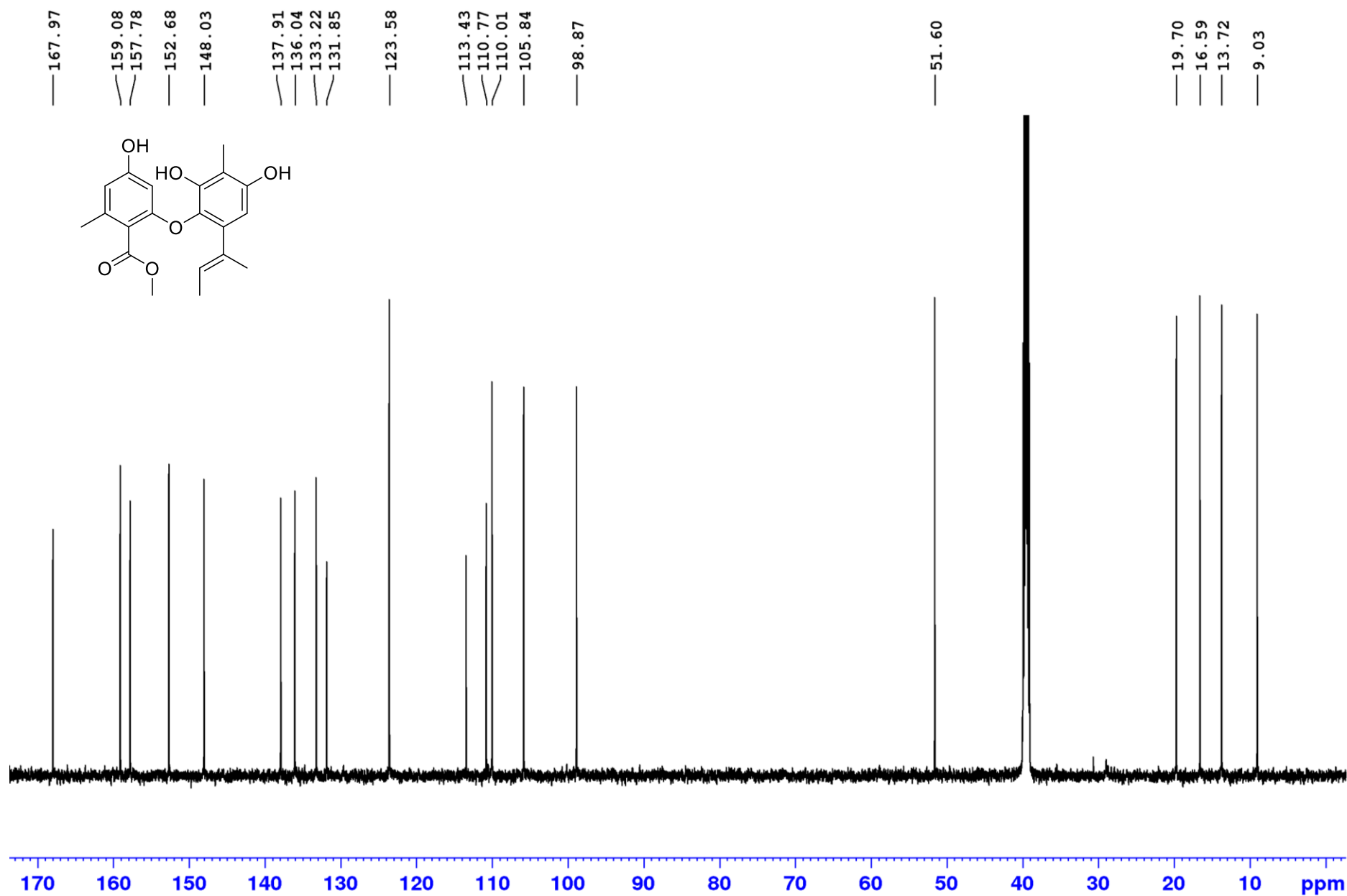


Figure S20. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) of methylunguinate (4a)

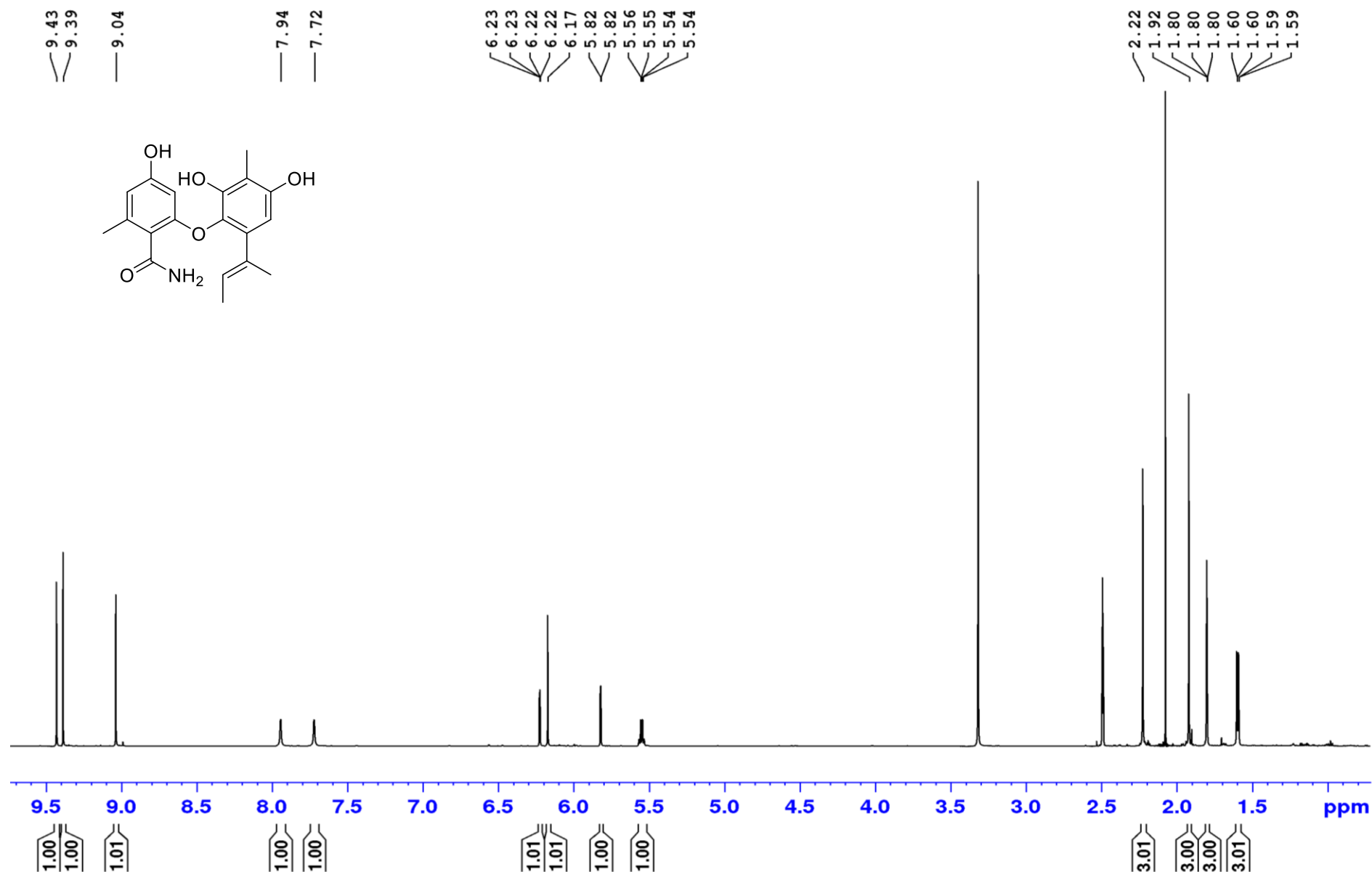


Figure S21. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of unguinolamide (4b)

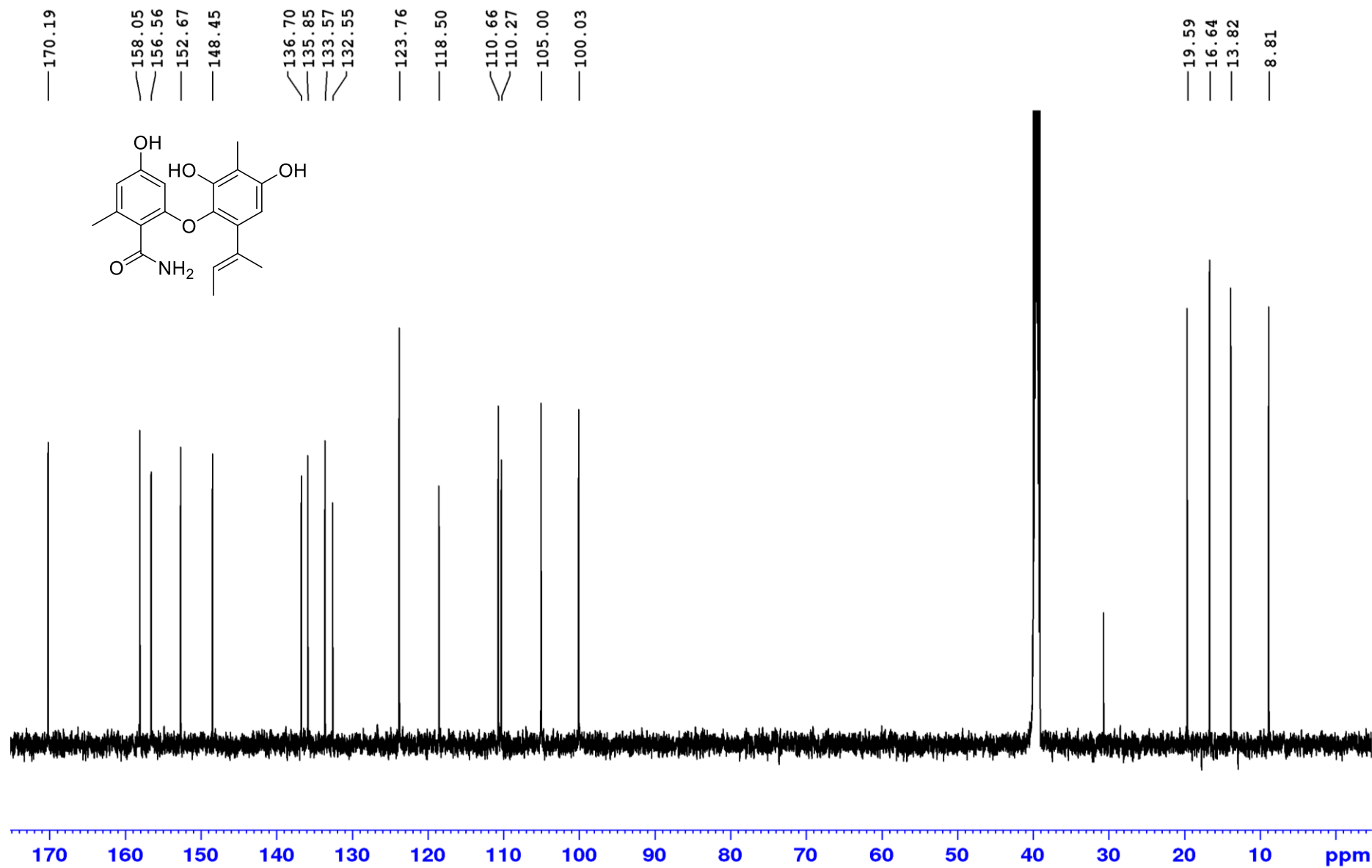


Figure S22. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) of unguinolamide (4b)

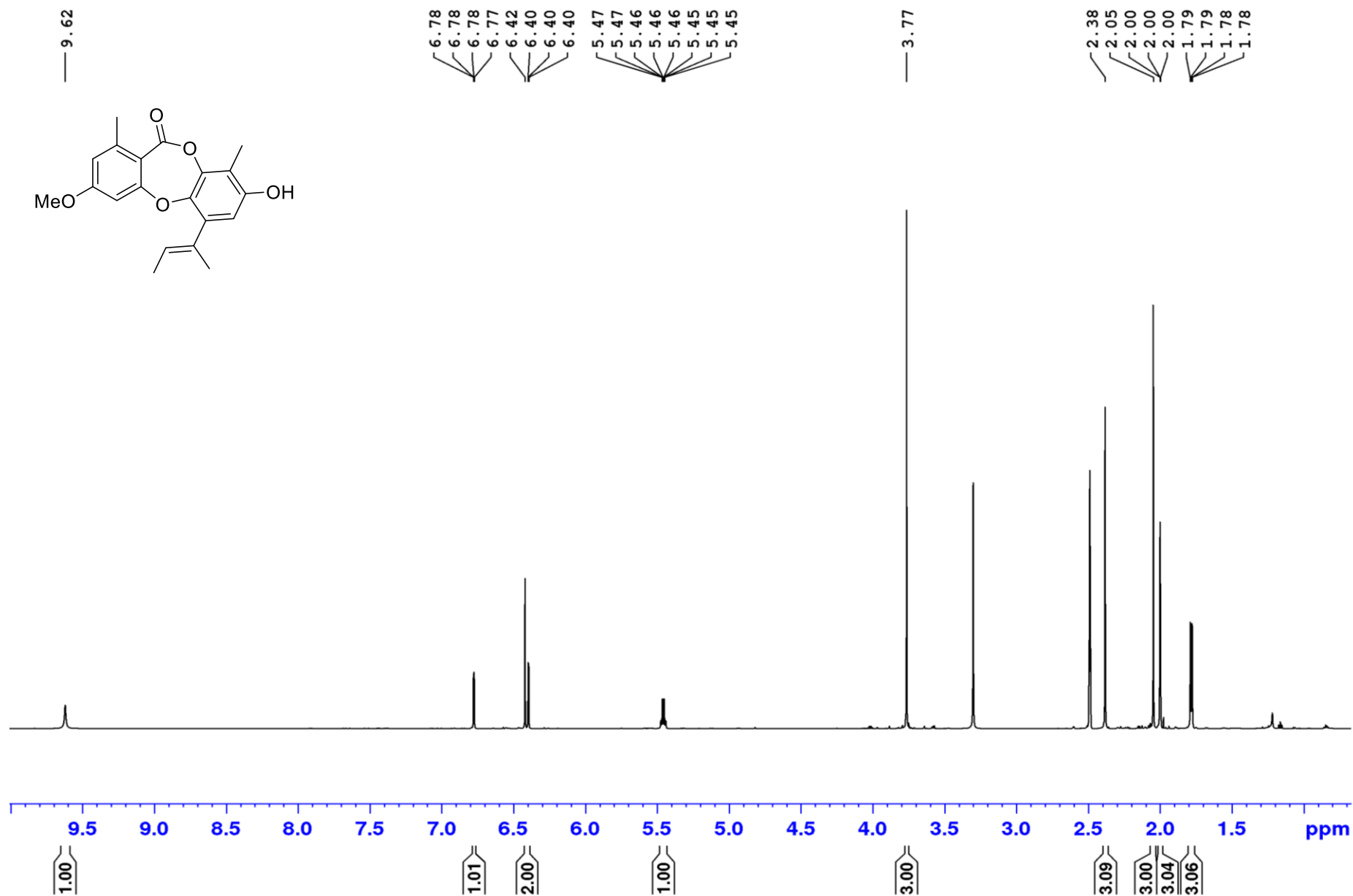


Figure S23. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of 3-O-methylunguinol (5a)

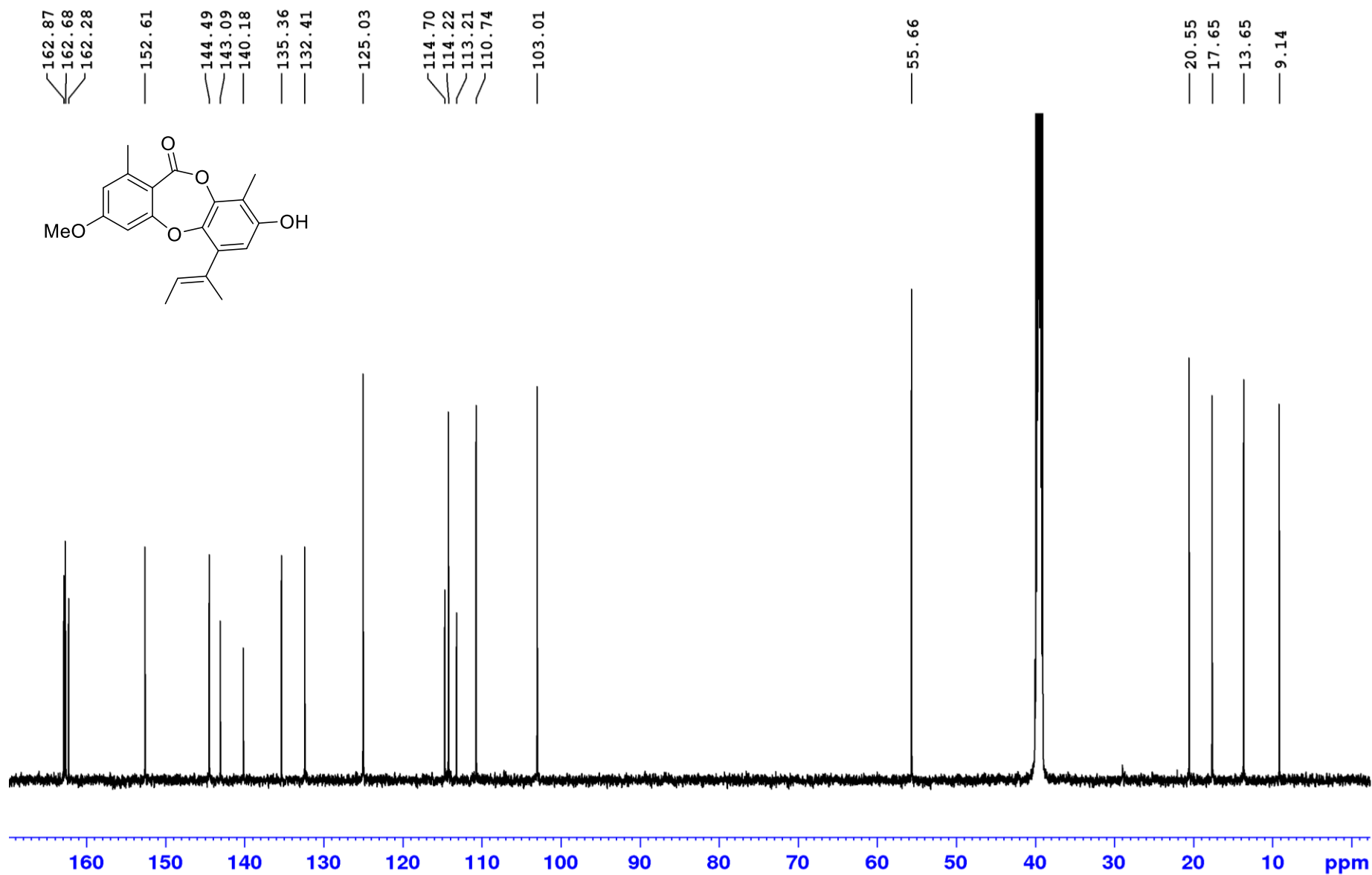


Figure S24. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) of 3-O-methylunguinal (5a)

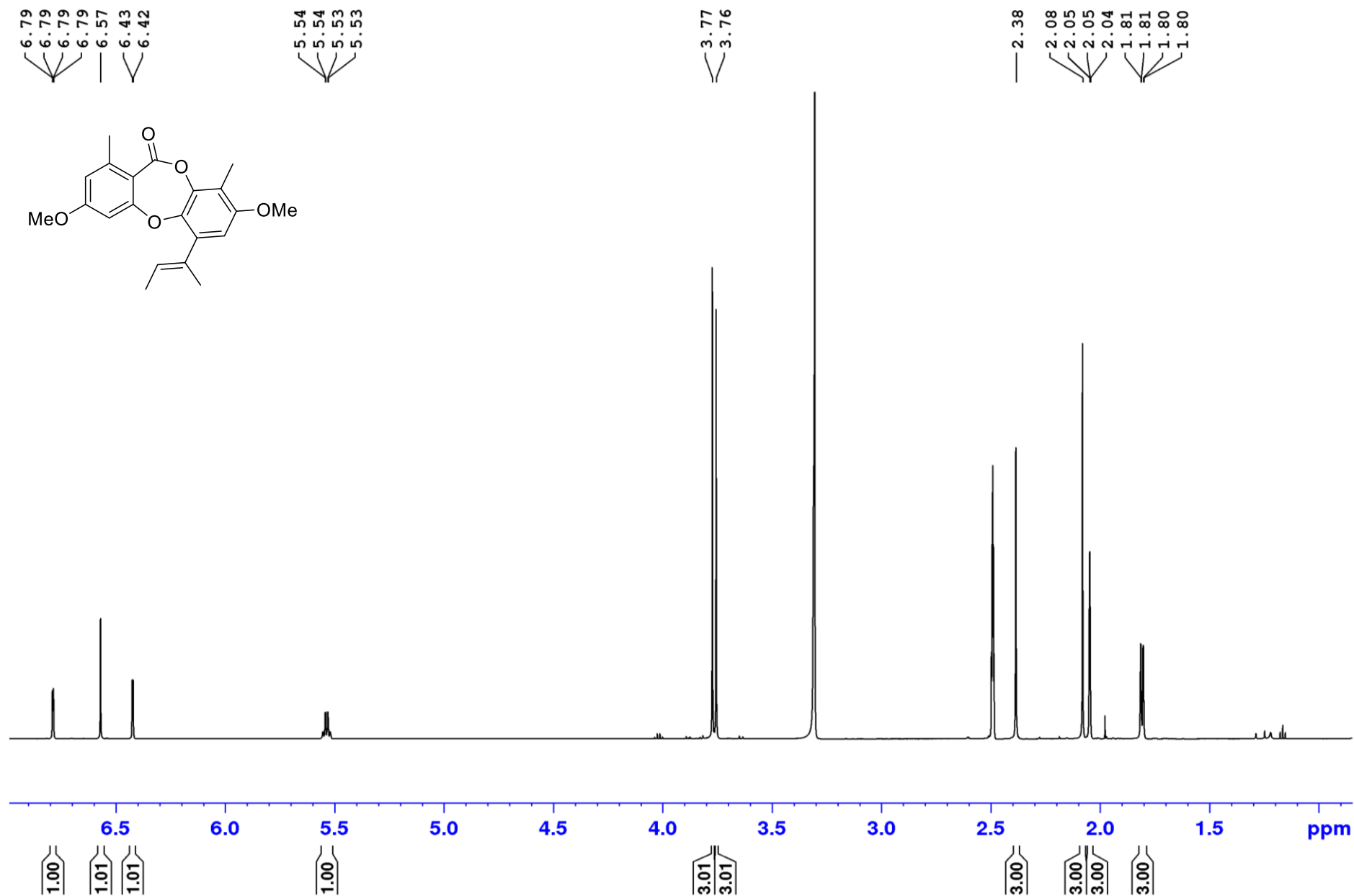


Figure S25. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of 3,8-di-O-methylunguinal (5b)

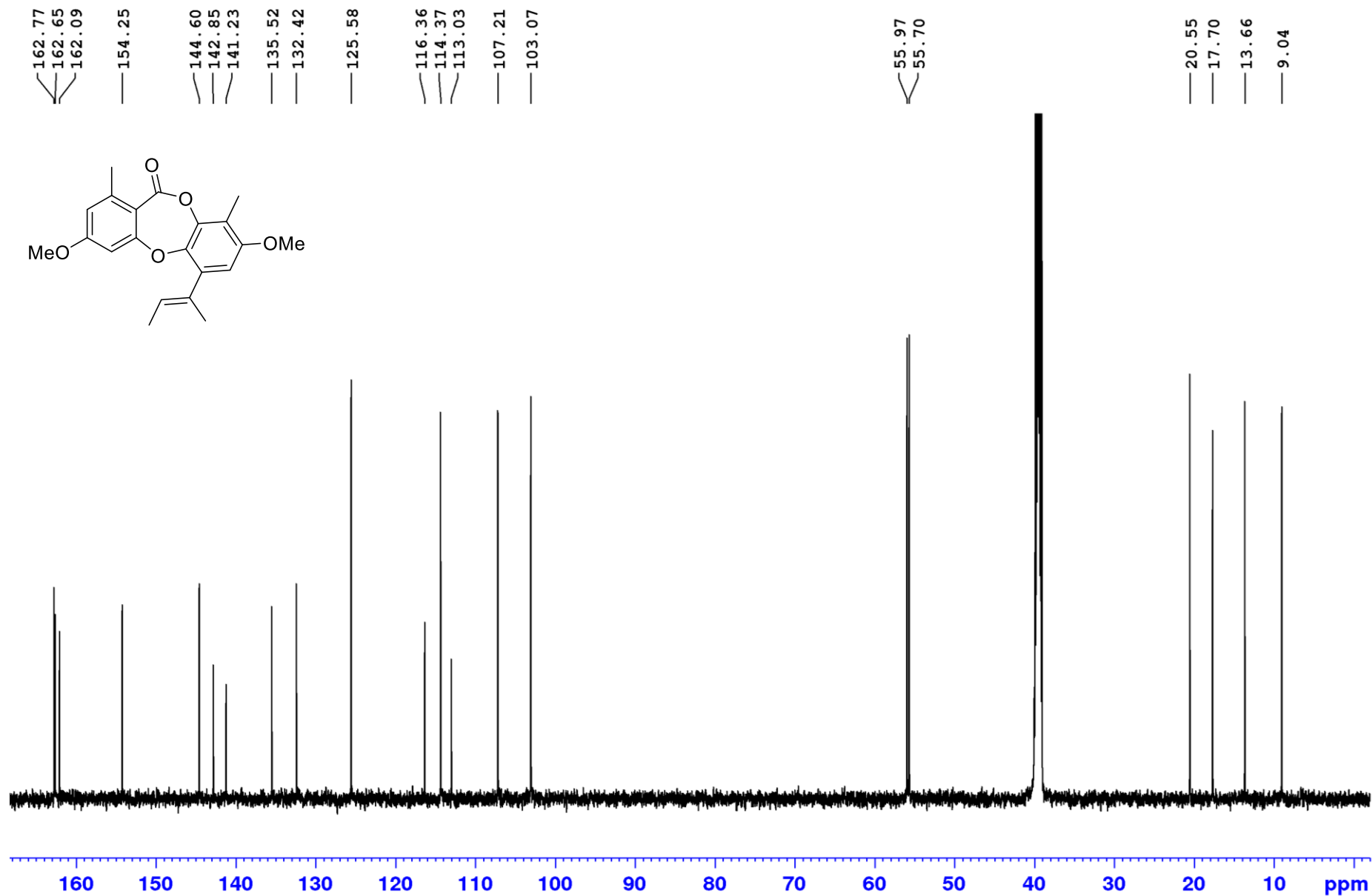


Figure S26. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) of 3,8-di-O-methylguinol (5b)

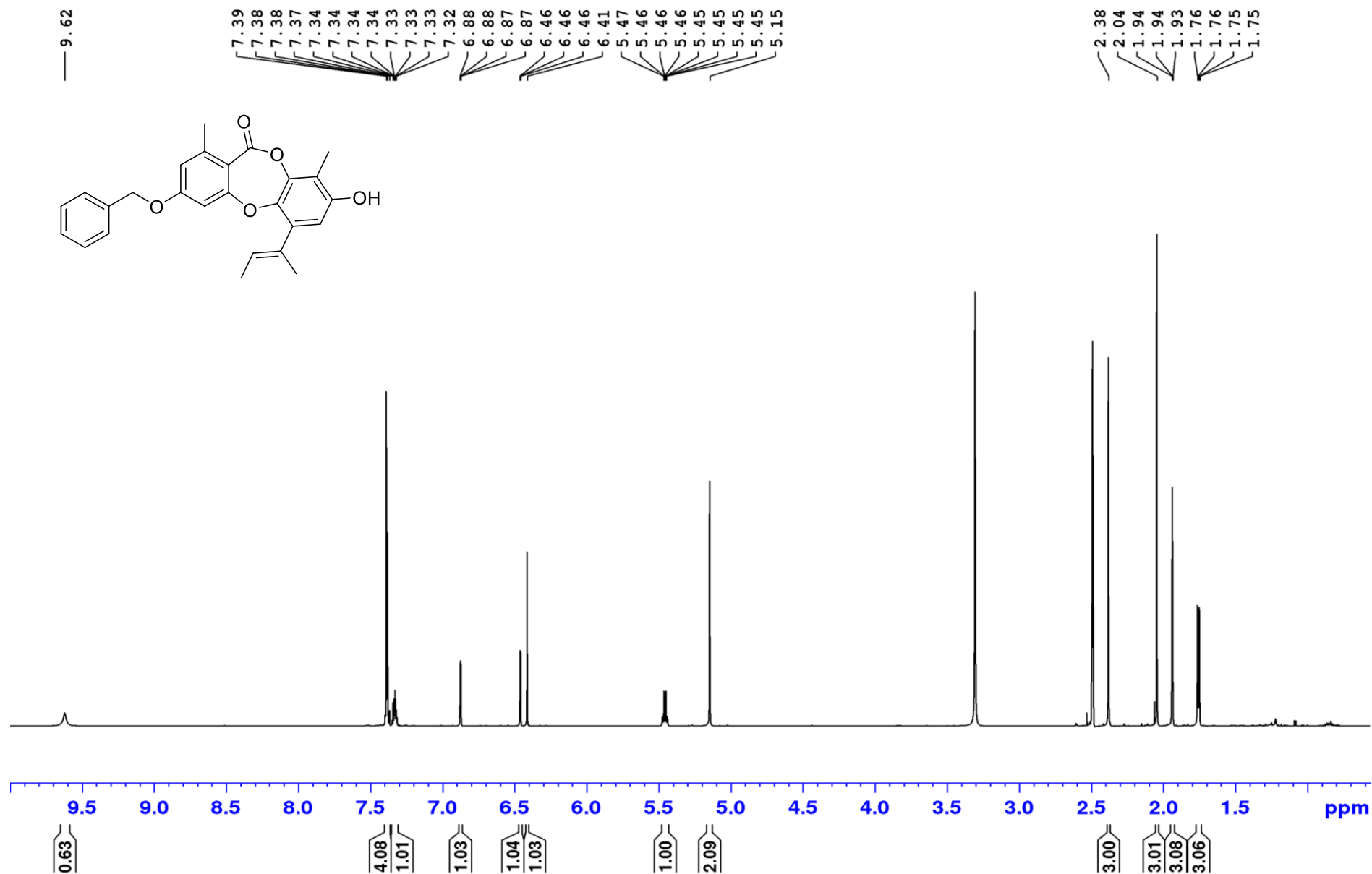


Figure S27. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of 3-O-benzylunguinol (6a)

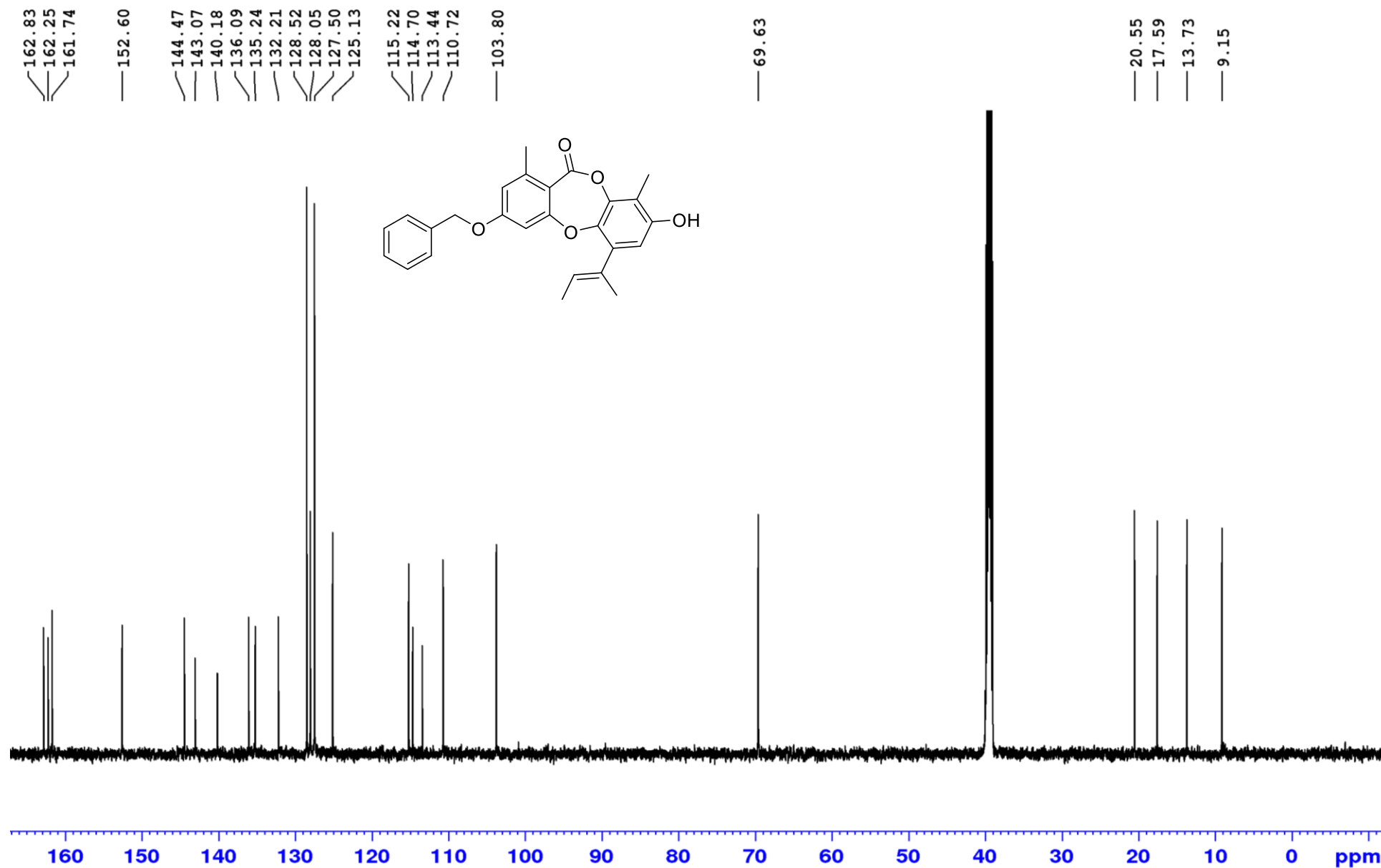


Figure S28. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) of 3-O-benzylguinol (6a)

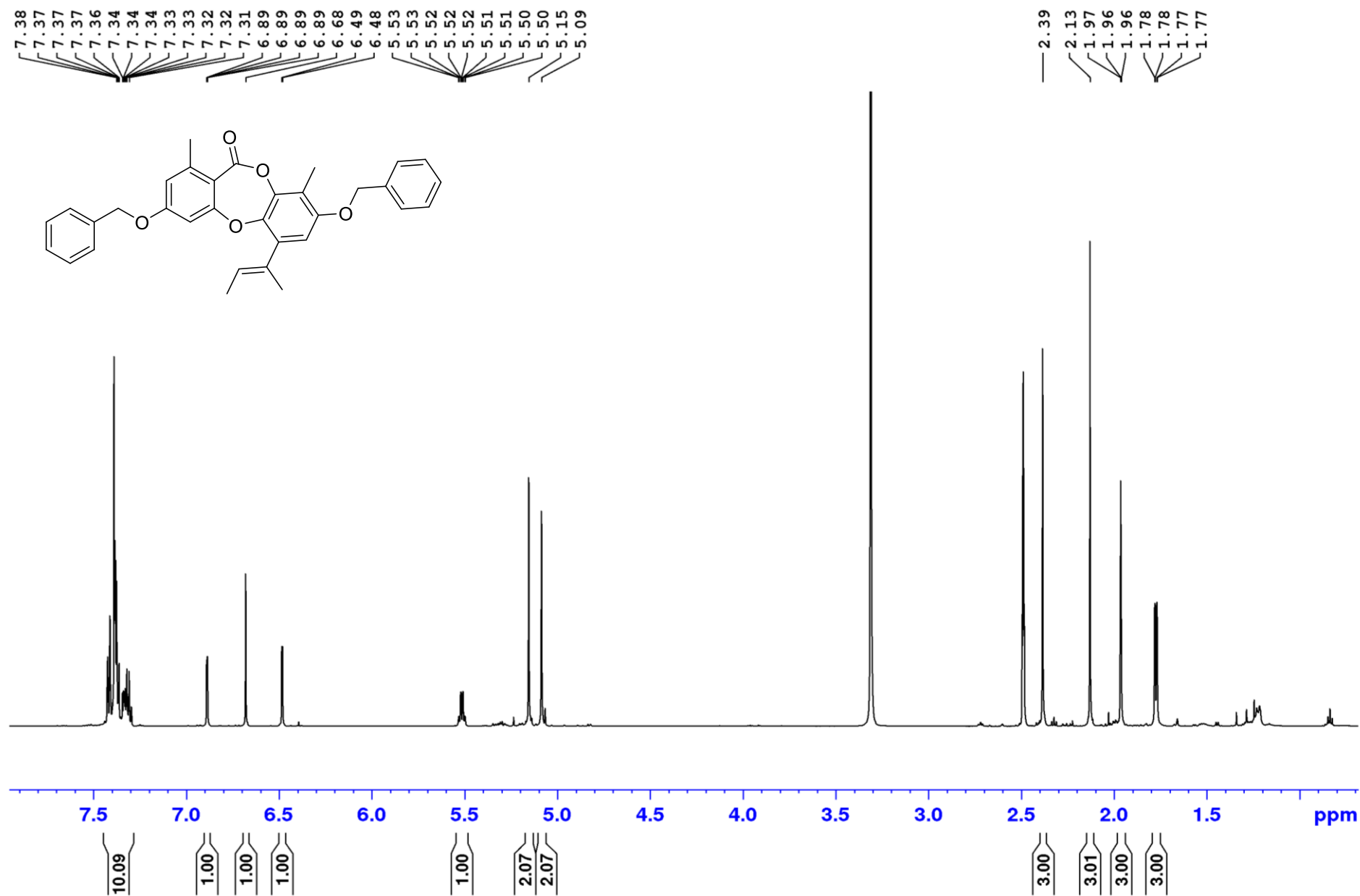


Figure S29. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of 3,8-O-dibenzylguinolinol (6b)

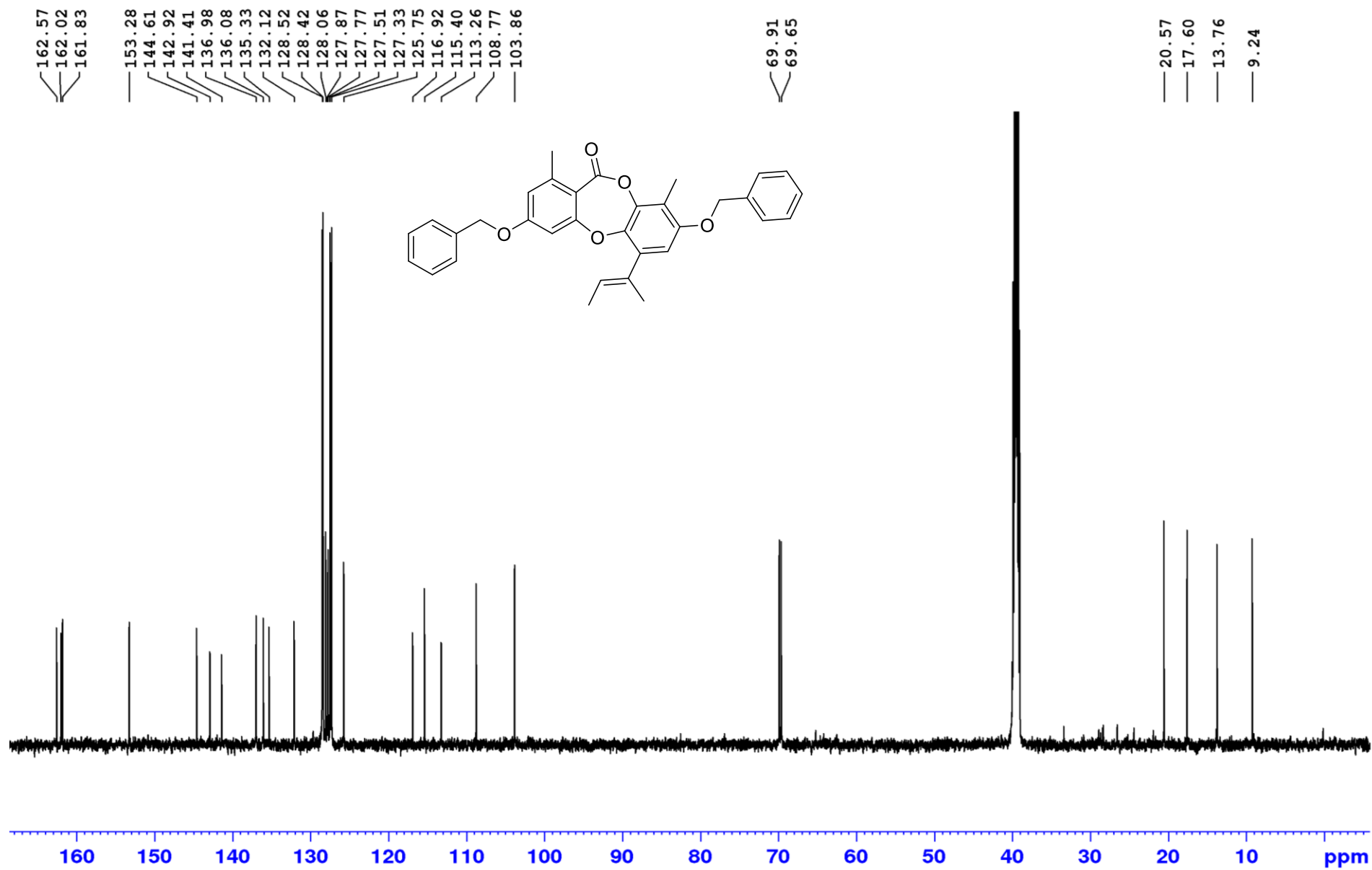


Figure S30. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) of 3,8-*O*-dibenzylguinol (6b)

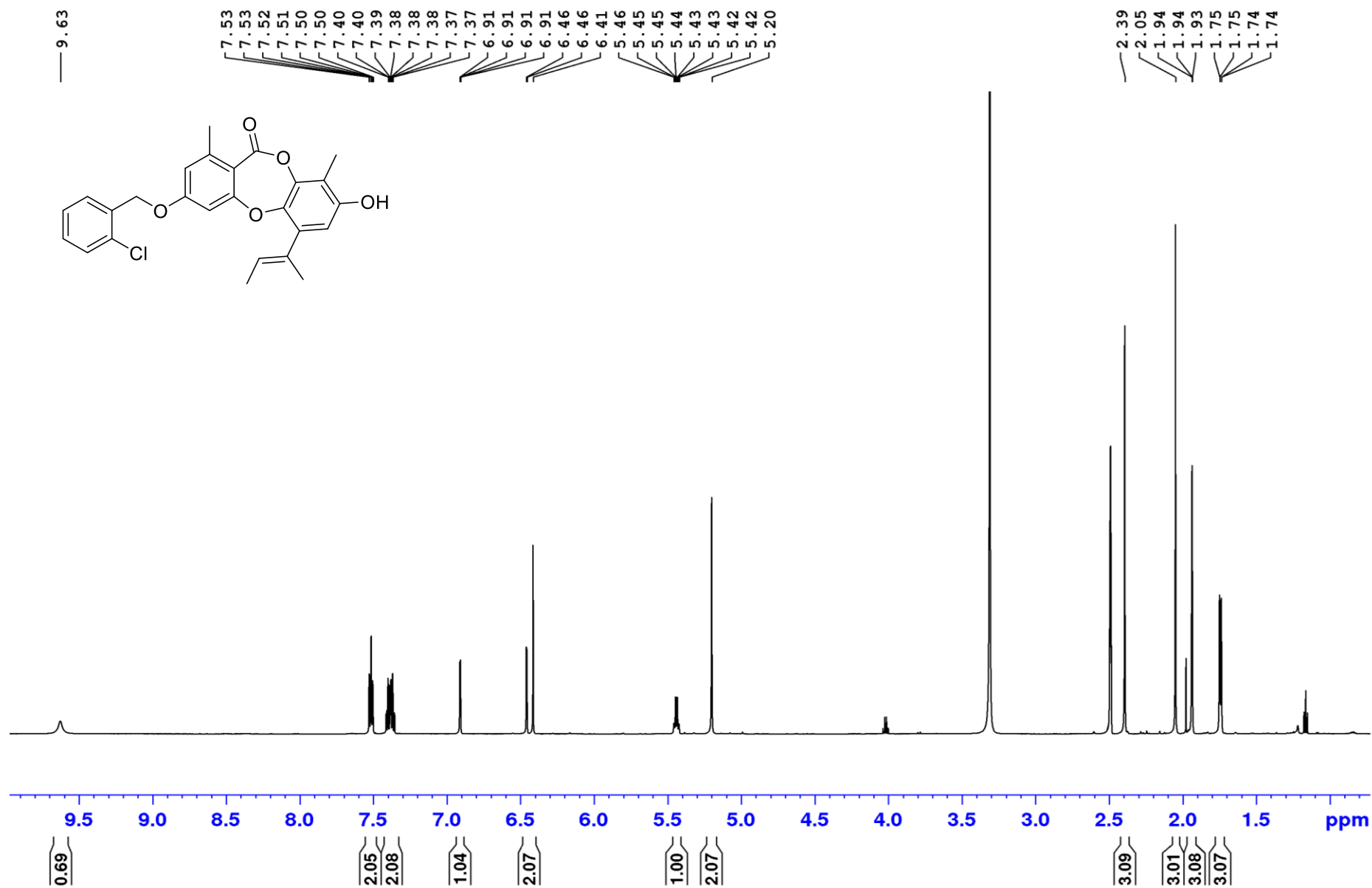


Figure S31. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of 3-O-(2-chlorobenzyl)unguinol (7a)

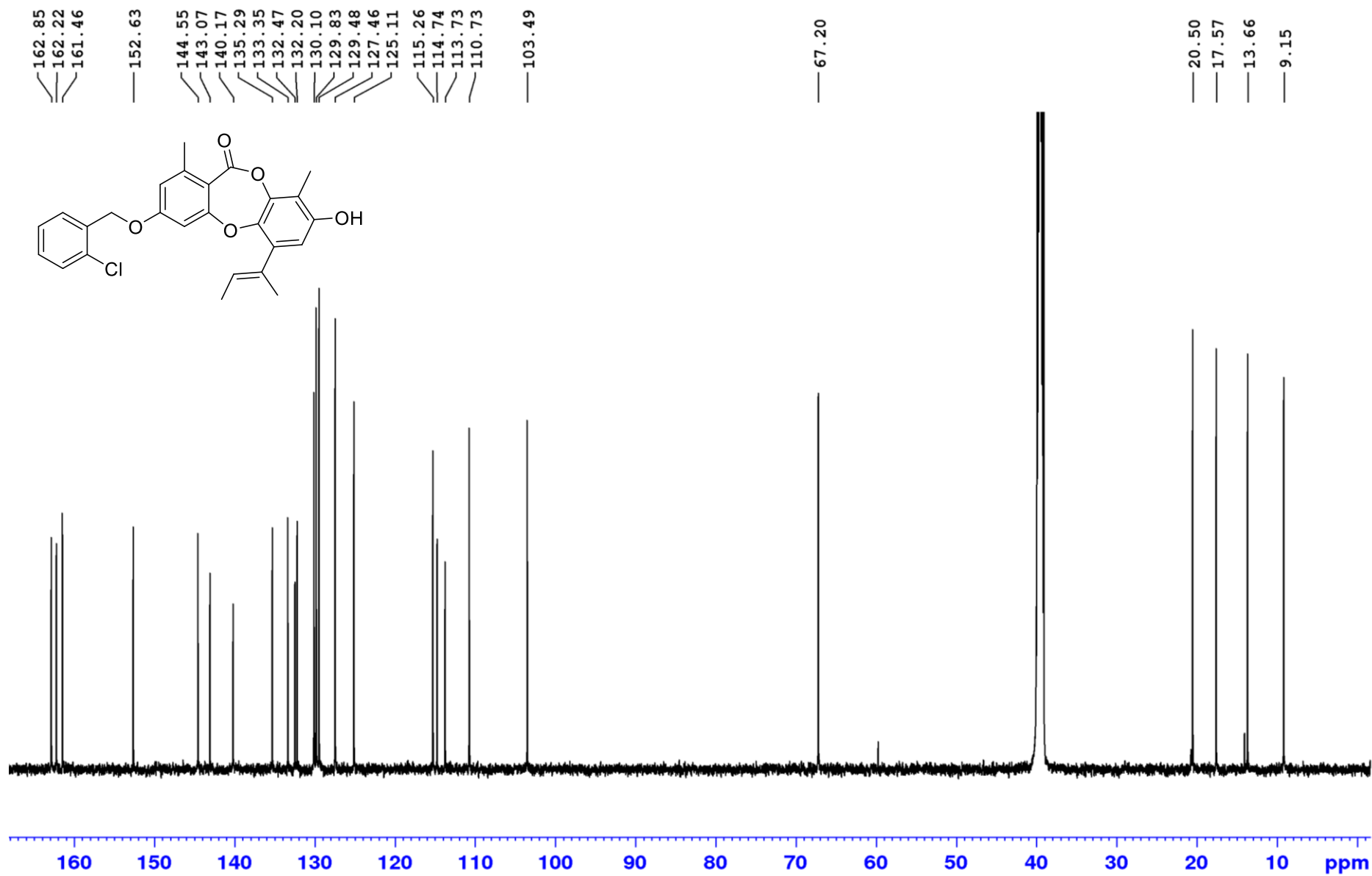


Figure S32. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) of 3-O-(2-chlorobenzyl)unguinol (7a)

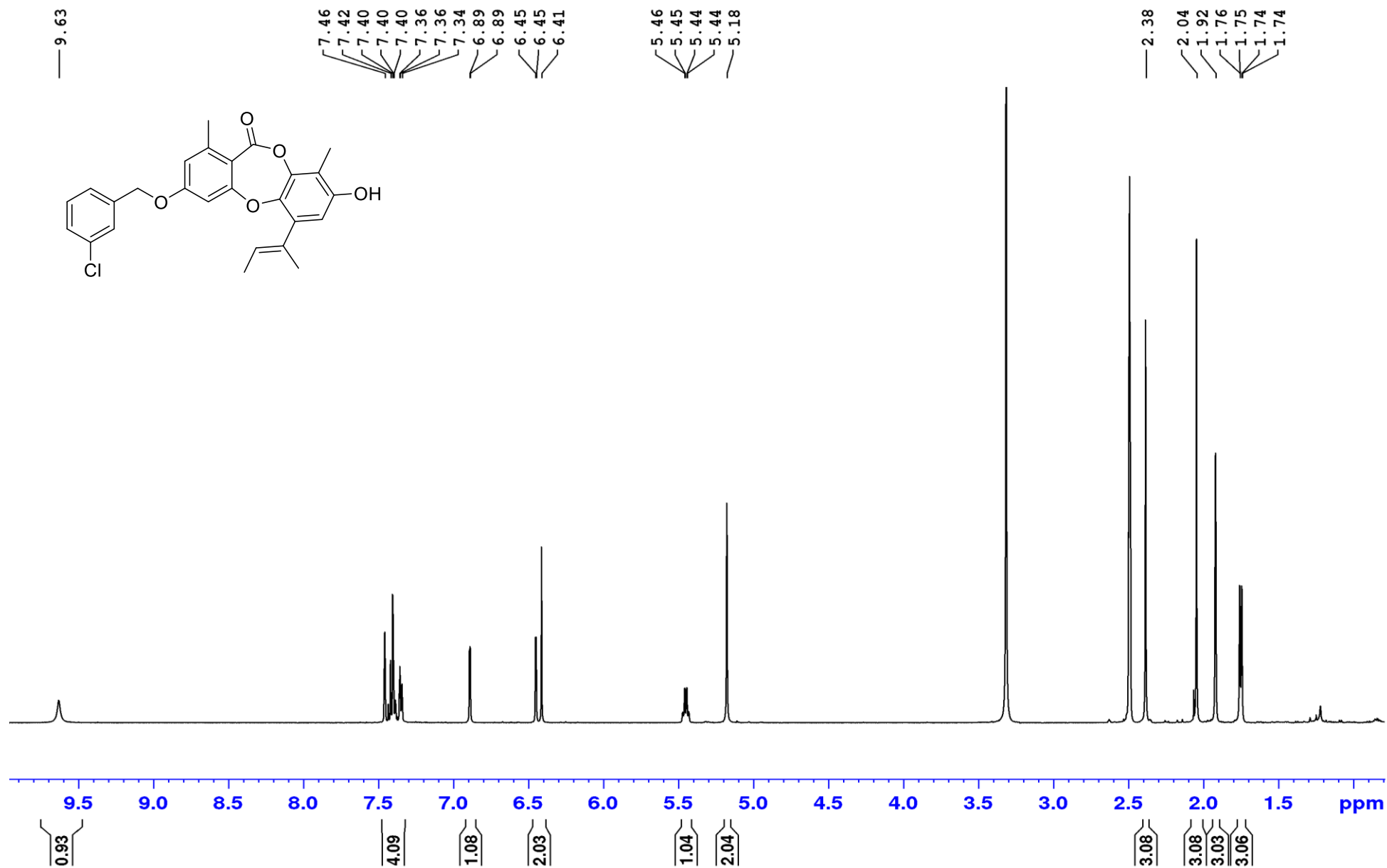


Figure S33. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of 3-O-(3-chlorobenzyl)unguinol (7b)

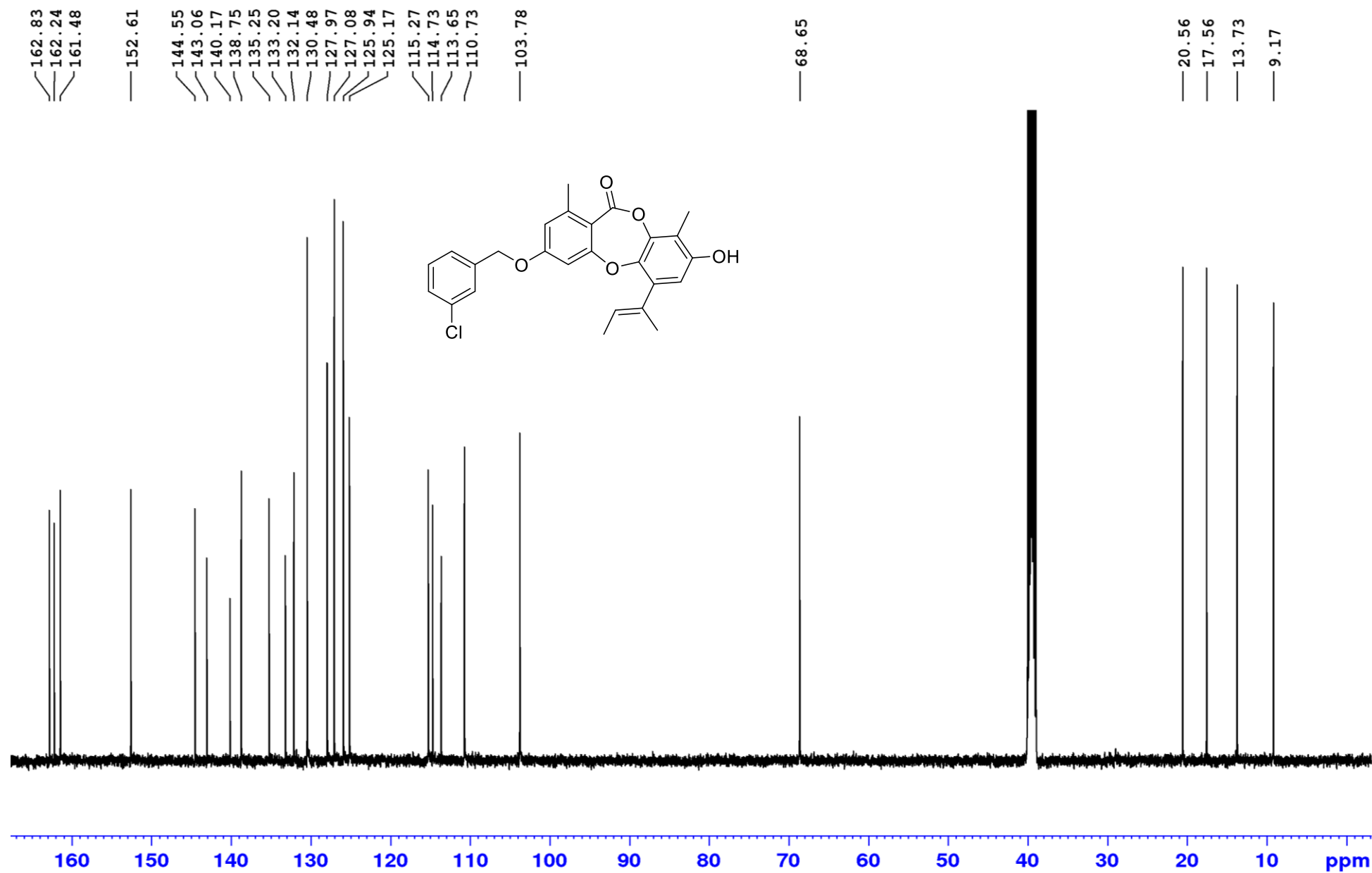


Figure S34. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) of 3-O-(3-chlorobenzyl)unguinol (7b)

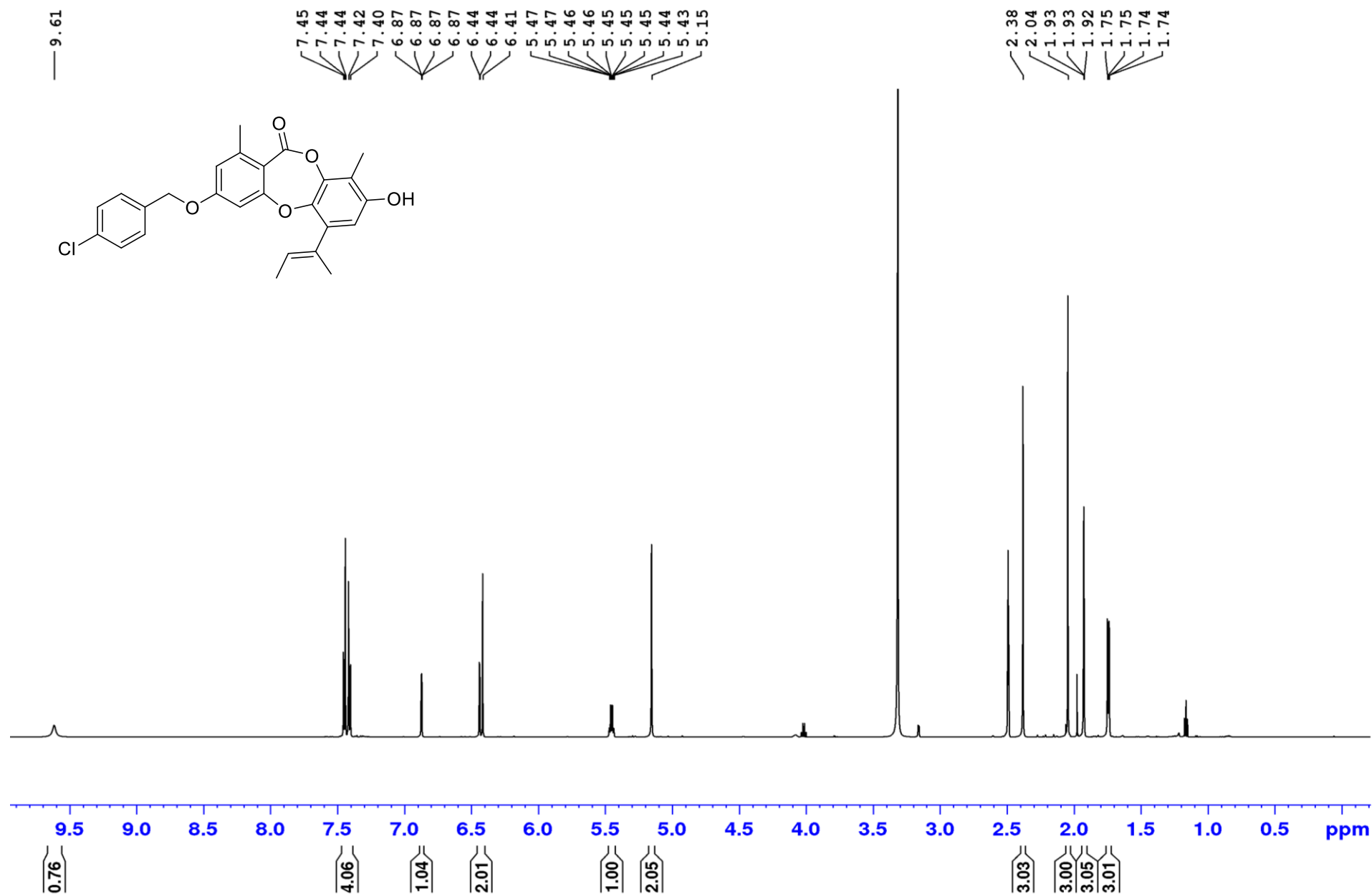


Figure S35. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of 3-O-(4-chlorobenzyl)unguinol (7c)

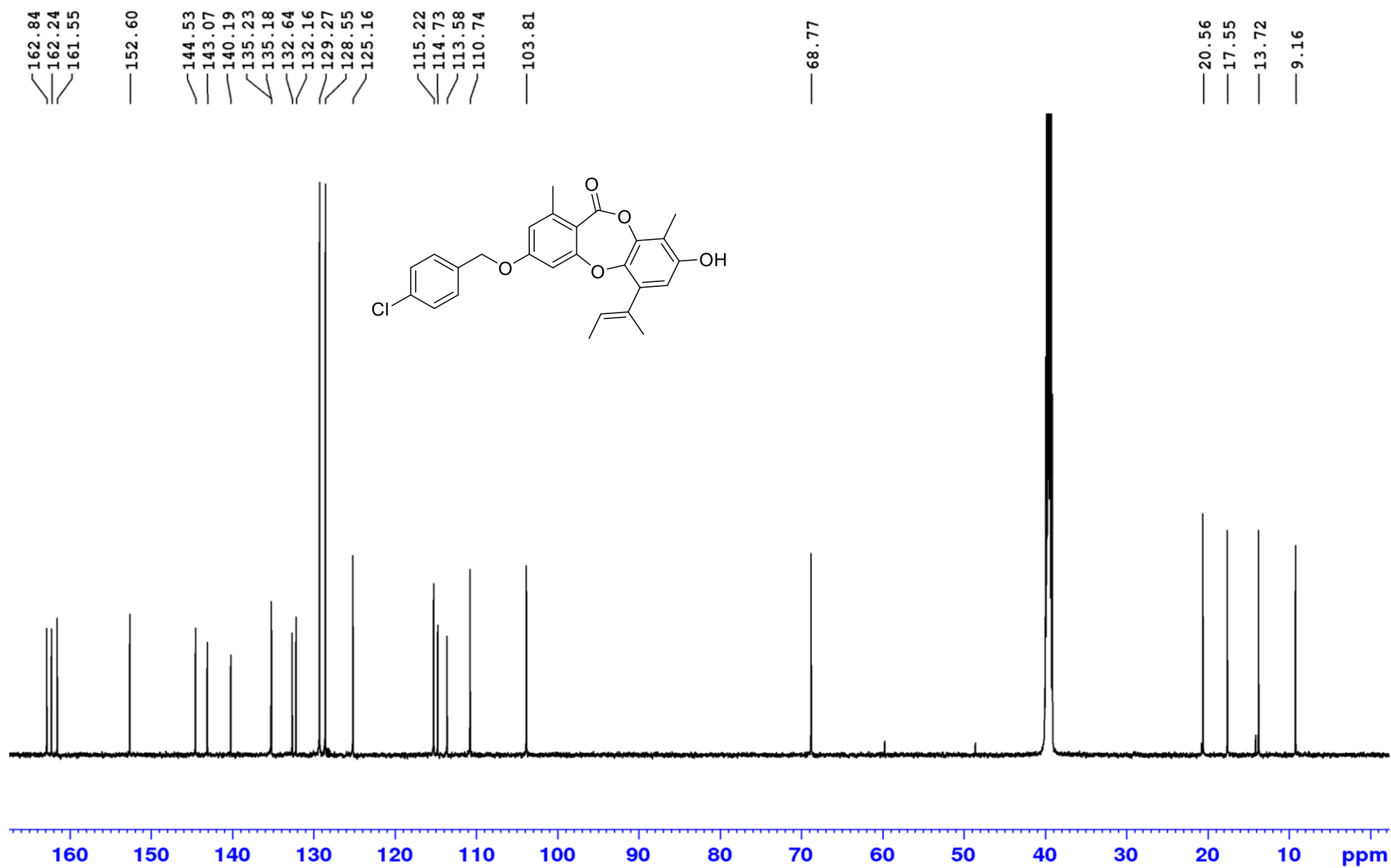


Figure S36. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) of 3-O-(4-chlorobenzyl)unguinol (7c)

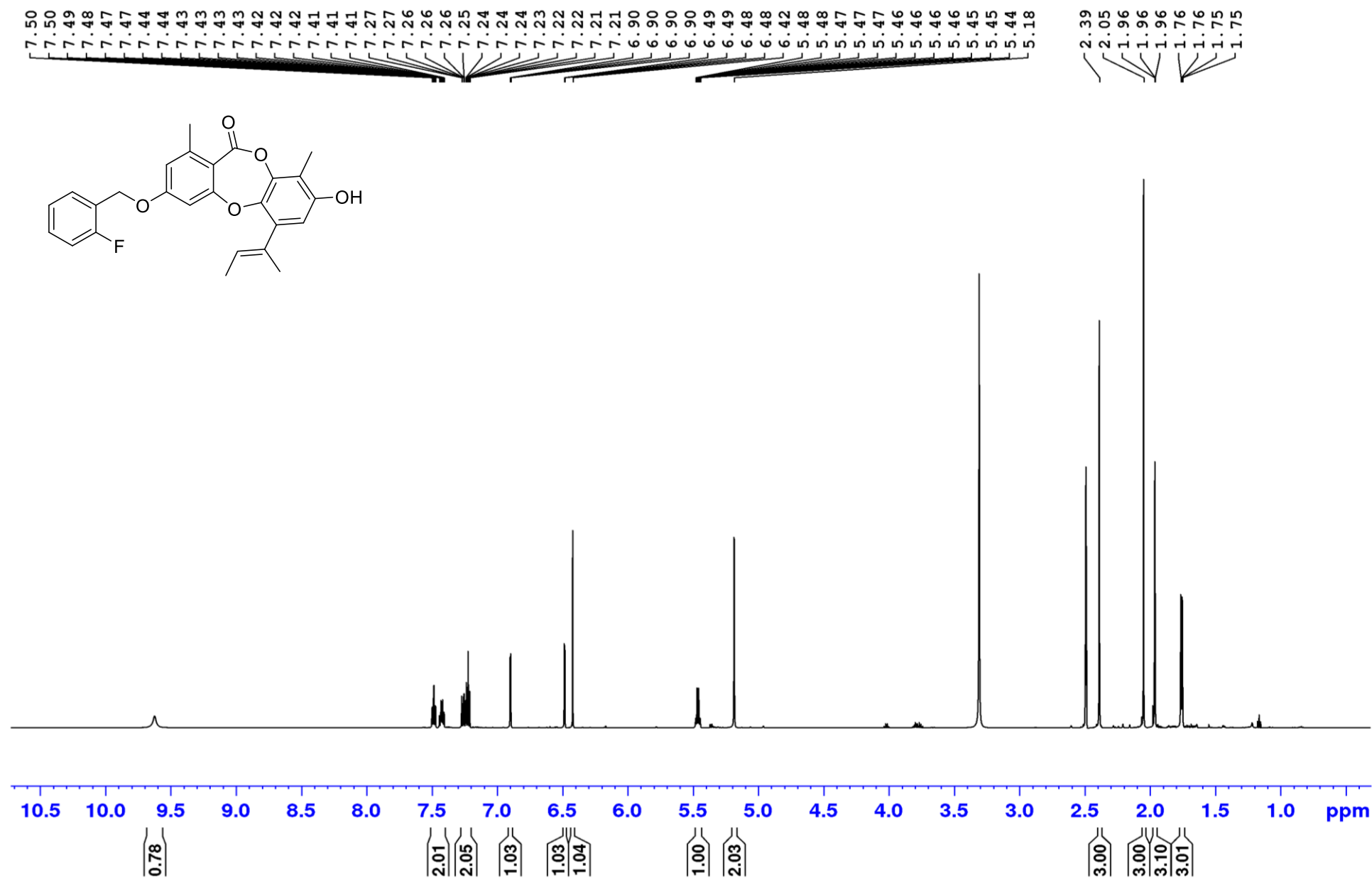


Figure S37. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of 3-O-(2-fluorobenzyl)unguinol (7d)

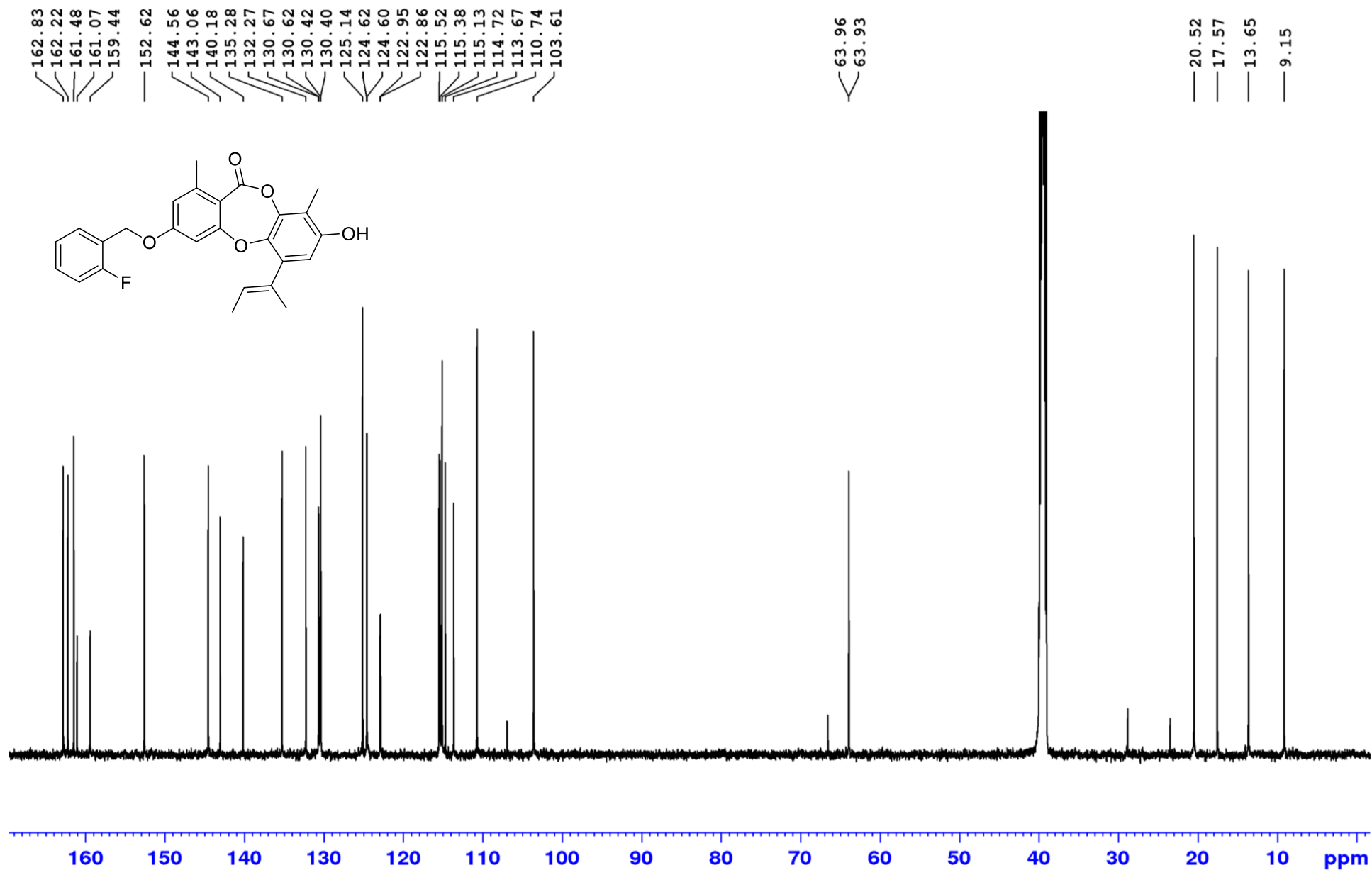


Figure S38. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) of 3-*O*-(2-fluorobenzyl)unguinol (7d)

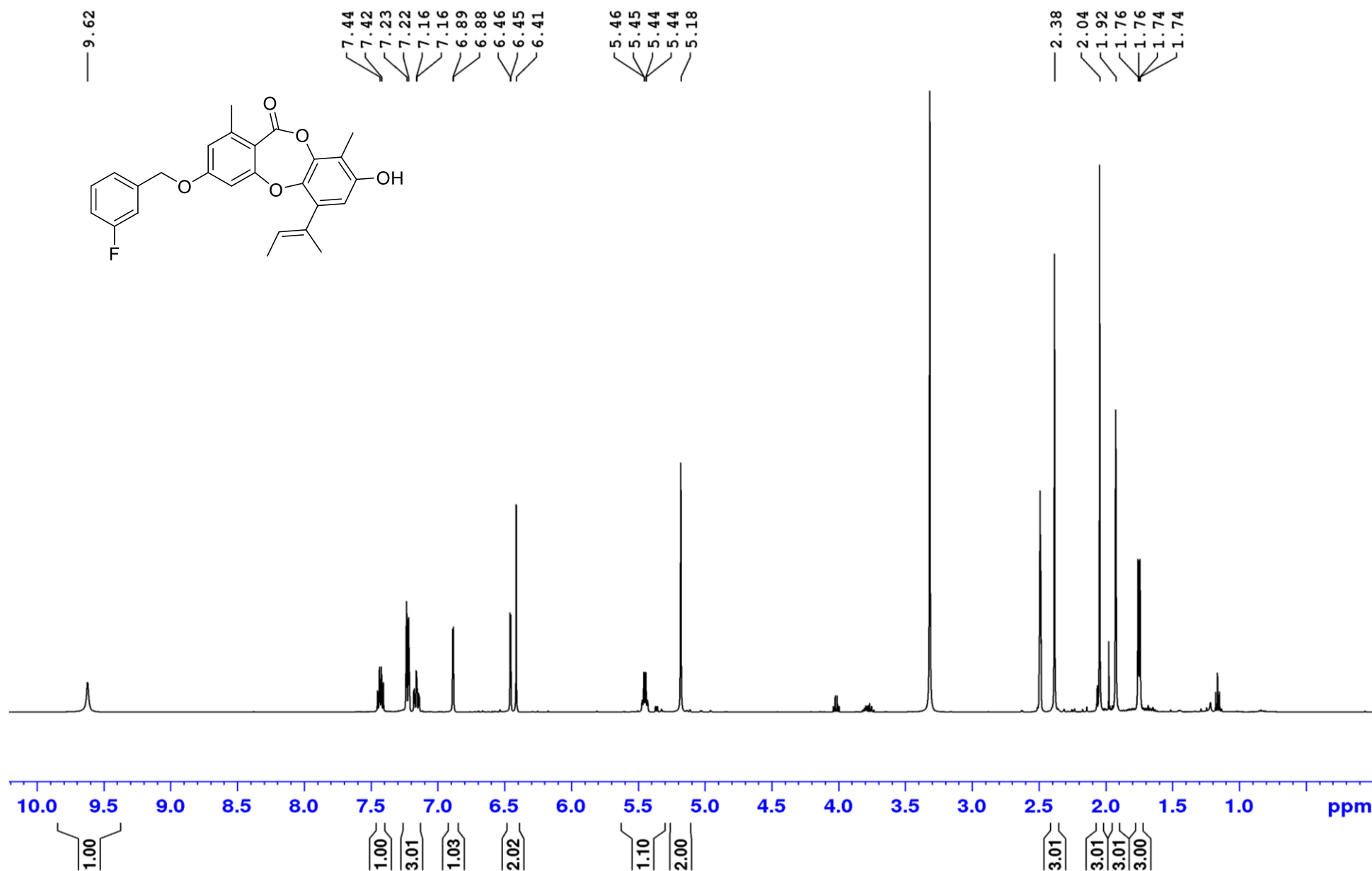


Figure S39. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of 3-O-(3-fluorobenzyl)unguinol (7e)

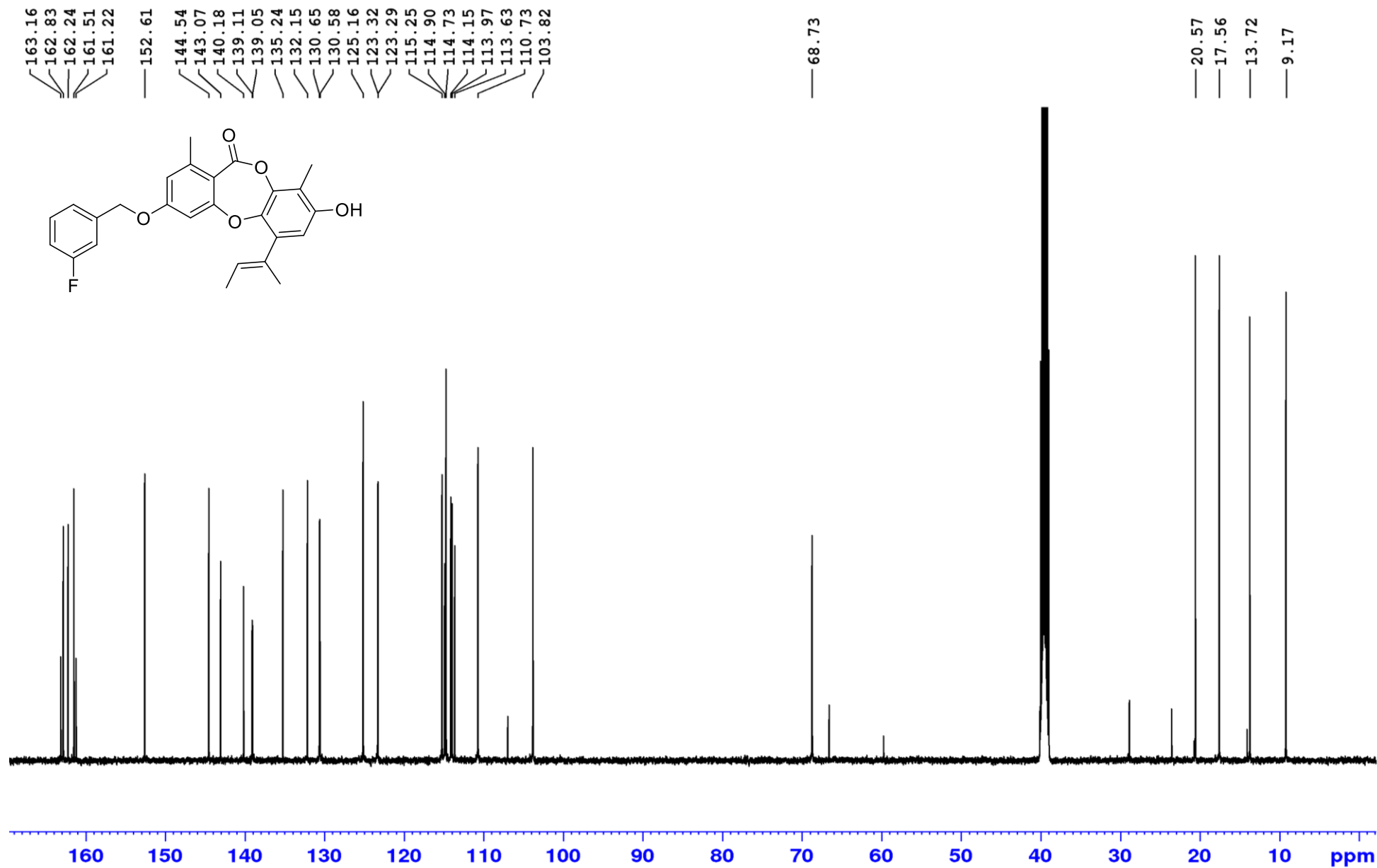


Figure S40. ^{13}C NMR spectrum (150 MHz, $\text{DMSO}-d_6$) of 3-O-(3-fluorobenzyl)unguinol (7e)

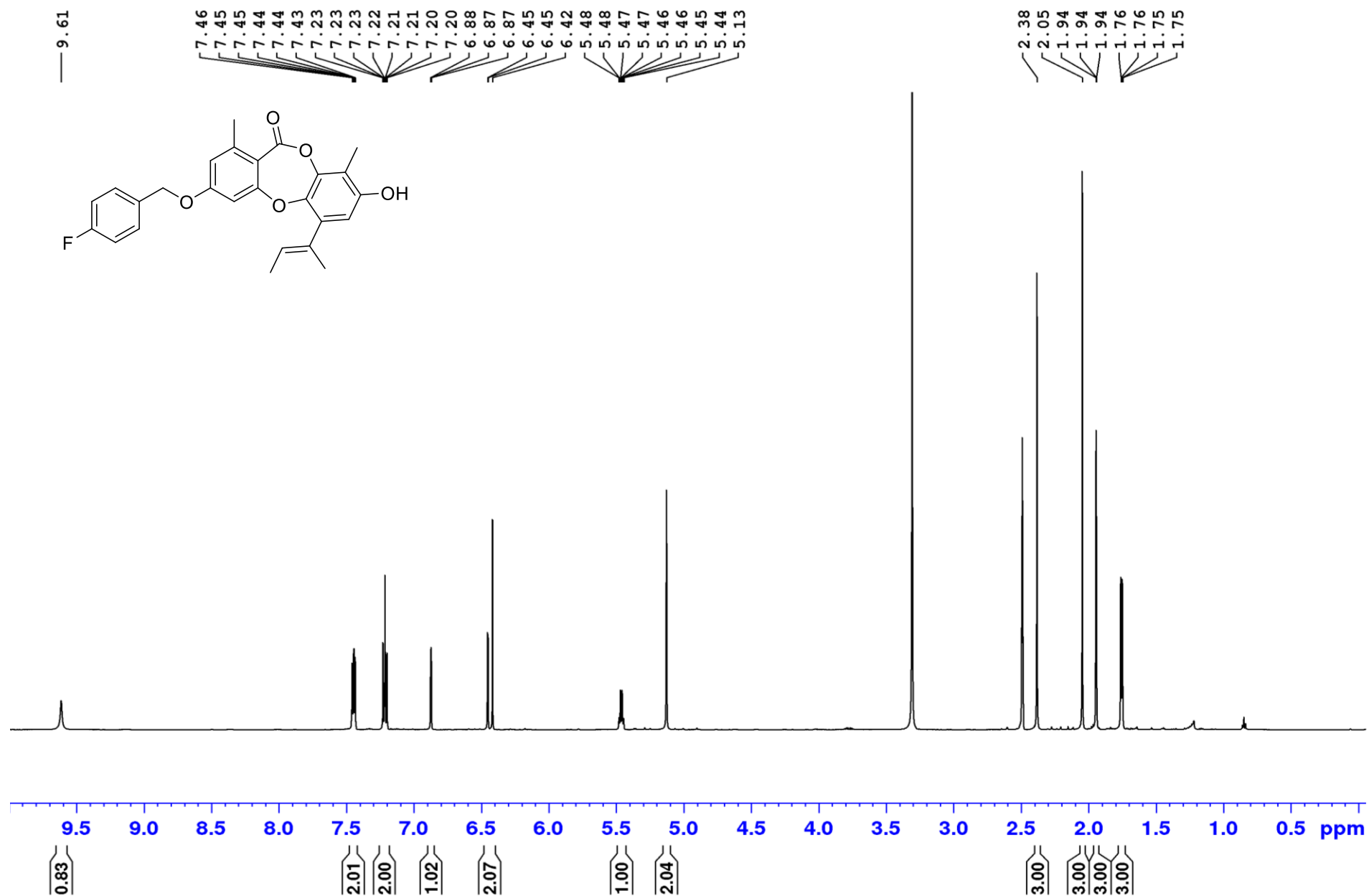


Figure S41. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of 3-O-(4-fluorobenzyl)unguinol (7f)

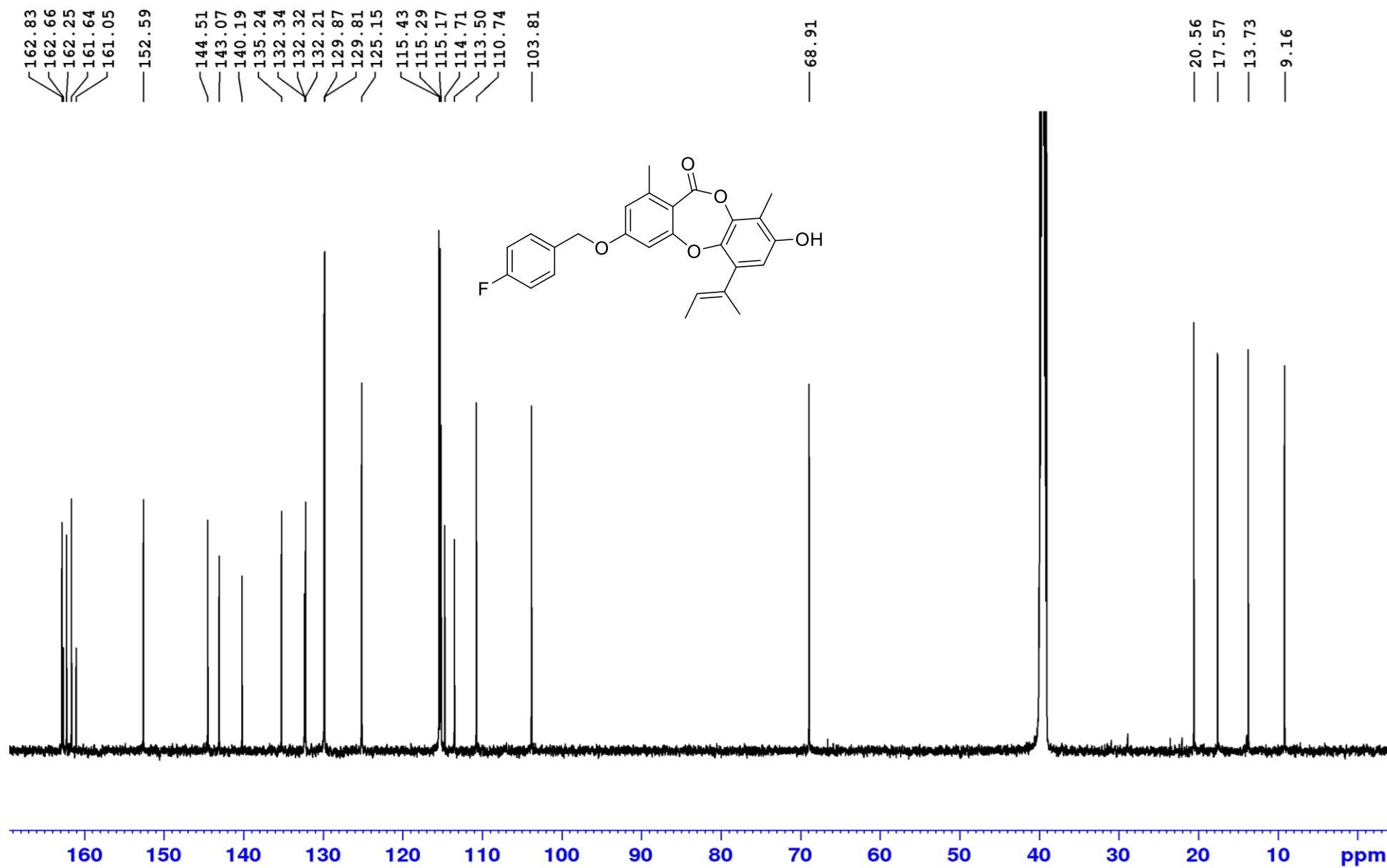


Figure S42. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) of 3-O-(4-fluorobenzyl)unguinol (7f)

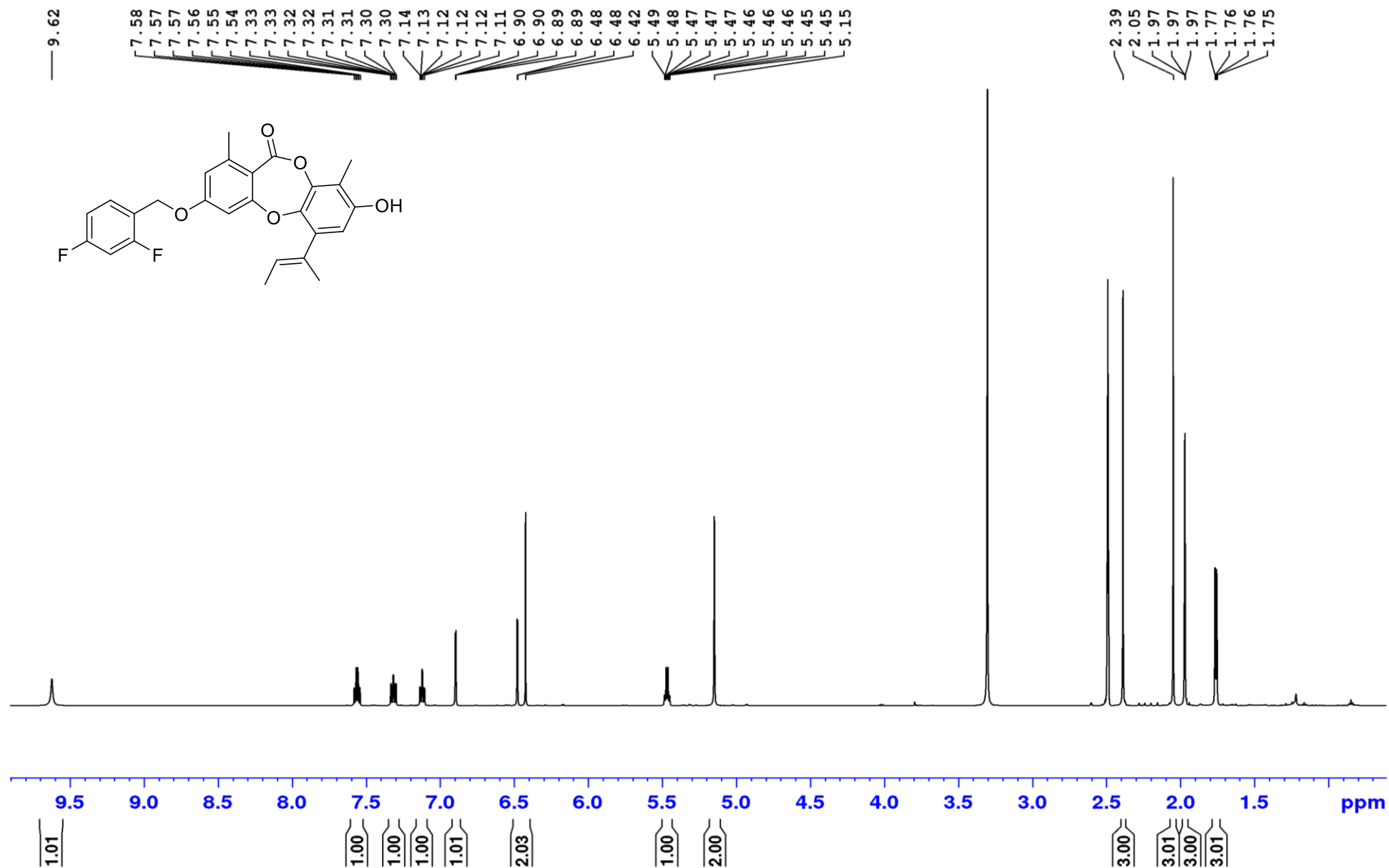


Figure S43. ¹H NMR spectrum (600 MHz, DMSO-d₆) of 3-O-(2,4-difluorobenzyl)unguinol (7g)

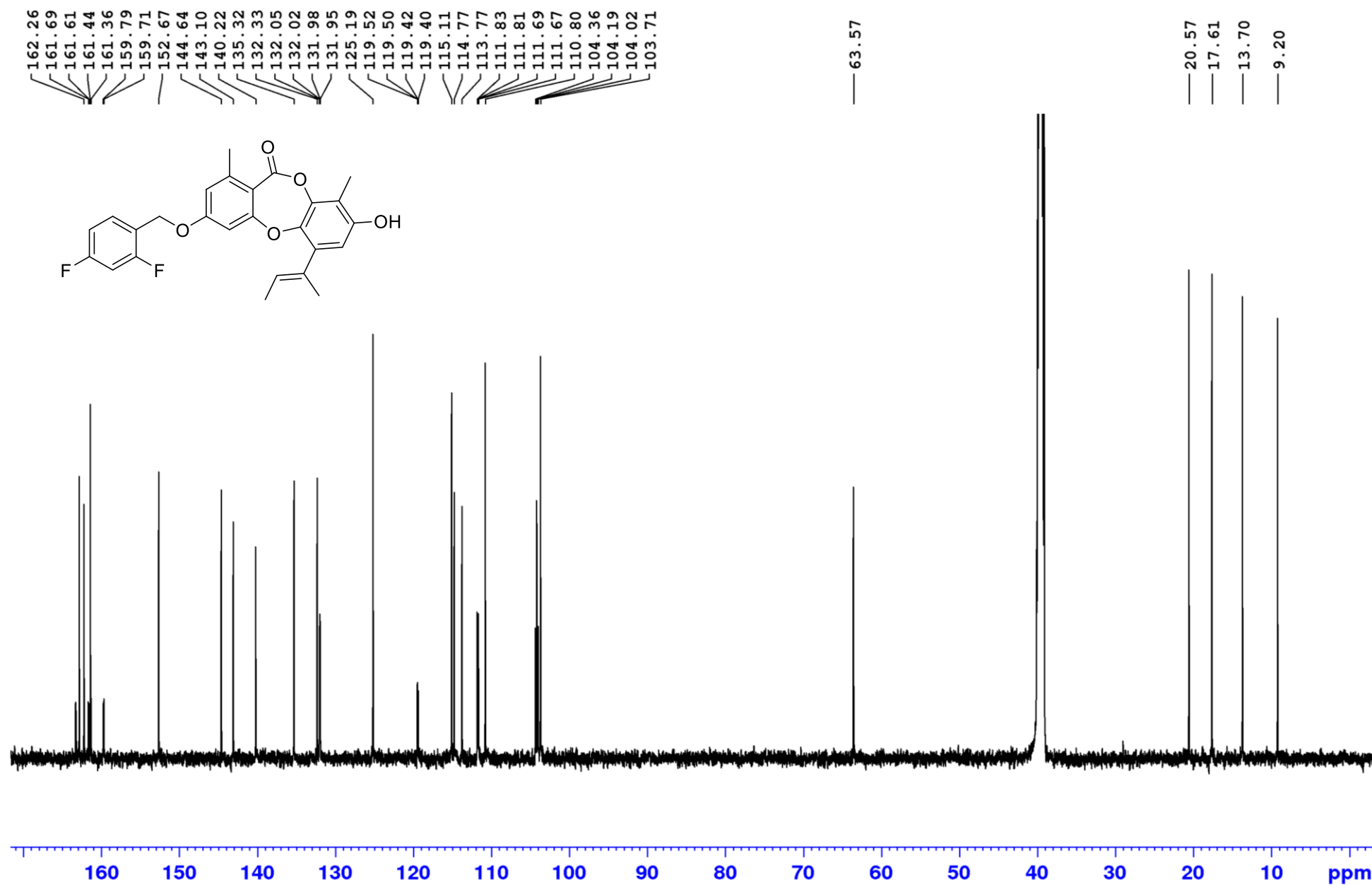


Figure S44. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) of 3-O-(2,4-difluorobenzyl)unguinol (7g)

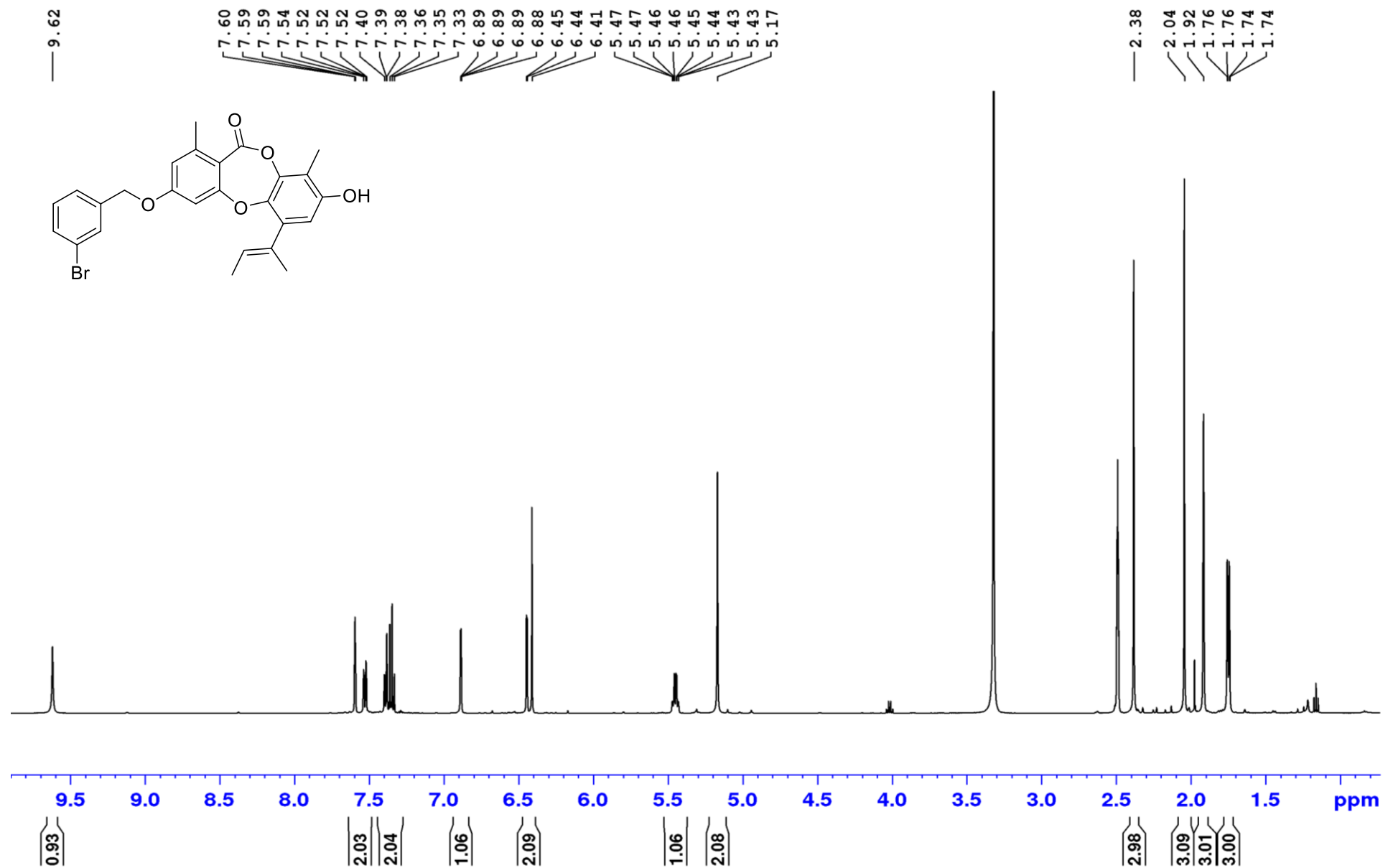


Figure S45. ¹H NMR spectrum (500 MHz, DMSO-*d*₆) of 3-O-(3-bromobenzyl)unguinol (7h)

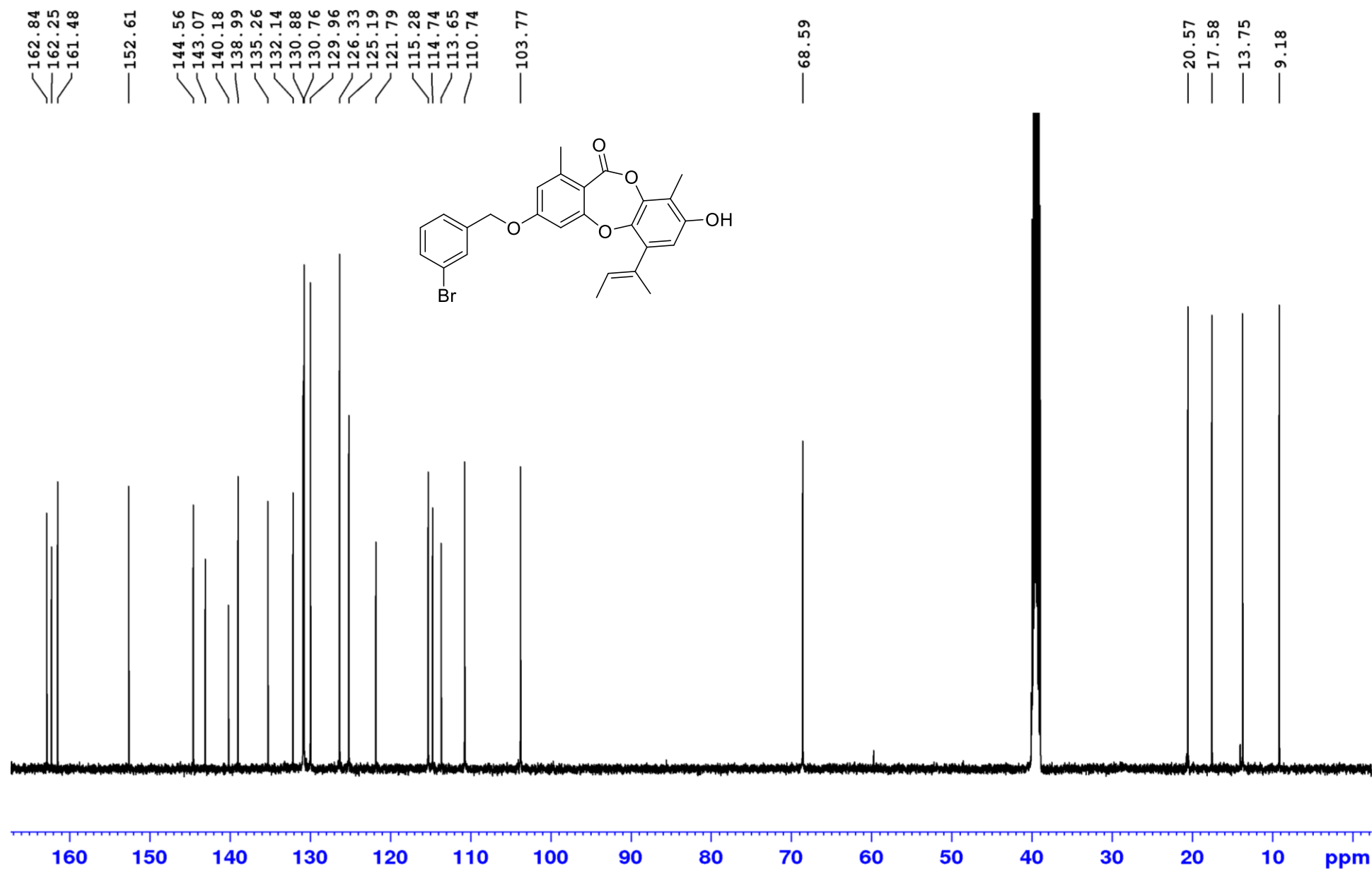


Figure S46. ¹³C NMR spectrum (125 MHz, DMSO-*d*₆) of 3-*O*-(3-bromobenzyl)unguinol (7h)

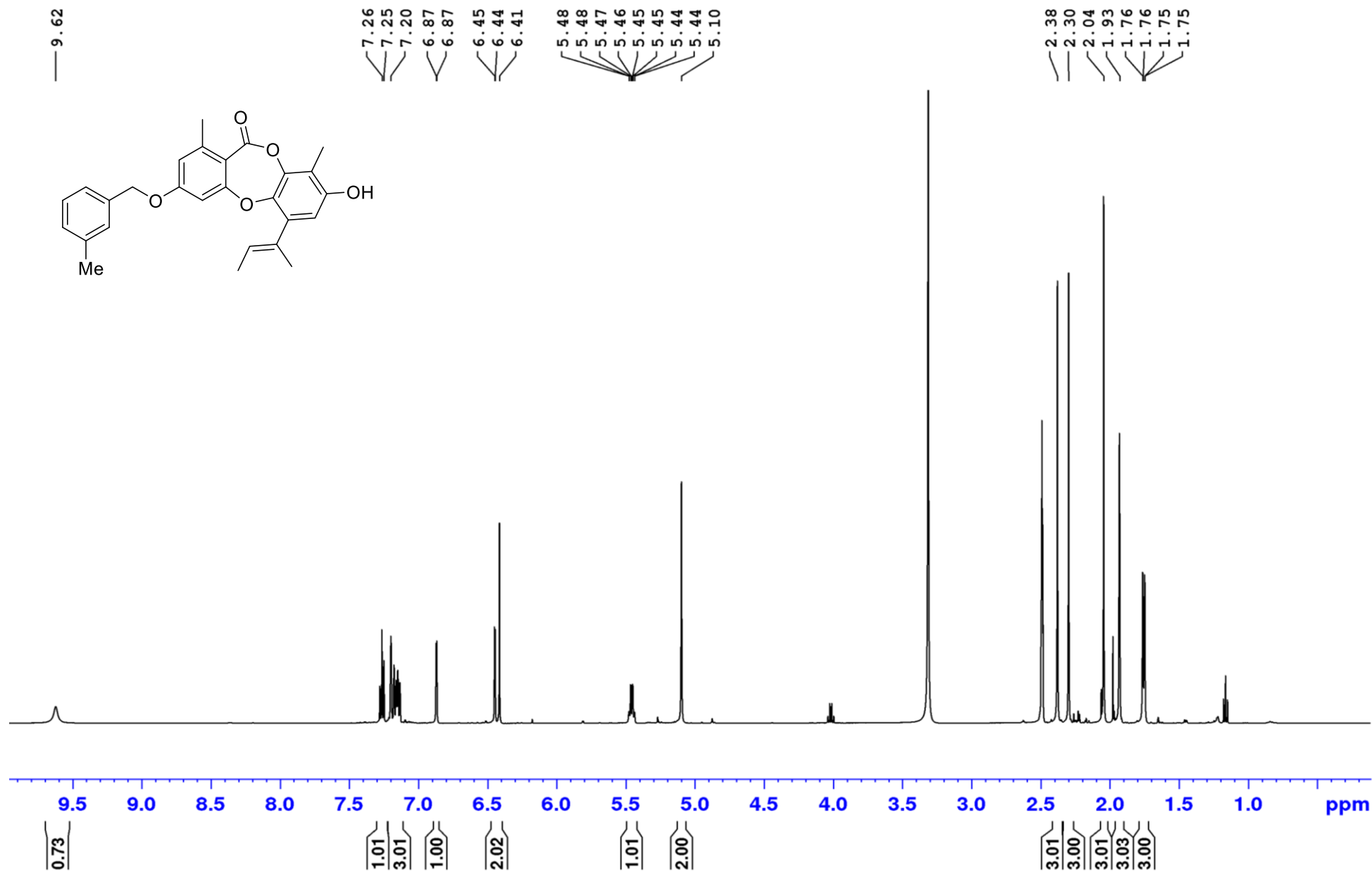


Figure S47. ¹H NMR spectrum (500 MHz, DMSO-*d*₆) of 3-O-(3-methylbenzyl)unguinol (7i)

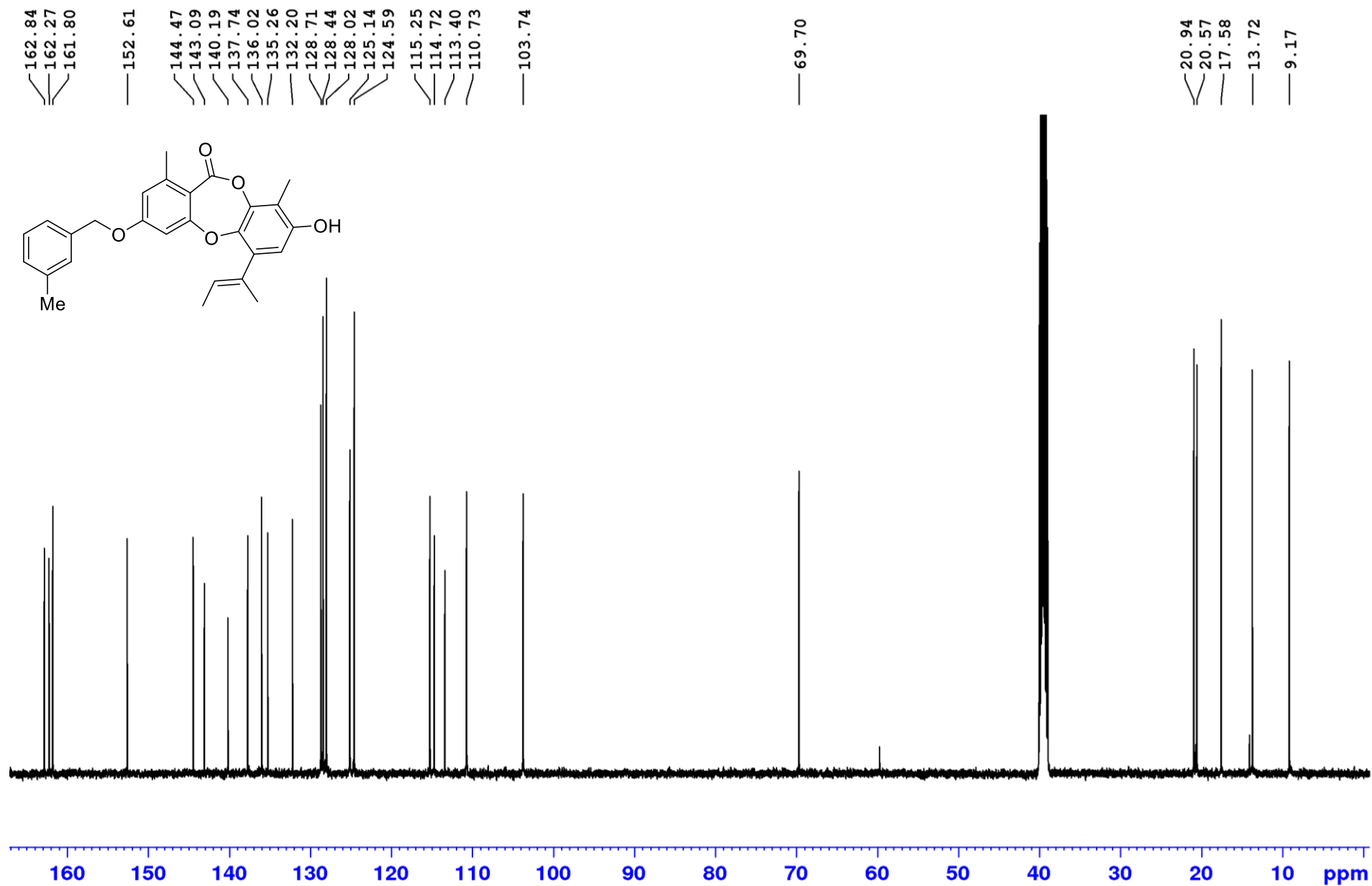


Figure S48. ¹³C NMR spectrum (125 MHz, DMSO-*d*₆) of 3-O-(3-methylbenzyl)unguinol (**7i**)

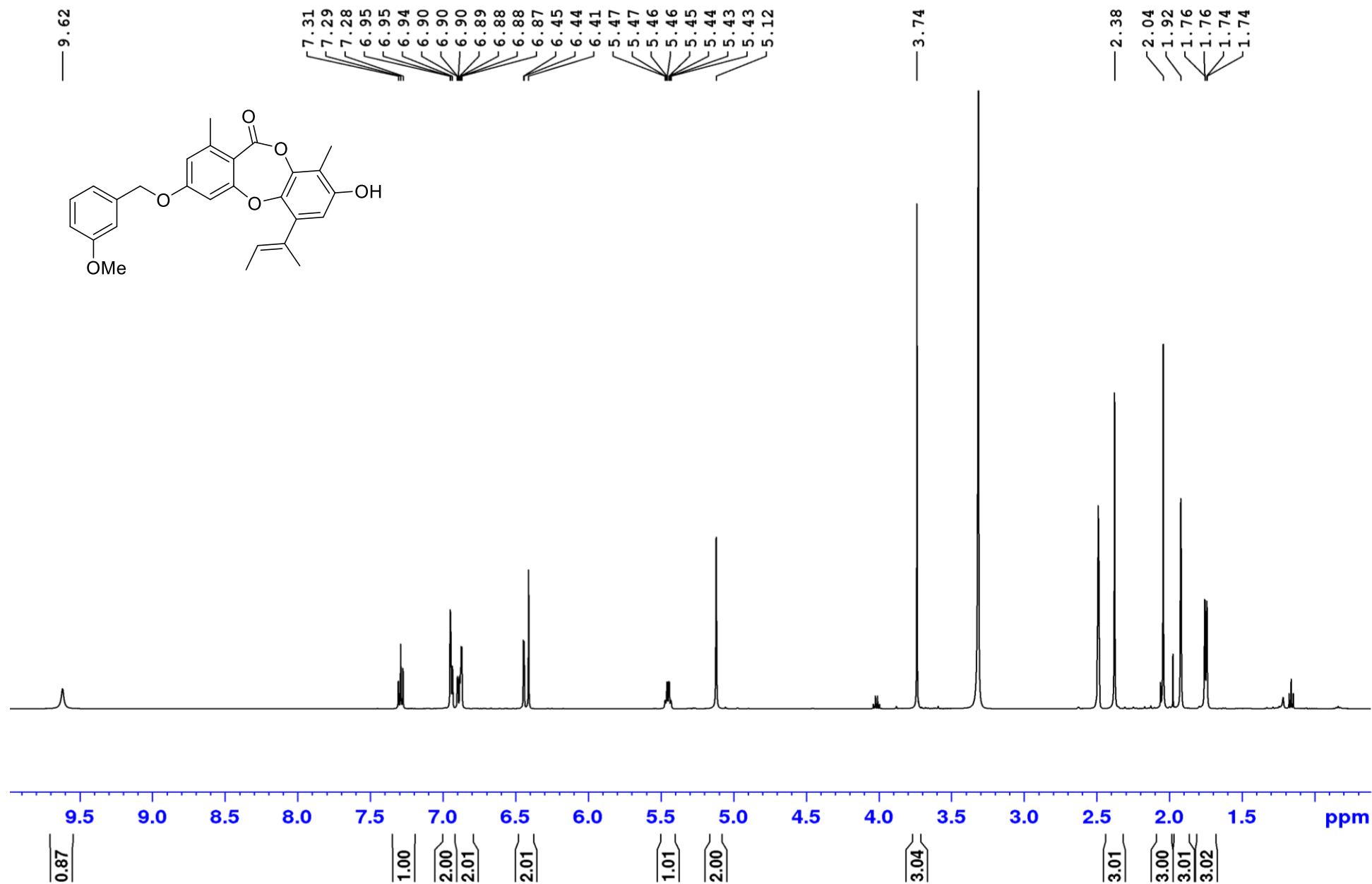


Figure S49. ¹H NMR spectrum (500 MHz, DMSO-*d*₆) of 3-O-(3-methoxybenzyl)unguinol (7j)

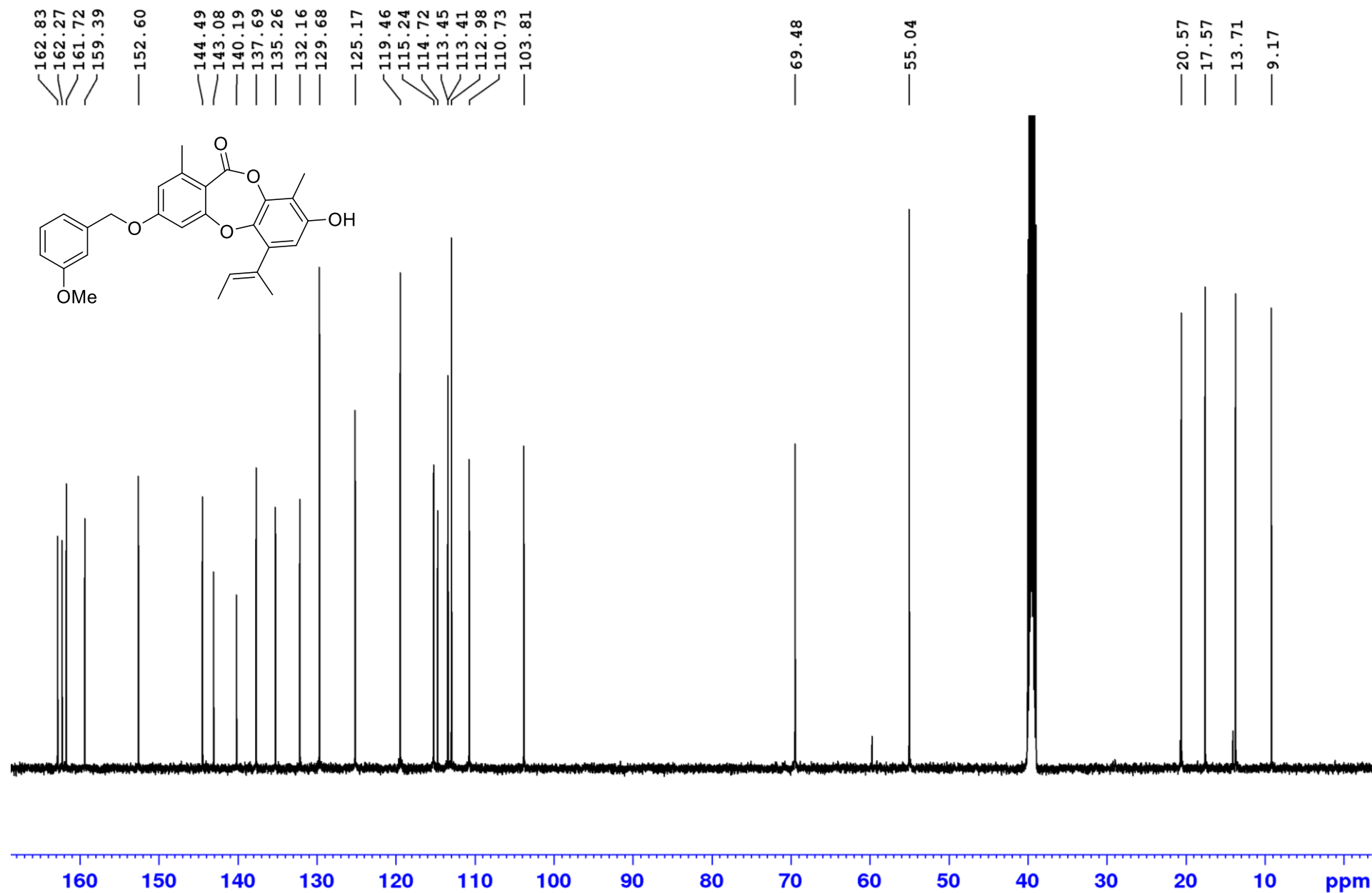


Figure S50. ¹³C NMR spectrum (125 MHz, DMSO-*d*₆) of 3-O-(3-methoxybenzyl)unguinol (7j)

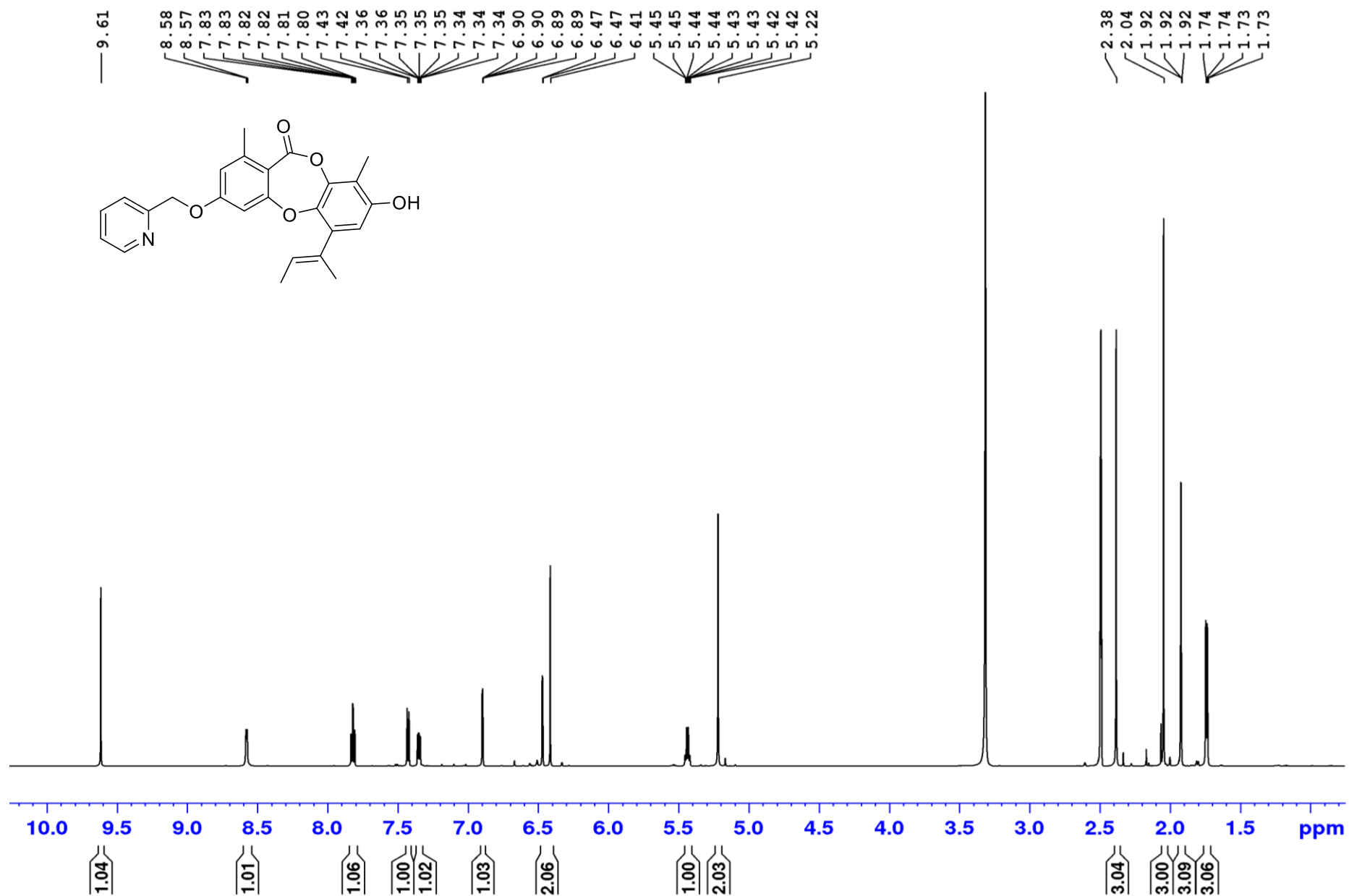


Figure S51. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of 3-O-(2-picolyl)unguinol (7k)

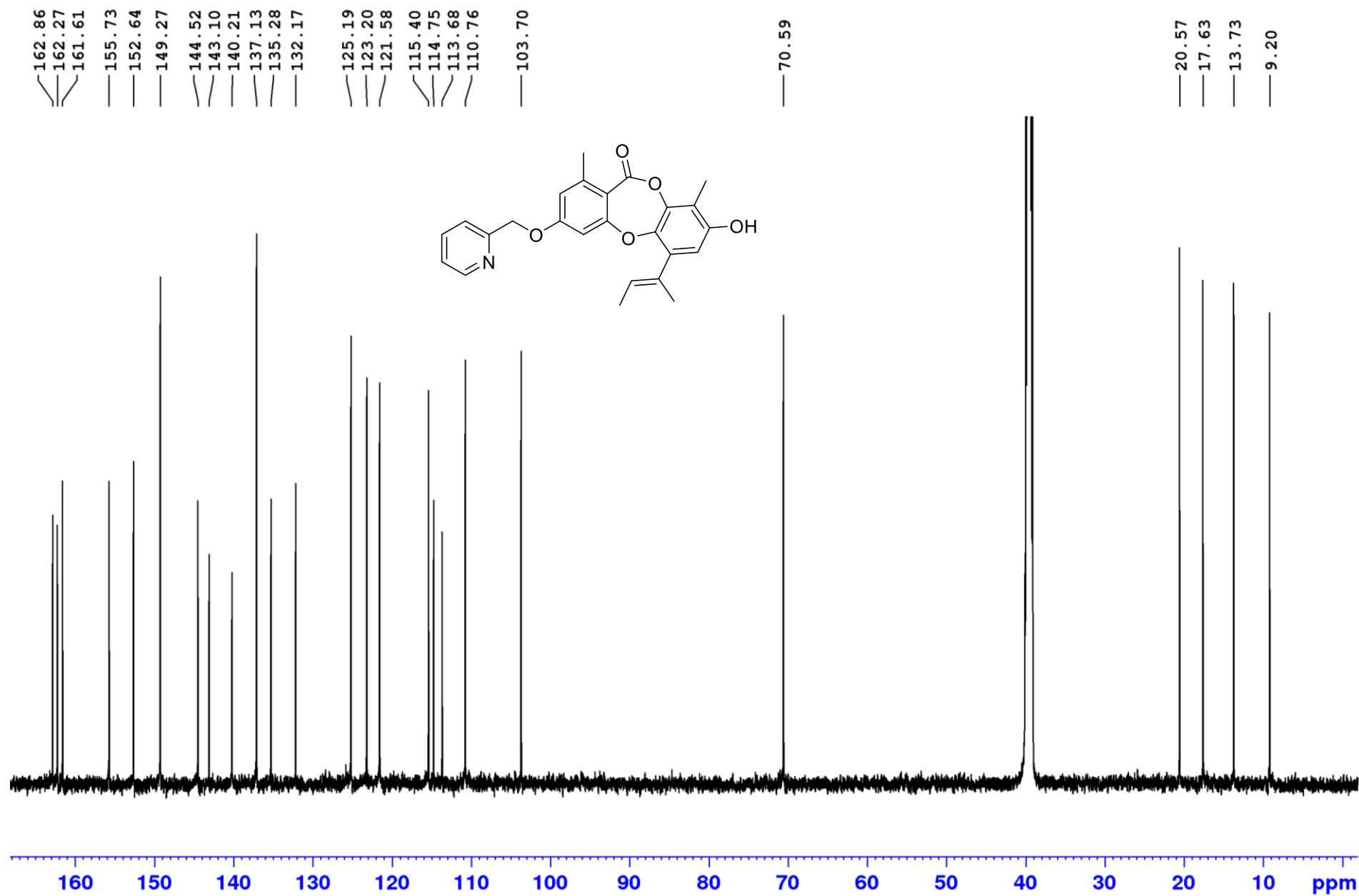


Figure S52. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) of 3-*O*-(2-picolyl)unguinol (7k)

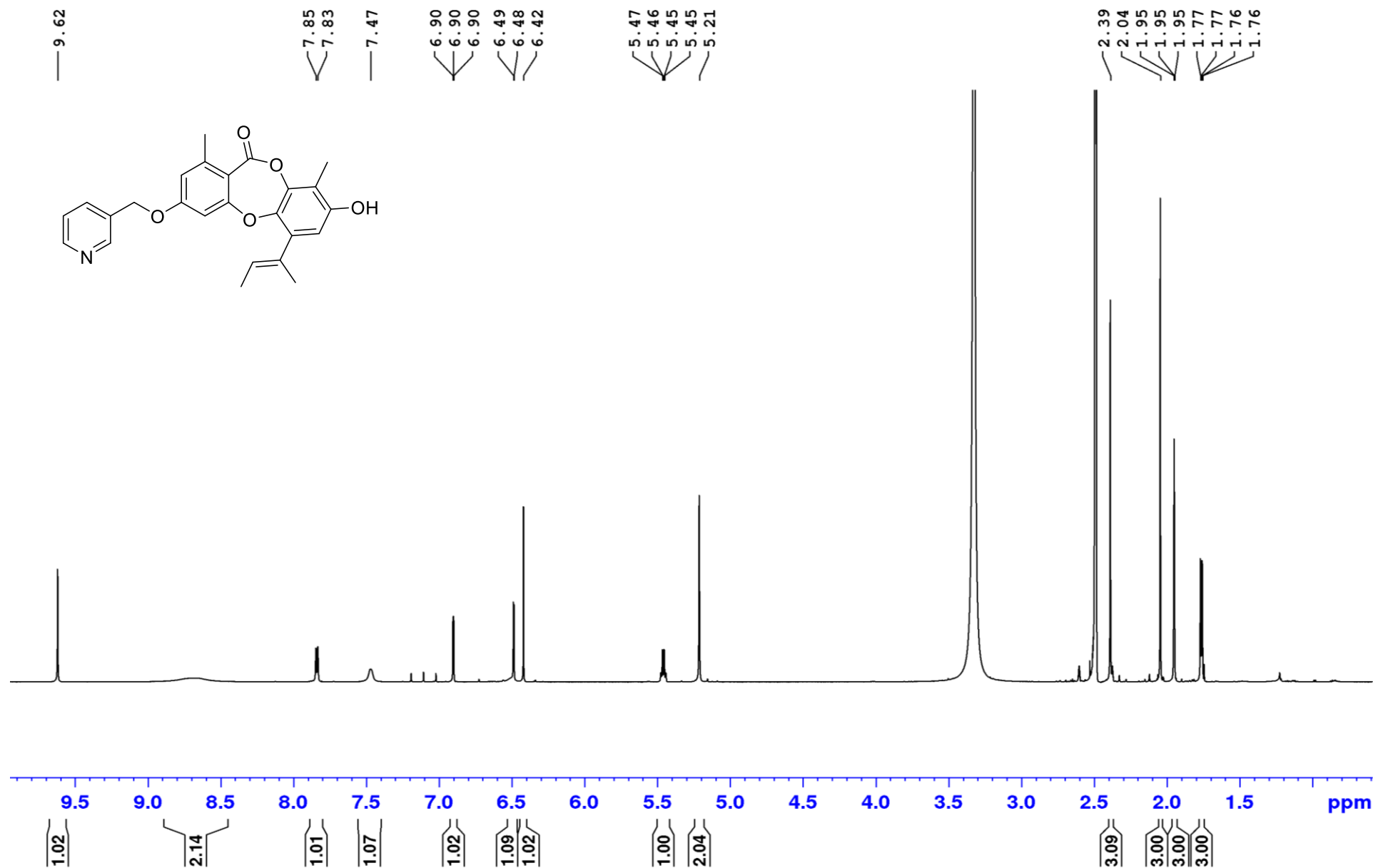


Figure S53. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of 3-O-(3-picolyl)unguinol (71)

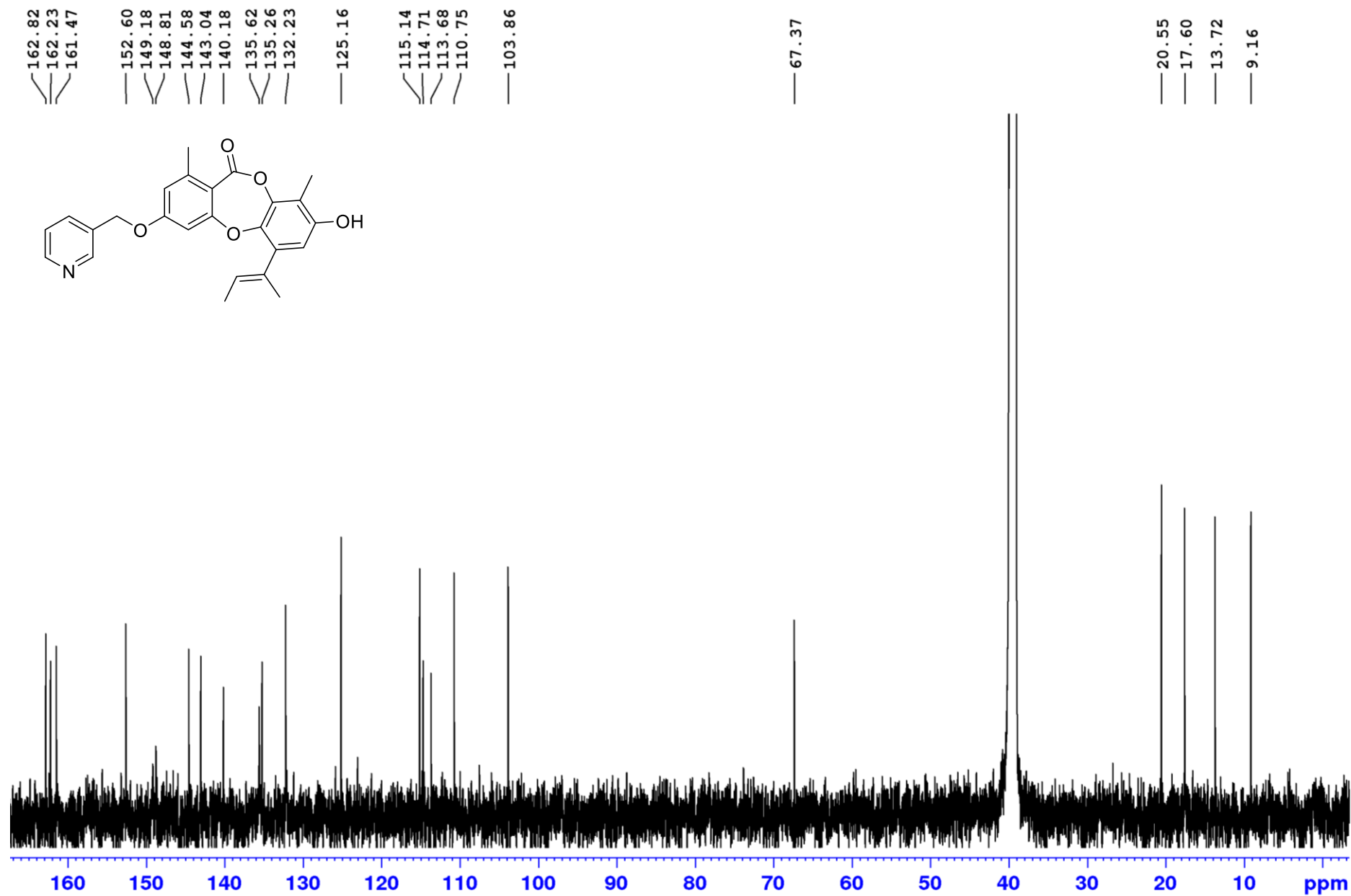


Figure S54. ^{13}C NMR spectrum (150 MHz, $\text{DMSO-}d_6$) of 3-*O*-(3-picolyl)unguinol (**71**)

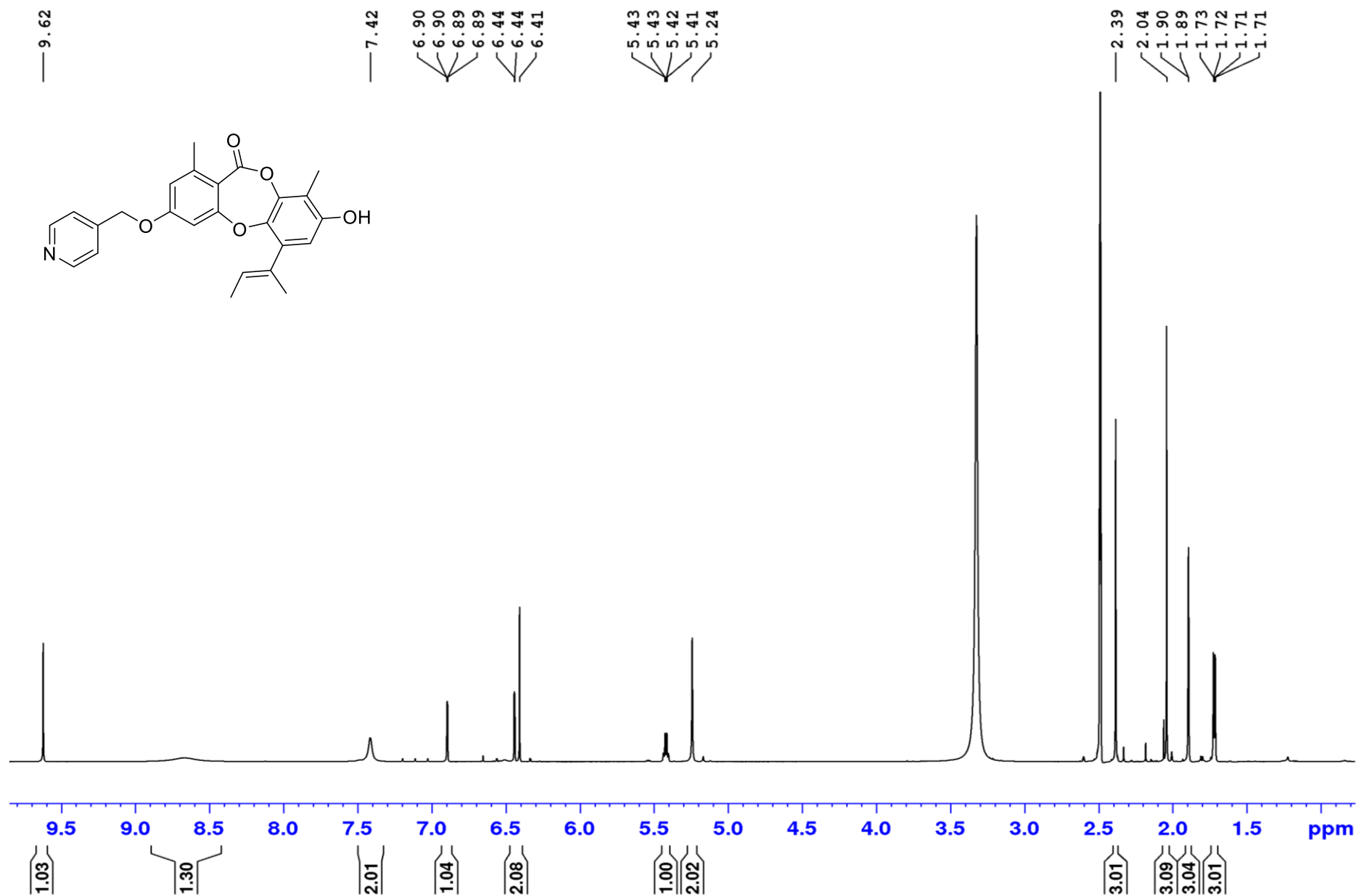


Figure S55. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of 3-O-(4-picolyl)unguinol (7m)

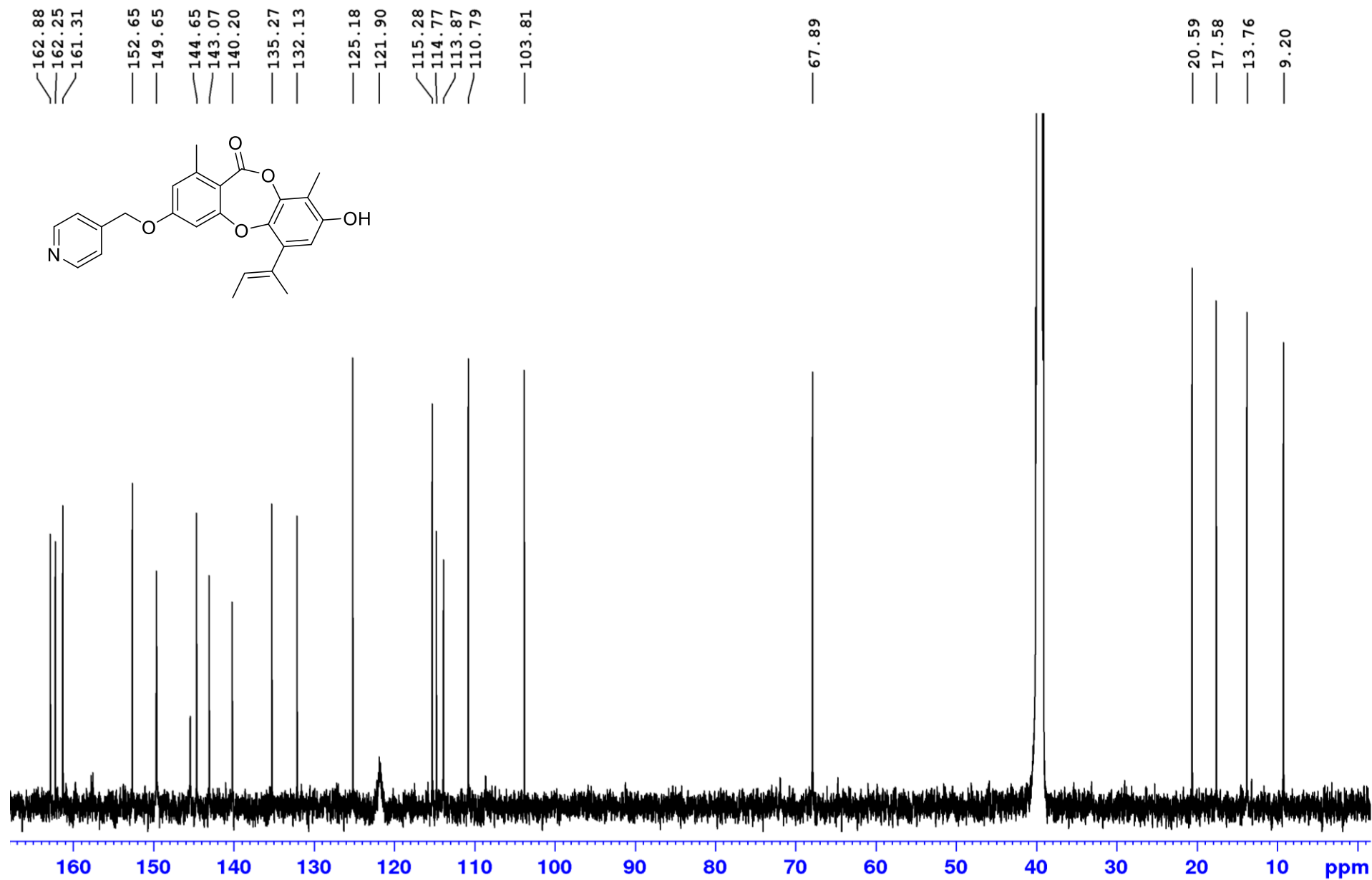


Figure S56. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) of 3-O-(4-picolyl)unguinol (7m)

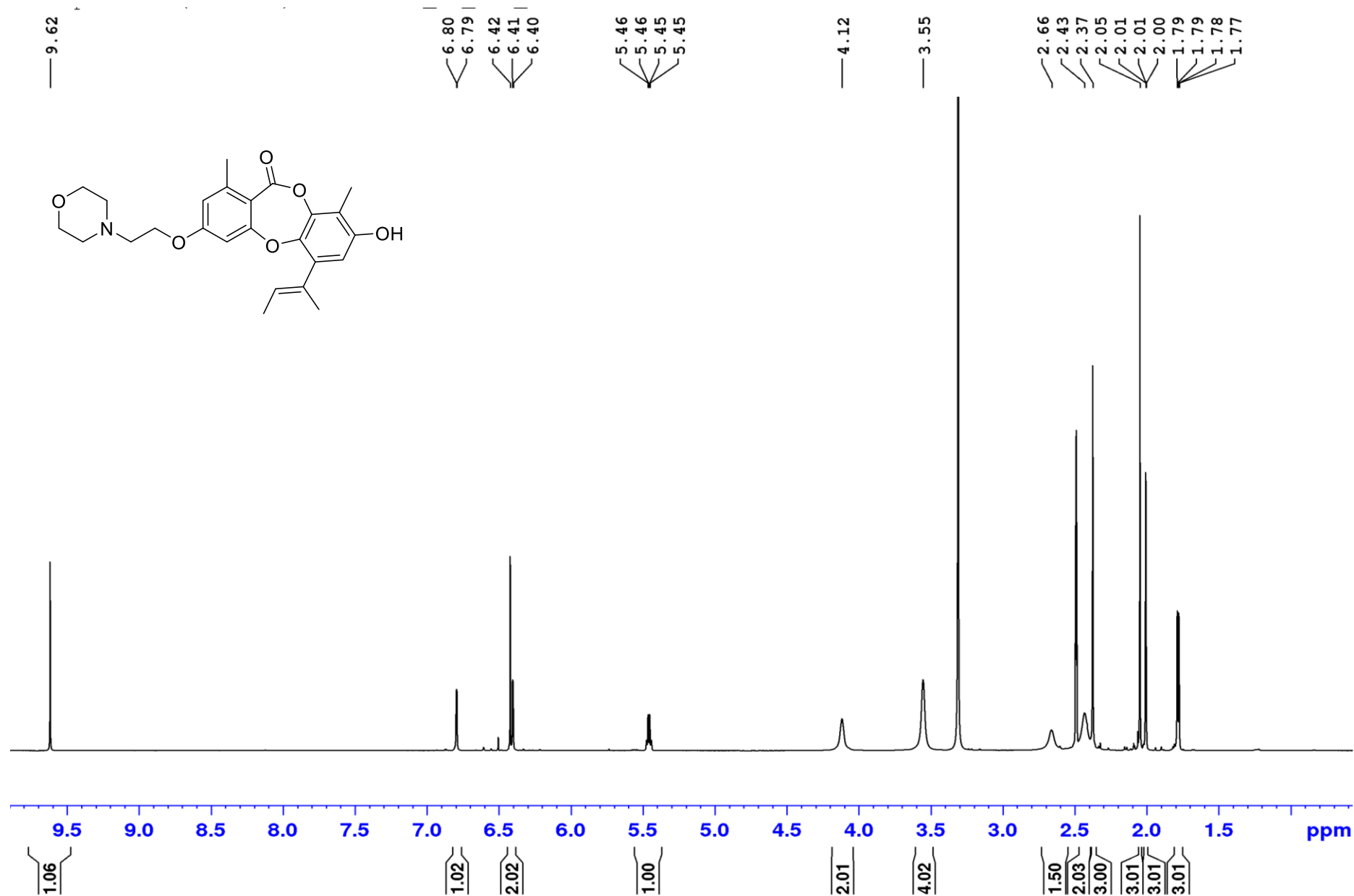


Figure S57. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of 3-O-(4-morpholinoethyl)unguinol (7n)

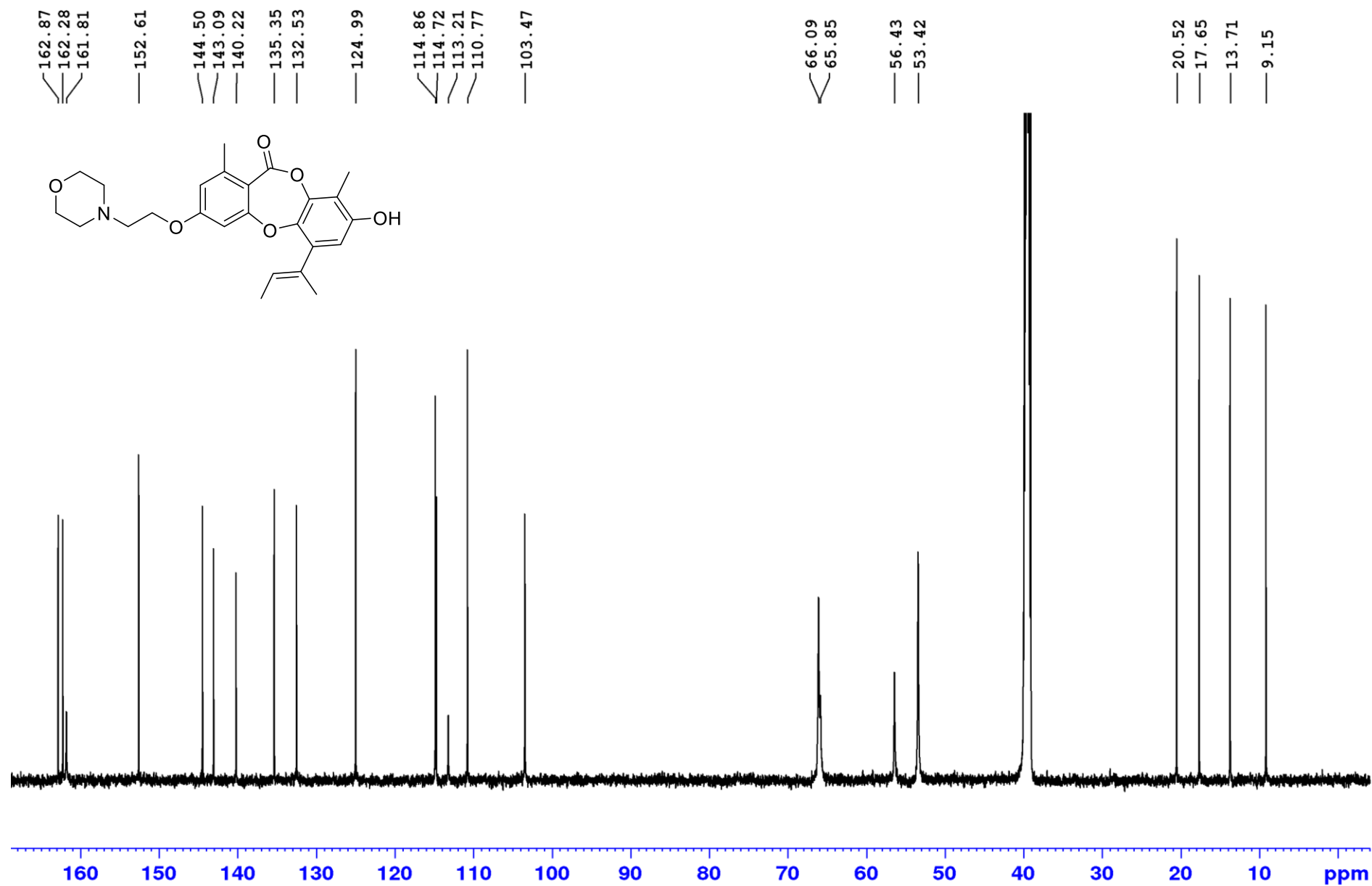


Figure S58. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) of 3-O-(4-morpholinoethyl)unguinol (7n)

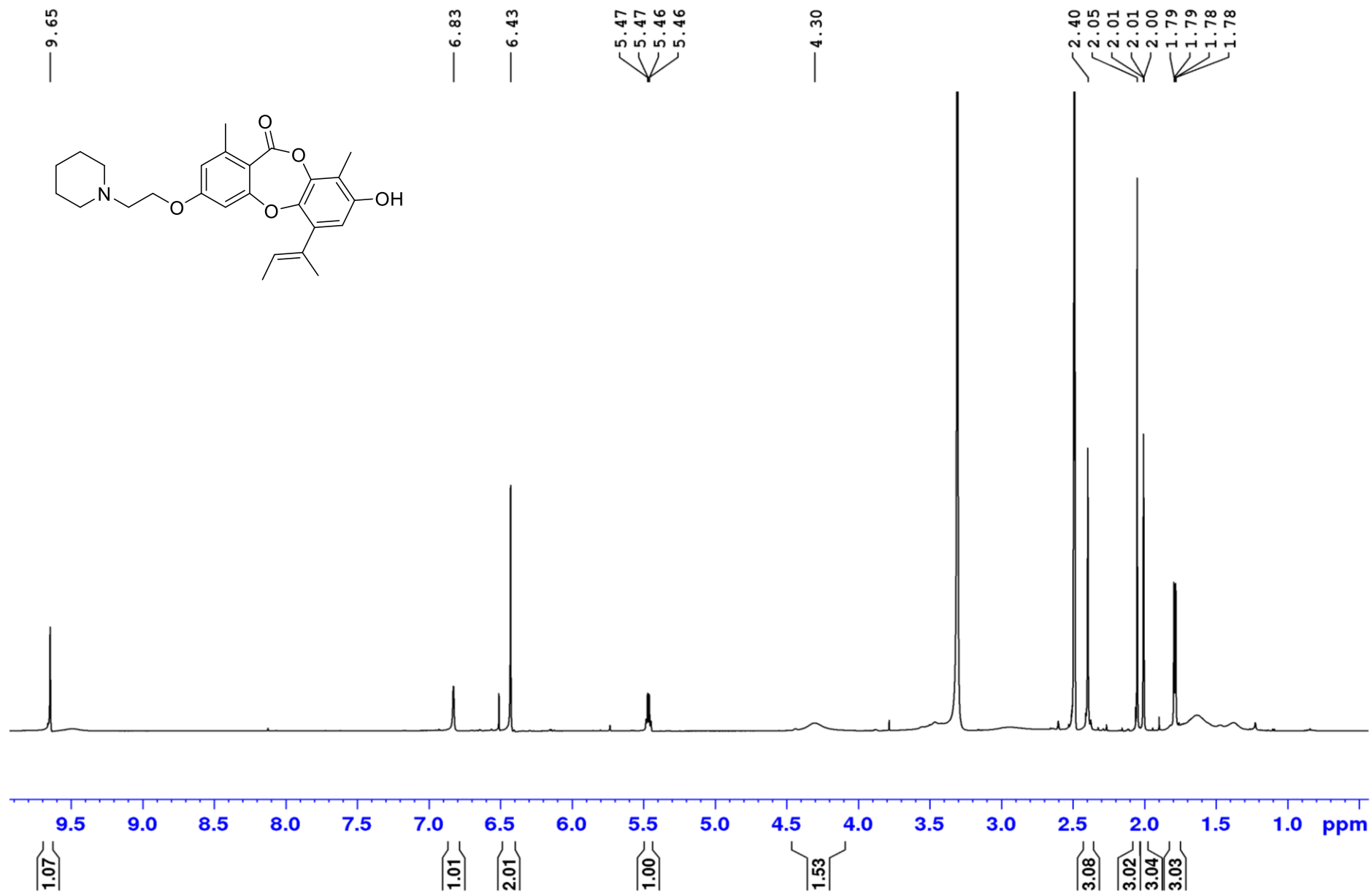


Figure S59. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of 3-O-(1-piperidinyethyl)unguinol (70)

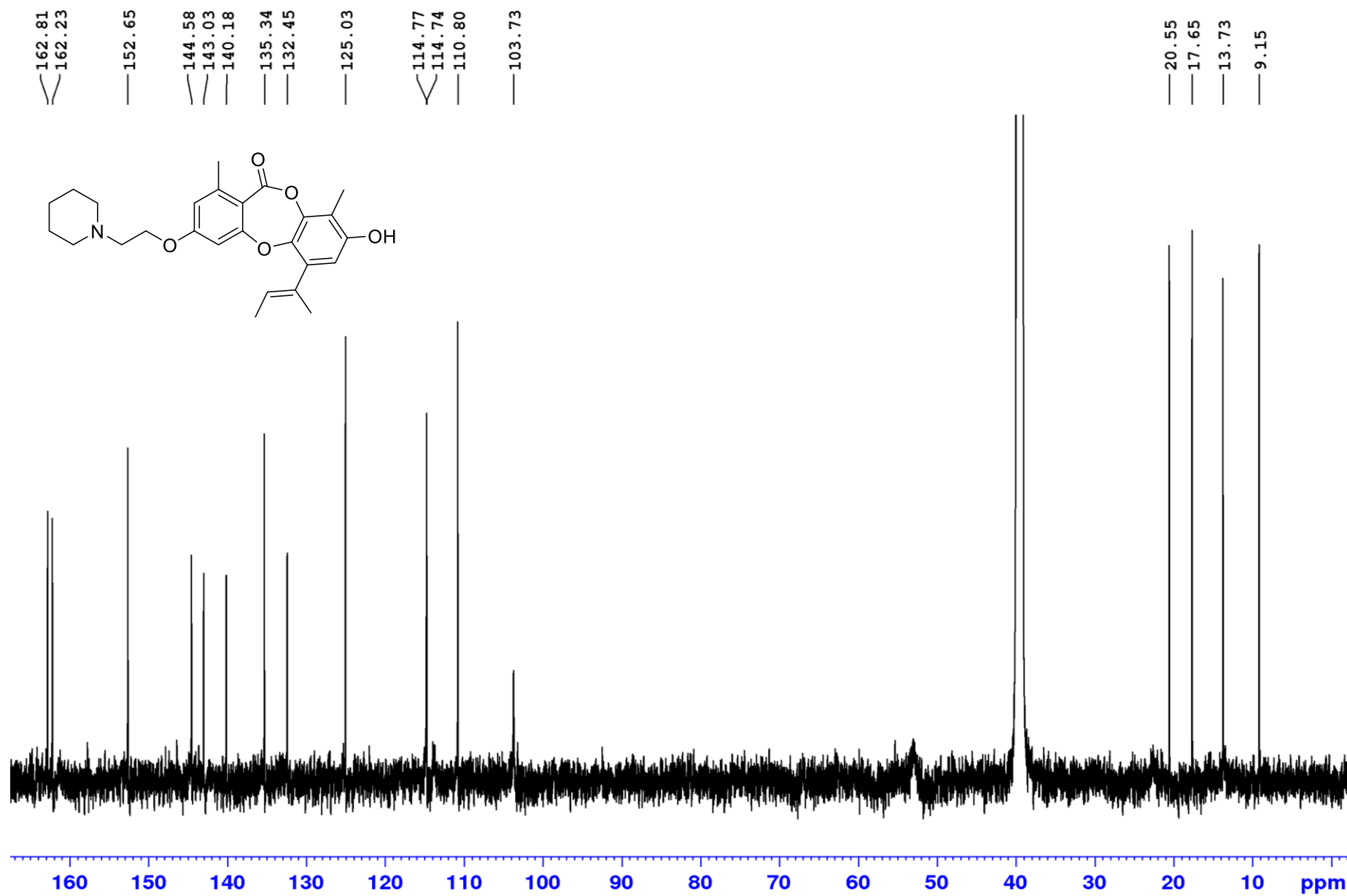


Figure S60. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) of 3-O-(1-piperidinyloxy)unguinol (7o)

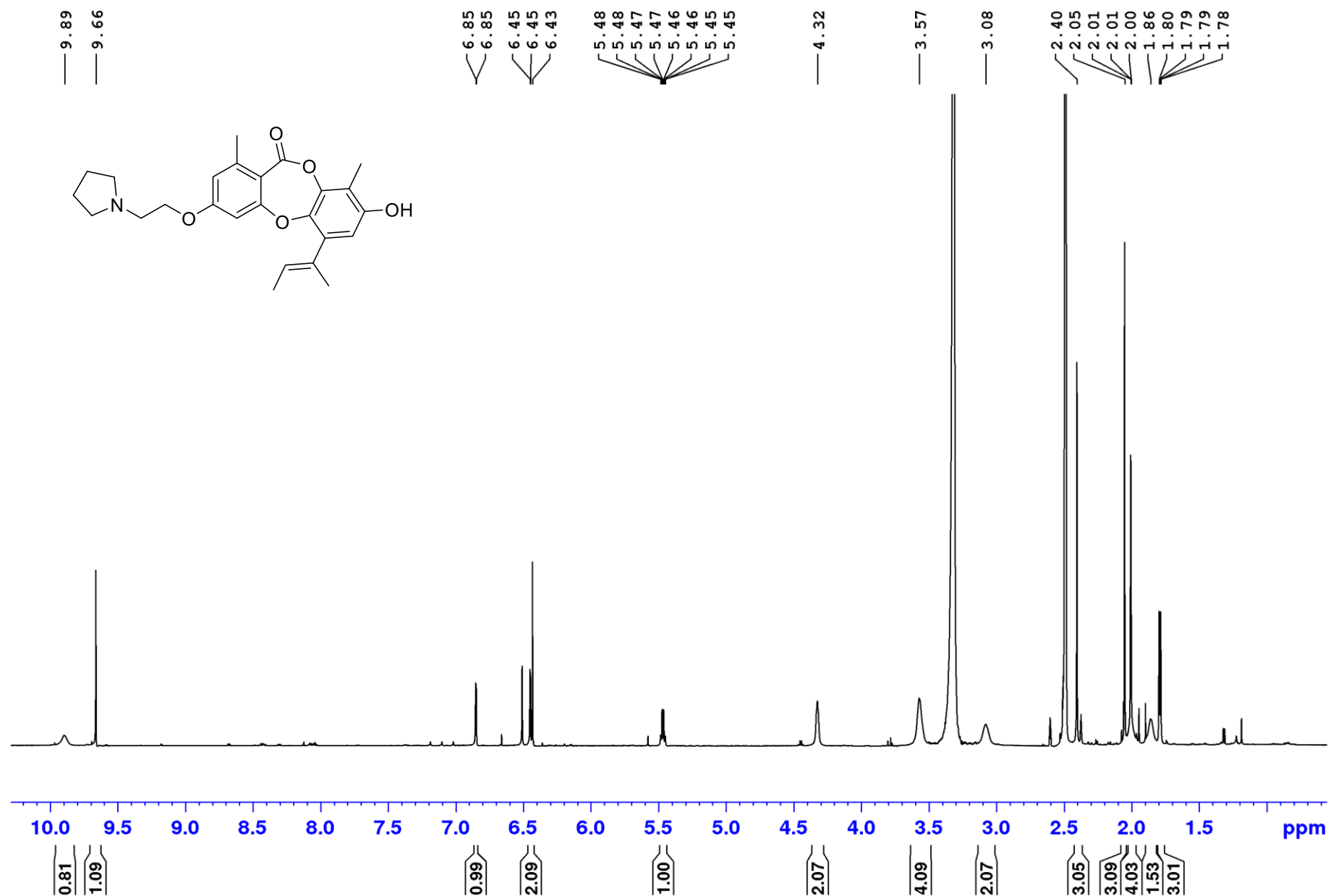


Figure S61. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of 3-O-(1-pyrrolidinyethyl)unguinol (7p)

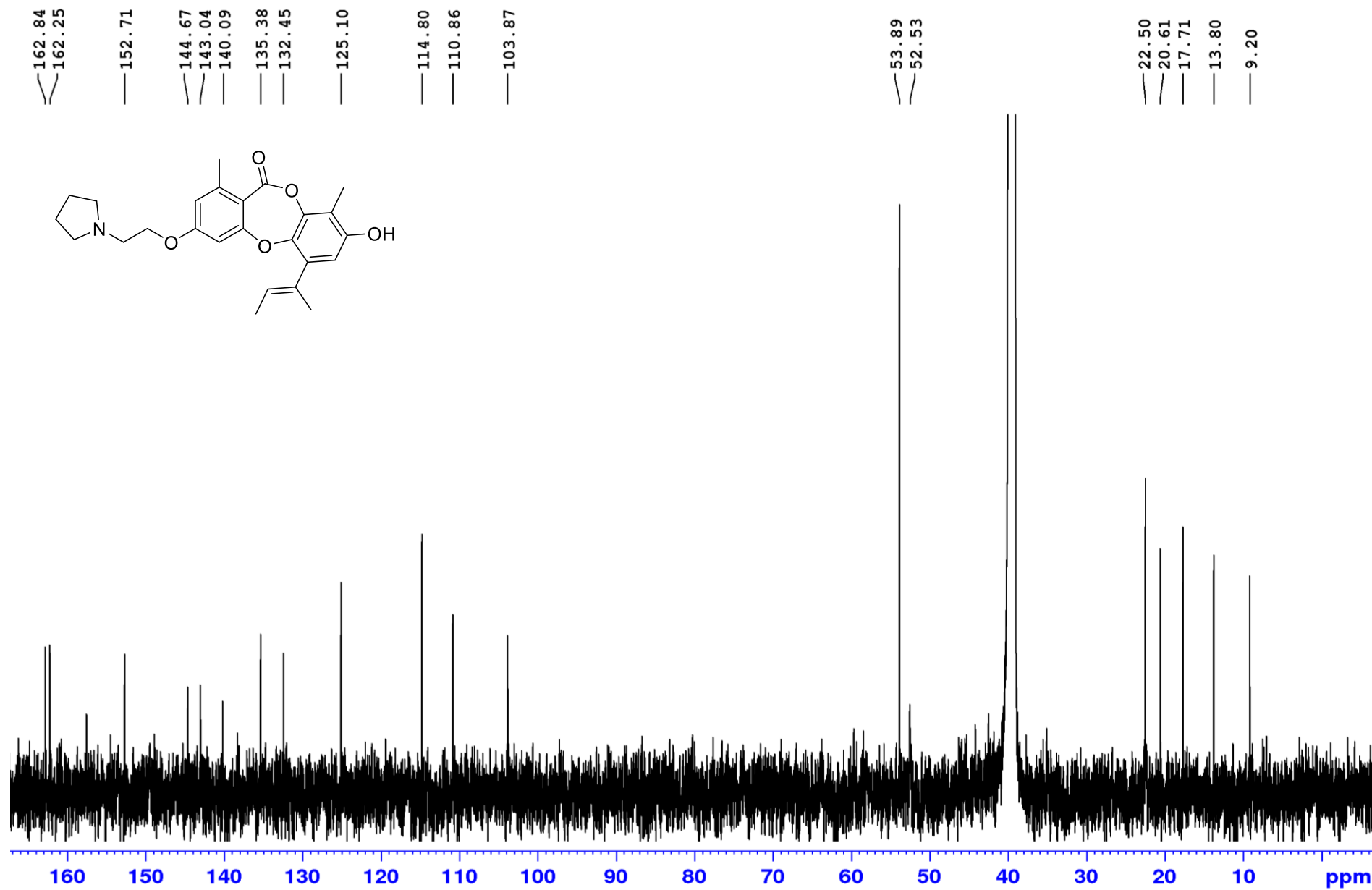


Figure S62. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) of 3-O-(1-pyrrolidinyloxy)guaiacol (7p)

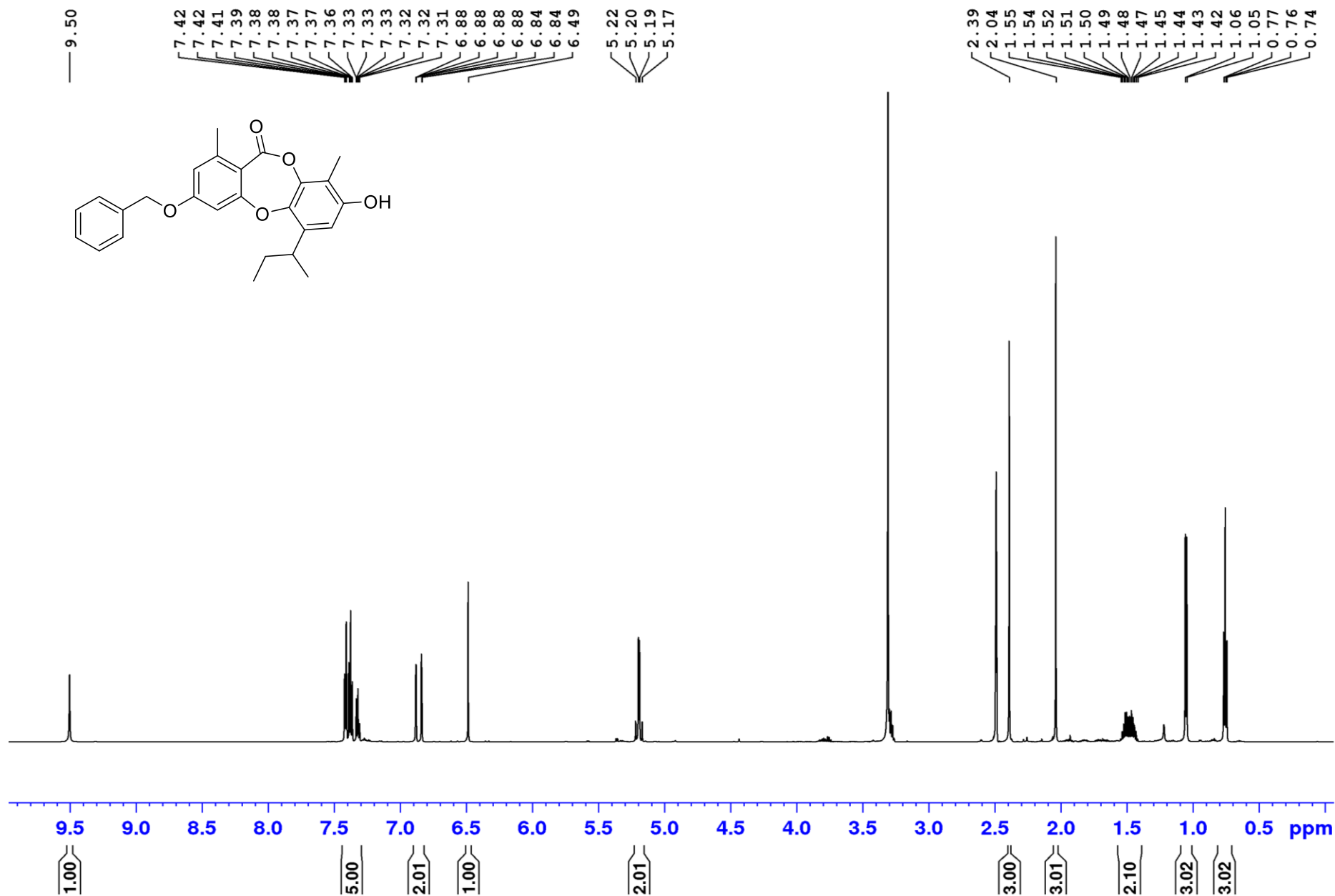


Figure S63. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of 3-O-benzyl-1',2'-dihydrounguinol (8a)

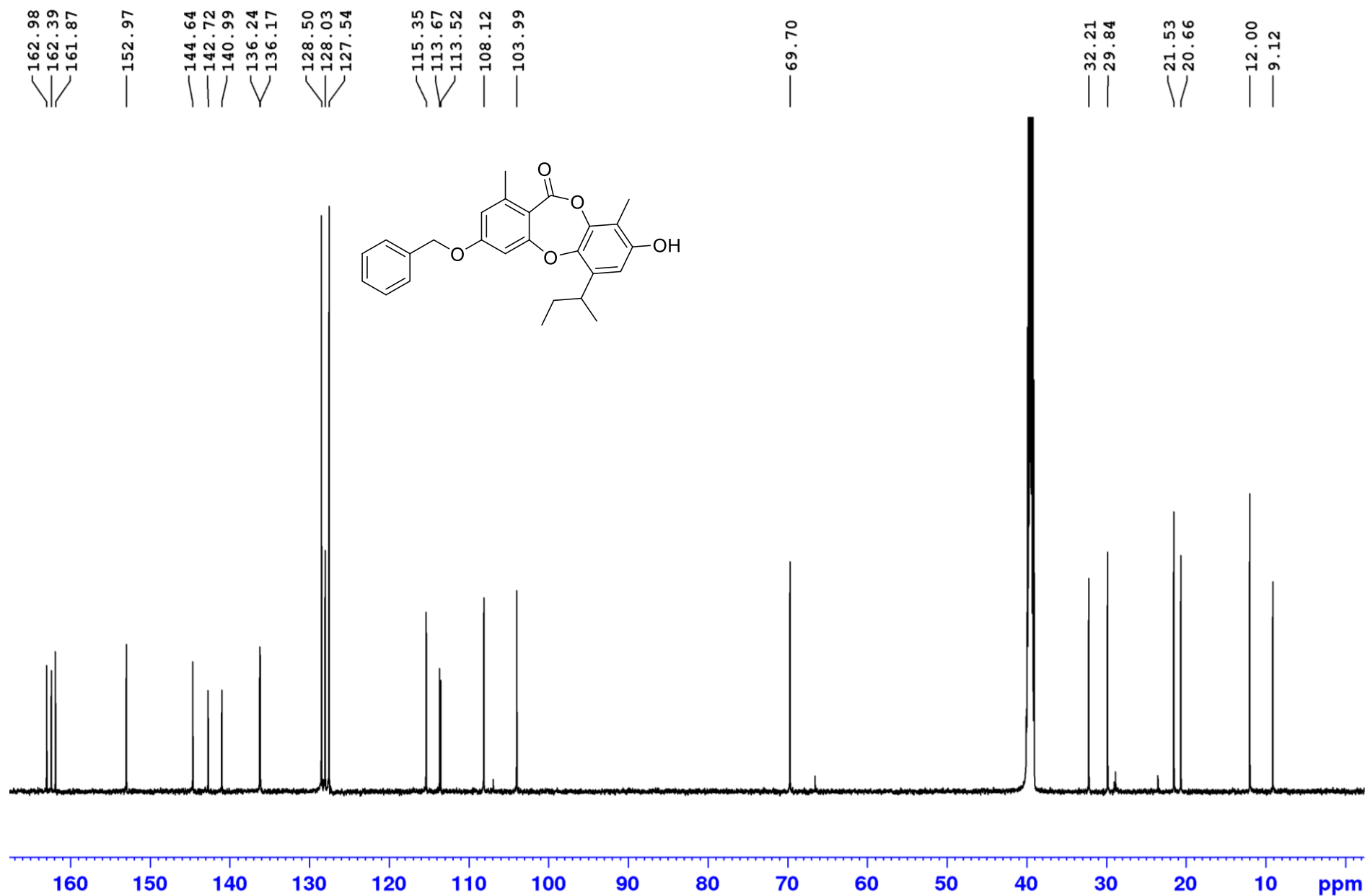


Figure S64. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) of 3-O-benzyl-1',2'-dihydroanguinol (8a)

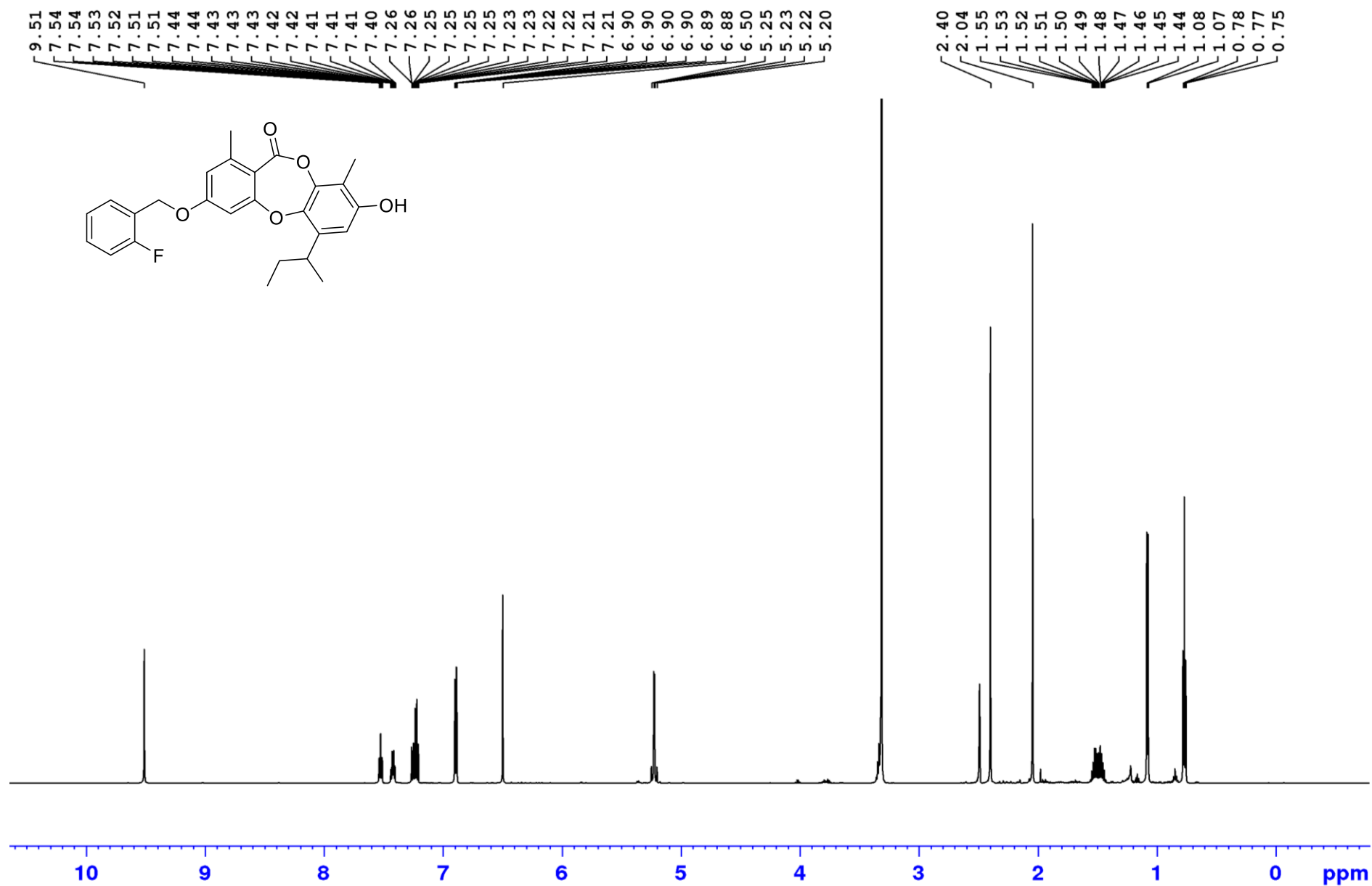


Figure S65. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of 3-O-(2-fluorobenzyl)-1',2'-dihydroquinol (8b)

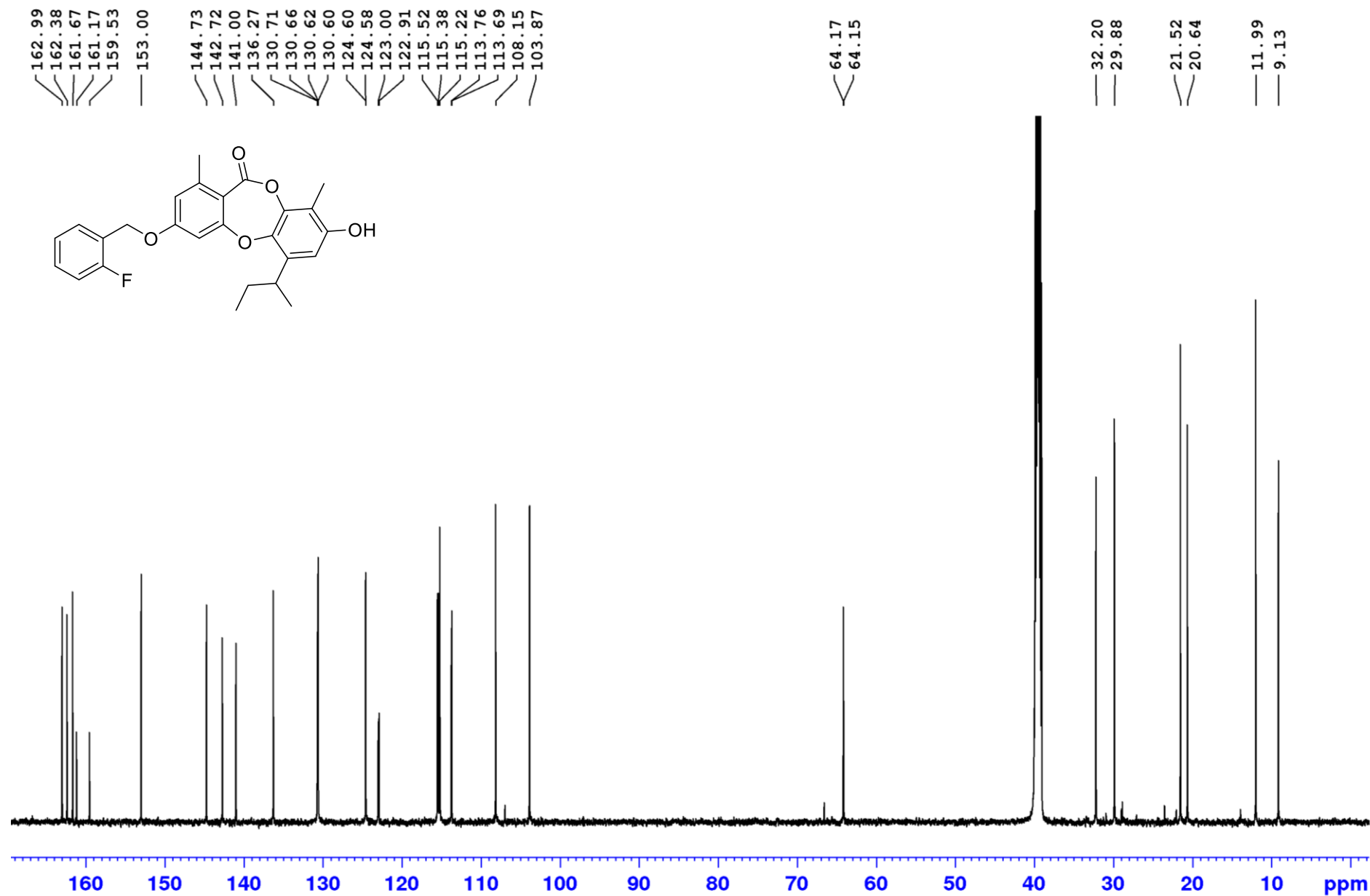


Figure S66. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) of 3-O-(2-fluorobenzyl)-1',2'-dihydrounguinol (8b)

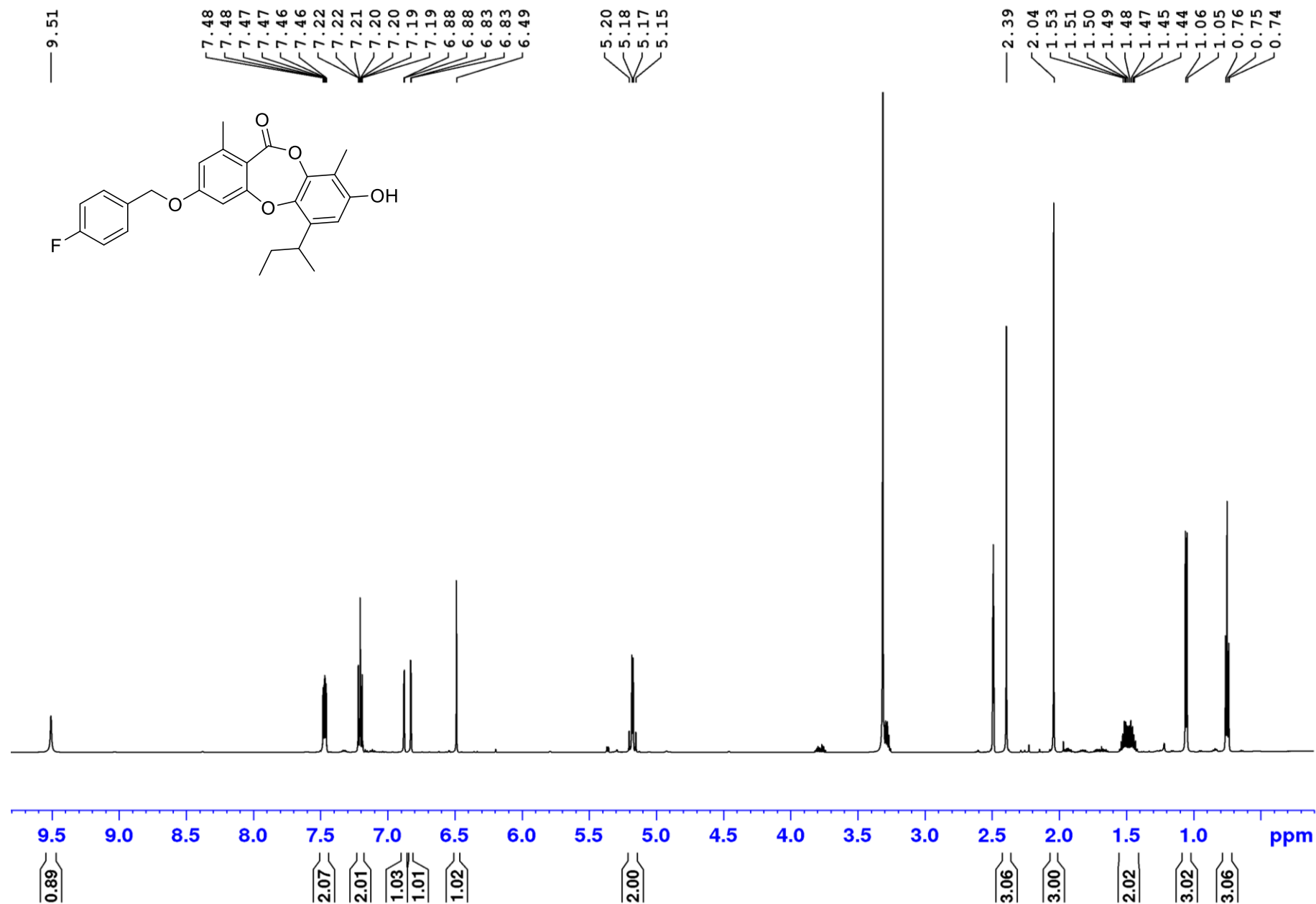


Figure S67. ¹H NMR spectrum (600 MHz, DMSO-*d*₆) of 3-O-(4-fluorobenzyl)-1',2'-dihydroquinol (8c)

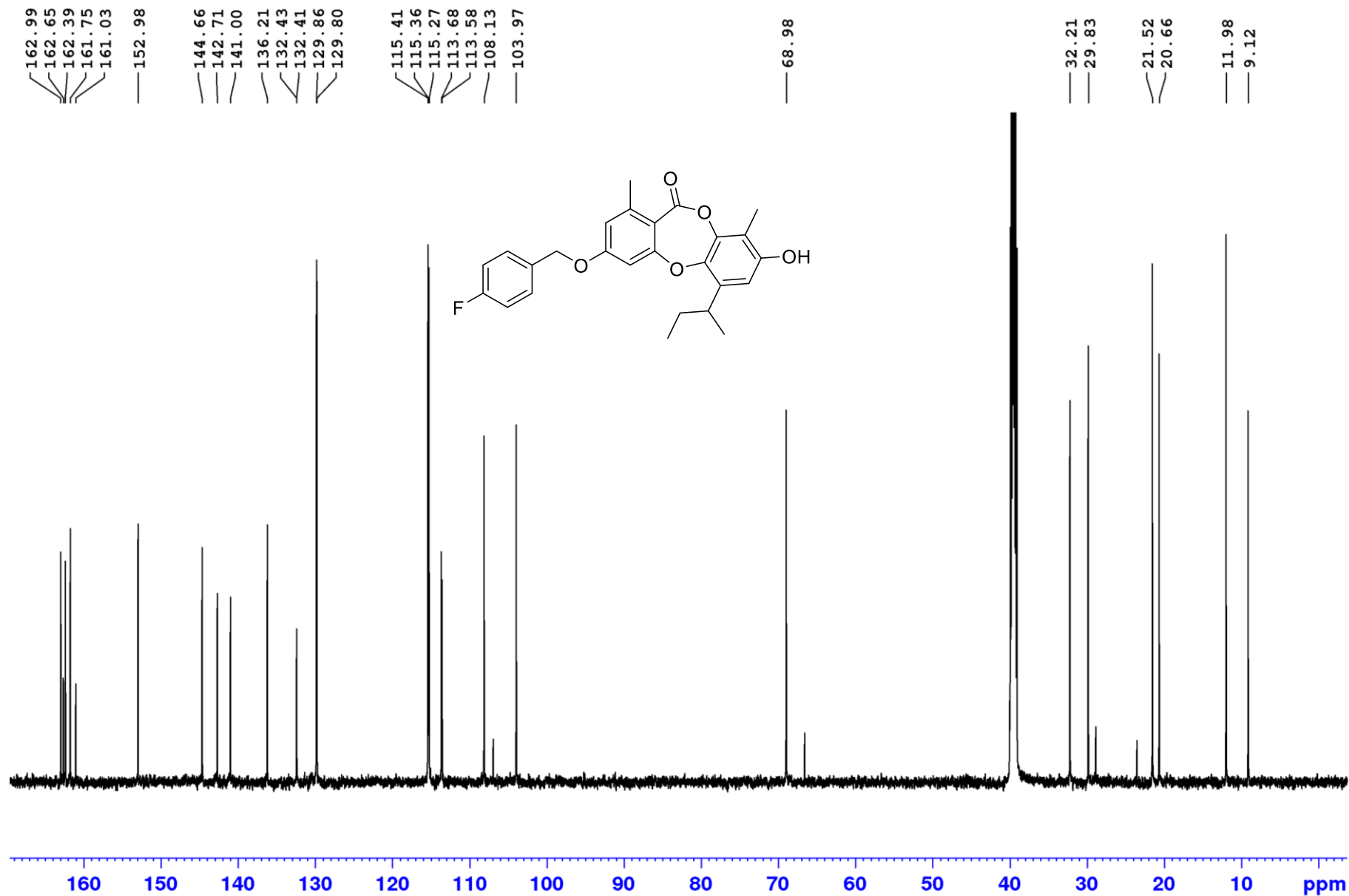


Figure S68. ¹³C NMR spectrum (150 MHz, DMSO-*d*₆) of 3-O-(4-fluorobenzyl)-1',2'-dihydrounguinol (8c)

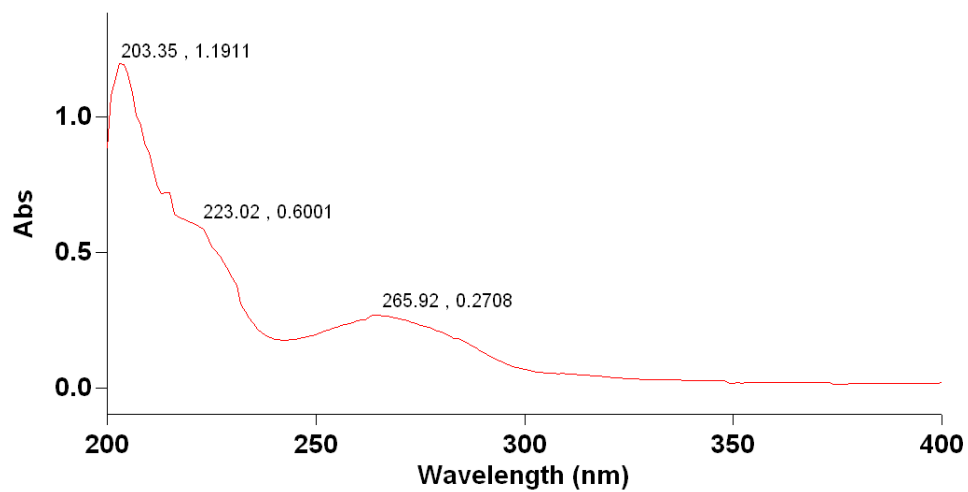


Figure S69. UV-vis spectrum of 1',2'-dihydroanguinol (**2a**) in MeOH

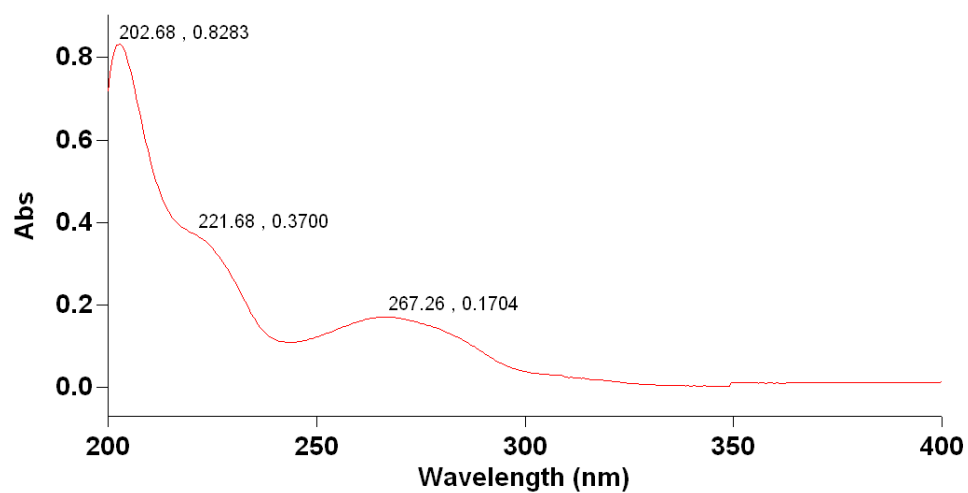


Figure S70. UV-vis spectrum of *cis*-1',2'-epoxyanguinol (**2b**) in MeOH

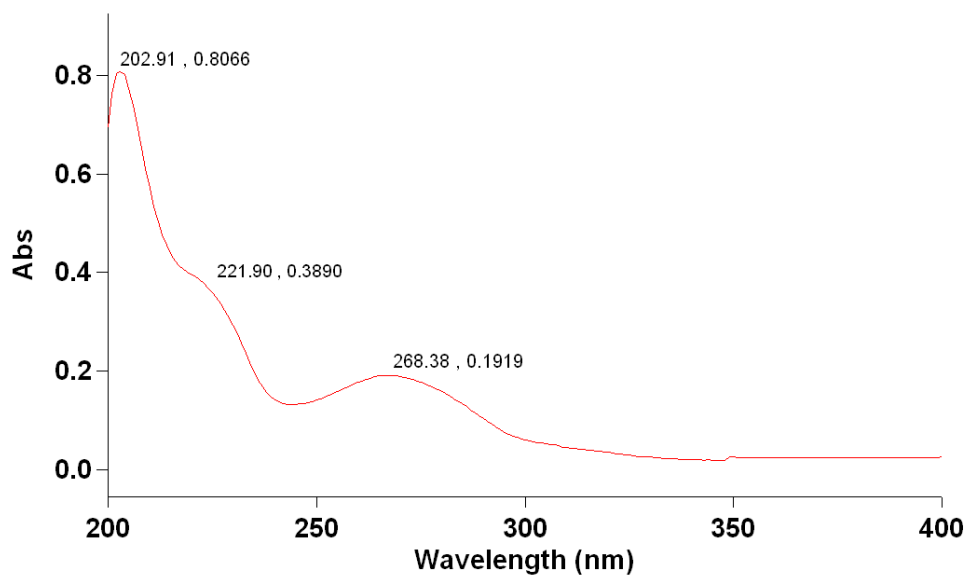


Figure S71. UV-vis spectrum of 1',2'-dihydroxyunguinol (**2c**) in MeOH

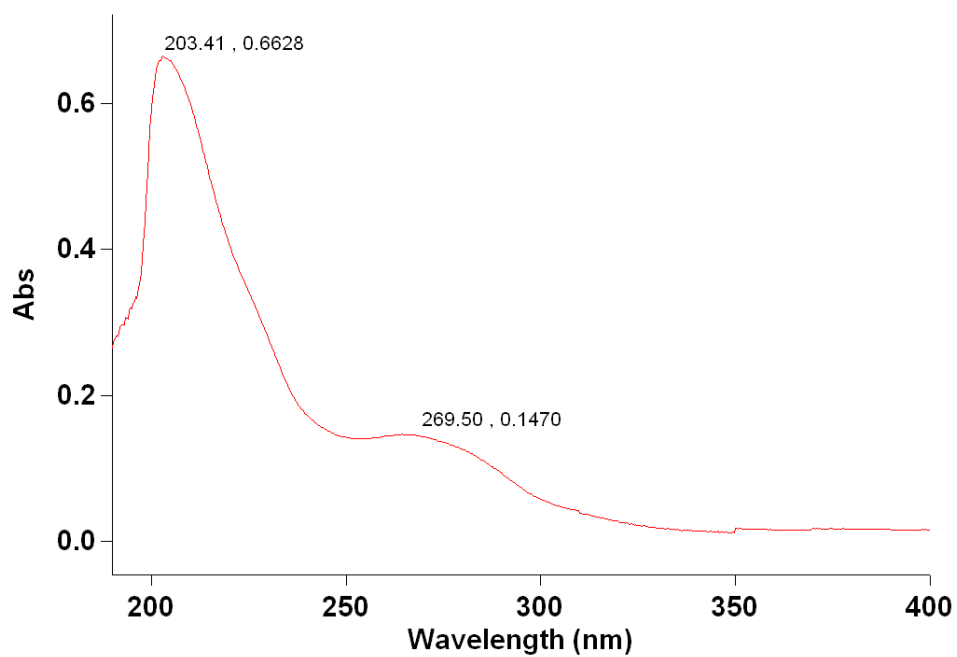


Figure S72. UV-vis spectrum of 2'-hydroxy- $\Delta^{1,4'}$ -unguinol (**2d**) in MeOH

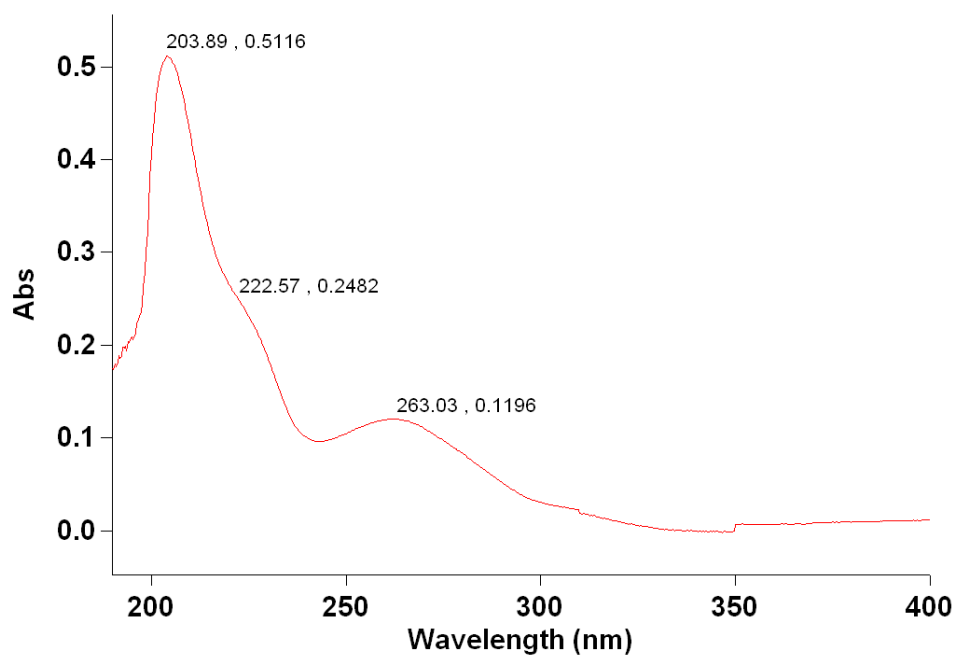


Figure S73. UV-vis spectrum of 2'-oxo- $\Delta^{1,4'}$ -unguinol (**2e**) in MeOH

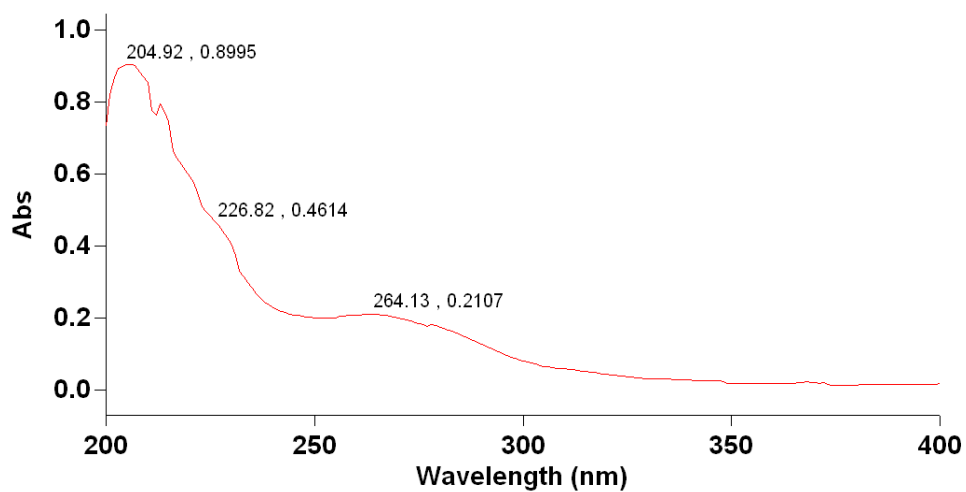


Figure S74. UV-vis spectrum of 2'-hydroperoxy- $\Delta^{1,4'}$ -unguinol (**2f**) in MeOH

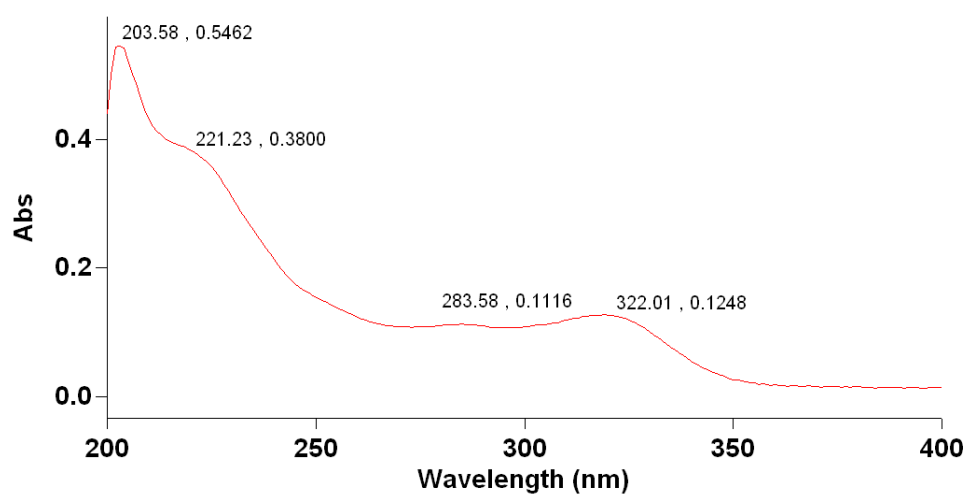


Figure S75. UV-vis spectrum of 2,7-dibromo-1',2'-dihydroanguinol (**3a**) in MeOH

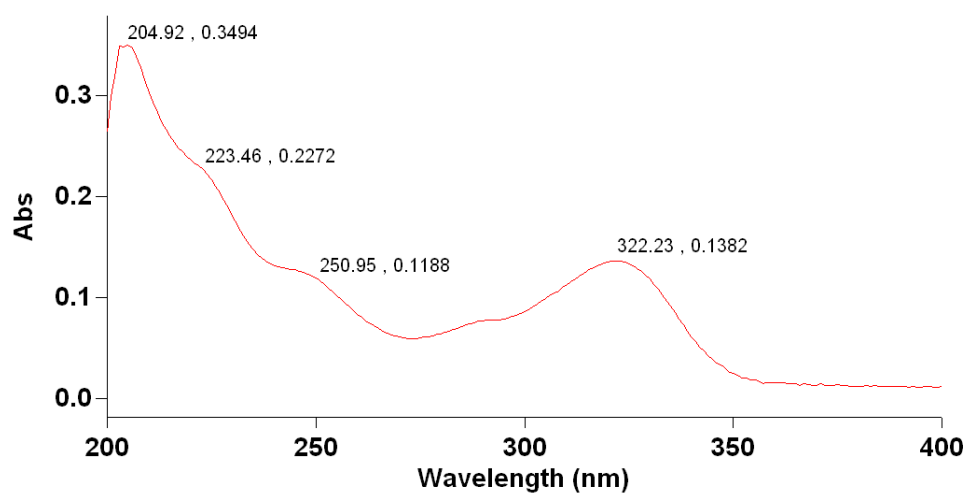


Figure S76. UV-vis spectrum of 2,4,7-tribromo-1',2'-dihydroanguinol (**3b**) in MeOH

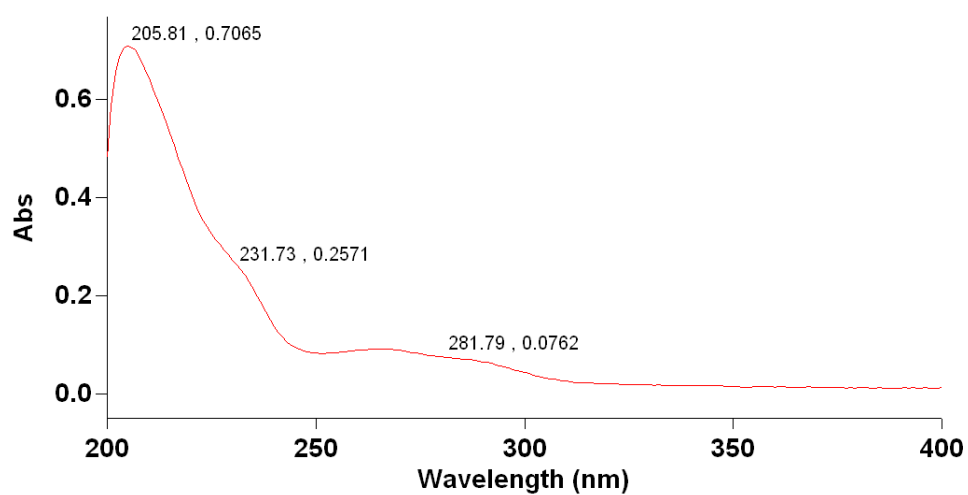


Figure S77. UV-vis spectrum of 2,4-diiodo-1',2'-dihydranguinol (**3c**) in MeOH

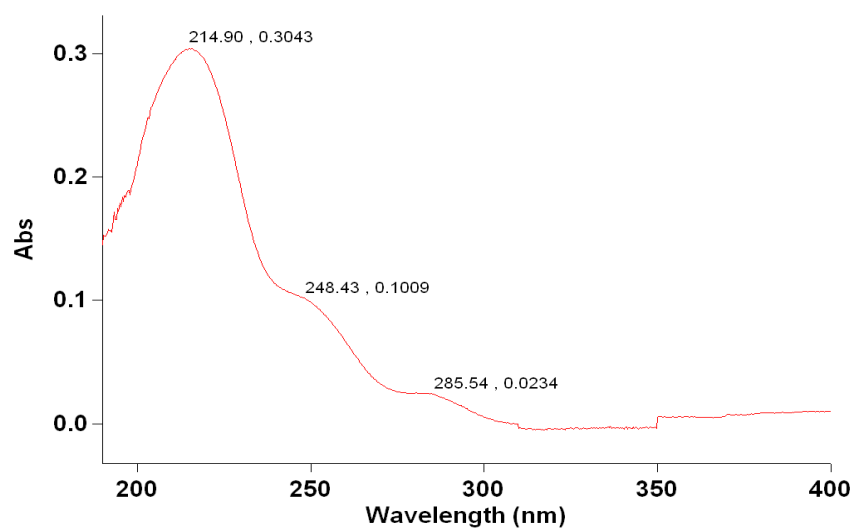


Figure S78. UV-vis spectrum of methylanguinol (**4a**) in MeOH

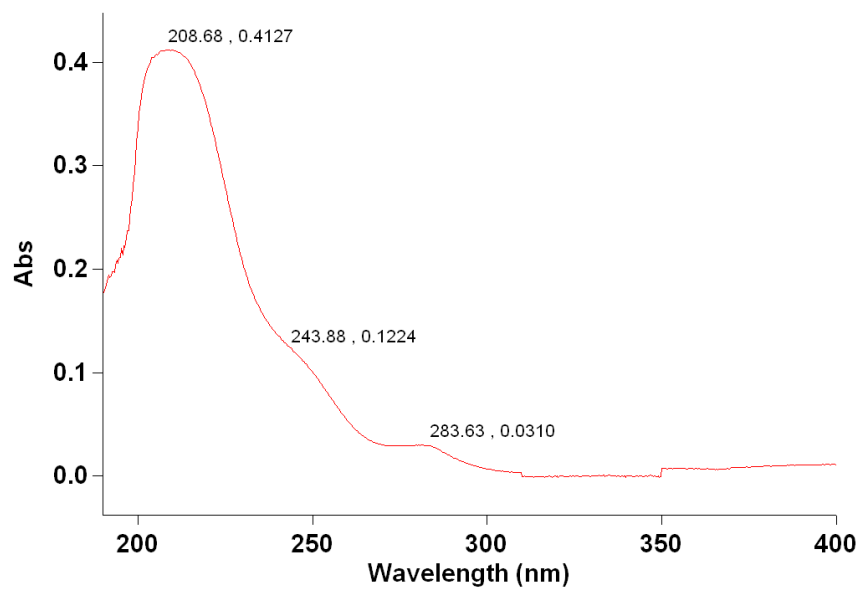


Figure S79. UV-vis spectrum of unguinolamide (4b) in MeOH

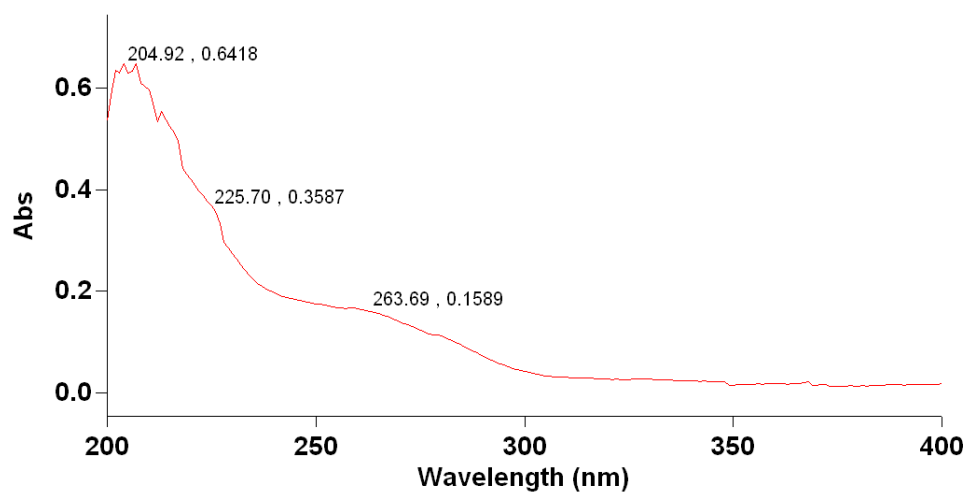


Figure S80. UV-vis spectrum of 3-O-methylunguinol (5a) in MeOH

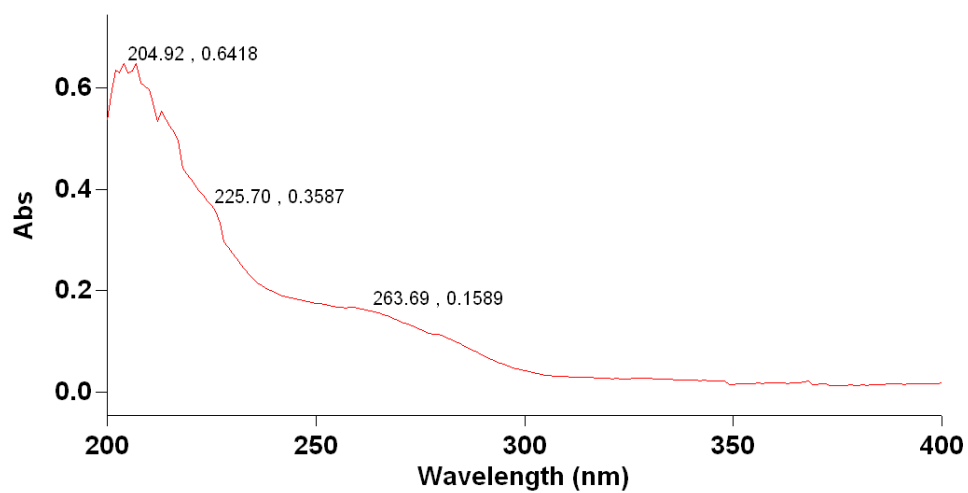


Figure S81. UV-vis spectrum of 3,8-di-*O*-methylunguinol (**5b**) in MeOH

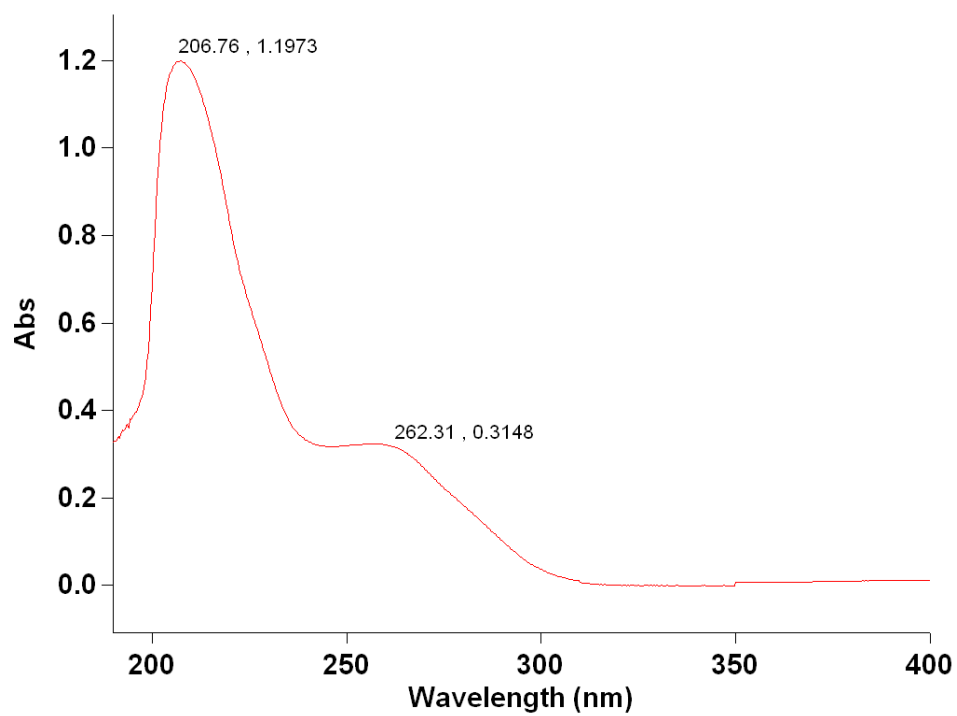


Figure S82. UV-vis spectrum of 3-*O*-benzylunguinol (**6a**) in MeOH

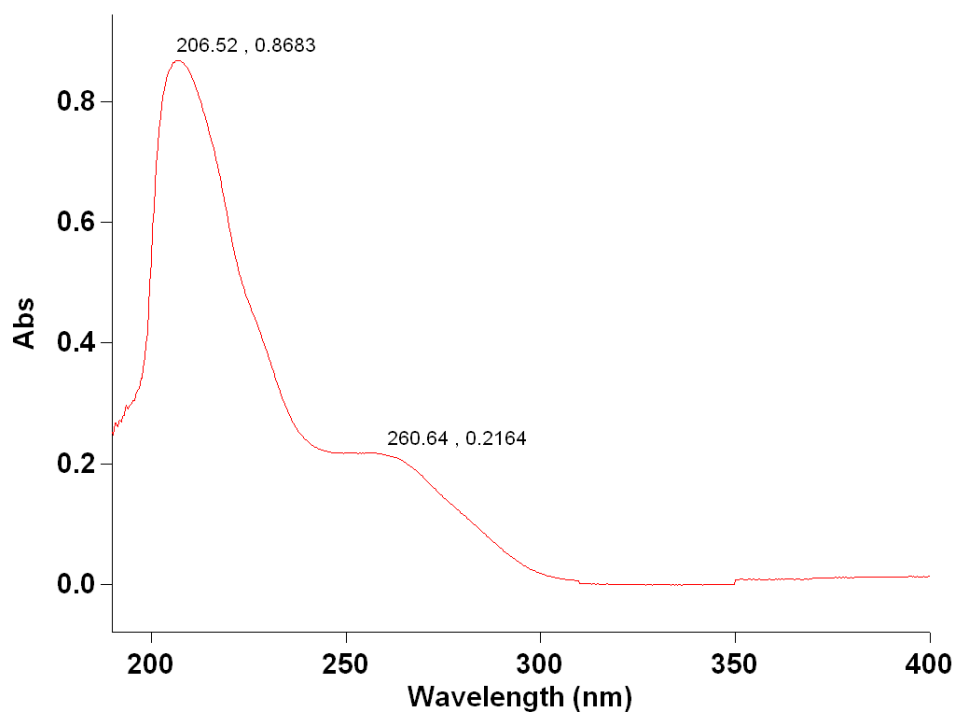


Figure S83. UV-vis spectrum of 3,8-di-O-benzylunguinol (**6b**) in MeOH

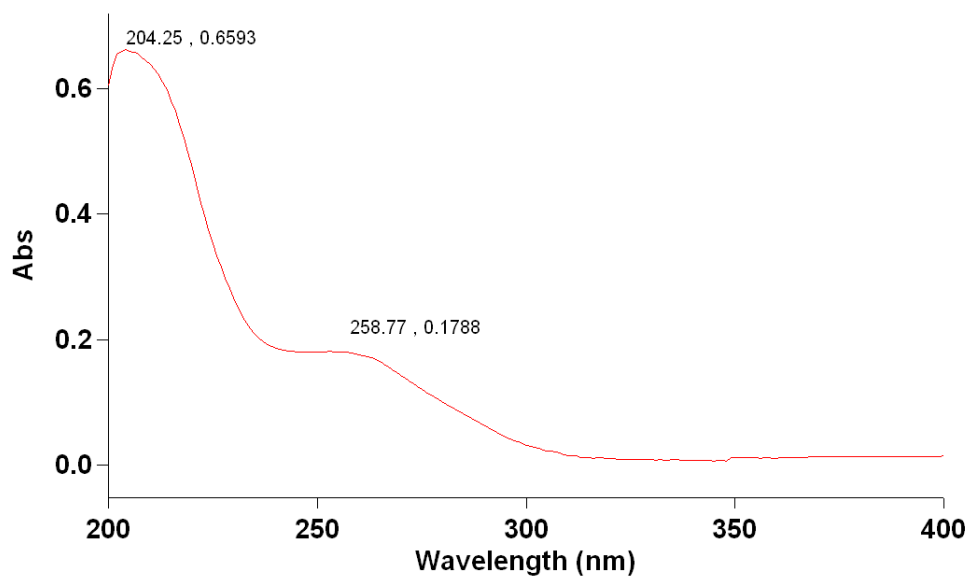


Figure S84. UV-vis spectrum of 3-O-(2-chlorobenzyl)unguinol (**7a**) in MeOH

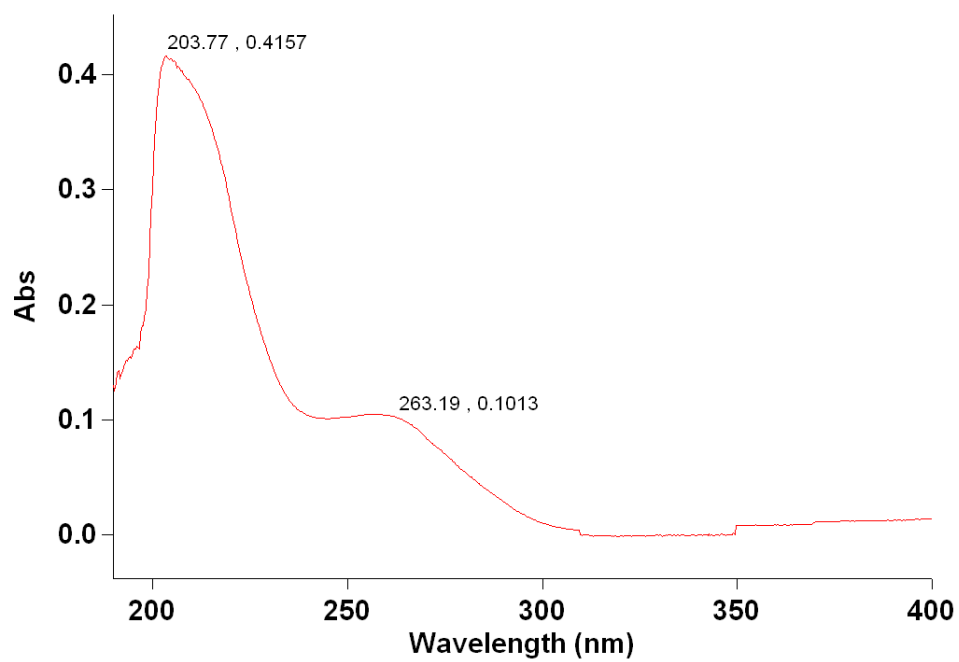


Figure S85. UV-vis spectrum of 3-O-(3-chlorobenzyl)unguinol (7b) in MeOH

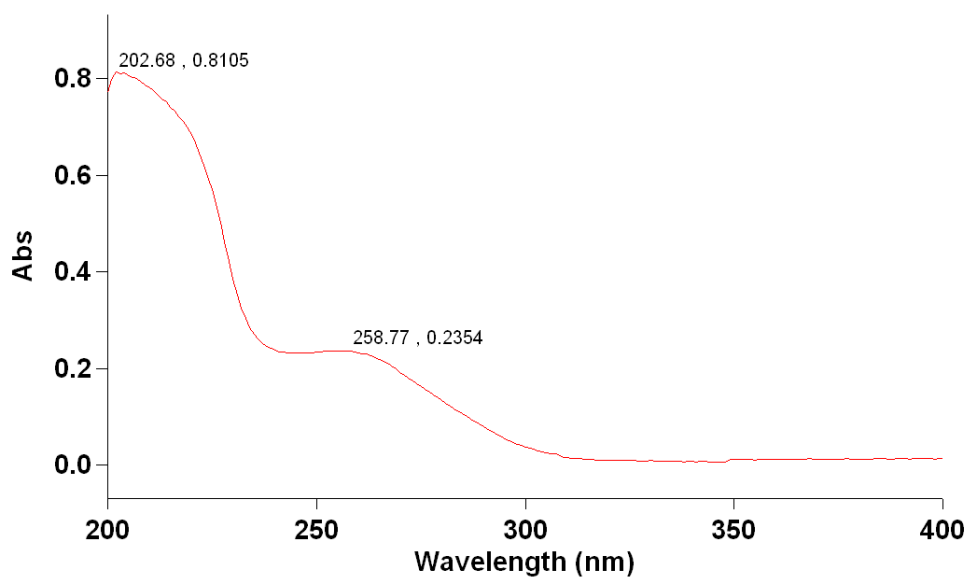


Figure S86. UV-vis spectrum of 3-O-(4-chlorobenzyl)unguinol (7c) in MeOH

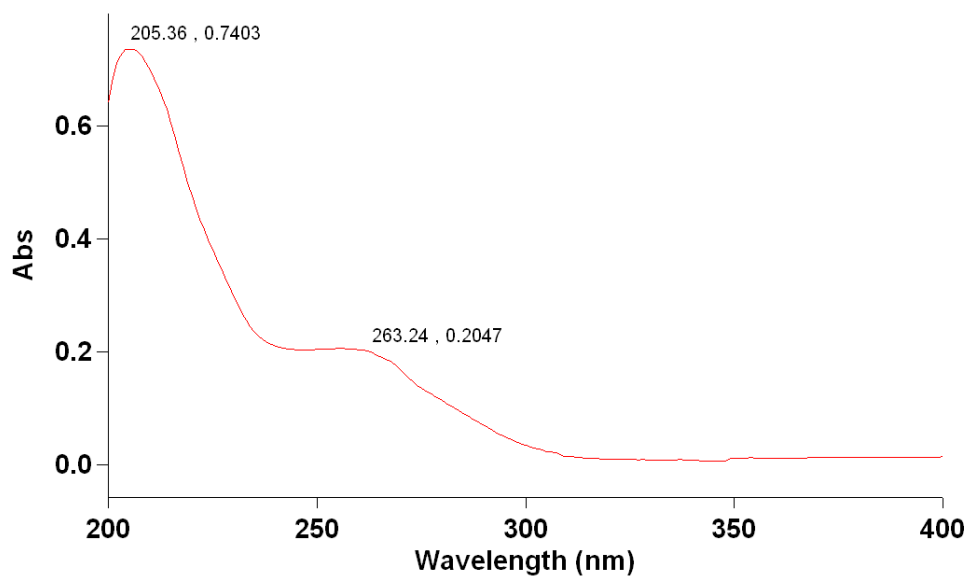


Figure S87. UV-vis spectrum of 3-O-(2-fluorobenzyl)unguinol (7d) in MeOH

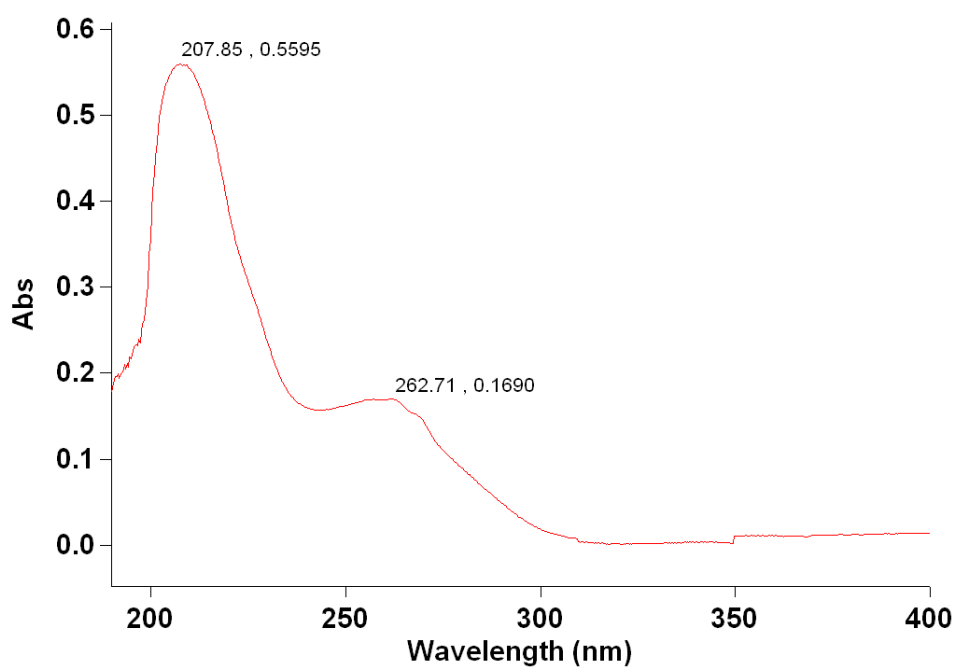


Figure S88. UV-vis spectrum of 3-O-(3-fluorobenzyl)unguinol (7e) in MeOH

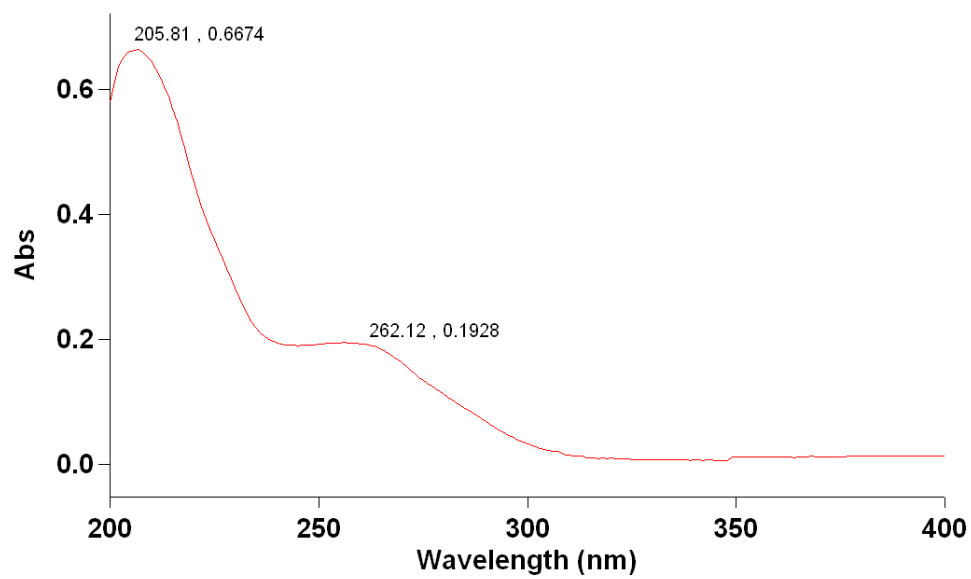


Figure S89. UV-vis spectrum of 3-O-(4-fluorobenzyl)unguinol (7f) in MeOH

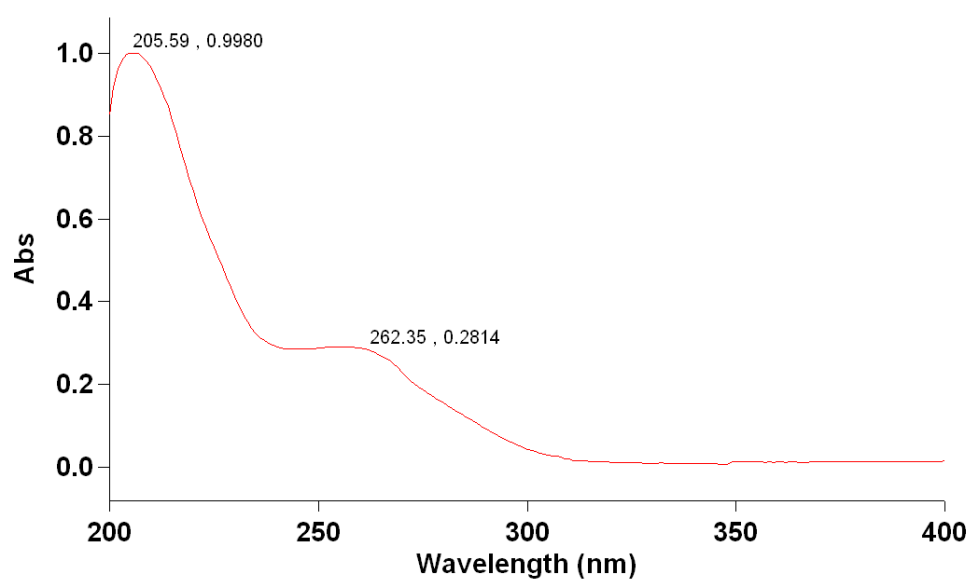


Figure S90. UV-vis spectrum of 3-O-(2,4-difluorobenzyl)unguinol (7g) in MeOH

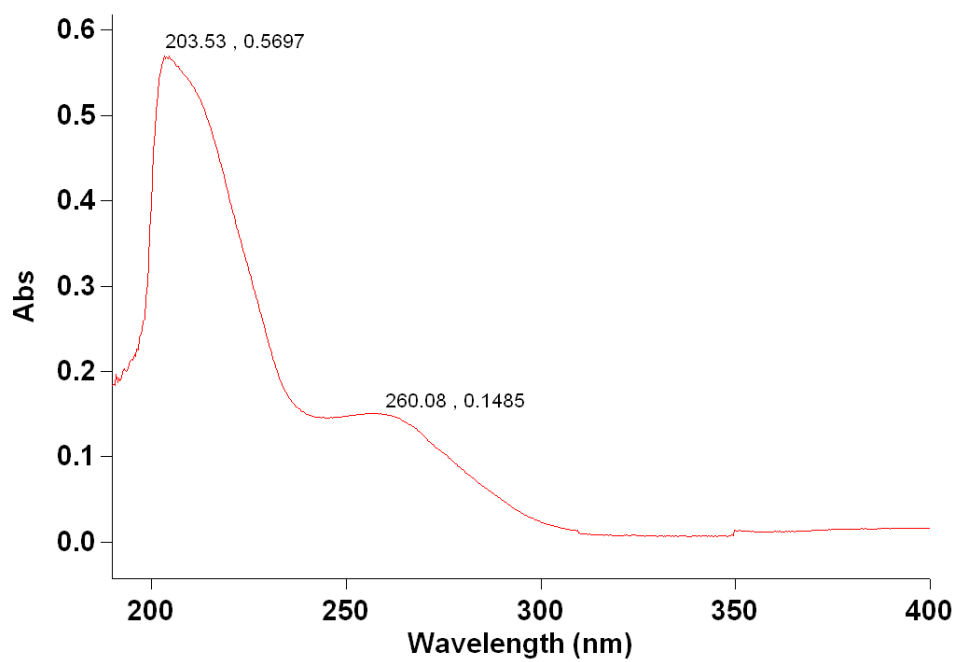


Figure S91. UV-vis spectrum of 3-O-(3-bromobenzyl)unguinol (7h) in MeOH

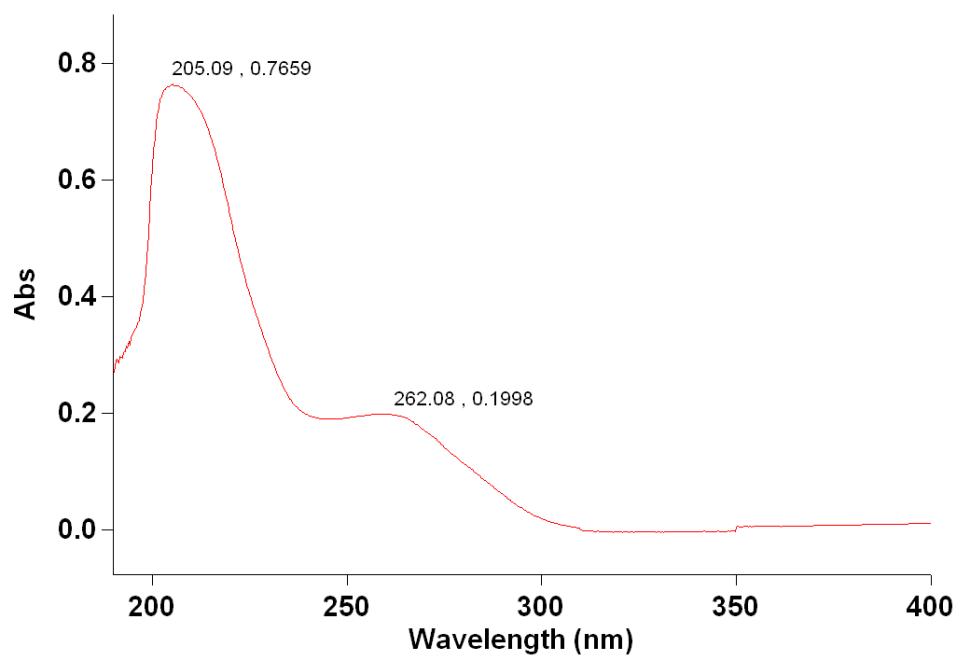


Figure S92. UV-vis spectrum of 3-O-(3-methylbenzyl)unguinol (7i) in MeOH

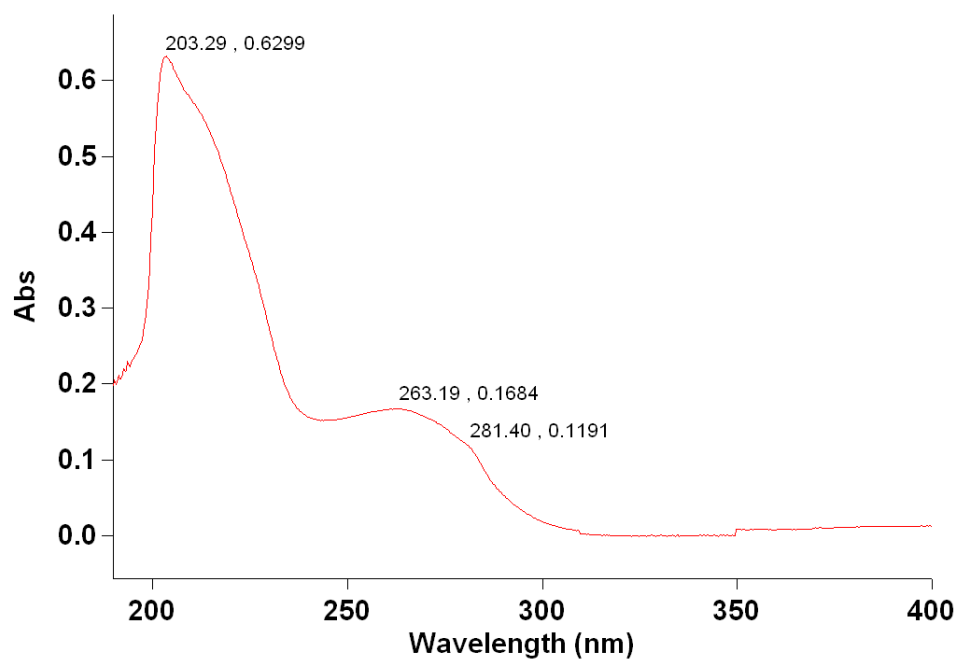


Figure S93. UV-vis spectrum of 3-O-(3-methoxybenzyl)unguinol (7j) in MeOH

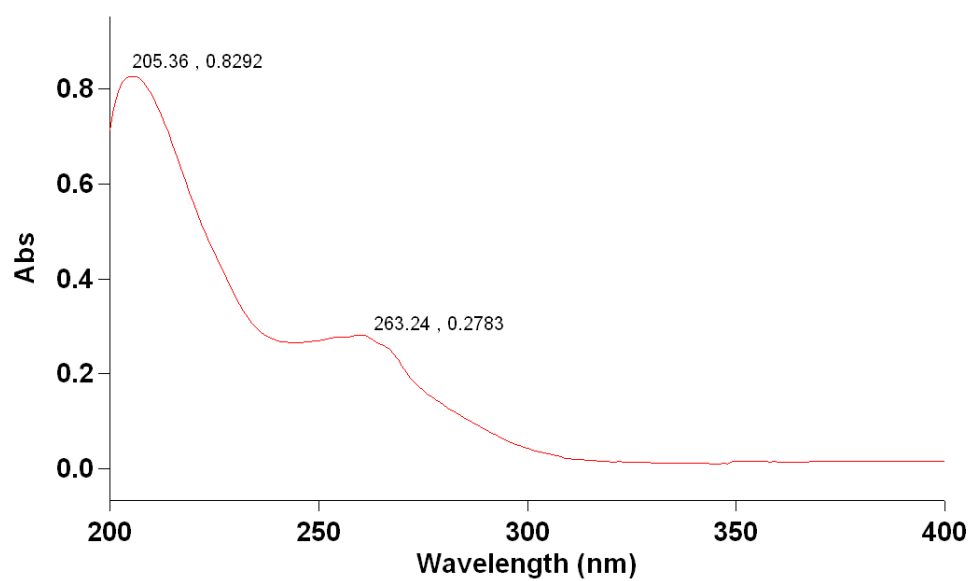


Figure S94. UV-vis spectrum of 3-O-(2-picolyl)unguinol (7k) in MeOH

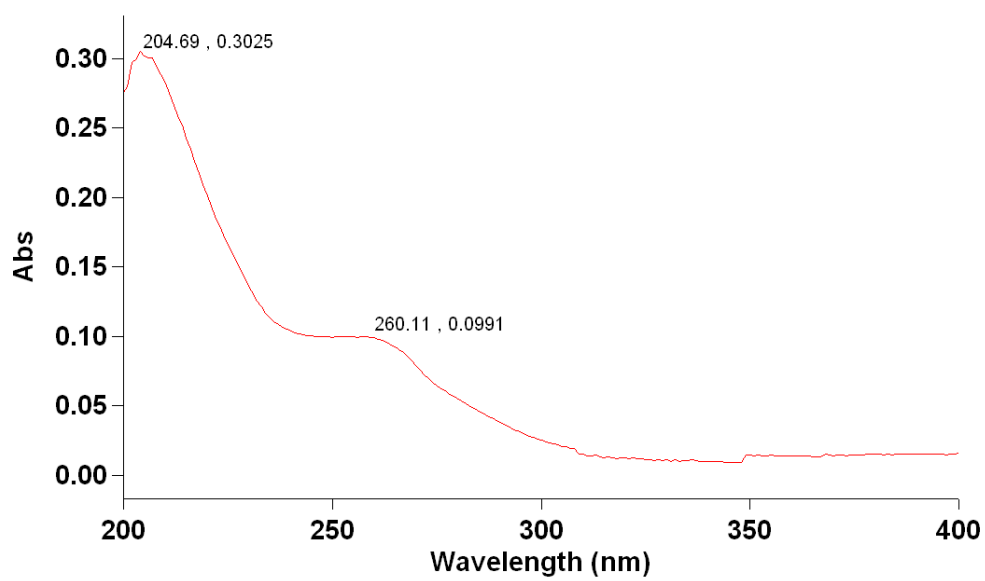


Figure S95. UV-vis spectrum of 3-O-(3-picolyl)unguinol (**7l**) in MeOH

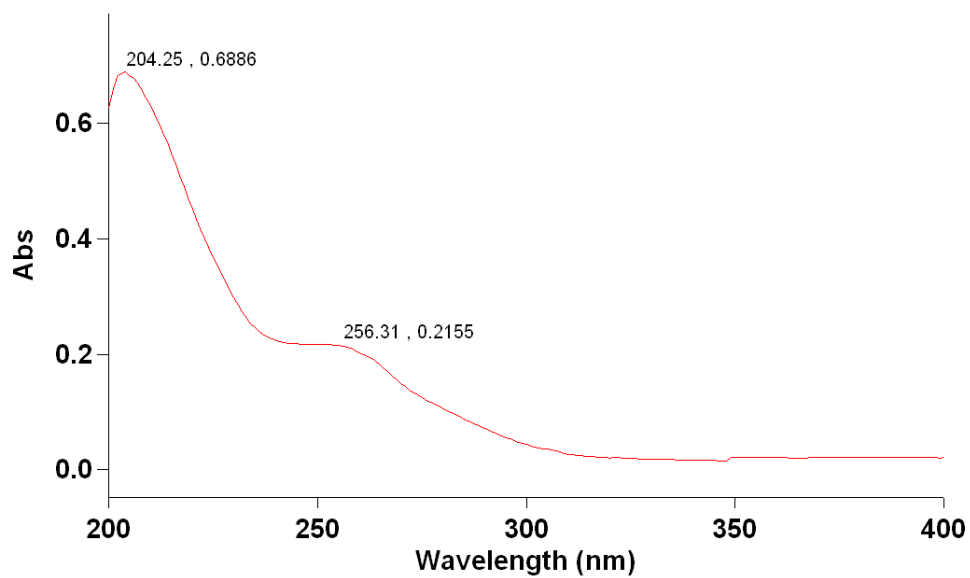


Figure S96. UV-vis spectrum of 3-O-(4-picolyl)unguinol (**7m**) in MeOH

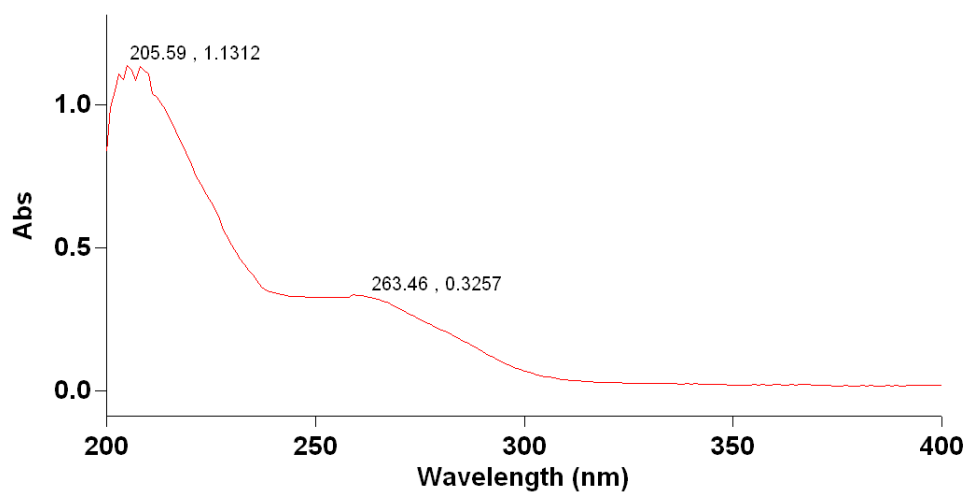


Figure S97. UV-vis spectrum of 3-O-(4-morpholinoethyl)unguinol (**7n**) in MeOH

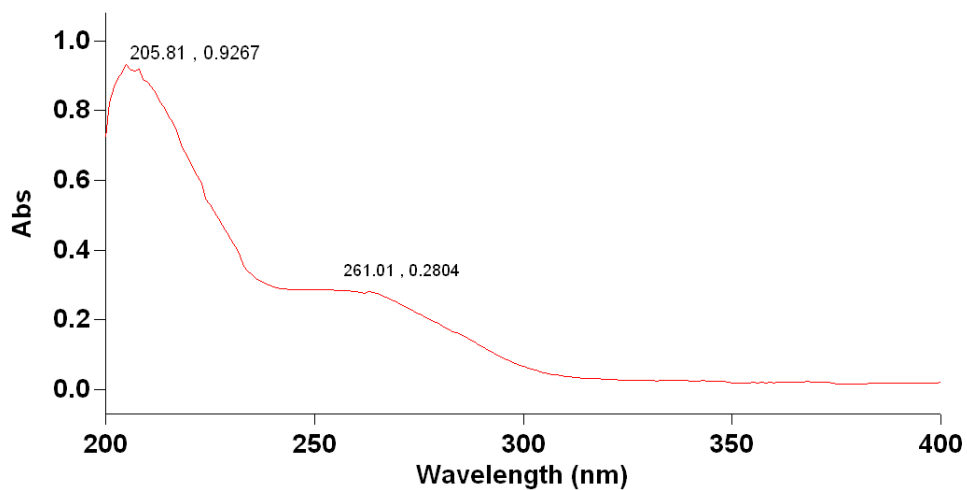


Figure S98. UV-vis spectrum of 3-O-(1-piperidinyethyl)unguinol (**7o**) in MeOH

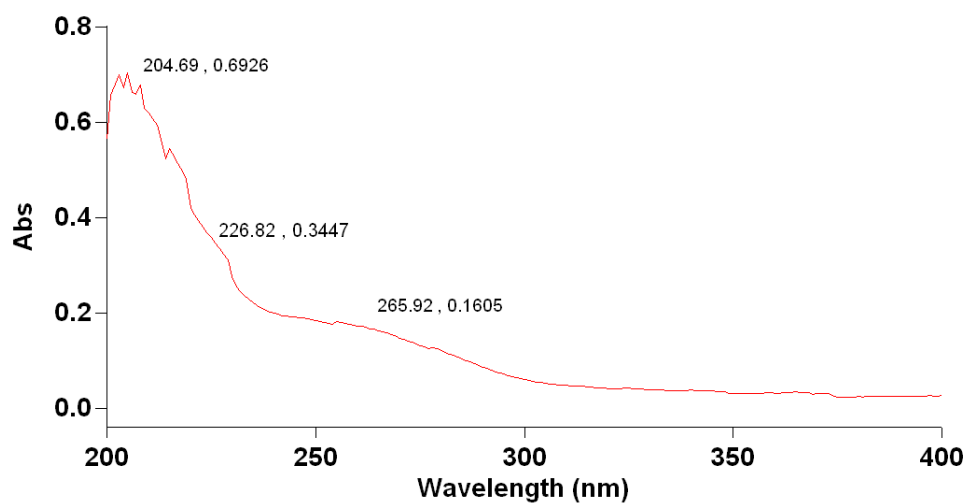


Figure S99. UV-vis spectrum of 3-O-(1-pyrrolidinyethyl)unguinol (**7p**) in MeOH

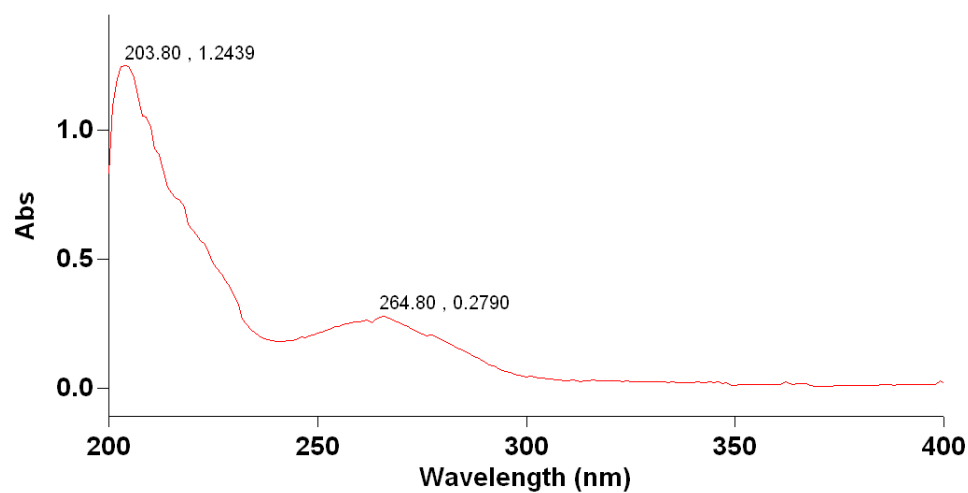


Figure S100. UV-vis spectrum of 3-O-1',2'-dihydrobenzylunguinol (**8a**) in MeOH

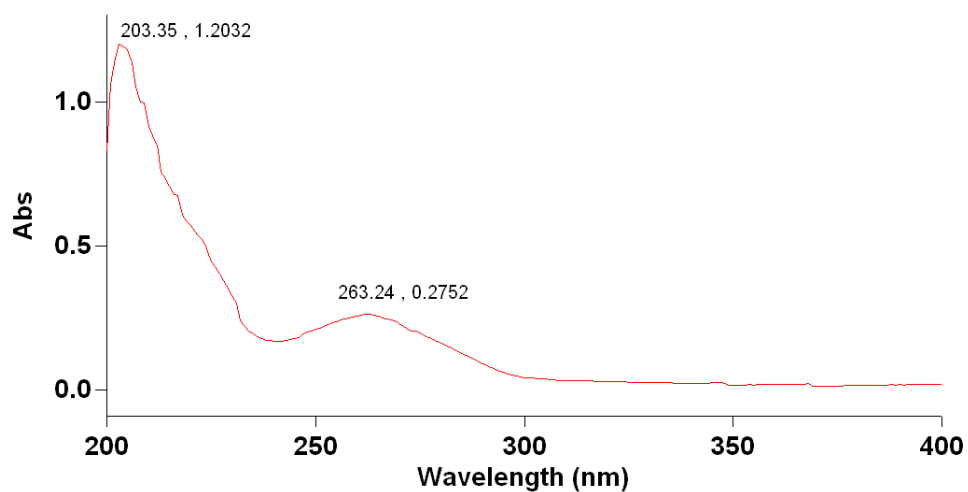


Figure S101. UV-vis spectrum of 3-O-(2-fluorobenzyl)-1',2'-dihydroanguinol (**8b**) in MeOH

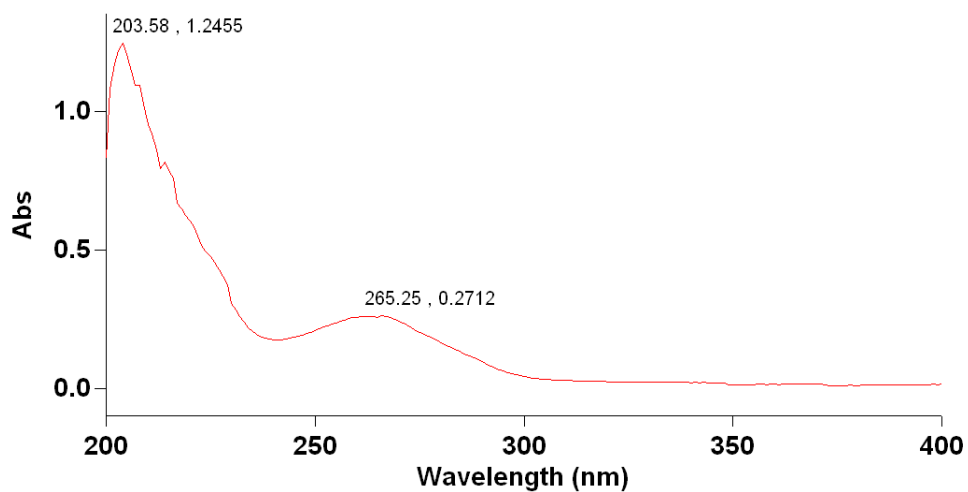


Figure S102. UV-vis spectrum of 3-O-(4-fluorobenzyl)-1',2'-dihydroanguinol (**8c**) in MeOH

180312_P21590_1-2-dihydroanguinol_Pos_1 #81 RT: 0.89 AV: 1 NL: 2.09E7
T: FTMS + p ESI Full ms [150.0000-1800.0000]

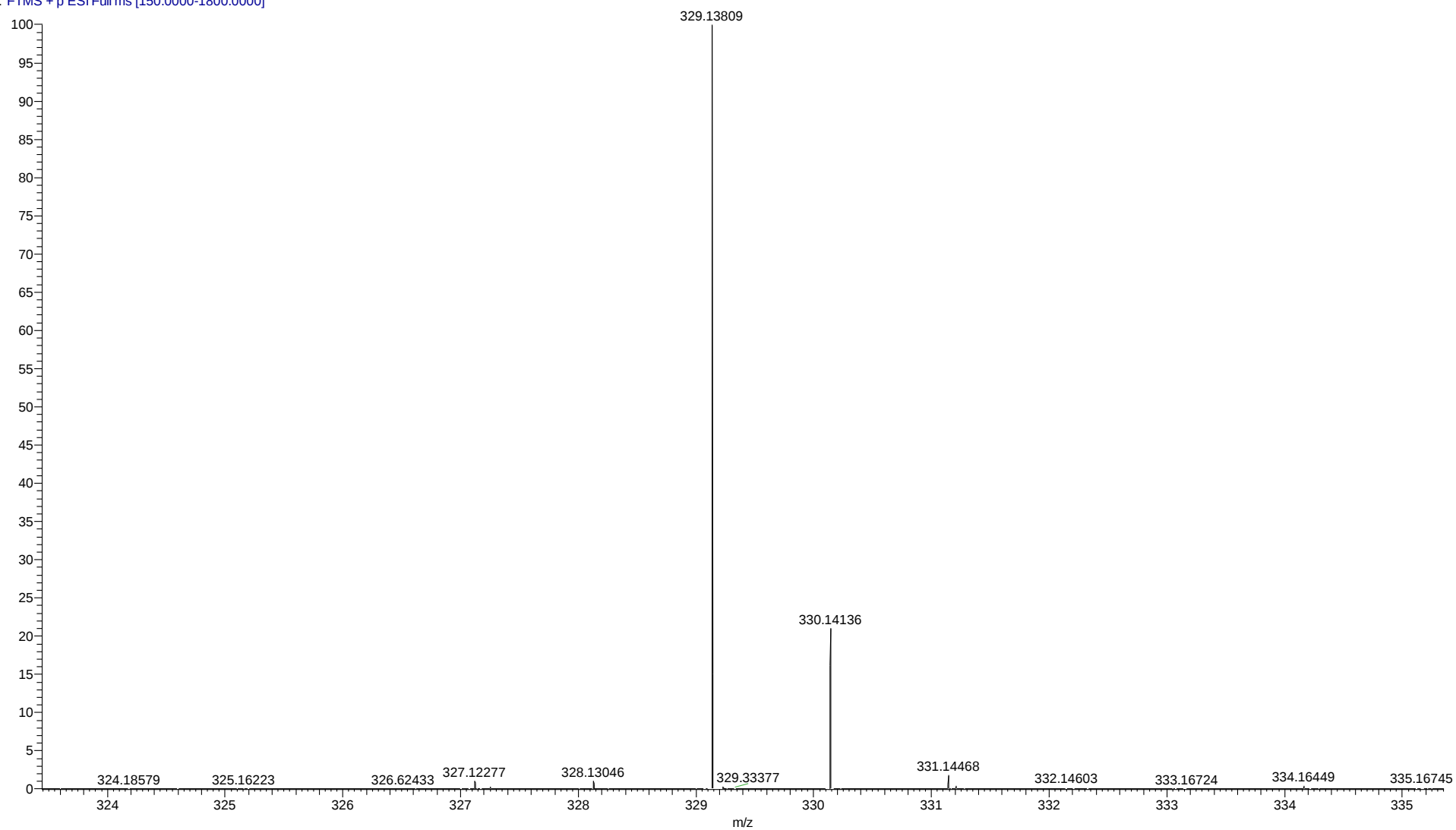


Figure S103. HRESI(+)-MS spectrum of 1',2'-dihydroanguinol (**2a**)

180502_P21590_1-2-epoxyunguinol_Neg_1 #51 RT: 0.61 AV: 1 NL: 7.47E8
T: FTMS - p ESI Full ms [150.0000-1800.0000]

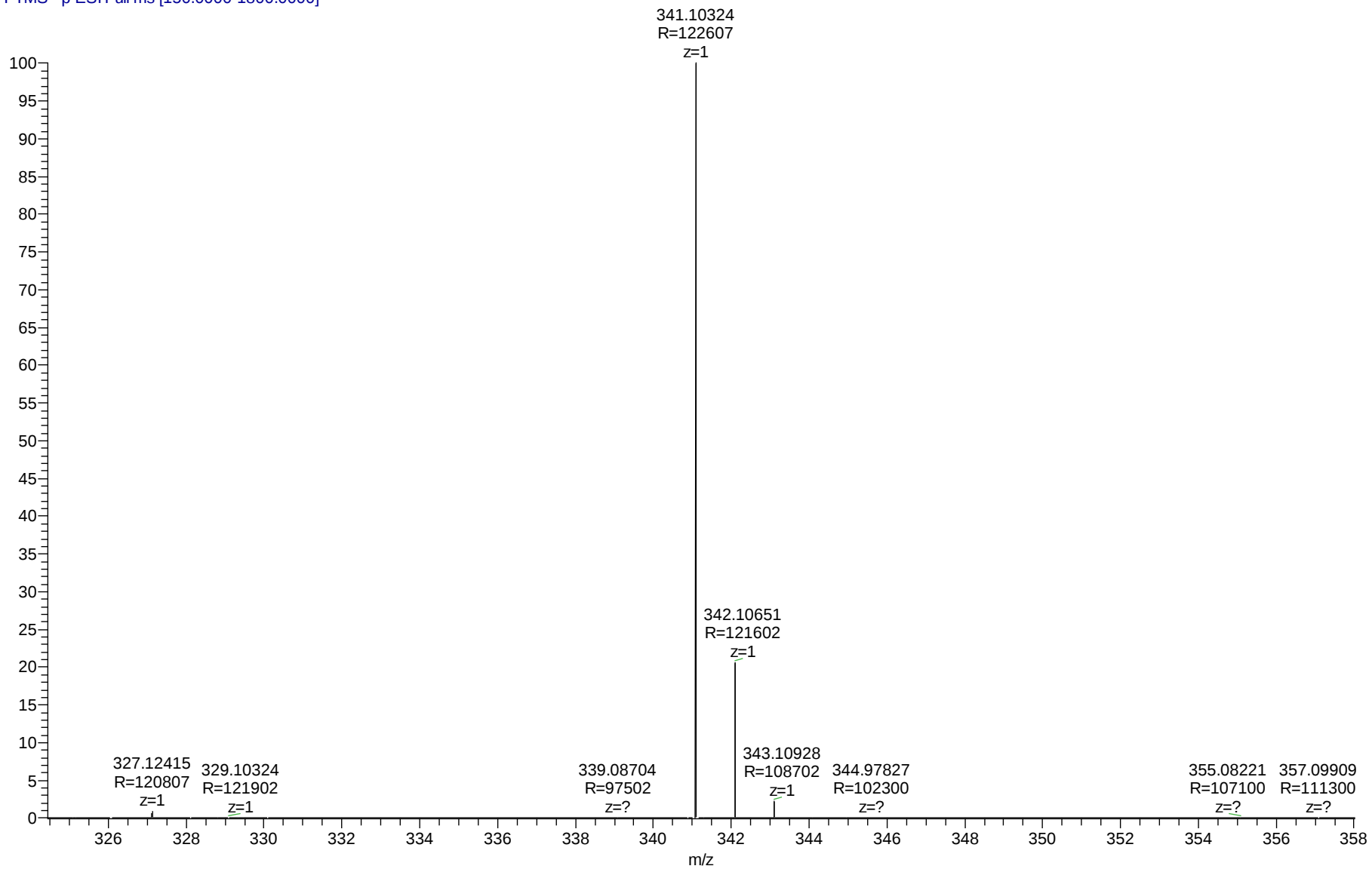


Figure S104. HRESI(-)-MS spectrum of *cis*-1',2'-epoxyunguinol (**2b**)

Epoxy Urguinol 1_Neg #44-51 RT: 0.51-0.58 AV: 8 NL: 1.12E8
T: FTMS - p ESI Full ms [150.0000-1800.0000]

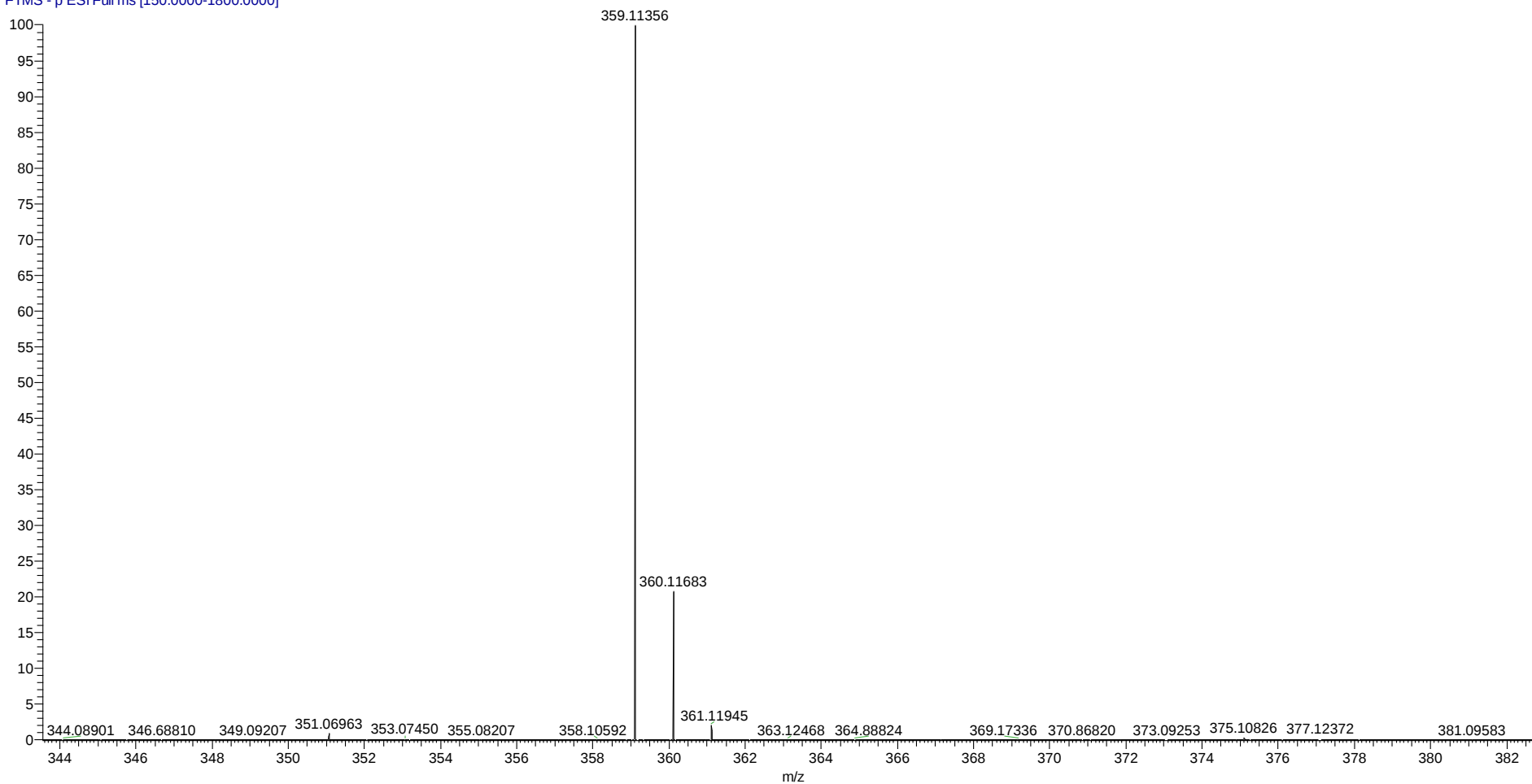


Figure S105. HRESI(-)-MS spectrum of 1',2'-dihydroxyunguinol (**2c**)

AC_15_169_4_Neg_D #41-57 RT: 0.47-0.62 AV: 17 NL: 1.94E8
T: FTMS - p ESI Full ms [150.0000-1800.0000]

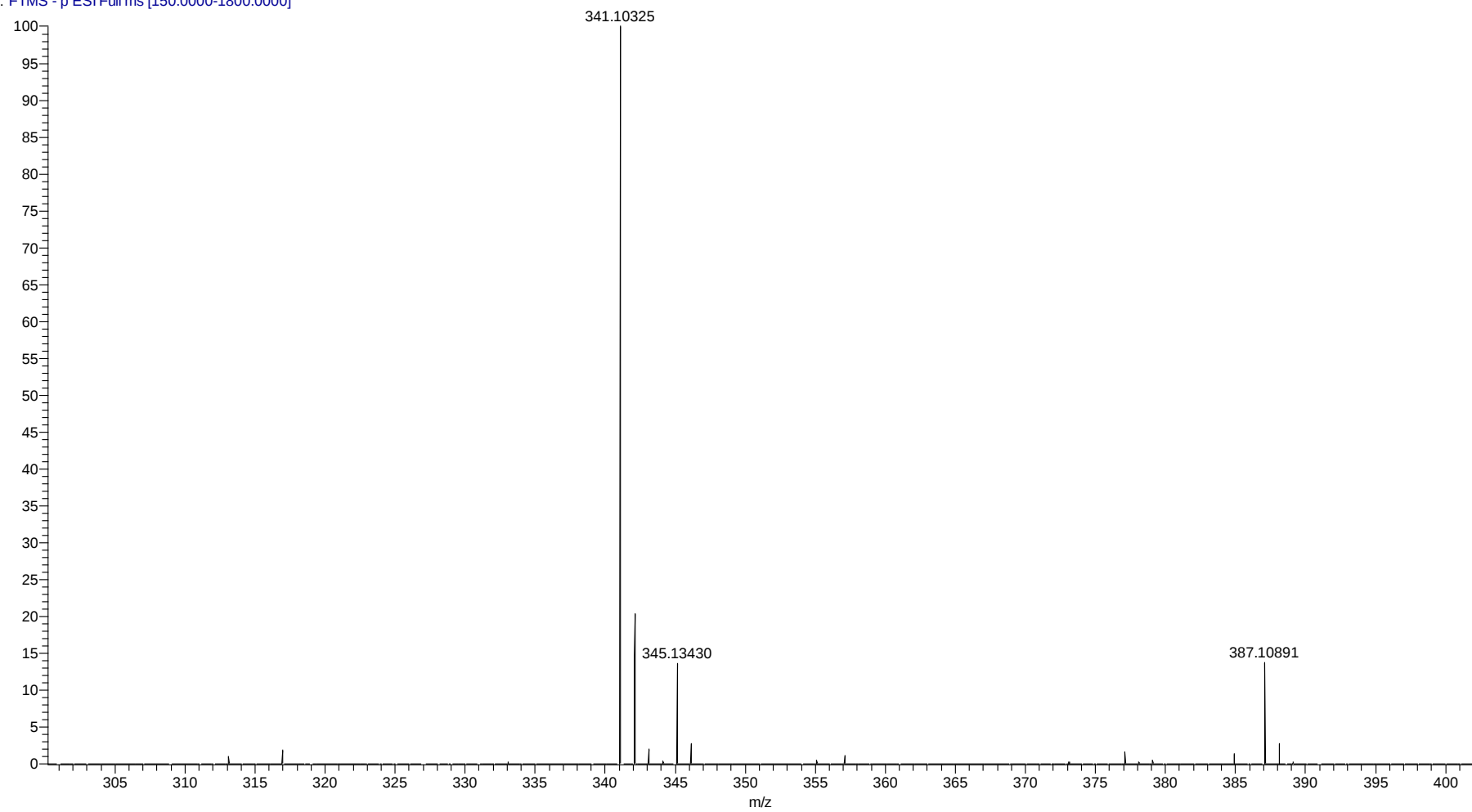


Figure S106. HR-ESI(-)-MS spectrum of 2'-hydroxy- $\Delta^{1',4'}$ -unguinol (2d)

AC_15_9_4_Neg #36-45 RT: 0.44-0.52 AV: 10 NL: 8.74E7
T: FTMS - p ESI Full ms [150.0000-1800.0000]

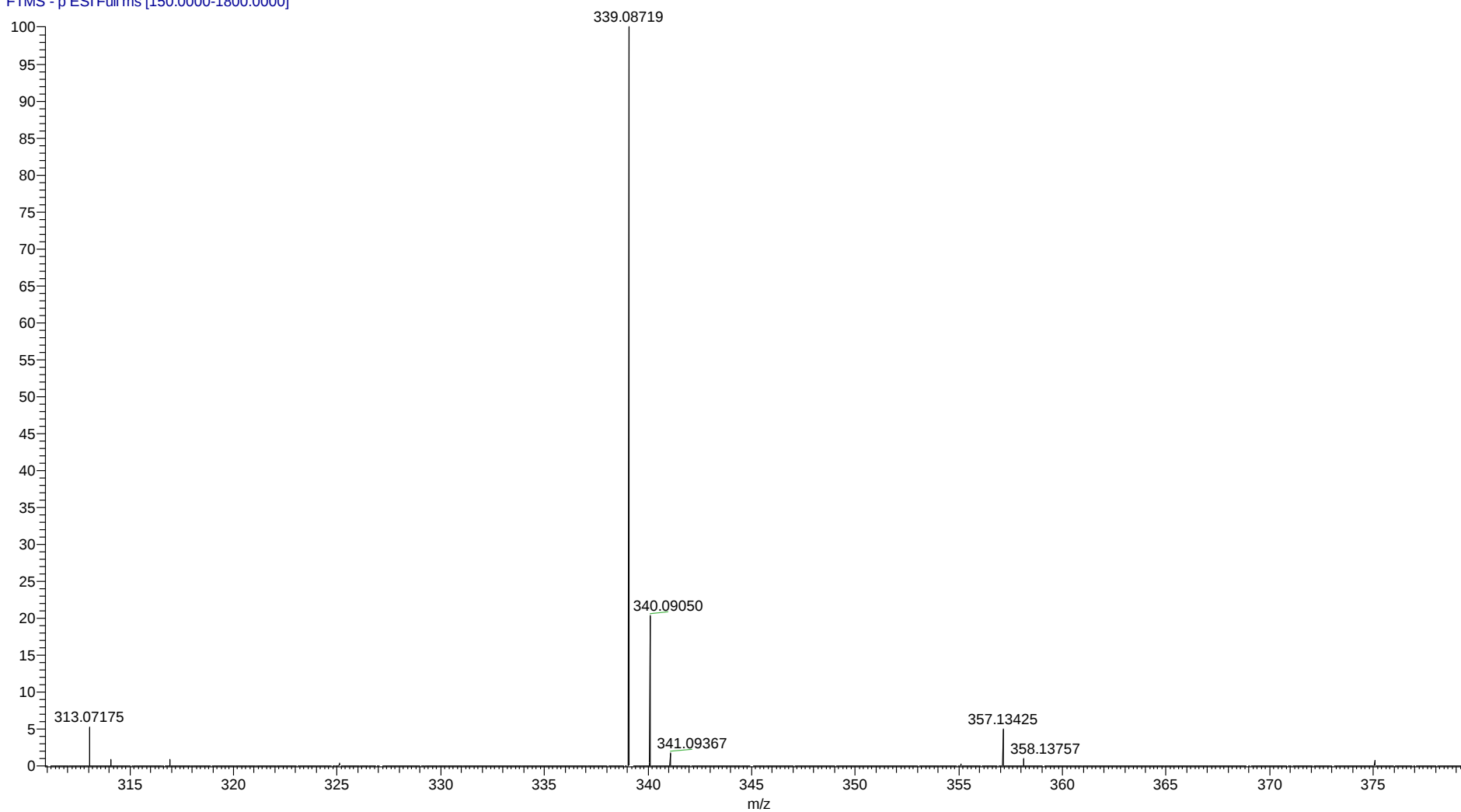


Figure S107. HRESI(-)-MS spectrum of 2'-oxo- $\Delta^{1,4'}$ -unguinol (**2e**)

AC_15_138_4_Neg#42-49 RT: 0.51-0.58 AV: 8 NL: 6.68E7
T: FTMS -p ESI Full ms [150.0000-1800.0000]

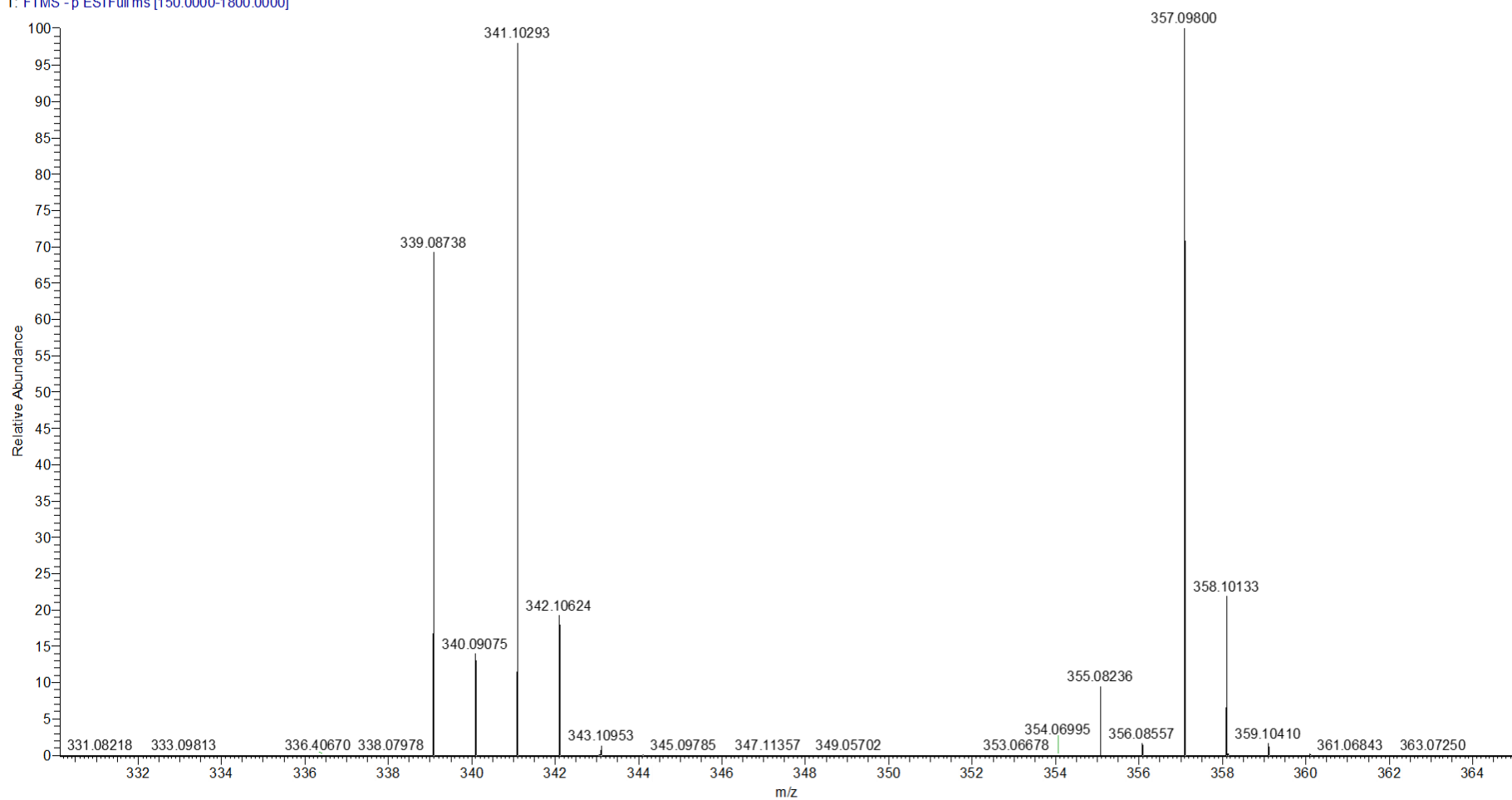


Figure S108. HR-ESI(-)-MS spectrum of 2'-hydroperoxy- $\Delta^{1,4'}$ -unguinol (2f)

Dibromo_1_2_dihydroanguinol_HRMS_NEG #27-402 RT: 0.03-0.48 AV: 376 NL: 4.20E7
T: FTMS - p ESI Full ms [200.00-1000.00]

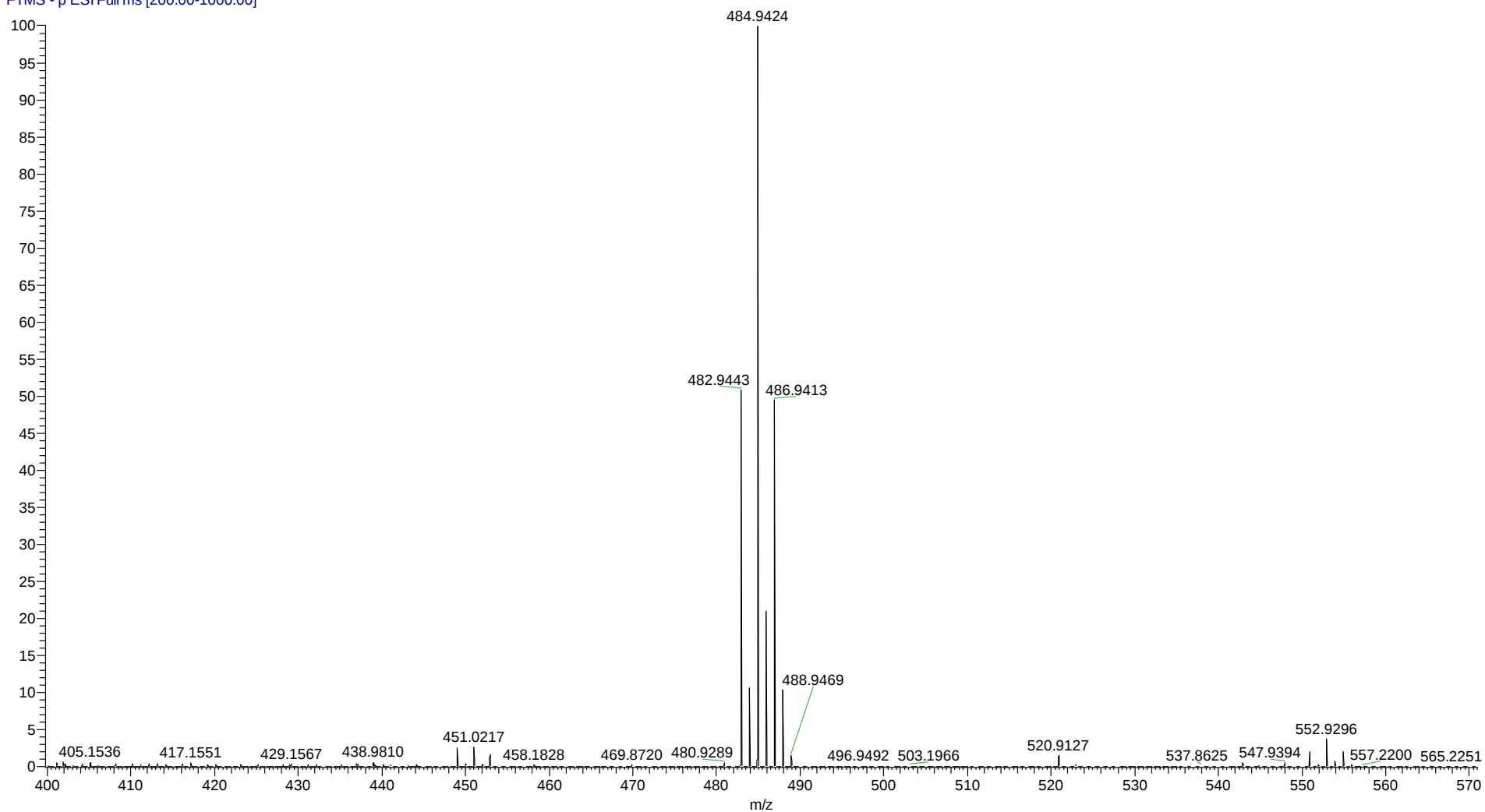


Figure S109. HRESI(-)-MS spectrum of 2,7-dibromo-1',2'-dihydroanguinol (**3a**)

2_4_7_1_2_dihydroanguinol_HRMS_NEG #74-362 RT: 0.09-0.43 AV: 289 NL: 5.27E7
T: FTMS - p ESI Full ms [200.00-1000.00]

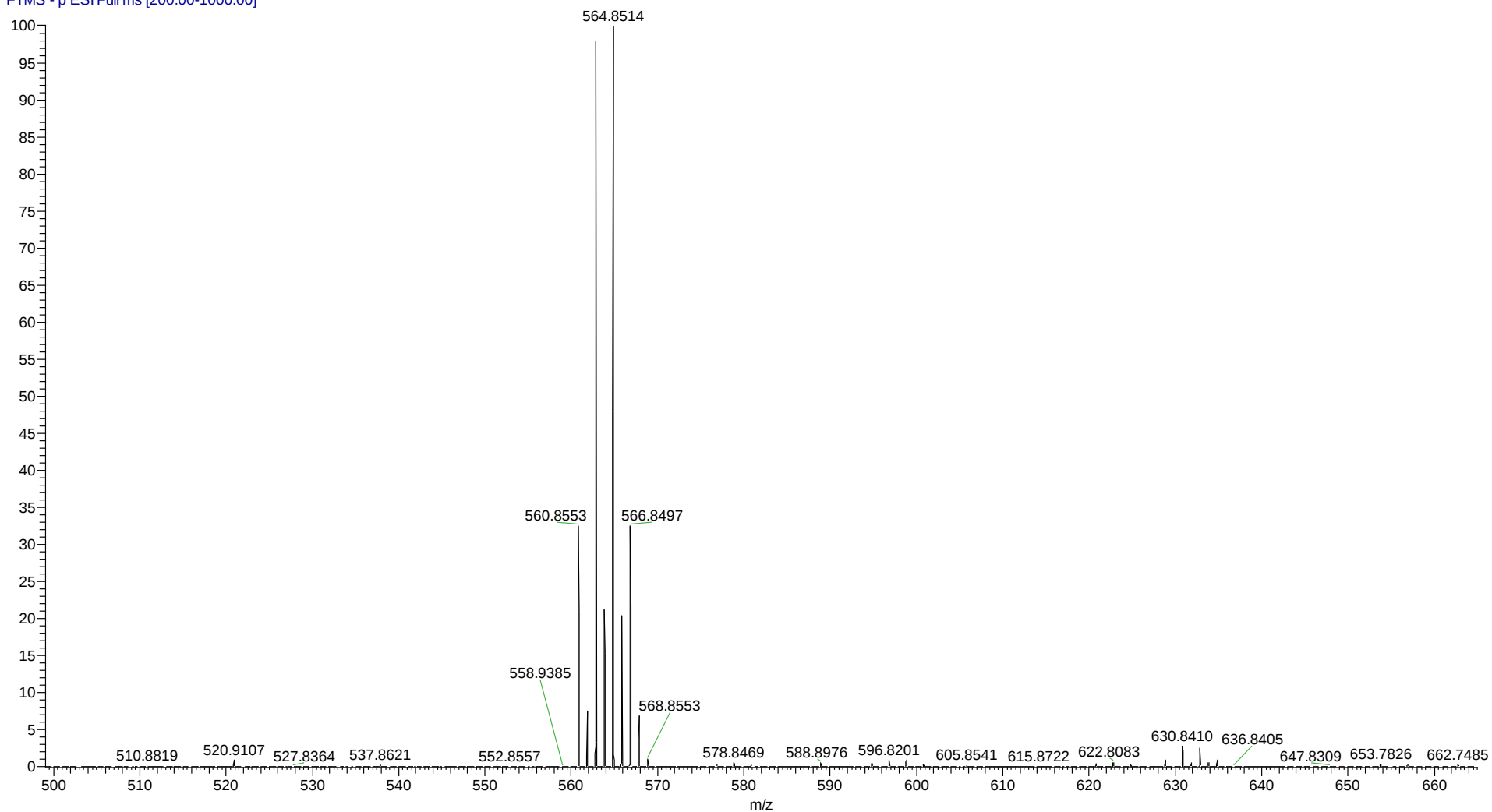


Figure S110. HRESI(-)-MS spectrum of 2,4,7-tribromo-1',2'-dihydroanguinol (**3b**)

2_4diiodo_1_2_dihydroanguinol_HRMS_NEG #23-393 RT: 0.03-0.47 AV: 371 NL: 8.31E7
T: FTMS - p ESI Full ms [200.00-1000.00]

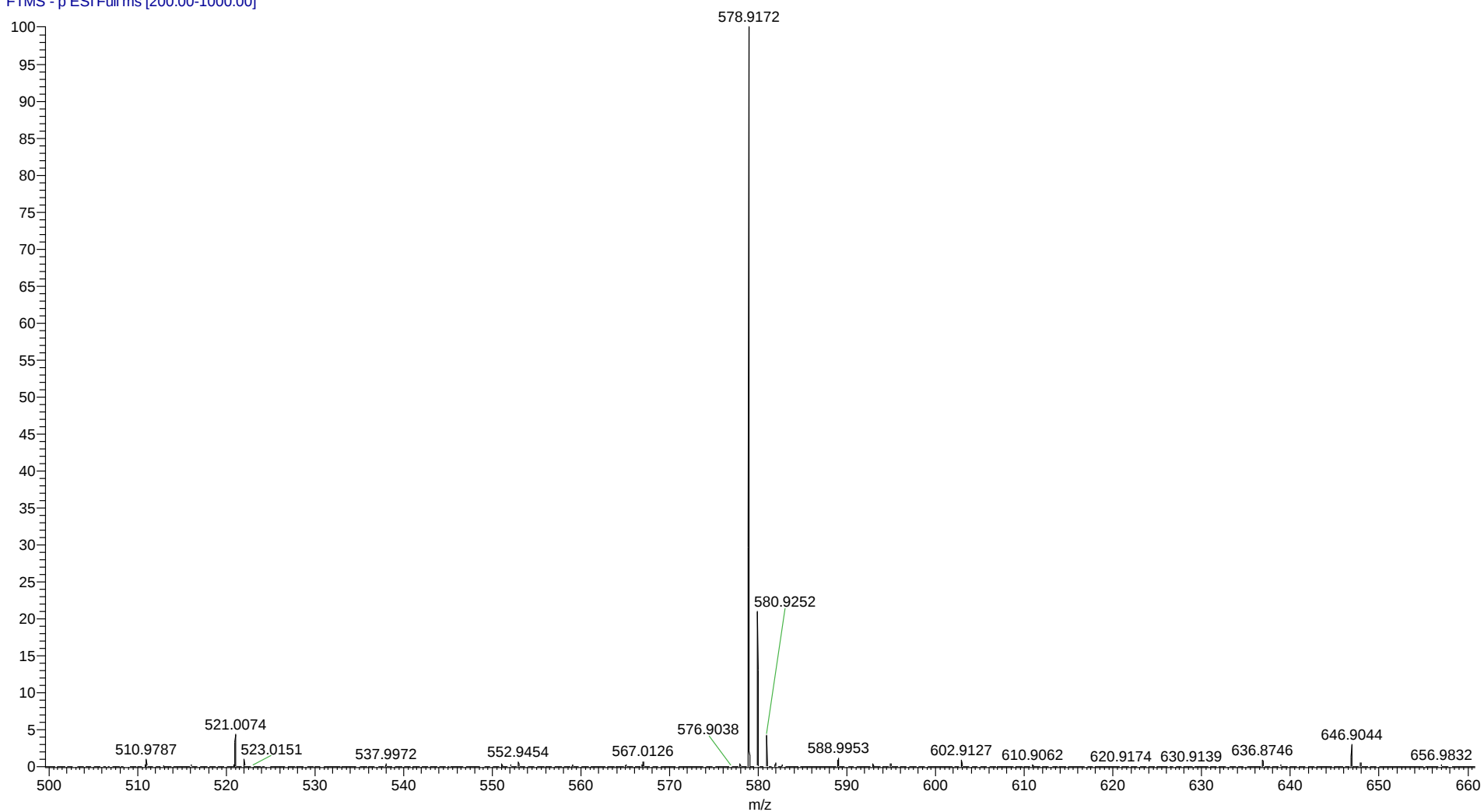


Figure S111. HRESI(-)-MS spectrum of 2,4-diiodo-1',2'-dihydroanguin (**3c**)

AC_14_175_6 Neg #34-48 RT: 0.41-0.54 AV: 15 NL: 3.02E8
T: FTMS - p ESI Full ms [150.0000-1800.0000]

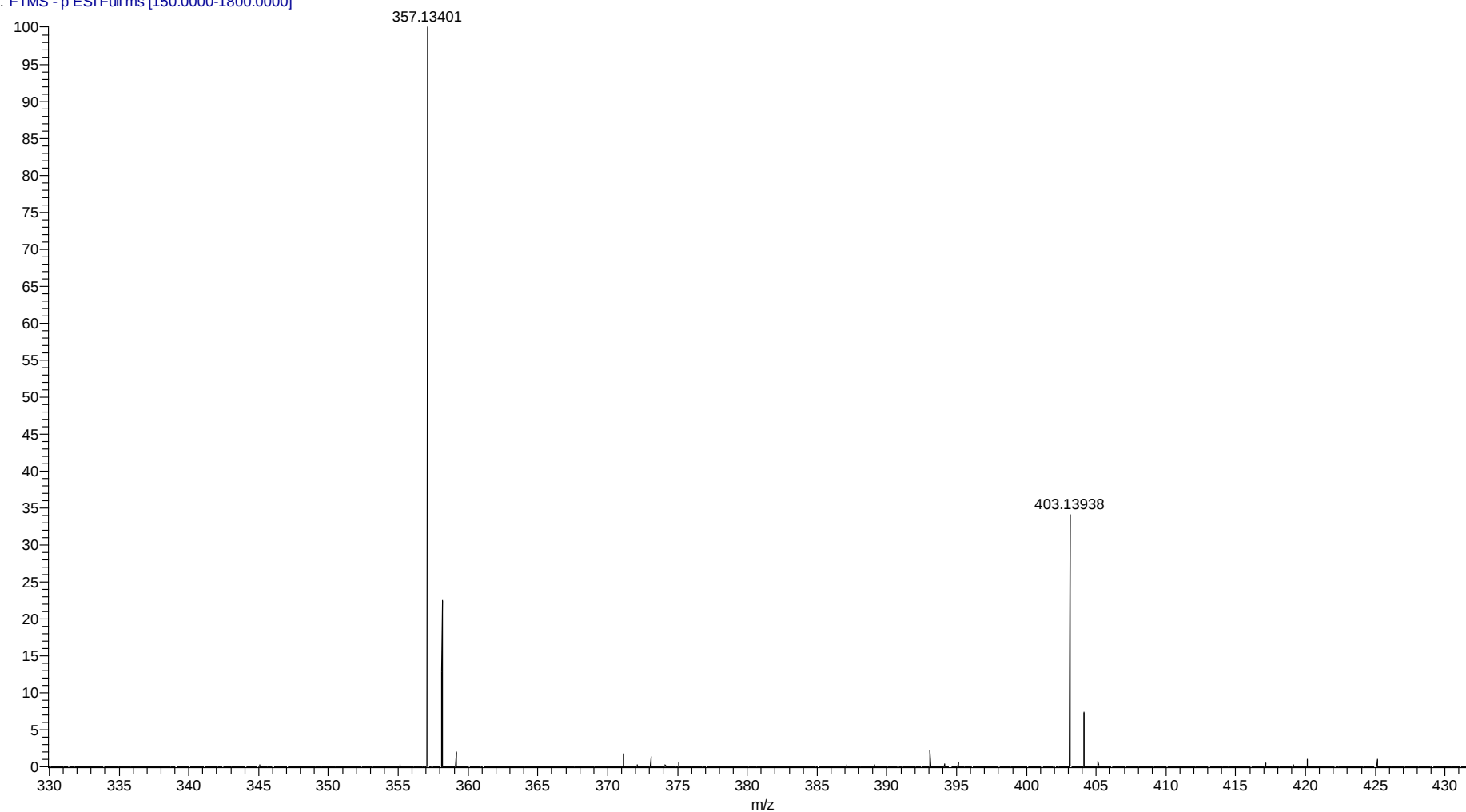


Figure S112. HRESI(-)-MS spectrum of methylunguinate (**4a**)

AC_14_184_2_Neg_F #43-65 RT: 0.50-0.70 AV: 23 NL: 3.49E8
T: FTMS - p ESI Full ms [150.0000-1800.0000]

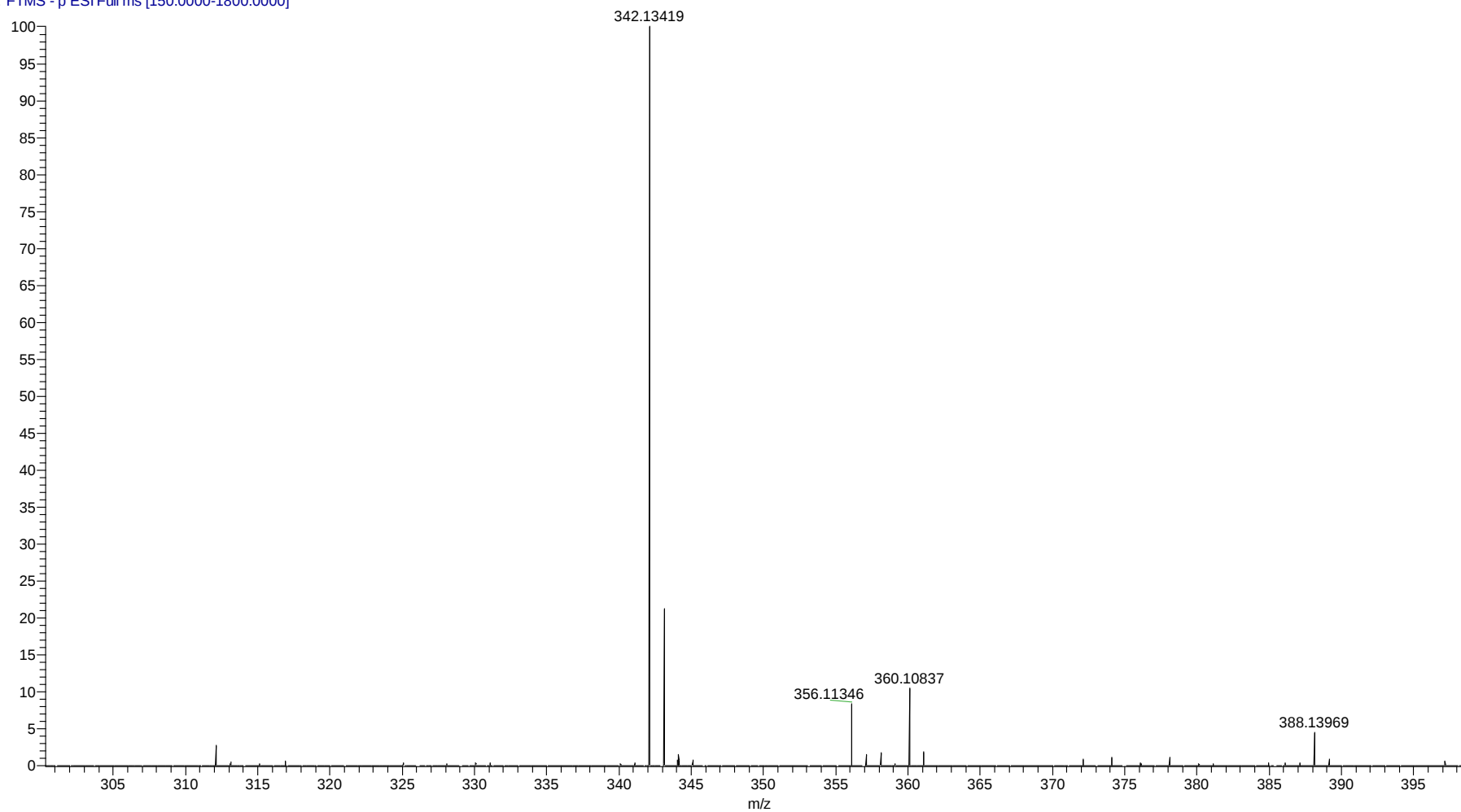


Figure S113. HRESI(-)-MS spectrum of unguinolamide (**4b**)

180823_3_O_methylunguinol_1_180823115213_#49 RT: 0.57 AV: 1 NL: 7.56E6
T: FTMS - p ESI Full ms [150.0000-1800.0000]

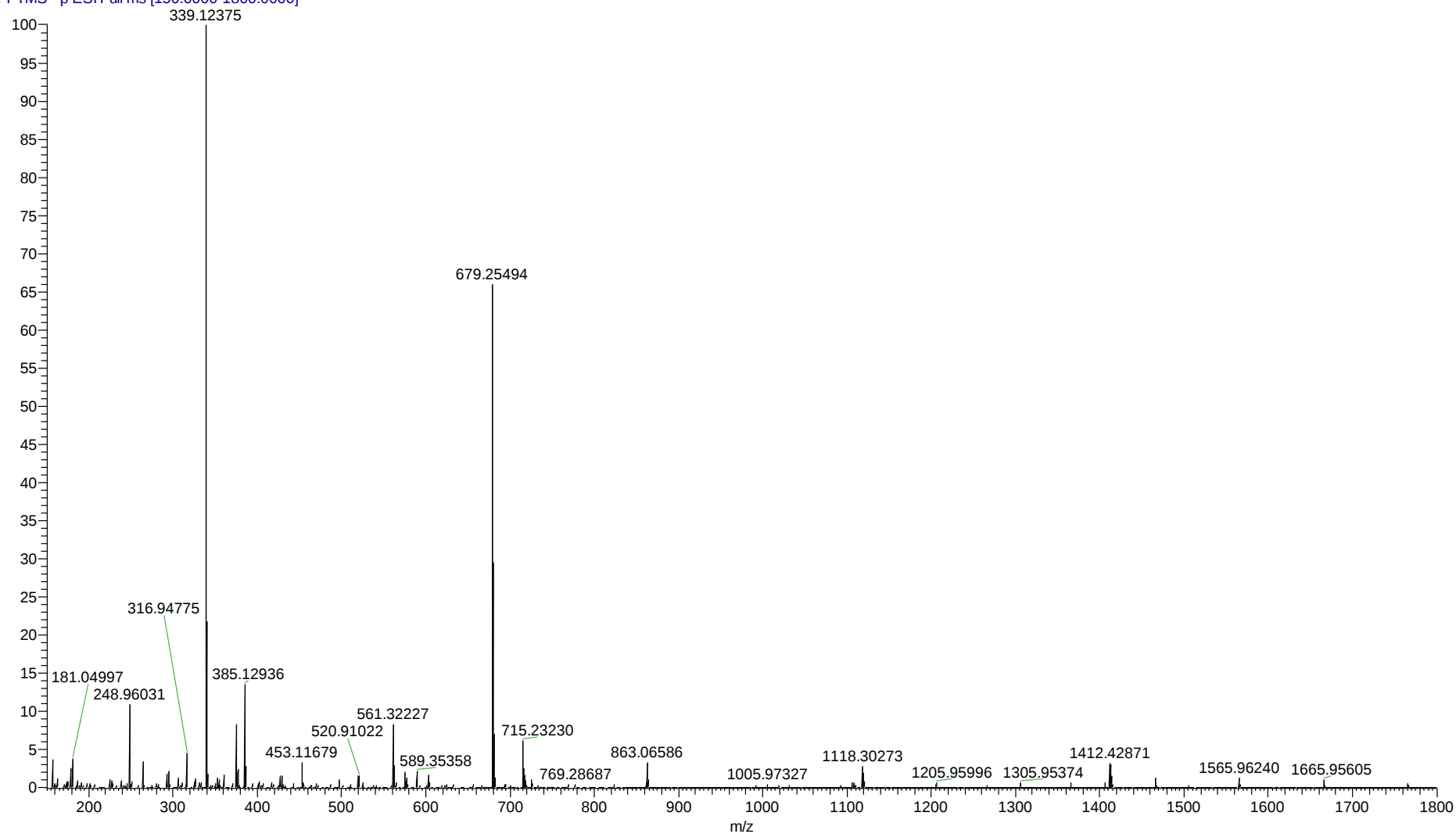


Figure S114. HRESI(-)-MS spectrum of 3-*O*-methylunguinol (**5a**)

3,8-di-O-methylunguinol_HRMS_POS #61-384 RT: 0.07-0.45 AV: 324 NL: 4.94E8
T: FTMS + p ESI Full ms [200.00-1000.00]

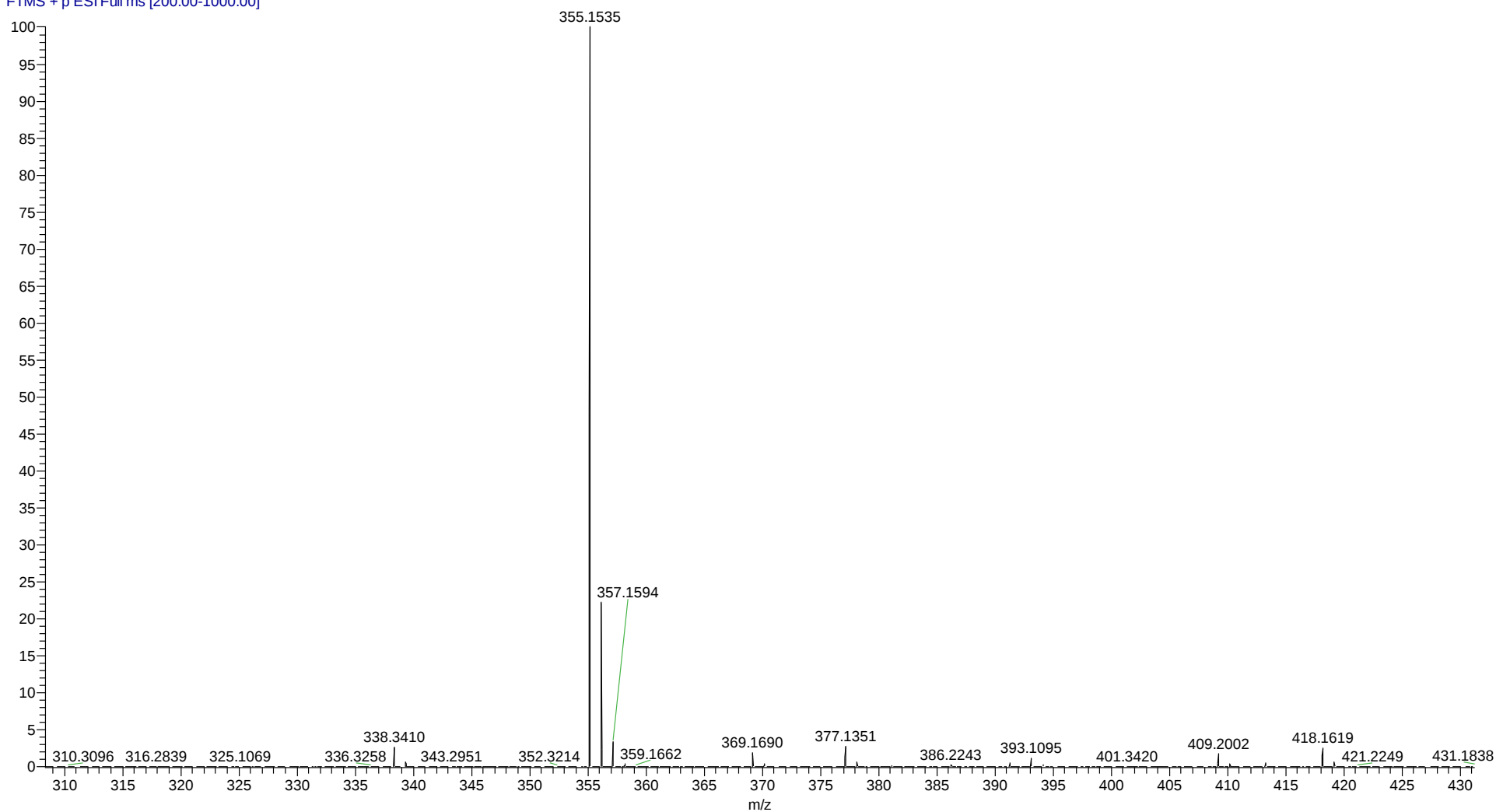


Figure S115. HRESI(+)-MS spectrum of 3,8-di-O-methylunguinol (5b)

monobenzylated_unguinol_HRMS_POS #47-384 RT: 0.06-0.45 AV: 338 NL: 1.96E8
T: FTMS + p ESI Full ms [200.00-1000.00]

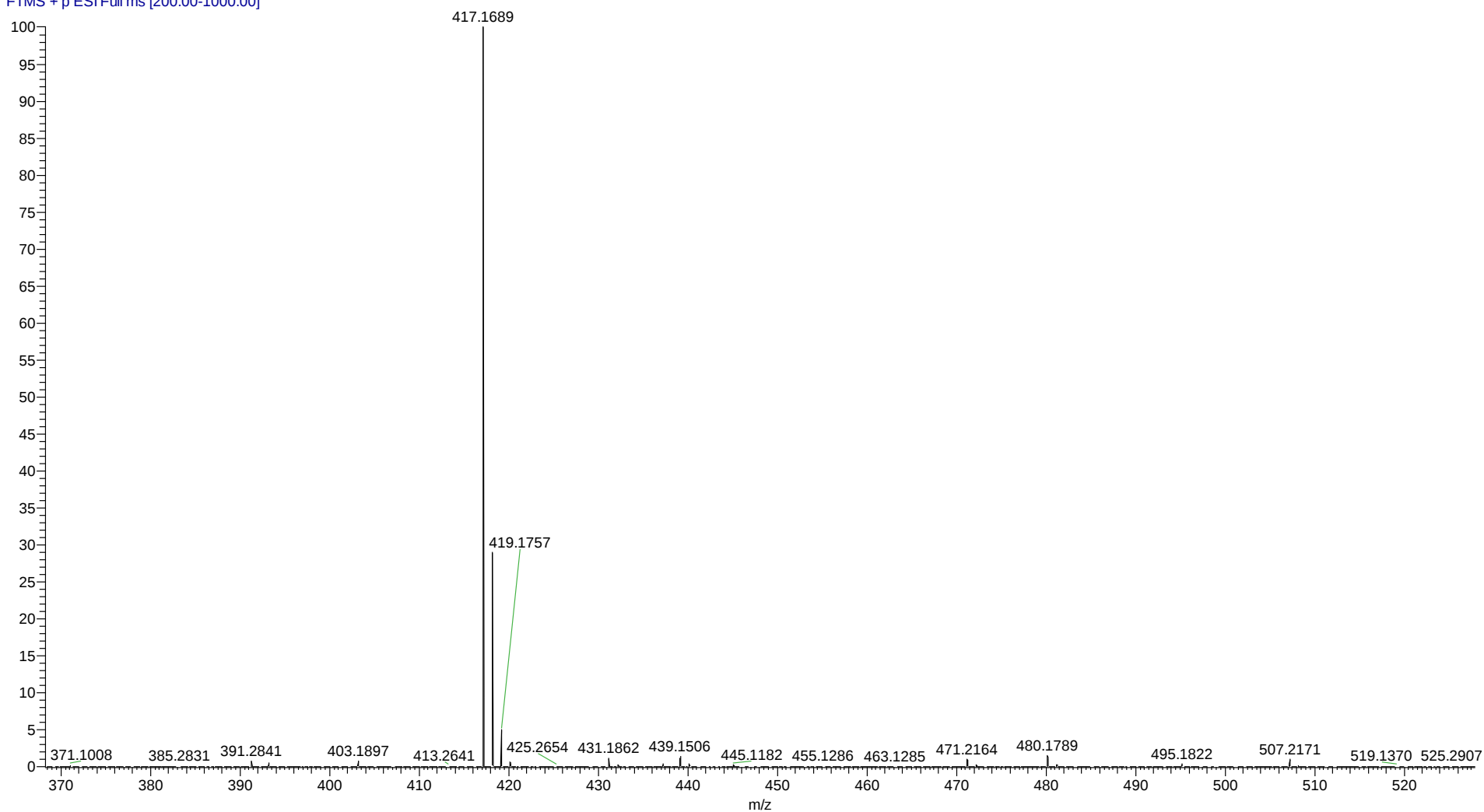


Figure S116. HRESI(+)-MS spectrum of 3-O-benzylunguinol (**6a**)

Dibenzylated_Unguinol_HRMS_POS #19-353 RT: 0.02-0.42 AV: 335 NL: 2.10E7
T: FTMS + p ESI Full ms [200.00-1000.00]

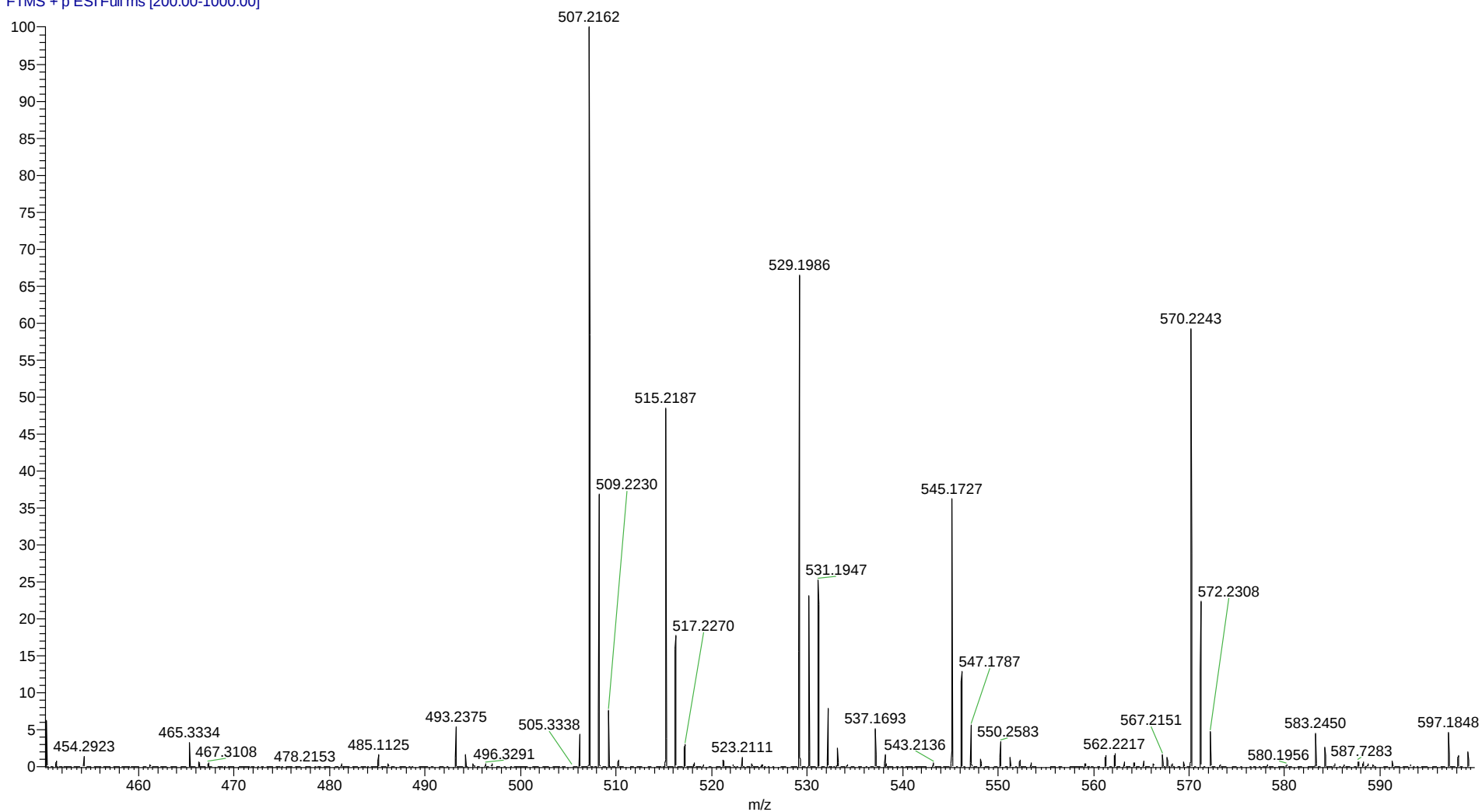


Figure S117. HRESI(+)-MS spectrum of 3,8-di-O-benzylunguinol (**6b**)

2_Cl_BnBr_Mono_Pos #39-47 RT: 0.52-0.60 AV: 9 NL: 1.01E6
T: FTMS + p ESI Full ms [150.0000-2200.0000]

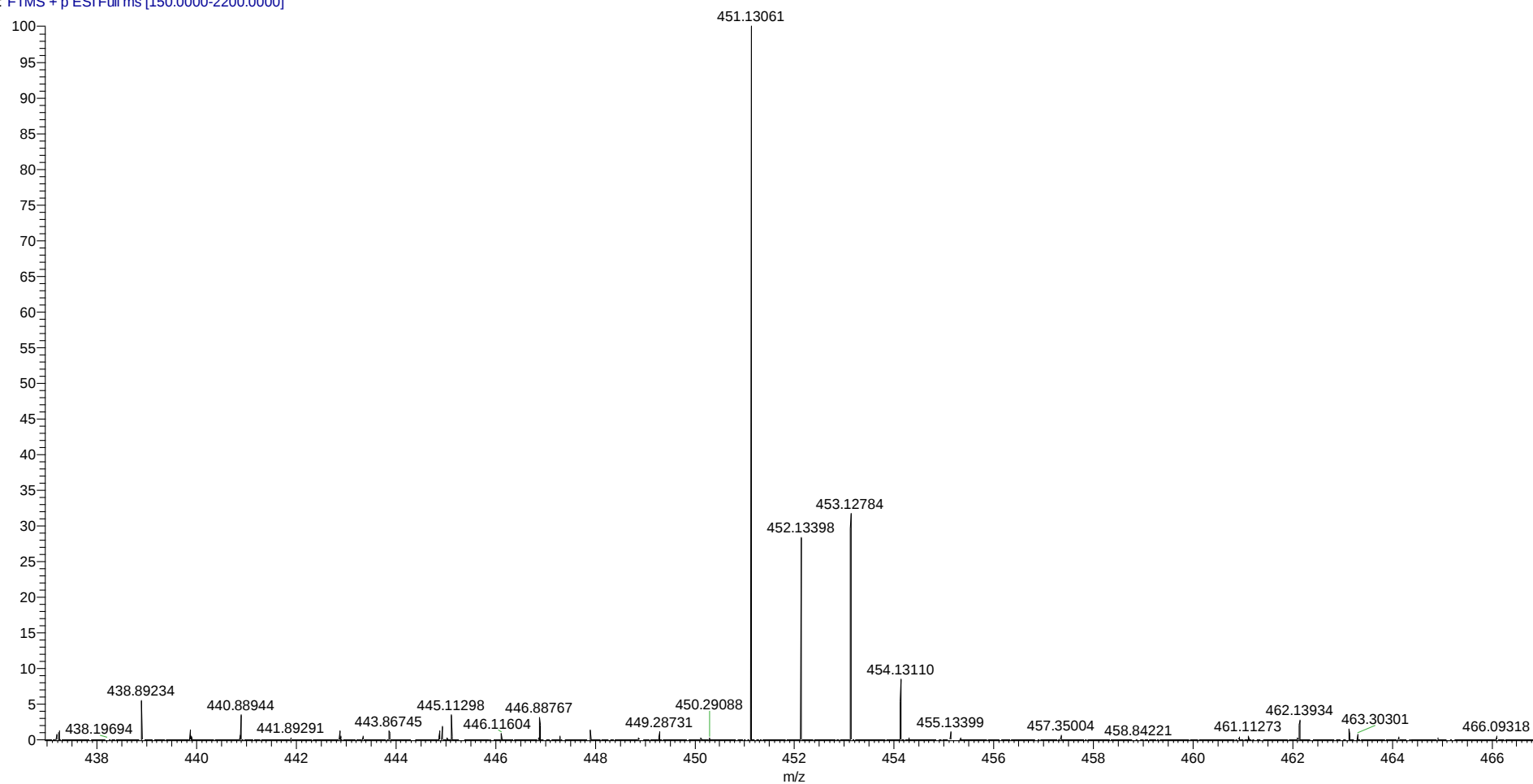


Figure S118. HRESI(+)-MS spectrum of 3-O-(2-chlorobenzyl)unguinol (**7a**)

3_Cl_Bn_Br_Mono_Neg #39-60 RT: 0.46-0.66 AV: 22 NL: 2.27E7
T: FTMS - p ESI Full ms [150.0000-1800.0000]

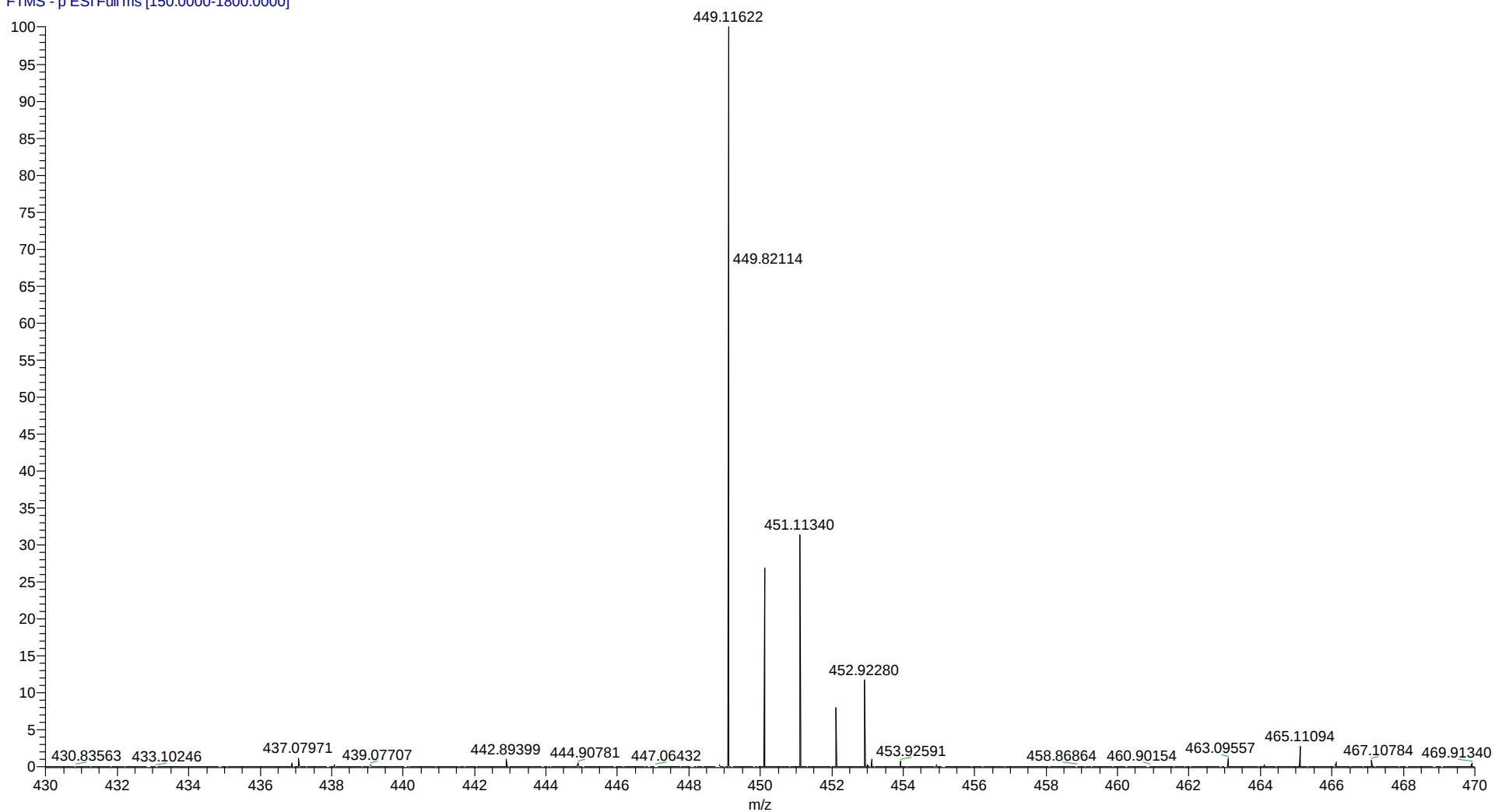


Figure S119. HRESI(-)-MS spectrum of 3-O-(3-chlorobenzyl)unguinol (**7b**)

4_Cl_BnBr_Mono_Neg #39-45 RT: 0.51-0.56 AV: 7 NL: 1.26E7
T: FTMS - p ESI Full ms [150.0000-1800.0000]

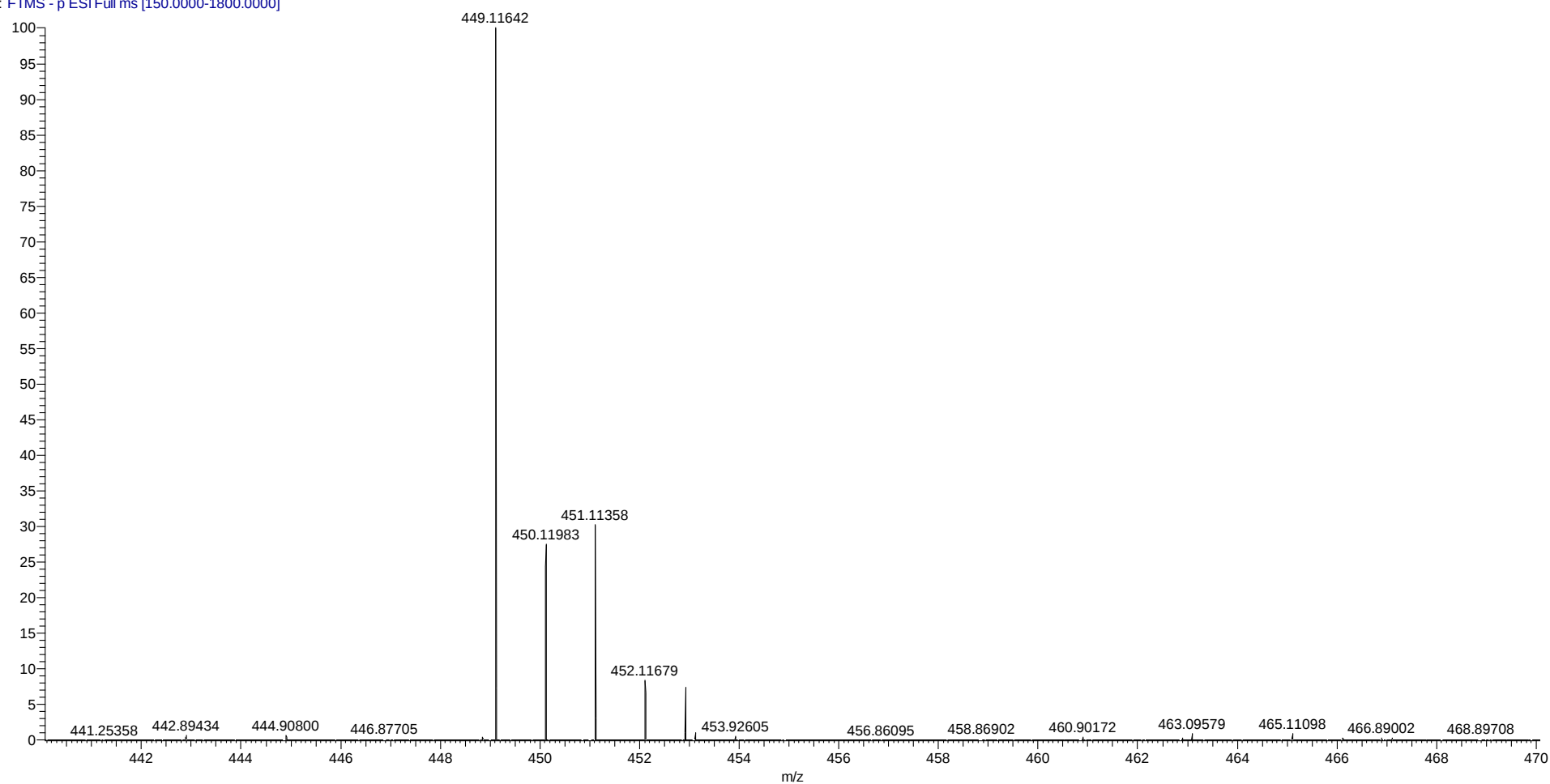


Figure S120. HRESI(-)-MS spectrum of 3-O-(4-chlorobenzyl)unguinol (7c)

2_F_BnBr_Mono_Pos #37-48 RT: 0.49-0.62 AV: 12 NL: 2.84E6
T: FTMS + p ESI Full ms [150.0000-2200.0000]

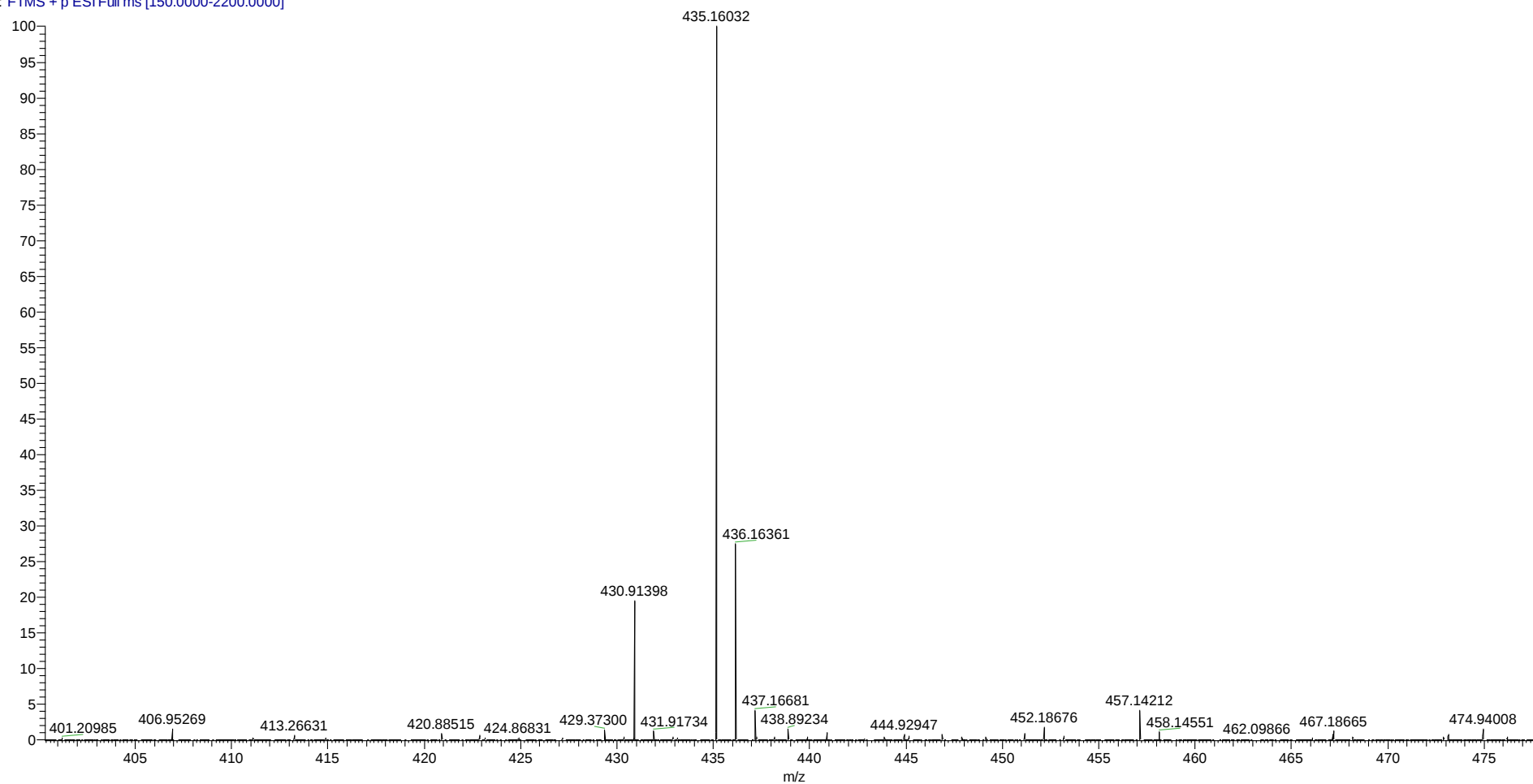


Figure S121. HRESI(+)-MS spectrum of 3-O-(2-fluorobenzyl)unguinol (**7d**)

3_F_Bn_Br_Mono_Neg #38-48 RT: 0.44-0.53 AV: 11 NL: 3.12E7
T: FTMS - p ESI Full ms [150.0000-1800.0000]

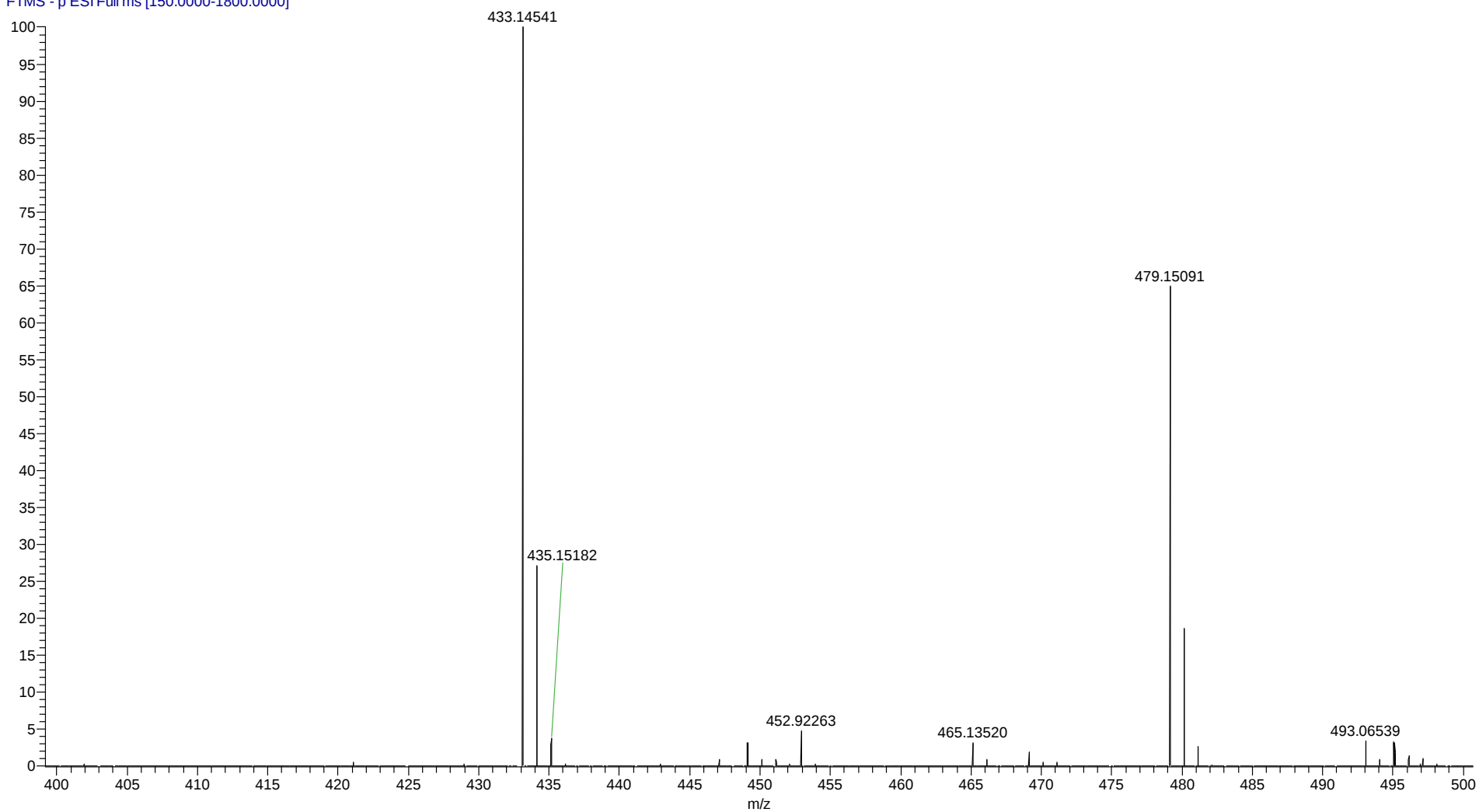


Figure S122. HRESI(-)-MS spectrum of 3-O-(3-fluorobenzyl)unguinol (**7e**)

4_F_BNBr_Mono_Neg #43-50 RT: 0.51-0.57 AV: 8 NL: 1.99E7
T: FTMS - p ESI Full ms [150.0000-1800.0000]

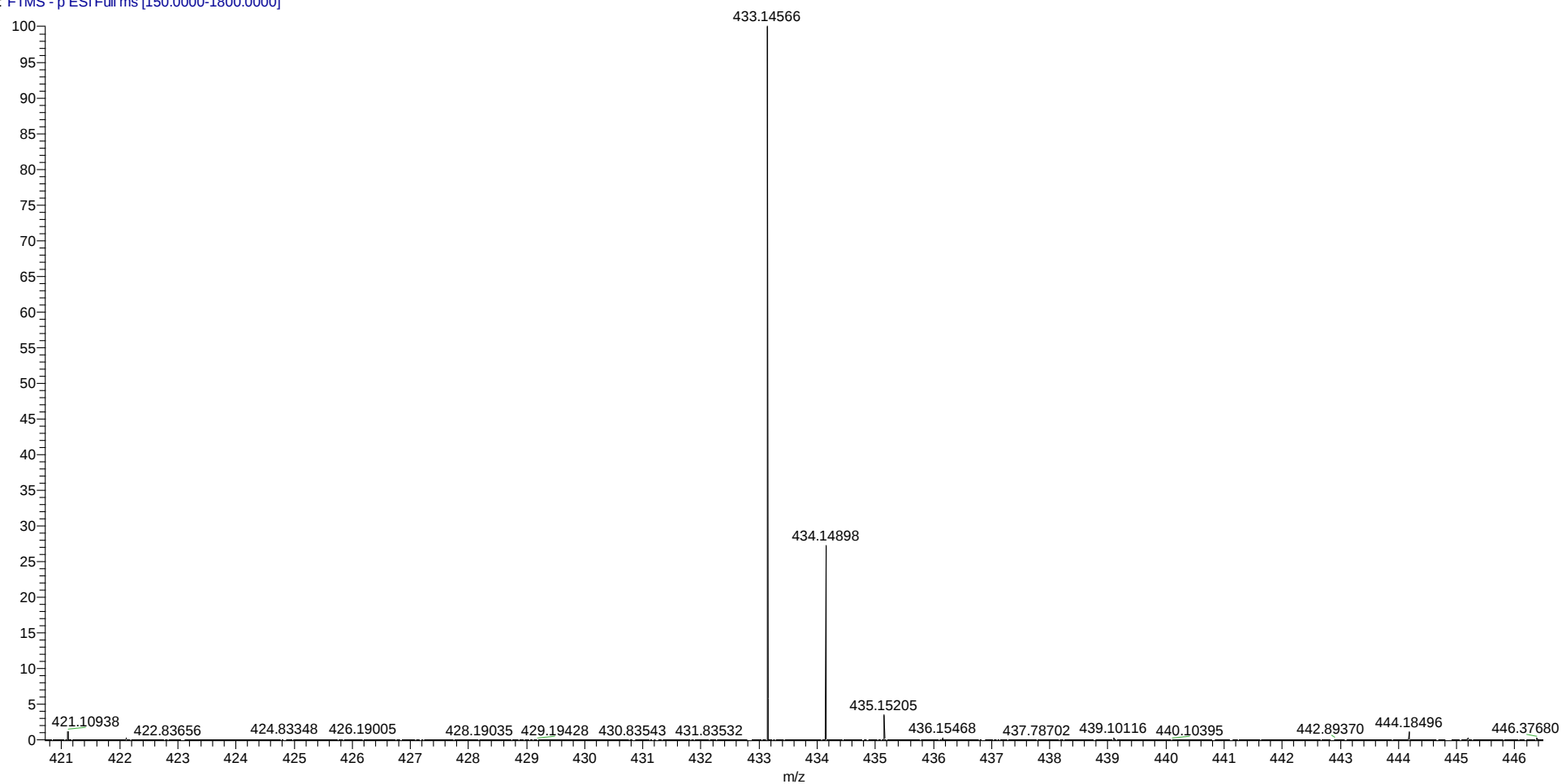


Figure S123. HRESI(–)-MS spectrum of 3-*O*-(4-fluorobenzyl)unguinol (**7f**)

2_4-Di-F_BnBr_Mono_Neg #40-47 RT: 0.51-0.57 AV: 8 NL: 3.27E7
T: FTMS - p ESI Full ms [150.0000-1800.0000]

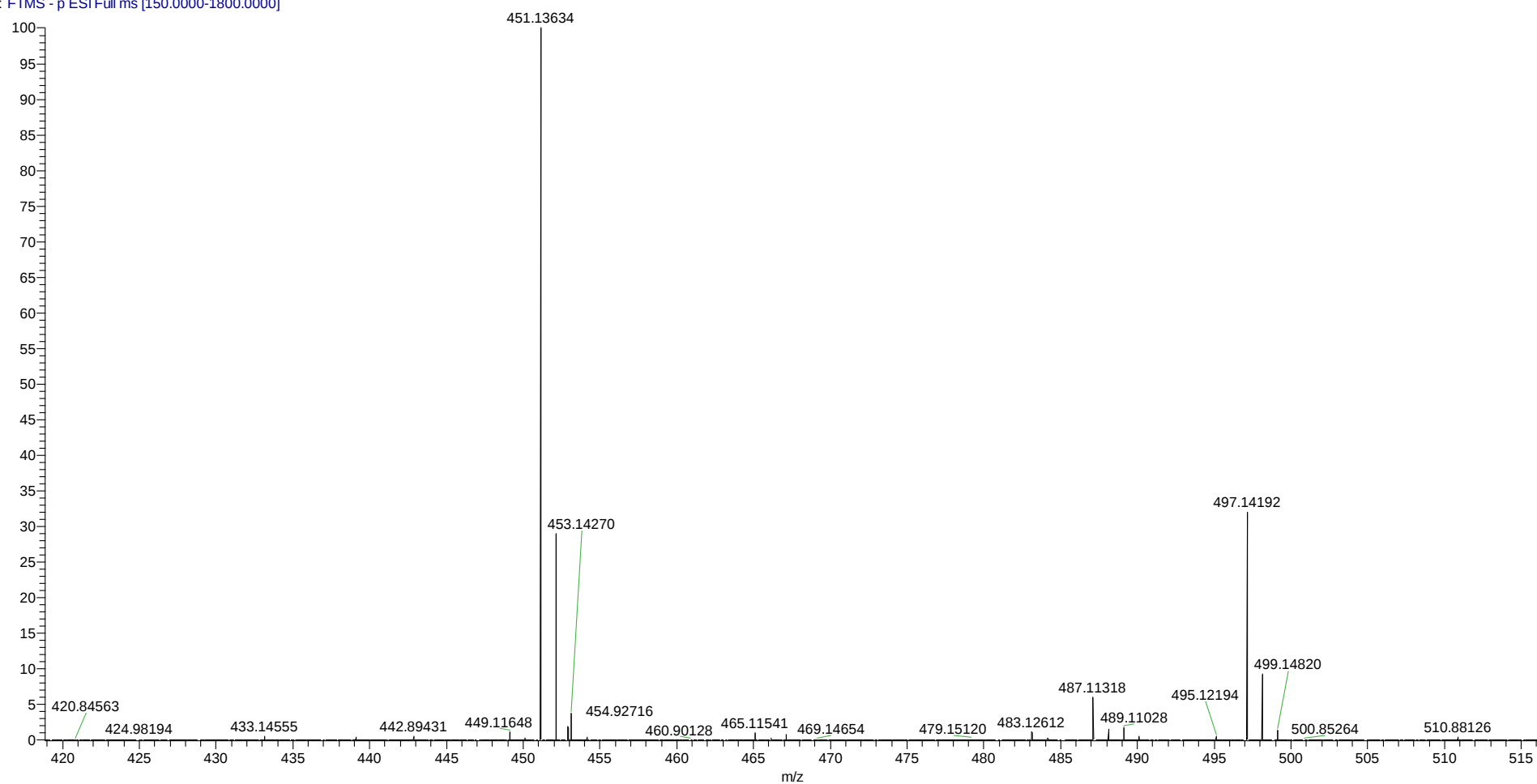


Figure S124. HRESI(-)-MS spectrum of 3-O-(2,4-difluorobenzyl)unguinol (7g)

3_Br_Bn_Br_Mono_Neg #40-50 RT: 0.45-0.54 AV: 11 NL: 1.17E7
T: FTMS - p ESI Full ms [150.0000-1800.0000]

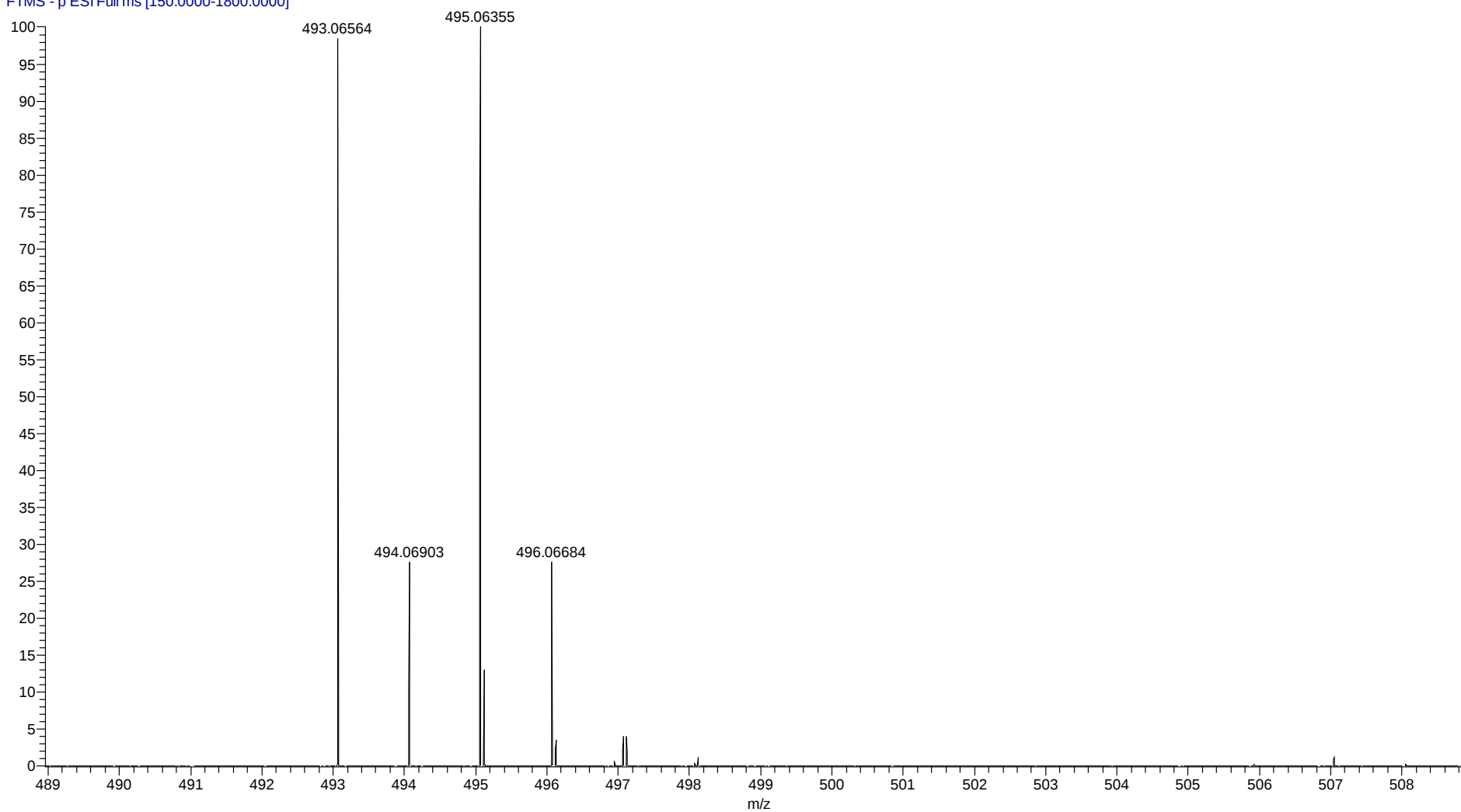


Figure S125. HRESI(-)-MS spectrum of 3-O-(3-bromobenzyl)unguinol (**7h**)

3_Methyl_Bn_Br_Mono_Neg #34-49 RT: 0.42-0.57 AV: 16 NL: 7.01E6
T: FTMS - p ESI Full ms [150.0000-1800.0000]

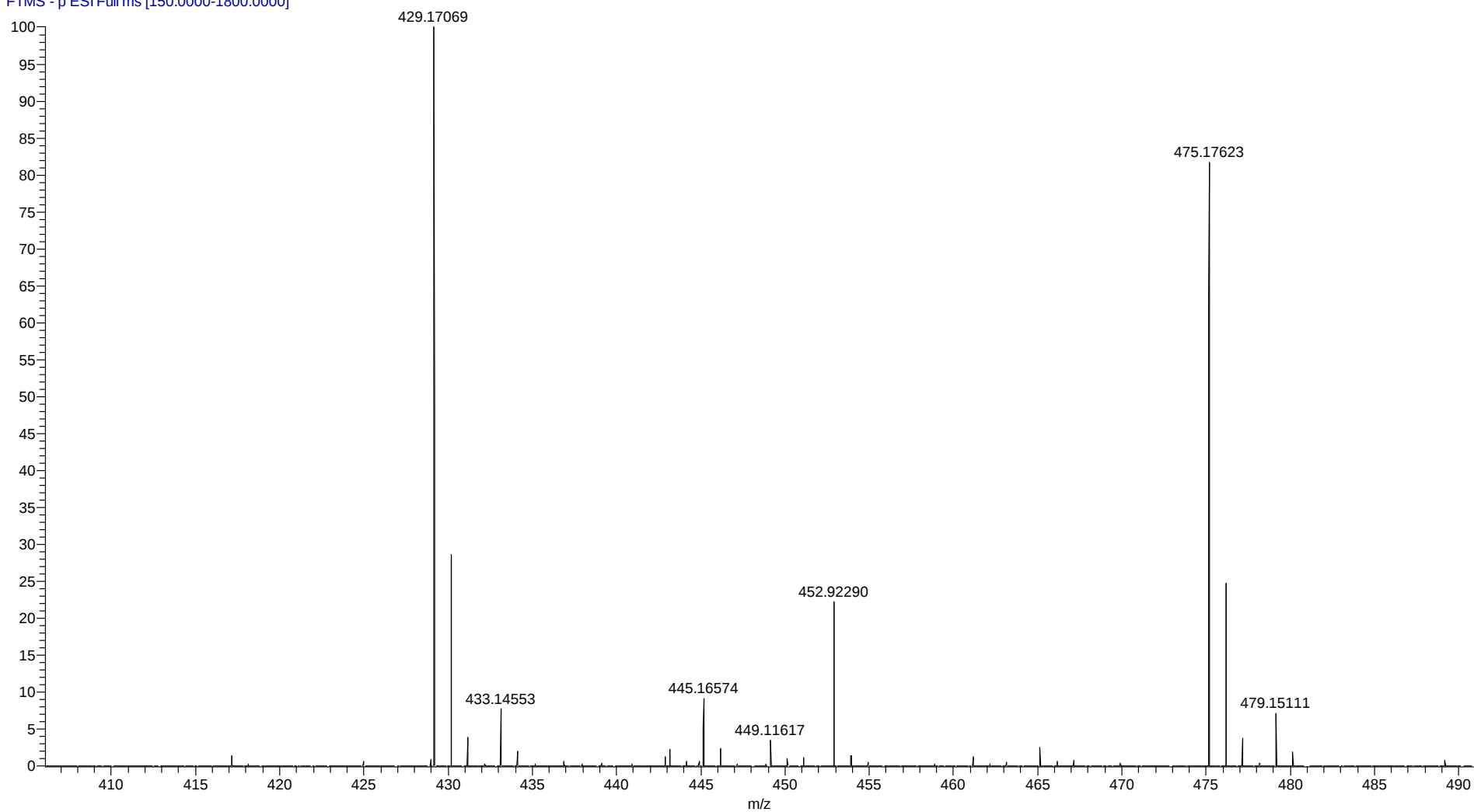


Figure S126. HRESI(-)-MS spectrum of 3-O-(3-methylbenzyl)unguinol (**7i**)

3_OMe_Bn_Br_Mono_Neg #34-48 RT: 0.41-0.55 AV: 15 NL: 1.76E7
T: FTMS - p ESI Full ms [150.0000-1800.0000]

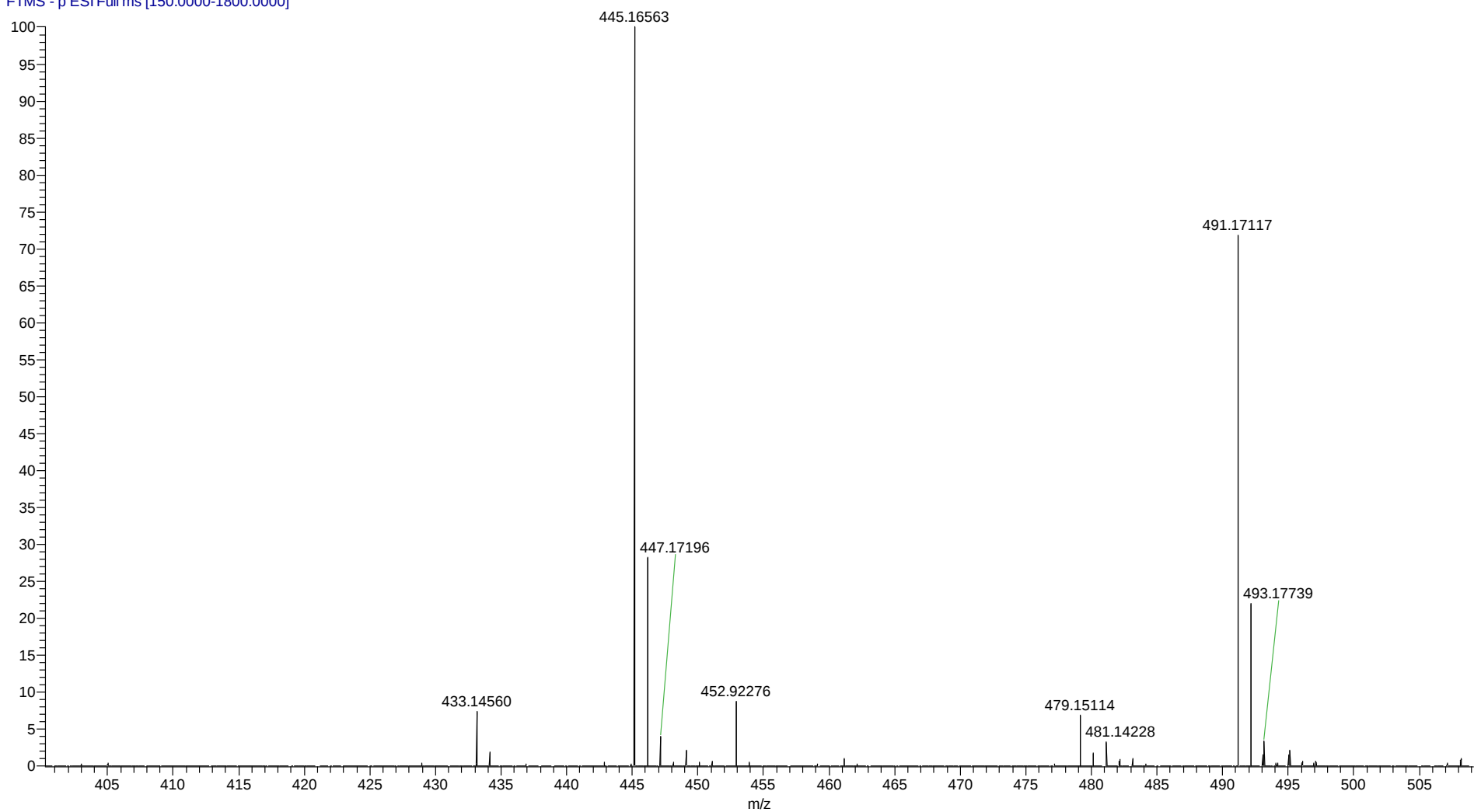


Figure S127. HRESI(-)-MS spectrum of 3-O-(3-methoxybenzyl)unguinol (**7j**)

2_Bromo_methyl_Pyridine_Mono_Pos #42-49 RT: 0.51-0.58 AV: 8 NL: 1.31E8
T: FTMS + p ESI Full ms [150.0000-2200.0000]

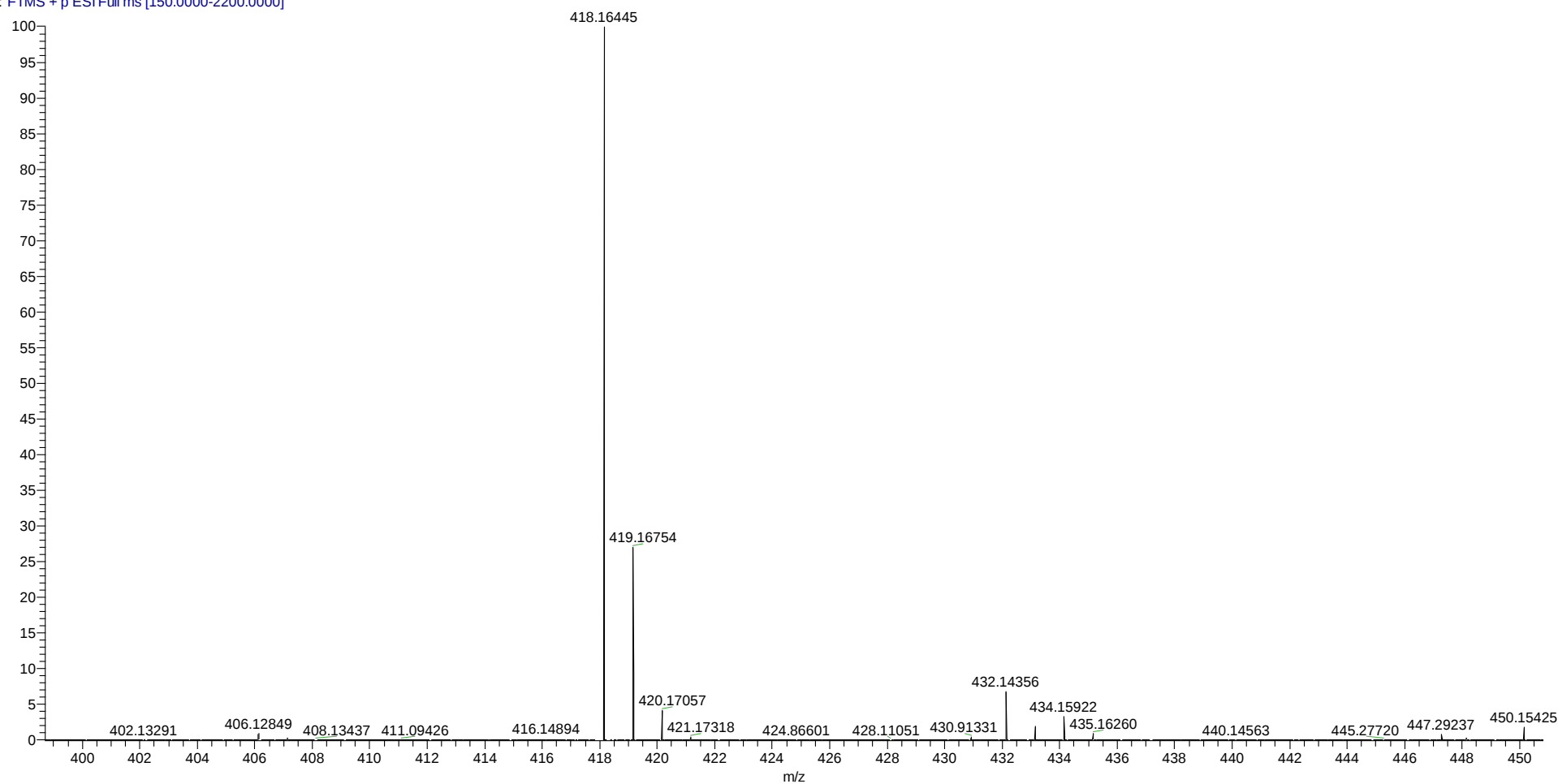


Figure S128. HRESI(+)-MS spectrum of 3-O-(2-picolyl)unguinol (**7k**)

3_Bromo_methyl_Pyridine_Mono_Pos #39-47 RT: 0.51-0.58 AV: 9 NL: 1.32E8
T: FTMS + p ESI Full ms [150.0000-2200.0000]

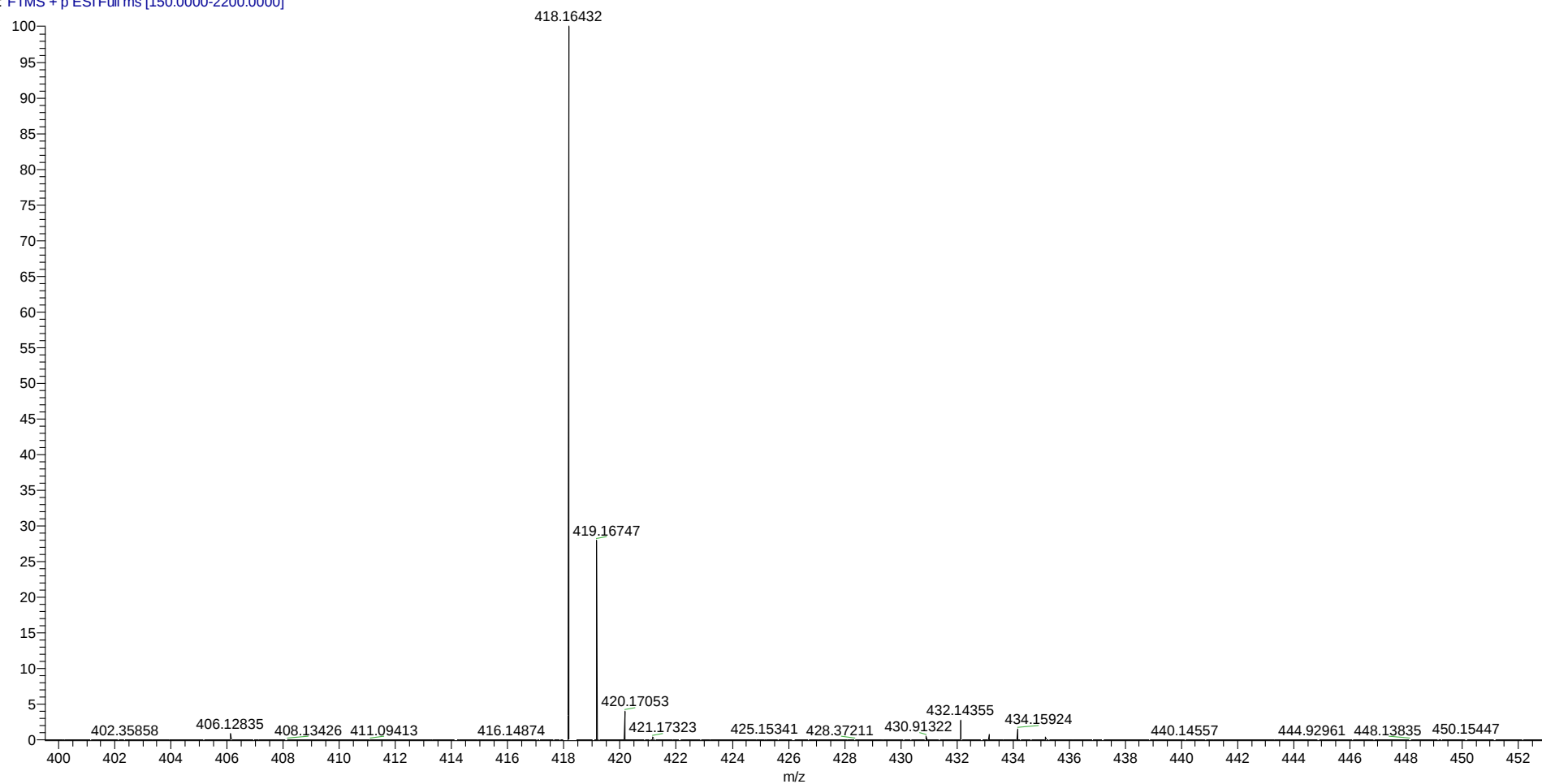


Figure S129. HRESI(+)-MS spectrum of 3-O-(3-picolyl)unguinol (71)

4_Bromo_methyl_Pyridine_Mono_Pos #39-47 RT: 0.51-0.58 AV: 9 NL: 2.20E8
T: FTMS + p ESI Full ms [150.0000-2200.0000]

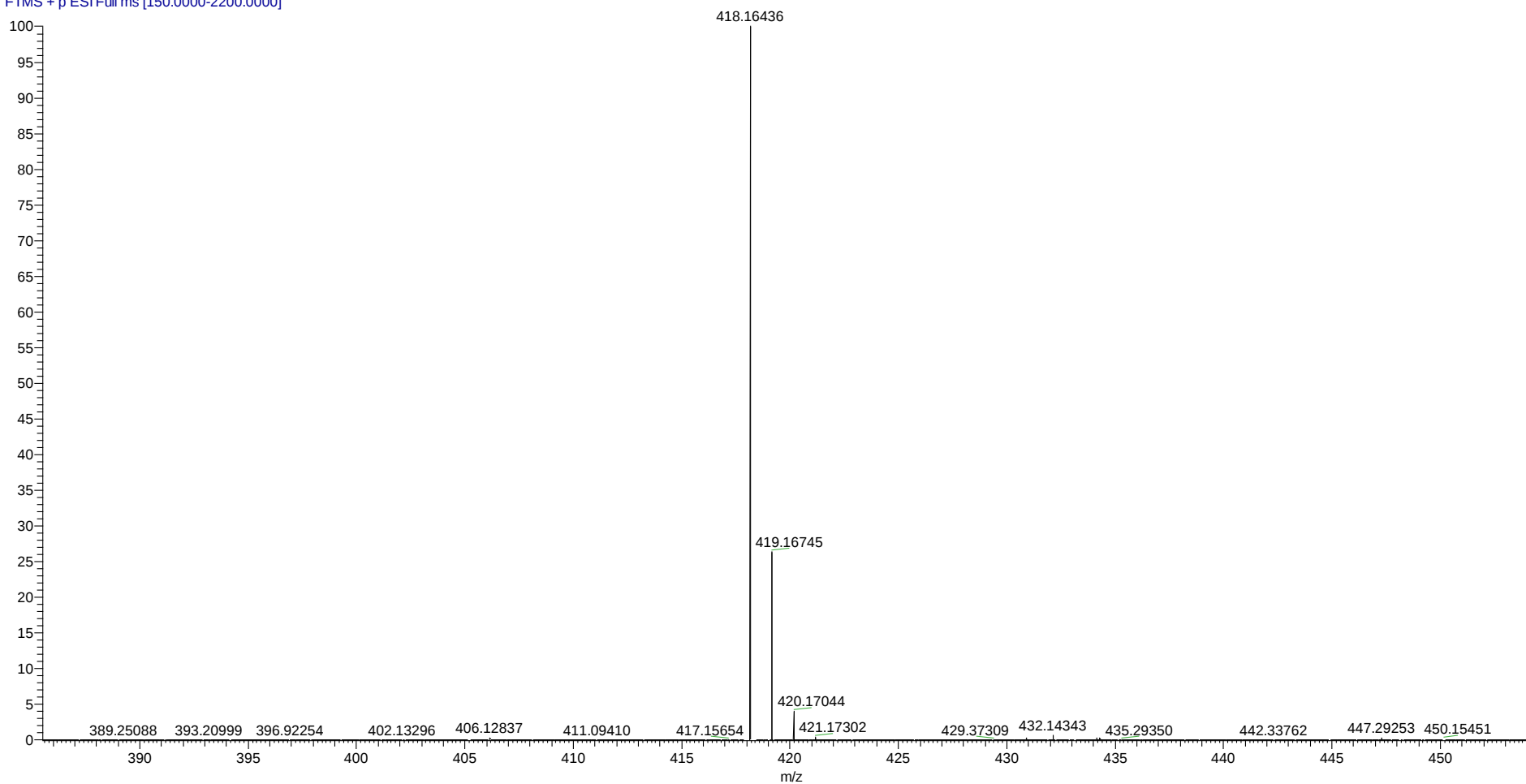


Figure S130. HRESI(+)-MS spectrum of 3-O-(4-picolyl)unguinol (**7m**)

180312 P21590 TM 119 5 Pos 1 #51 RT: 0.59 AV: 1 NL: 3.71E9
T: FTMS + p ESI Full ms [150.0000-1800.0000]

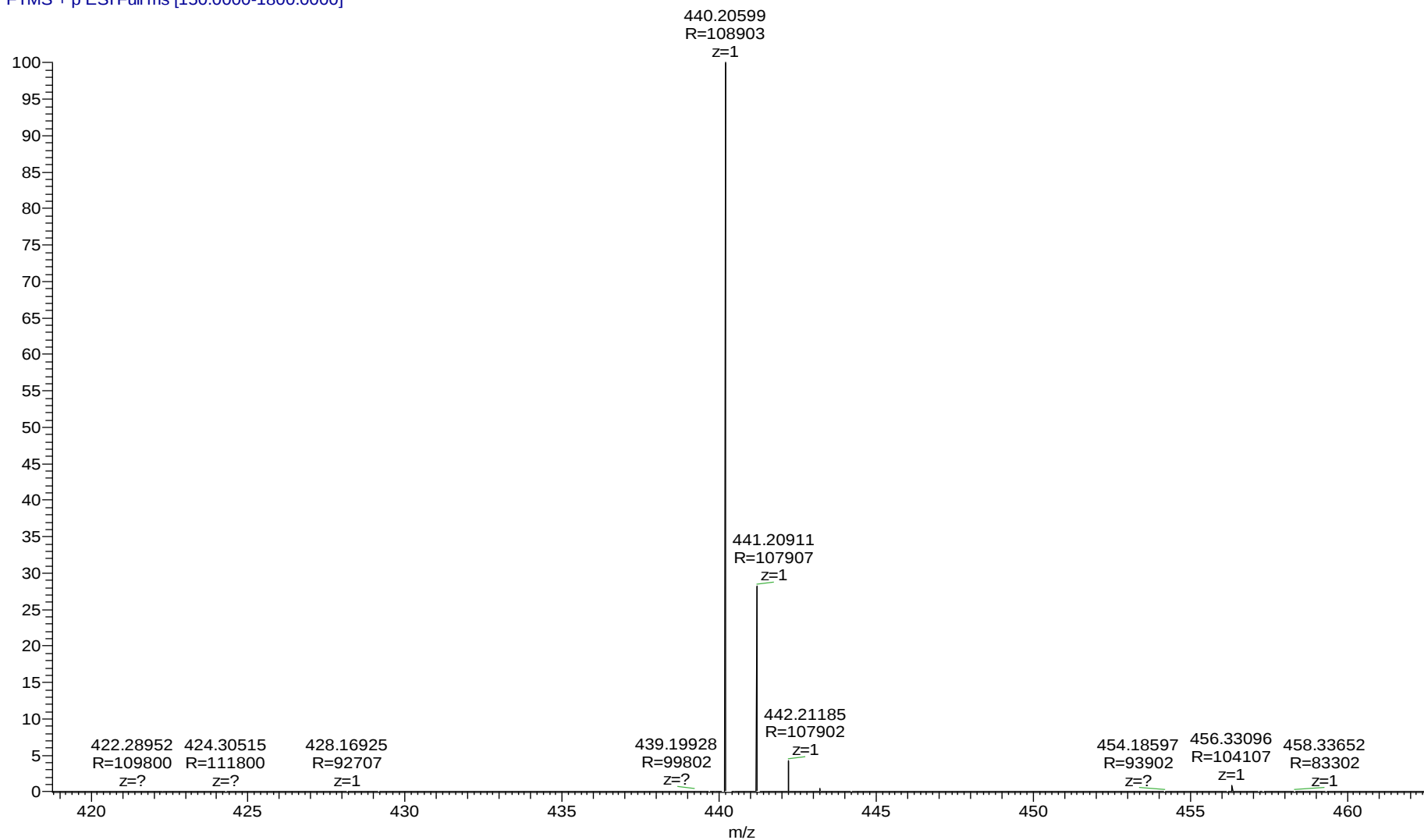


Figure S131. HRESI(+)-MS spectrum of 3-O-(4-morpholinoethyl)unguinol (**7n**)

180312 P21590 TM 119 4 Pos 1 #187 RT: 2.01 AV: 1 NL: 1.12E7
T: FTMS + p ESI Full ms [150.0000-1800.0000]

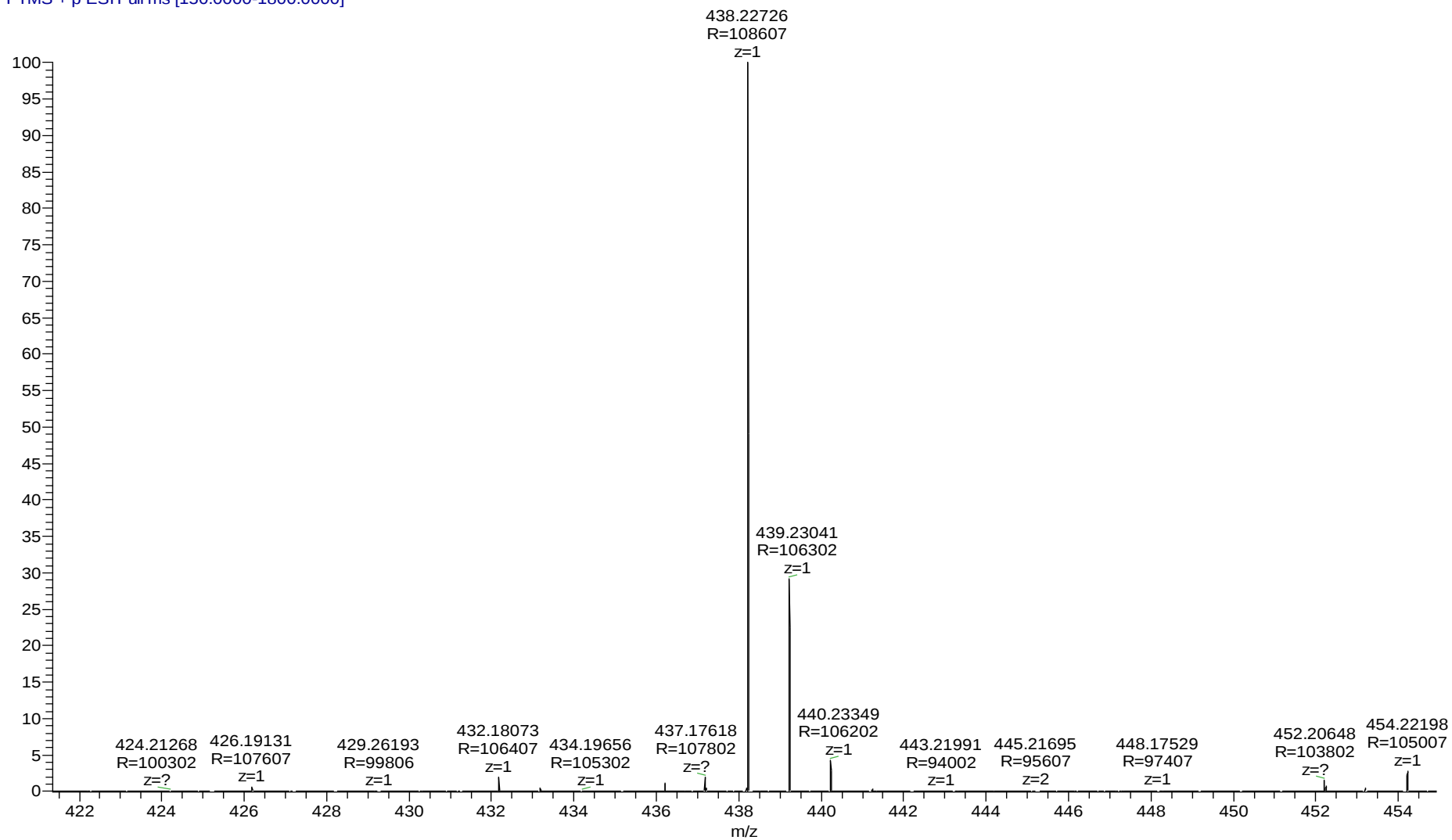


Figure S132. HRESI(+)-MS spectrum of 3-O-(1-piperidinylethyl)unguinol (**7o**)

180312 P21590 TM 119 6 Pos 1 #48 RT: 0.58 AV: 1 NL: 1.79E9
T: FTMS + p ESI Full ms [150.0000-1800.0000]

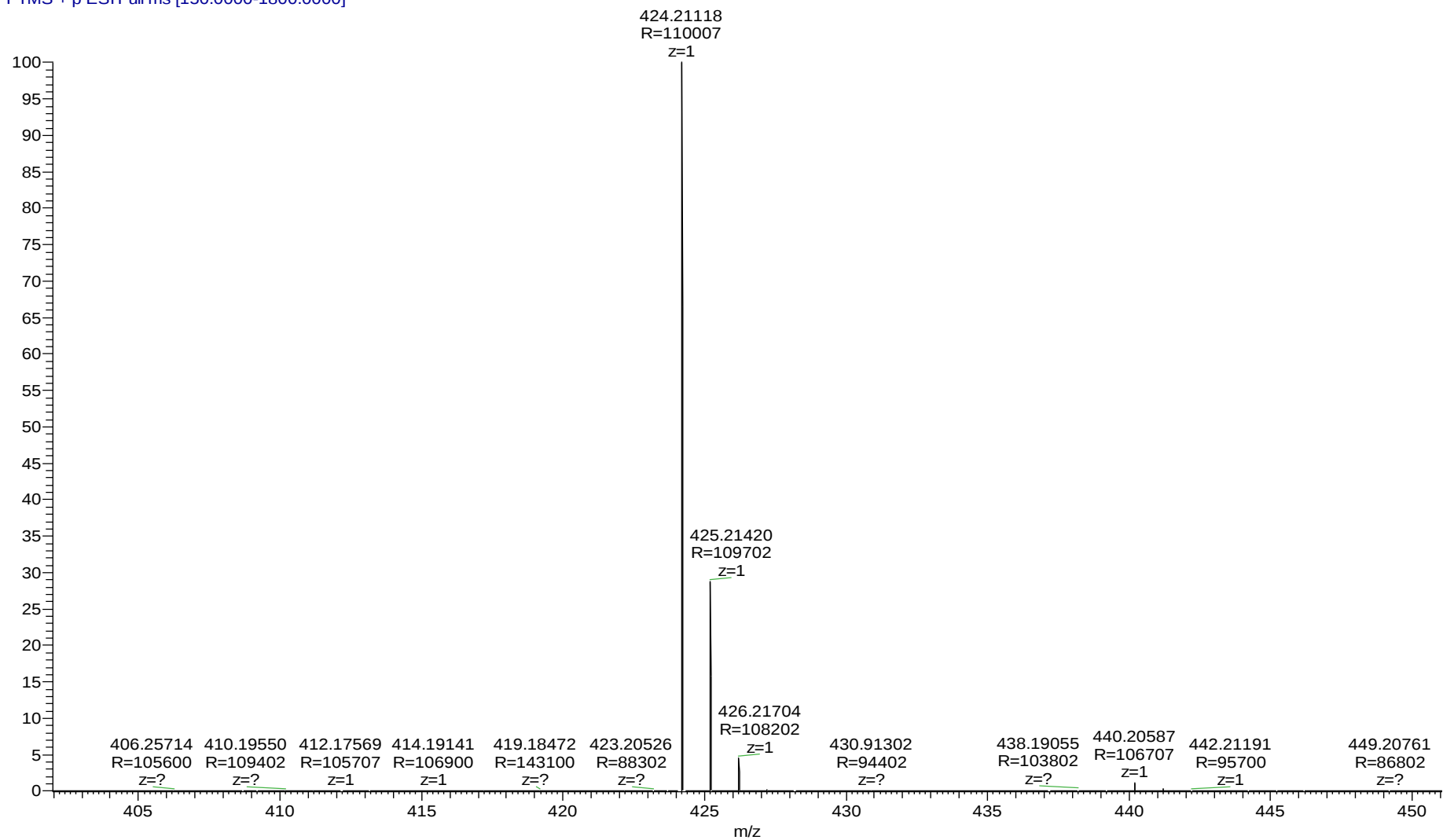


Figure S133. HRESI(+)-MS spectrum of 3-O-(1-pyrrolidinyethyl)unguinol (7p)

180312_P21590_TM_119_1_Pos_1 #54 RT: 0.60 AV: 1 NL: 8.04E7
T: FTMS + p ESI Full ms [150.0000-1800.0000]

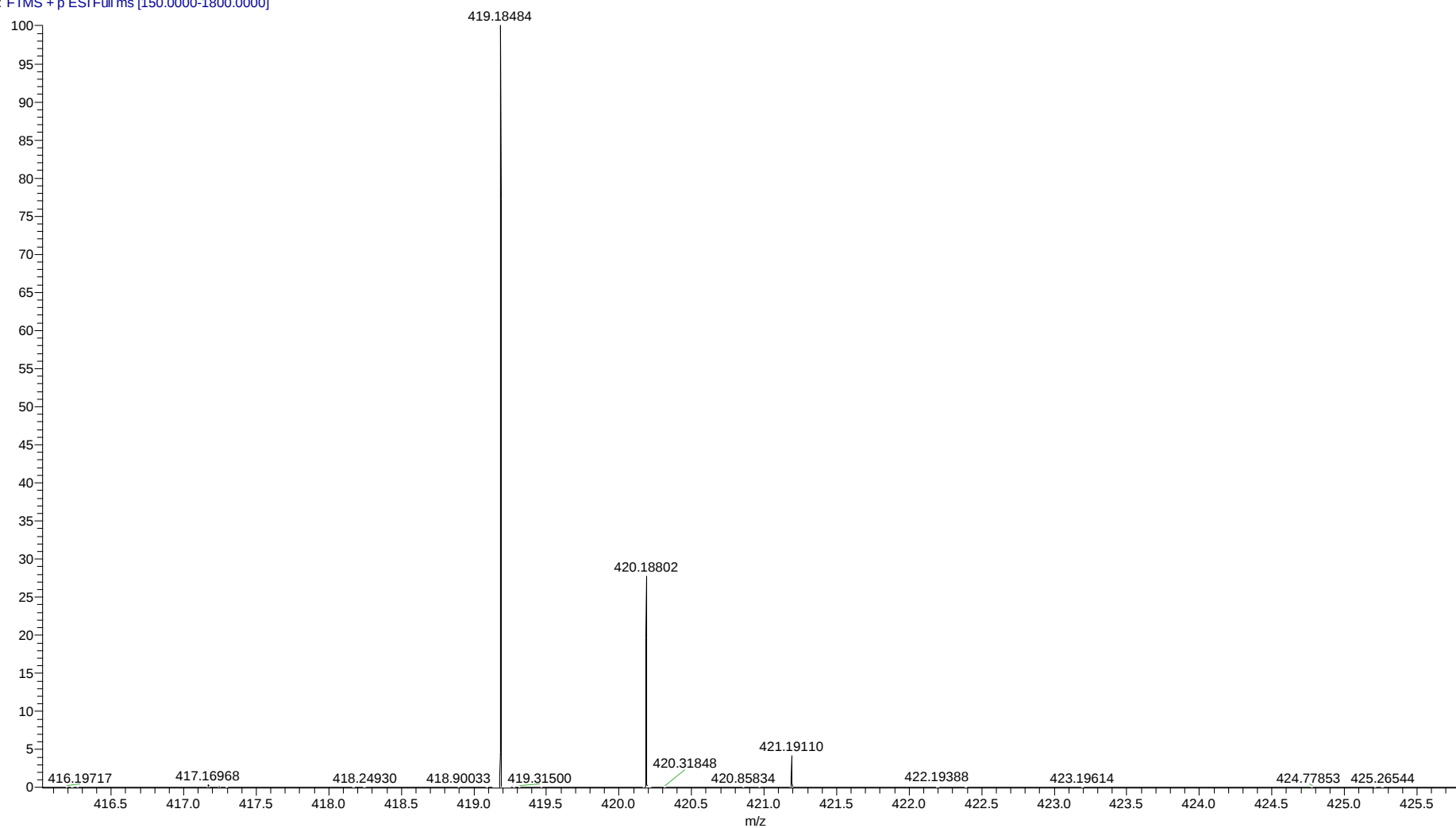


Figure S134. HRESI(+)-MS spectrum of 3-O-1',2'-dihydrobenzylunguinol (**8a**)

180312_P21590_TM_119_2_Pos_1 #54 RT: 0.64 AV: 1 NL: 4.66E7
T: FTMS + p ESI Full ms [150.0000-1800.0000]

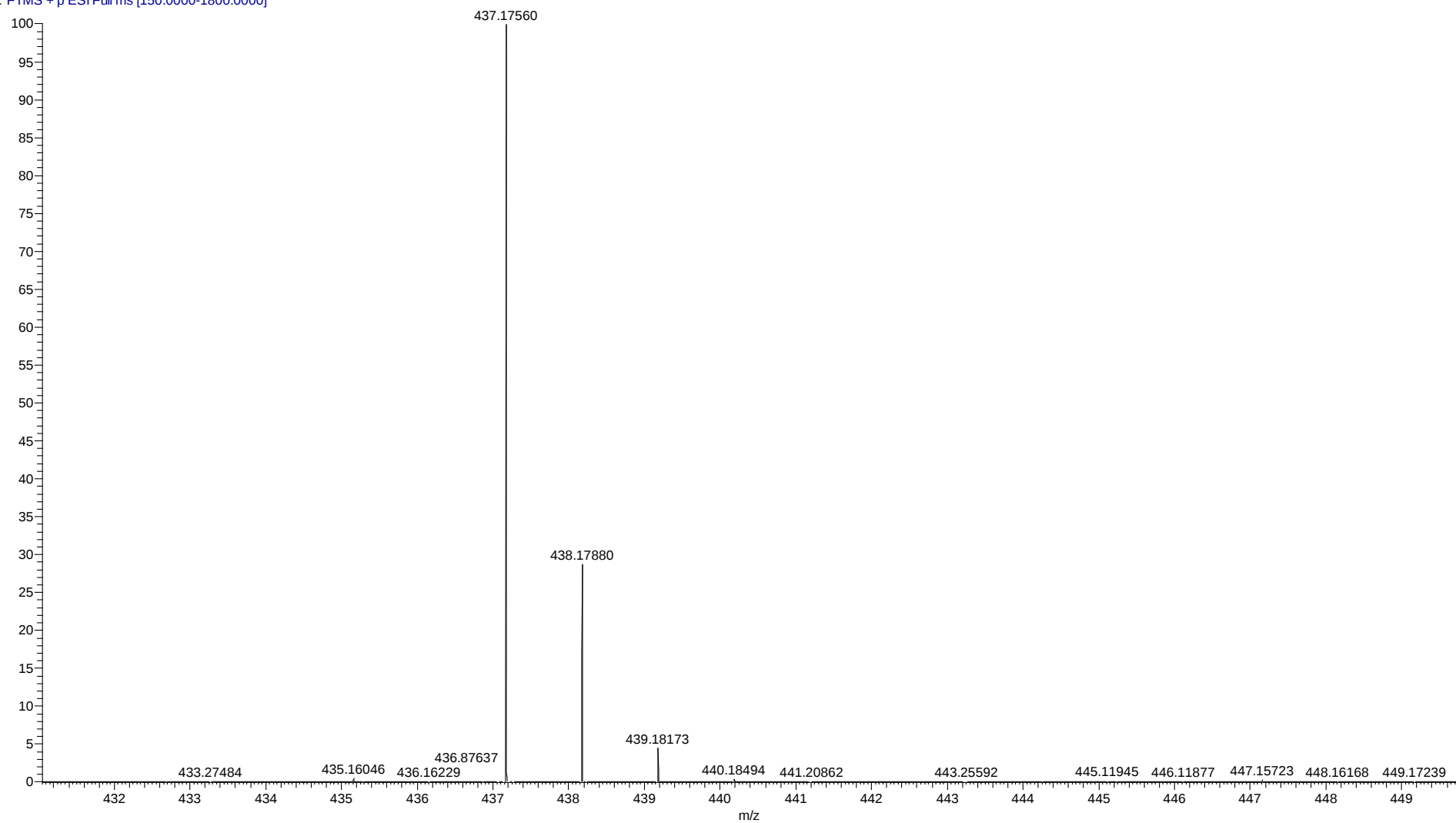


Figure S135. HRESI(+)-MS spectrum of 3-O-(2-fluorobenzyl)-1',2'-dihydroquinol (**8b**)

180312 P21590 TM 119 3 Pos 1 #51 RT: 0.62 AV: 1 NL: 2.44E7
T: FTMS + p ESI Full ms [150.0000-1800.0000]

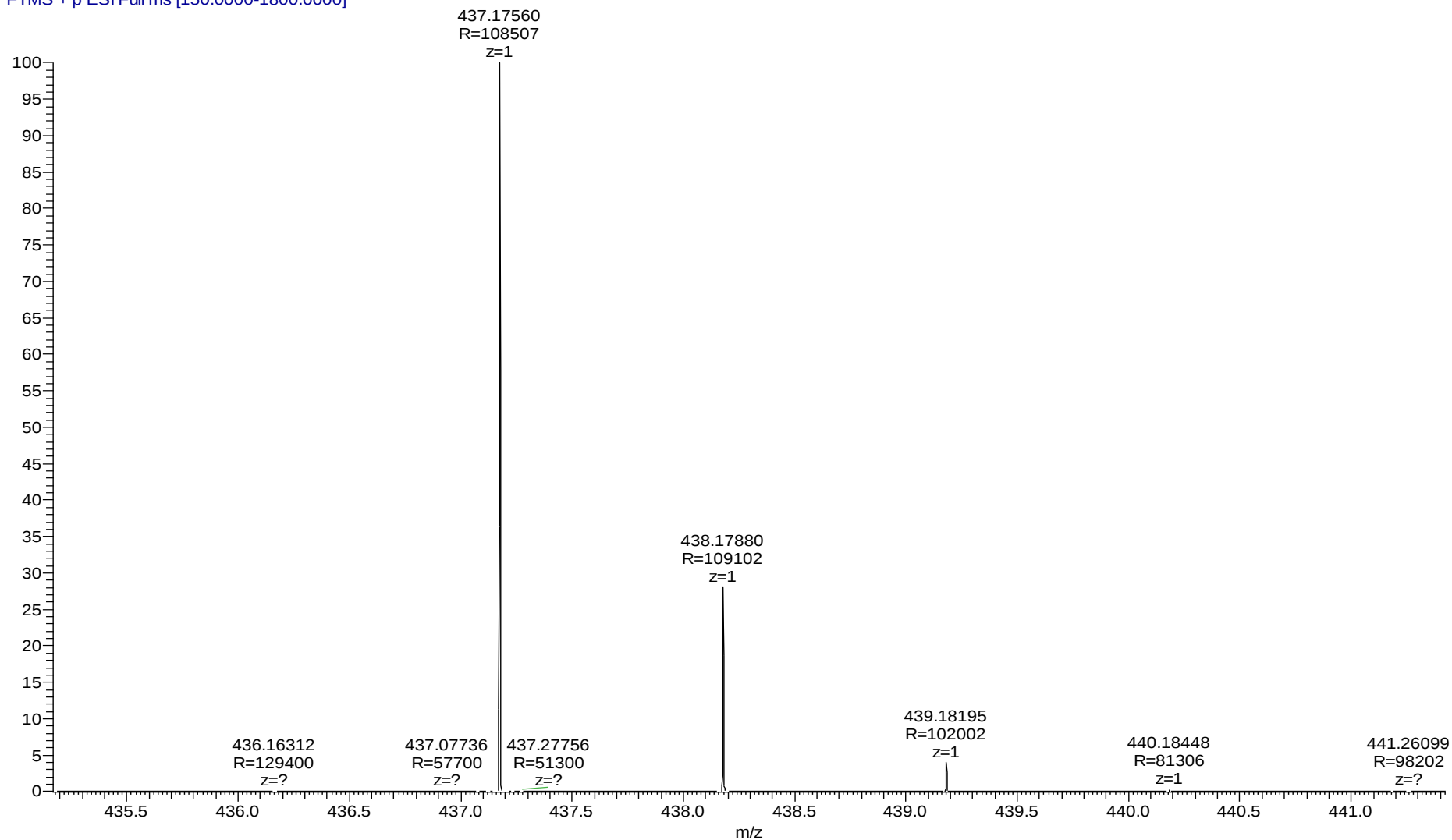


Figure S136. HRESI(+)-MS spectrum of 3-O-(4-fluorobenzyl)-1',2'-dihydroanguinol (**8c**)