

Supplementary Materials

Benzylated Dihydroflavones and Isoquinoline-Derived Alkaloids from the Bark of *Diclinanona calycina* (Annonaceae) and Their Cytotoxicities

Emmanoel V. Costa ^{1,*}, Liviane do N. Soares ¹, Jamal da S. Chaar ¹, Valdenizia R. Silva ², Luciano de S. Santos ², Hector H. F. Koolen ³, Felipe M. A. da Silva ¹, Josean F. Tavares ⁴, Gokhan Zengin ⁵, Milena B. P. Soares ² and Daniel P. Bezerra ^{2,*}

¹ Department of Chemistry, Federal University of Amazonas (UFAM), Manaus 69080-900, AM, Brazil; evc@ufam.edu.br (E.V.C.); BeM.Liviane@gmail.com (L.d.N.S.); jchaar@ufam.edu.br (J.d.S.C.); felipemourams@gmail.com (F.M.A.d.S.)

² Gonçalo Moniz Institute, Oswaldo Cruz Foundation (IGM-FIOCRUZ/BA), Salvador 40296-710, BA, Brazil; valdeniziar@gmail.com (V.R.S.); luciano.biomed@gmail.com (L.d.S.S.); milenabpsoares@gmail.com (M.B.P.S.); daniel.bezerra@fiocruz.br (D.P.B.)

³ Metabolomics and Mass Spectrometry Research Group, Amazonas State University (UEA), Manaus 690065-130, AM, Brazil; hkoolen@uea.edu.br

⁴ Health Sciences Center, Postgraduate Program in Natural and Synthetic Bioactive Products, Federal University of Paraíba (UFPB), João Pessoa 58051-970, PA, Brazil; josean@ltf.ufpb.br

⁵ Department of Biology, Science Faculty, Selcuk University, Konya 42130, Turkey; gokhanzengin@selcuk.edu.tr

* Correspondence: evc@ufam.edu.br (E.V.C.); daniel.bezerra@fiocruz.br (D.P.B.); Tel./Fax: +55-92-3305-1181 Ramal 2870 (E.V.C.); +55-71-3176-2272 (D.P.B.)

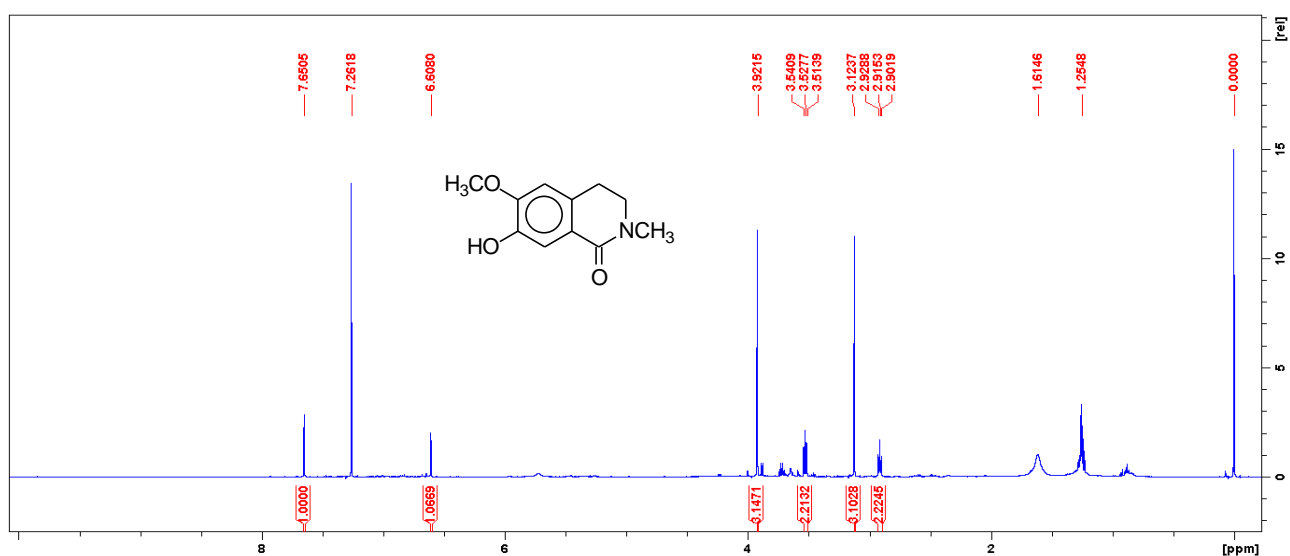


Figure S1. ¹H NMR spectrum of *thalifoline* (**1**) in CDCl₃ at 500 MHz.

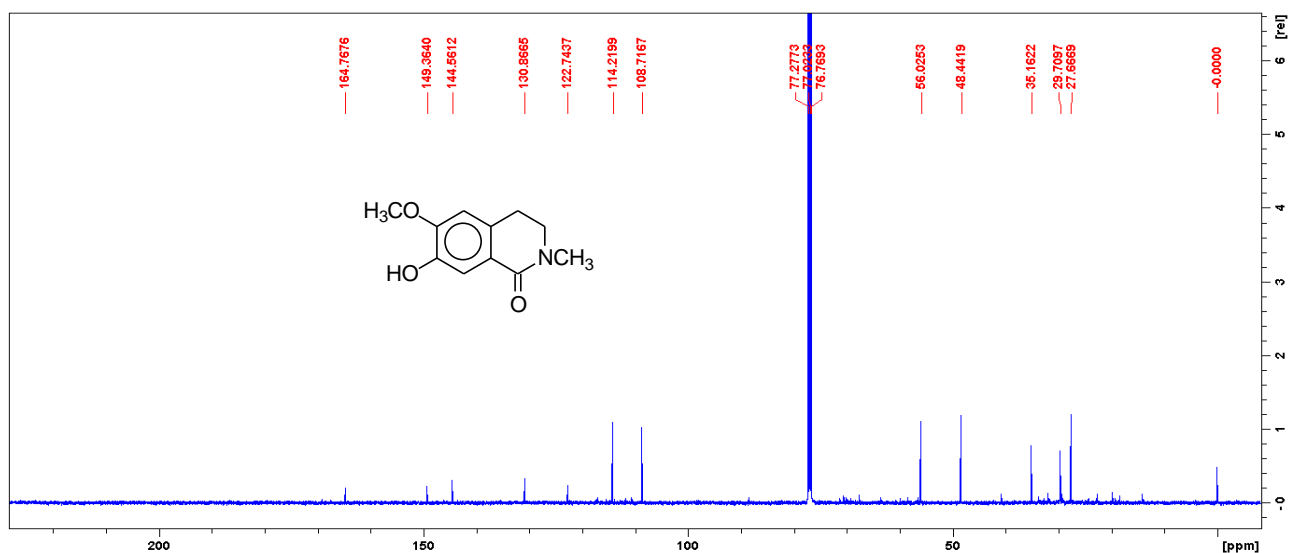


Figure S2. ¹³C NMR spectrum of *thalifoline* (**1**) in CDCl₃ at 100 MHz.

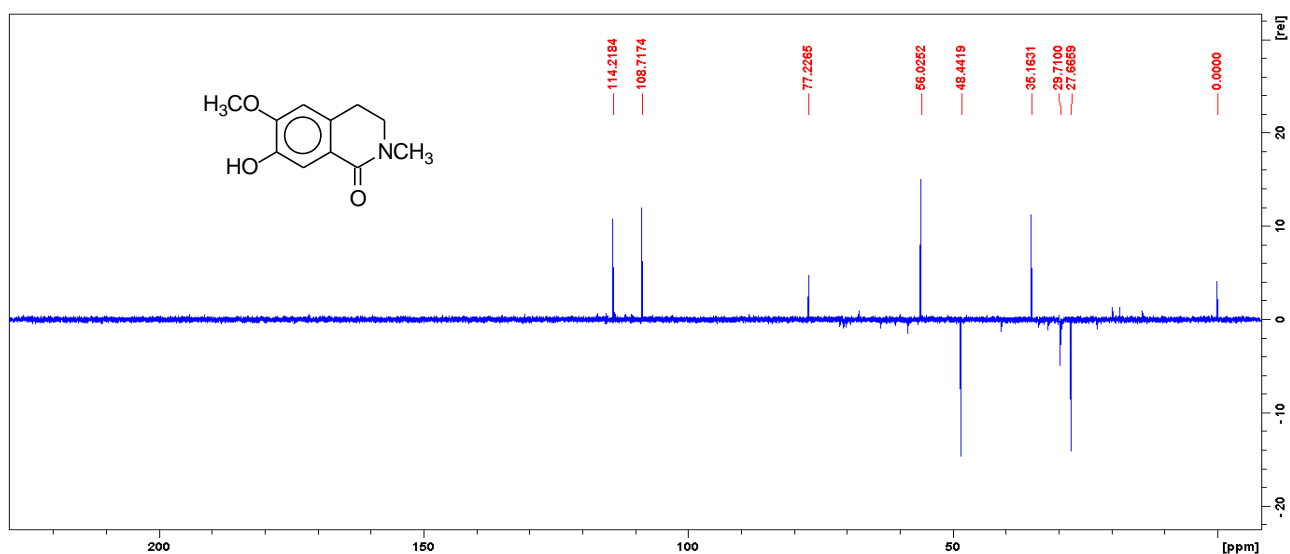


Figure S3. DEPT 135 spectrum of *thalifoline* (**1**) in CDCl₃ at 125 MHz.

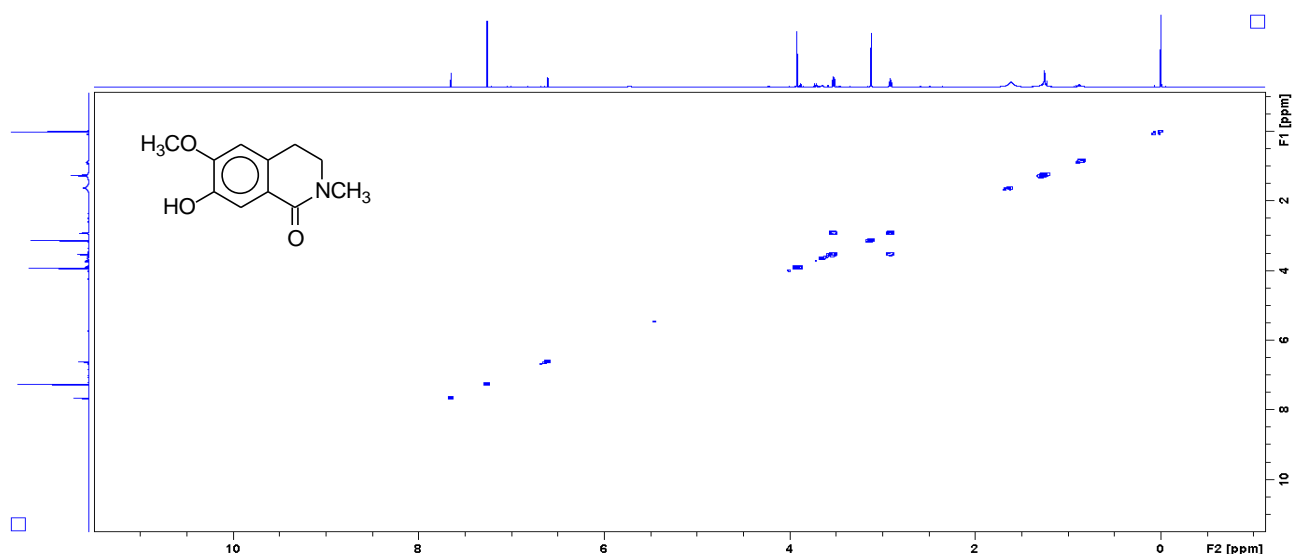


Figure S4. ^1H - ^1H correlation map from COSY NMR experiment of *thalifoline* (**1**) in CDCl_3 at 500 MHz.

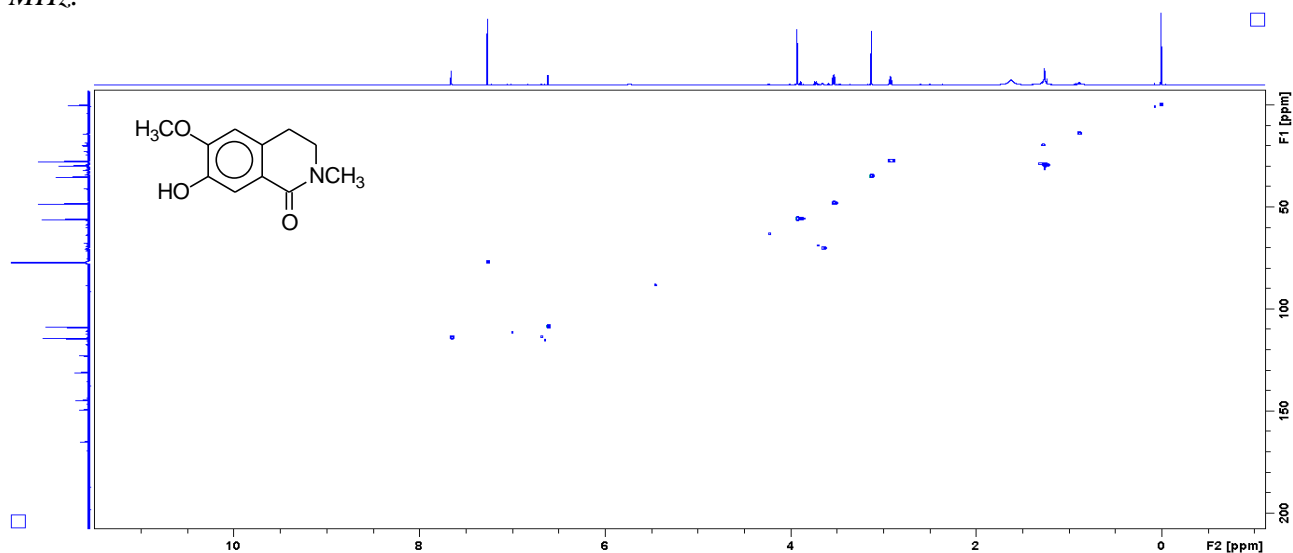


Figure S5. One-bond ^1H - ^{13}C correlation map from HSQC NMR experiment of *thalifoline* (**1**) in CDCl_3 at 500 (^1H) and 125 MHz (^{13}C), respectively.

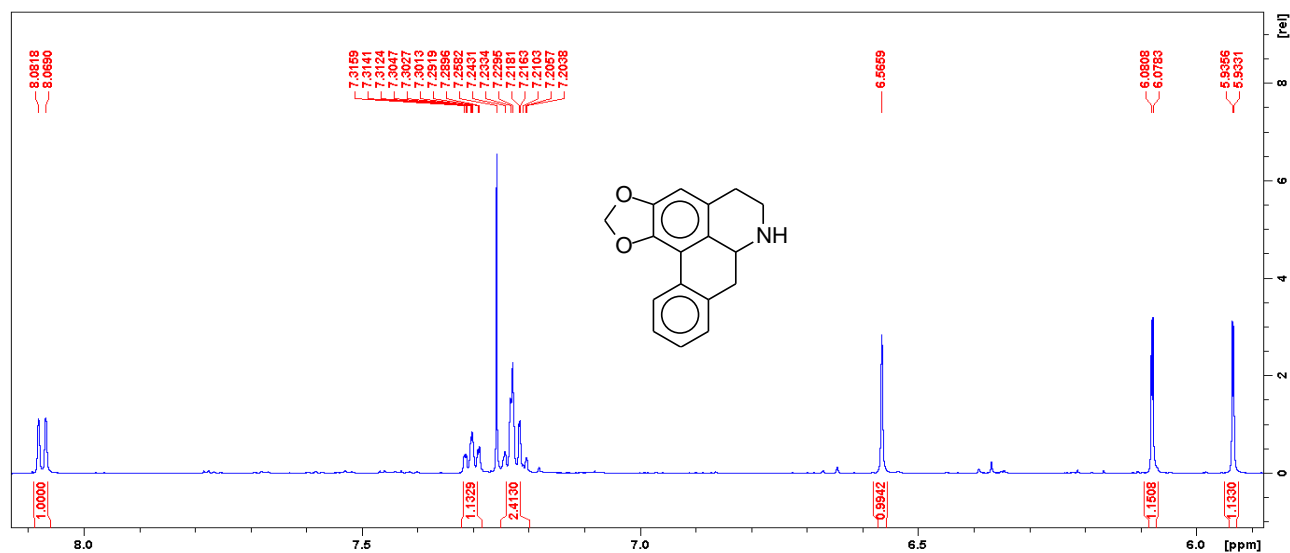


Figure S9. Expansion (δ 8.12 – 5.88) of the ^1H NMR spectrum of anonaine (2) in CDCl_3 at 600 MHz.

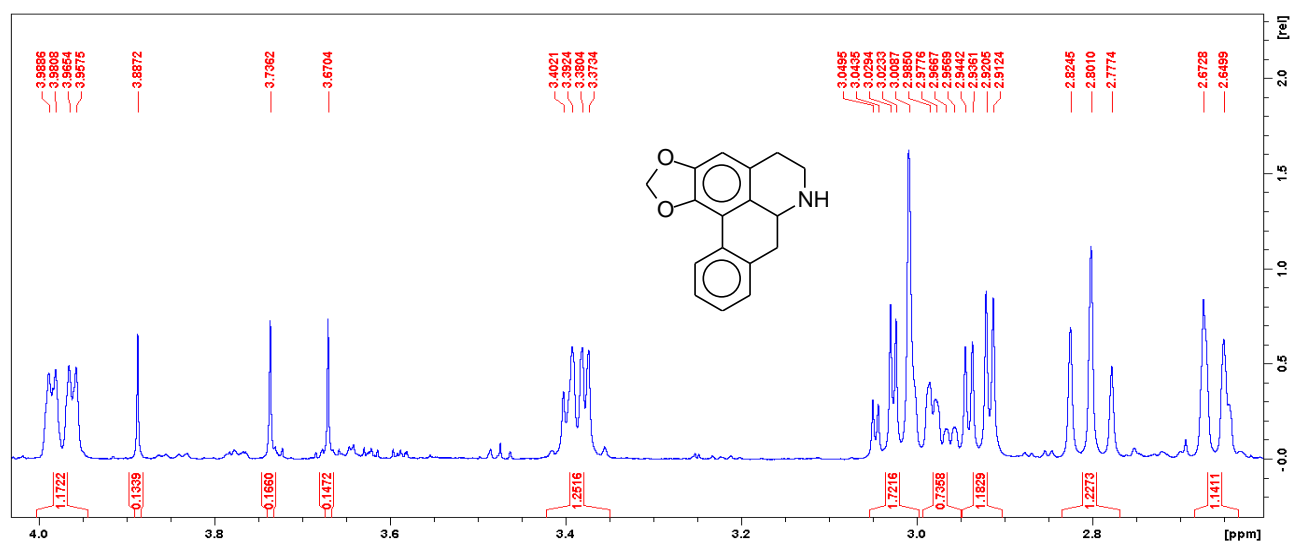


Figure S10. Expansion (δ 4.02 – 2.61) of the ^1H NMR spectrum of anonaine (2) in CDCl_3 at 600 MHz.

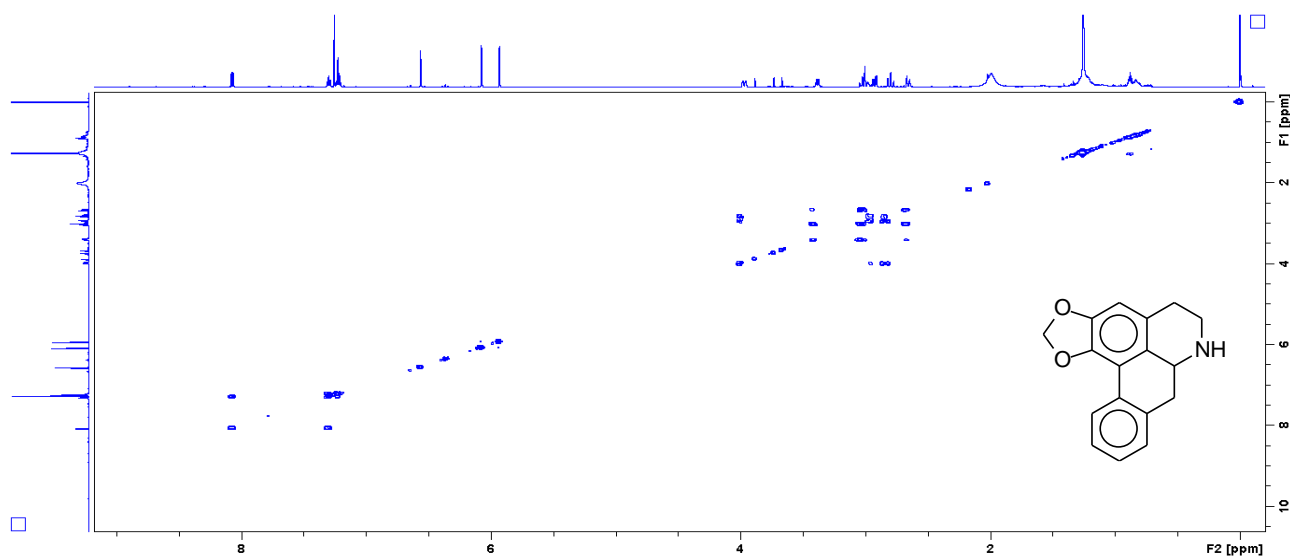


Figure S11. ^1H - ^1H correlation map from COSY NMR experiment of anonaine (2) in CDCl_3 at 600 MHz.

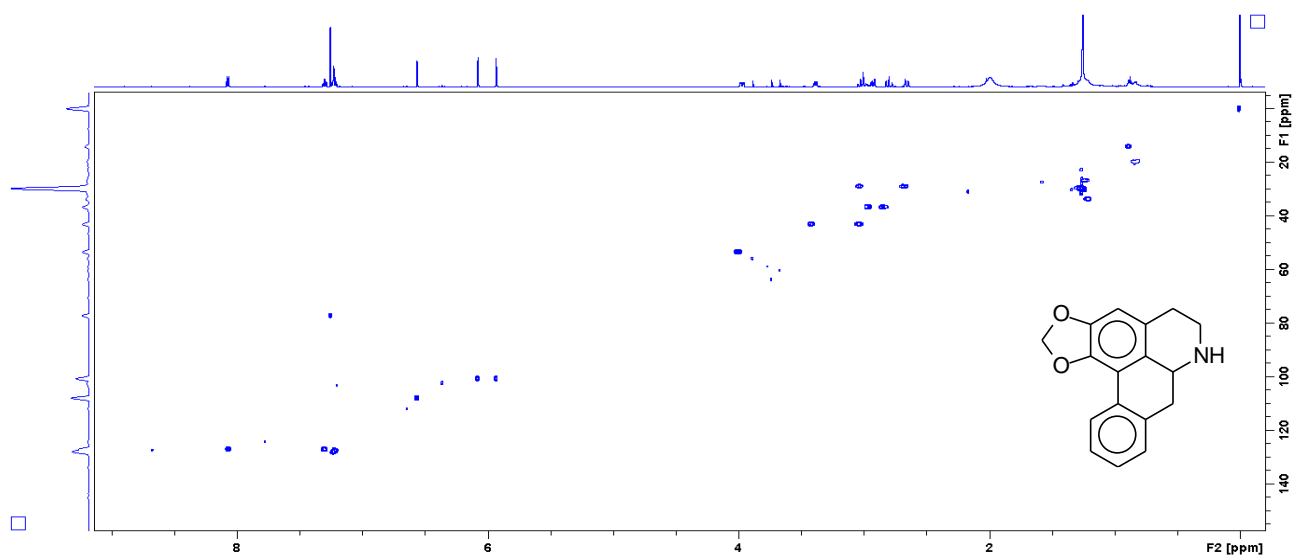


Figure S12. One-bond ^1H - ^{13}C correlation map from HSQC NMR experiment of **anonaine (2)** in CDCl_3 at 600 (^1H) and 150 MHz (^{13}C), respectively.

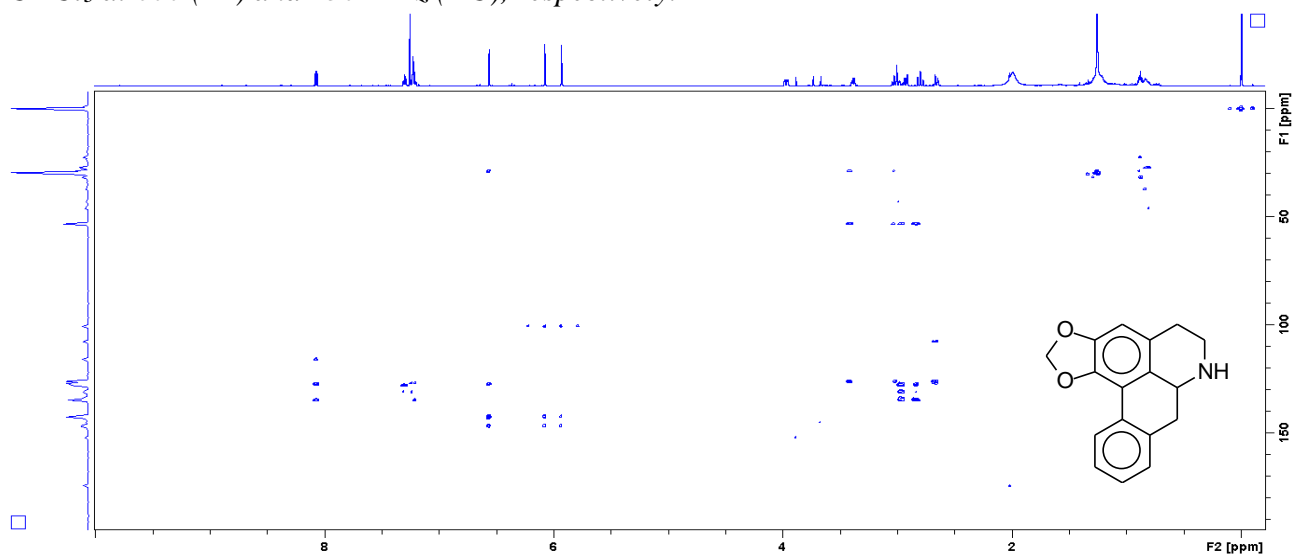


Figure S13. Long-range ^1H - ^{13}C correlation map from HMBC NMR experiment of **anonaine (2)** in CDCl_3 at 600 (^1H) and 150 MHz (^{13}C), respectively.

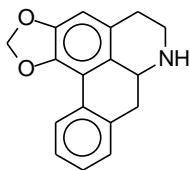


Figure S14. LR-ESI(+)-MS spectrum of anonaine (**2**) (m/z 266 $[M+H]^+$).

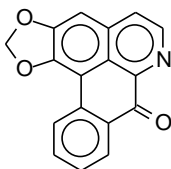


Figure S15. ^1H NMR spectrum of **liriodenine** (**3**) in CDCl_3 plus drop of CD_3OD at 600 MHz.

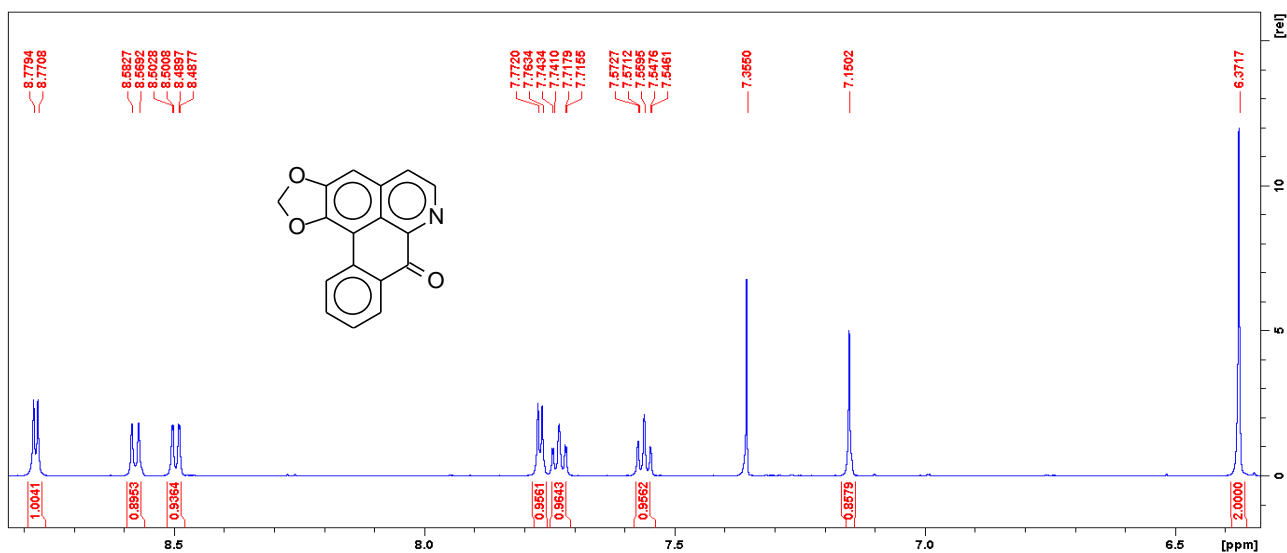


Figure S16. Expansion (δ 8.82 – 6.33) of the ^1H NMR spectrum of **liriodenine** (**3**) in CDCl_3 plus drop of CD_3OD at 600 MHz.

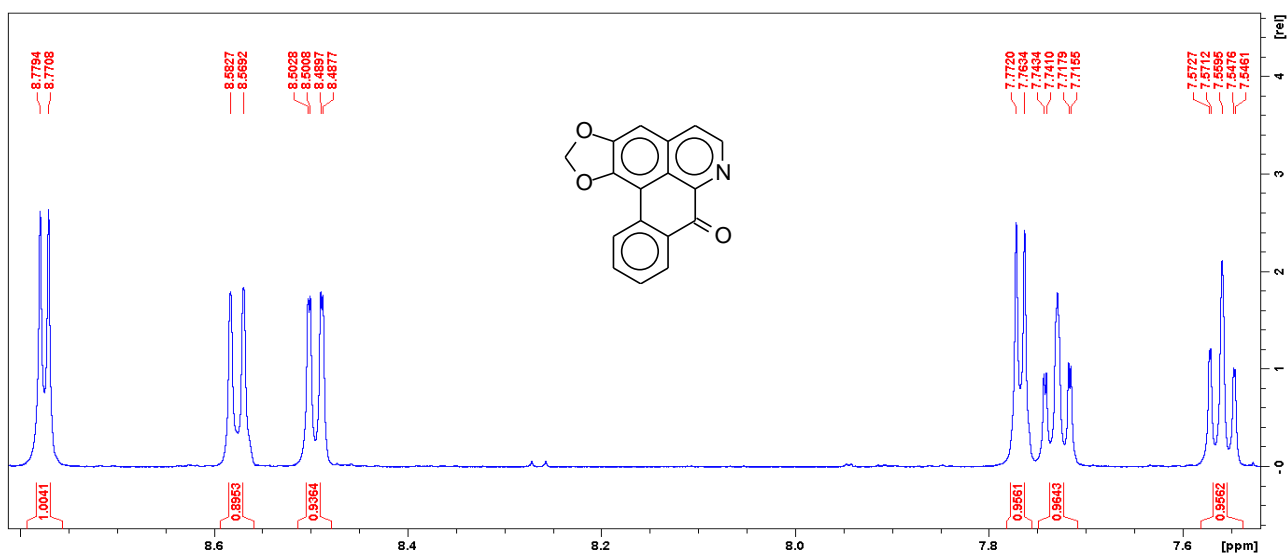


Figure S17. Expansion (δ 8.81 – 7.52) of the ^1H NMR spectrum of **liriodenine** (**3**) in CDCl_3 plus drop of CD_3OD at 600 MHz.

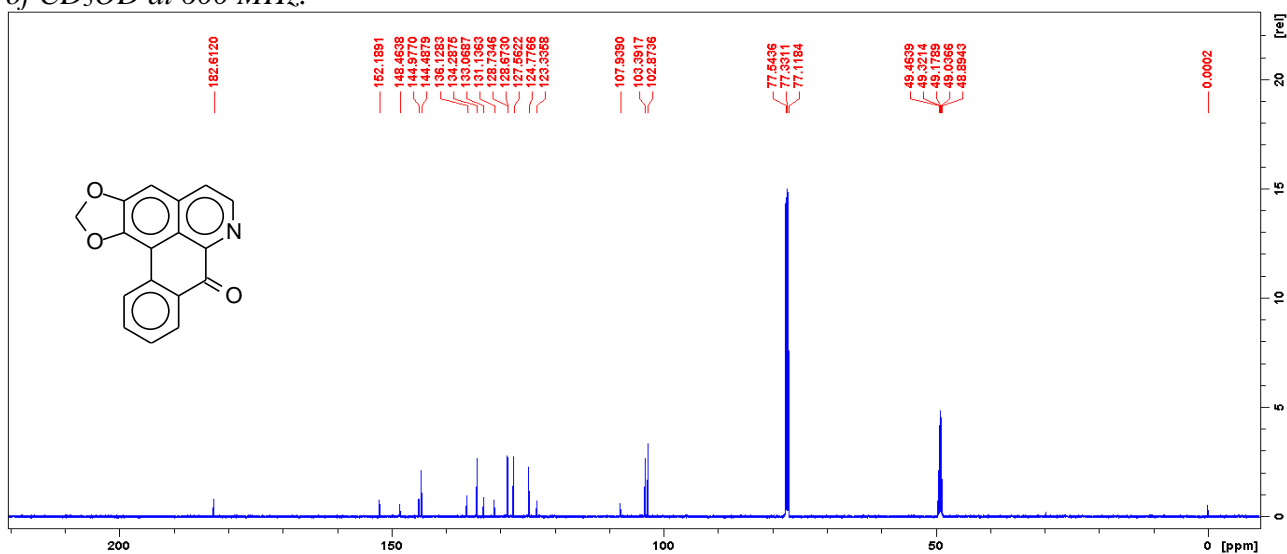


Figure S18. ^{13}C NMR spectrum of **liriodenine** (**3**) in CDCl_3 plus drop of CD_3OD at 150 MHz.

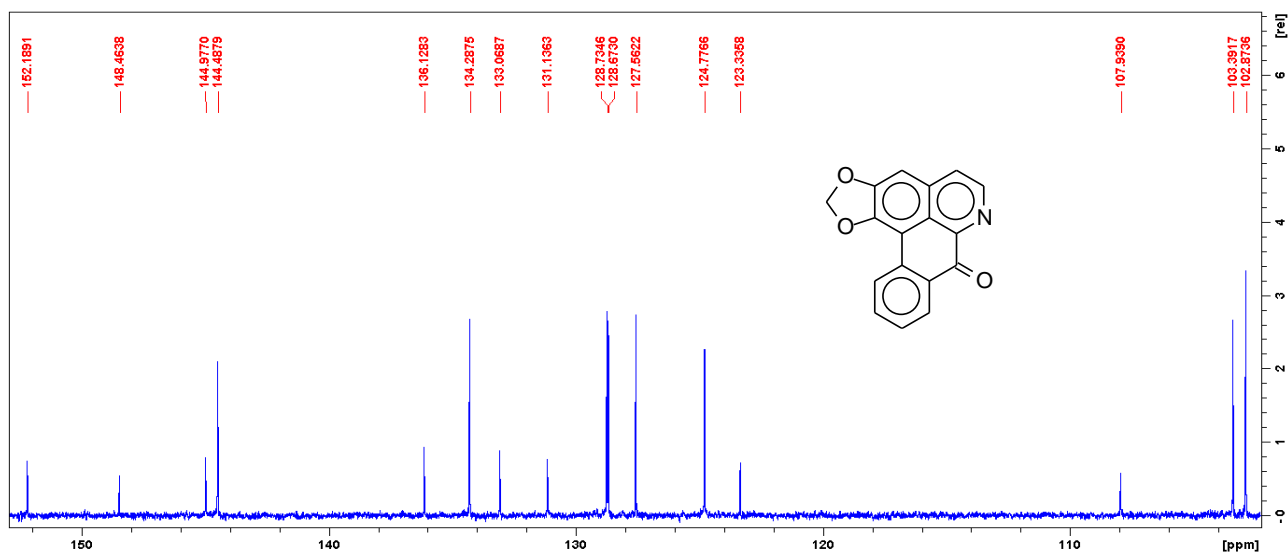


Figure S19. Expansion (δ 152.1 – 102.4) of the ^{13}C NMR spectrum of **liriodenine** (3) in CDCl_3 plus drop of CD_3OD at 150 MHz.

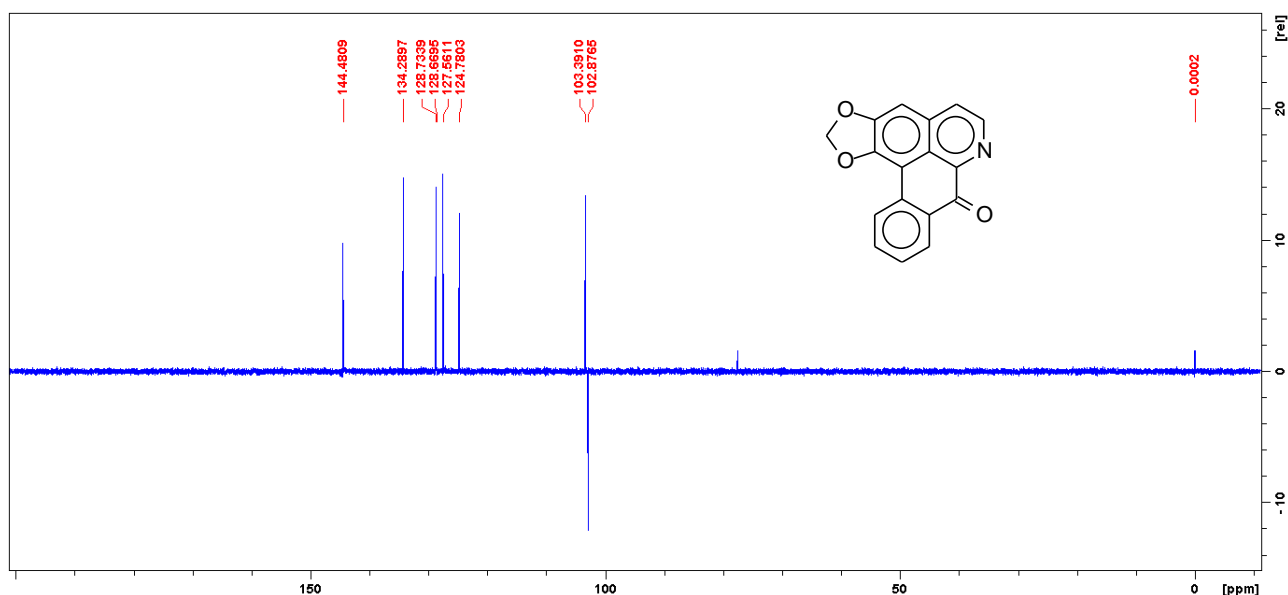


Figure S20. DEPT 135 spectrum of **liriodenine** (3) in CDCl_3 plus drop of CD_3OD at 150 MHz.

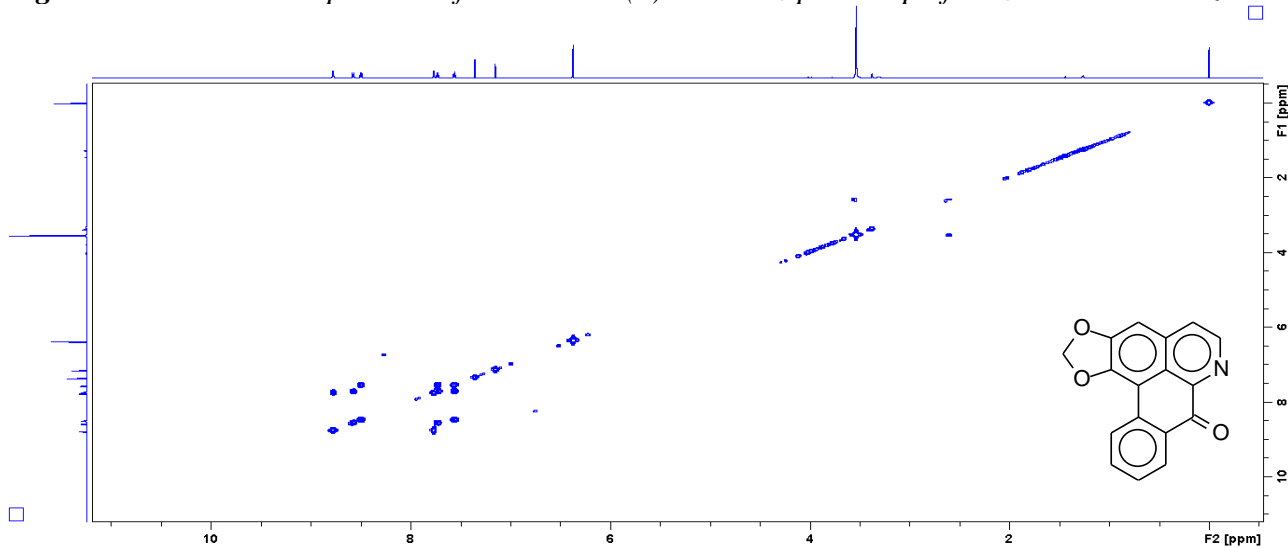


Figure S21. ^1H - ^1H correlation map from COSY NMR experiment of **liriodenine** (3) in CDCl_3 plus drop of CD_3OD at 600 MHz.

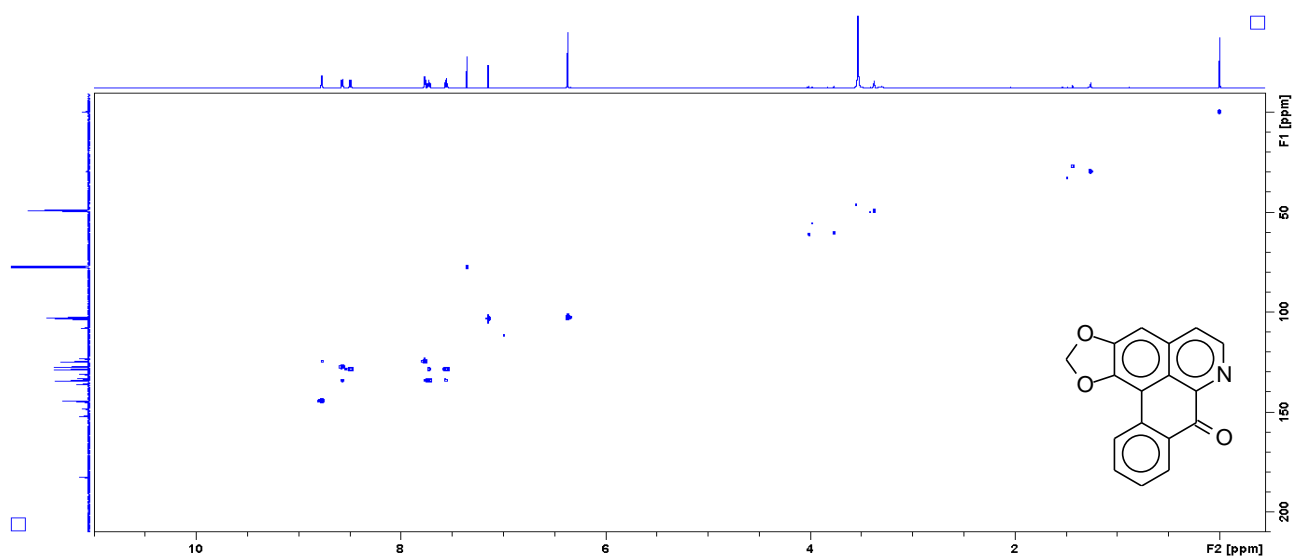


Figure S22. One-bond ^1H - ^{13}C correlation map from HSQC NMR experiment of **liriodenine (3)** in CDCl_3 plus drop of CD_3OD at 600 (^1H) and 150 MHz (^{13}C), respectively.

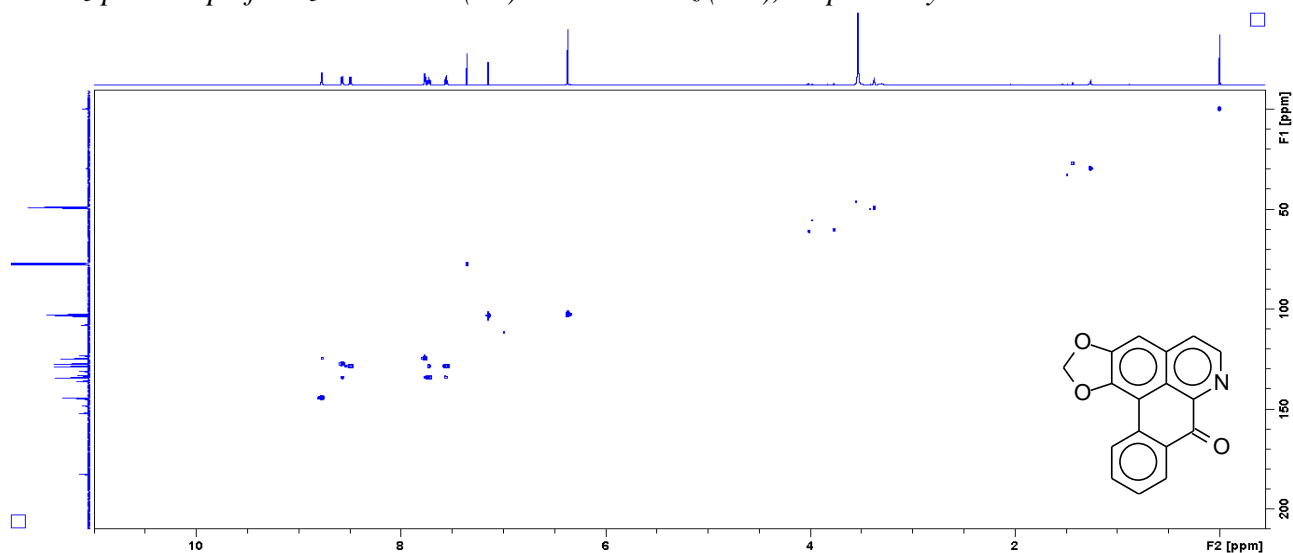


Figure S23. Long-range ^1H - ^{13}C correlation map from HMBC NMR experiment of **liriodenine (3)** in CDCl_3 plus drop of CD_3OD at 600 (^1H) and 150 MHz (^{13}C), respectively.

padres_posi_esi #243 RT: 3,31 AV: 1 NL: 3,41E4
T: ITMS + c ESI Full ms [100,00-1000,00]

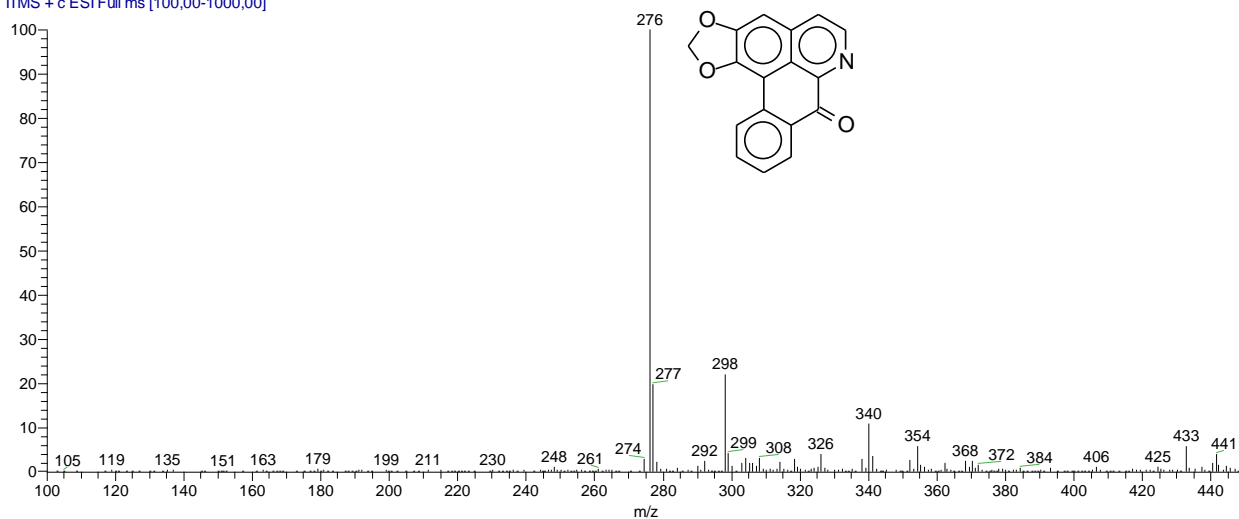


Figure S24. LR-ESI(+)-MS spectrum of **liriodenine (3)** (m/z 276 [$M+H$] $^+$).

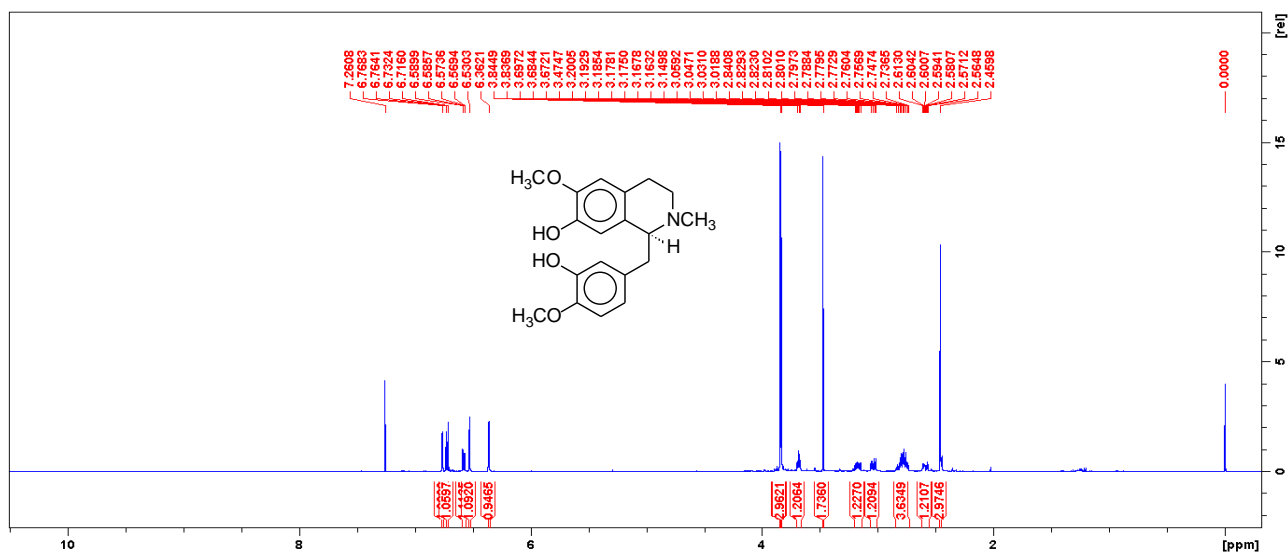


Figure S25. ^1H NMR spectrum of reticuline (4) in CDCl_3 at 500 MHz.

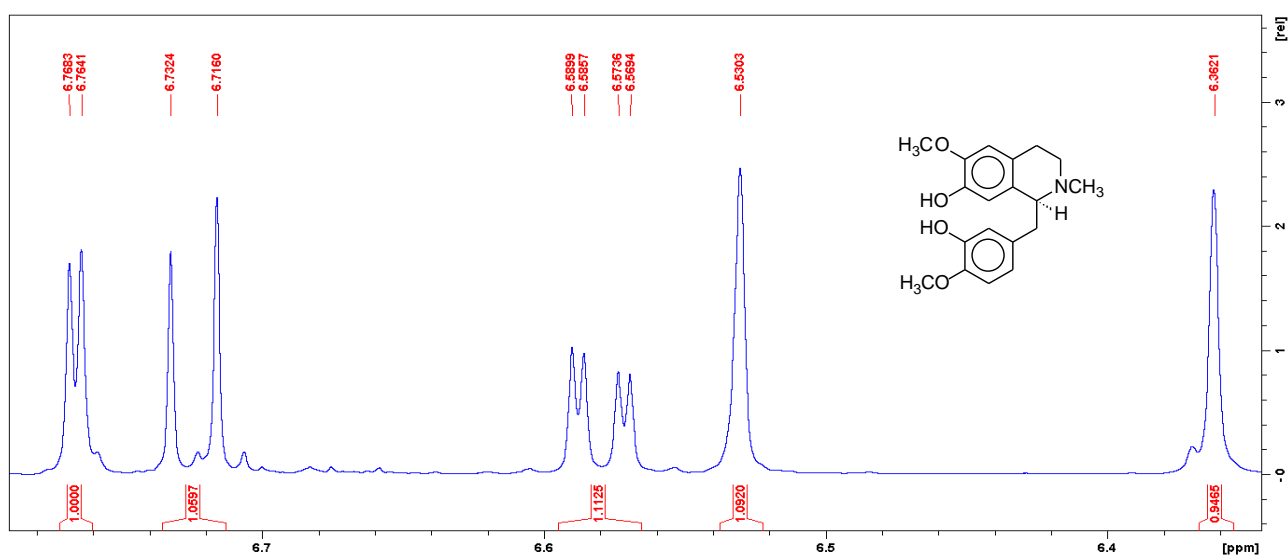


Figure S26. Expansion (δ 6.78 – 6.34) of the ^1H NMR spectrum of reticuline (4) in CDCl_3 at 500 MHz.

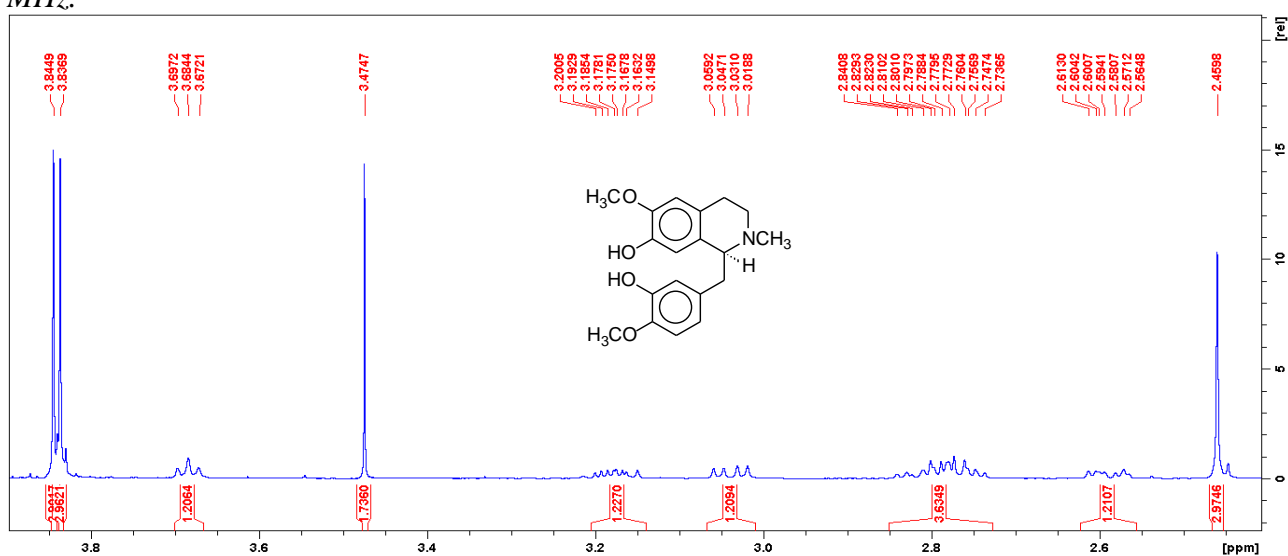


Figure S27. Expansion (δ 3.88 – 2.41) of the ^1H NMR spectrum of reticuline (4) in CDCl_3 at 500 MHz.

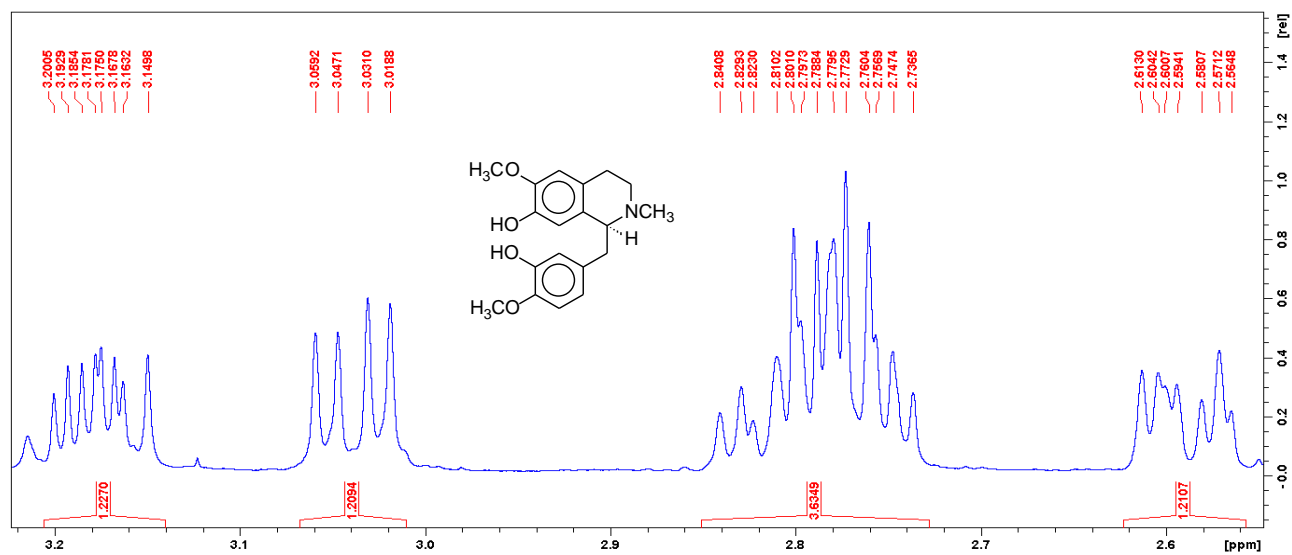


Figure S28. Expansion (δ 3.22 – 2.55) of the ^1H NMR spectrum of *reticuline* (4) in CDCl_3 at 500 MHz.

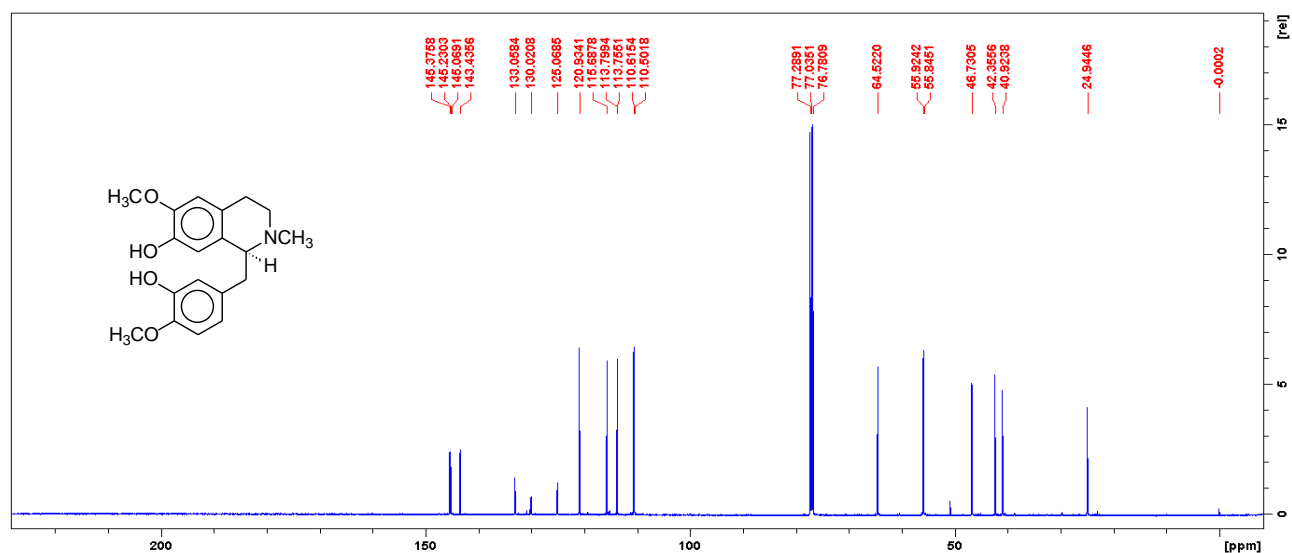


Figure S29. ^{13}C NMR spectrum of *reticuline* (4) in CDCl_3 at 125 MHz.

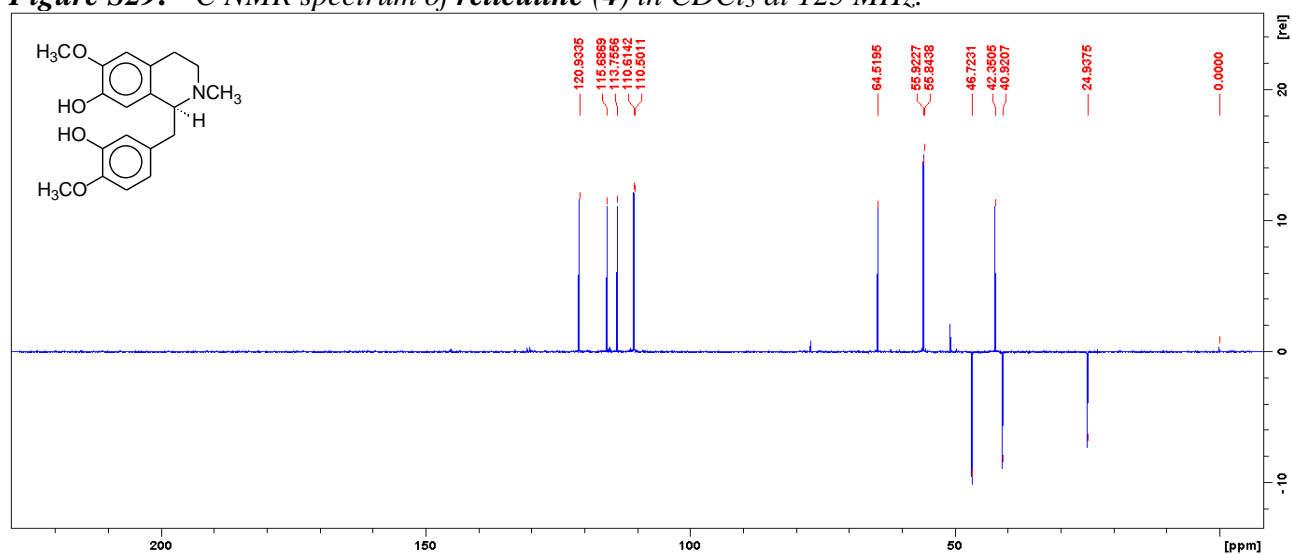


Figure S30. DEPT 135 spectrum of *reticuline* (4) in CDCl_3 at 125 MHz.

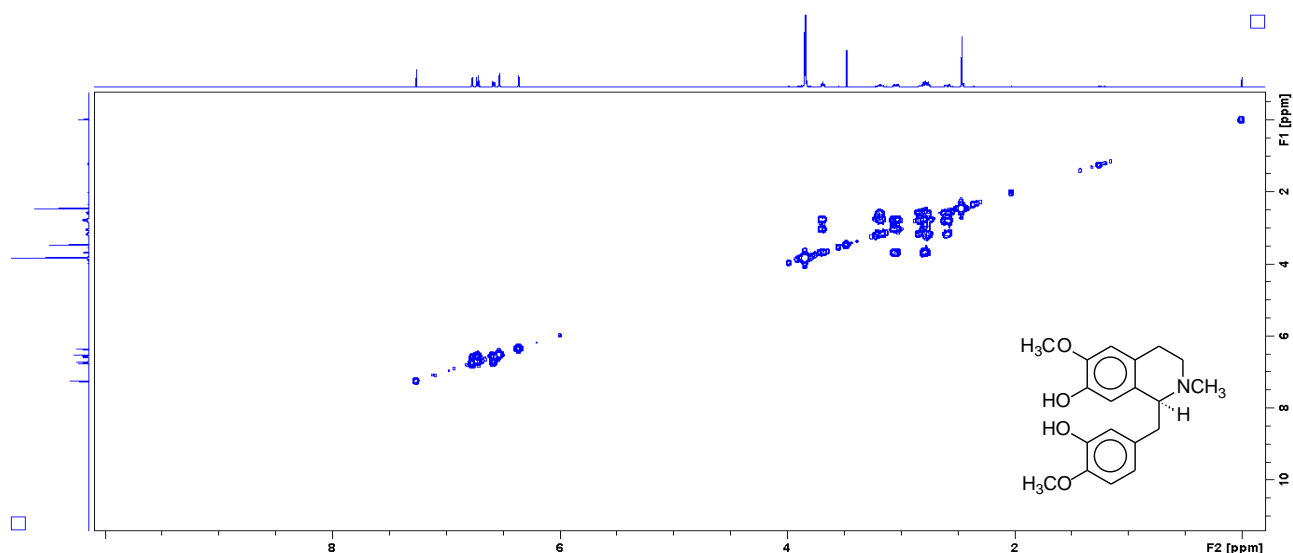


Figure S31. ^1H - ^1H correlation map from COSY NMR experiment of **reticuline (4)** in CDCl_3 at 500 MHz.

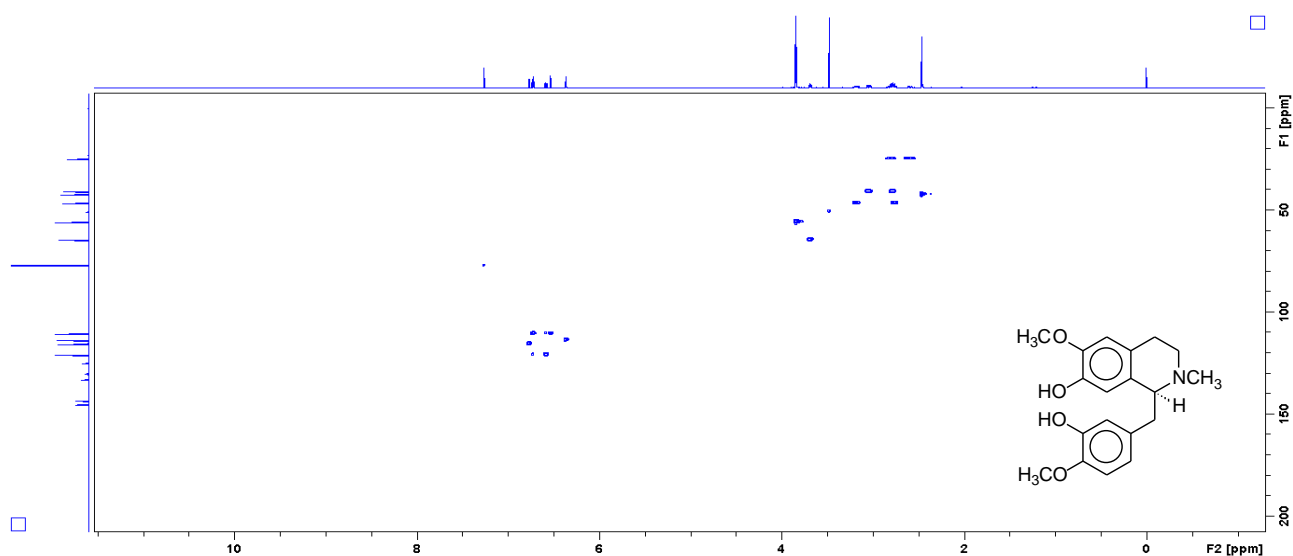


Figure S32. One-bond ^1H - ^{13}C correlation map from HSQC NMR experiment of **reticuline (4)** in CDCl_3 at 500 (^1H) and 125 MHz (^{13}C), respectively.

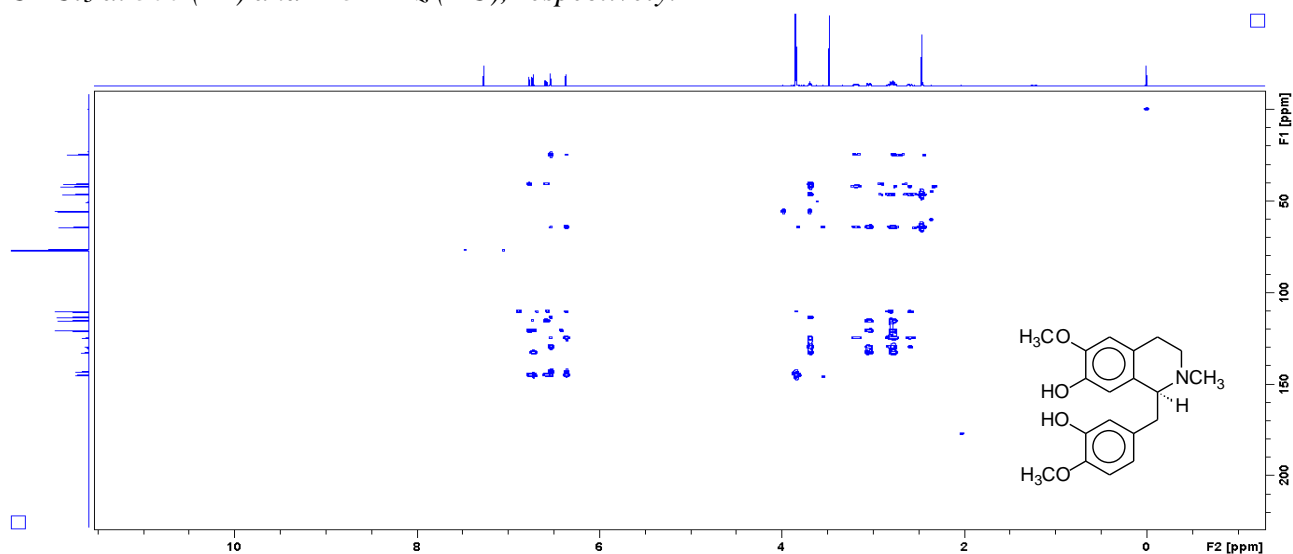


Figure S33. Long-range ^1H - ^{13}C correlation map from HMBC NMR experiment of **reticuline (4)** in CDCl_3 at 500 (^1H) and 125 MHz (^{13}C), respectively.

padroes_posi_esi #1031 RT: 14,32 AV: 1 NL: 8,07E4
T: FTMS + c ESI Full ms [100,00-1000,00]

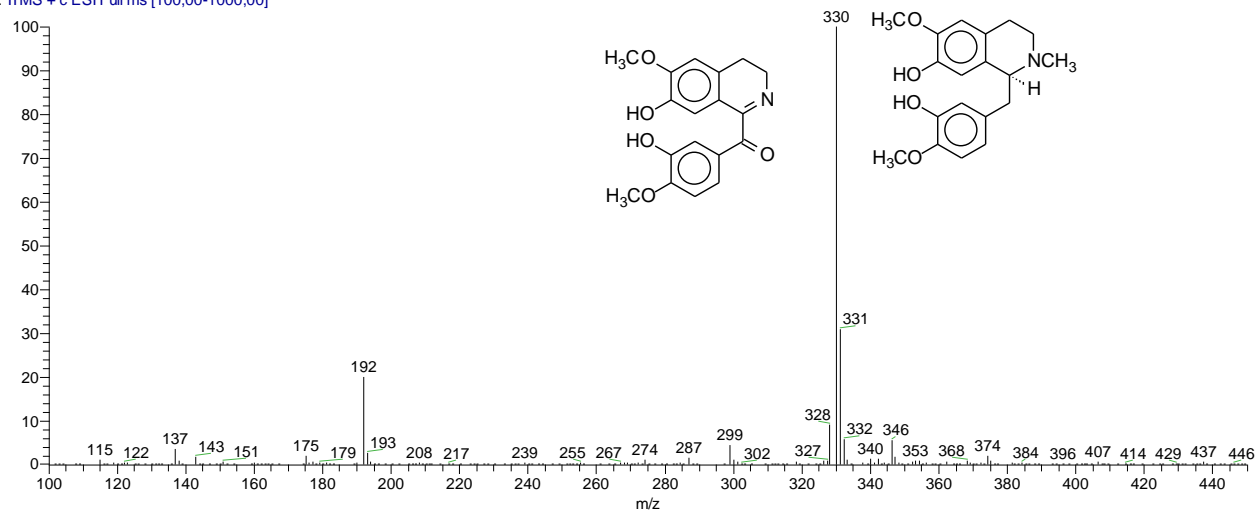


Figure S34. LR-ESI(+)-MS spectrum of *reticuline* (**4**) (m/z 330 $[M+H]^+$).

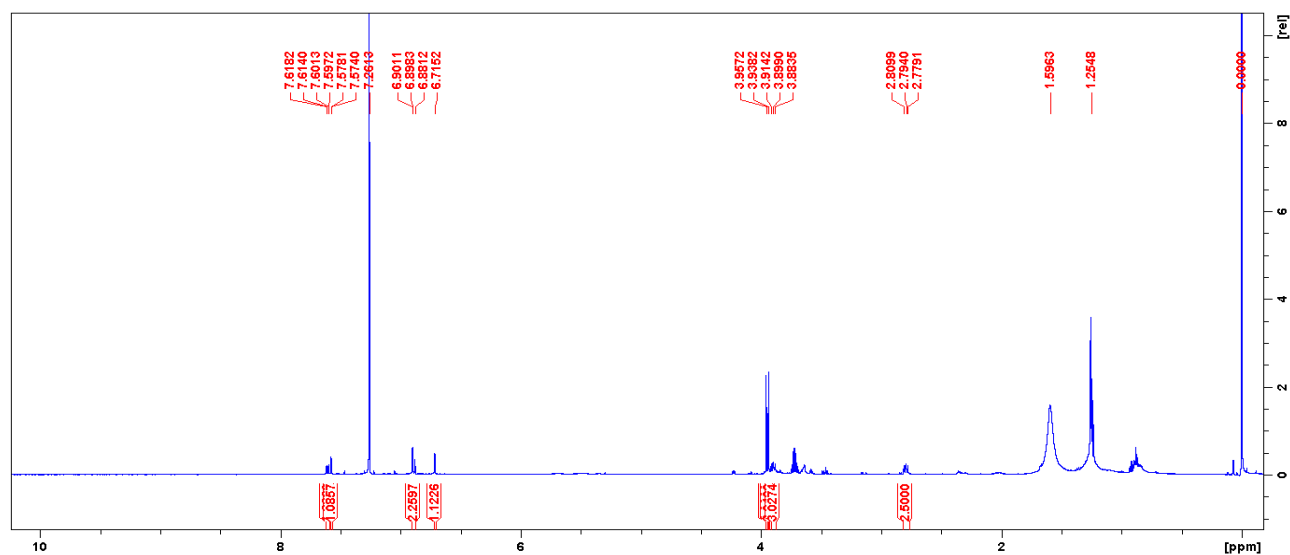


Figure S35. ^1H NMR spectrum of *dehydro-oxonorreticuline* (**5**) in CDCl_3 at 500 MHz.

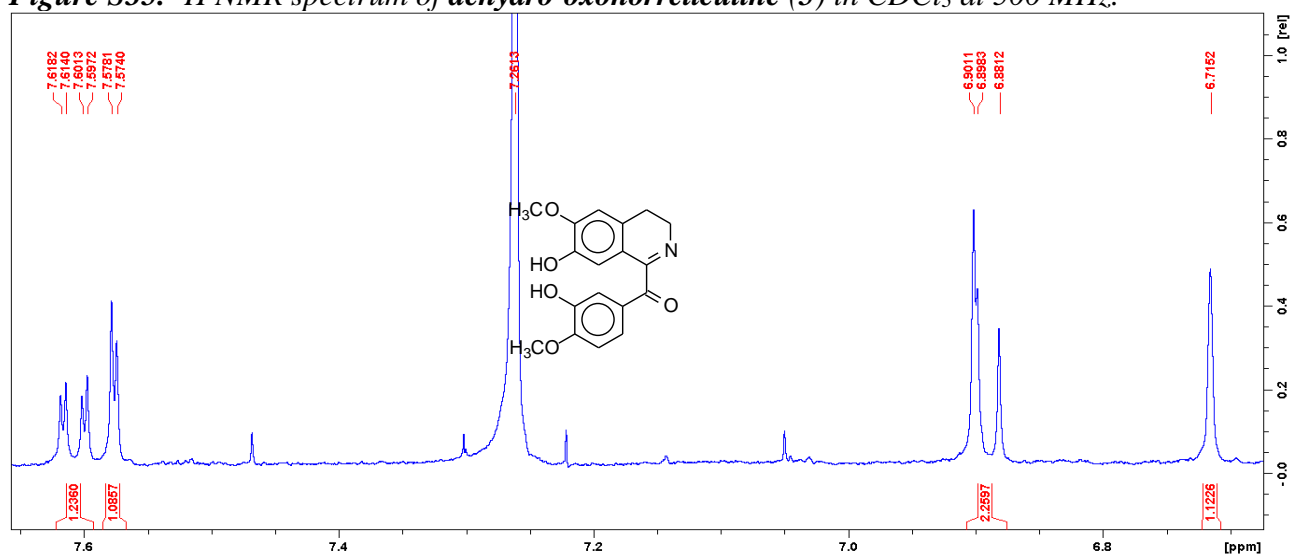


Figure S36. Expansion (δ 7,65 – 6,68) of the ^1H NMR spectrum of *dehydro-oxonorreticuline* (**5**) in CDCl_3 at 500 MHz.

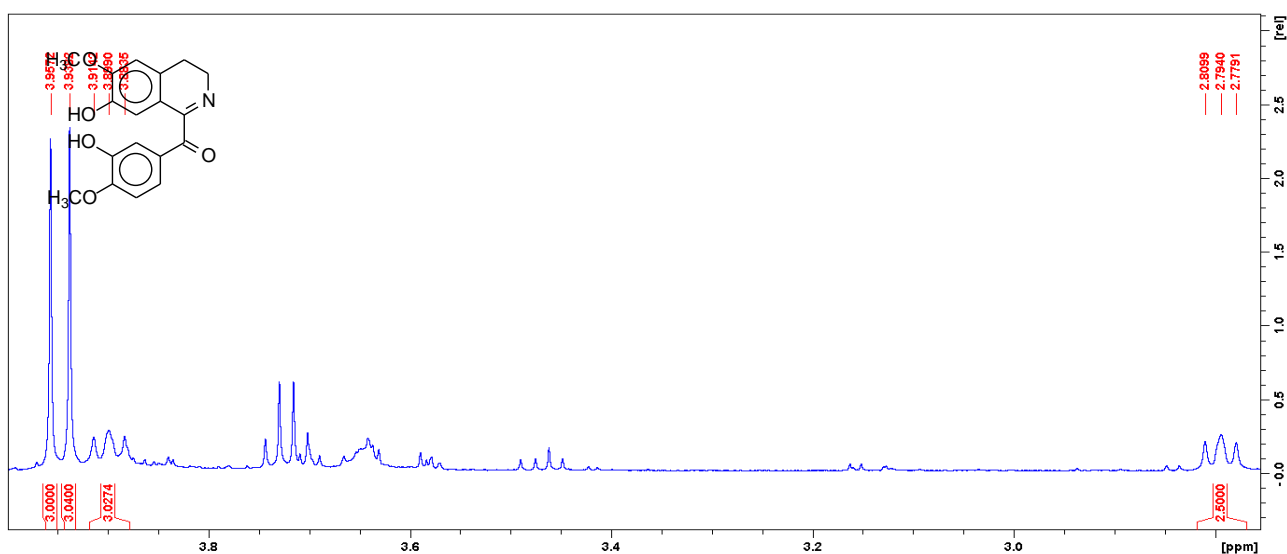


Figure S37. Expansion (δ 3.99 – 2.76) of the ¹H NMR spectrum of *dehydro-oxonorreticuline* (5) in CDCl₃ at 500 MHz.

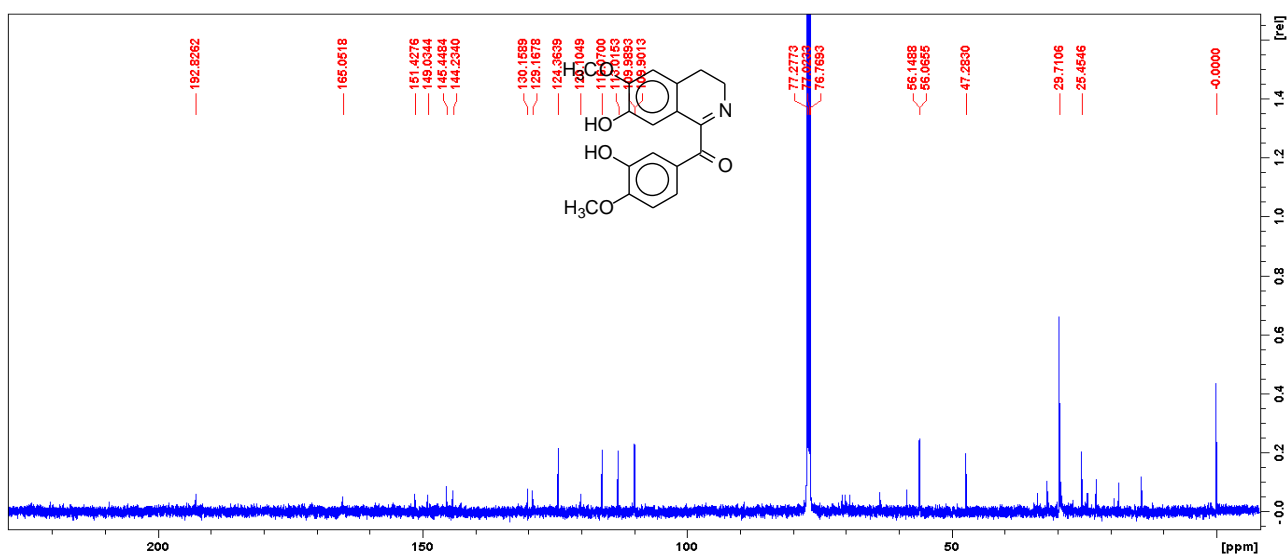


Figure S38. ¹³C NMR spectrum of *dehydro-oxonorreticuline* (5) in CDCl₃ at 125 MHz.

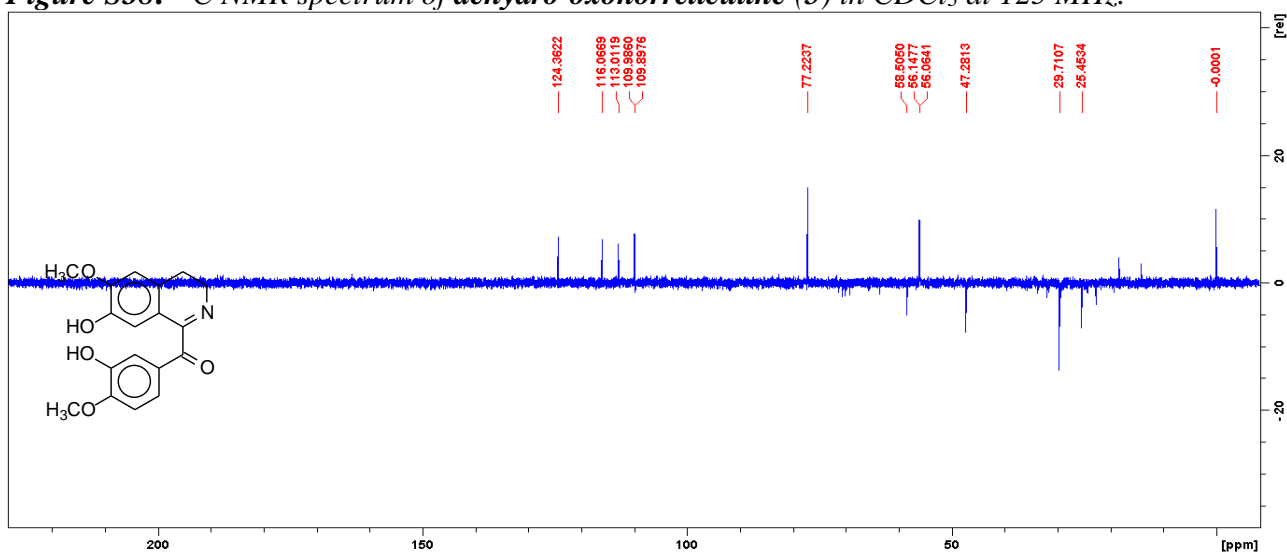


Figure S39. DEPT 135 spectrum of *dehydro-oxonorreticuline* (5) in CDCl₃ at 125 MHz.

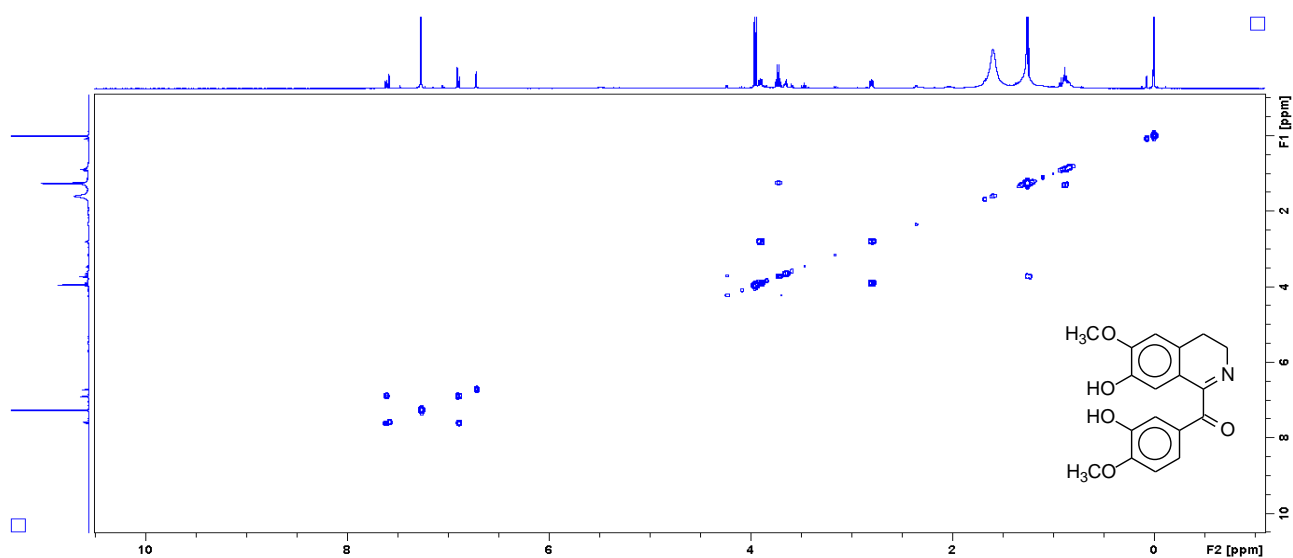


Figure S40. ^1H - ^1H correlation map from COSY NMR experiment of *dehydro-oxonorreticuline* (**5**) in CDCl_3 at 500 MHz.

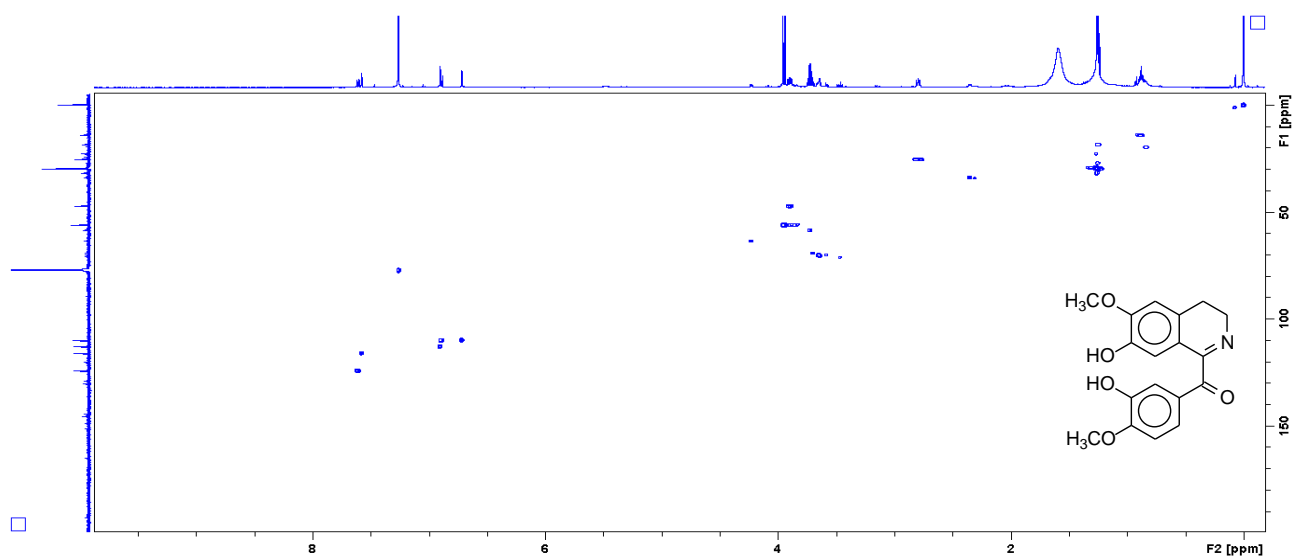


Figure S41. One-bond ^1H - ^{13}C correlation map from HSQC NMR experiment of *dehydro-oxonorreticuline* (**5**) in CDCl_3 at 500 (^1H) and 125 MHz (^{13}C), respectively.

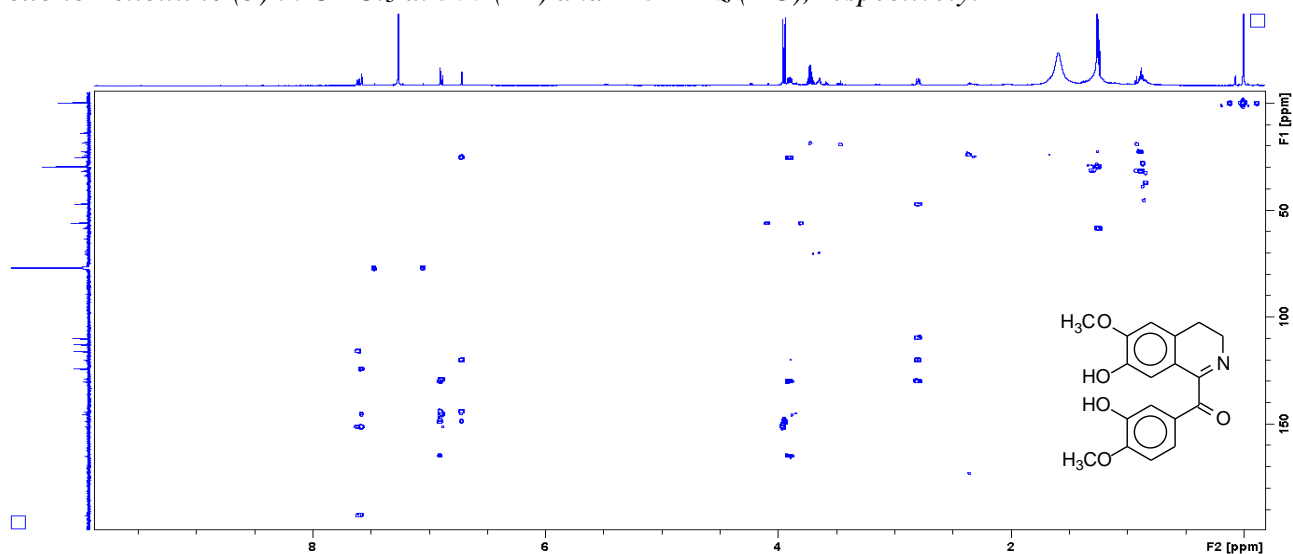


Figure S42. Long-range ^1H - ^{13}C correlation map from HMBC NMR experiment of *dehydro-oxonorreticuline* (**5**) in CDCl_3 at 500 (^1H) and 125 MHz (^{13}C), respectively.

DEFESA_16_04_2019 #826 RT: 16,65 AV: 1 NL: 2,03E8
T: + c ESI Q1MS [100,000-1000,000]

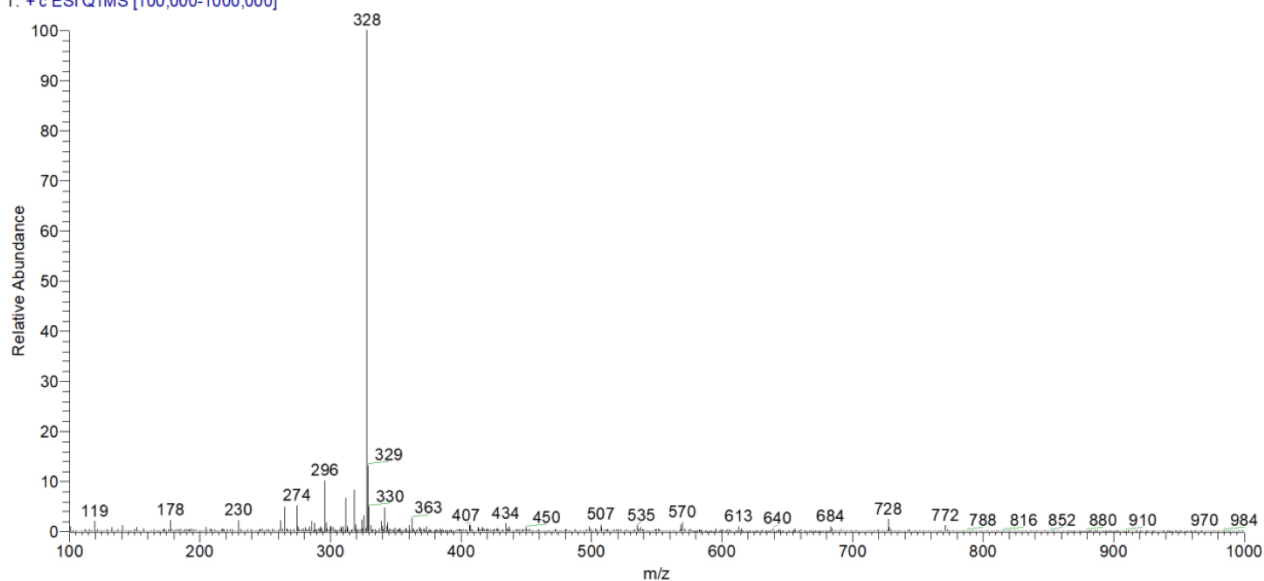


Figure S43. LR-ESI(+)-MS spectrum of *dehydro-oxonorreticuline* (**5**) (m/z 328 $[M+H]^+$).

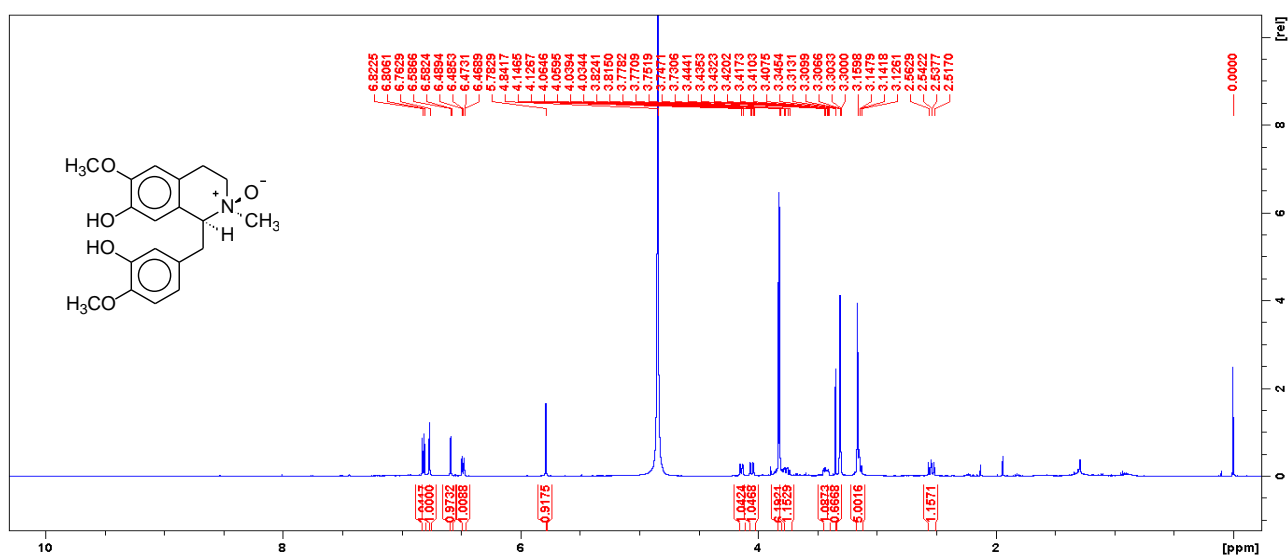
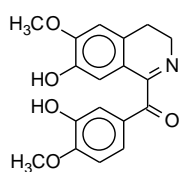


Figure S44. ^1H NMR spectrum of *(+)-1S,2R-reticuline-N β -oxide* (**6**) in CD_3OD at 500 MHz.

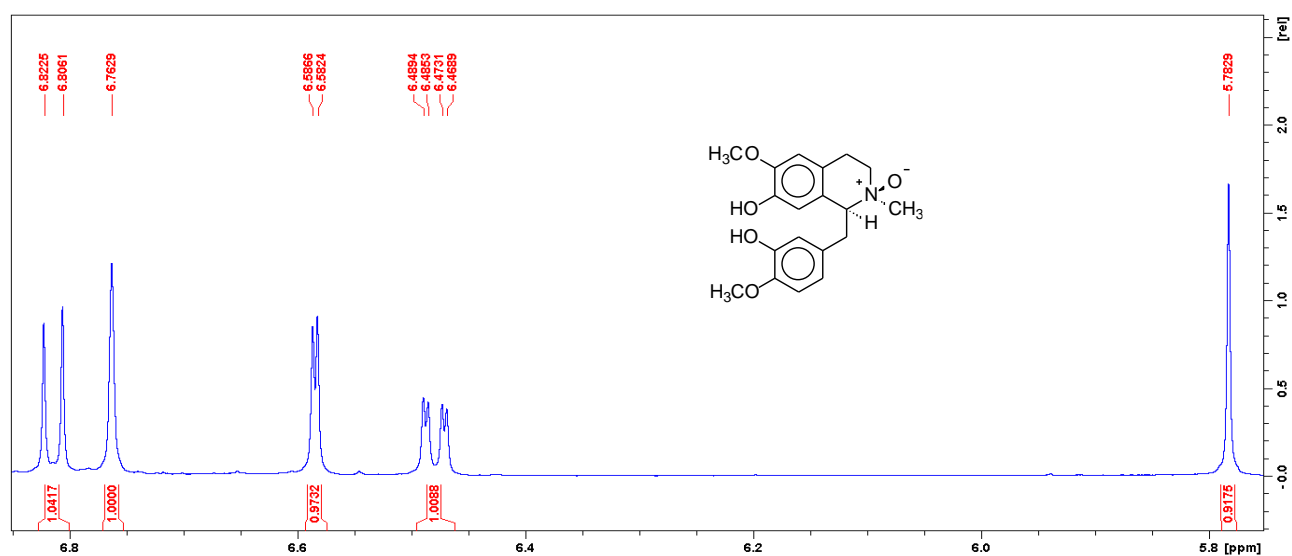


Figure S45. Expansion (δ 6.84 – 5.75) of the ^1H NMR spectrum of (+)-1S,2R-reticuline-N β -oxide (6) in CD_3OD at 500 MHz.

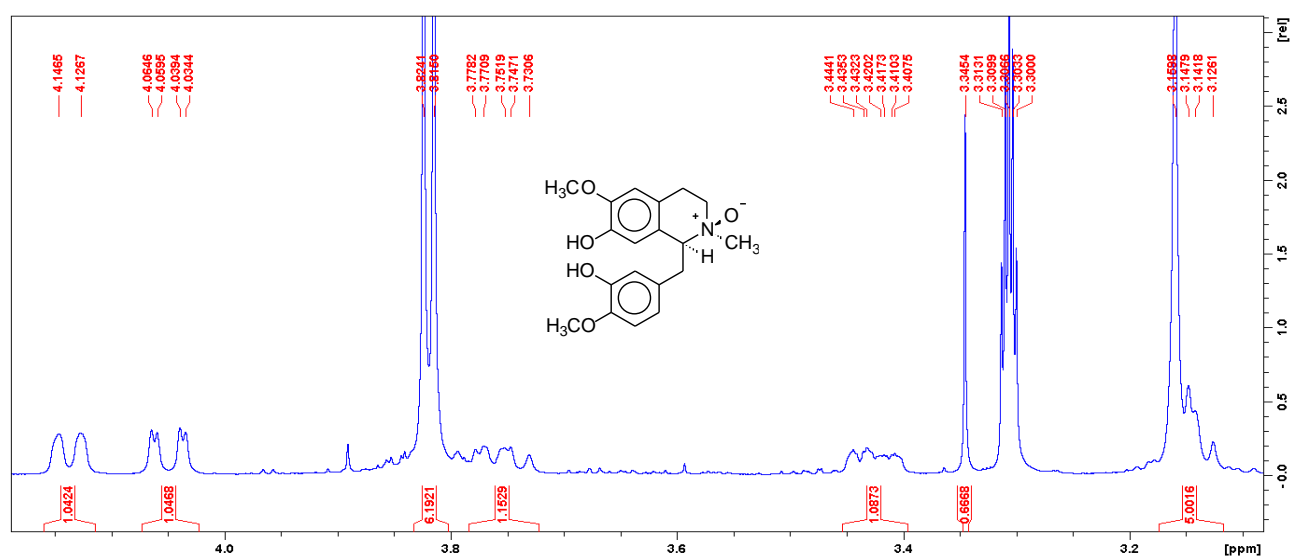


Figure S46. Expansion (δ 3.88 – 2.41) of the ^1H NMR spectrum of (+)-1S,2R-reticuline-N β -oxide (6) in CD_3OD at 500 MHz.

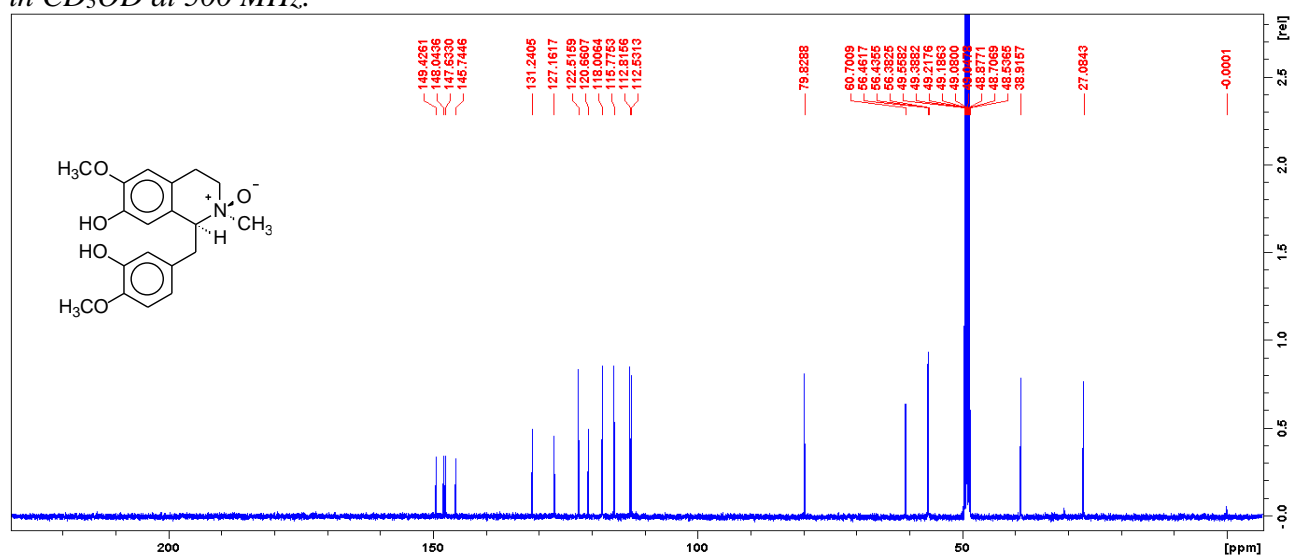


Figure S47. ^{13}C NMR spectrum of (+)-1S,2R-reticuline-N β -oxide (6) in CD_3OD at 125 MHz.

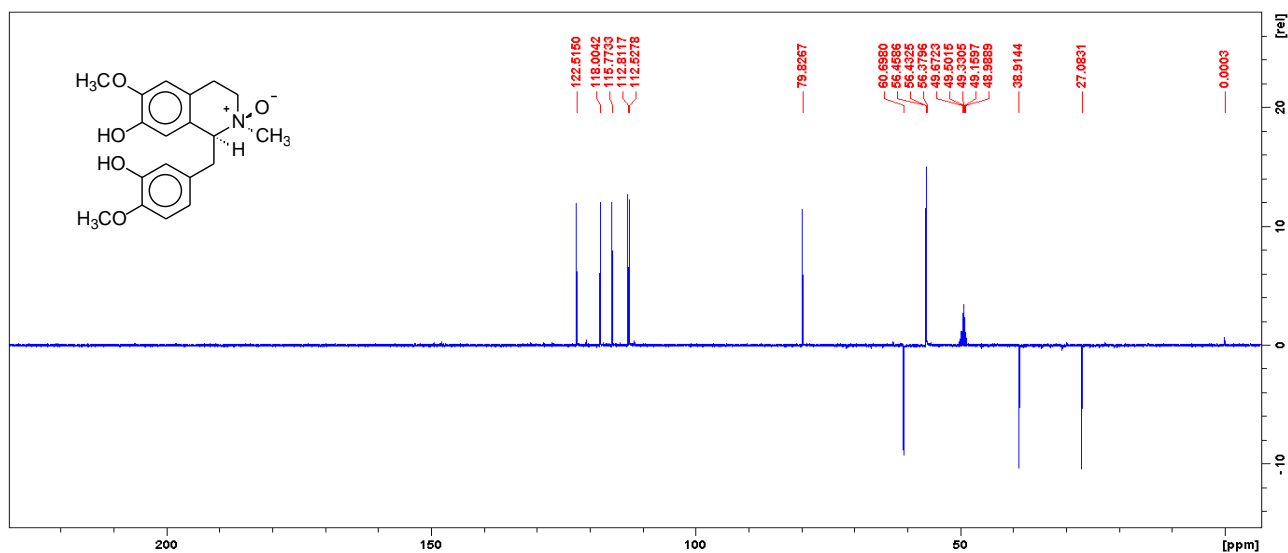


Figure S48. DEPT 135 spectrum of (+)-1S,2R-reticuline-N β -oxide (6) in CD₃OD at 125 MHz.

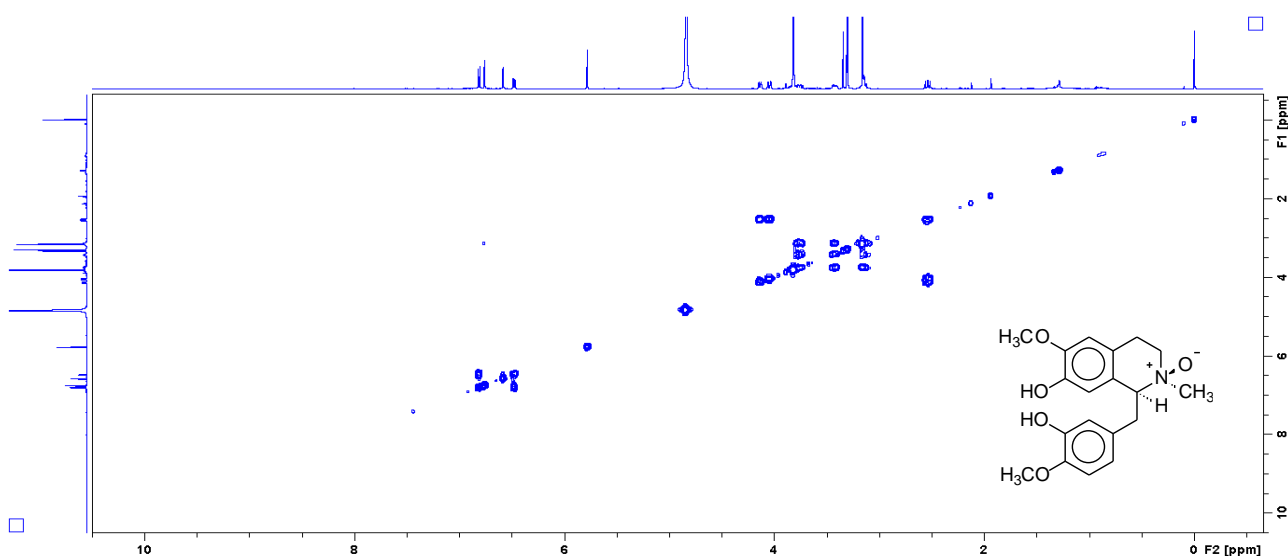


Figure S49. ^1H - ^1H correlation map from COSY NMR experiment of (+)-1S,2R-reticuline-N β -oxide (6) in CD₃OD at 500 MHz.

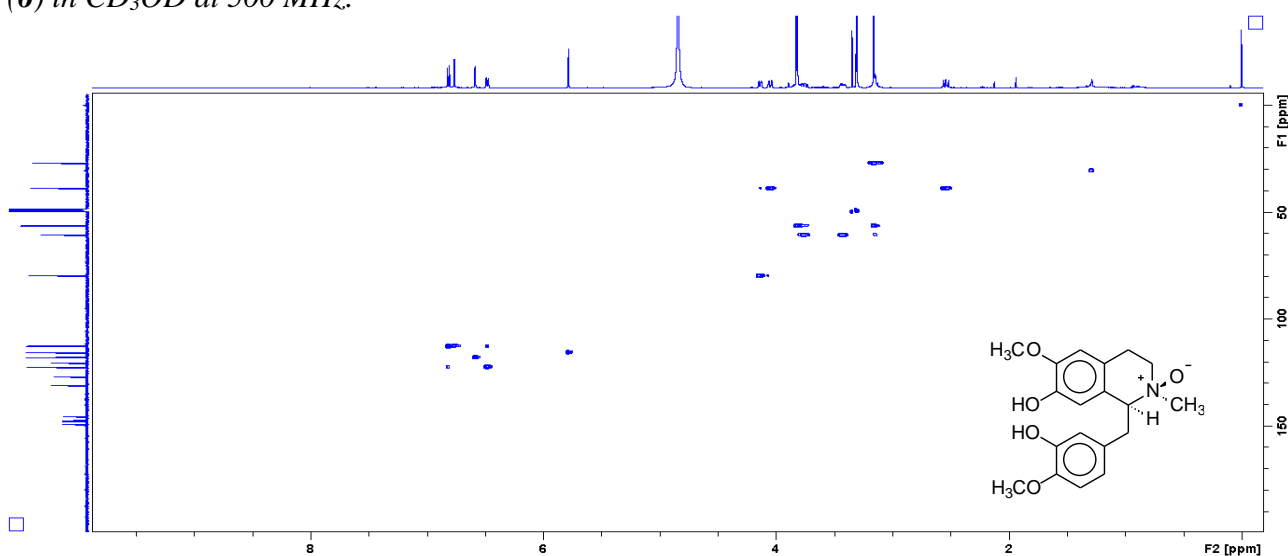


Figure S50. One-bond ^1H - ^{13}C correlation map from HSQC NMR experiment of (+)-1S,2R-reticuline-N β -oxide (6) in CD₃OD at 500 (^1H) and 125 MHz (^{13}C), respectively.

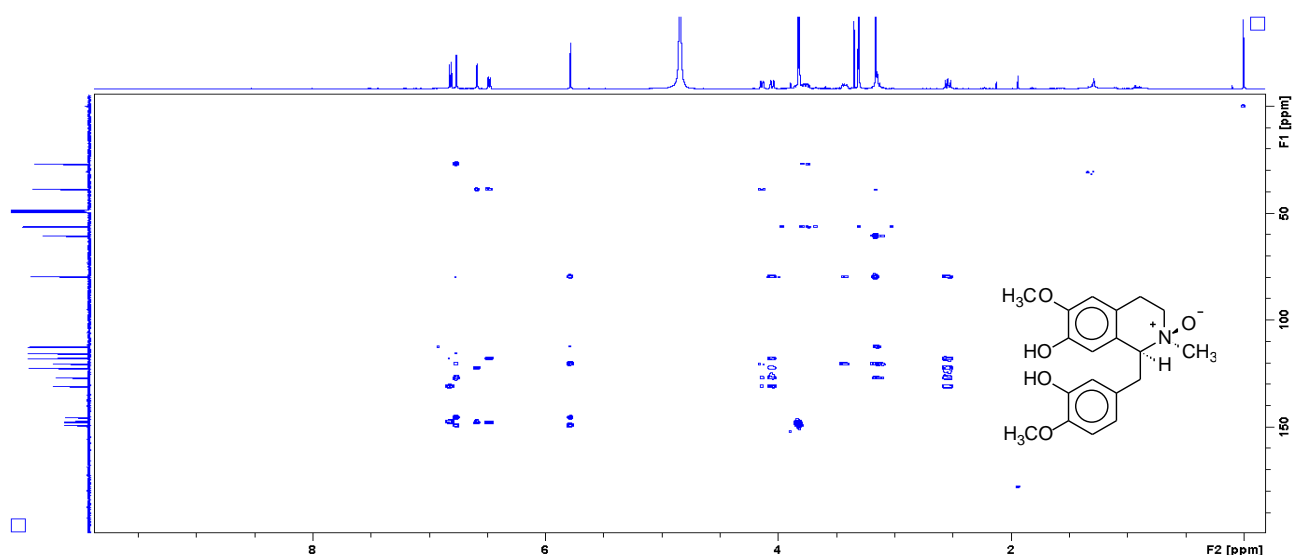


Figure S51. Long-range ^1H - ^{13}C correlation map from HMBC NMR experiment of (+)-1S,2R-reticuline- $\text{N}\beta$ -oxide (**6**) in CD_3OD at 500 (^1H) and 125 MHz (^{13}C), respectively.

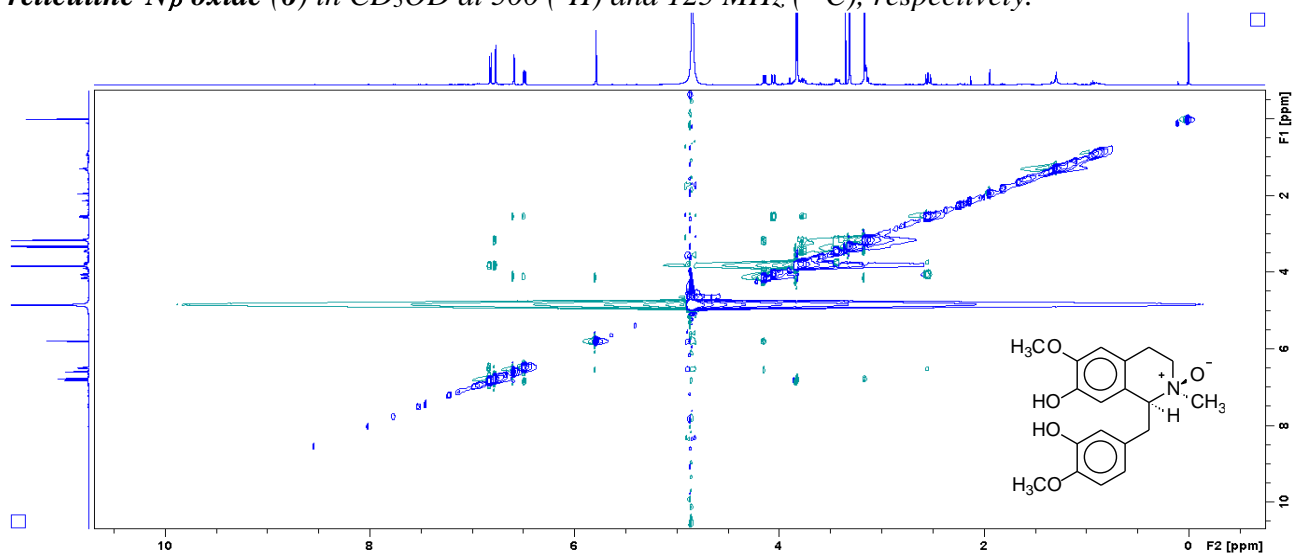


Figure S52. ^1H - ^1H correlation map from NOESY NMR experiment of (+)-1S,2R-reticuline- $\text{N}\beta$ -oxide (**6**) in CD_3OD at 500 (^1H) and 125 MHz (^{13}C), respectively.

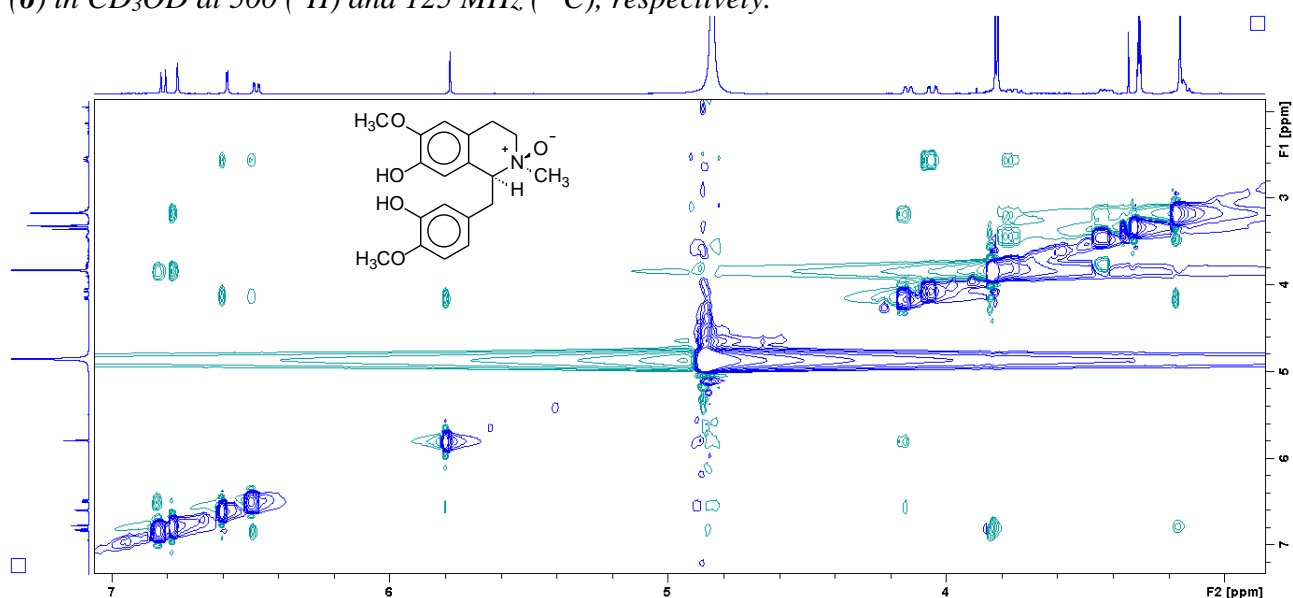


Figure S53. Expansion of ^1H - ^1H correlation map from NOESY NMR experiment of (+)-1S,2R-reticuline- $\text{N}\beta$ -oxide (**6**) in CD_3OD at 500 (^1H) and 125 MHz (^{13}C), respectively.

DC_08_05 #216-257 RT: 1.68-1.98 AV: 42 NL: 5,37E8
T: + c APCI Q1MS [150,000-1000,000]

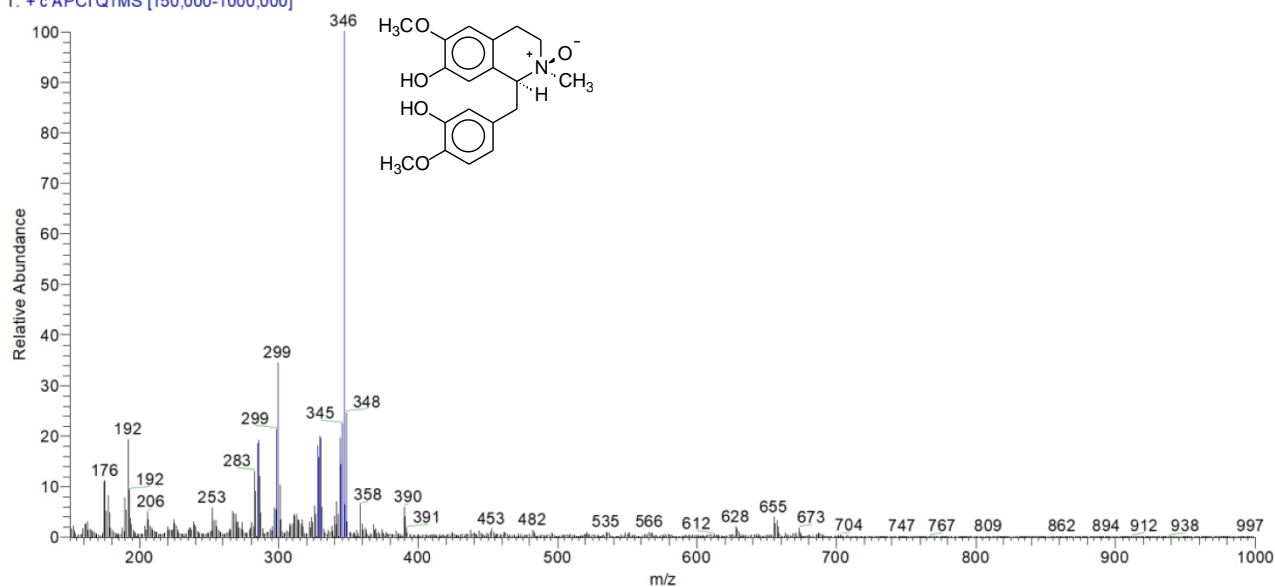


Figure S54. LR-APCI(+)-MS spectrum of (+)-1S,2R-reticuline-N β -oxide (6) (m/z 346 [$M+H$] $^+$).

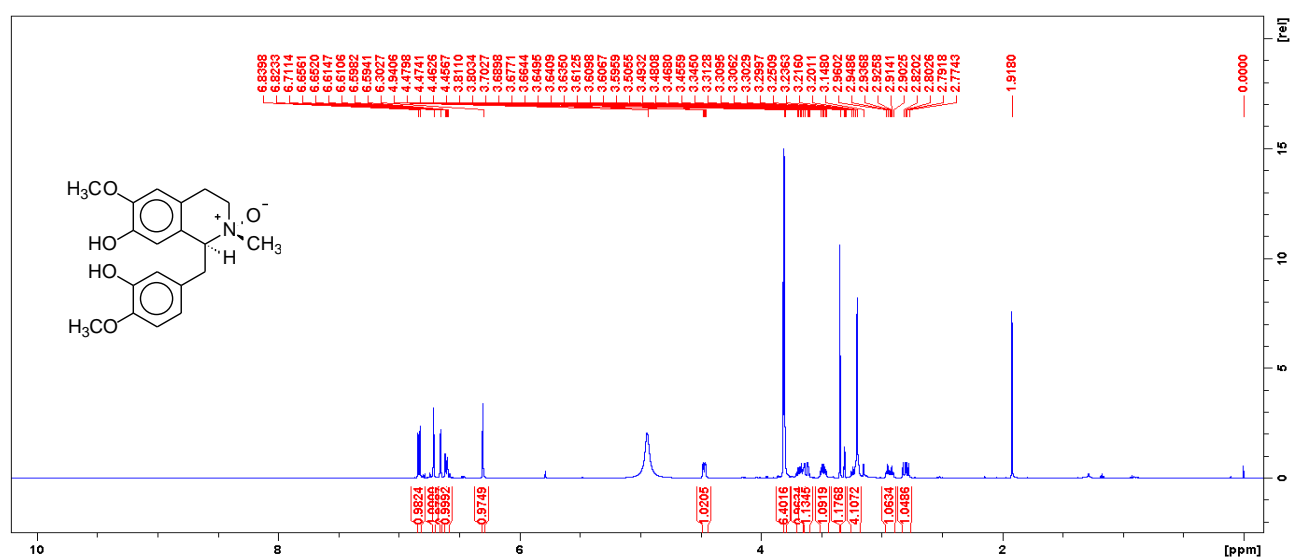


Figure S55. ^1H NMR spectrum of (+)-1S,2S-reticuline-N α -oxide (7) in CD_3OD at 500 MHz.

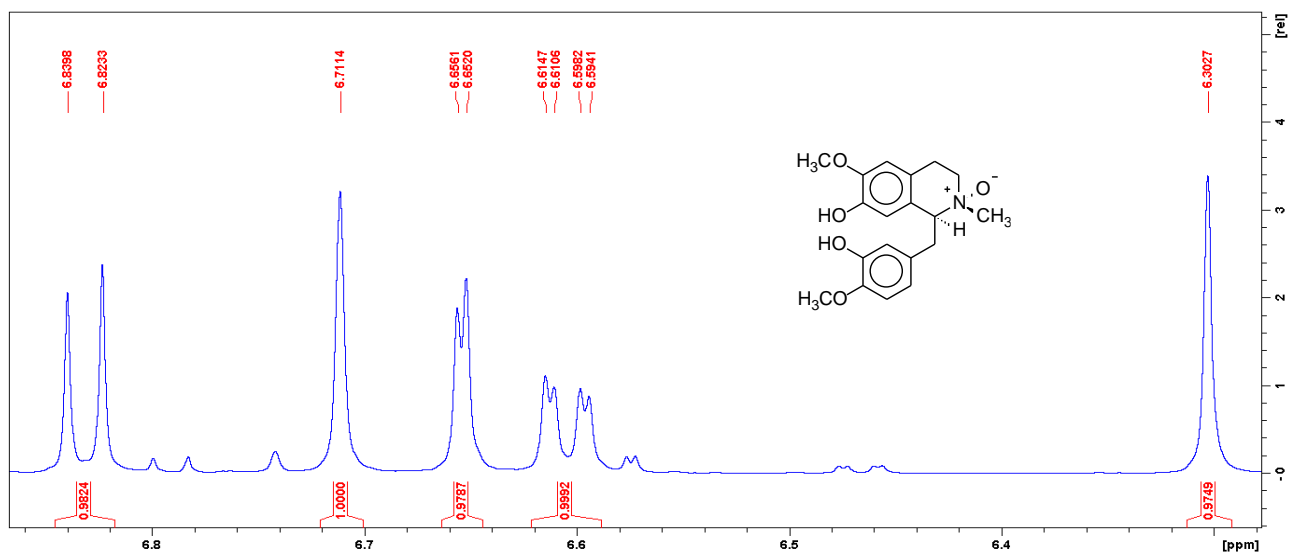


Figure S56. Expansion (δ 6.86 – 6.28) of the ^1H NMR spectrum of (+)-1S,2S-reticuline-N α -oxide (7) in CD_3OD at 500 MHz.

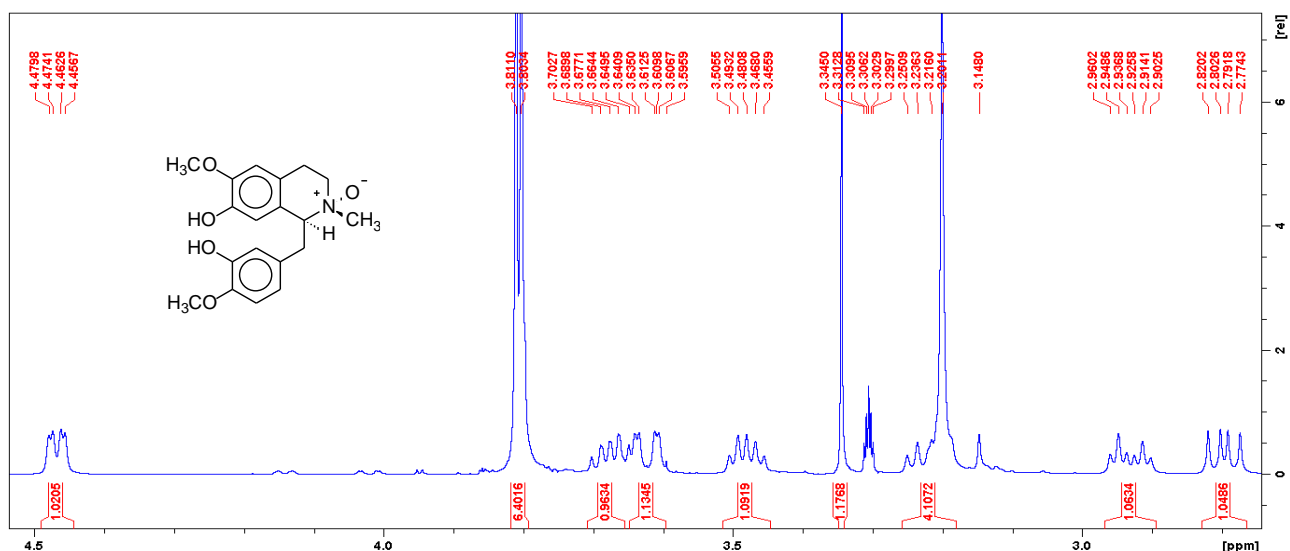


Figure S57. Expansion (δ 4.53 – 2.75) of the ^1H NMR spectrum of (+)-1S,2S-reticuline-N α -oxide (7) in CD_3OD at 500 MHz.

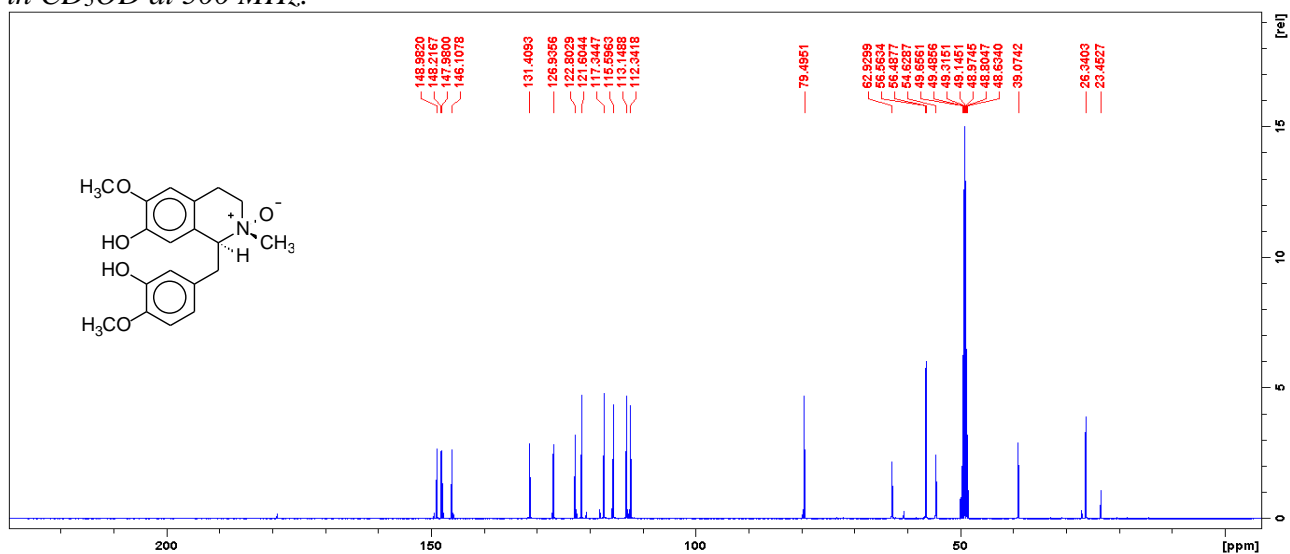


Figure S58. ^{13}C NMR spectrum of (+)-1S,2S-reticuline-N α -oxide (7) in CD_3OD at 125 MHz.

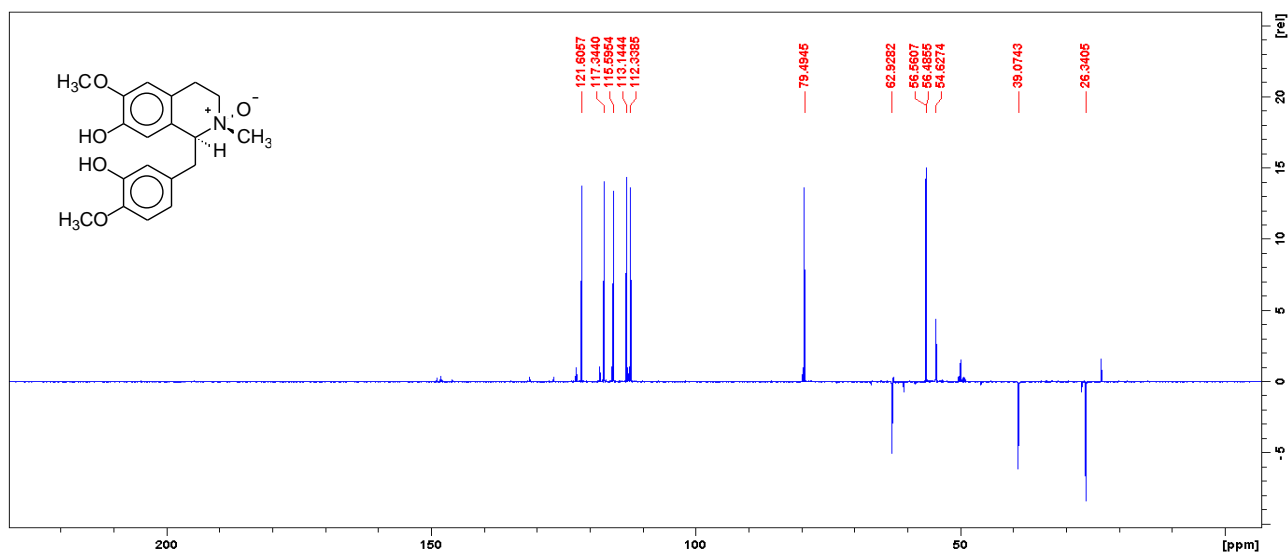


Figure S59. DEPT 135 spectrum of (+)-1S,2S-reticuline-N α -oxide (7) in CD₃OD at 125 MHz.

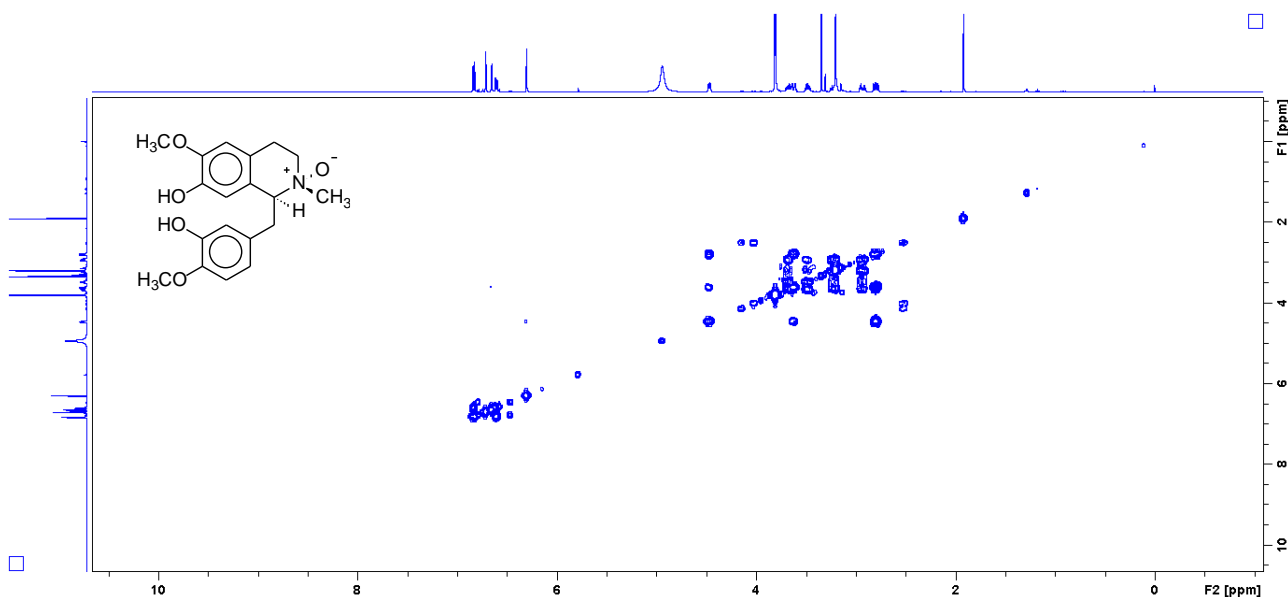


Figure S60. ^1H - ^1H correlation map from COSY NMR experiment of (+)-1S,2S-reticuline-N α -oxide (7) in CD₃OD at 500 MHz.

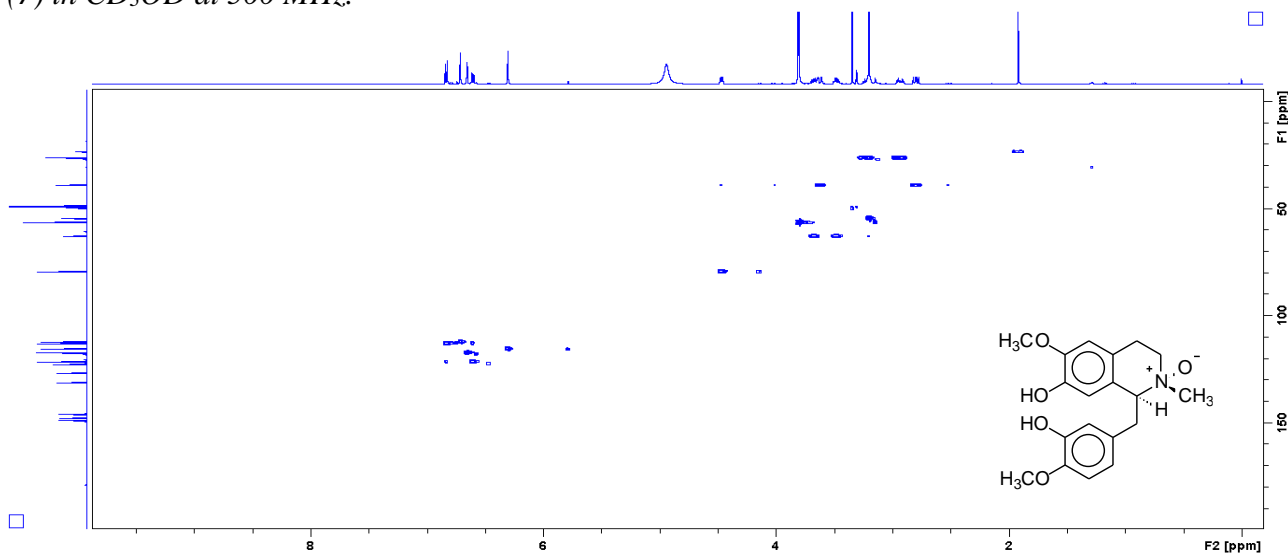


Figure S61. One-bond ^1H - ^{13}C correlation map from HSQC NMR experiment of (+)-1S,2S-reticuline-N α -oxide (7) in CD₃OD at 500 (^1H) and 125 MHz (^{13}C), respectively.

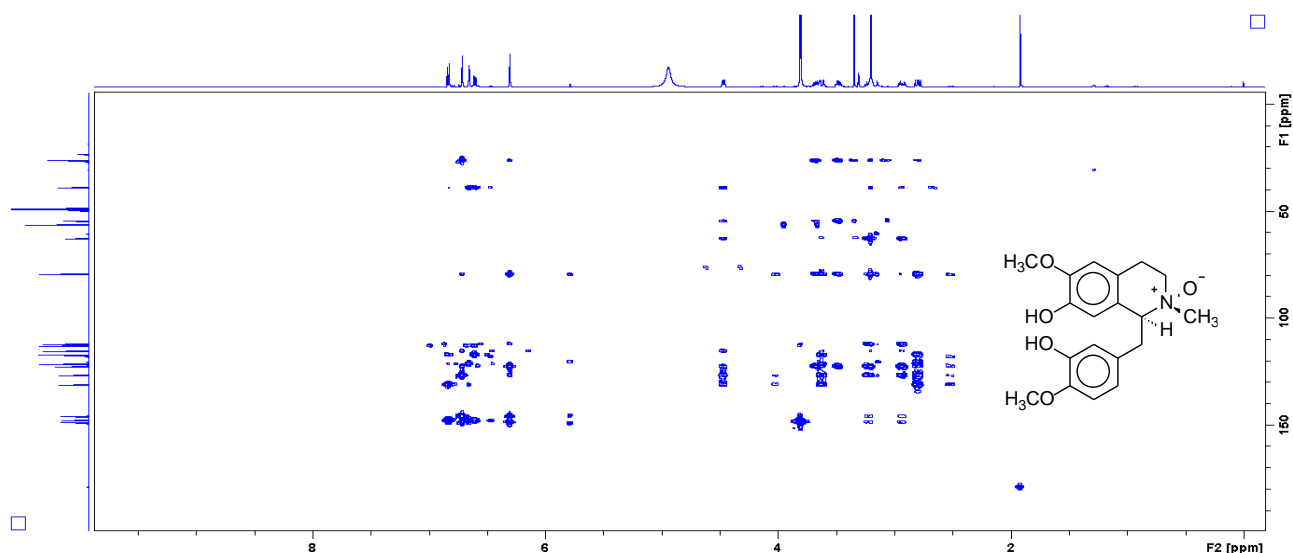


Figure S62. Long-range ^1H - ^{13}C correlation map from HMBC NMR experiment of (+)-1S,2S-reticuline- N_α -oxide (7) in CD_3OD at 500 (^1H) and 125 MHz (^{13}C), respectively.

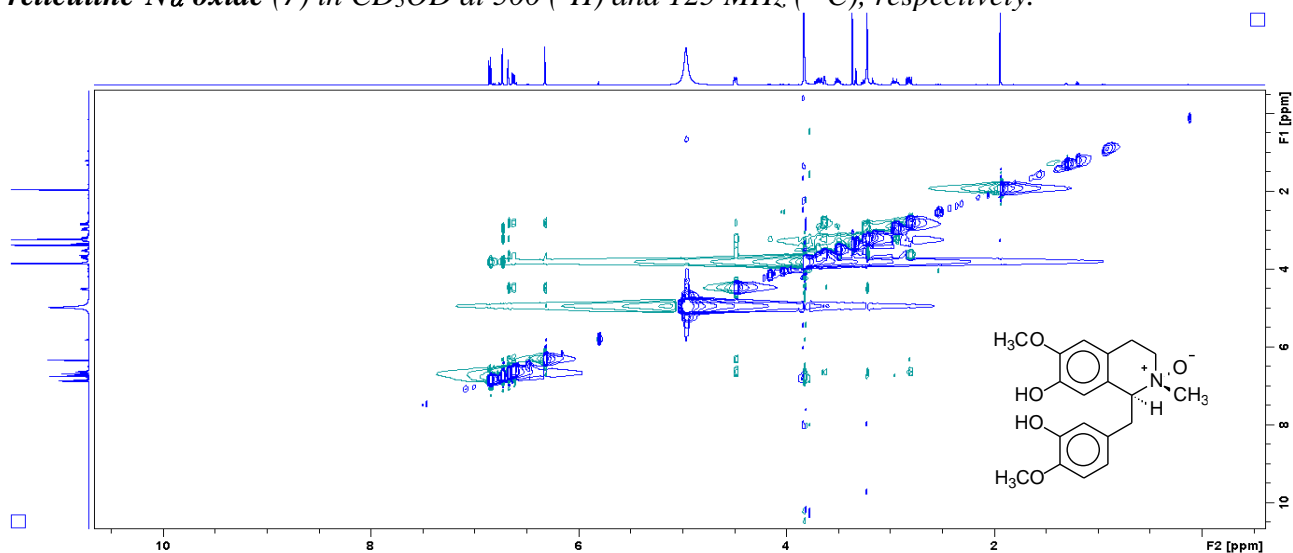


Figure S63. ^1H - ^1H correlation map from NOESY NMR experiment of (+)-1S,2S-reticuline- N_α -oxide (7) in CD_3OD at 500 (^1H) and 125 MHz (^{13}C), respectively.

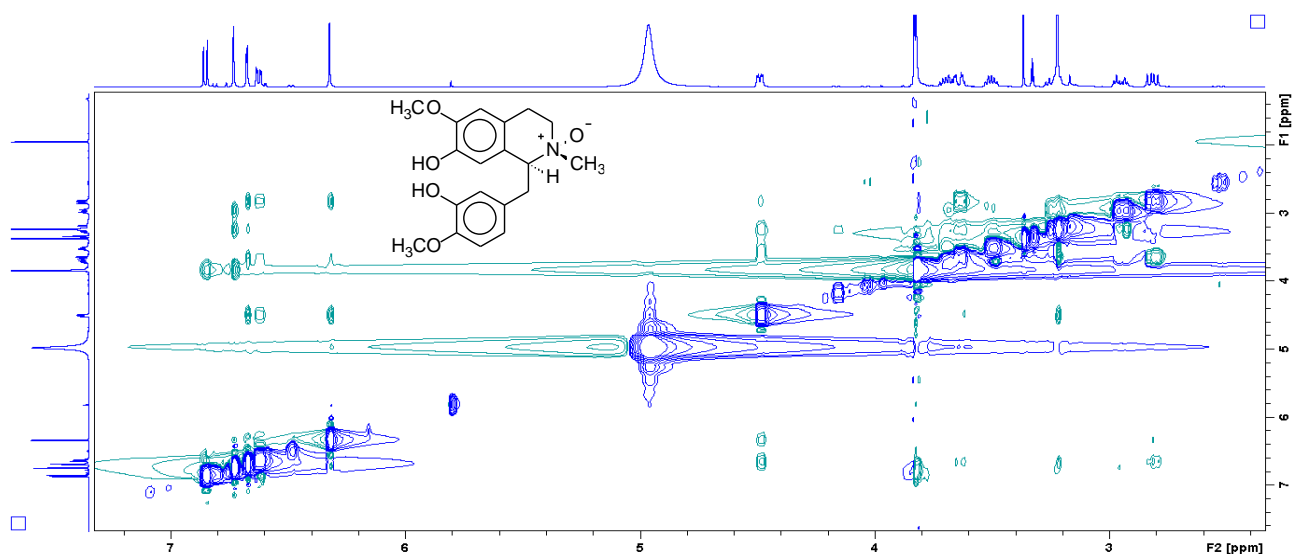


Figure S64. Expansion of ^1H - ^1H correlation map from NOESY NMR experiment of (+)-1S,2S-reticuline- N_α -oxide (7) in CD_3OD at 500 (^1H) and 125 MHz (^{13}C), respectively.

DC_08_05#361 RT: 2.78 AV: 1 NL: 7.76E8
T: +c APCI Q1MS [150,000-1000,000]

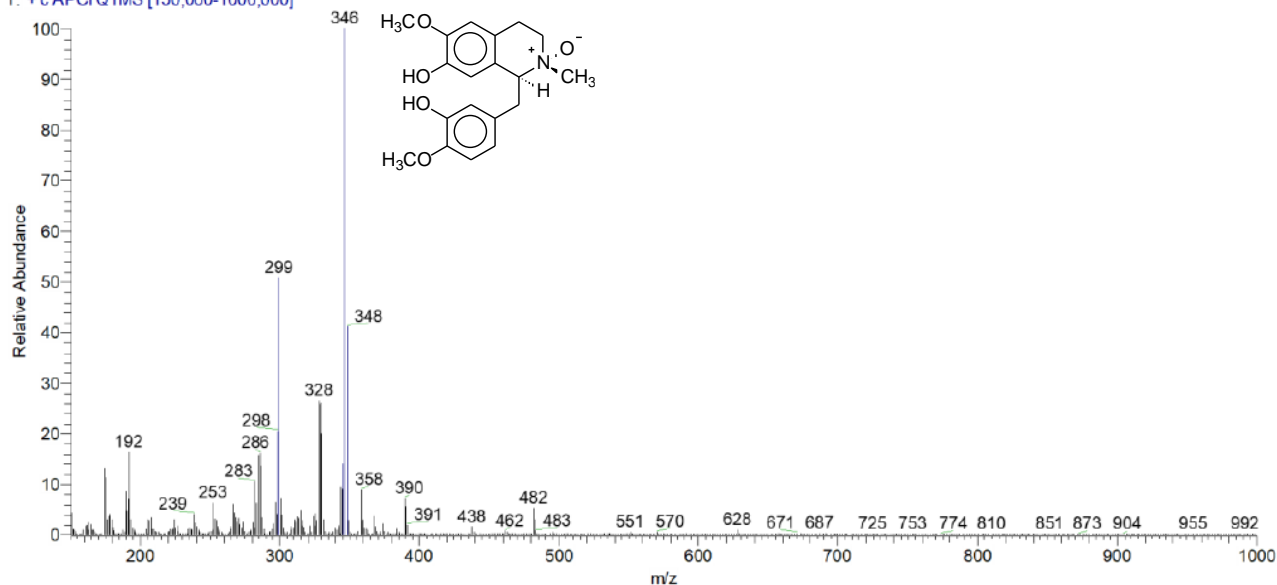


Figure S65. LR-APCI(+)-MS spectrum of (+)-1S,2S-reticuline-N-oxide (7) (m/z 345 $[M+H]^+$).

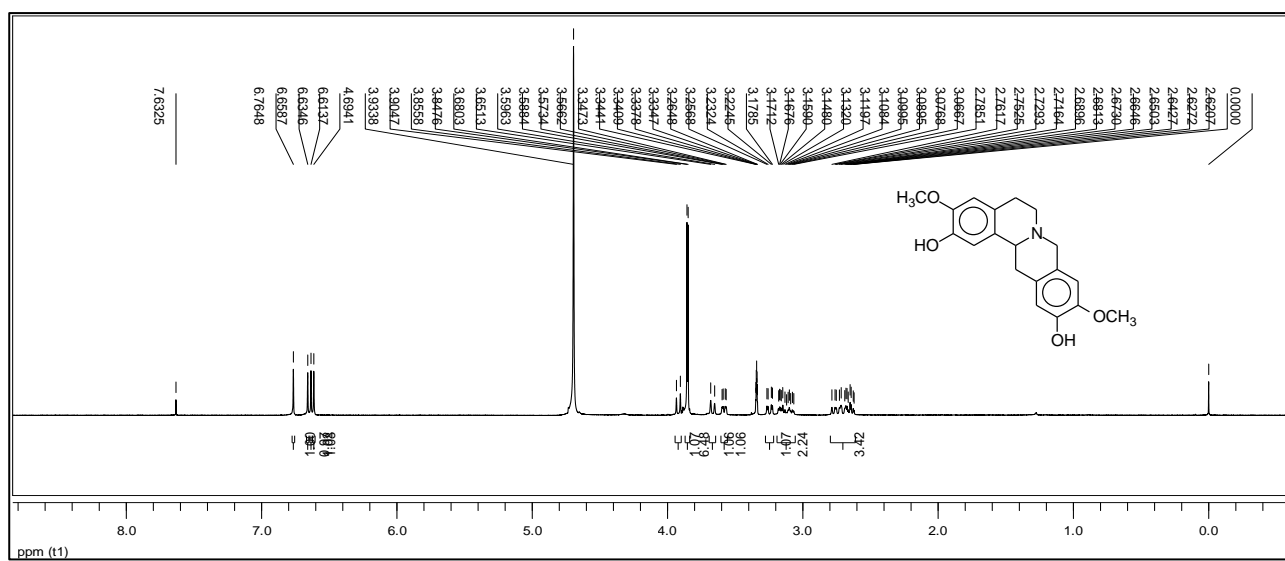


Figure S66. ^1H NMR spectrum of coreximine (8) in CDCl_3 plus drops of CD_3OD at 500 MHz.

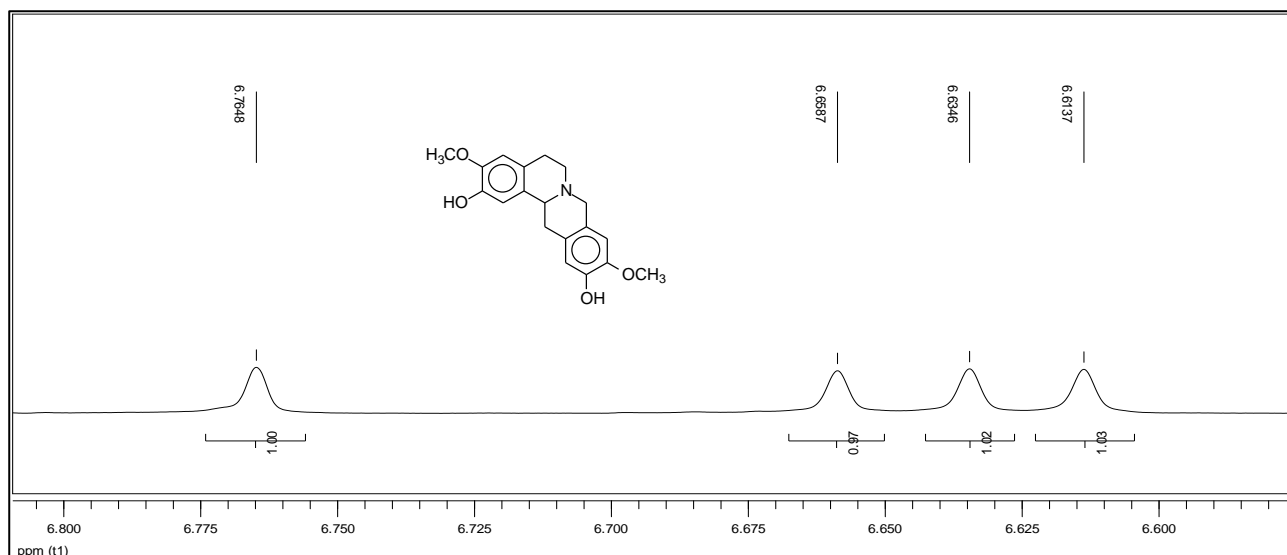


Figure S67. Expansion (δ 6.80 – 6.57) of the ^1H NMR spectrum of **coreximine** (**8**) in CDCl_3 plus drops of CD_3OD at 500 MHz.

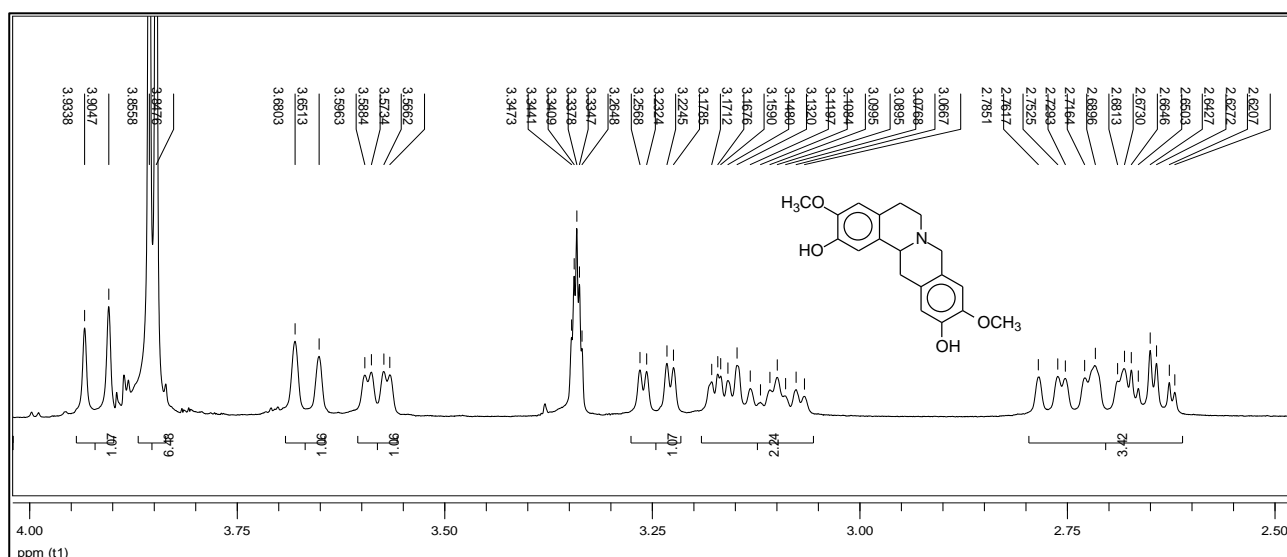


Figure S68. Expansion (δ 4.00 – 2.49) of the ^1H NMR spectrum of **coreximine** (**8**) in CDCl_3 plus drops of CD_3OD at 500 MHz.

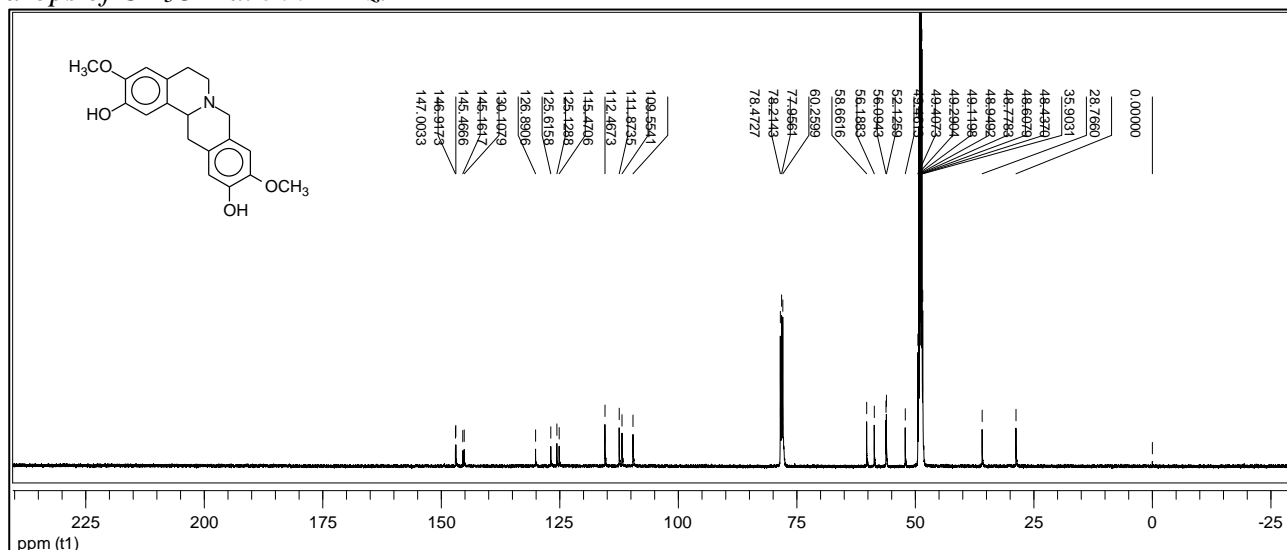


Figure S69. ^{13}C NMR spectrum of **coreximine** (**8**) in CDCl_3 plus drops of CD_3OD at 125 MHz.

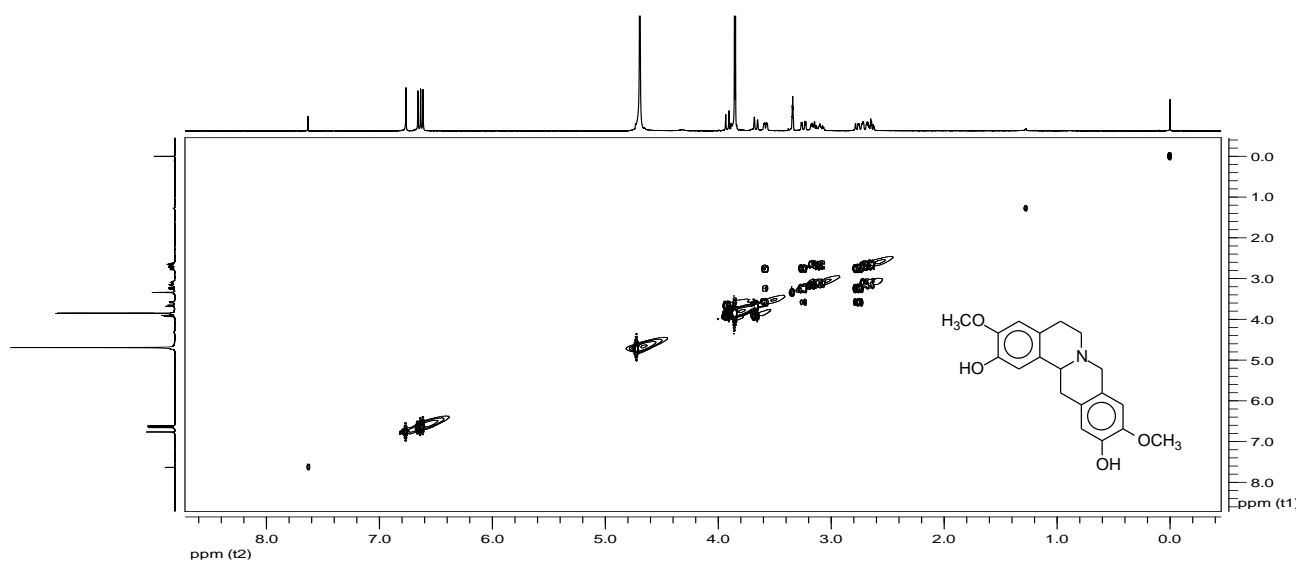


Figure S70. ^1H - ^1H correlation map from COSY NMR experiment of **coreximine (8)** in CDCl_3 plus drops of CD_3OD in CD_3OD at 500 MHz.

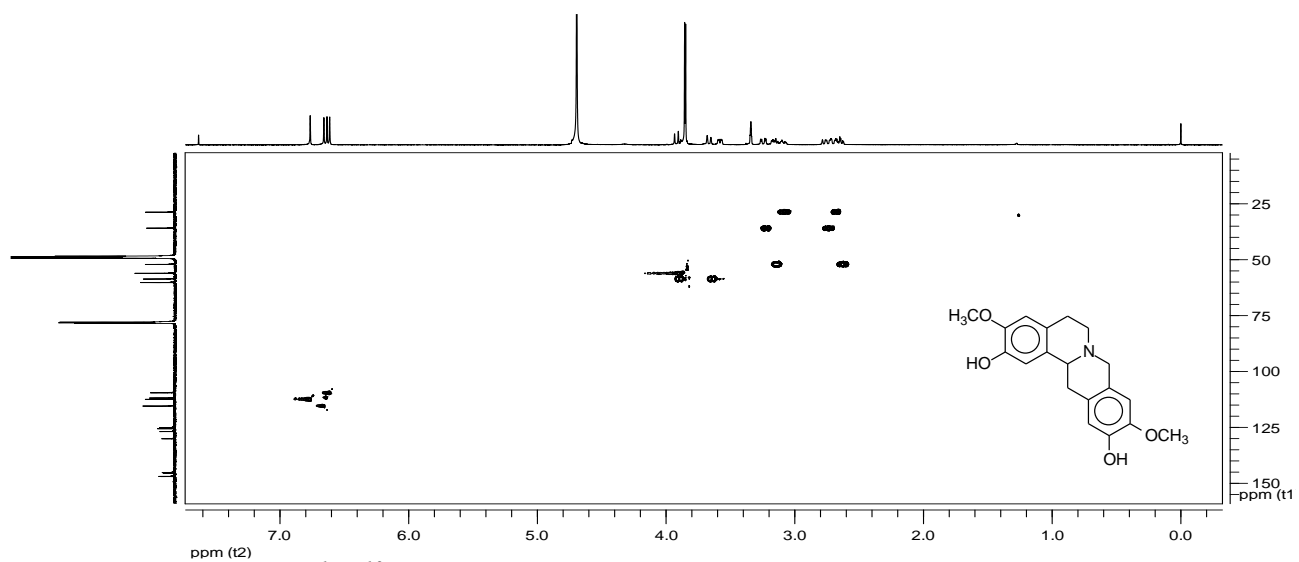


Figure S71. One-bond ^1H - ^{13}C correlation map from HSQC NMR experiment of **coreximine (8)** in CDCl_3 plus drops of CD_3OD at 500 (^1H) and 125 MHz (^{13}C), respectively.

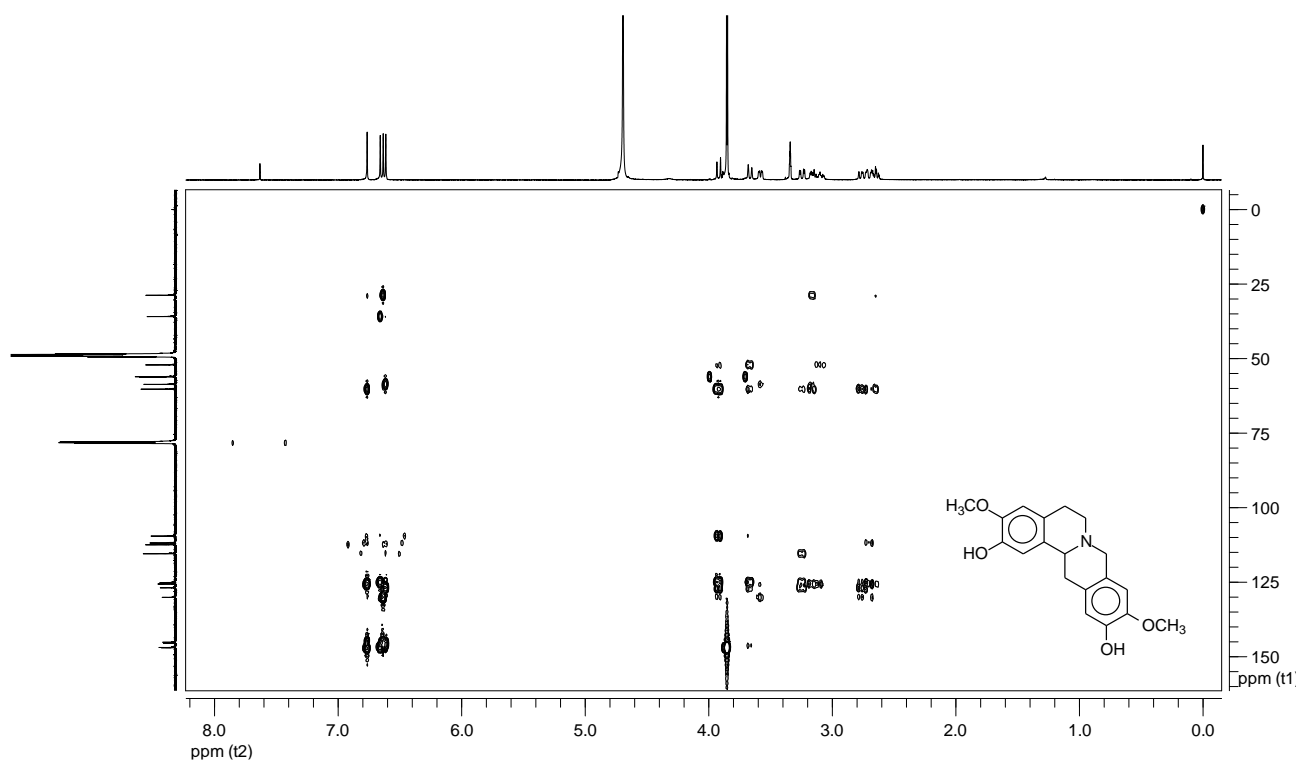


Figure S72. Long-range ^1H - ^{13}C correlation map from HMBC NMR experiment of **coreximine (8)** in CDCl_3 plus drops of CD_3OD at 500 (^1H) and 125 MHz (^{13}C), respectively.

DEFESA_16_04_2019#823-841 RT: 16.59-16.79 AV: 11 NL: 5,00E7
T: + c ESI Q1 MS [100,000-1000,000]

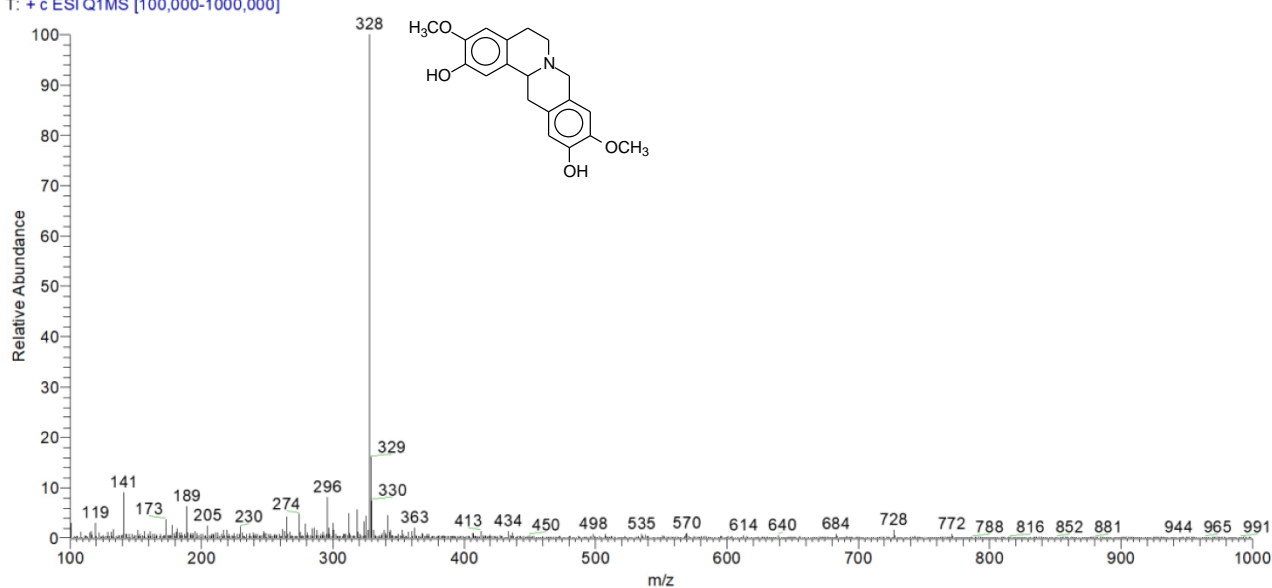


Figure S73. LR-ESI(+)-MS spectrum of **coreximine (8)** (m/z 328 [$M+H$] $^+$).

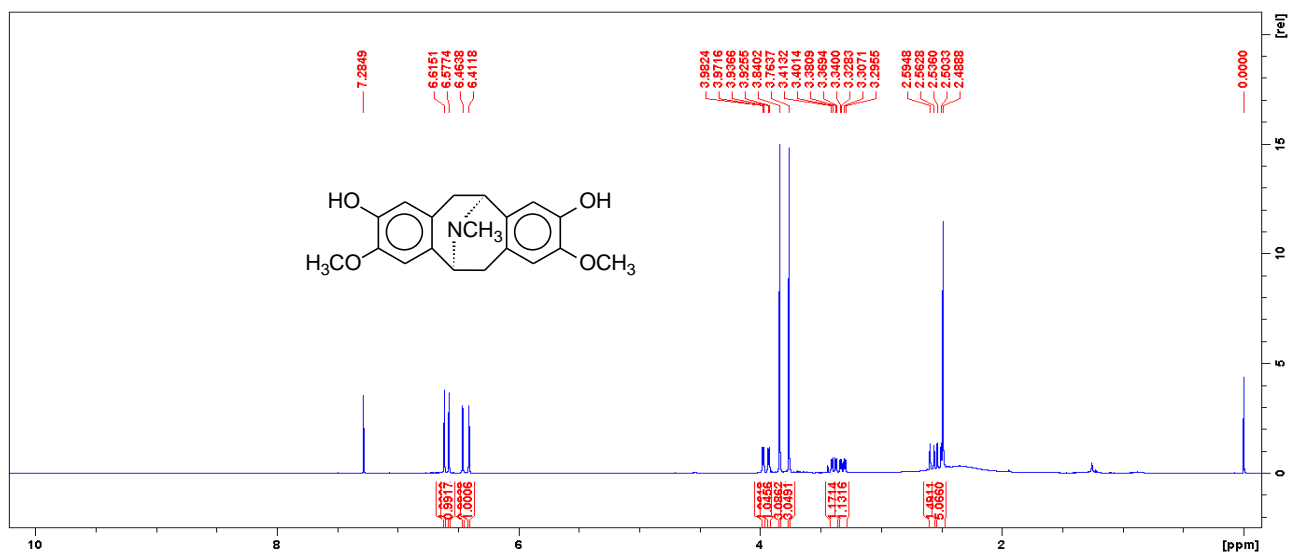


Figure S74. ^1H NMR spectrum of *bisnorargemonine* (9) in CDCl_3 plus drop of CD_3OD at 500 MHz.

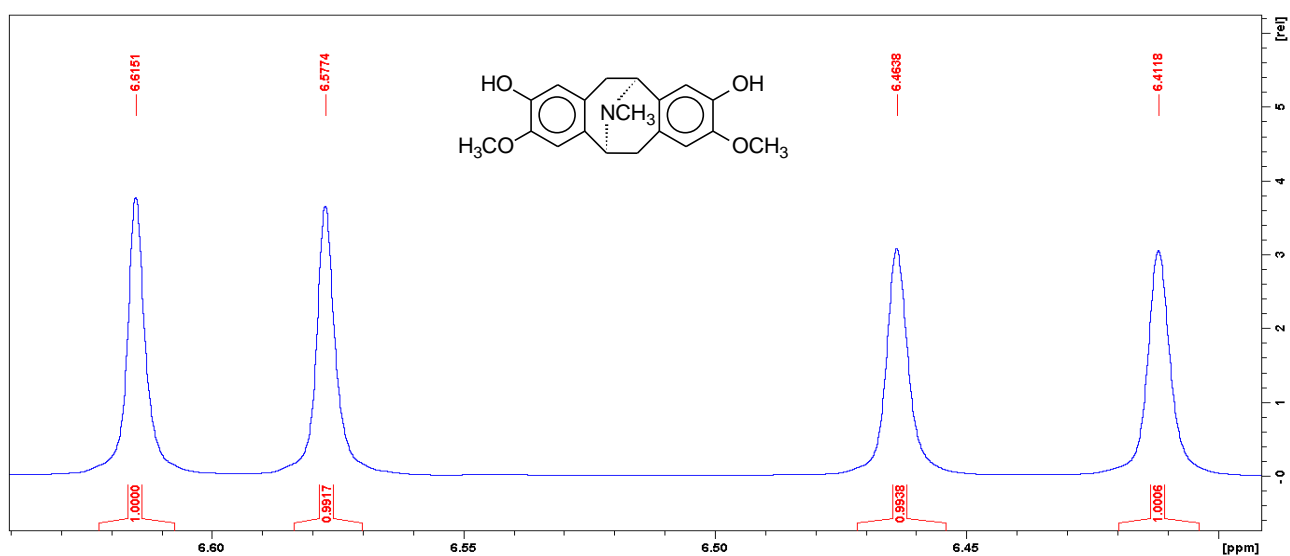


Figure S75. Expansion (δ 6.63 – 6.39) of the ^1H NMR spectrum of *bisnorargemonine* (9) in CDCl_3 plus drop of CD_3OD at 500 MHz.

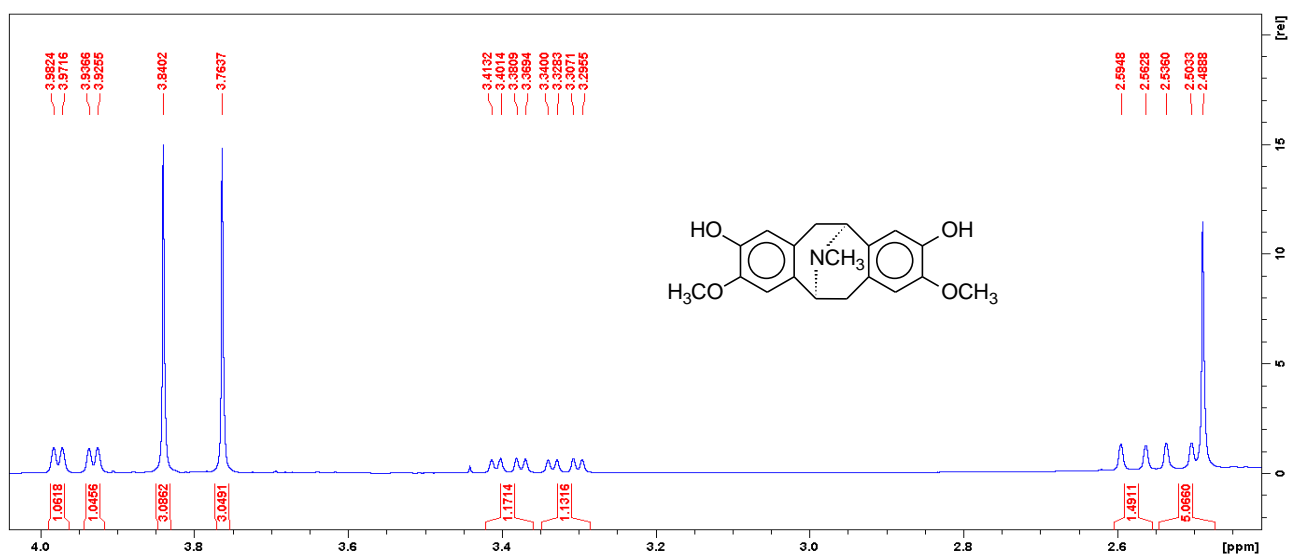


Figure S76. Expansion (δ 4.03 – 2.42) of the ^1H NMR spectrum of *bisnorargemonine* (9) in CDCl_3 plus drop of CD_3OD at 500 MHz.

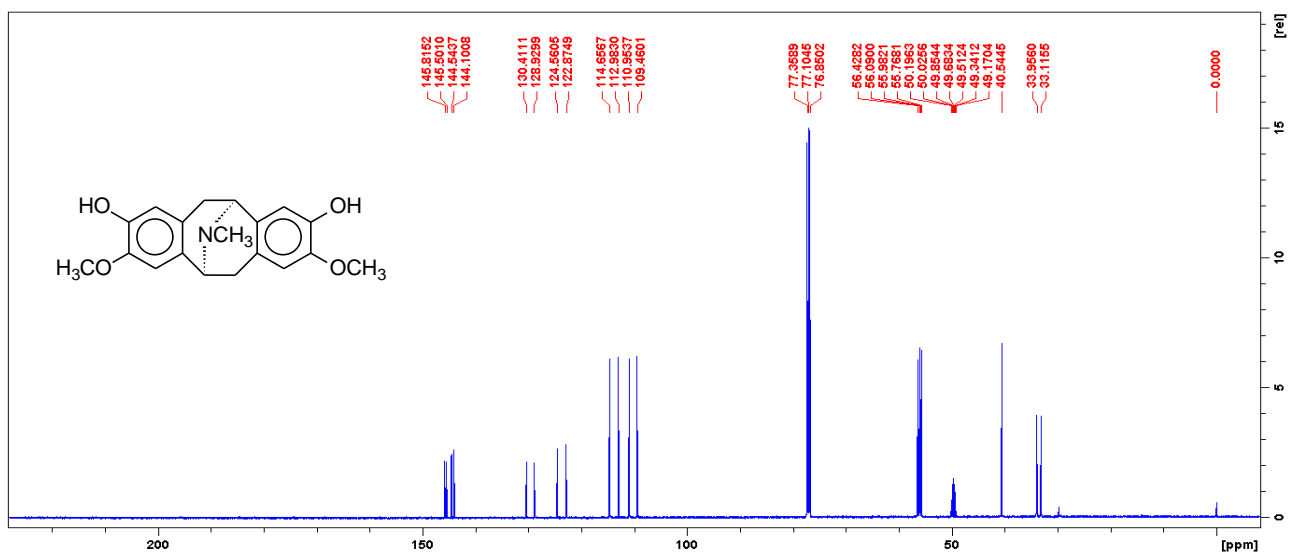


Figure S77. ¹³C NMR spectrum of *bisnorargemonine* (9) in CDCl₃ plus drop of CD₃OD at 125 MHz.

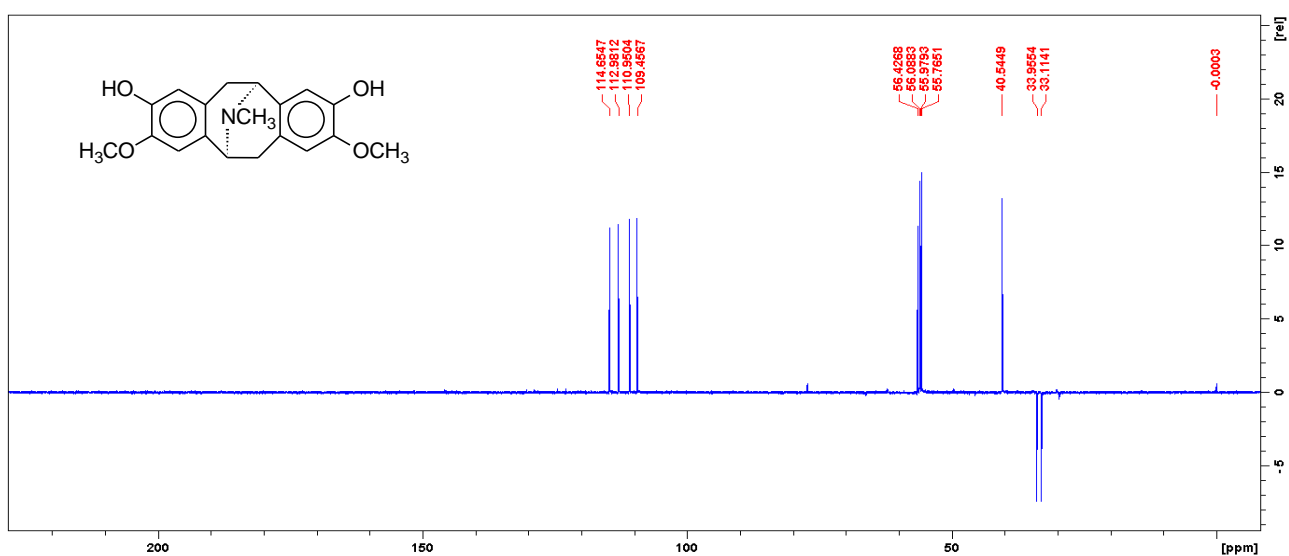


Figure S78. DEPT 135 spectrum of *bisnorargemonine* (9) in CDCl₃ plus drop of CD₃OD at 125 MHz.

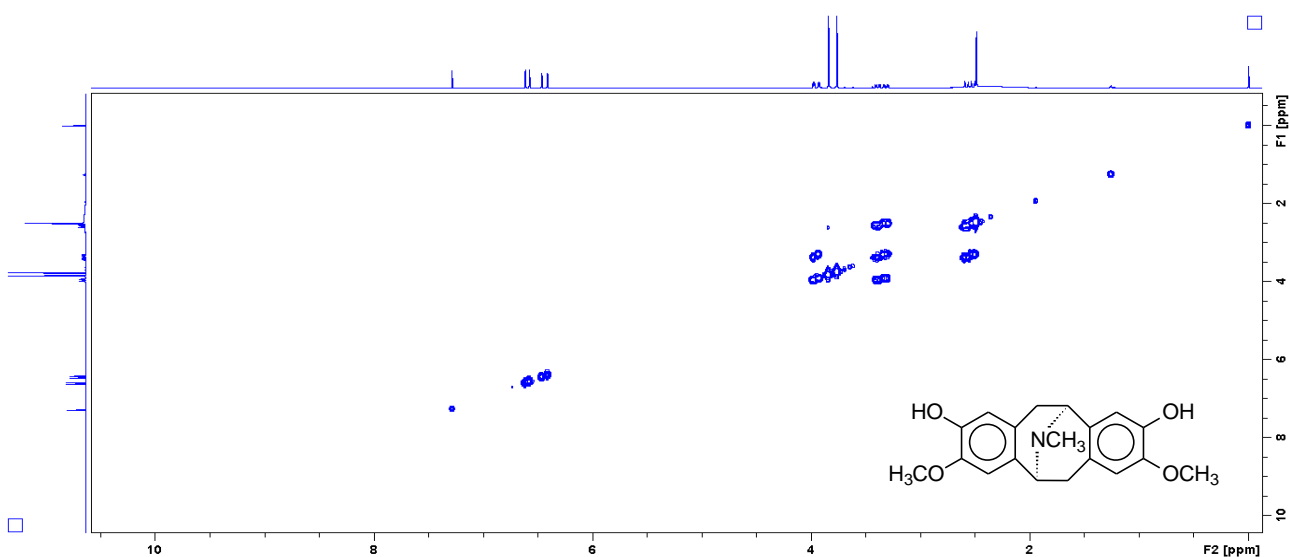


Figure S79. ¹H-¹H correlation map from COSY NMR experiment of *bisnorargemonine* (9) in CDCl₃ plus drop of CD₃OD at 500 MHz.

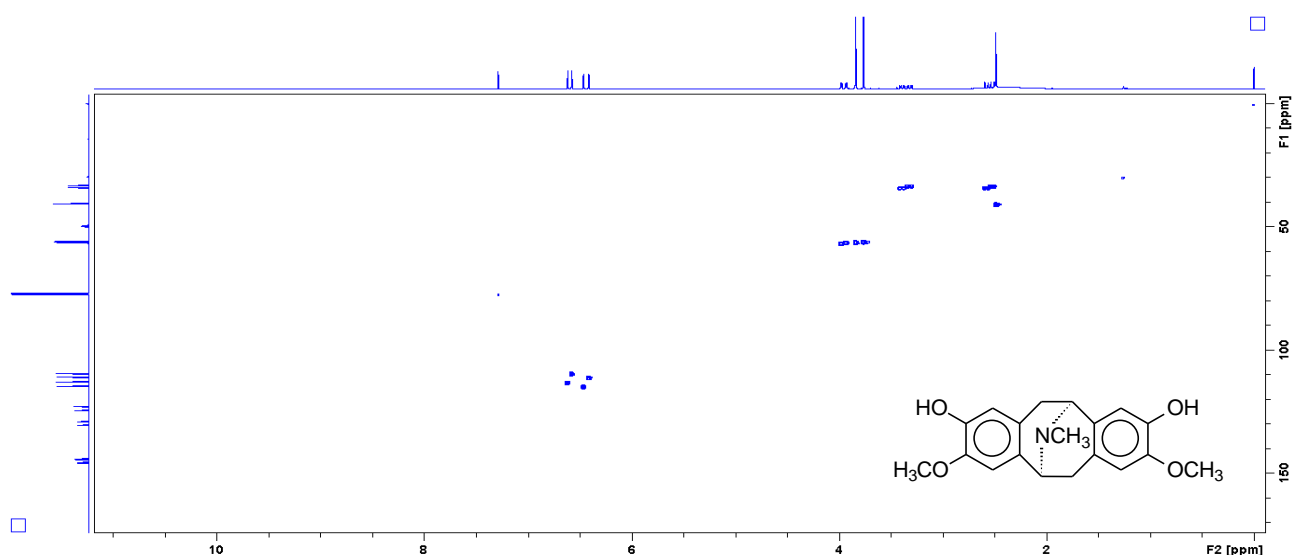


Figure S80. One-bond ^1H - ^{13}C correlation map from HSQC NMR experiment of *bisnorargemonine* (**9**) in CDCl_3 plus drop of CD_3OD at 500 (^1H) and 125 MHz (^{13}C), respectively.

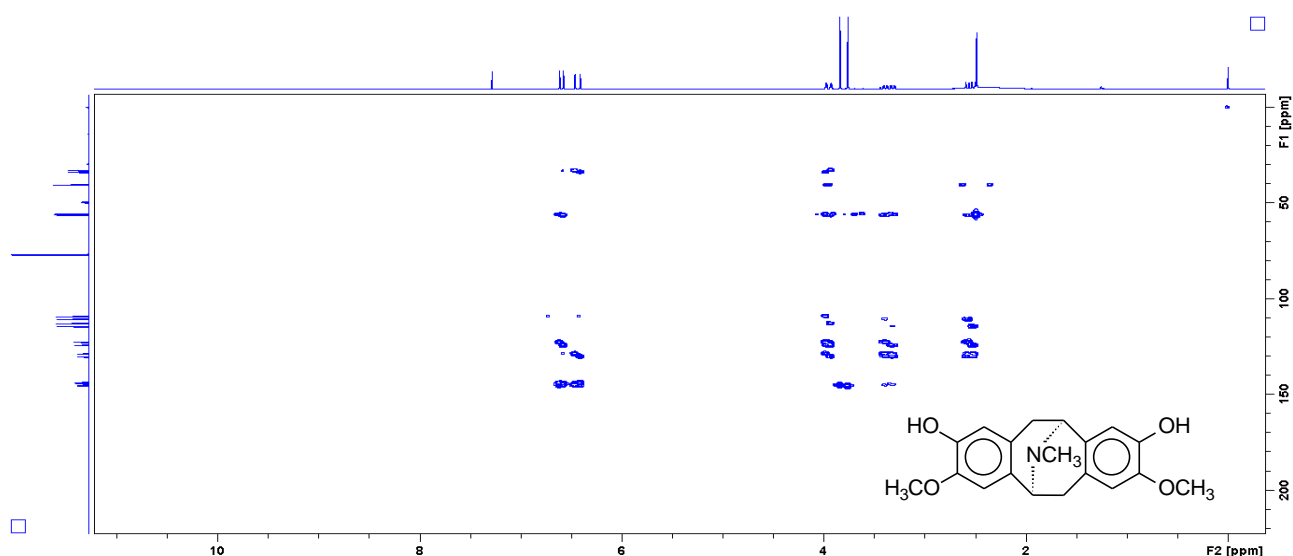


Figure S81. Long-range ^1H - ^{13}C correlation map from HMBC NMR experiment of *bisnorargemonine* (**9**) in CDCl_3 plus drop of CD_3OD at 500 (^1H) and 125 MHz (^{13}C), respectively.

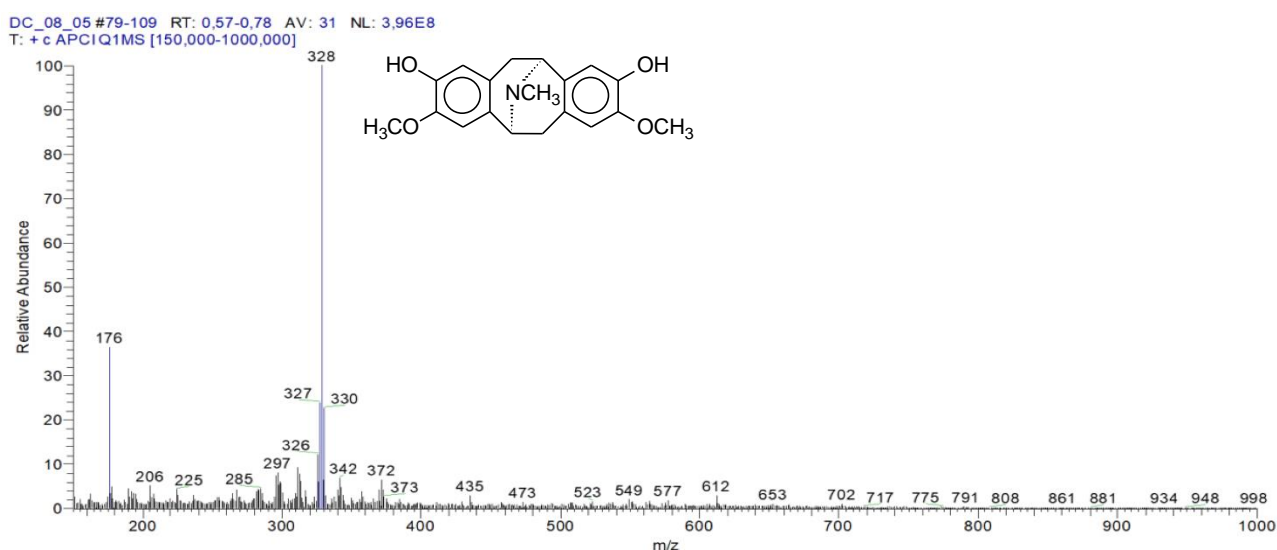


Figure S82. LR-APCI(+)-MS spectrum of *bisnorargemonine* (**9**) (m/z 328 [$M+H$] $^+$).

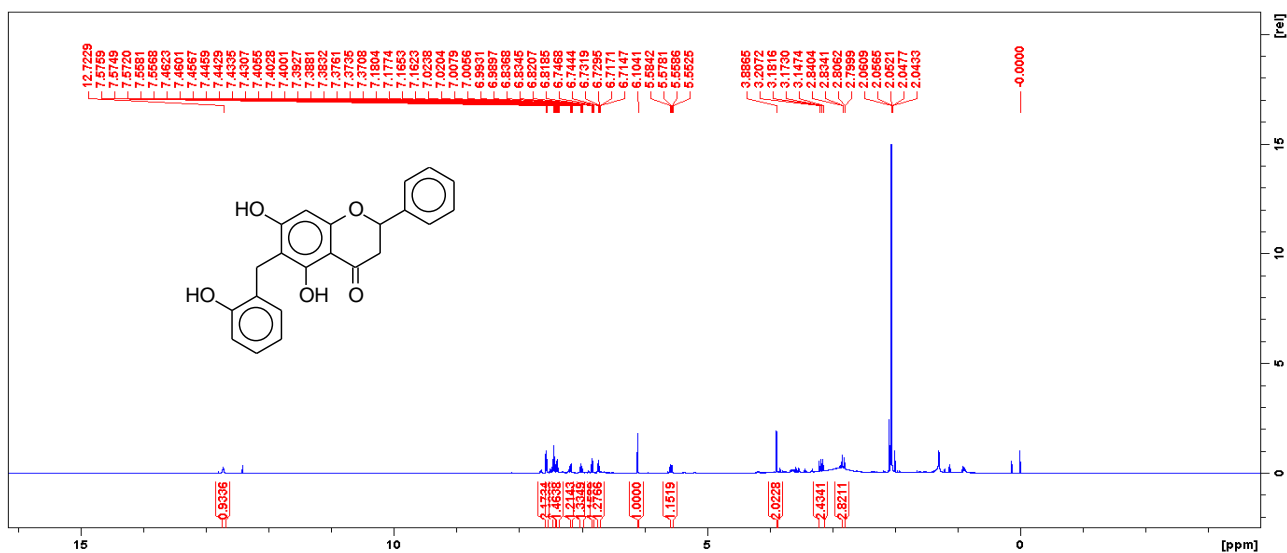


Figure S83. ^1H NMR spectrum of isochamanetin (10) in acetone- d_6 at 500 MHz.

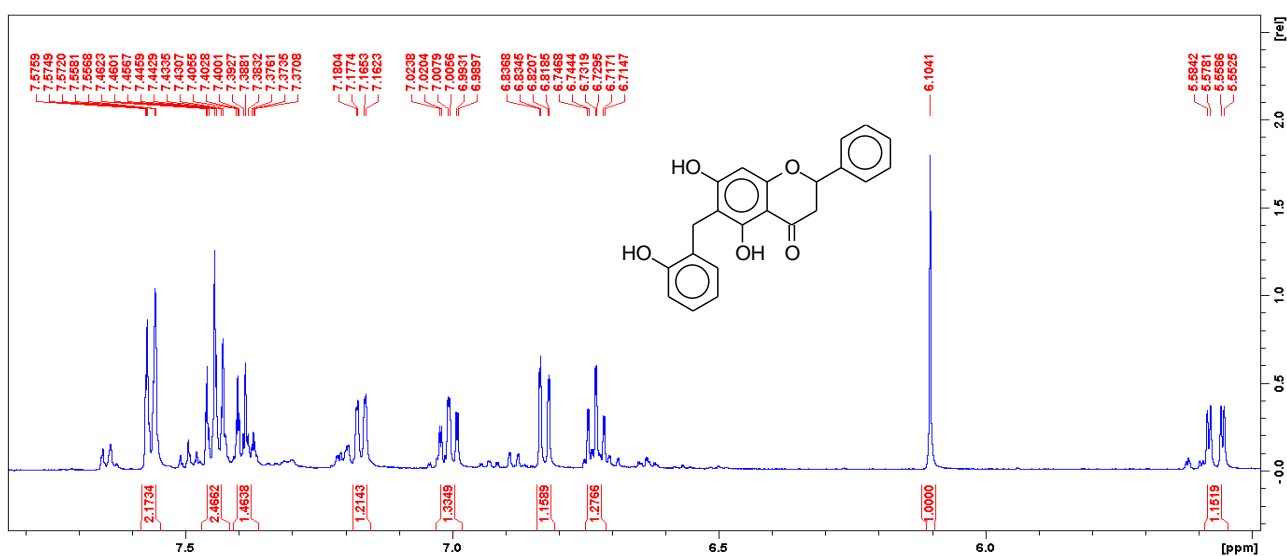


Figure S84. Expansion (δ 7.82 – 7.49) of the ^1H NMR spectrum of isochamanetin (10) in acetone- d_6 at 500 MHz.

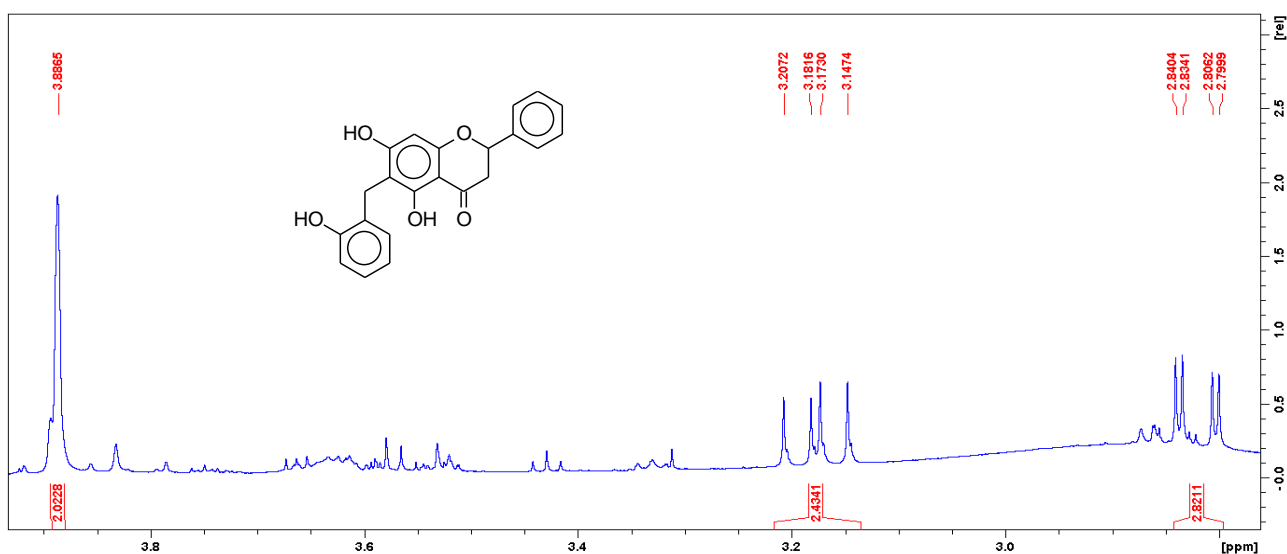


Figure S85. Expansion (δ 3.92 – 2.76) of the ^1H NMR spectrum of isochamanetin (10) in acetone- d_6 at 500 MHz.

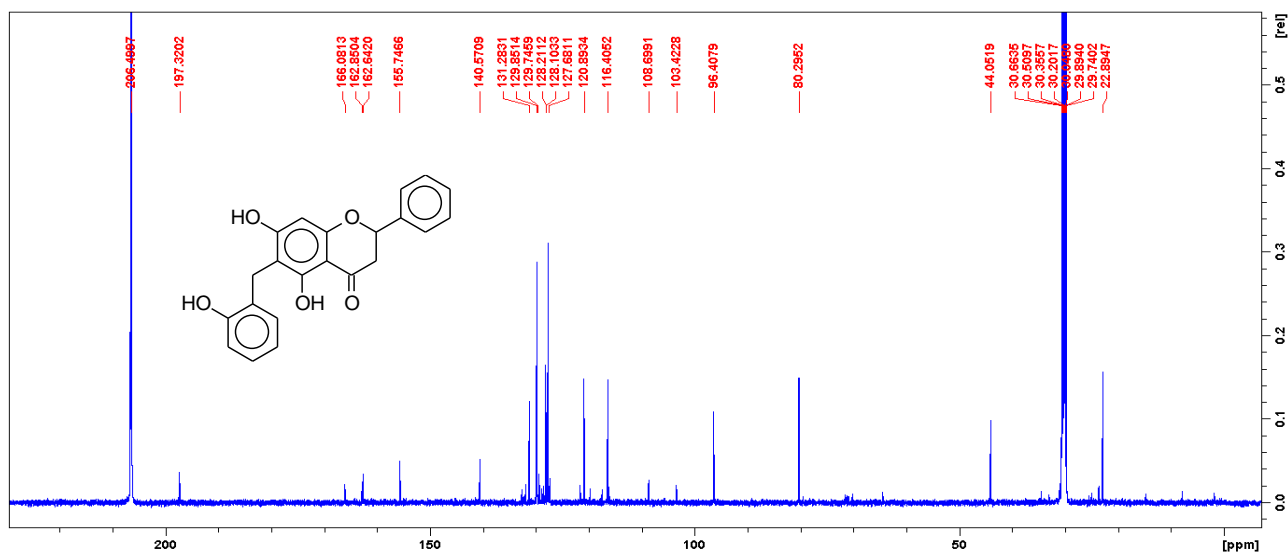


Figure S86. ^{13}C NMR spectrum of *isochamanetin* (**10**) in acetone- d_6 at 125 MHz.

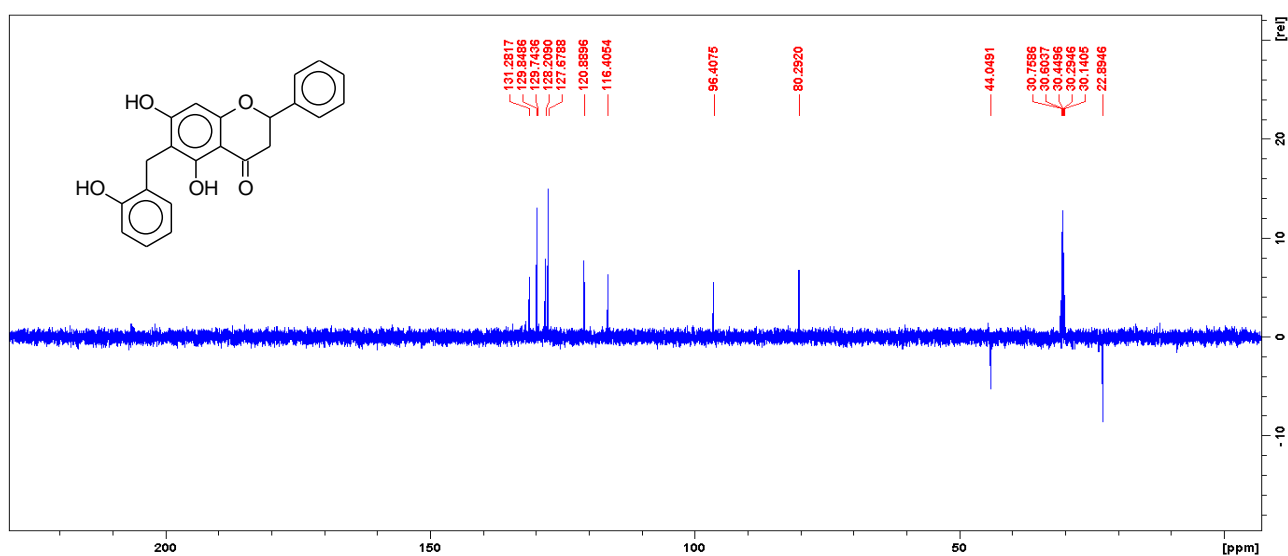


Figure S87. DEPT 135 spectrum of *isochamanetin* (**10**) in acetone- d_6 at 125 MHz.

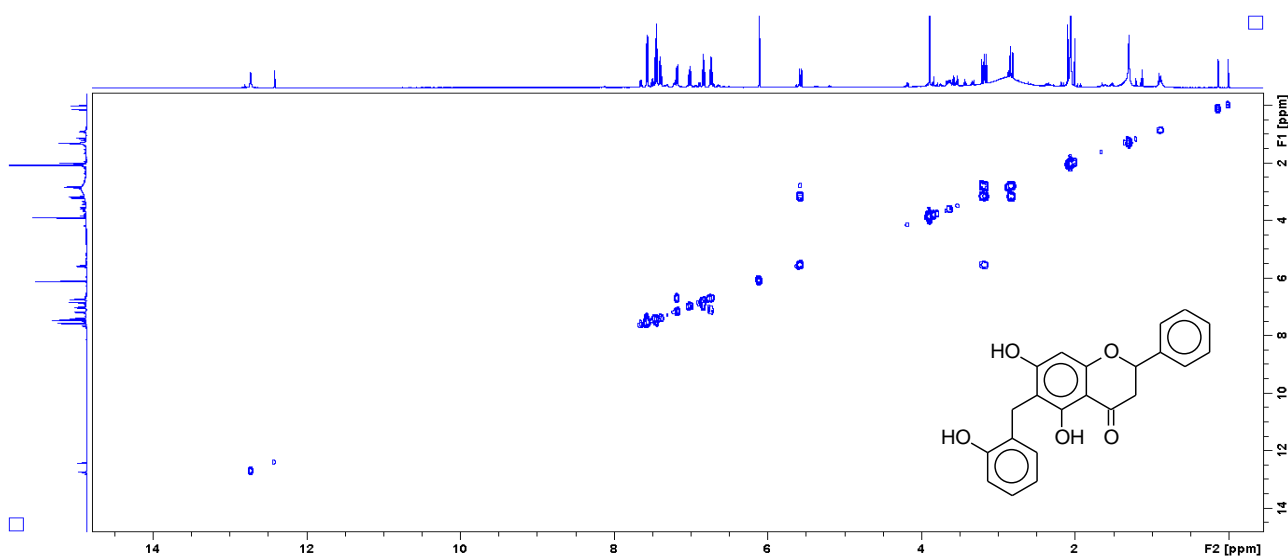


Figure S88. ^1H - ^1H correlation map from COSY NMR experiment of *isochamanetin* (**10**) in acetone- d_6 at 500 MHz.

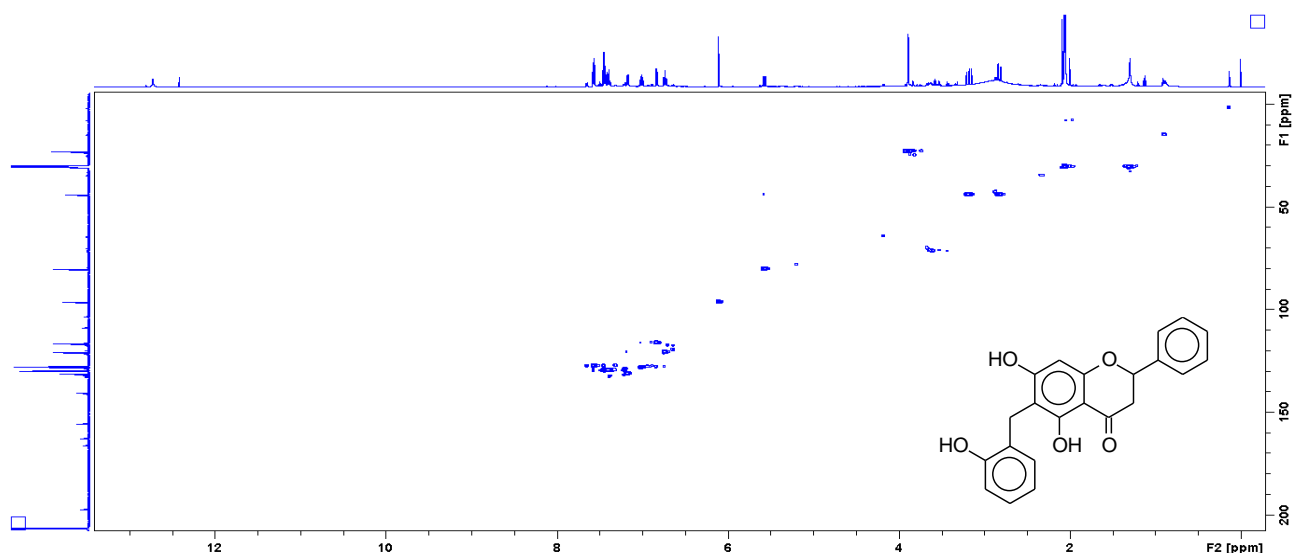


Figure S89. One-bond ^1H - ^{13}C correlation map from HSQC NMR experiment of **isochamanetin (10)** in acetone- d_6 at 500 (^1H) and 125 MHz (^{13}C), respectively.

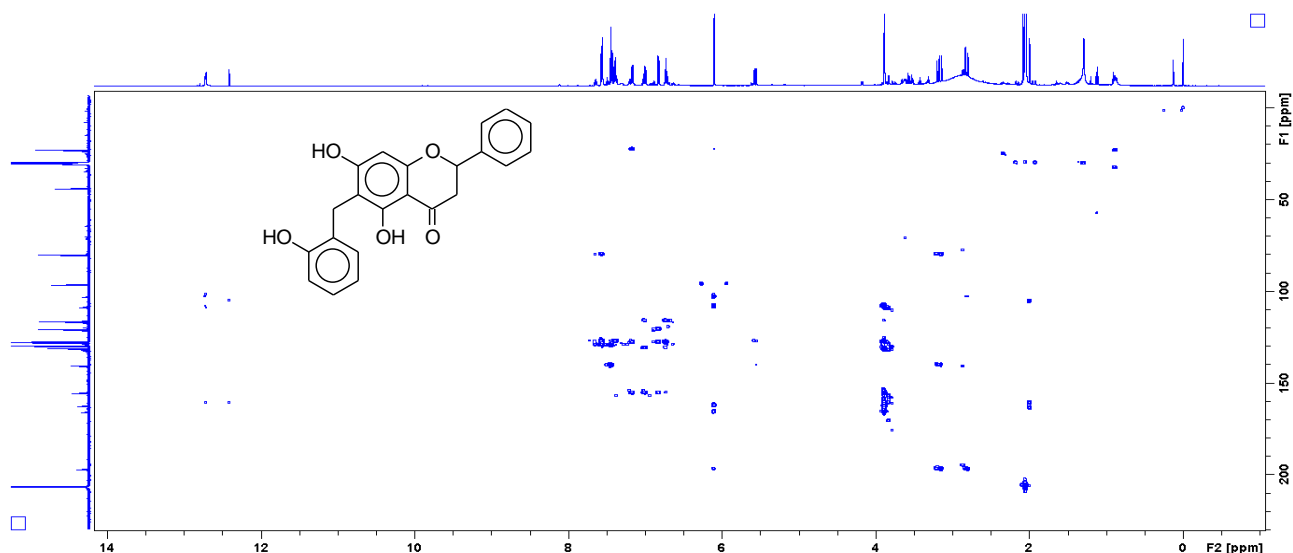


Figure S90. Long-range ^1H - ^{13}C correlation map from HMBC NMR experiment of **isochamanetin (10)** in acetone- d_6 at 500 (^1H) and 125 MHz (^{13}C), respectively.

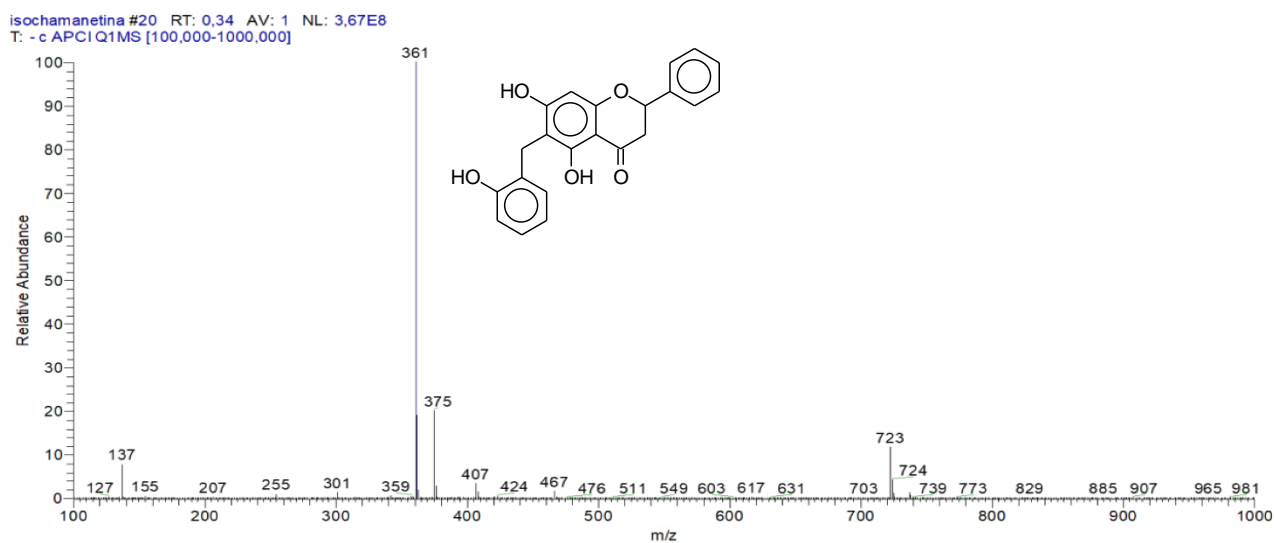


Figure S91. LR-APCI(-)-MS spectrum of **isochamanetin (10)** (m/z 361 [$M-H$] $^-$).

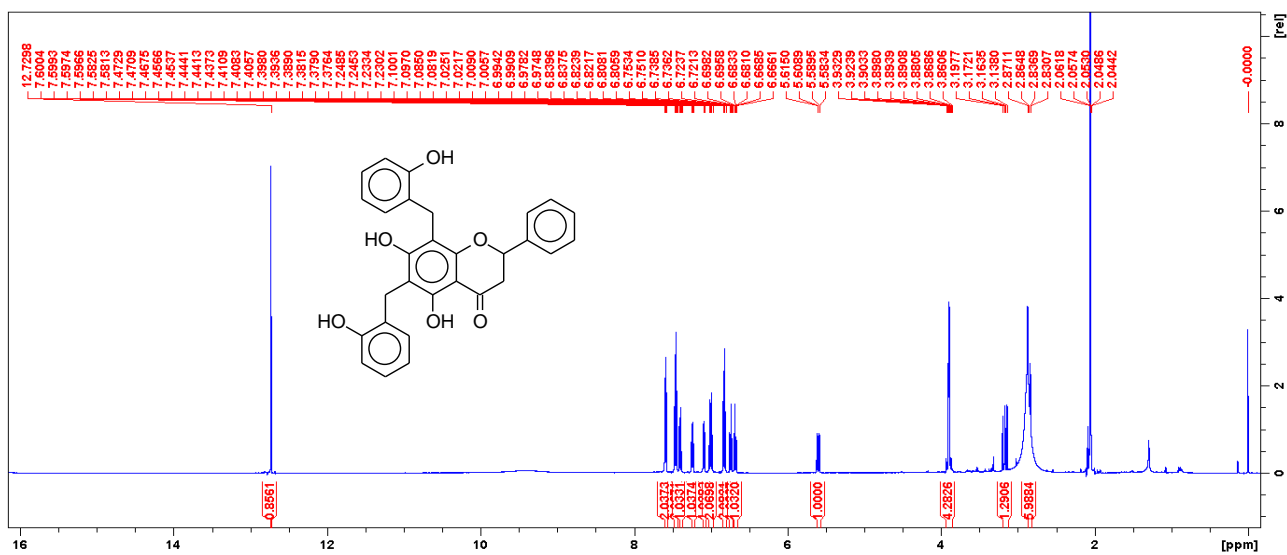


Figure S92. ^1H NMR spectrum of dichamanetin (11) in acetone- d_6 at 500 MHz.

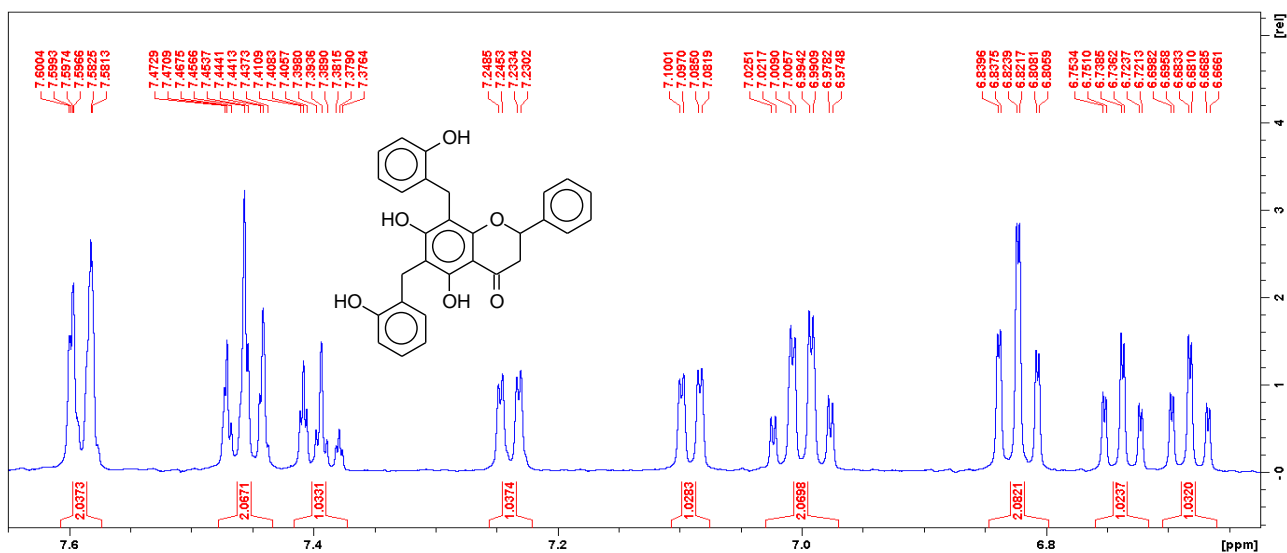


Figure S93. Expansion (δ 7.64 – 6.63) of the ^1H NMR spectrum of dichamanetin (11) in acetone- d_6 at 500 MHz.

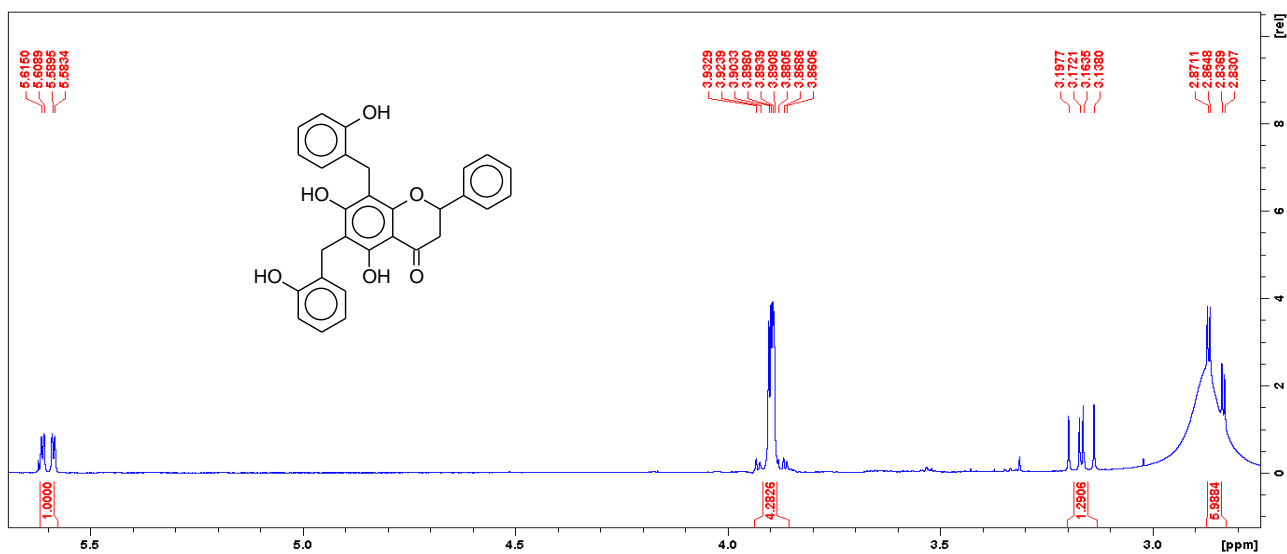


Figure S94. Expansion (δ 5.68 – 2.75) of the ^1H NMR spectrum of dichamanetin (11) in acetone- d_6 at 500 MHz.

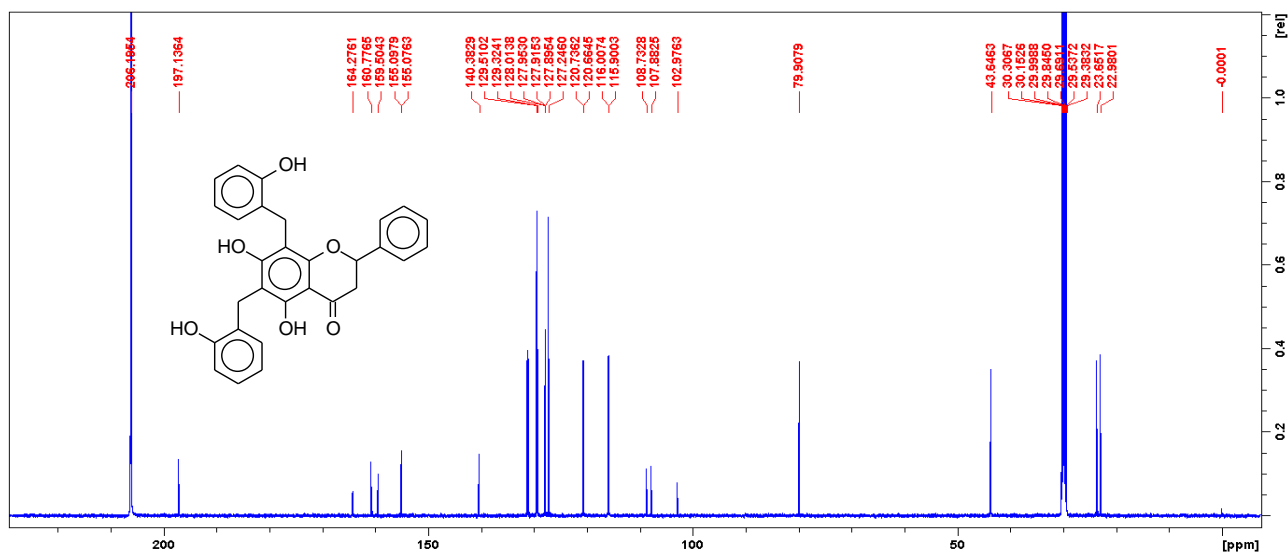


Figure S95. ^{13}C NMR spectrum of *dichamanetin* (**11**) in acetone- d_6 at 125 MHz.

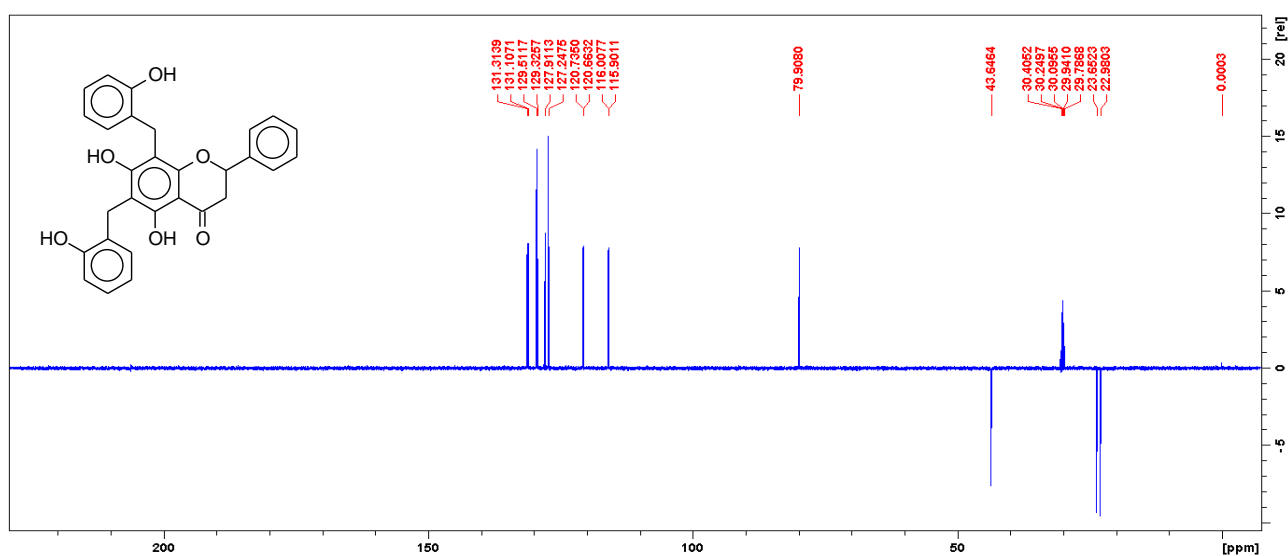


Figure S96. DEPT 135 spectrum of *dichamanetin* (**11**) in acetone- d_6 at 125 MHz.

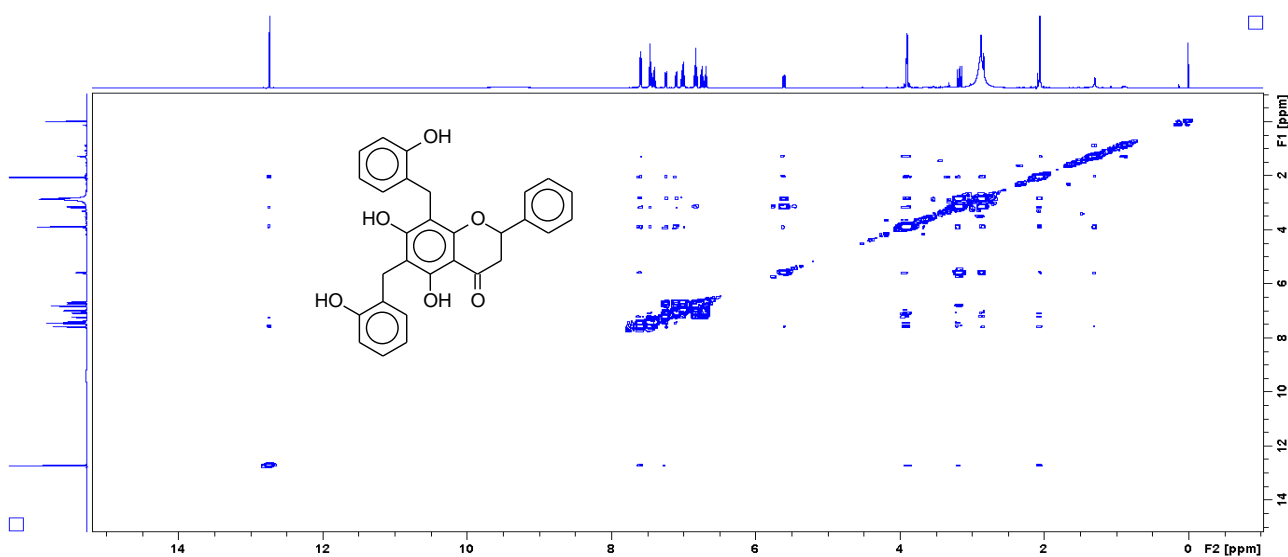


Figure S97. ^1H - ^1H correlation map from COSY NMR experiment of *dichamanetin* (**11**) in acetone- d_6 at 500 MHz.

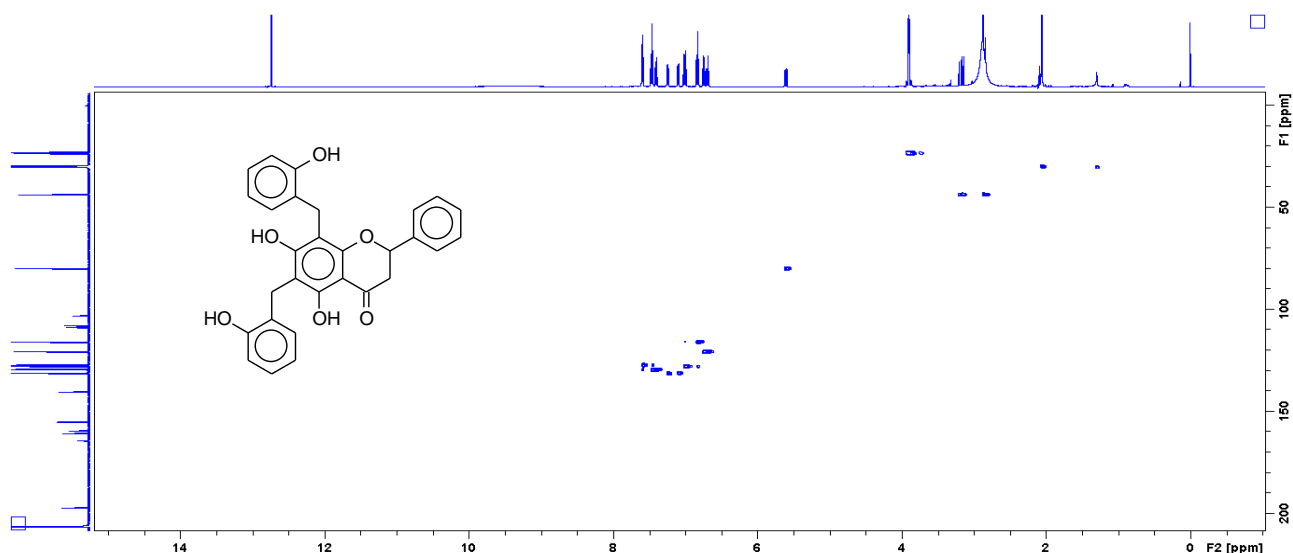


Figure S98. One-bond ^1H - ^{13}C correlation map from HSQC NMR experiment of *dichamanetin* (**11**) in acetone- d_6 at 500 (^1H) and 125 MHz (^{13}C), respectively.

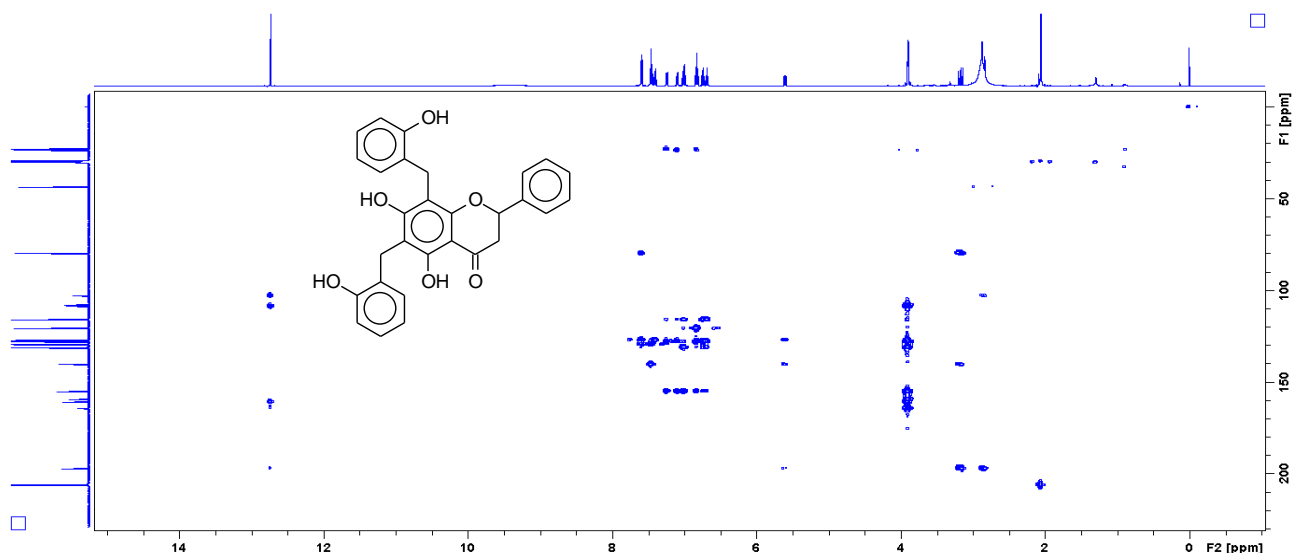


Figure S99. Long-range ^1H - ^{13}C correlation map from HMBC NMR experiment of *dichamanetin* (**11**) in acetone- d_6 at 500 (^1H) and 125 MHz (^{13}C), respectively.

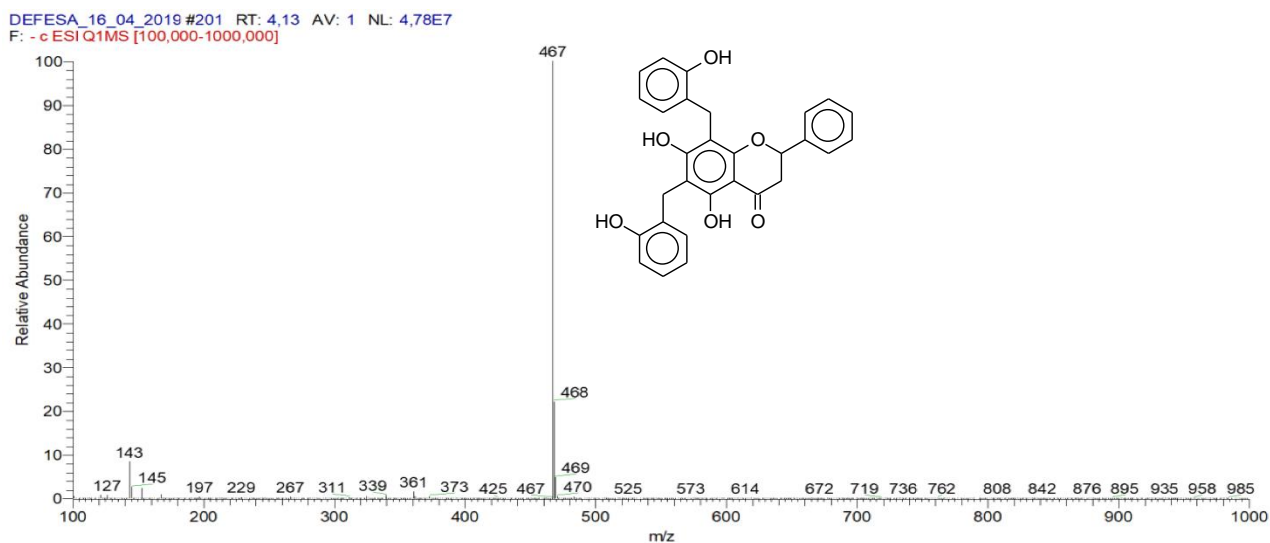


Figure S100. LR-ESI(-)-MS spectrum of *dichamanetin* (**11**) (m/z 467 [$\text{M}-\text{H}$] $^-$).

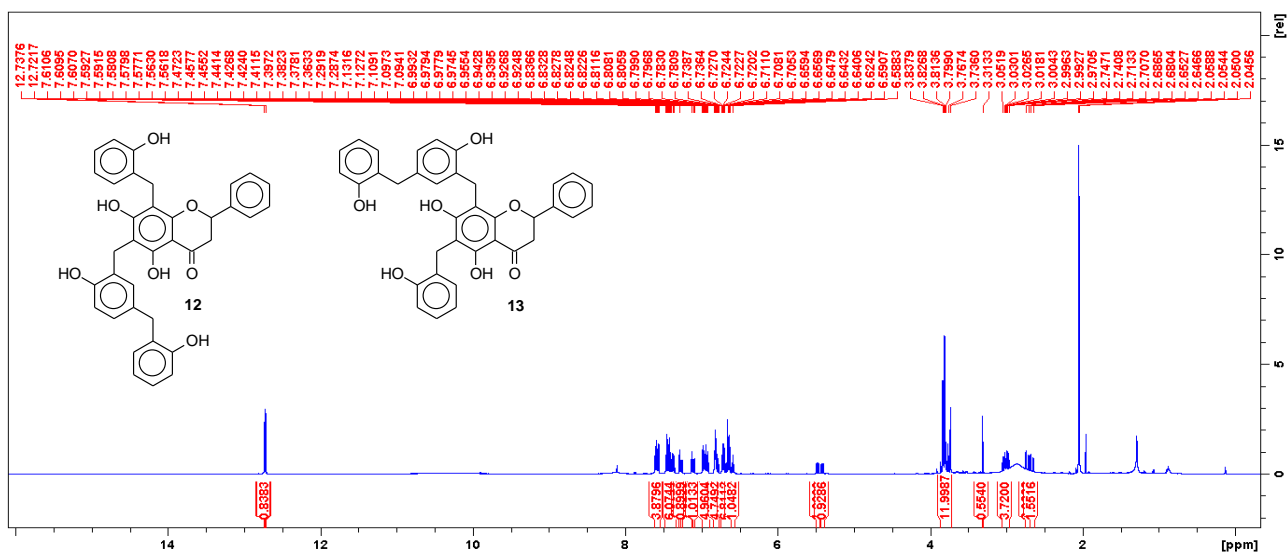


Figure S101. ^1H NMR spectrum of the mixture of **uvarinol** (12) and **isouvarinol** (13) in acetone- d_6 at 500 MHz.

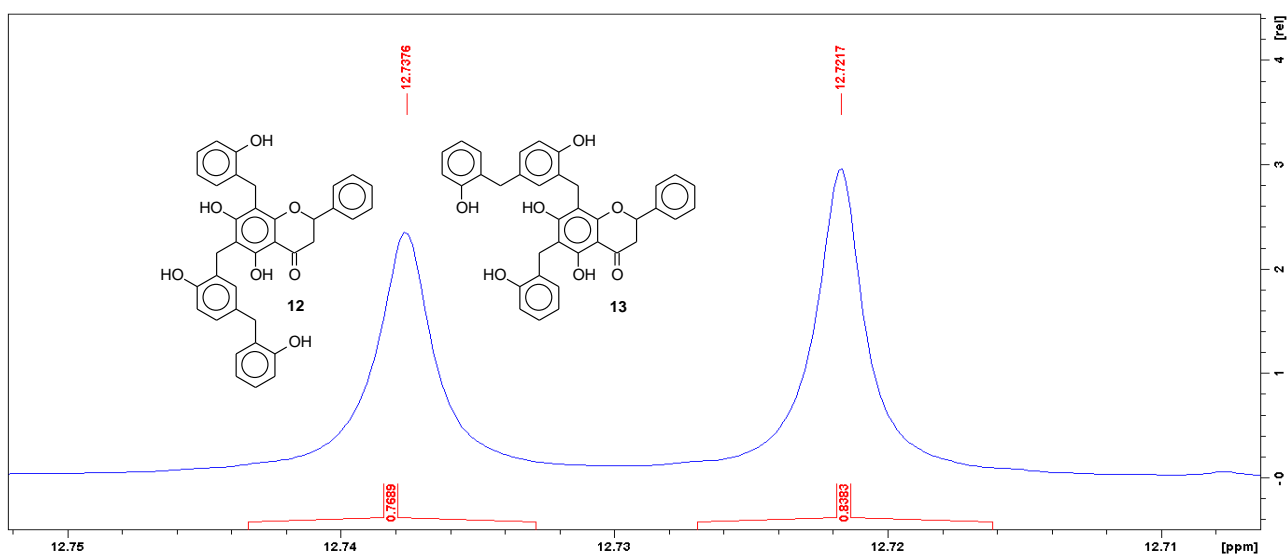


Figure S102. Expansion (δ 12.75 – 12.70) of the ^1H NMR spectrum of the mixture of **uvarinol** (12) and **isouvarinol** (13) in acetone- d_6 at 500 MHz.

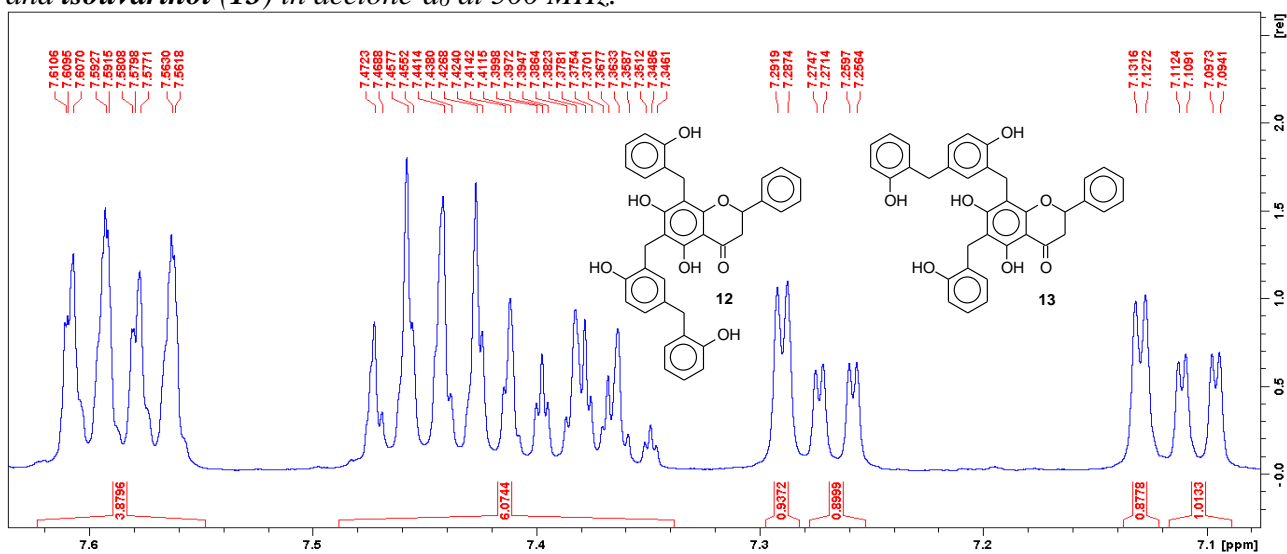


Figure S103. Expansion (δ 7.63 – 7.07) of the ^1H NMR spectrum of the mixture of **uvarinol** (12) and **isouvarinol** (13) in acetone- d_6 at 500 MHz.

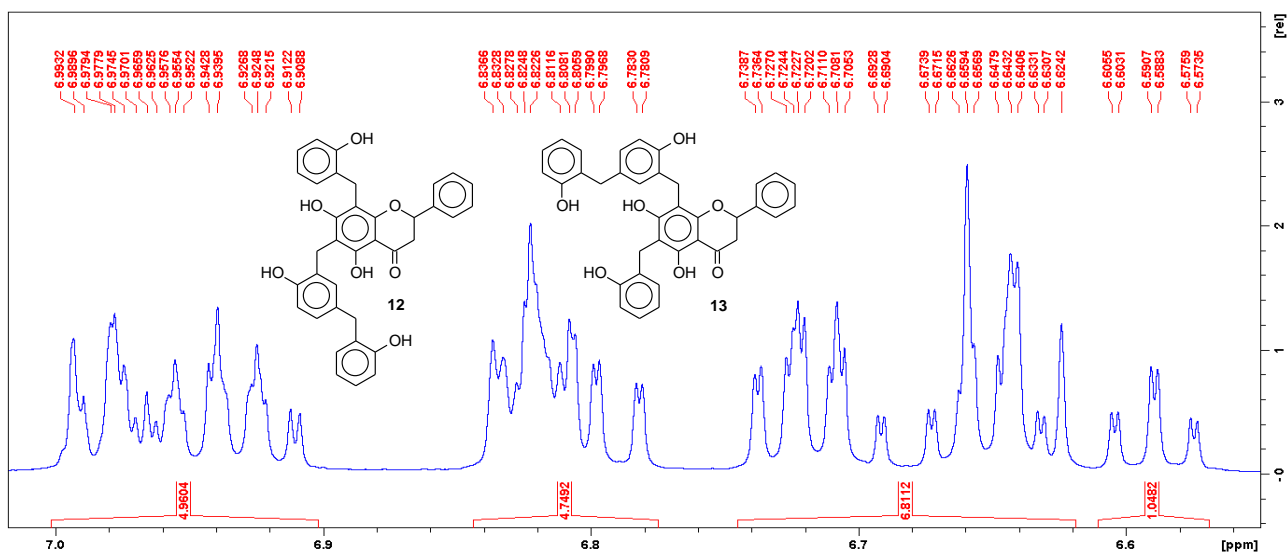


Figure S104. Expansion (δ 7.01 – 6.55) of the ^1H NMR spectrum of the mixture of **uvarinol** (**12**) and **isouvarinol** (**13**) in acetone- d_6 at 500 MHz.

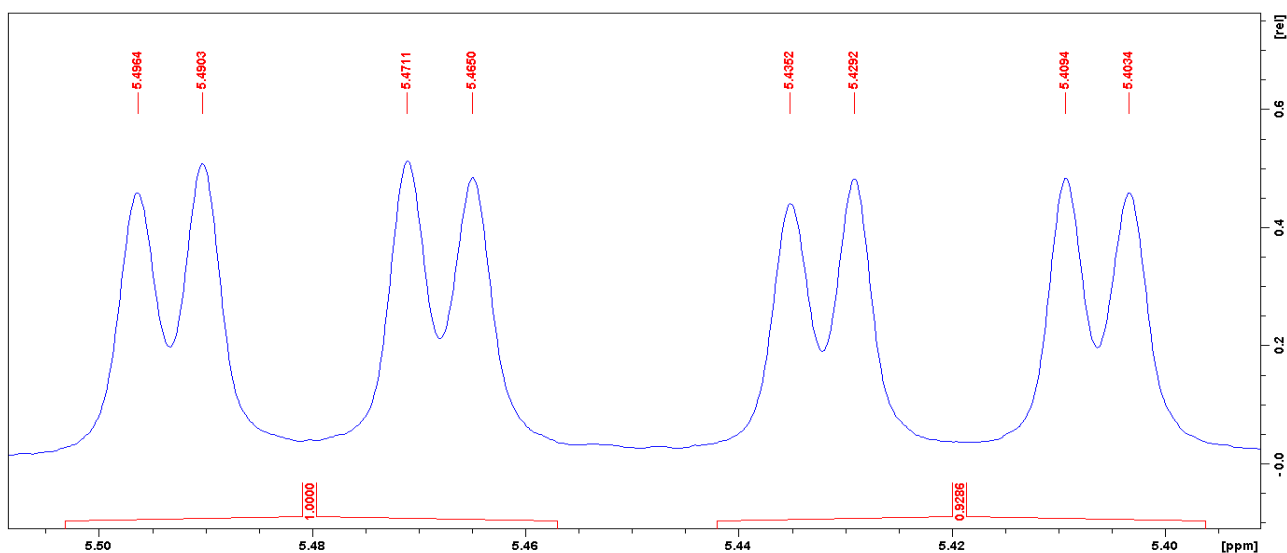


Figure S105. Expansion (δ 5.50 – 5.39) of the ^1H NMR spectrum of the mixture of **uvarinol** (**12**) and **isouvarinol** (**13**) in acetone- d_6 at 500 MHz.

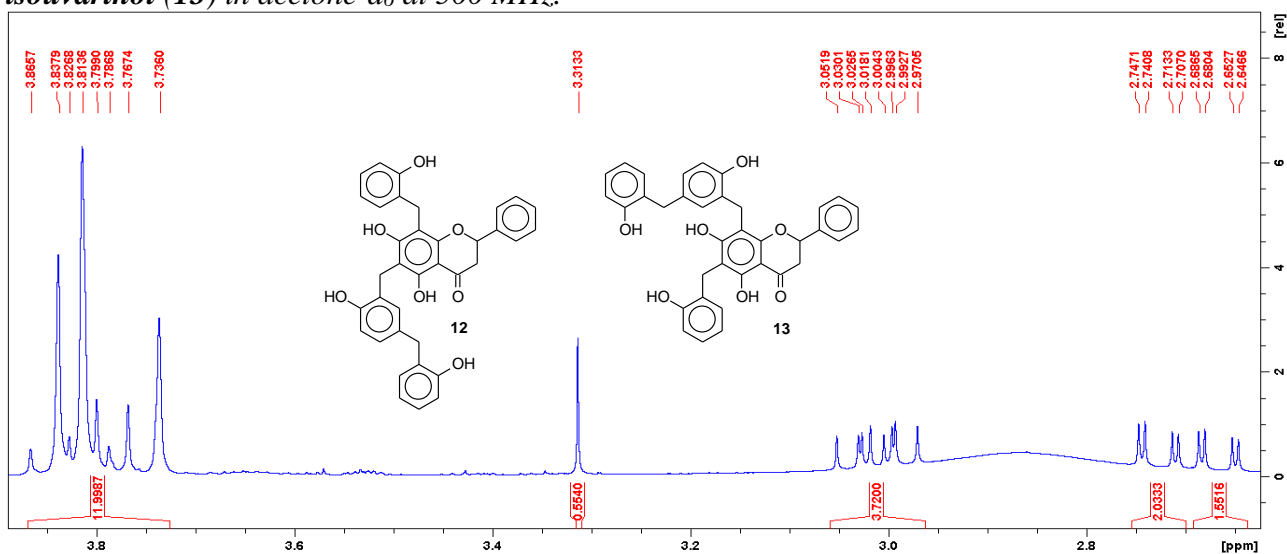


Figure S106. Expansion (δ 5.50 – 5.39) of the ^1H NMR spectrum of the mixture of **uvarinol** (**12**) and **isouvarinol** (**13**) in acetone- d_6 at 500 MHz.

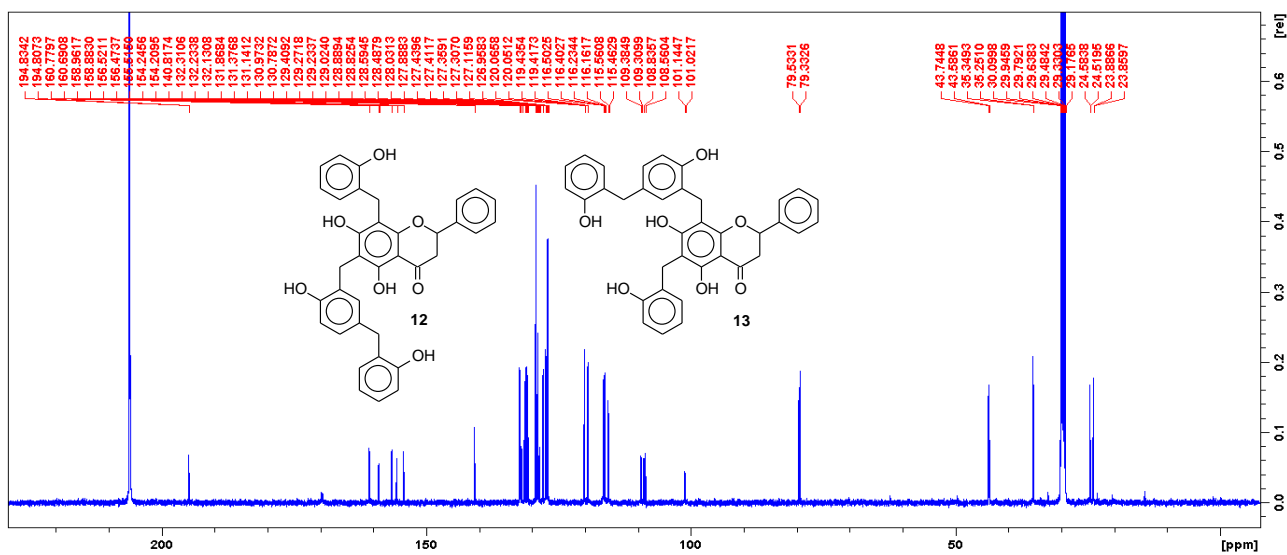


Figure S107. ^{13}C NMR spectrum of the mixture of uvarinol (12) and isouvarinol (13) in acetone- d_6 at 125 MHz.

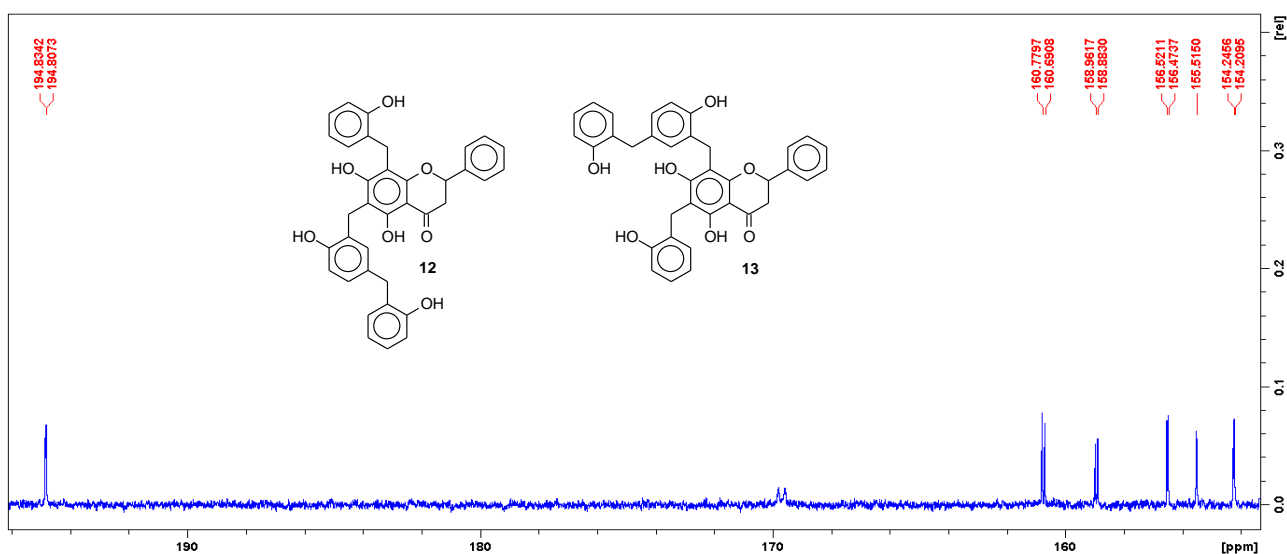


Figure S108. Expansion (δ 196.0 – 153.4) of the ^{13}C NMR spectrum of the mixture of uvarinol (12) and isouvarinol (13) in acetone- d_6 at 125 MHz.

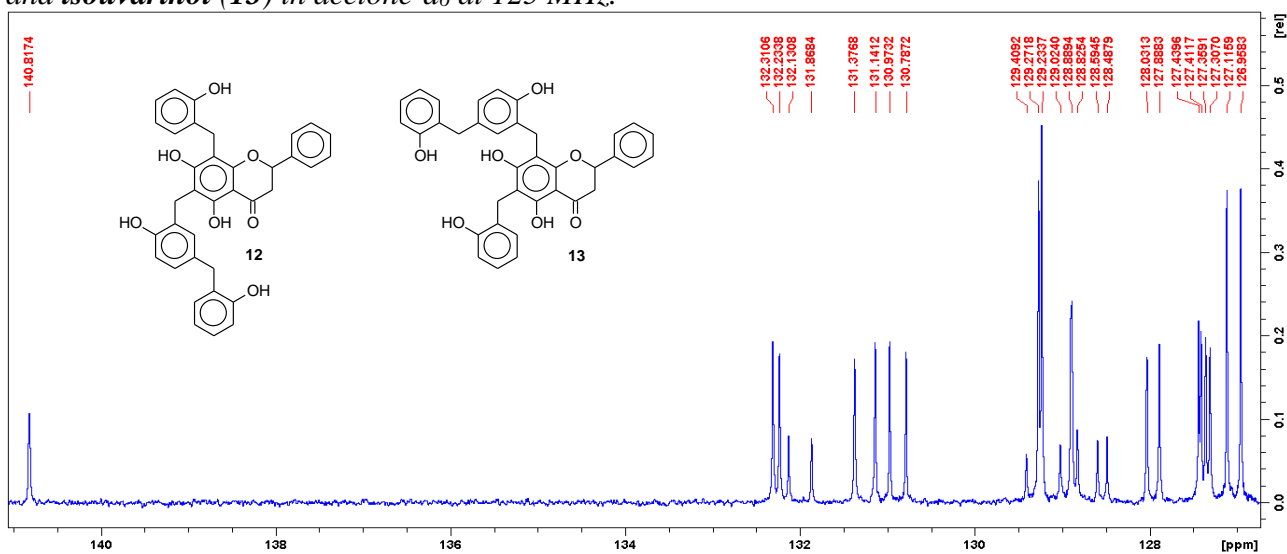


Figure S109. Expansion (δ 141.0 – 126.7) of the ^{13}C NMR spectrum of the mixture of uvarinol (12) and isouvarinol (13) in acetone- d_6 at 125 MHz.

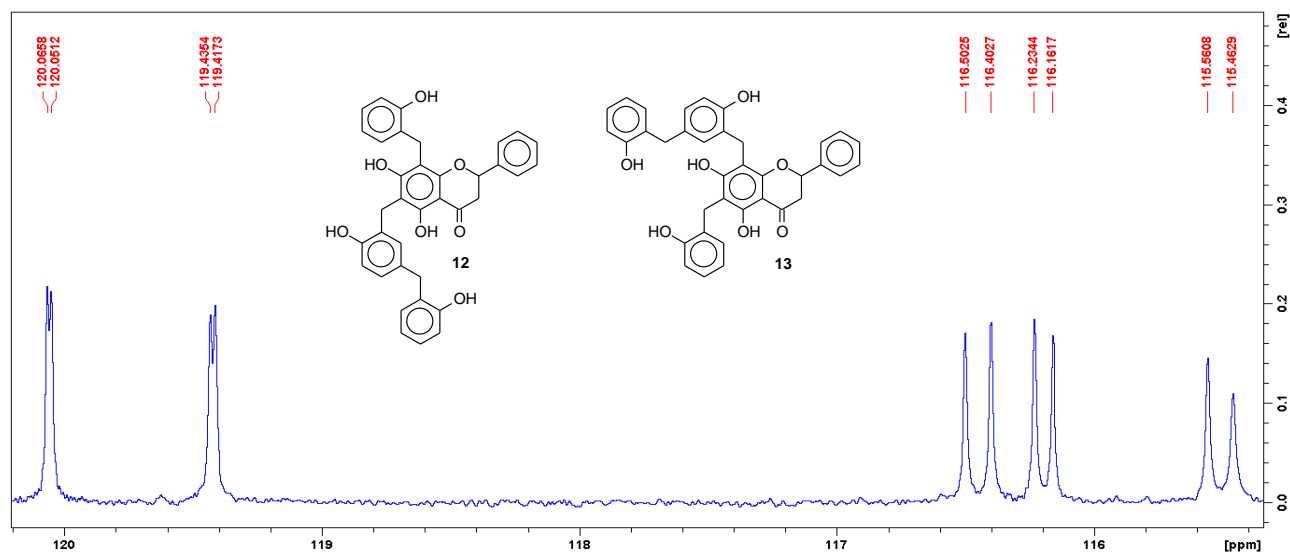


Figure S110. Expansion (δ 120.1 – 115.3) of the ^{13}C NMR spectrum of the mixture of **uvarinol** (**12**) and **isouvarinol** (**13**) in acetone- d_6 at 125 MHz.

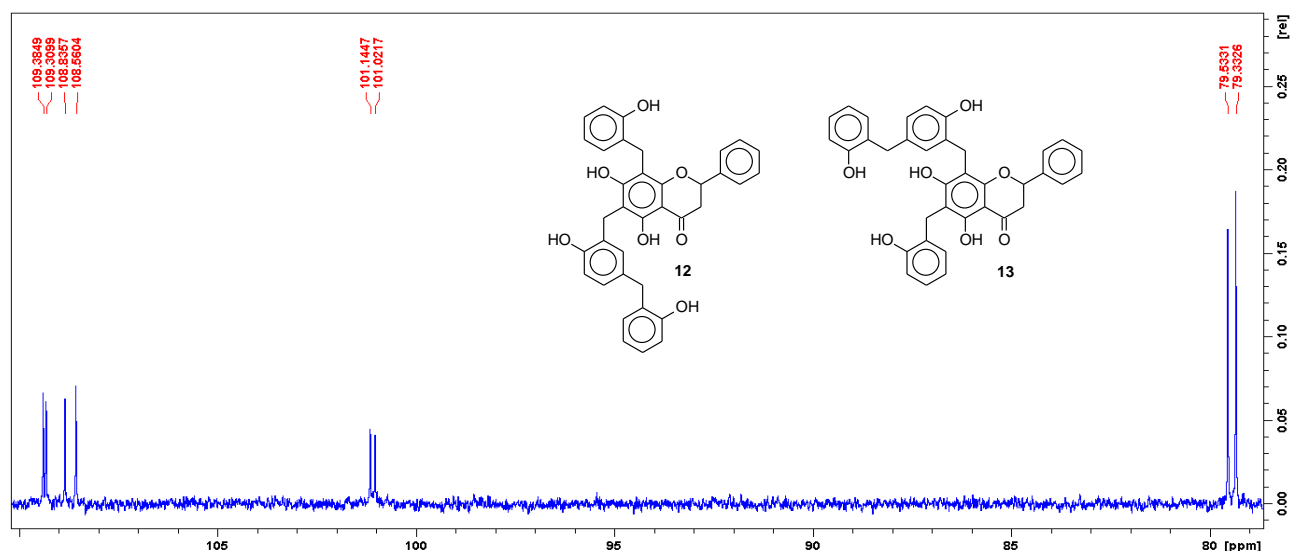


Figure S111. Expansion (δ 110.1 – 78.7) of the ^{13}C NMR spectrum of the mixture of **uvarinol** (**12**) and **isouvarinol** (**13**) in acetone- d_6 at 125 MHz.

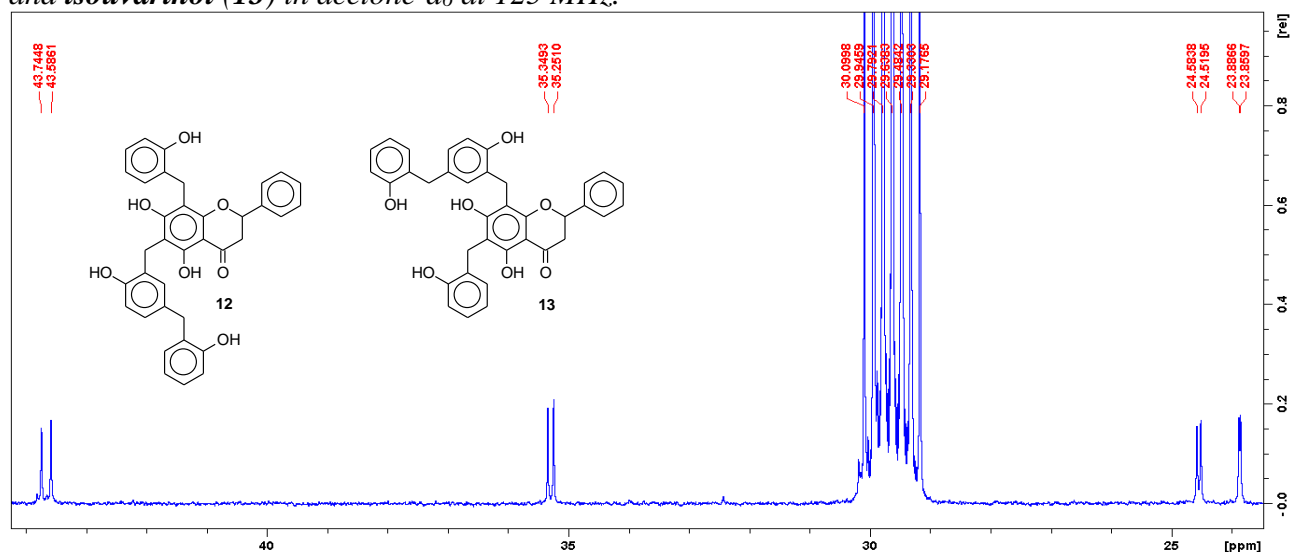


Figure S112. Expansion (δ 44.2 – 23.5) of the ^{13}C NMR spectrum of the mixture of **uvarinol** (**12**) and **isouvarinol** (**13**) in acetone- d_6 at 125 MHz.

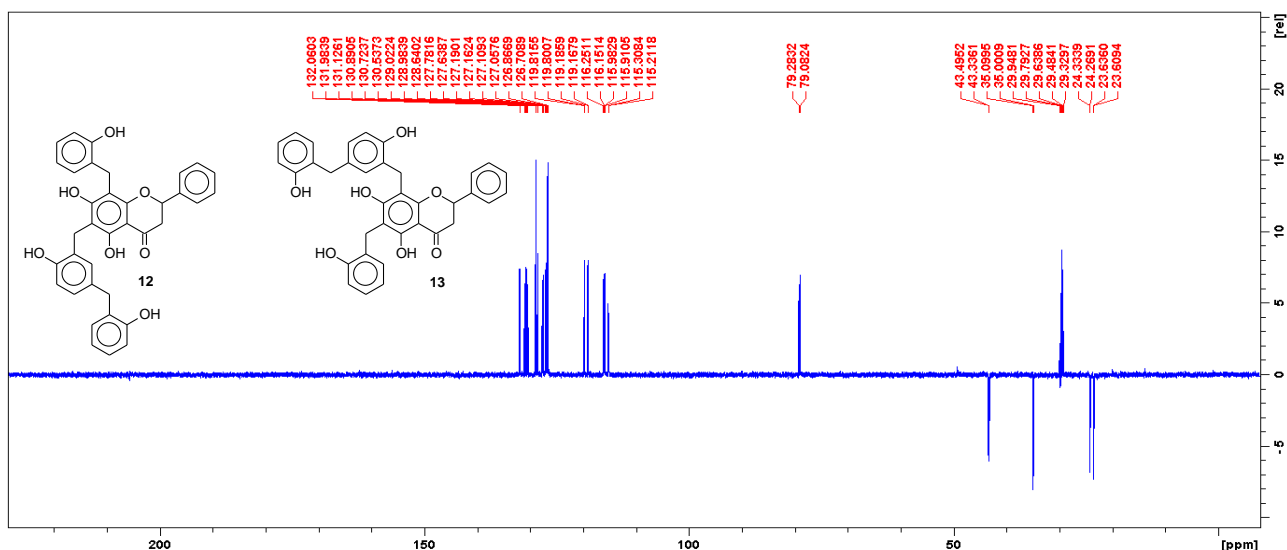


Figure S113. DEPT 135 spectrum of the mixture of **uvarinol** (**12**) and **isouvarinol** (**13**) in acetone- d_6 at 125 MHz.

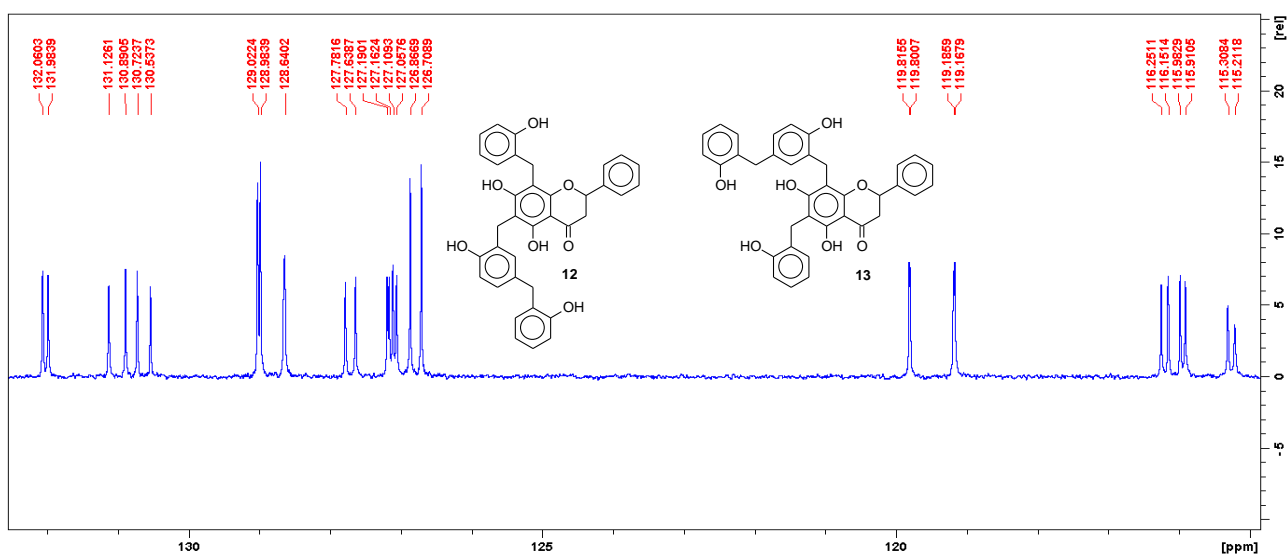


Figure S114. Expansion (δ 132.4 – 114.9) of the DEPT 135 spectrum of the mixture of **uvarinol** (**12**) and **isouvarinol** (**13**) in acetone- d_6 at 125 MHz.

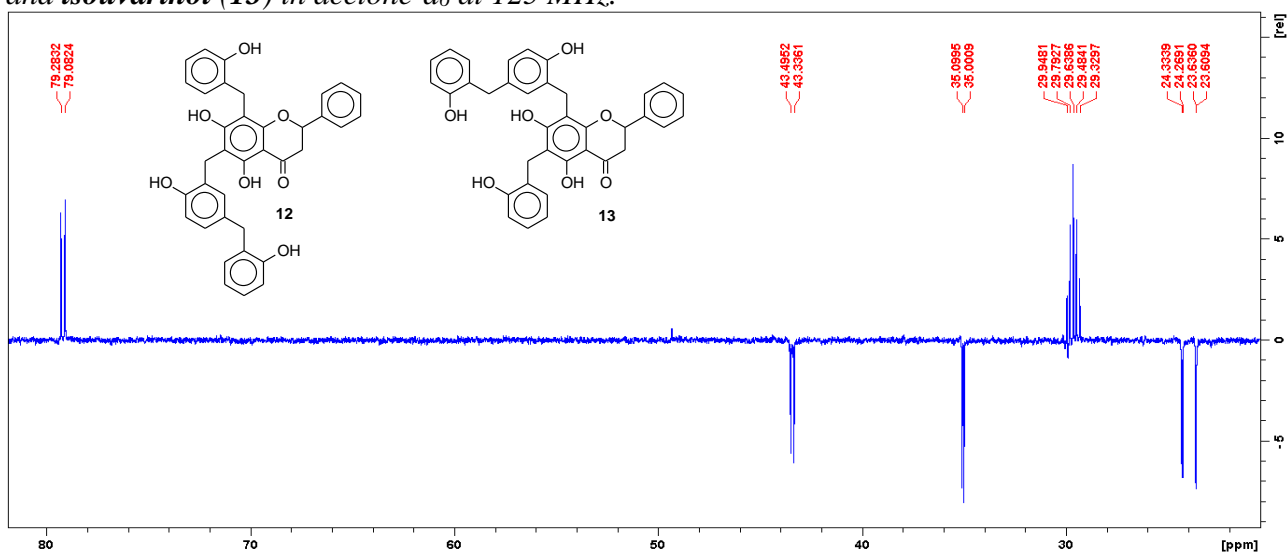


Figure S115. Expansion (δ 81.7 – 20.7) of the DEPT 135 spectrum of the mixture of **uvarinol** (**12**) and **isouvarinol** (**13**) in acetone- d_6 at 125 MHz.

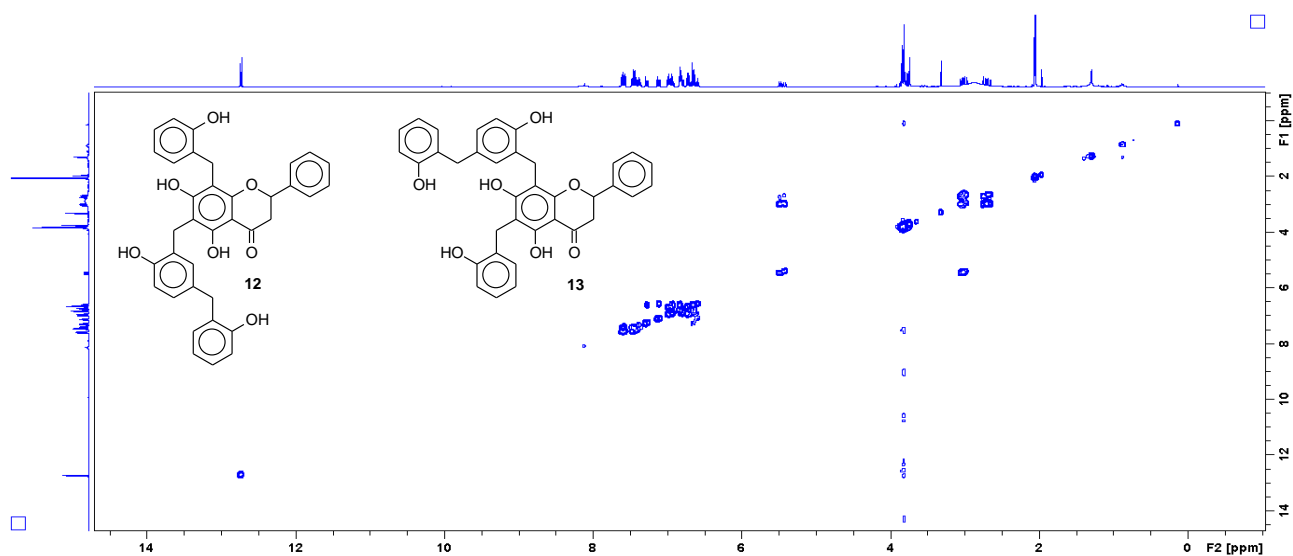


Figure S116. ^1H - ^1H correlation map from COSY NMR experiment of the mixture of *uvarinol* (12) and *isouvarinol* (13) in acetone- d_6 at 500 MHz.

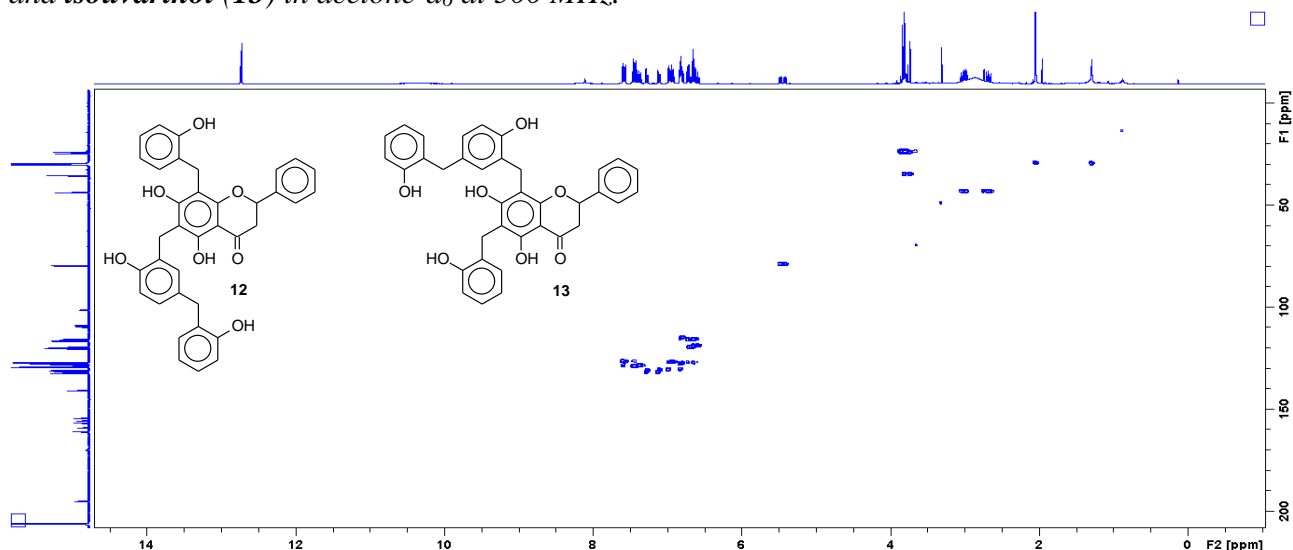


Figure S117. One-bond ^1H - ^{13}C correlation map from HSQC NMR experiment of the mixture of *uvarinol* (12) and *isouvarinol* (13) in acetone- d_6 at 500 (^1H) and 125 MHz (^{13}C), respectively.

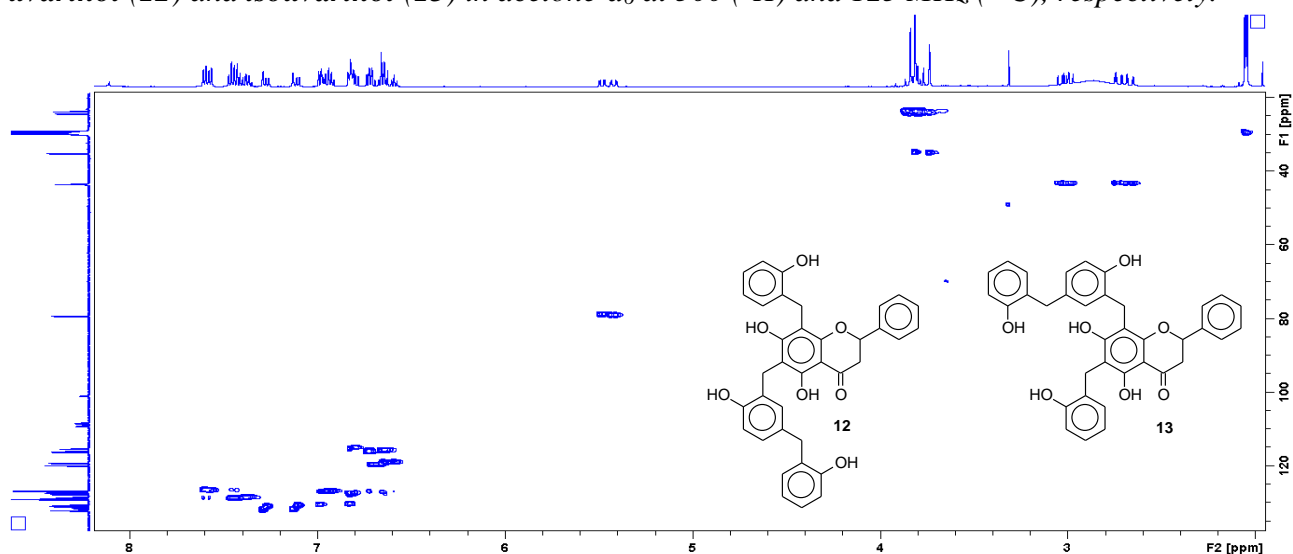


Figure S118. Expansion of the one-bond ^1H - ^{13}C correlation map from HSQC NMR experiment of the mixture of *uvarinol* (12) and *isouvarinol* (13) in acetone- d_6 at 500 (^1H) and 125 MHz (^{13}C), respectively.

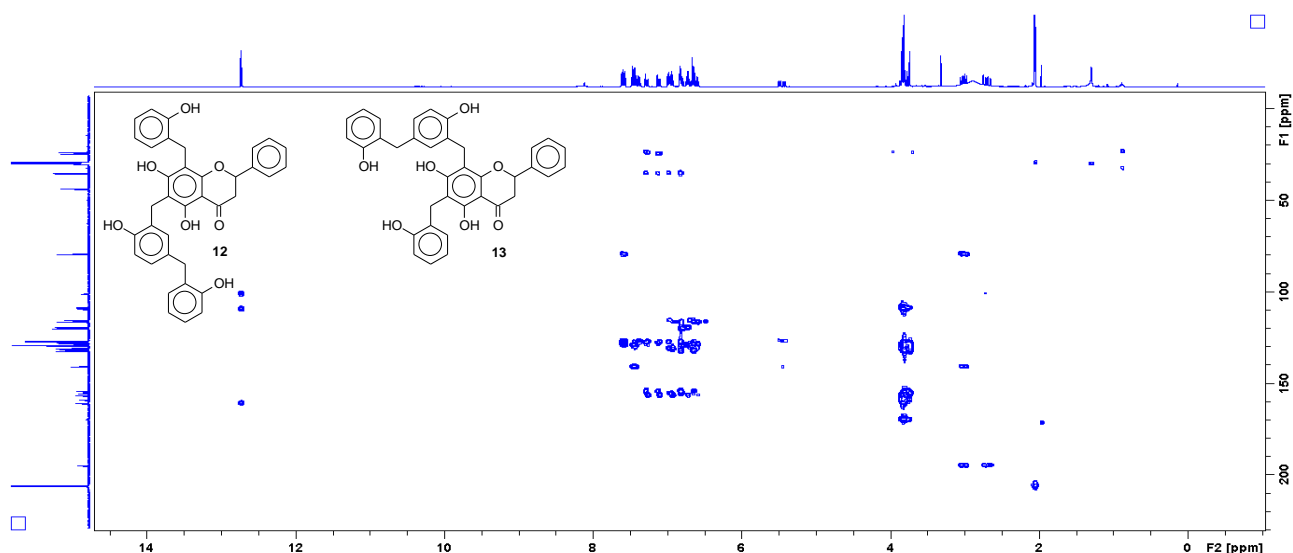


Figure S119. Long-range ^1H - ^{13}C correlation map from HMBC NMR experiment of the mixture of **uvarinol** (**12**) and **isouvarinol** (**13**) in acetone- d_6 at 500 (^1H) and 125 MHz (^{13}C), respectively.

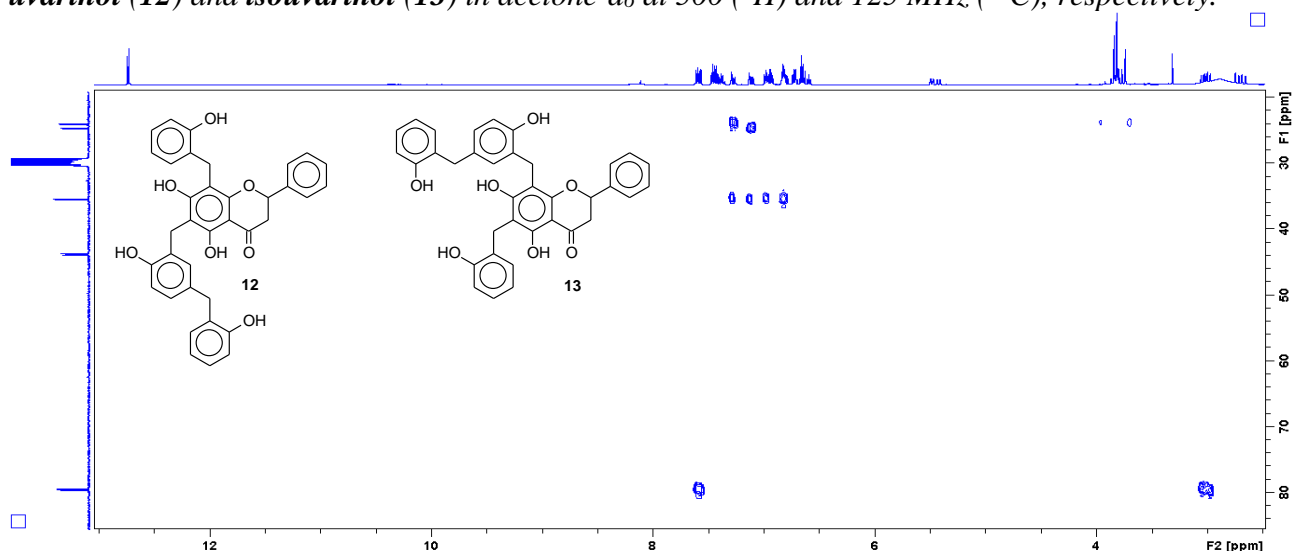


Figure S120. Expansion of the long-range ^1H - ^{13}C correlation map from HMBC NMR experiment of the mixture of **uvarinol** (**12**) and **isouvarinol** (**13**) in acetone- d_6 at 500 (^1H) and 125 MHz (^{13}C), respectively.

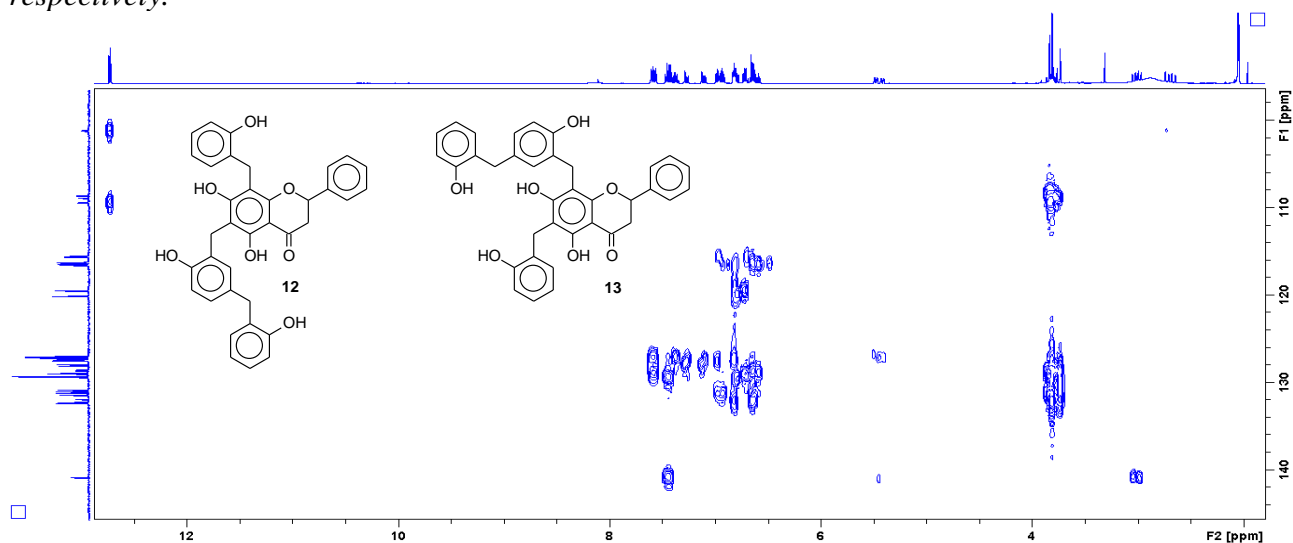


Figure S121. Expansion of the long-range ^1H - ^{13}C correlation map from HMBC NMR experiment of the mixture of **uvarinol** (**12**) and **isouvarinol** (**13**) in acetone- d_6 at 500 (^1H) and 125 MHz (^{13}C), respectively.

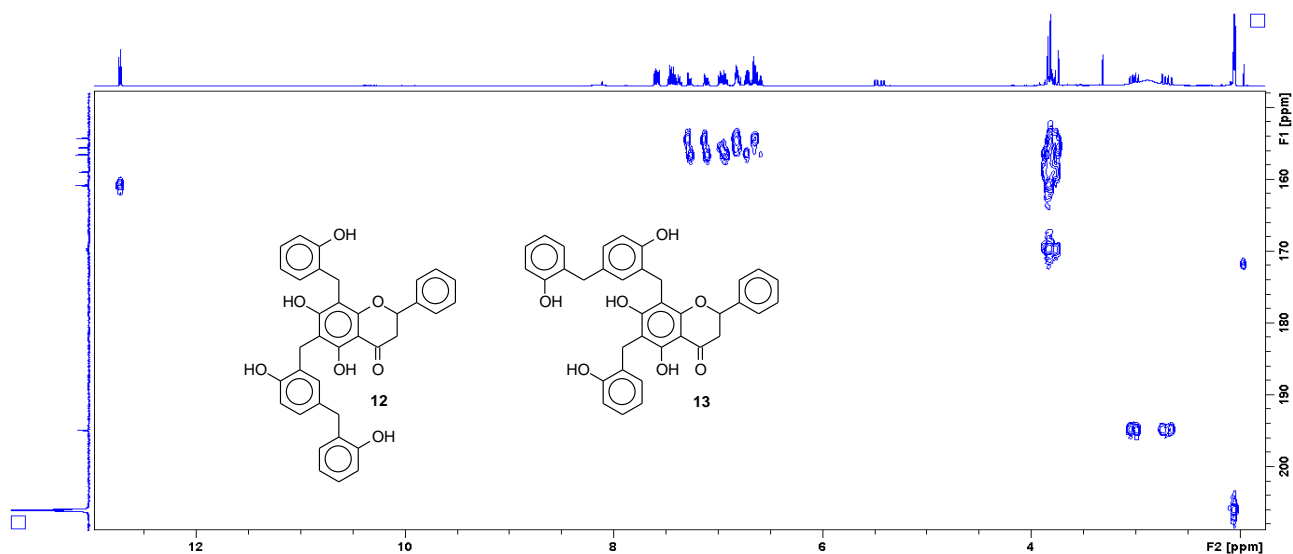


Figure S122. Expansion of the long-range ^1H - ^{13}C correlation map from HMBC NMR experiment of the mixture of **uvarinol** (**12**) and **isouvarinol** (**13**) in acetone- d_6 at 500 (^1H) and 125 MHz (^{13}C), respectively.

DEFESA_16_04_2019 #399 RT: 8,16 AV: 1 NL: 1,05E7
F: -c ESI Q1MS [100,000-1000,000]

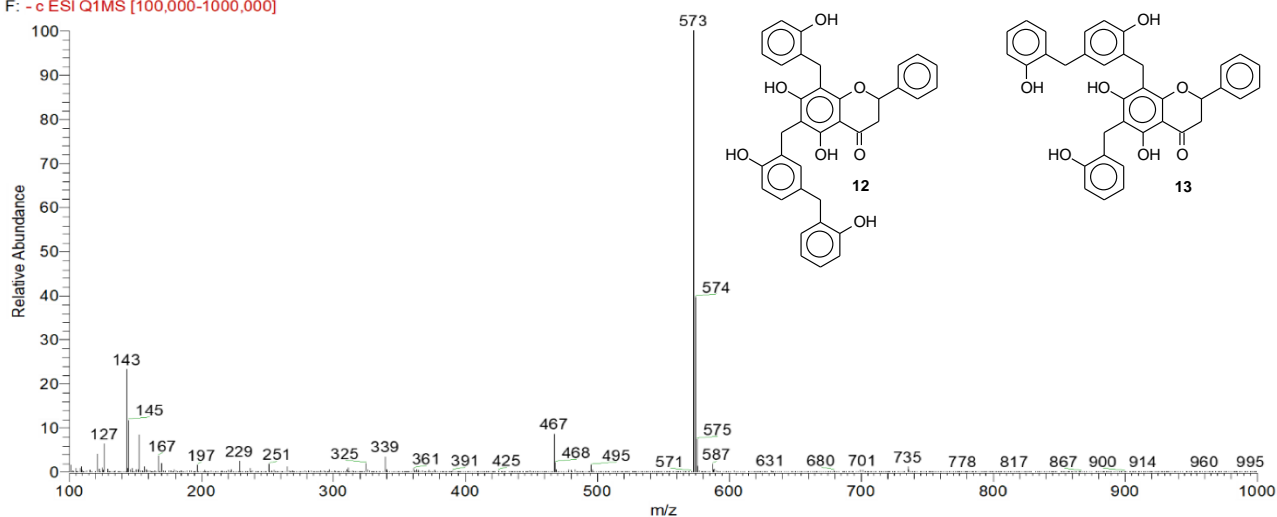


Figure S123. LR-ESI(-)-MS spectrum of the mixture of **uvarinol** (**12**) and **isouvarinol** (**13**) (m/z 573 $[\text{M}-\text{H}]^-$).