Supporting Information

***Rec. Nat. Prod.* 10:5 (2016) 654-658**

Lignoids Isolated from *Nectandra turbacensis* (Kunth) Nees (Lauraceae)

Víctor Macías-Villamizar[1, *,§], Luís Cuca-Suárez[1,*], Florenci V. González[2], Santiago Rodríguez[2].

[1]Departamento Química, Laboratorio de Productos Naturales, Universidad Nacional de Colombia. Av. Carrera 30 # 45-03. Cód. postal 111321; Edificio 476-Oficina 11; Bogotá D.C., Colombia. [§]Profesor Universidad del Magdalena, Colombia

[2]Departament de Química Inorgànica i Orgànica, Universitat Jaume I, Campus Riu Sec, Escola Superior de Tecnologia i ciències Experimentals, Dept. Química Inorgánica i Orgánica; Avda. Sos Baynat; PO BOX 12071, Castelló, Spain

Table of Contents **Page**

S1: IR [cm^{-1}, KBr pellets] Spectrum of Compound **1** (turbacenlignan) **4**

S2: ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **1** (turbacenlignan) **4**

S3: Expansion of the ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **1** (turbacenlignan A) **5**

S4: ^{13}C NMR (100 MHz, $CDCl_3$) Spectrum of Compound **1** (turbacenlignan A) **5**

S5: DEPT-135° Spectrum of Compound **1** (turbacenlignan A) **6**

S6: HMBC Spectrum of Compound **1** (turbacenlignan A) **6**

S7: Expansion of the HMBC Spectrum of Compound **1** (turbacenlignan A) (From 95.0 to 45.0) **7**

S8: Expansion of the HMBC Spectrum of Compound **1** (turbacenlignan A) (From 17.0 to 125.0) **8**

S9: Expansion of the HMBC Spectrum of Compound **1** (turbacenlignan A) (From 105.0 to 75.0) **9**

S10: HMQC Spectrum of Compound **1** (turbacenlignan A) **10**

S11: Expansion of the HMQC Spectrum of Compound **1** (turbacenlignan A) (From 75.0 to 5.0) **11**

* Corresponding author: E-Mail: vemaciasv@unal.edu.co; Phone (57)(1) 3165000 - Ext: 14476.

S12: Expansion of the HMQC Spectrum of Compound **1** (turbacenlignan A) (From 7.00 to 5.80) **12**

S13: COSY Spectrum of Compound **1** (turbacenlignan A) **13**

S14: ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **2** (*meso*-monomethyl dihydroguaiaretic acid) **14**

S15: Expansion of the ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **2** (*meso*-monomethyl dihydroguaiaretic acid) **15**

S16: ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **3** (*threo*-dihydroguaiaretic acid) **15**

S17: Expansion of the ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **3** (*threo*-dihydroguaiaretic acid) **16**

S18: ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **4** (schineolignin B) **16**

S19: Expansion of ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **4** (schineolignin B) **17**

S20: ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **5** (austrobailignan-5) **18**

S21: Expansion of ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **5** (austrobailignan-5) **19**

S22: ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **6** (henricine) **20**

S23: Expansion of ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **6** (henricine) **21**

S24: ^{13}C NMR (100 MHz, $CDCl_3$) Spectrum of Compound **6** (henricine) **21**

S25: NOESY Spectrum of Compound **6** (henricine) **22**

S26: Expansion of NOESY Spectrum of Compound **6** (henricine) **23**

S27: Expansion of NOESY Spectrum of Compound **6** (henricine) (From 3.00 to 0.40) **24**

S28: Expansion of NOESY Spectrum of Compound **6** (henricine) (From 5.20 to 3.20) **25**

S29: Expansion of NOESY Spectrum of Compound **6** (henricine) (From 5.00 to 4.30) **26**

S30: COSY Spectrum of Compound **6** (henricine) **27**

S31: Expansion of **C**OSY Spectrum of Compound **6** (henricine) (From 1.60 to 0.30) **28**

S32: Expansion of **C**OSY Spectrum of Compound **6** (henricine) (From 2.60 to 0.50) **29**

S33: DEPT-135° Spectrum of Compound **6** (henricine) **30**

S34: HMQC Spectrum of Compound 6 (henricine) **30**

S35: HMBC Spectrum of Compound **6** (henricine) **31**

S36: ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **7-8** (veraguensin and galgravin) **32**

S37: Expansion of ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **7-8** (veraguensin and galgravin) **33**

S38: ^{13}C NMR (100 MHz, $CDCl_3$) Spectrum of Compound **7-8** (veraguensin and galgravin) **33**

S39: DEPT-135° Spectrum of Compound **7-8** (veraguensin and galgravin) **34**

S40: COSY Spectrum of Compound **7-8** (veraguensin and galgravin) **35**

S41: HMQC Spectrum of Compound **7-8** (veraguensin and galgravin) **36**

S42: HSQC Spectrum of Compound **7-8** (veraguensin and galgravin) **37**

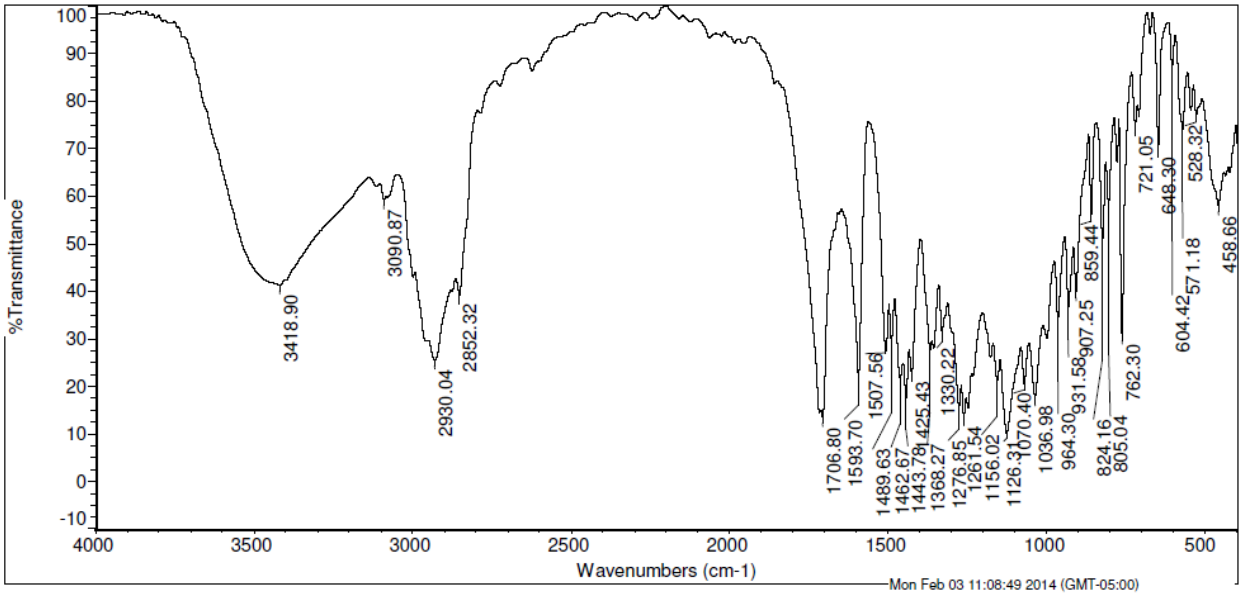
S43: HMBC Spectrum of Compound **7-8** (veraguensin and galgravin) **38**

S44: Total Ion Current of ethanol extract **39**

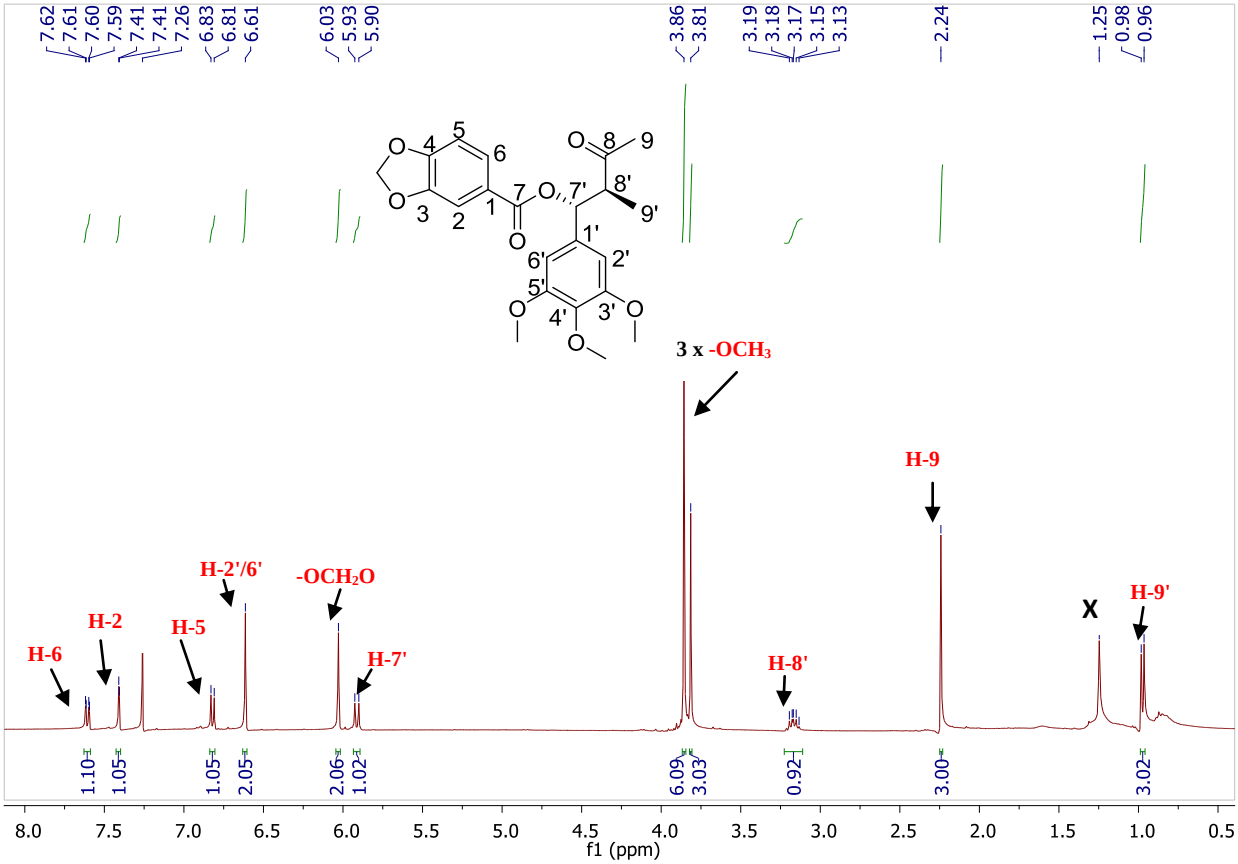
S45: Mass spectra of Compound **5** (austrobailignan-5, in the ethanol extract) **40**

S46: Mass spectra of Compound **8** (galgravin, in the ethanol extract) **40**

S47: Mass spectra of Compound **3** (*threo*-dihydroguaiaretic acid, in the ethanol extract) **40**

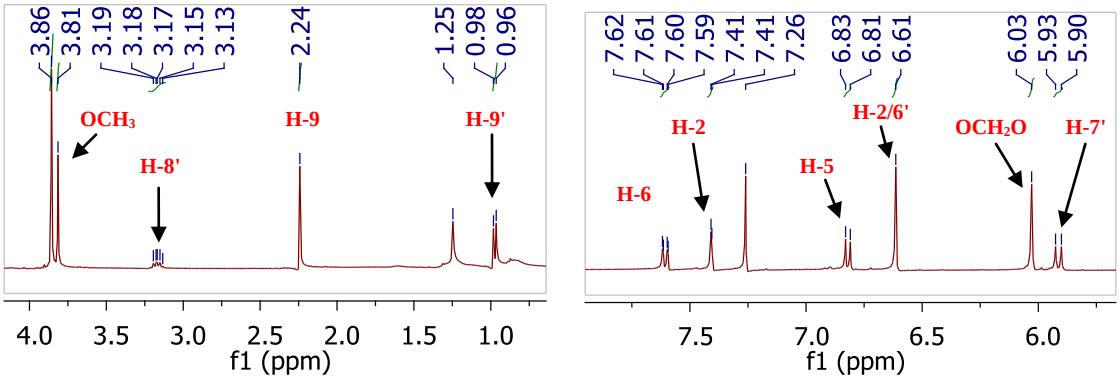


S1: IR [cm^{-1}, KBr pellets] Spectrum of Compound **1** (turbacenlignan A)

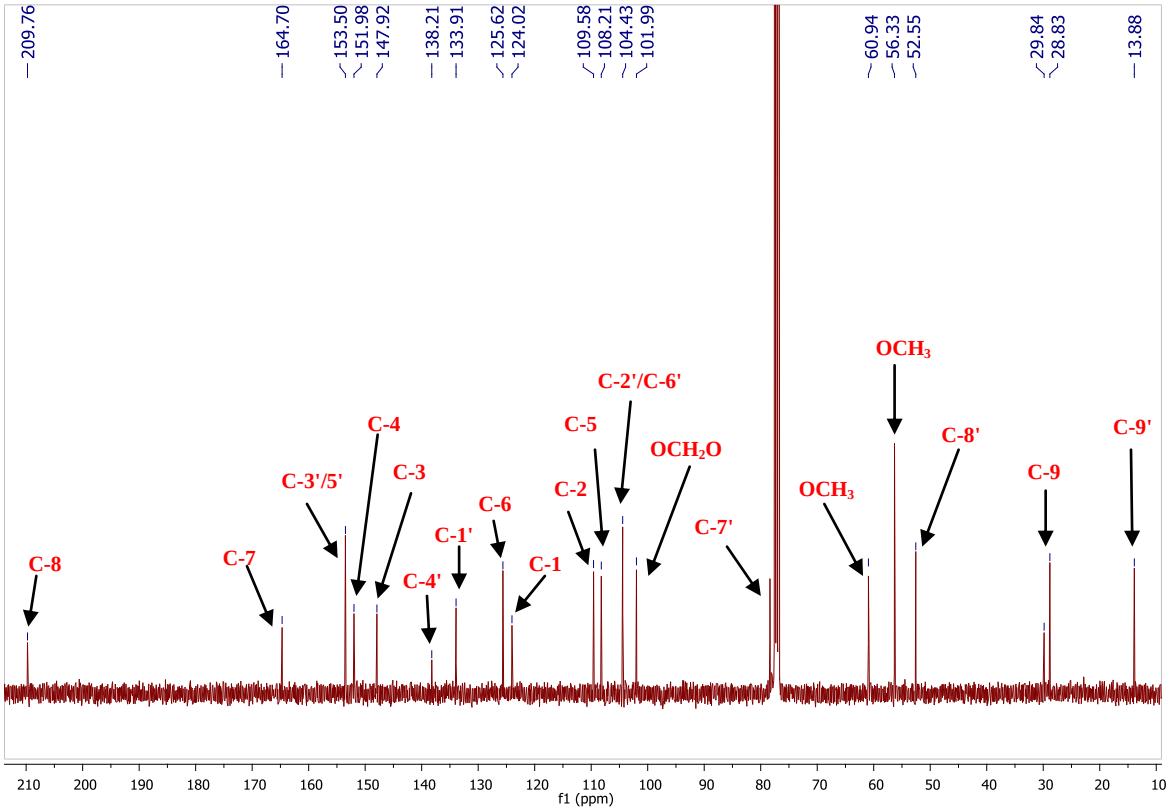


S2: ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **1** (turbacenlignan A)

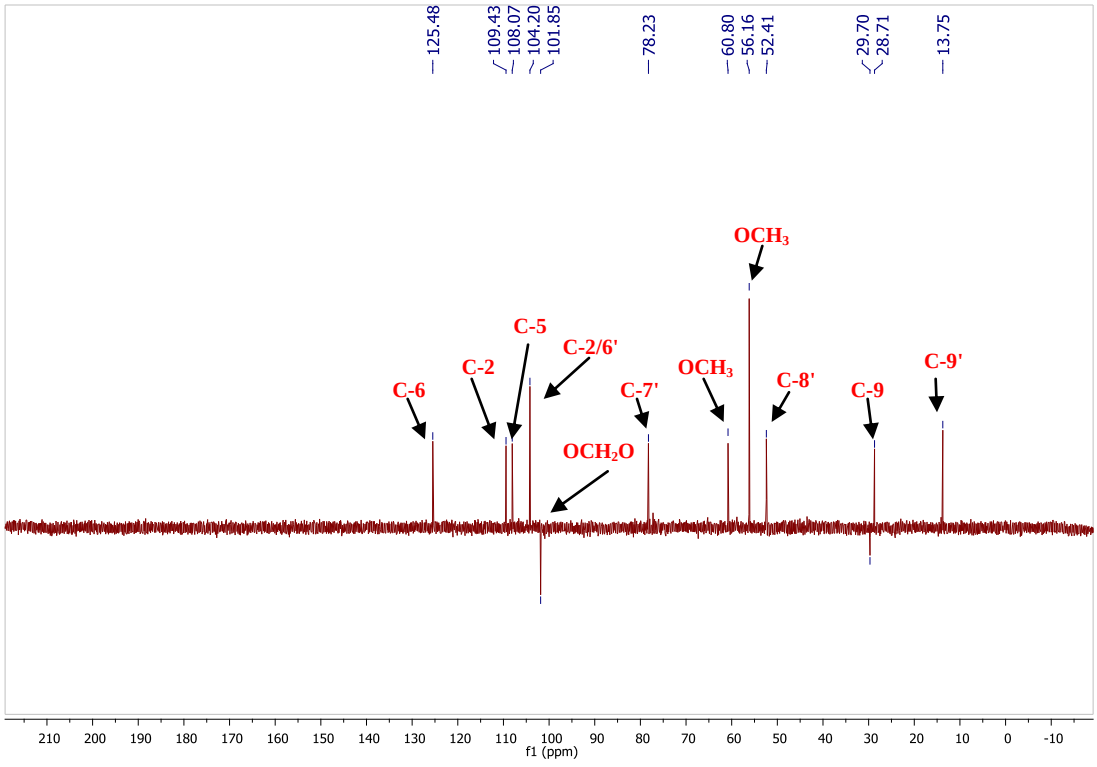
Turbacenlignan A ***(1)*** *(=rel-(7'S,8'R)-3',4',5'-trimethoxy-3,4-methylenedioxy-7,8-seco-7,7'-epoxylignan-7,8-dione*): White amorphous powder. $[\alpha]_D^{24}$ +33 (*c*=0.5,$CHCl_3$). IR (KBr): 3419, 3091, 2930, 2852, 1707, 1594, 1507, 1489, 1444, 1368, 1276, 1126, 1070, 824. ^{1}H NMR (400 MHz, $CDCl_3$), δ: 7.60 (1H, *dd*, *J*= 8.2, 1.6, H-6), 7.40 (1H, *d*, *J*= 1.6, H-2), 6.81 (1H, *d*, *J*= 8.2, H-2'/6'), 6.02 (2H, *s*, OCH_2O), 5.91 (1H, *d*, 10.1, H-7'), 3.86 (6H, *s*, OCH_3), 3.81 (3H, *s*, OCH_3), 3.17 (1H, dq, *J*= 10.1, 7.1, H-8'), 2.24 (3H, *s*, H-9), 0.96 (3H, *d*, *J*= 7.2, H-9').



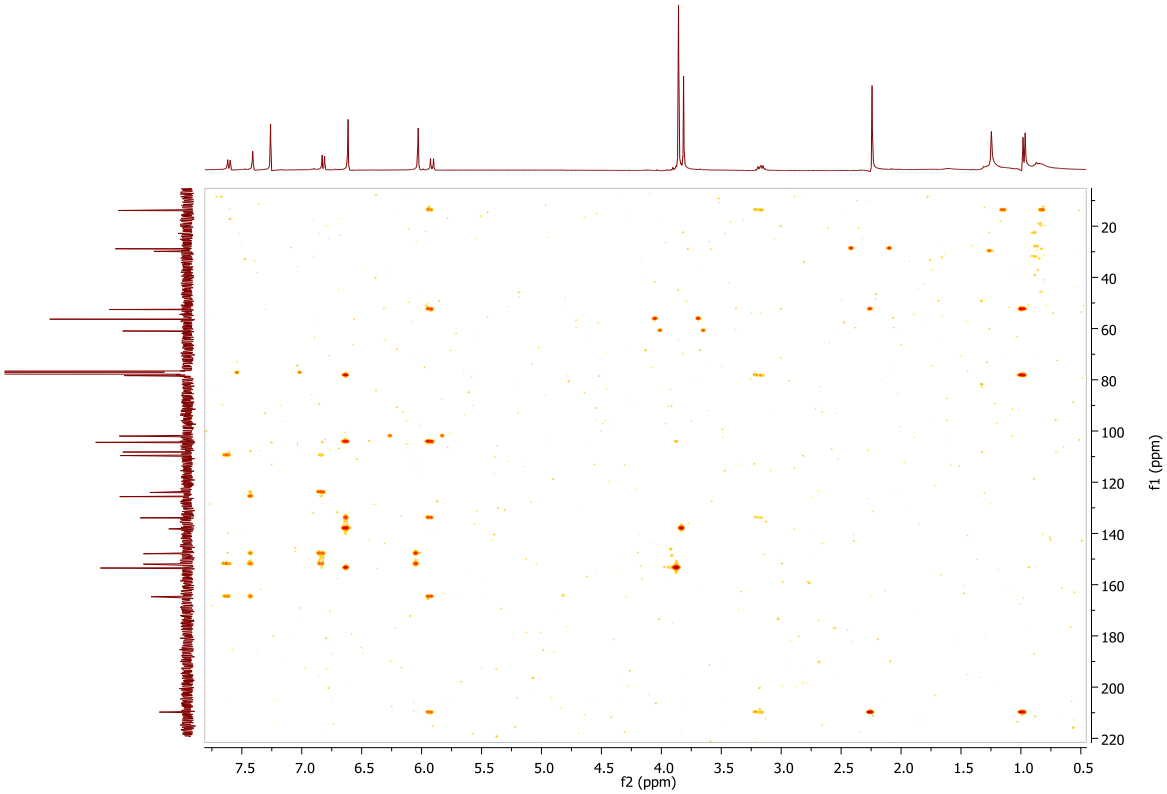
S3: ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **1** (turbacenlignan A) (From 4.00 to 1.00) and (From 7.60 to 5.80)



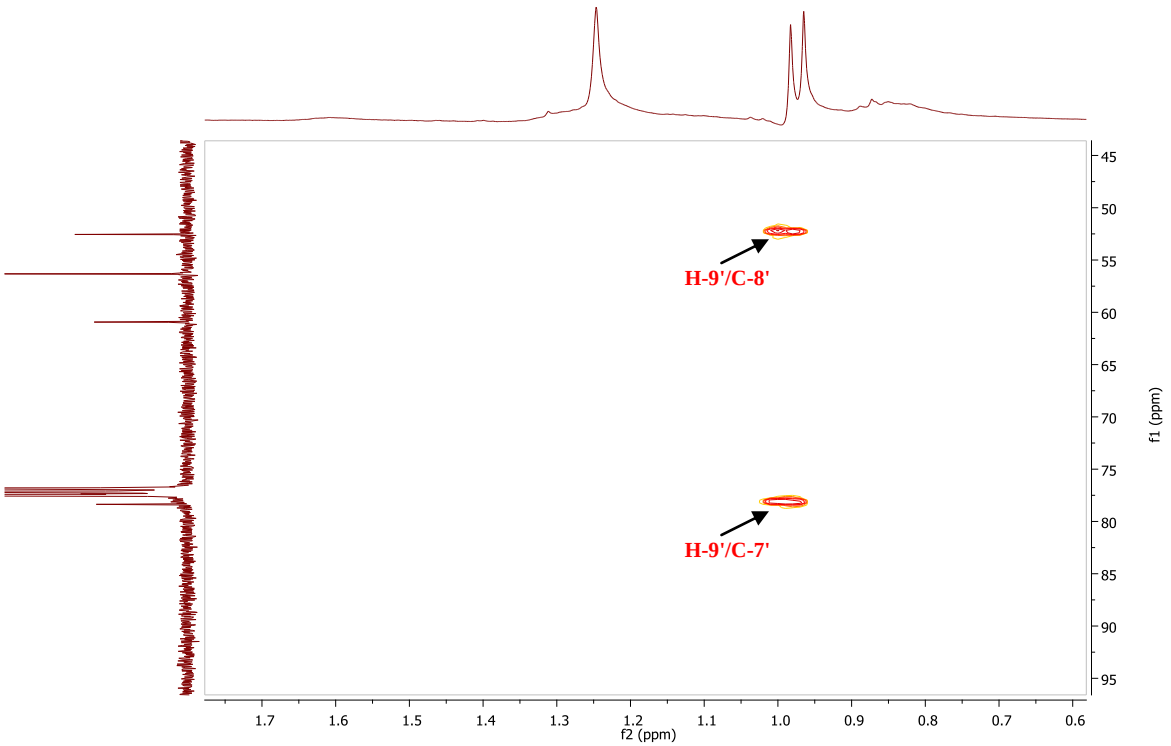
S4: ^{13}C NMR (100 MHz, $CDCl_3$) Spectrum of Compound **1** (turbacenlignan A)



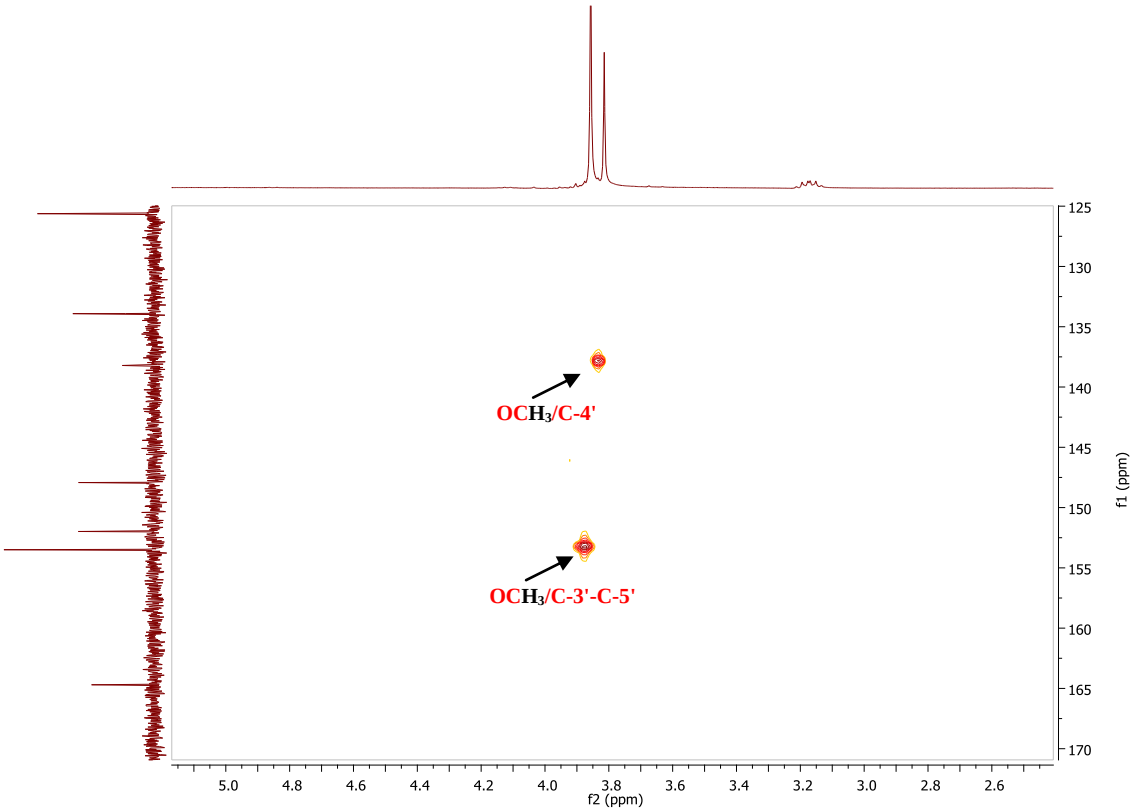
S5: DEPT-135° Spectrum of Compound **1** (turbacenlignan A)



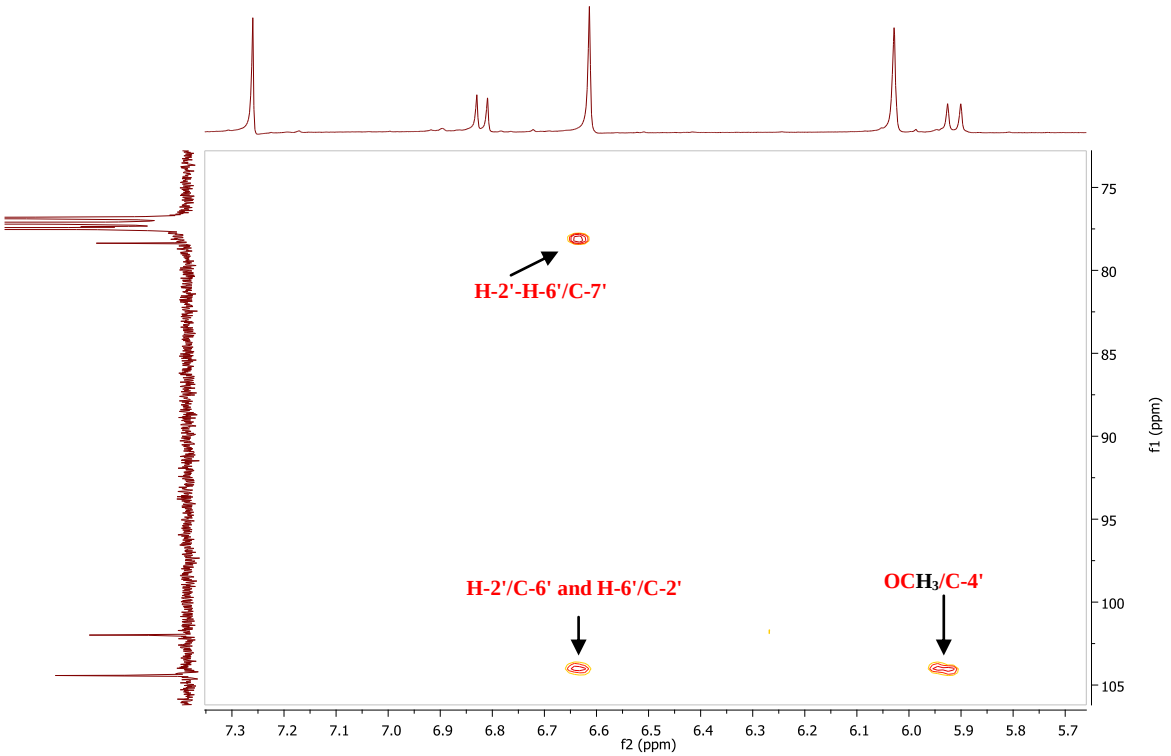
S6: HMBC Spectrum of Compound **1** (turbacenlignan A)



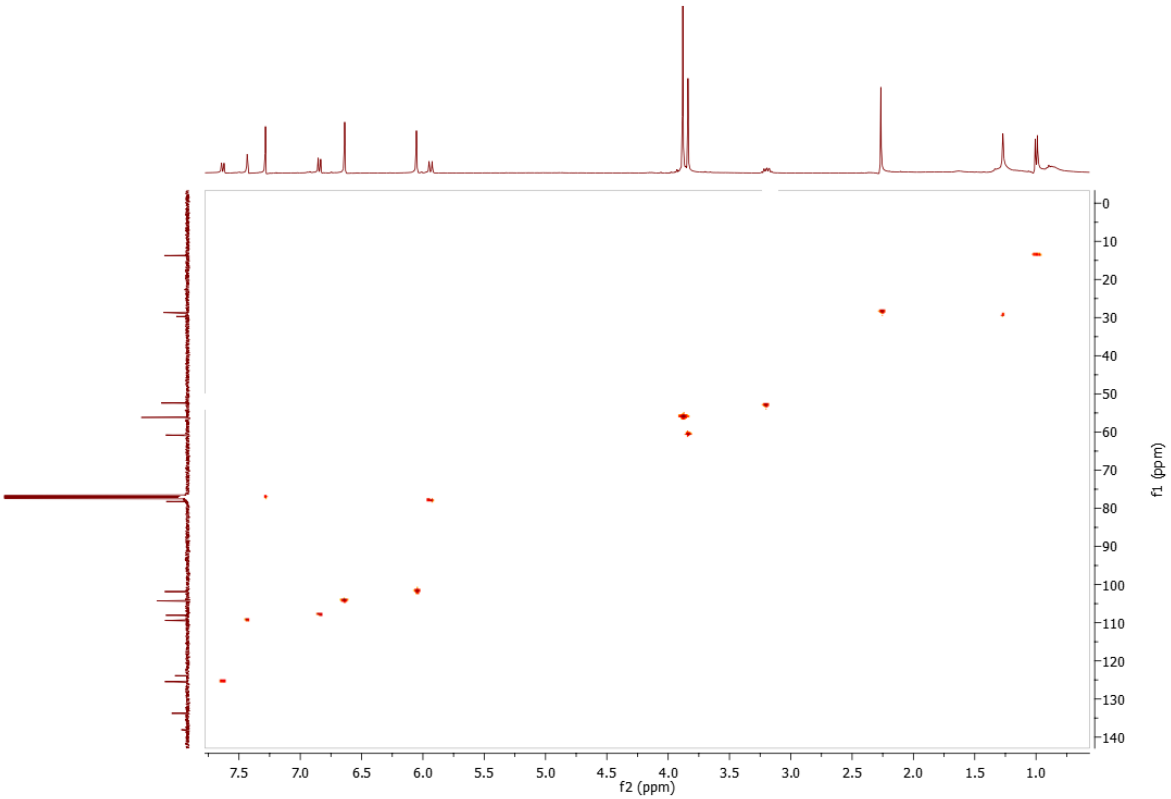
S7: HMBC Spectrum of Compound **1** (turbacenlignan A) (^{1}H NMR, from 1.70 to 0.60 f2) (^{13}C NMR, From 45.0 to 95.0 f1)



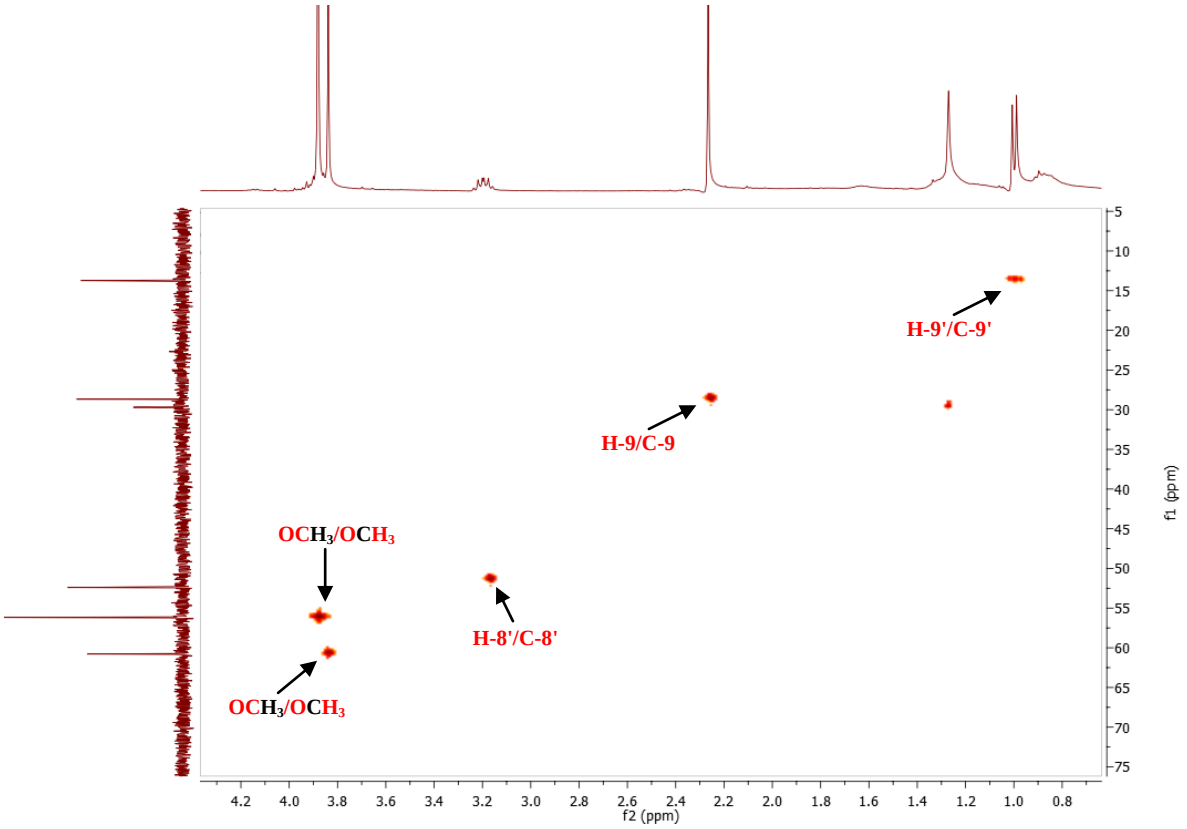
S8: HMBC Spectrum of Compound **1** (turbacenlignan A) (^{1}H NMR, from 5.00 to 2.60 f2) (^{13}C NMR, From 170.0 to 125.0 f1)



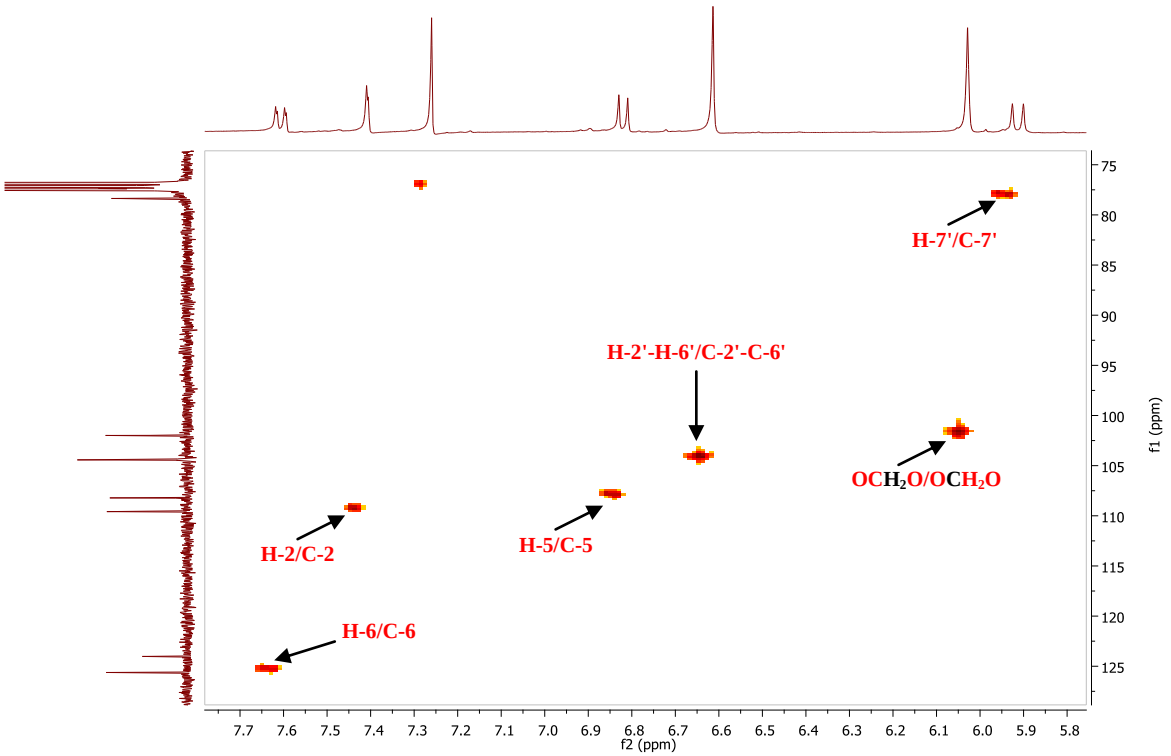
S9: HMBC Spectrum of Compound **1** (turbacenlignan A) (^{1}H NMR, from 7.00 to 5.80 f2) (^{13}C NMR, From 105.0 to 75.0 f1)



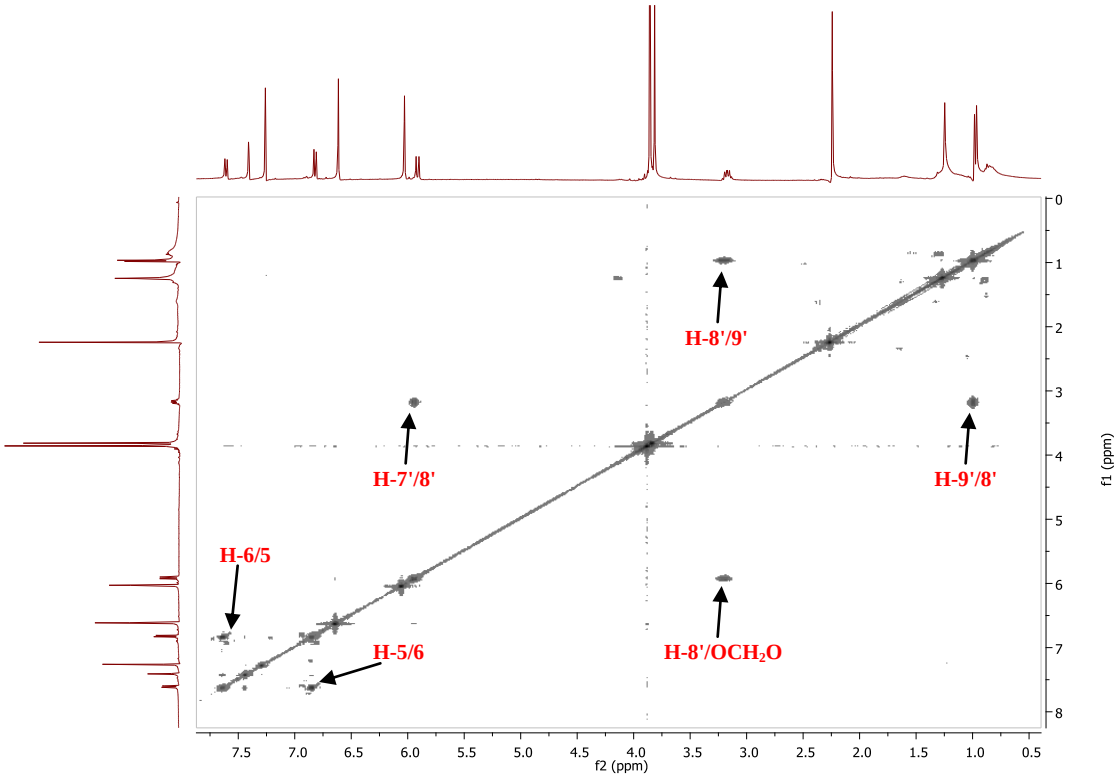
S10: HMQC Spectrum of Compound **1** (turbacenlignan A)



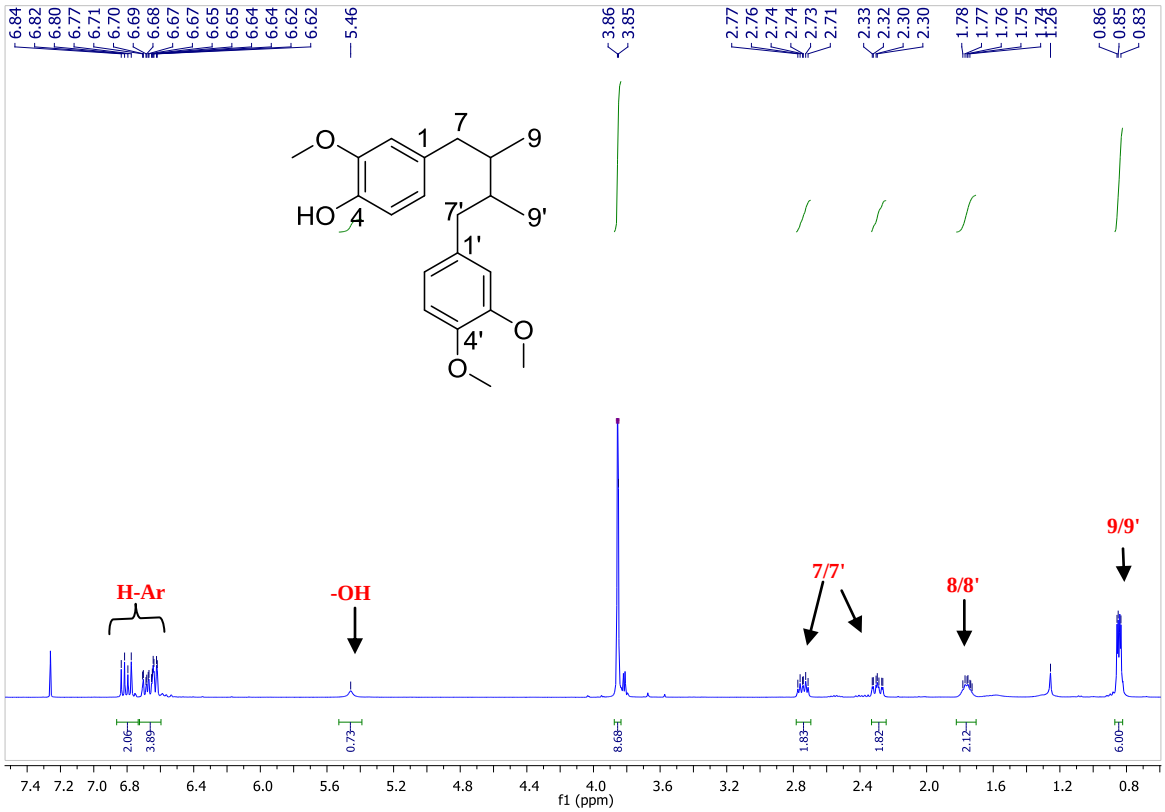
S11: HMQC Spectrum of Compound **1** (turbacenlignan A) (^{1}H NMR, from 4.20 to 0.80 f2) (^{13}C NMR, From 75.0 to 5.0 f1)



S12: HMQC Spectrum of Compound **1** (turbacenlignan A) (^{1}H NMR, from 7.70 to 5.8 f2) (^{13}C NMR, From 125.0 to 75.0 f1)

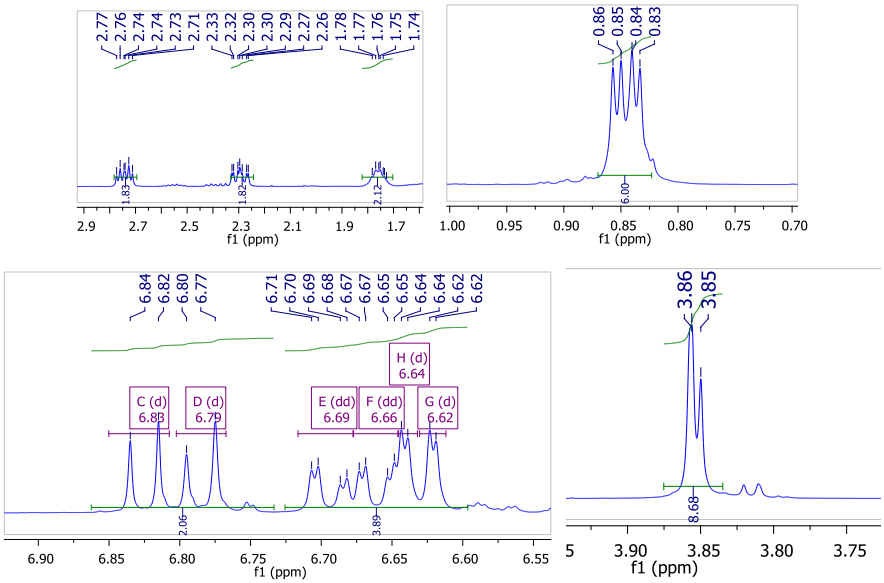


S13: COSY Spectrum of Compound **1** (turbacenlignan A)

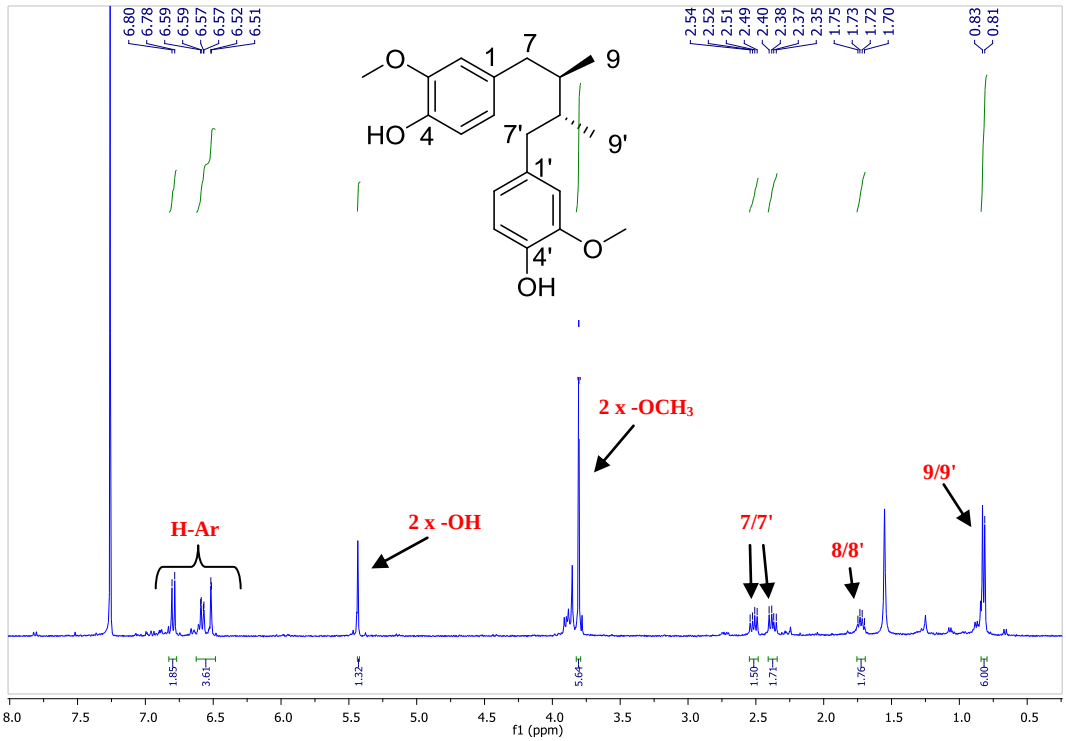


S14: ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **2** (*meso*-monomethyl dihydroguaiaretic acid)

Meso-monomethyl dihydroguaiaretic acid (**2**): Colourless oil. ^{1}H NMR (400 MHz, $CDCl_3$), δ: 6.82 (1H, *d*, *J* = 8.0, H-5), 6.79 (1H, *d*, *J* = 8.1, H-5'), 6.70 (1H, *dd*, *J* = 8.1, 1.8, H-6'), 6.65 (1H, *dd*, *J* = 8.0, H-6), 6.62 (1H, d, 1.8, H-2), 6.64 (1H, d, 2.0, H-2'), 5.46 (1H, *s*, OH), 3.85-3.84 (9H, *s*, 3 x OCH_3), 2.75 (2H *dd*, *J* = 13.4, 4.9, H-7b/7'b), 2.30 (2H, *dd*, *J* = 13.4, 9.3, H-7a/7'a), 1.77 (2H, *dd*, *J* = 12.8, 6.3, H-8/8'), 0.85 (6H, *d*, *J* = 6.6, H-9'), 0.84 (d, 6.7, H-9).



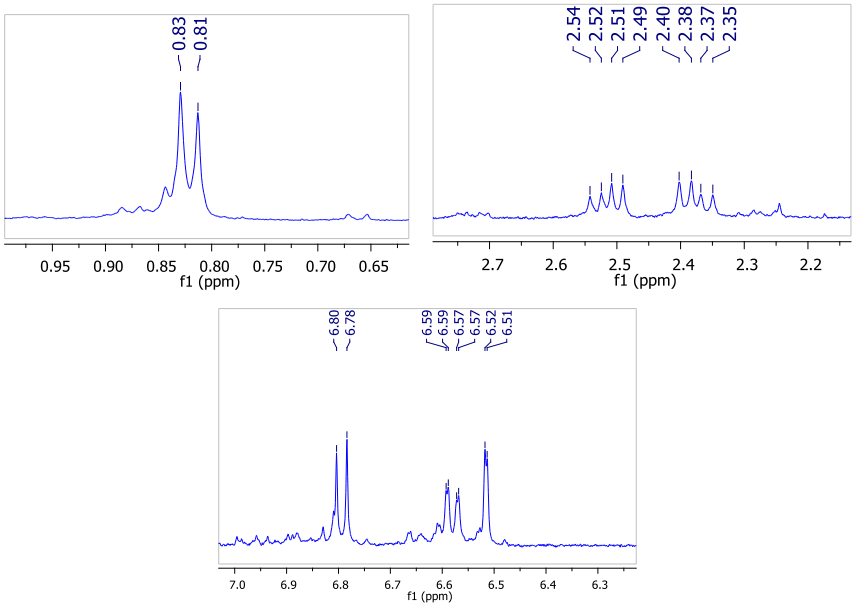
S15: ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **2** (*meso*-monomethyl dihydroguaiaretic acid) (From 1.00 to 0.70), (From 2.90 to 1.70), (From 5.00 to 3.75) and (From 6.90 to 6.55)



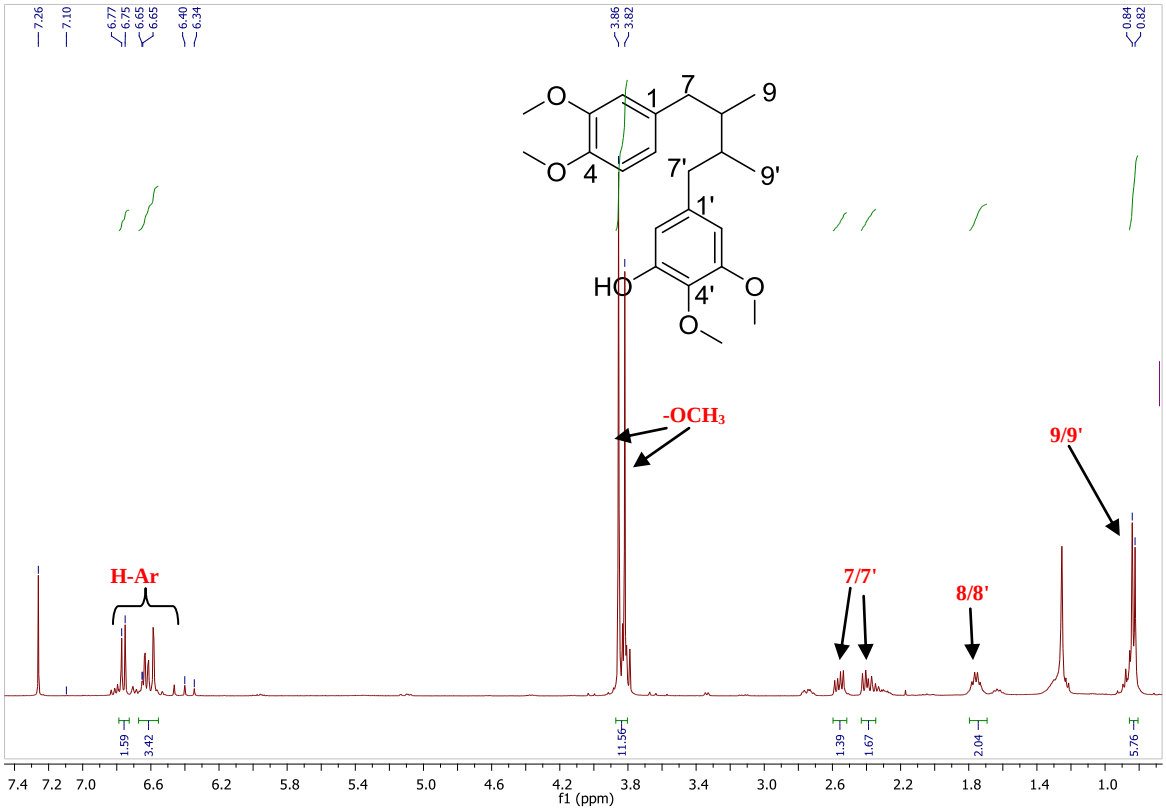
S16: ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **3** (*threo*-dihydroguaiaretic acid)

*Threo-dihydroguaiaretic acid (**3**)*: ^{1}H NMR (400 MHz, $CDCl_3$), δ: 6.80 (2H, *d*, *J*=7.9, H-5,5´), 6.58 (2H, *dd*, *J*=7.0, 1.6, H-6,6´), 6.52 (2H, *d*, *J*=1.6, H-2,2´), 5.43 (2H, *s*, Ar-OH), 3.81 (6H, *s*, OMe),

2.52 (2H, *dd*, *J*=13.6, 7.1, H-7b, 7′b), 2.38 (2H, *dd*, *J*=13.5, 7.5, H-7a, 7′a), 1.73 (2H, *dd*, *J*=12.9, 6.5, H-8, 8′), 0.83 (6H, *d*, *J*=6.6, H-9, 9′).



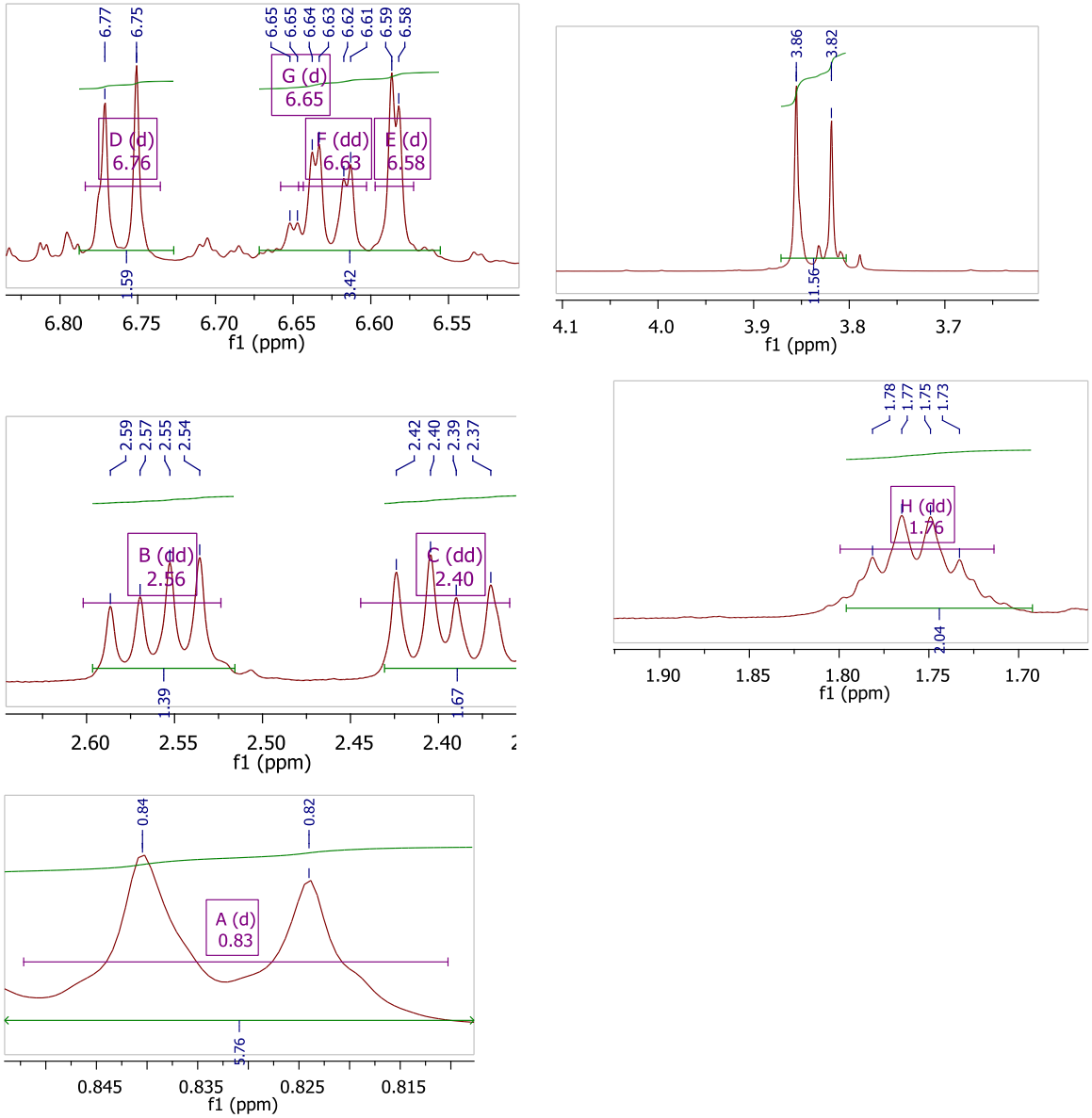
S17: ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **3** (*threo*-dihydroguaiaretic acid) (From 0.95 to 0.65), (From 2.70 to 2.20), and (From 6.90 to 6.40)



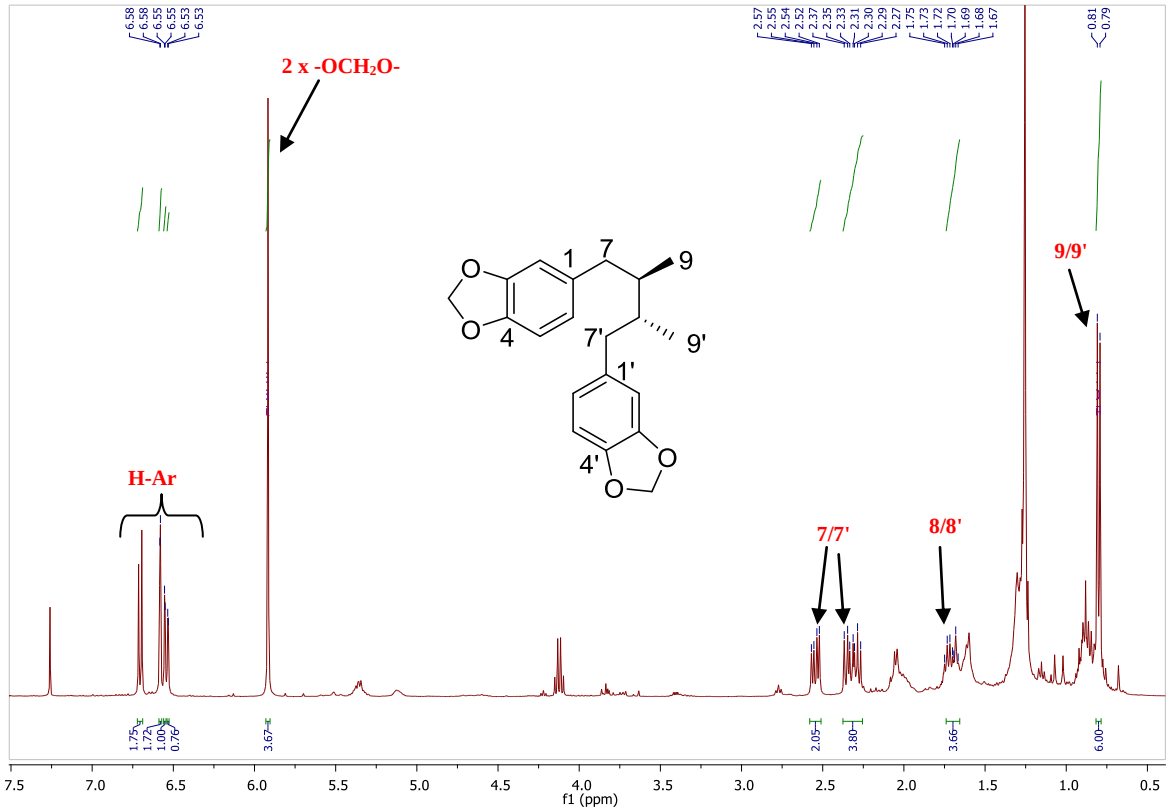
S18: ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **4** (schineolignin B)

*Schineolignin B (**4**):* White amorphous solid, $[\alpha]_D^{24}$= +14.8 (*c*=0.4, CH_3OH). ^{1}H NMR (400 MHz, $CDCl_3$), δ: 6.76 (1H, *d*, *J* = 8.1, H-), 6.65 (1H, *d*, *J* = 1.9, H-), 6.63 (1H, *dd*, *J* = 8.1, 1.8, H-), 6.58

(1H, *d*, *J* = 1.8, H-), 3.86-3.82 (12H, *s*, *2* x OCH_3), 2.56 (2H, *dd*, *J* = 13.5, 6.8, H-7b/7'b), 2.40 (2H, *dd*, *J* = 13.7, 7.8, H-7a/7'a), 1.76 (2H, *m*, H-8/8'), 0.83 (d, *J* = 6.6, H-9/9').

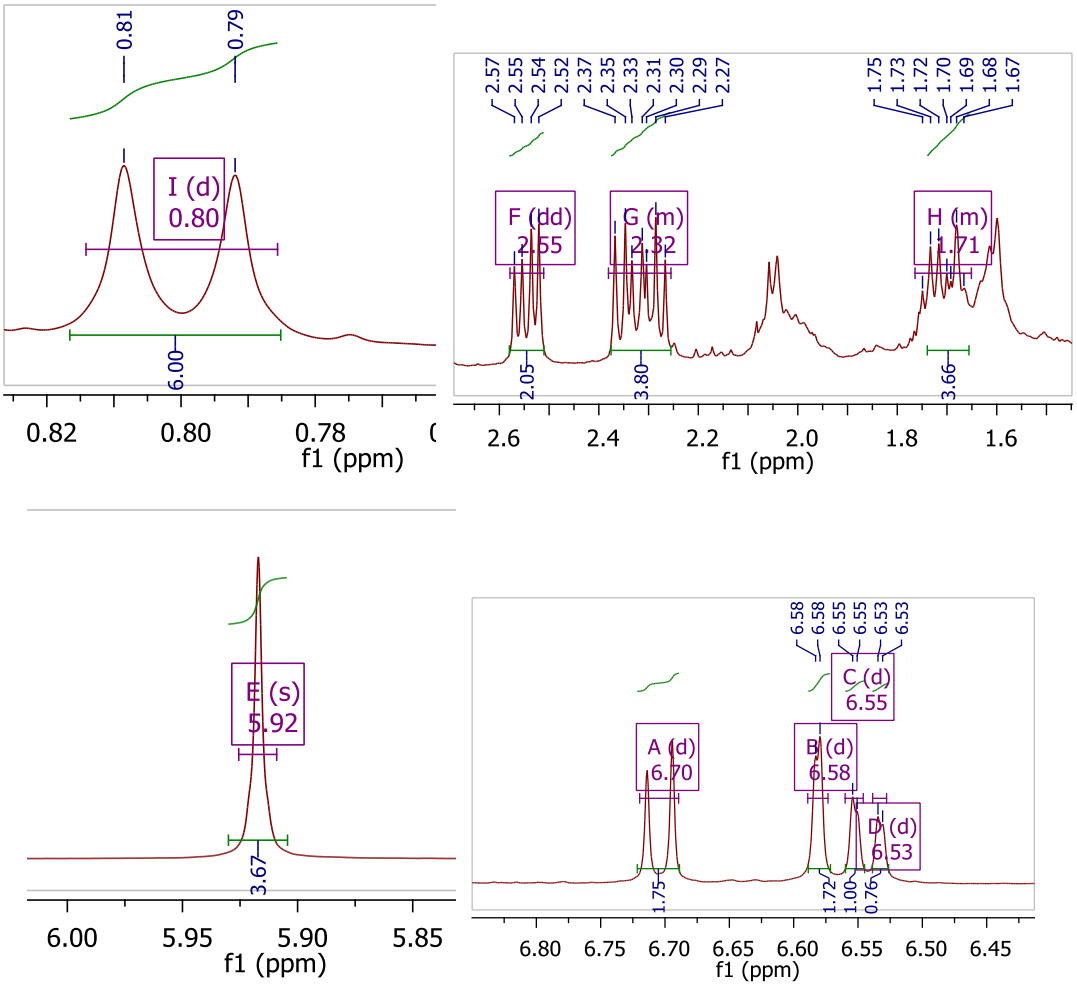


S19: ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **4** (schineolignin B) (From 0.84 to 0.82), (From 1.85 to 1.70), (From 2.60 to 2.35), (From 3.90 to 3.70), and (From 6.80 to 6.55)

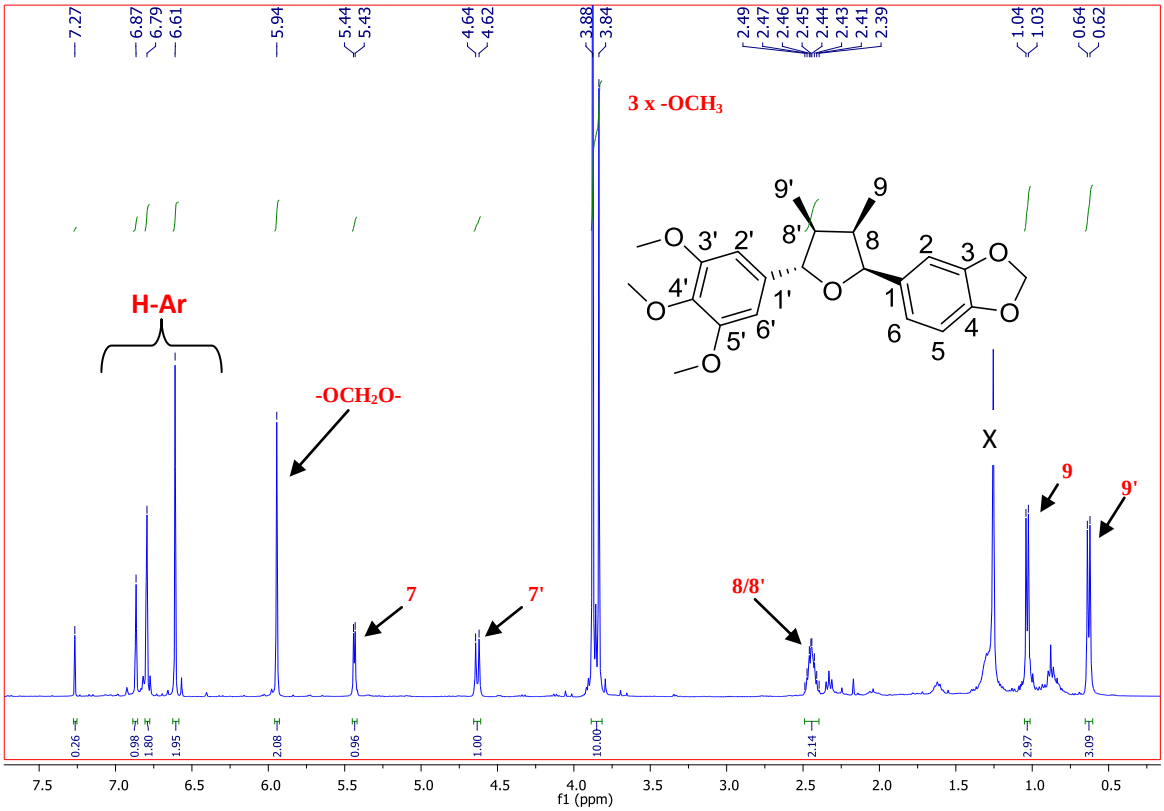


S20: ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **5** (austrobailignan-5)

*Austrobailignan-5 (**5**):* Crystalline solid, m.p. 44–45 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.70 (2H, *d*, *J* = 7.8, H-5/5'), 6.58 (2H, *d*, *J* = 1.4, H-6/6'), 6.54 (2H, *dd*, *J* = 7.9, 1.4, H-2/2'), 5.92 (4H, *s*, 2 x OCH_2O), 2.55 (2H, *dd*, *J* = 13.5, 6.1, H-7b/7'b), 2.34 (2H, *dd*, *J* = 13.6, 8.3, H-7a/7'a), 1.79 – 1.64 (2H, *m*, H-8/8'), 0.80 (6H, *d*, *J* = 6.6 Hz, H-9/9').

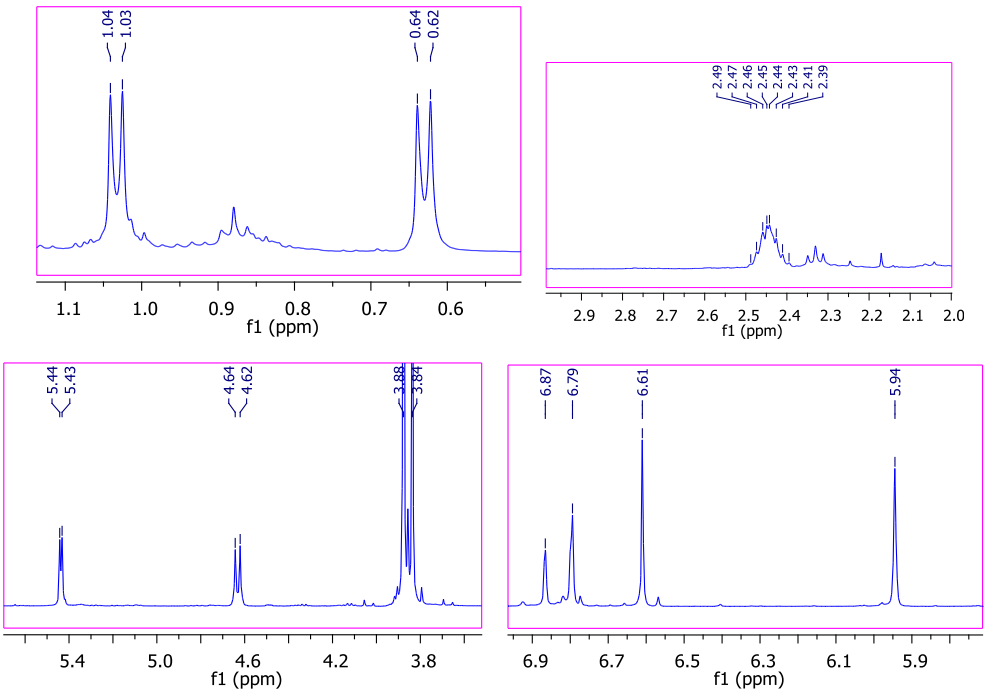


S21: ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **5** (austrobailignan-5) (From 0.82 to 0.78), (From 2.60 to 1.60), (From 6.00 to 5.85), and (From 6.80 to 6.50)

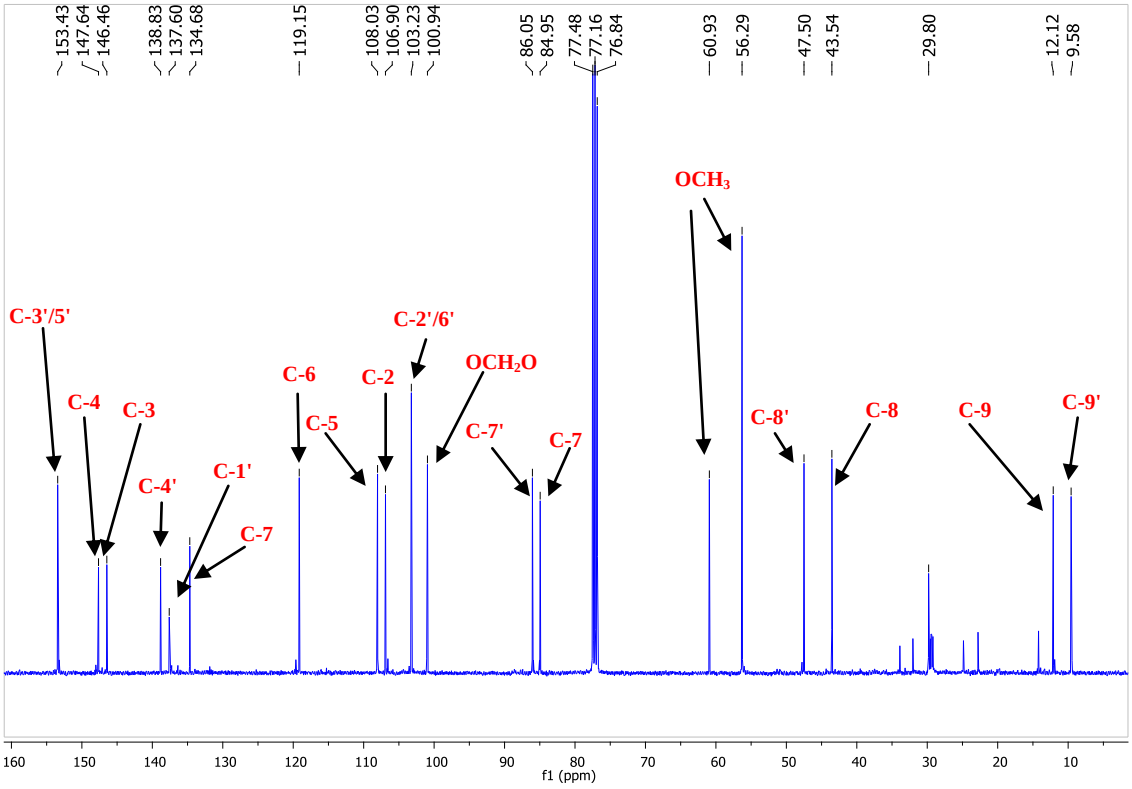


S22: ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **6** (henricine)

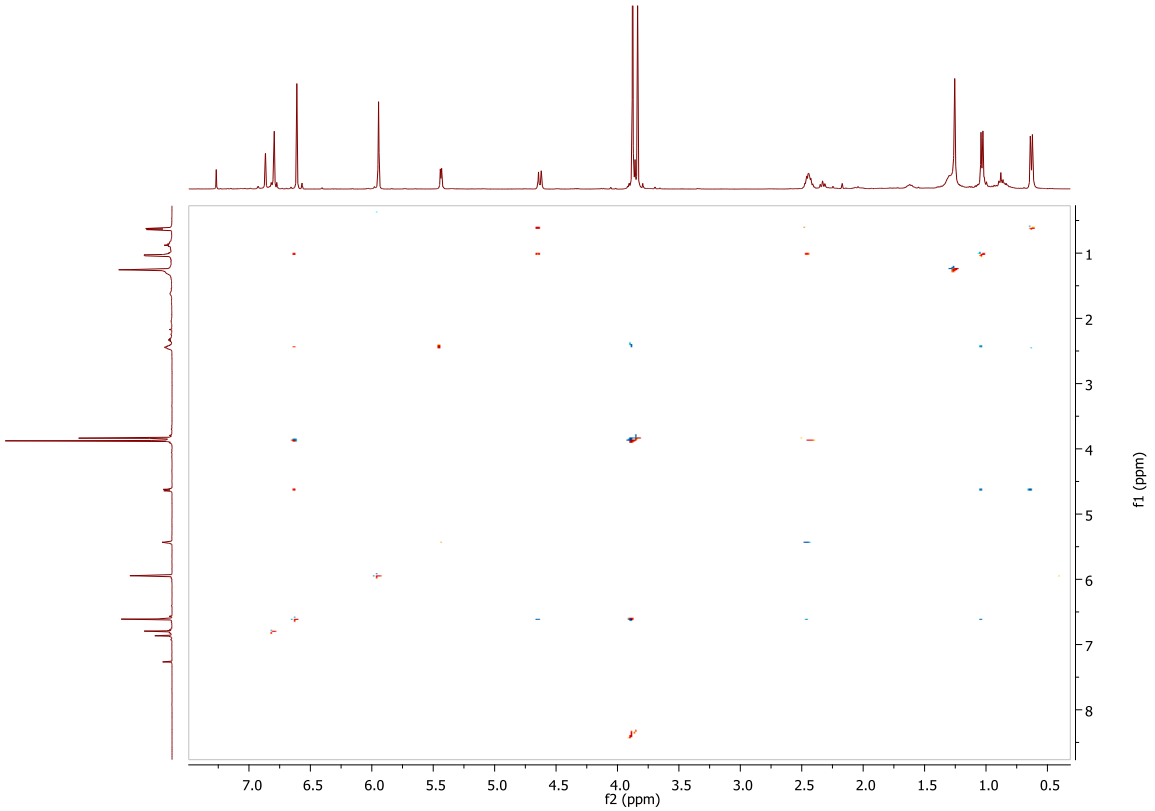
*Henricine (**6**):* Crystalline solid (colorless needles), m.p= 76°C. $[\alpha]_D^{24.3} = +15°$ (*c*=0.5, $CHCl_3$). ^{1}H NMR (400 MHz, $CDCl_3$), δ: 1.03 (3H, *d*, *J*= 6.8 Hz , H-9'), 1.05 (3H, *d*, *J*= 7.6, H-9), 2.30 (2H, *m*, H-8/8'), 4.47 (1H, *d*, J= 6.0, H-7'), 4.50 (1H, *d*, J= 6.4, H-7), 6.63 (1H, *s*, H-2'), 6.66 (1H, *s*, H-6'), 6.87 (1H, *d*, J= 8.0, H-5), 6.96 (1H, *s*, H-6), 6.99 (1H, *d*, *J*= 4.4, H-2), 5.96 (2H, *s*, 3,4-OCH_2O), 3.89-3.91 (9H, *s*, 3',4',5'-OCH_3).



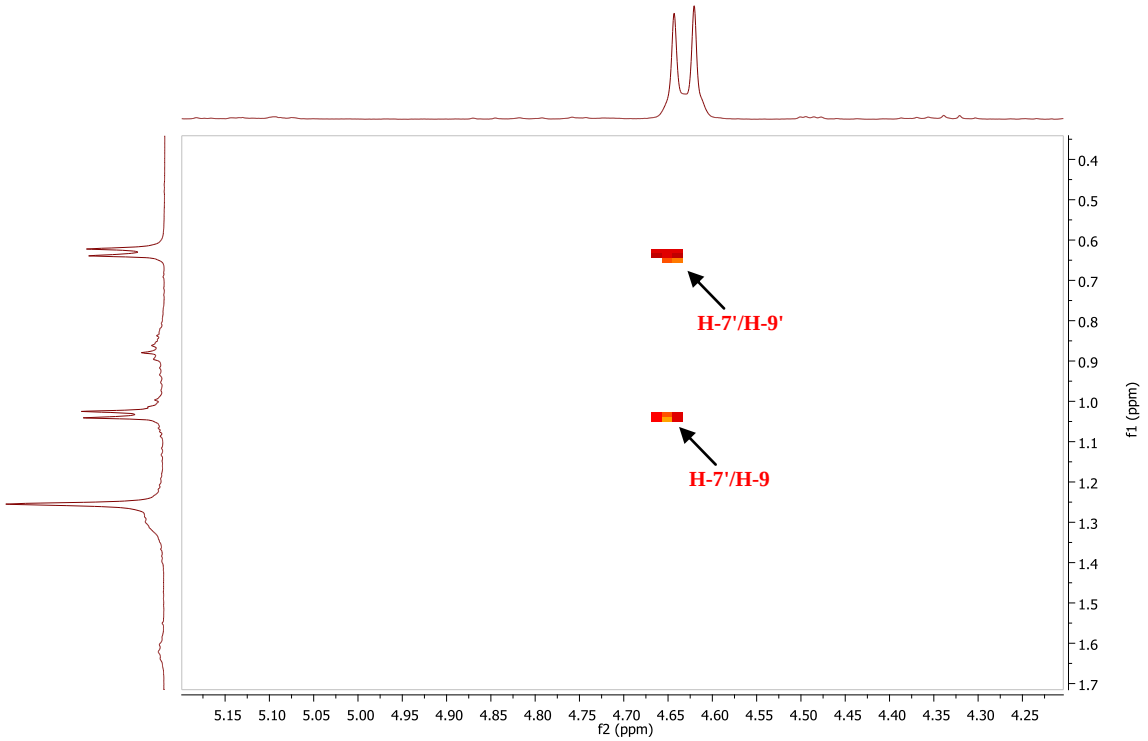
S23: ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **6** (henricine) (From 1.10 to 0.60), (From 2.0 to 2.10), (From 5.50 to 3.70), and (From 6.90 to 5.90)



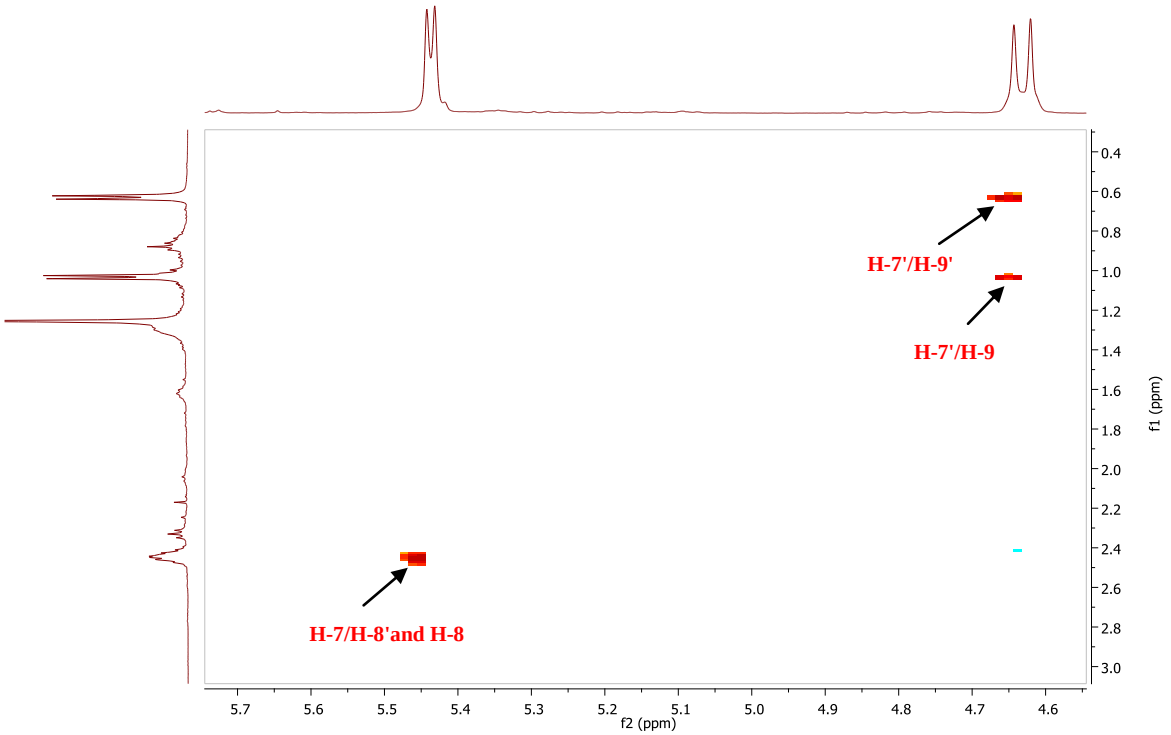
S24: ^{13}C NMR (100 MHz, $CDCl_3$) Spectrum of Compound **6** (henricine)



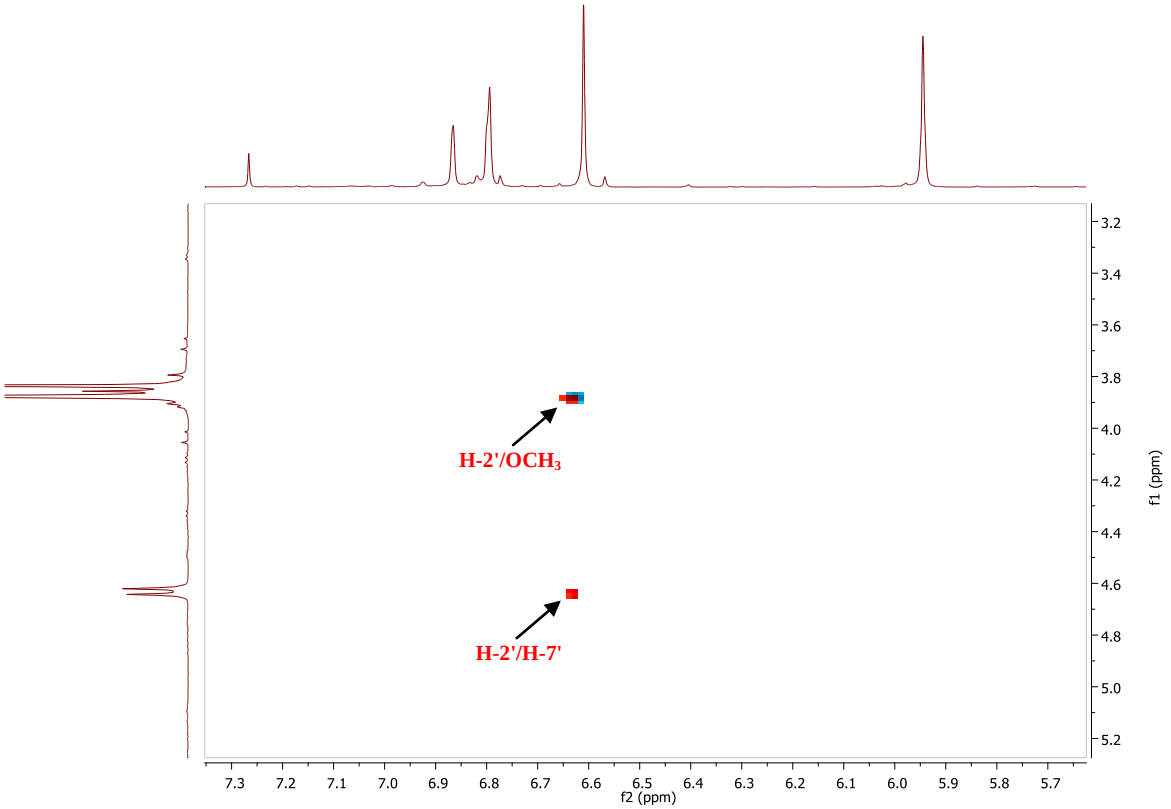
S25: NOESY Spectrum of Compound **6** (henricine)



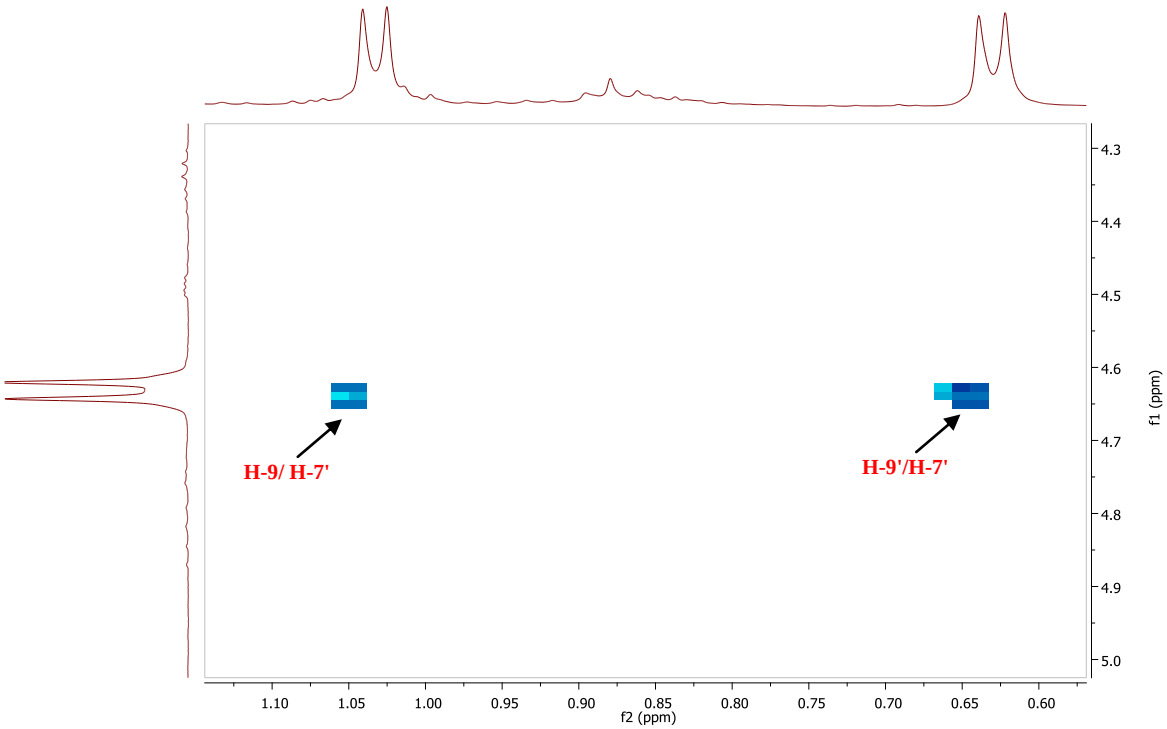
S26: NOESY Spectrum of Compound **6** (henricine) (^{1}H NMR, from 1.70 to 0.40 f1) (^{1}H NMR, From 5.25 to 4.25 f2)



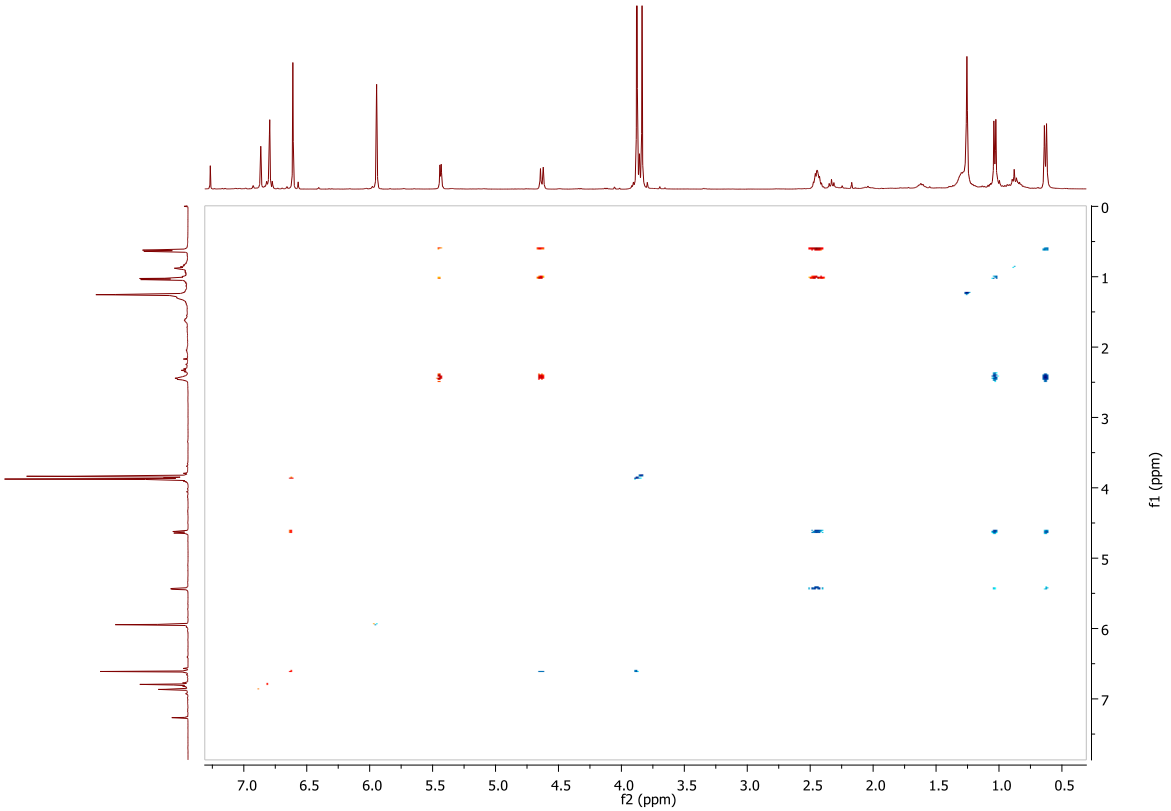
S27: NOESY Spectrum of Compound **6** (henricine) (^{1}H NMR, from 3.00 to 0.40 f1) (^{1}H NMR, From 5.7 to 4.6 f2)



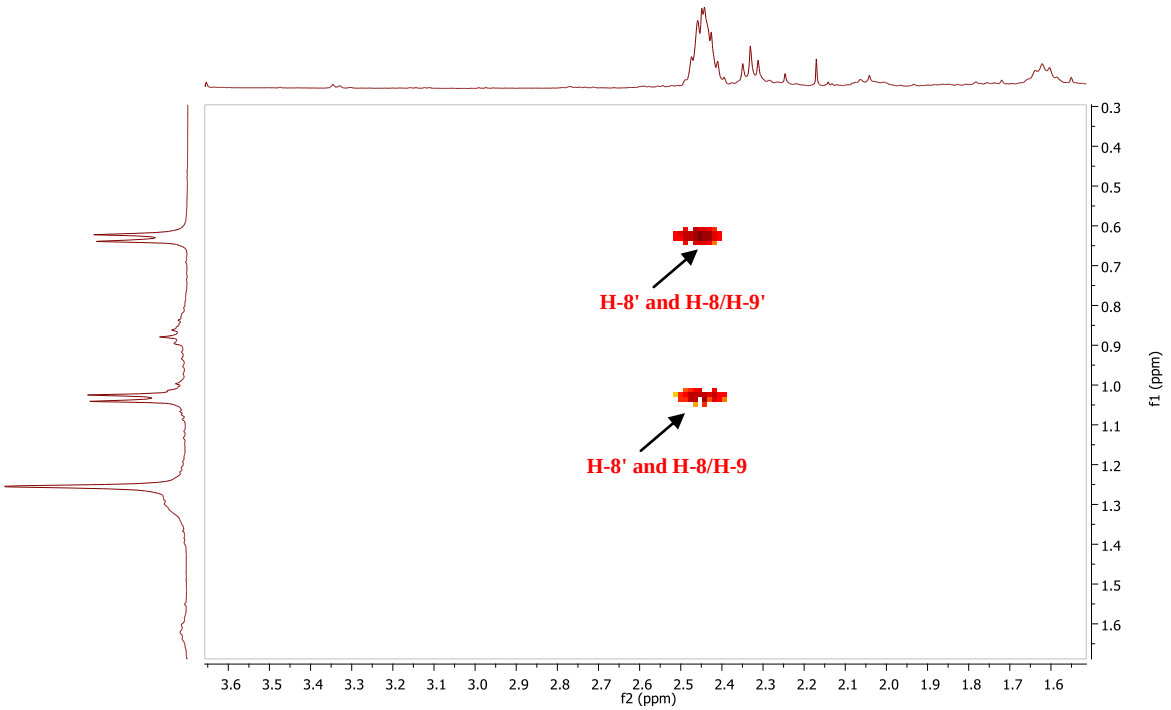
S28: NOESY Spectrum of Compound **6** (henricine) (^{1}H NMR, from 5.20 to 3.20 f1) (^{1}H NMR, From 7.30 to 5.70 f2)



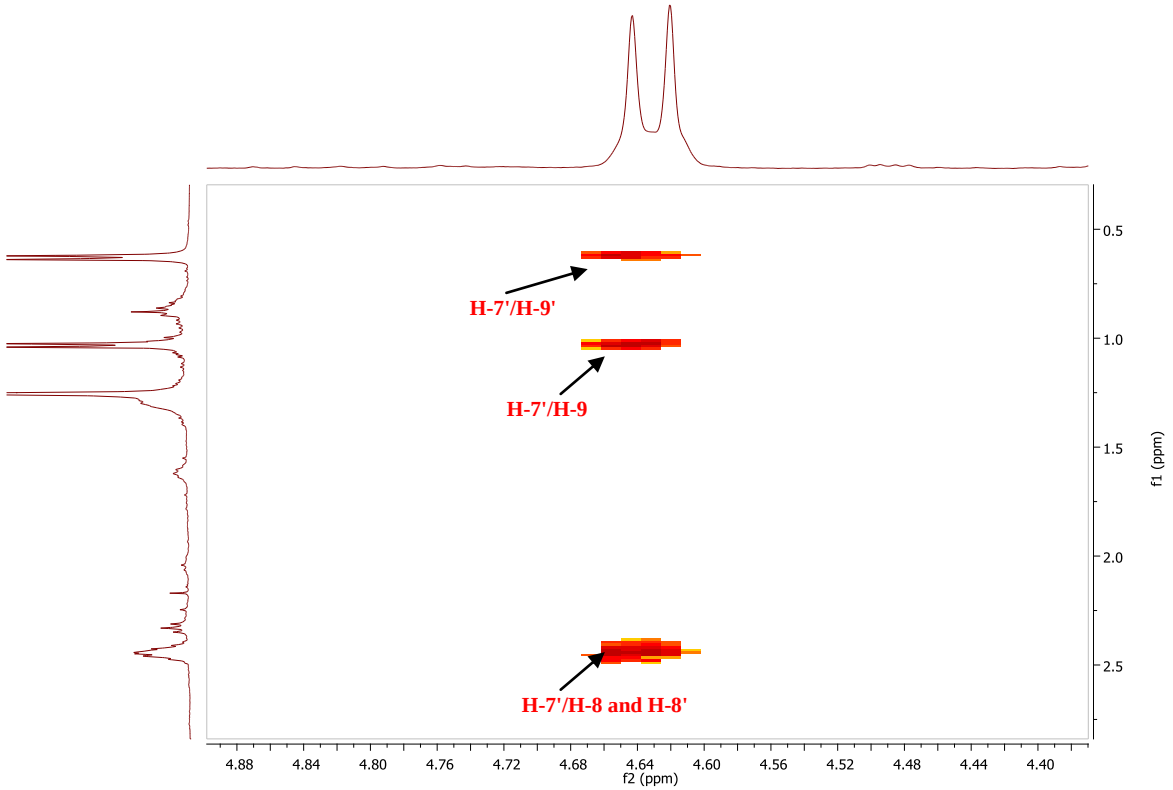
S29: NOESY Spectrum of Compound **6** (henricine) (^{1}H NMR, from 4.30 to 5.00 f1) (^{1}H NMR, From 1.10 to 0.60 f2)



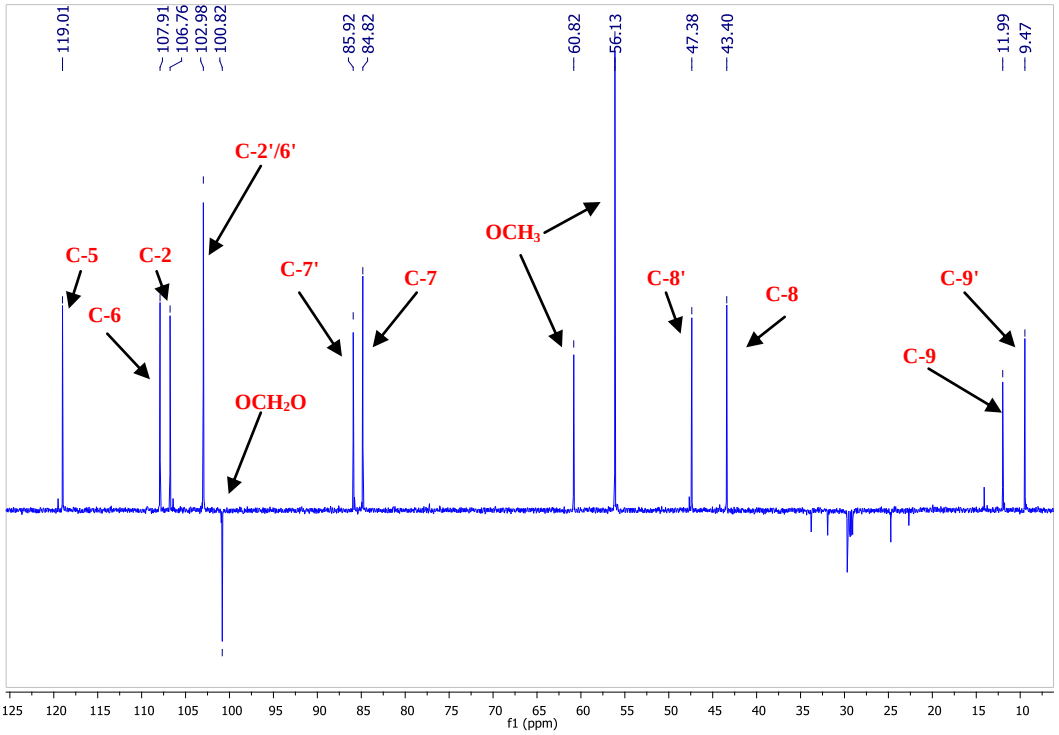
S30: COSY Spectrum of Compound **6** (henricine)



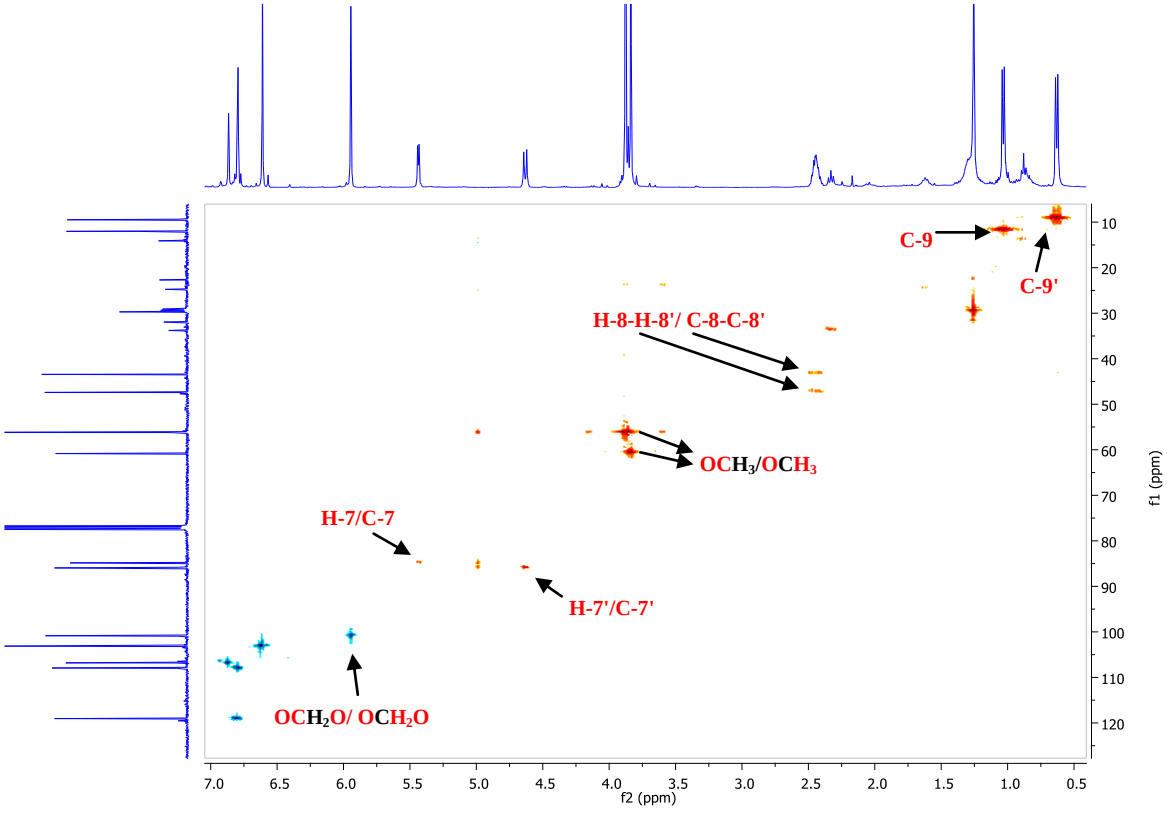
S31: COSY Spectrum of Compound **6** (henricine) (^{1}H NMR, from 1.60 to 0.30 f1) (^{1}H NMR, From 3.60 to 1.60 f2)



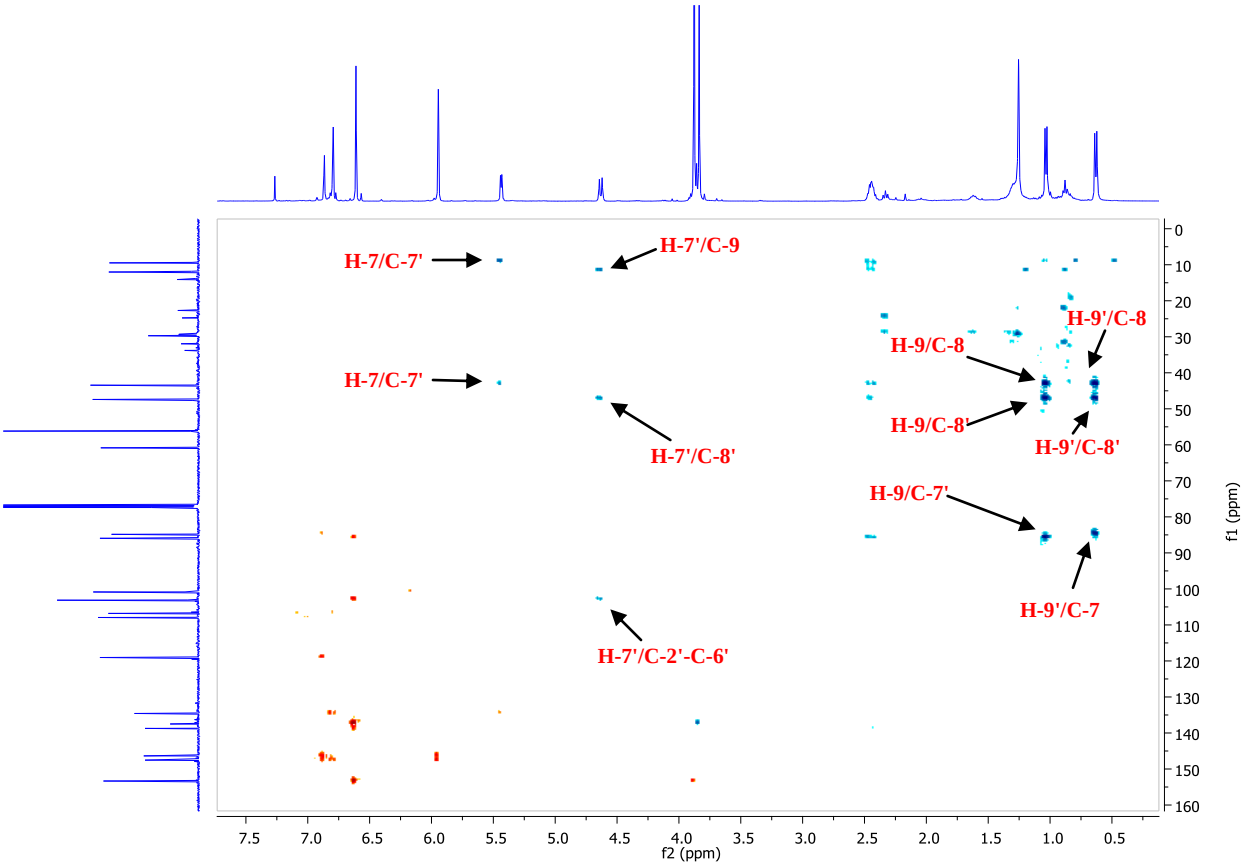
S32: COSY Spectrum of Compound **6** (henricine) (^{1}H NMR, from 2.60 to 0.50 f1) (^{1}H NMR, From 4.88 to 4.40 f2)



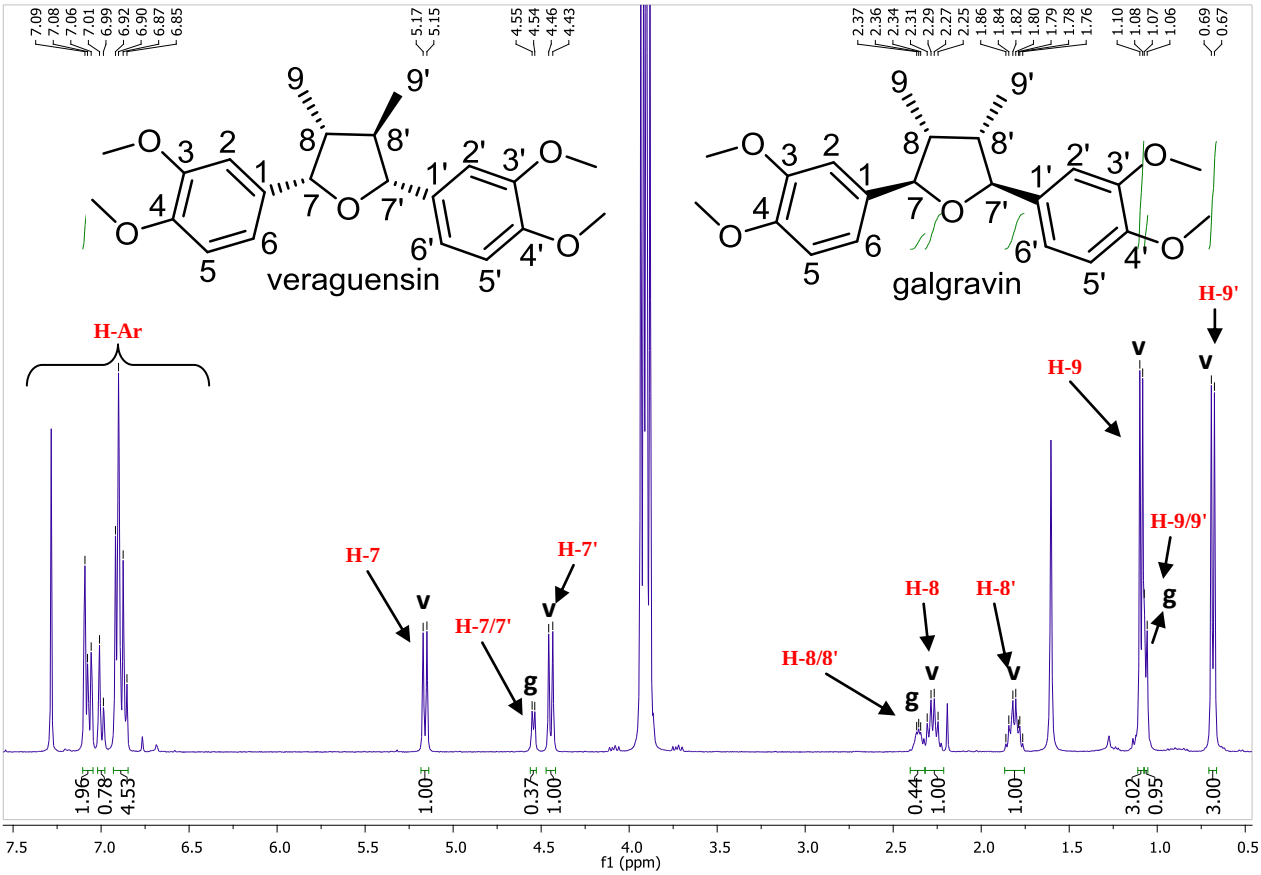
S33: DEPT-135° Spectrum of Compound **6** (henricine)



S34: HMQC Spectrum of Compound **6** (henricine)



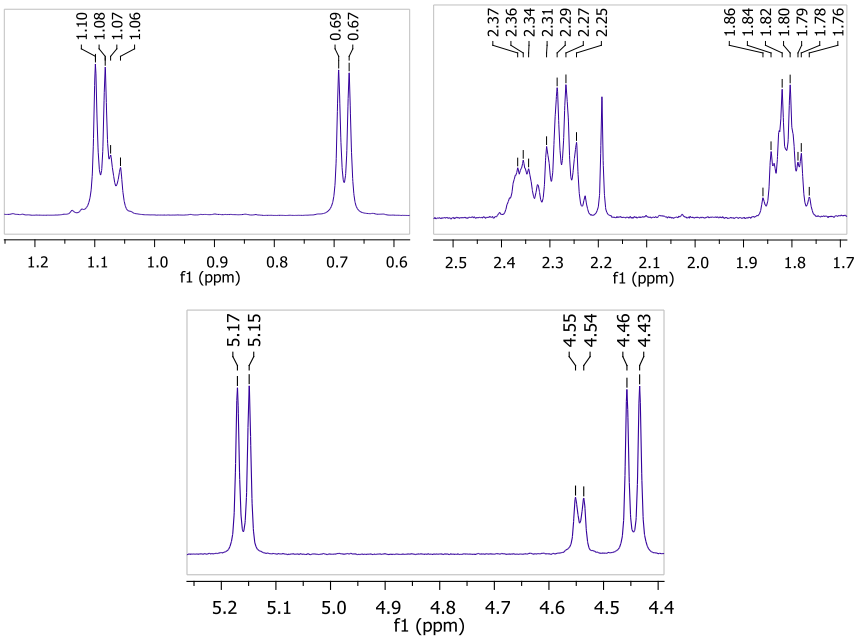
S35: HMBC Spectrum of Compound **6** (henricine)



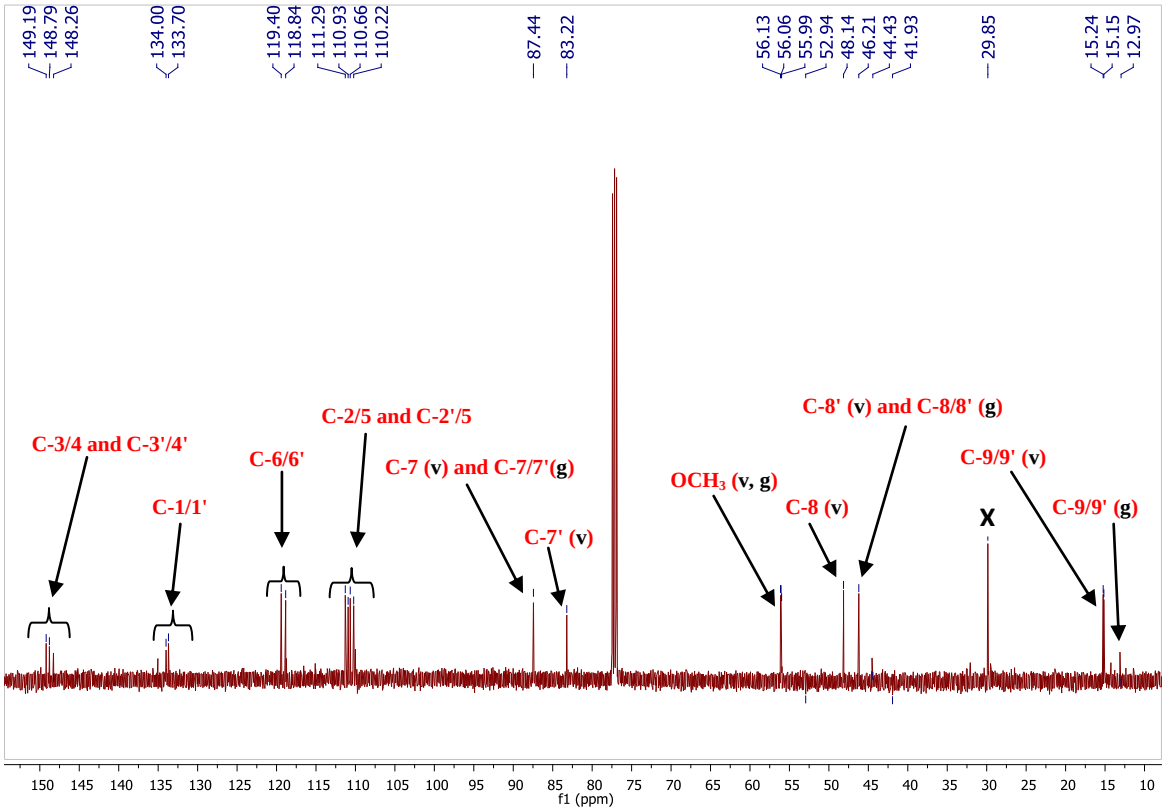
S36: ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **7**-**8** (veraguensin and galgravin)

*Veraguensin (**7**):* ^{1}H NMR (400 MHz, $CDCl_3$), δ: 0.67 (3H, *d*, *J* = 7.0, H-9'), 1.07 (3H, *d*, *J* = 6.6, H-9), 1.79 (1H, *m*, H-8), 2.25 (1H, *m*, H-8'), 3.86 (*s*, OCH_3), 3.88 (*s*, OCH_3), 3.89 (*s*, OCH_3), 3.91 (*s*, OCH_3), 4.42 (1H, *d*, *J* = 9.3, H-7), 5.14 (1H, *d*, *J* = 8.6, H-7'), 6.86-7.08 (6H, *m*, H-2/5/6, H-2'/5'/6'). [**v**=*veraguensin*].

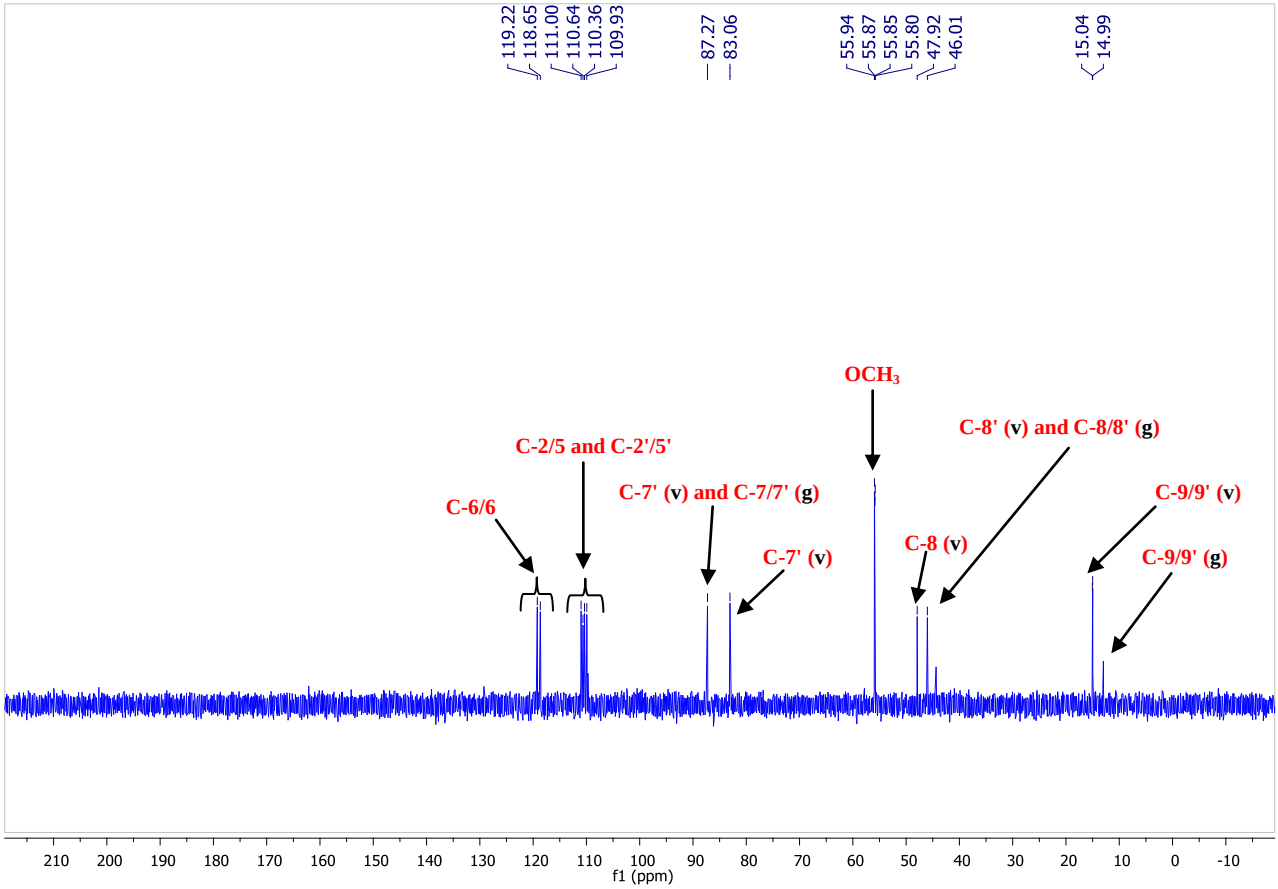
*Galgravin (**8**):* ^{1}H NMR (400 MHz, $CDCl_3$), δ: 1.05 (6H, *d*, *J* = 6.7, H-9/9'), 2.34 (2H, *m*, H-8/8'), 3.87 (*s*, OCH_3), 3.88 (*s*, OCH_3), 4.52 (2H, *d*, *J* = 6.4, H-7/7'), 6.85-6.99 (6H, *m*, H-2/5/6, H-2'/5'/6'). [**g**=*galgravin*].



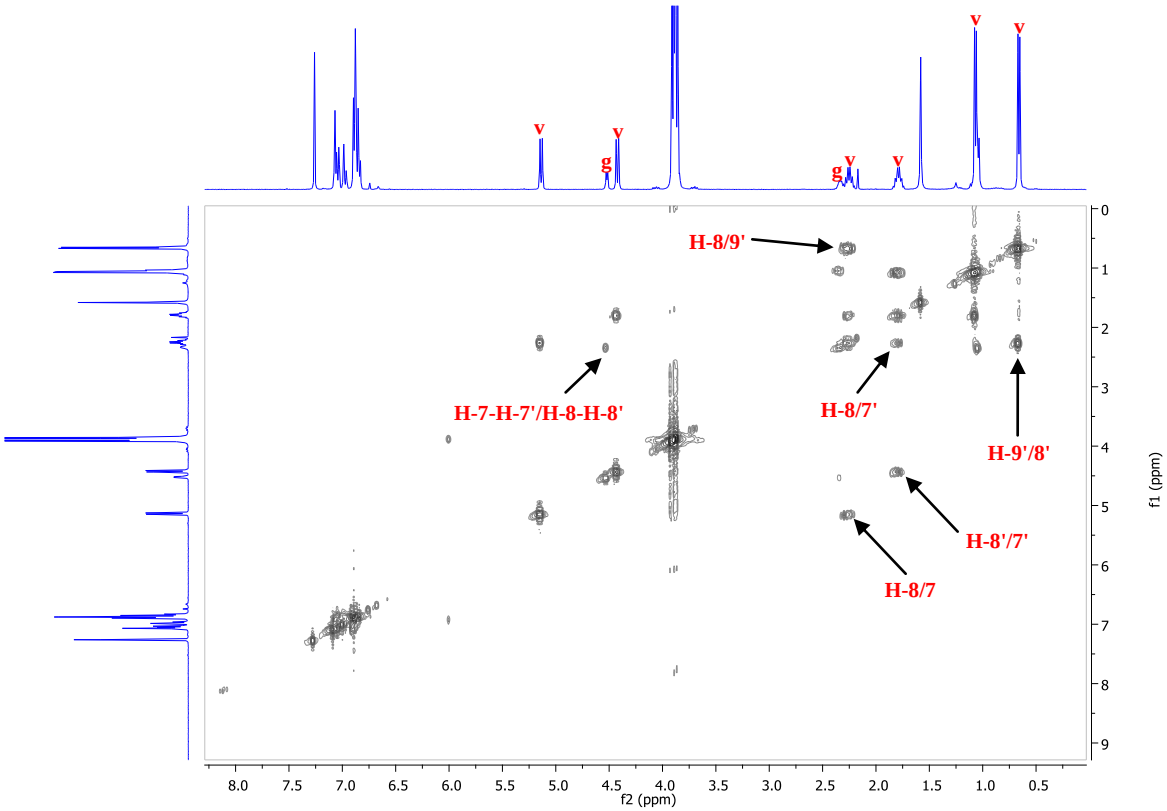
S37: ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **7-8** (veraguensin and galgravin) (From 1.20 to 0.60), (From 2.5 to 1.70), and (From 5.20 to 4.40)



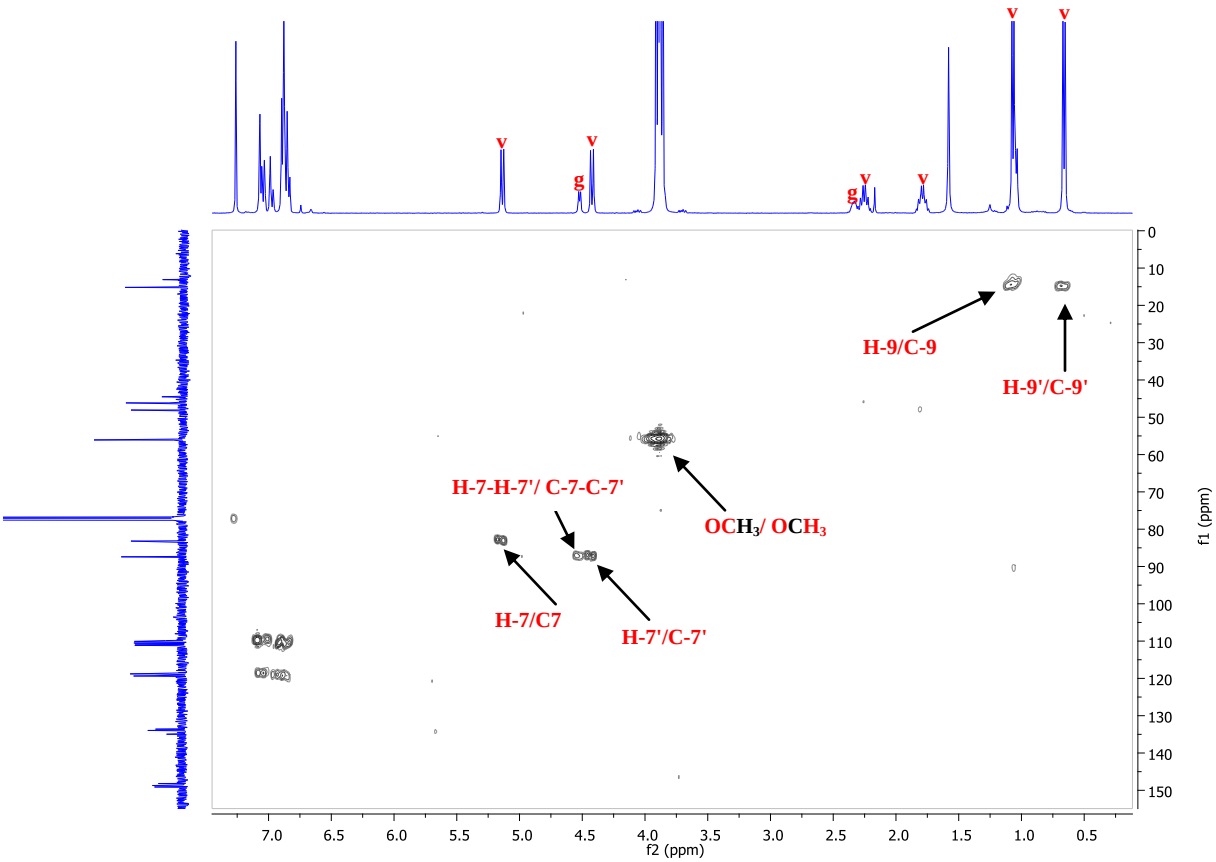
S38: ^{13}C NMR (100 MHz, $CDCl_3$) Spectrum of Compound **7-8** (veraguensin and galgravin)



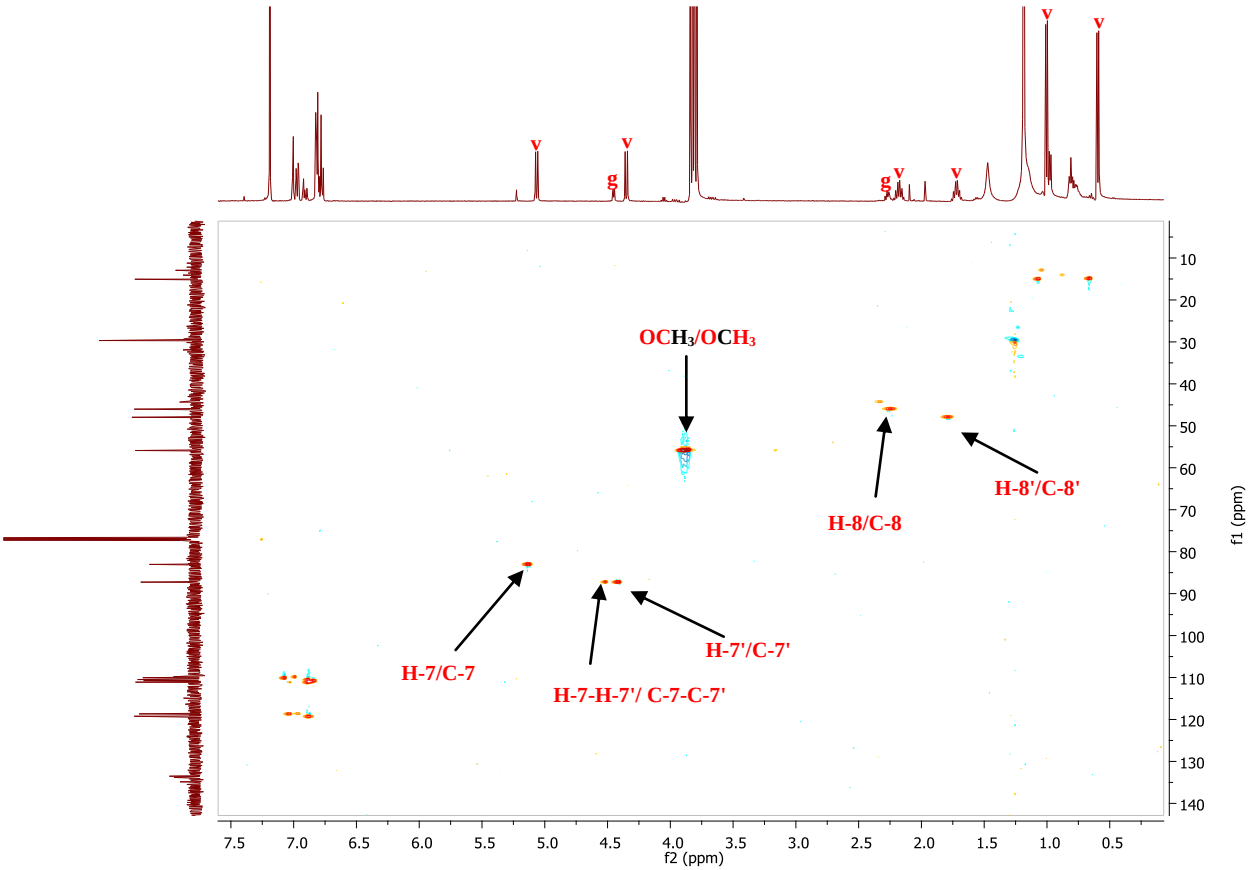
S39: DEPT-135° Spectrum of Compound **7-8** (veraguensin and galgravin)



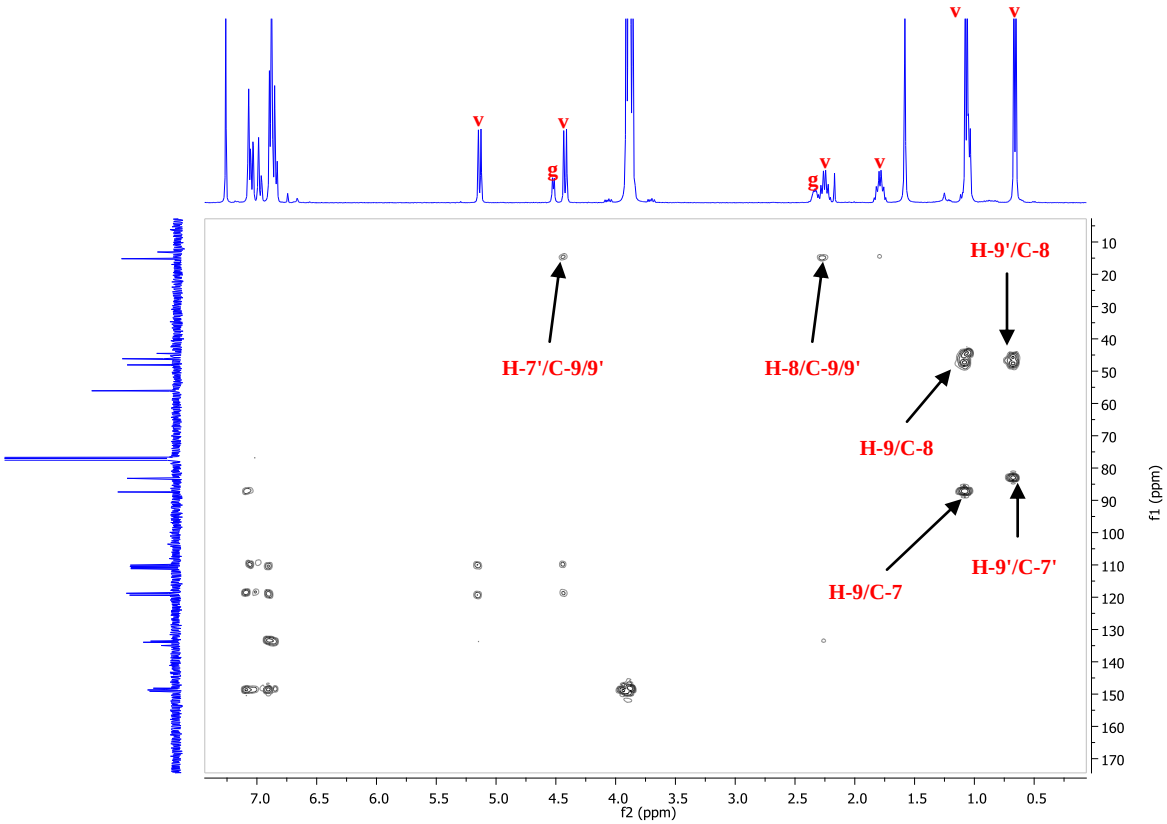
S40: COSY Spectrum of Compound **7-8** (veraguensin and galgravin)



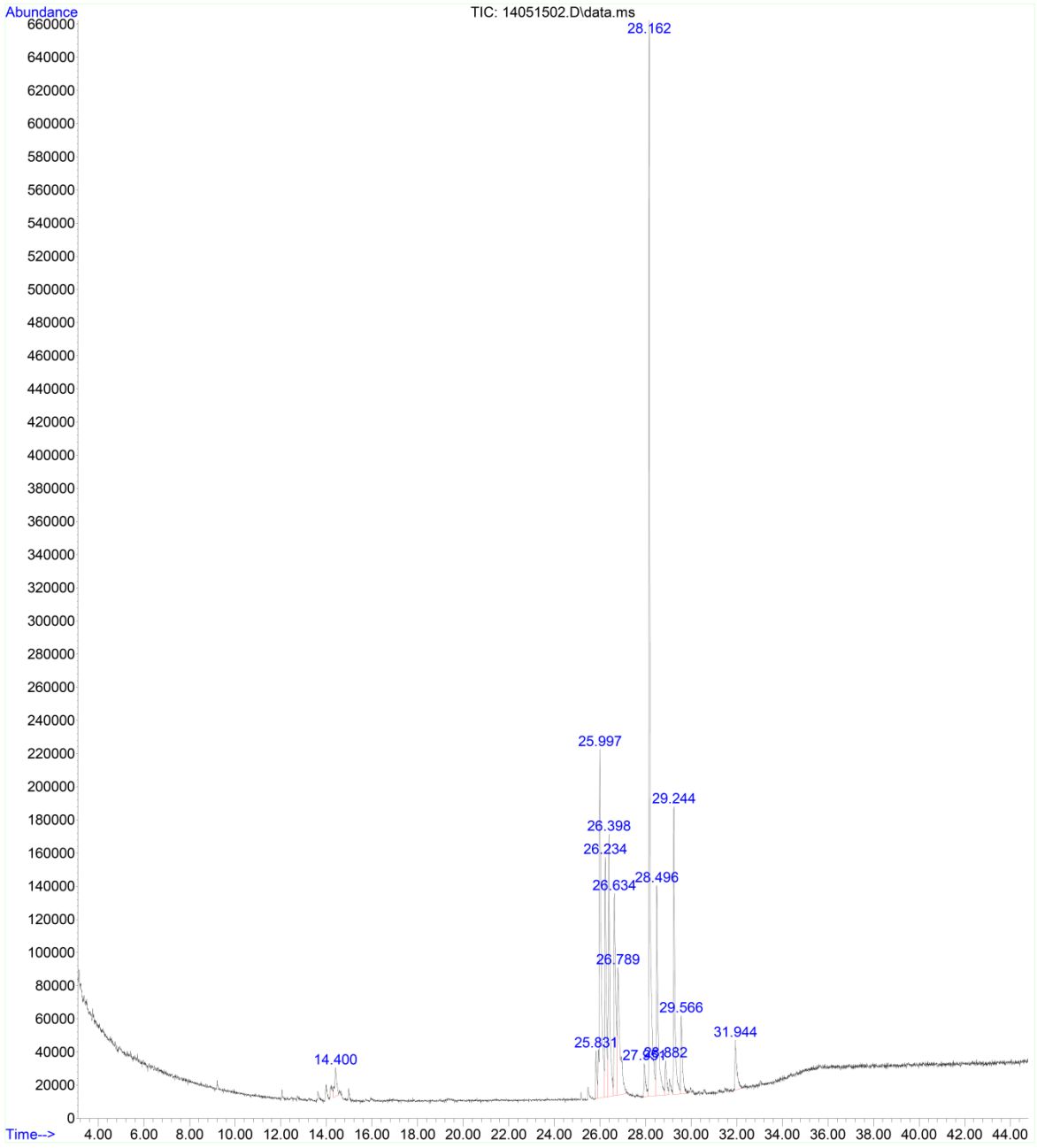
S41: HMQC Spectrum of Compound **7-8** (veraguensin and galgravin)



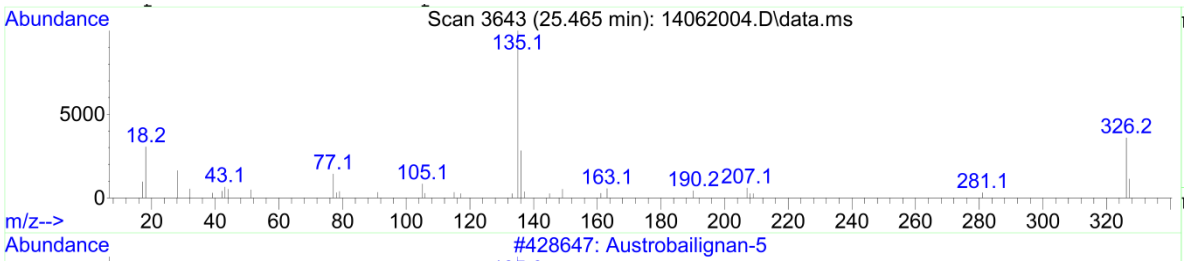
S42: HSQC Spectrum of Compound **7-8** (veraguensin and galgravin)



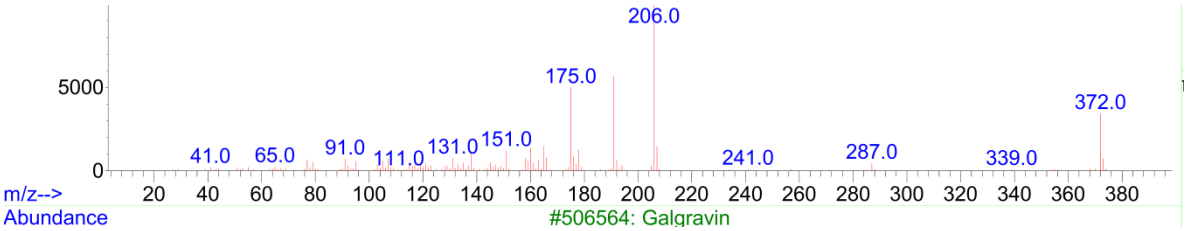
S43: HMBC Spectrum of Compound **7-8** (veraguensin and galgravin)



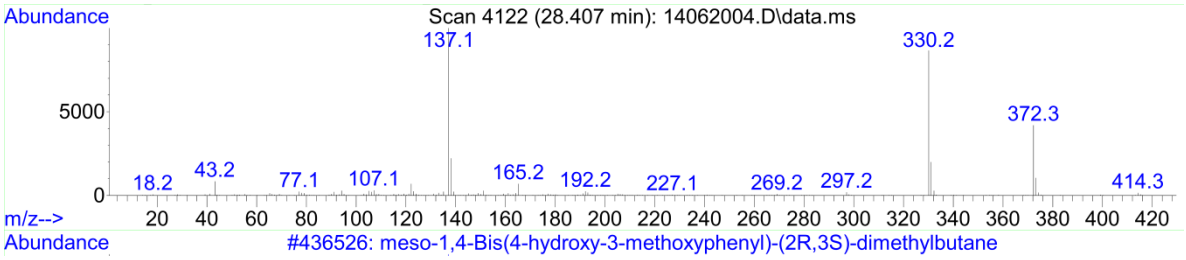
S44: Total Ion Current of ethanol extract



S45: Mass spectra of austrobailignan-5 in the ethanol extract



S46: Mass spectra of galgravin in the ethanol extract



S47: Mass spectra of *threo*-dihydroguaiaretic acid