

Supporting Information

Rec. Nat. Prod. 16:1 (2022) 66-73

Three New Phenolic Sulfates from *Acrostichum aureum* Collected from Coastal Area of Thai Binh Province, Vietnam and Their Cytotoxic Activity

Tran Thi Minh^{1*}, Nguyen Hoai Thu¹, Ho Khanh Toan¹,

Tran Thuong Quang¹, Nguyen Thi Viet Thanh¹, Tran Thu Huong¹ and

Tran Van Sung²

¹School of Chemical Engineering, Hanoi University of Science and Technology, Hanoi 112456, Vietnam

²Institute of Chemistry, Vietnam Academy of Science and Technology, Hanoi 122102, Vietnam

Table of Contents	Page
Figure S1: HR-ESI Mass Spectrum of 1 (4-(3'- <i>O</i> -sulfate-4'-hydroxyphenyl)-2-butanone)	3
Figure S2: ¹ H-NMR (500 MHz, DMSO) Spectrum of 1	4
Figure S3: ¹³ C-NMR (125 MHz, DMSO) Spectrum of 1	5
Figure S4: DEPT90 and 135 (125 MHz, DMSO) Spectrum of 1	6
Figure S5: HSQC Spectrum of 1 (4-(3'- <i>O</i> -sulfate-4'-hydroxyphenyl)-2-butanone)	7
Figure S6: ¹ H- ¹ H COSY Spectrum of 1 (4-(3'- <i>O</i> -sulfate-4'-hydroxyphenyl)-2-butanone)	8
Figure S7: HMBC Spectrum of 1 (4-(3'- <i>O</i> -sulfate-4'-hydroxyphenyl)-2-butanone)	9
Figure S8: HMBC Spectrum of 1 (From δ_C 120 ppm to δ_C 210 ppm)	10
Figure S9: HMBC Spectrum of 1 (From δ_C 110 ppm to δ_C 150 ppm)	11
Figure S10: HMBC Spectrum of 1 (From δ_C 25 ppm to δ_C 45 ppm)	12
Figure S11: FT-IR Spectrum of 1 (4-(3'- <i>O</i> -sulfate-4'-hydroxyphenyl)-2-butanone)	13
Figure S12: HR-ESI Mass Spectrum of 2 (4-(3'- <i>O</i> -sulfate-4'-hydroxyphenyl)-2(<i>R</i>)-butanol)	14
Figure S13: ¹ H-NMR (500 MHz, DMSO) Spectrum of 2	15
Figure S14: ¹³ C-NMR (125 MHz, DMSO) Spectrum of 2	16
Figure S15: DEPT90 and 135 (125 MHz, DMSO) Spectrum of 2	17
Figure S16: HSQC Spectrum of 2 (4-(3'- <i>O</i> -sulfate-4'-hydroxyphenyl)-2(<i>R</i>)-butanol)	18
Figure S17: ¹ H- ¹ H COSY Spectrum of 2 (4-(3'- <i>O</i> -sulfate-4'-hydroxyphenyl)-2(<i>R</i>)-butanol)	19
Figure S18: HMBC Spectrum of 2 (4-(3'- <i>O</i> -sulfate-4'-hydroxyphenyl)-2(<i>R</i>)-butanol)	20
Figure S19: HMBC Spectrum of 2 (From δ_C 115 ppm to δ_C 150 ppm)	21
Figure S20: HMBC Spectrum of 2 (From δ_C 20 ppm to δ_C 135 ppm)	22

* Corresponding author: E-Mail: minh.tranthi@hust.edu.vn; Phone:0084-988557877 Fax: 0084-24-38690070

Figure S21: FT-IR Spectrum of 2 (4-(3'- <i>O</i> -sulfate-4'-hydroxyphenyl)-2(<i>R</i>)-butanol)	23
Figure S22: HR-ESI Mass Spectrum of 3 (dihydrodehydrodiconiferyl alcohol-9- <i>O</i> -sulfate)	24
Figure S23: ¹ H-NMR (500 MHz, CD ₃ OD) Spectrum of 3	25
Figure S24: ¹ H-NMR (500 MHz, CD ₃ OD) Spectrum of 3 (From δ _C 1.5 ppm to δ _C 4.5 ppm)	25
Figure S25: ¹³ C-NMR (125 MHz, CD ₃ OD) Spectrum of 3	26
Figure S26: DEPT90 and 135 (125 MHz, CD ₃ OD) Spectrum of 3	27
Figure S27: HSQC Spectrum of 3 (dihydrodehydrodiconiferyl alcohol-9- <i>O</i> -sulfate)	28
Figure S28: HSQC Spectrum of 3 (From δ _C 85 ppm to δ _C 120 ppm)	29
Figure S29: HSQC Spectrum of 3 (From δ _C 30 ppm to δ _C 70 ppm)	30
Figure S30: ¹ H- ¹ H COSY Spectrum of 3 (dihydrodehydrodiconiferyl alcohol-9- <i>O</i> -sulfate)	31
Figure S31: HMBC Spectrum of 3 (dihydrodehydrodiconiferyl alcohol-9- <i>O</i> -sulfate)	32
Figure S32: HMBC Spectrum of 3 (From δ _C 30 ppm to δ _C 90 ppm)	33
Figure S33: HMBC Spectrum of 3 (From δ _C 30 ppm to δ _C 90 ppm)	34
Figure S34: HMBC Spectrum of 3 (From δ _C 90 ppm to δ _C 150 ppm)	35
Figure S35: NOESY Spectrum of 3 (dihydrodehydrodiconiferyl alcohol-9- <i>O</i> -sulfate)	36
Figure S36: FT-IR Spectrum of 3 (dihydrodehydrodiconiferyl alcohol-9- <i>O</i> -sulfate)	37
Figure S37: CD Spectrum (CH ₃ OH) of 3 (dihydrodehydrodiconiferyl alcohol-9- <i>O</i> -sulfate)	38
Figure S38: ¹ H-NMR (500 MHz, DMSO) Spectrum of (+)-pinoresinol-4- <i>O</i> -sulfate (4)	39
Figure S39: ¹³ C-NMR (125 MHz, DMSO) Spectrum of (+)-pinoresinol-4- <i>O</i> -sulfate (4)	40
Figure S40: ¹ H-NMR (500 MHz, CD ₃ OD) Spectrum of (+)-pinoresinol-4- <i>O</i> -glucoside (5)	41
Figure S41: ¹³ C-NMR (125 MHz, CD ₃ OD) Spectrum of (+)-pinoresinol-4- <i>O</i> -glucoside (5)	42
Figure S42: ¹ H-NMR (500 MHz, CD ₃ OD) Spectrum of dihydrodehydrodiconiferyl alcohol-4- <i>O</i> -glucoside (6)	43
Figure S43: ¹³ C-NMR (125 MHz, CD ₃ OD) Spectrum of dihydrodehydrodiconiferyl alcohol-4- <i>O</i> -glucoside (6)	44
Figure S44: ¹ H-NMR (500 MHz, CD ₃ OD) Spectrum of (+)-isolarisiresinol-9- <i>O</i> -sulfate (7)	45
Figure S45: ¹³ C-NMR (125 MHz, CD ₃ OD) Spectrum of (+)-isolarisiresinol-9- <i>O</i> -sulfate (7)	46
Figure S46: ¹ H-NMR (500 MHz, CD ₃ OD) Spectrum of isotachioside (8)	47
Figure S47: ¹³ C-NMR (125 MHz, CD ₃ OD) Spectrum of isotachioside (8)	48
Figure S48: SciFinder Search Results of 1	49
Figure S49: SciFinder Search Results of 2	50
Figure S50: SciFinder Search Results of 3	51
Table S1: ¹³ C NMR (125 MHz) data for compounds 1 , 1a and 2 in DMSO	52
Table S2: ¹³ C NMR (125 MHz) data for compounds 3-7	53
Table S3 : ¹ H NMR (500 MHz) and ¹³ C NMR (125 MHz) data for compounds 3 and 3a in CD ₃ OD	54

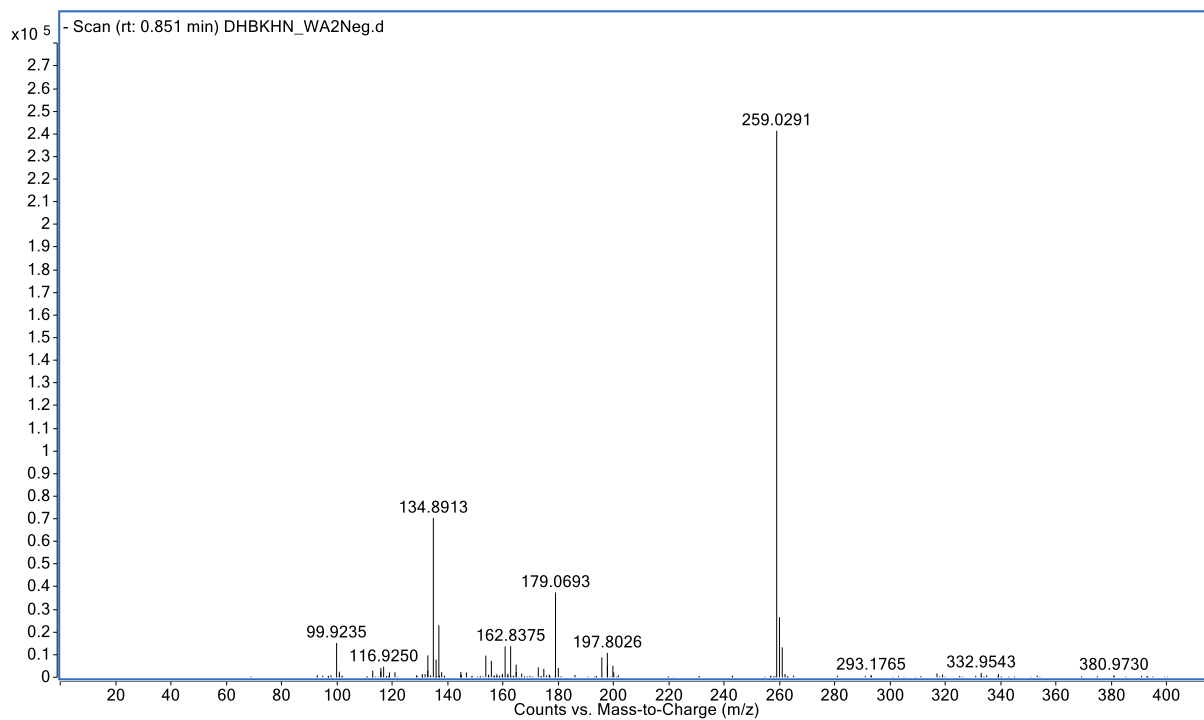


Figure S1: HR-ESI Mass Spectrum of **1** (4-(3'-O-sulfate-4'-hydroxyphenyl)-2-butanone)

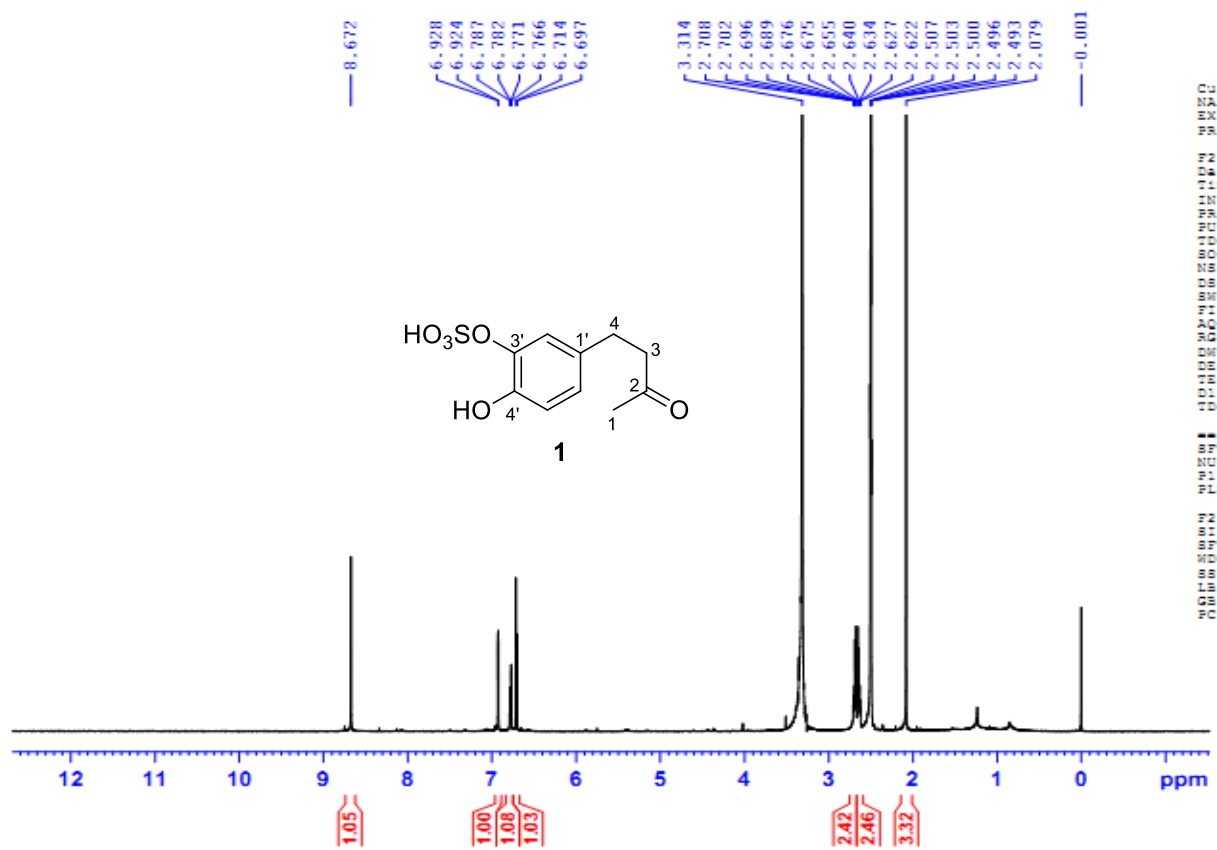


Figure S2: $^1\text{H-NMR}$ (500 MHz, DMSO) Spectrum of **1**

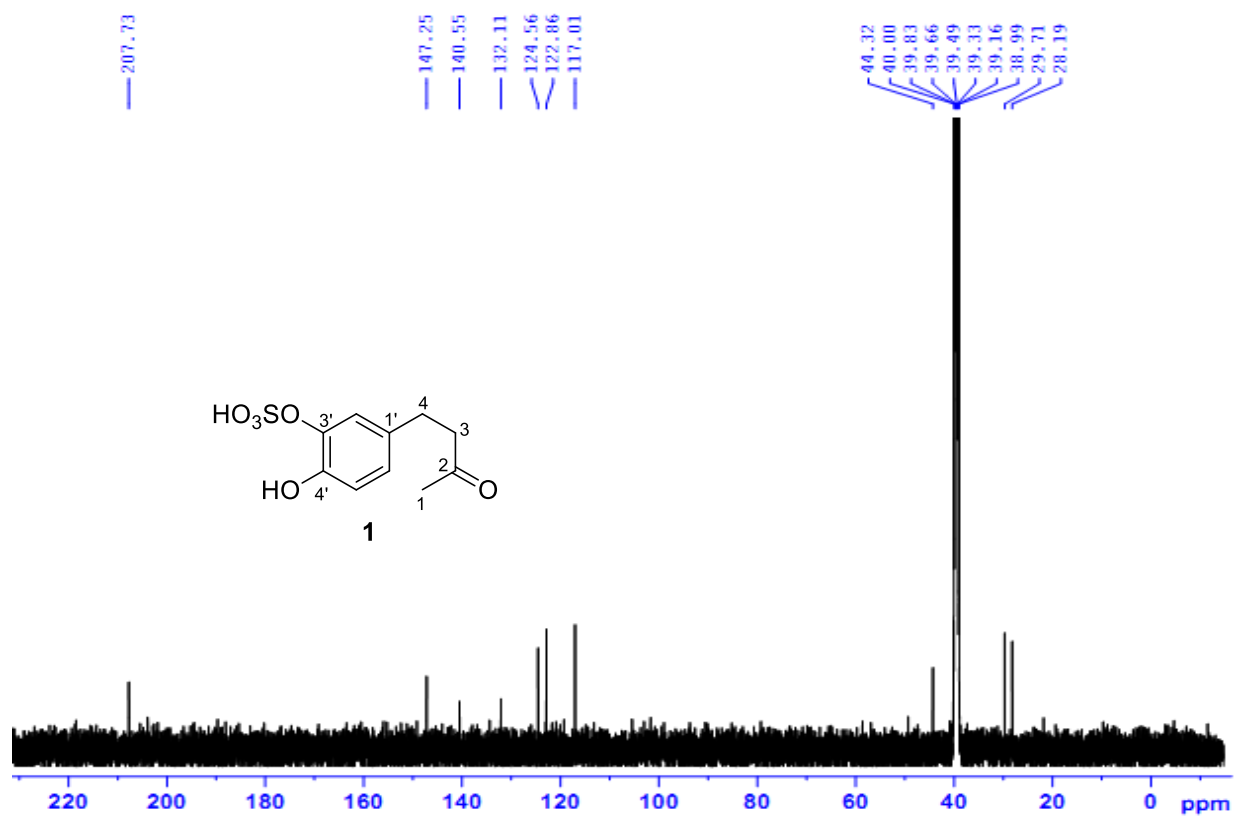
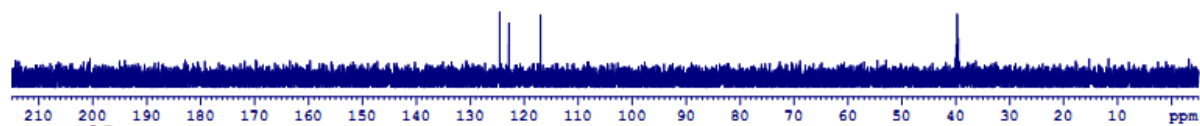


Figure S3: ¹³C-NMR (125 MHz, DMSO) Spectrum of **1**

DEPT90

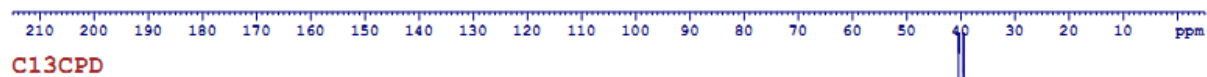


DEPT135



CH&CH3

CH2



C13CPD

Figure S4: DEPT90 and 135 (125 MHz, DMSO) Spectrum of **1**

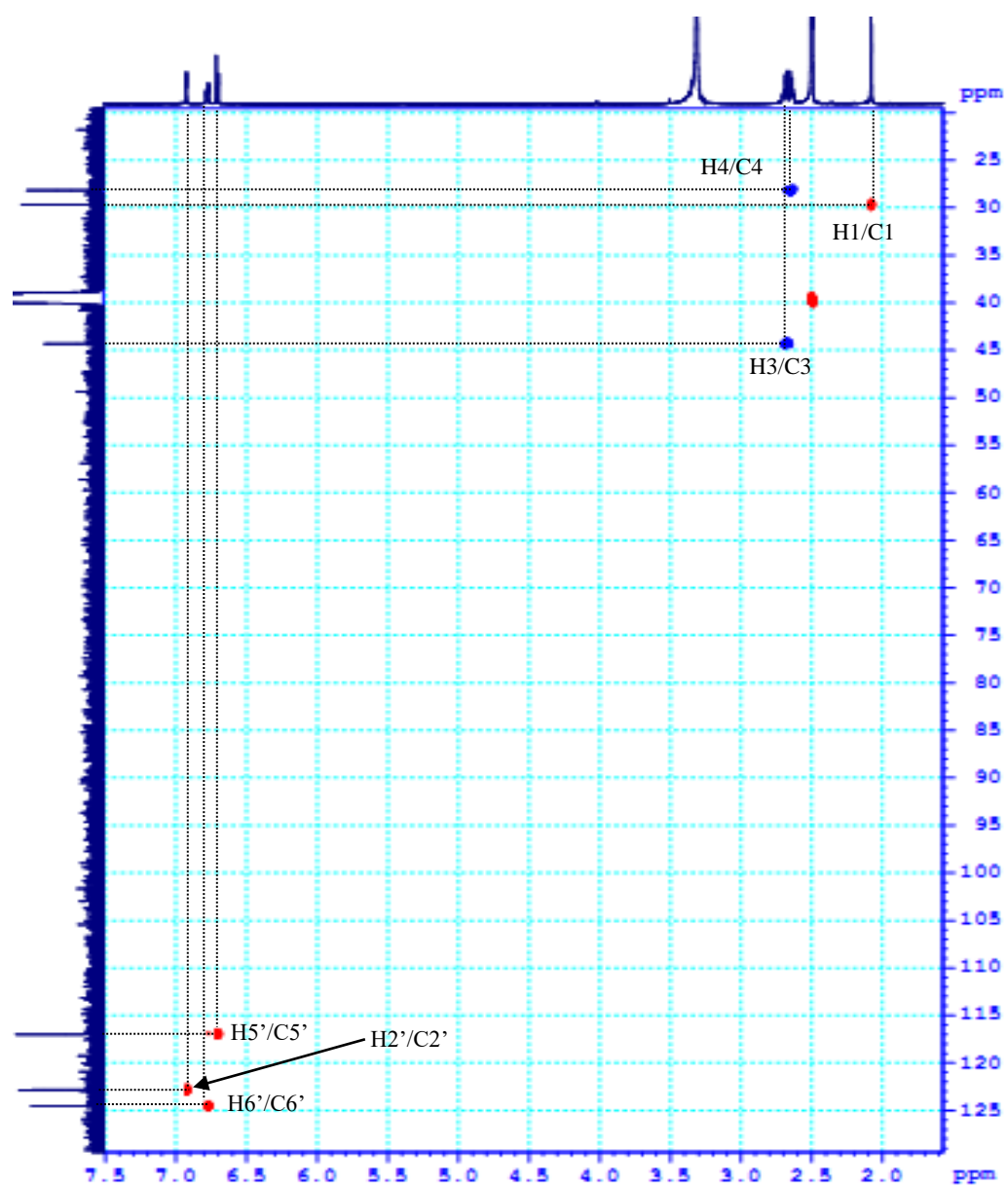


Figure S5: HSQC Spectrum of **1** (4-(3'-*O*-sulfate-4'-hydroxyphenyl)-2-butanone)

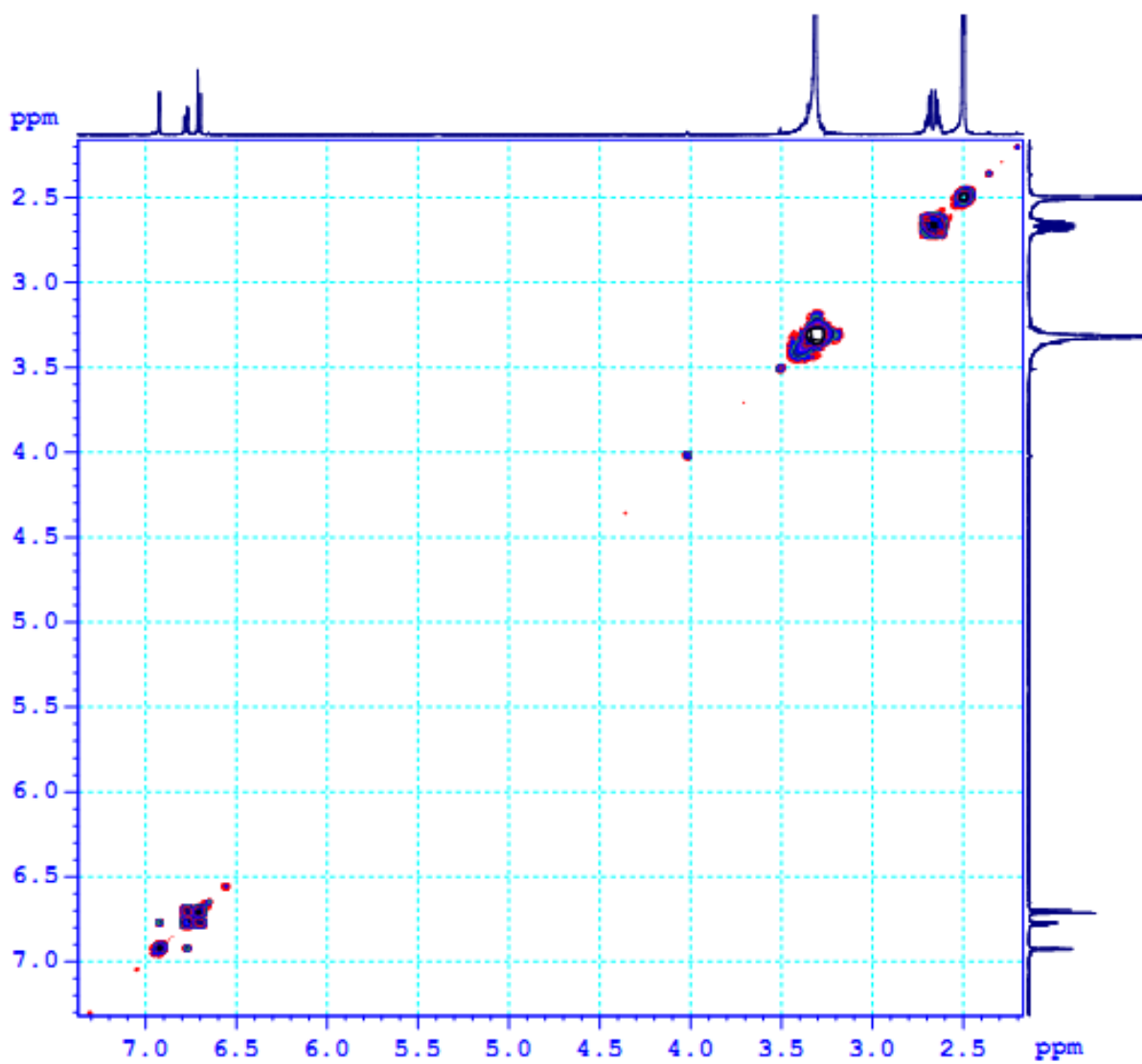


Figure S6: ^1H - ^1H COSY Spectrum of **1** (4-(3'-*O*-sulfate-4'-hydroxyphenyl)-2-butanone)

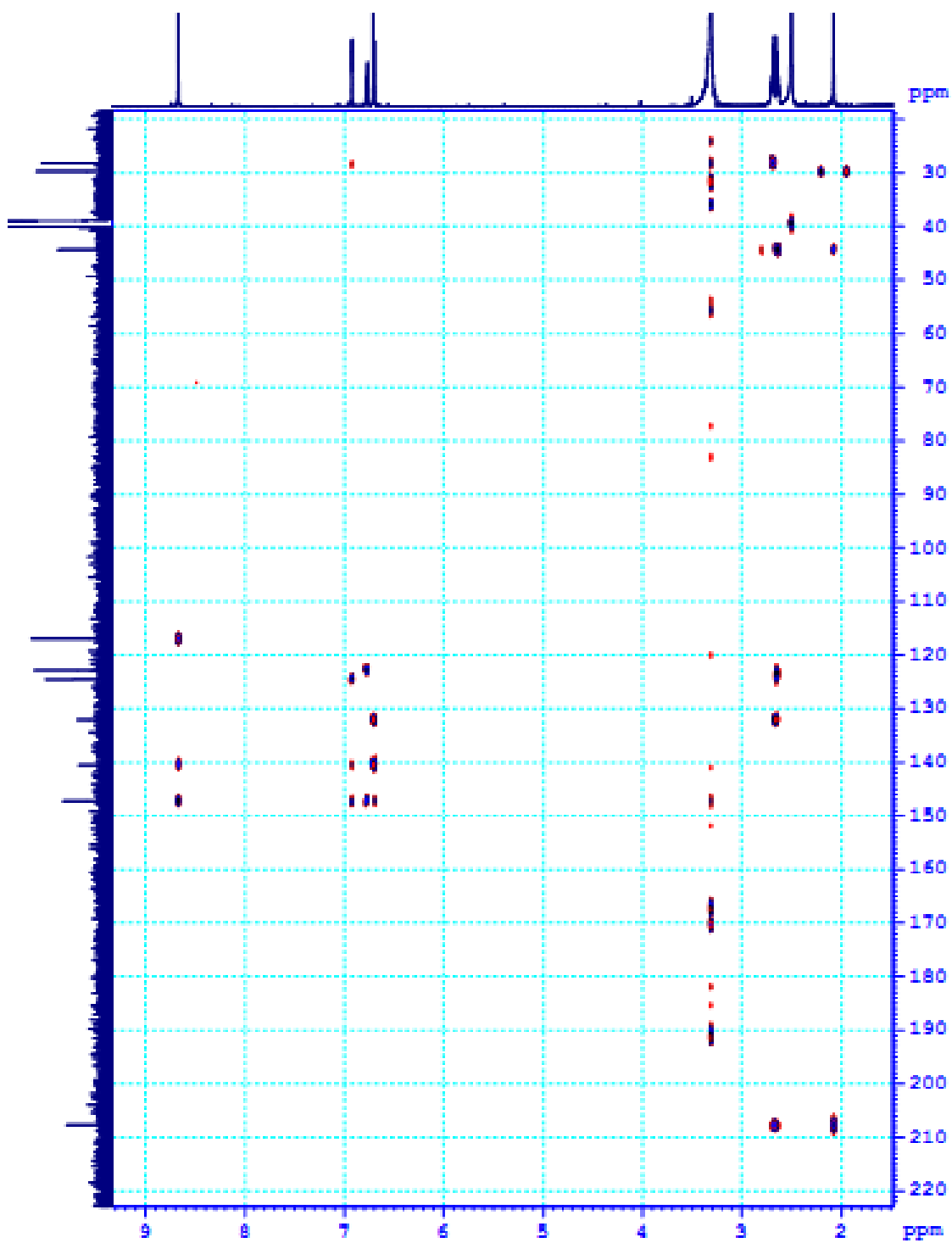


Figure S7: HMBC Spectrum of HMBC of **1** (4-(3'-*O*-sulfate-4'-hydroxyphenyl)-2-butanone)

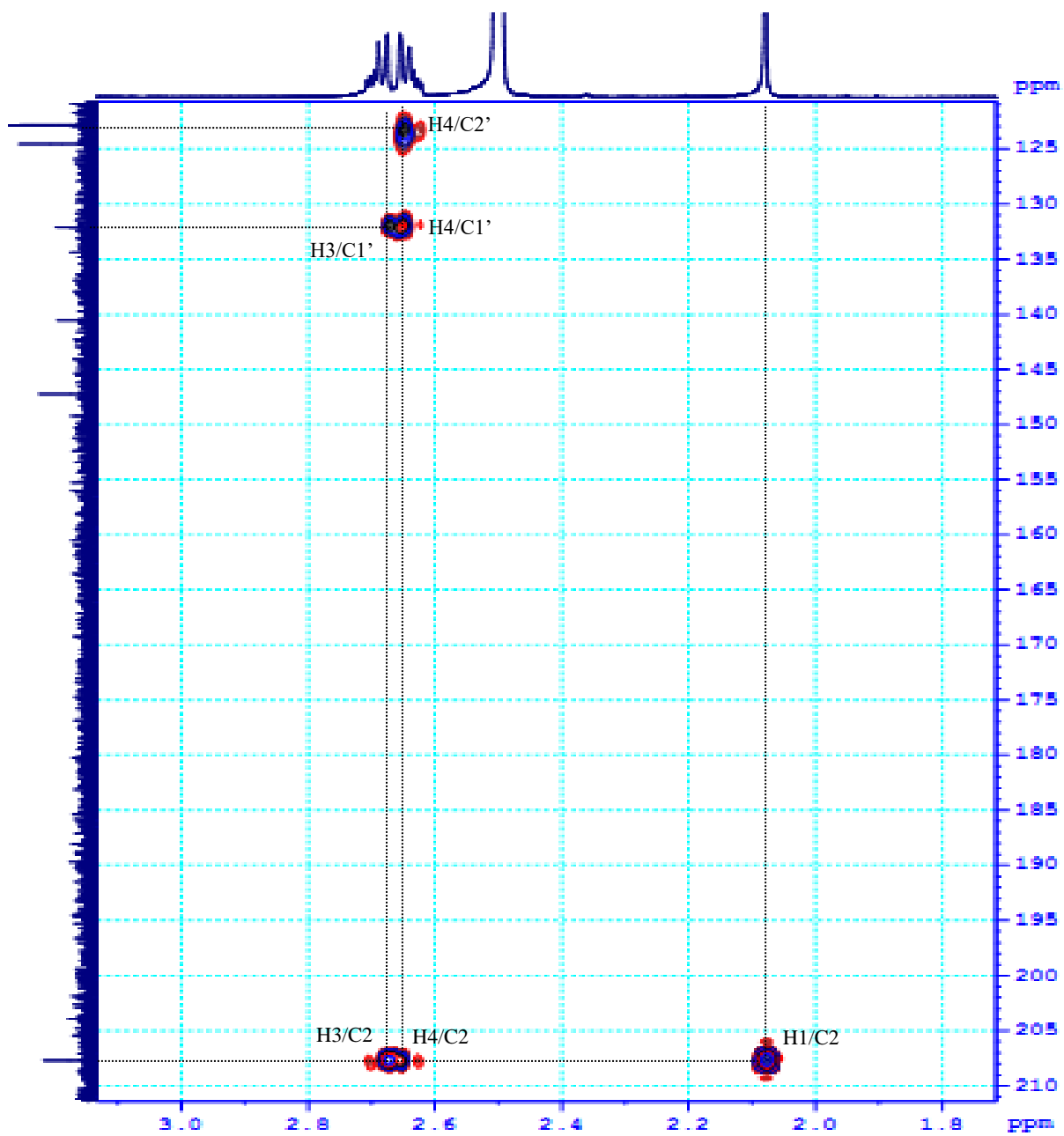


Figure S8: HMBC Spectrum of 1 (From δ_C 120 ppm to δ_C 210 ppm)

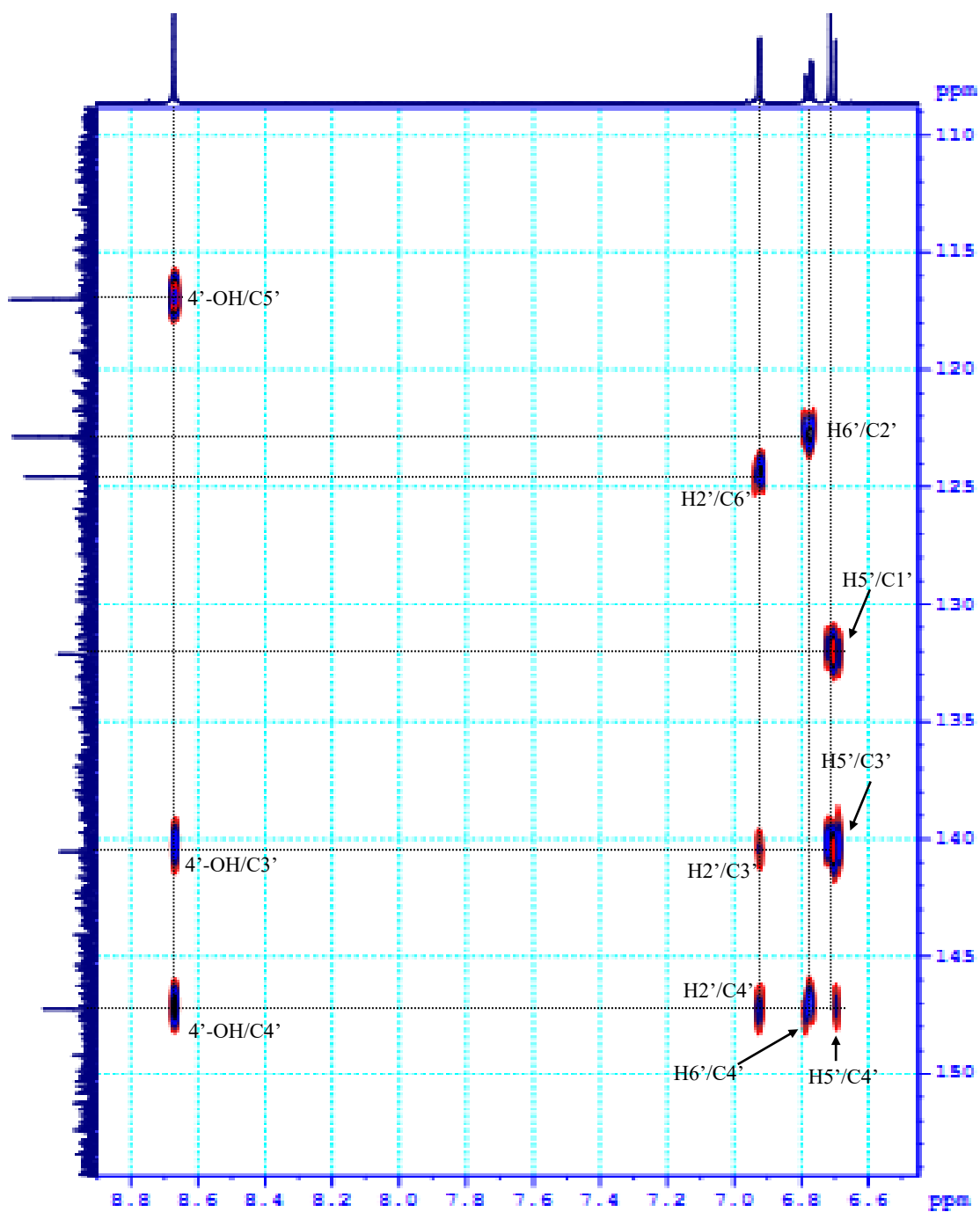


Figure S9: HMBC Spectrum of 1 (From δ_c 110 ppm to δ_c 150 ppm)

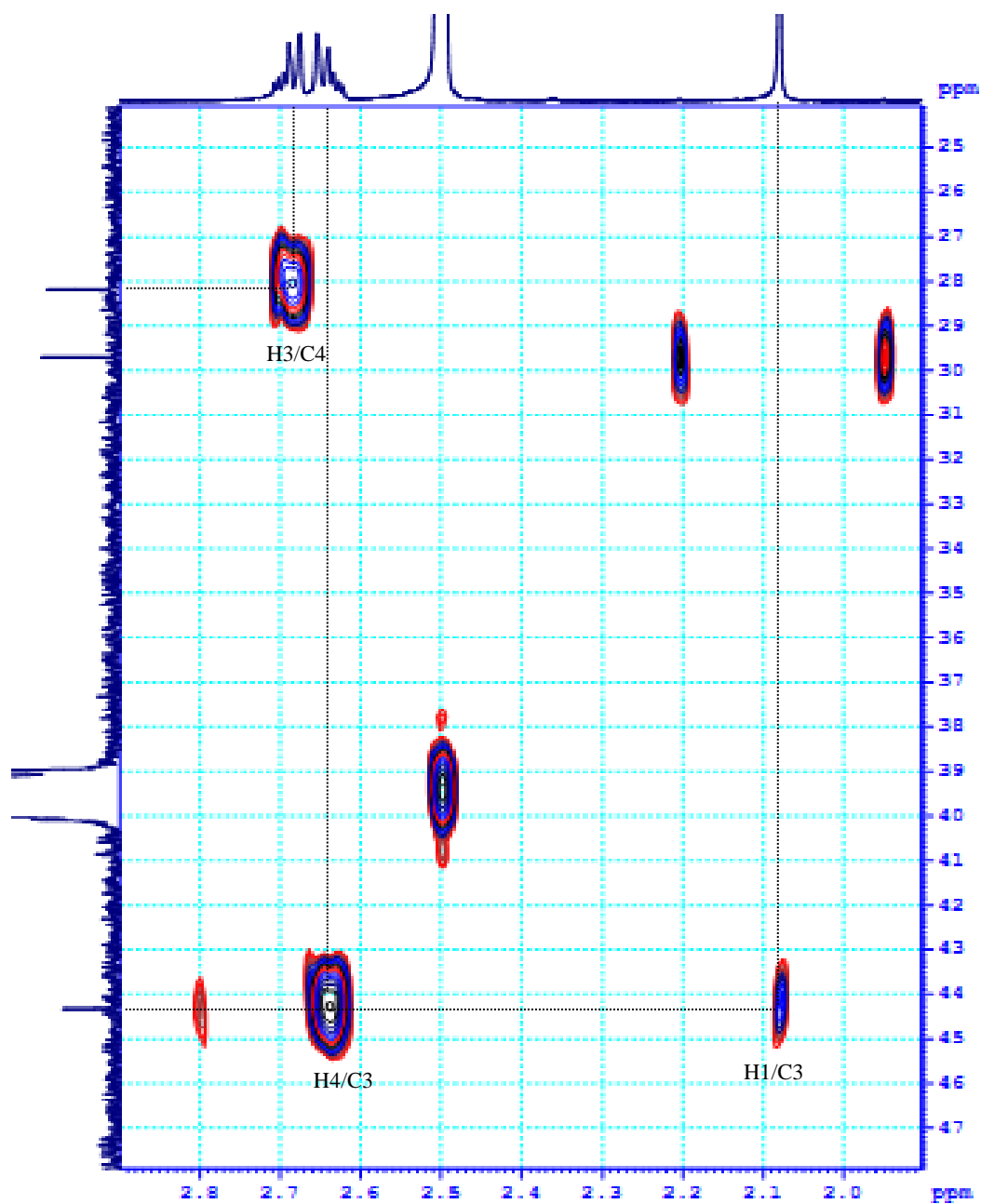


Figure S10: HMBC Spectrum of **1** (From δ_c 25 ppm to δ_c 45 ppm)

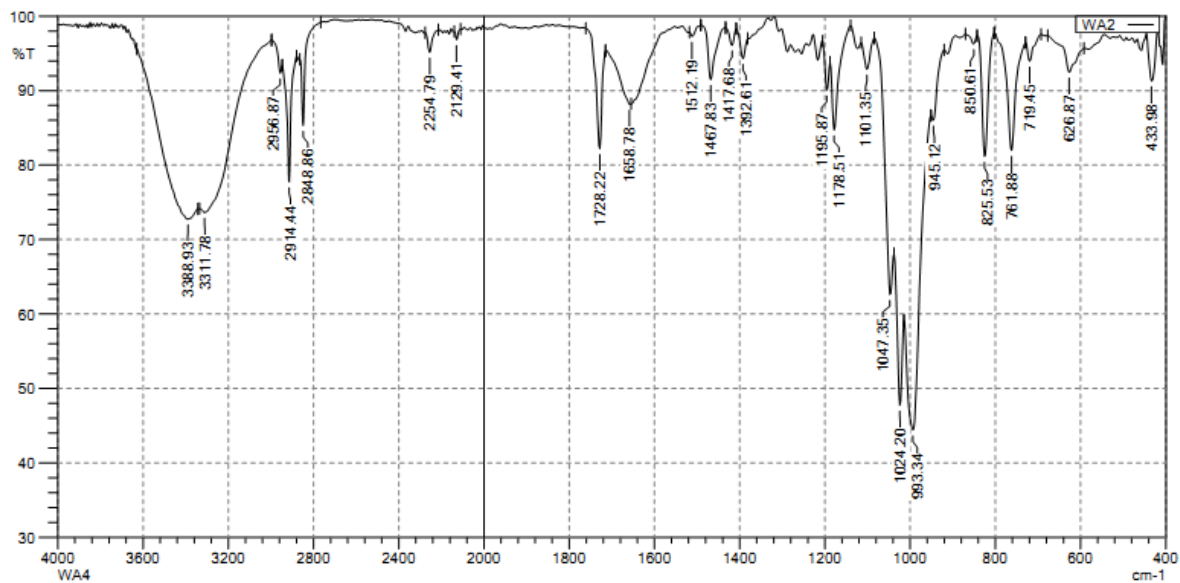


Figure S11: FT-IR Spectrum of **1** (4-(3'-*O*-sulfate-4'-hydroxyphenyl)-2-butanone)

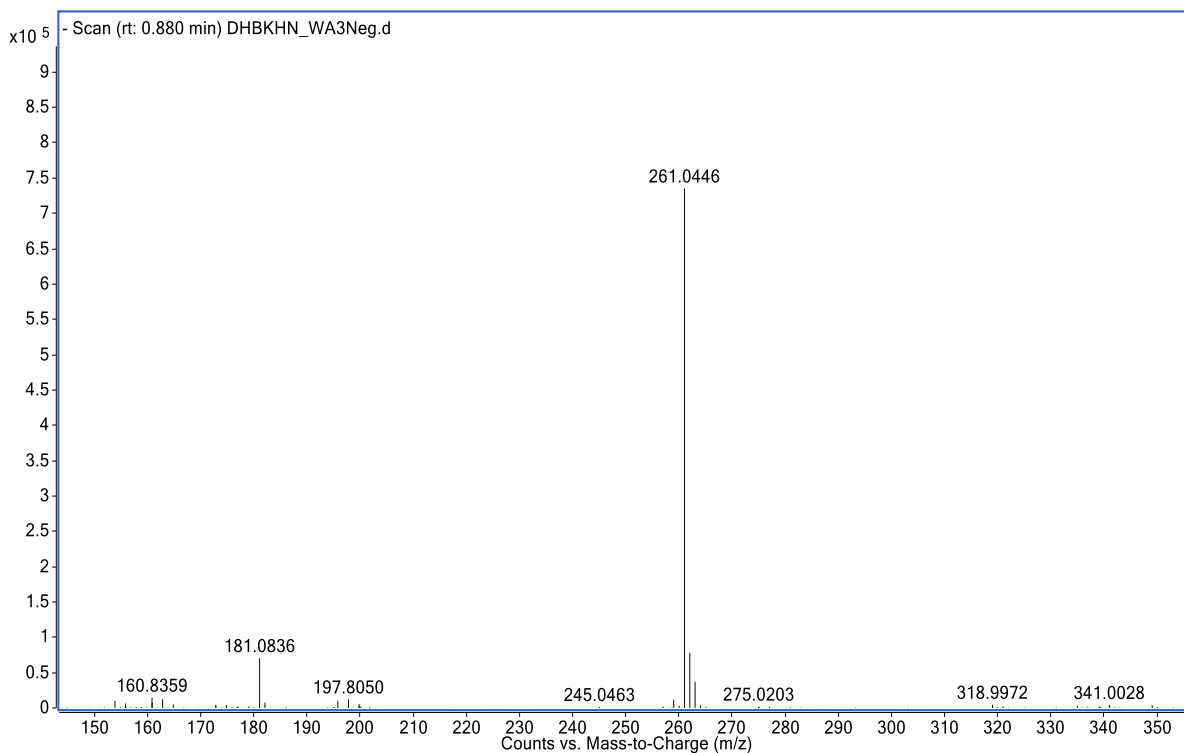


Figure S12: HR-ESI Mass Spectrum of **2** (4-(3'-*O*-sulfate-4'-hydroxyphenyl)-2(*R*)-butanol)

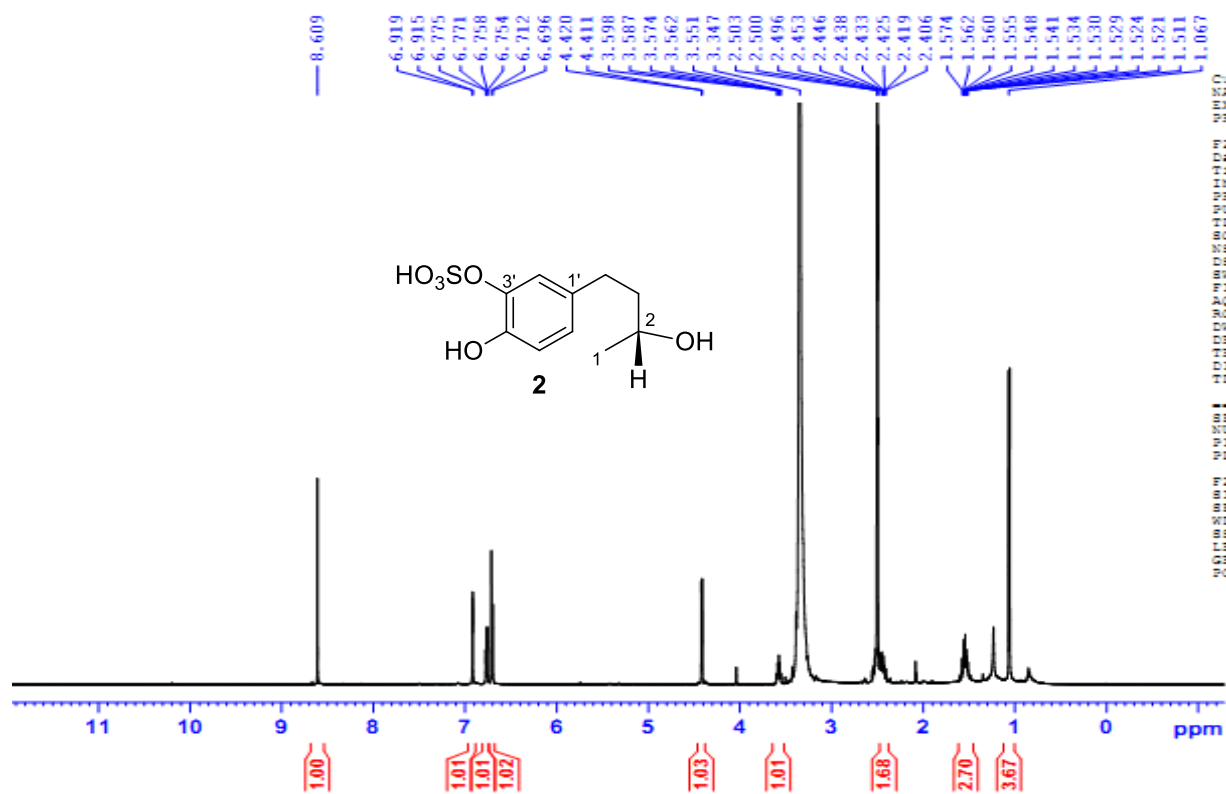


Figure S13: ¹H-NMR (500 MHz, DMSO) Spectrum of **2**

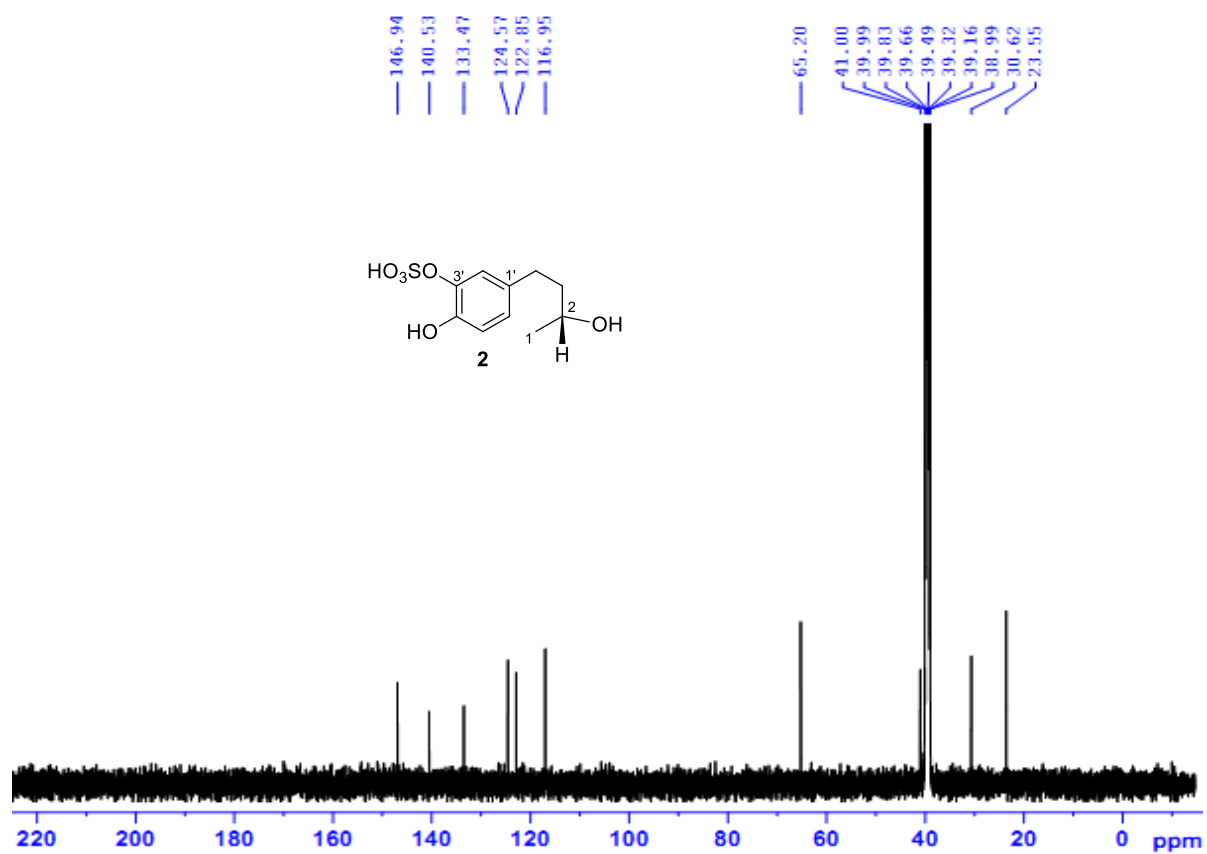


Figure S14: ¹³C-NMR (125 MHz, DMSO) Spectrum of **2**

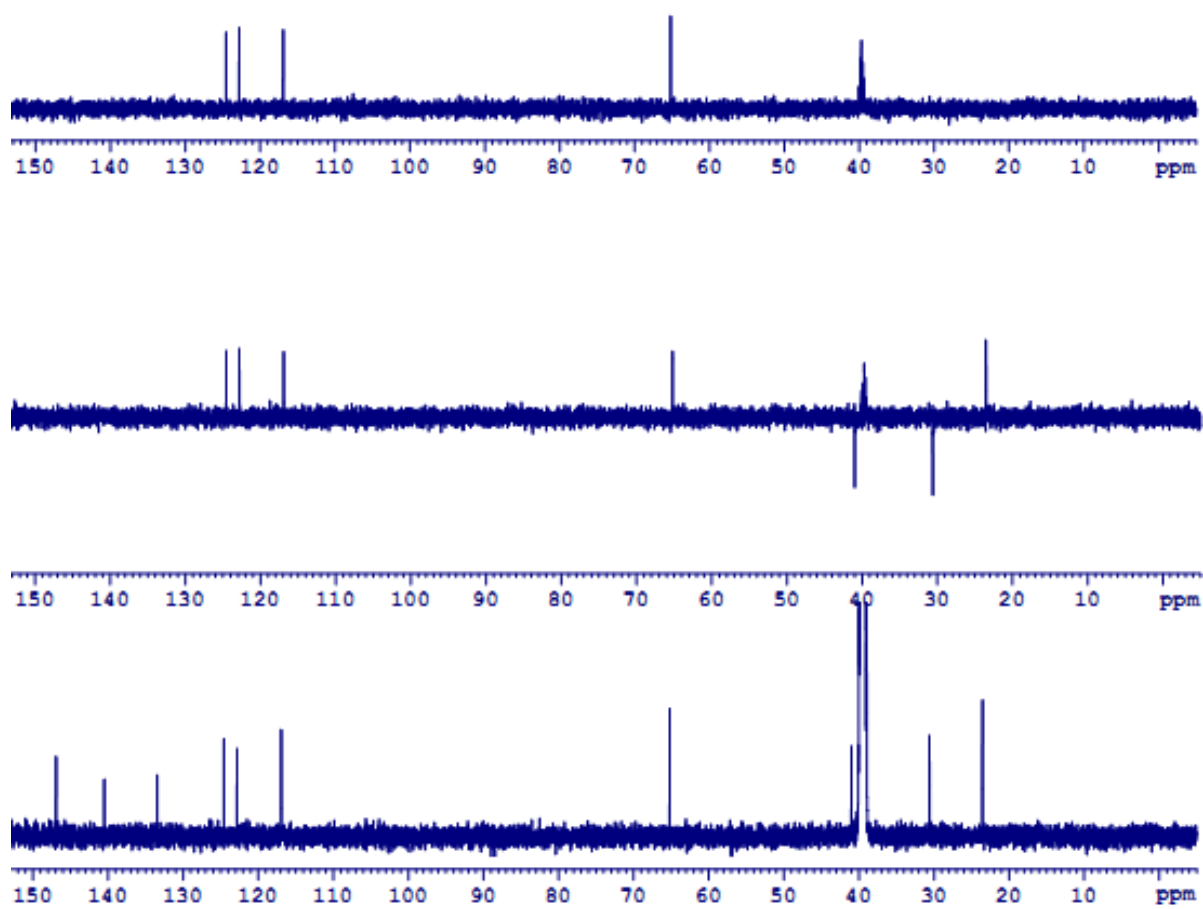


Figure S15: DEPT90 and 135 (125 MHz, DMSO) Spectrum of **2**

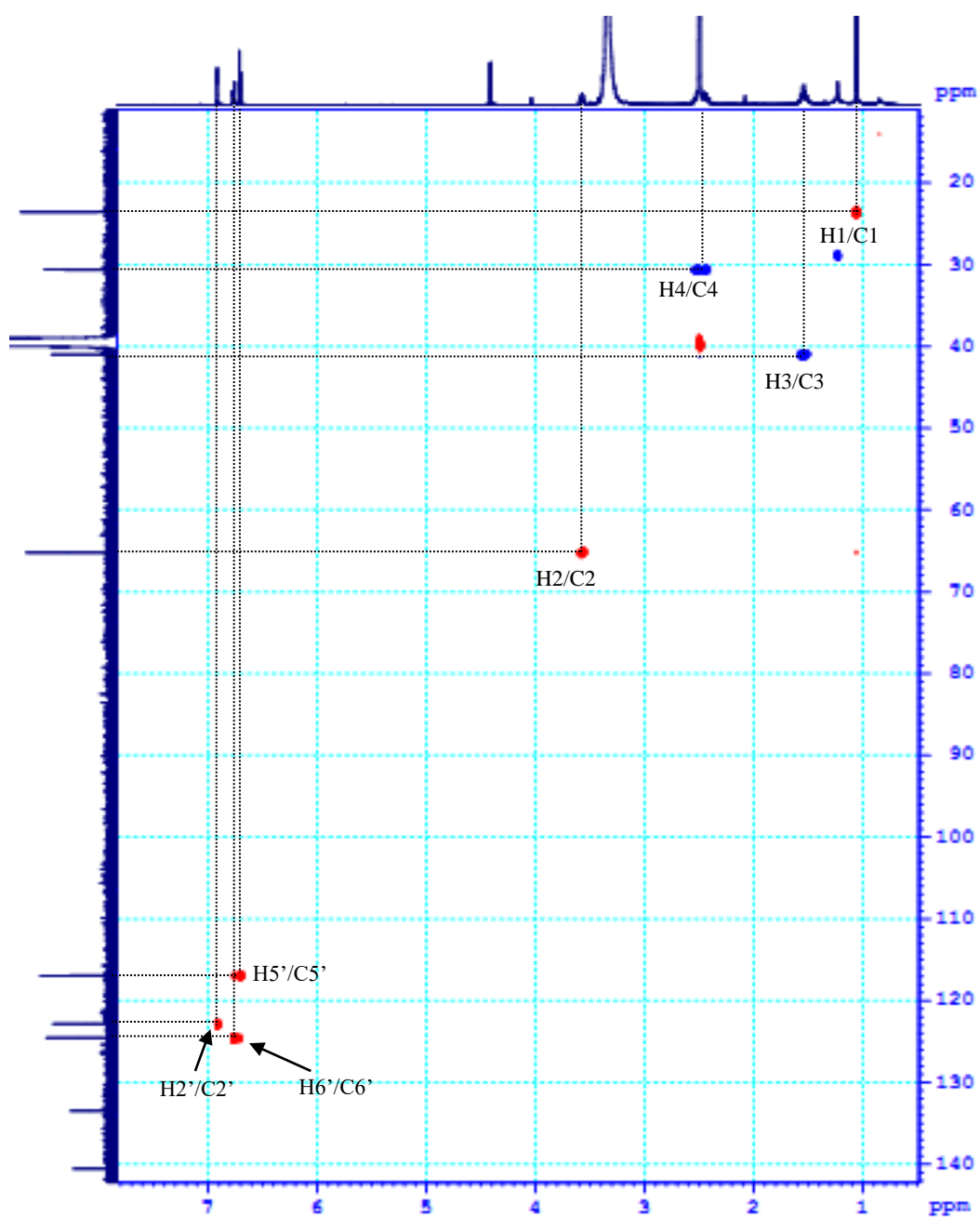


Figure S16: HSQC Spectrum of 2 (4-(3'-*O*-sulfate-4'-hydroxyphenyl)-2(*R*)-butanol)

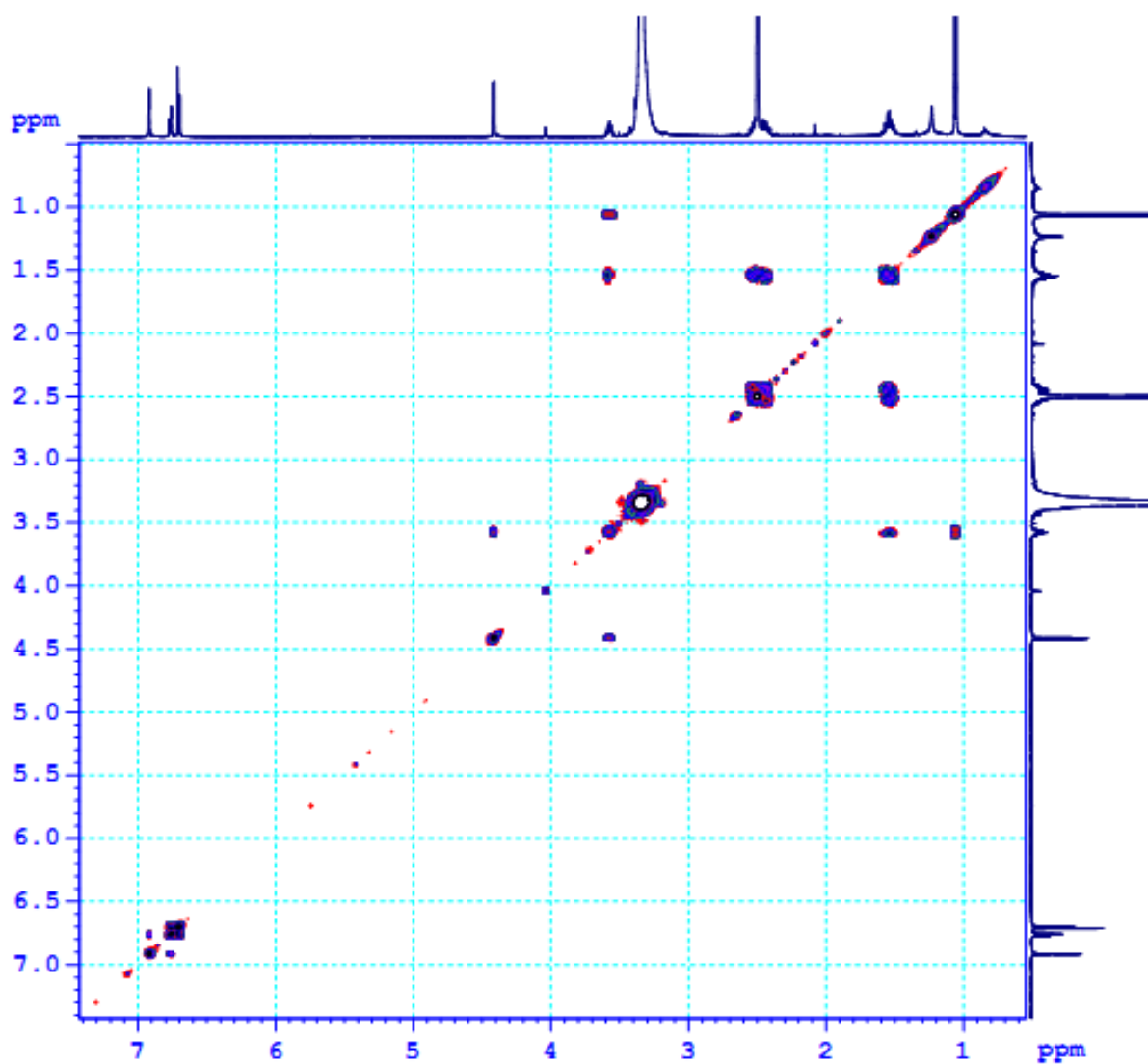


Figure S17: ^1H - ^1H COSY Spectrum of **2** (4-(3'-*O*-sulfate-4'-hydroxyphenyl)-2(*R*)-butanol)

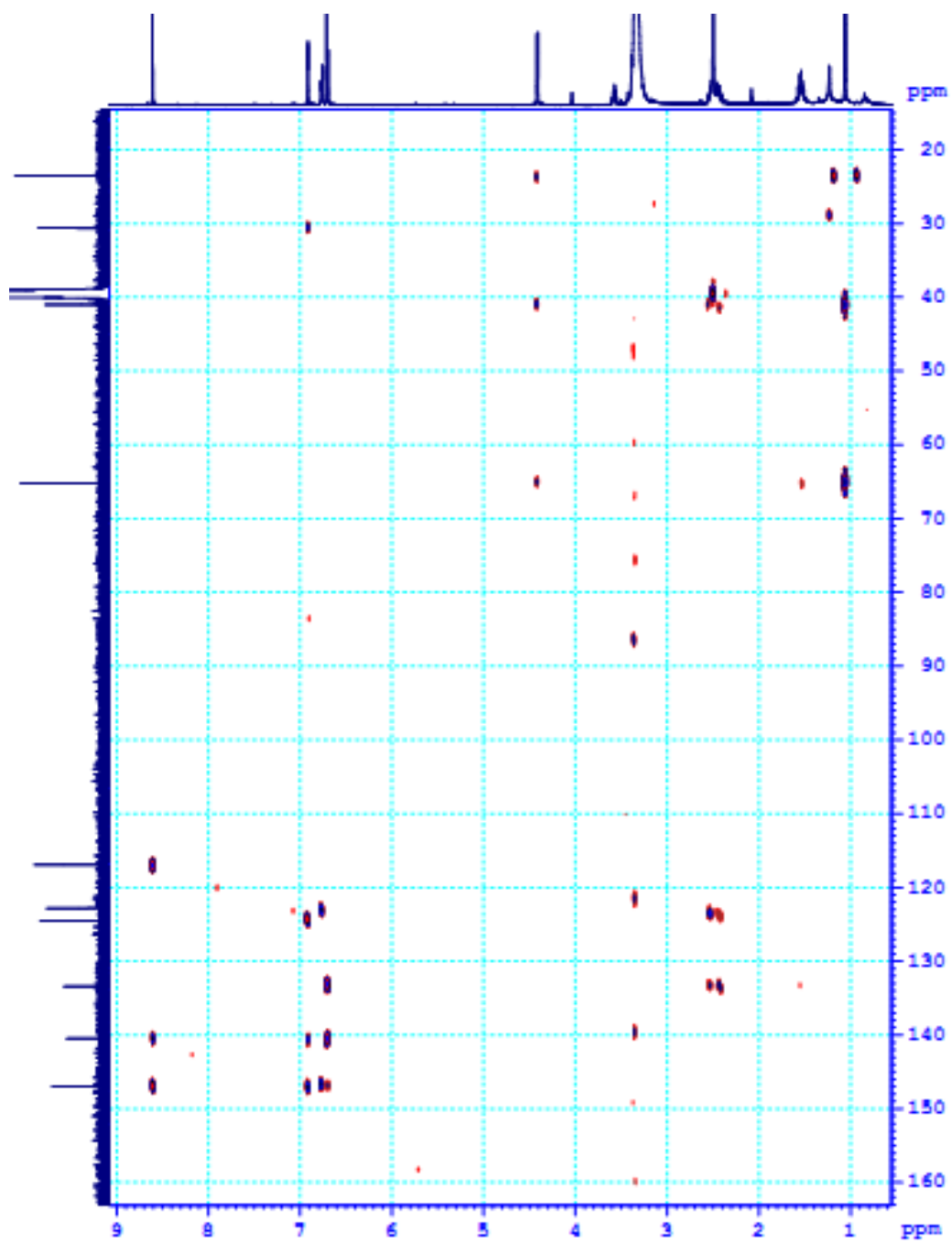


Figure S18: HMBC Spectrum of **2** (4-(3'-*O*-sulfate-4'-hydroxyphenyl)-2(*R*)-butanol)

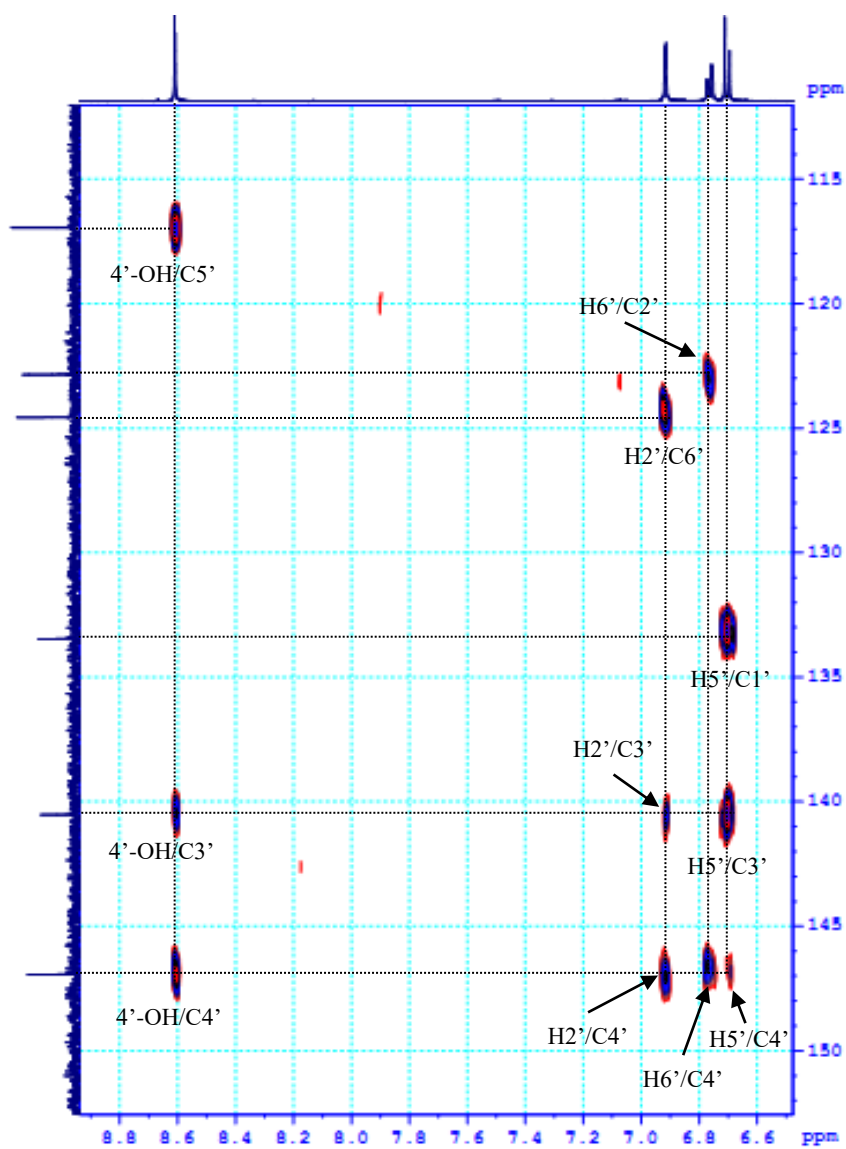


Figure S19: HMBC Spectrum of **2** (From δ_c 115 ppm to δ_c 150 ppm)

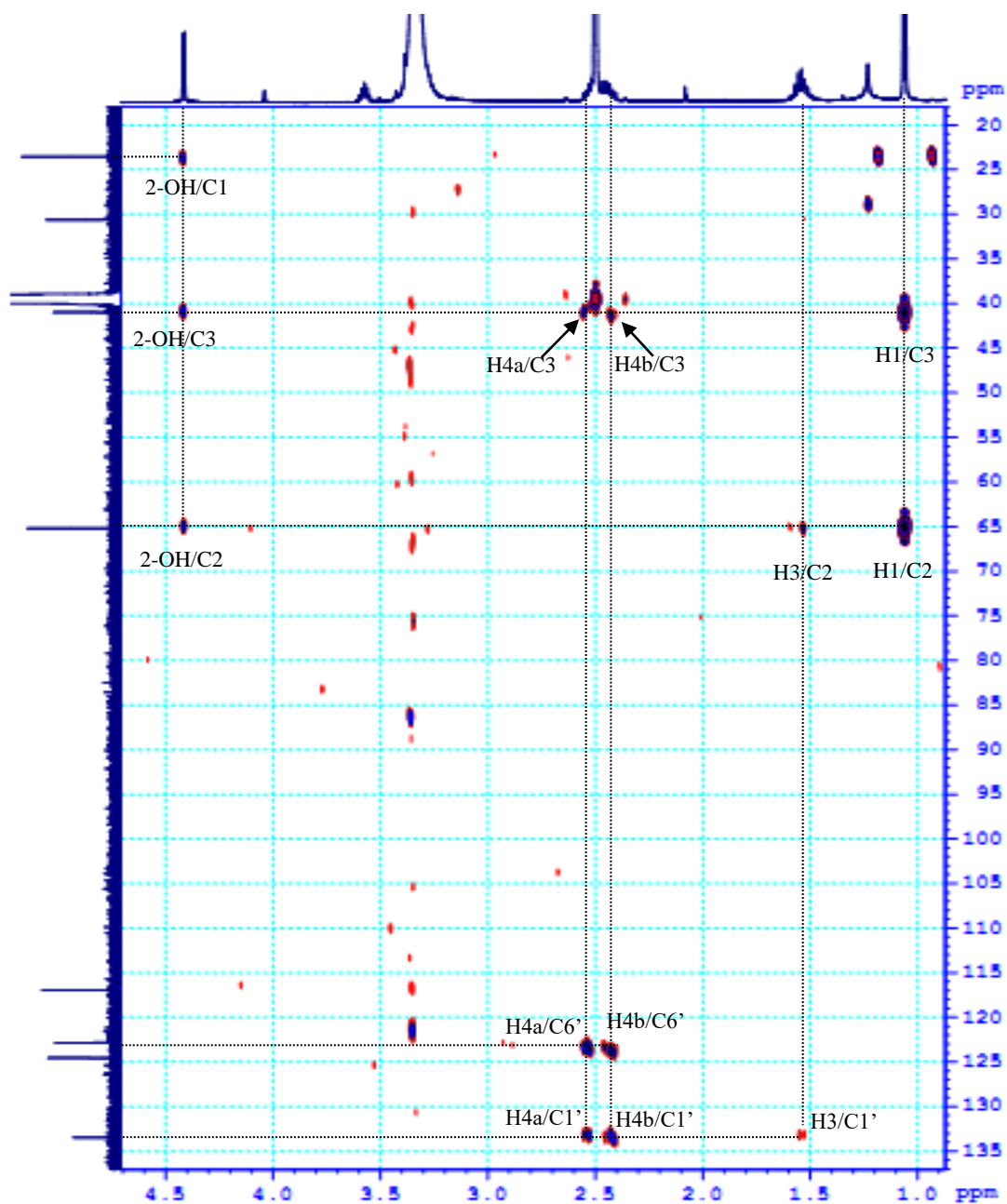


Figure S20: HMBC Spectrum of **2** (From δ_c 20 ppm to δ_c 135 ppm)

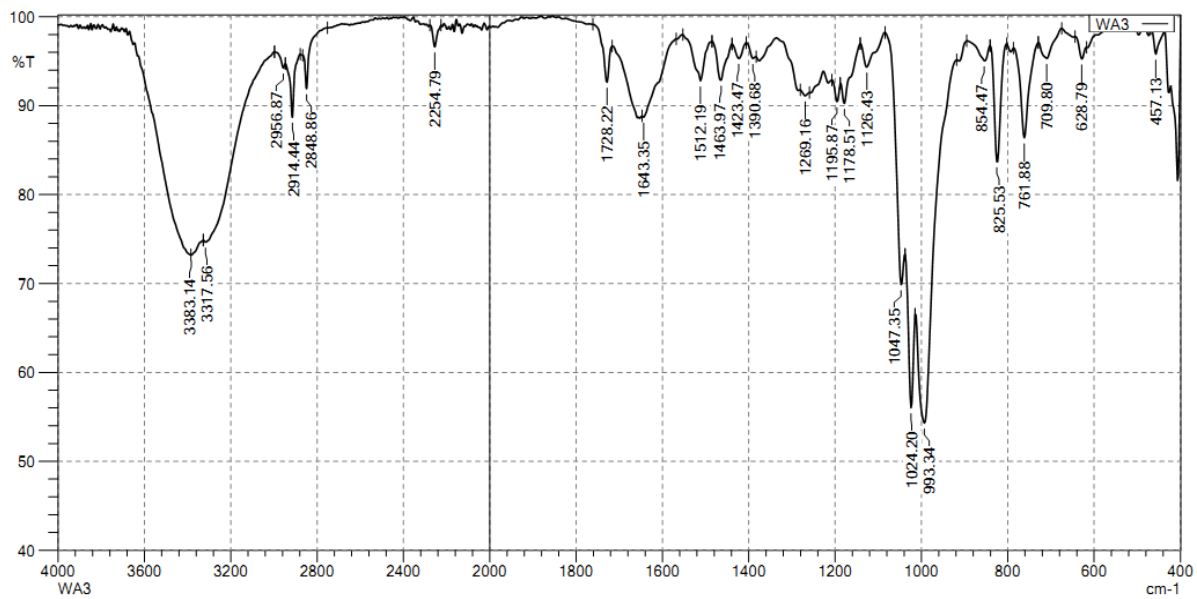


Figure S21: FT-IR Spectrum of 2 (4-(3'-O-sulfate-4'-hydroxyphenyl)-2(R)-butanol)

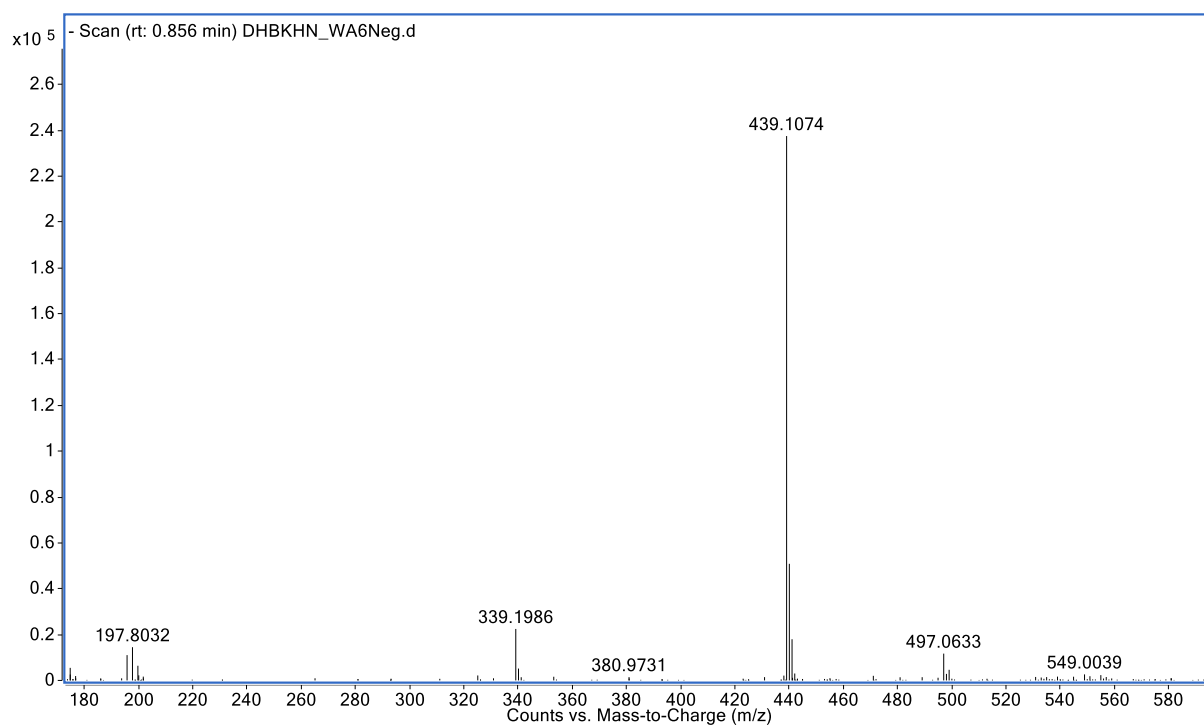


Figure S22: HR-ESI Mass Spectrum of **3** (dihydrodehydrodiconiferyl alcohol-9-*O*-sulfate)

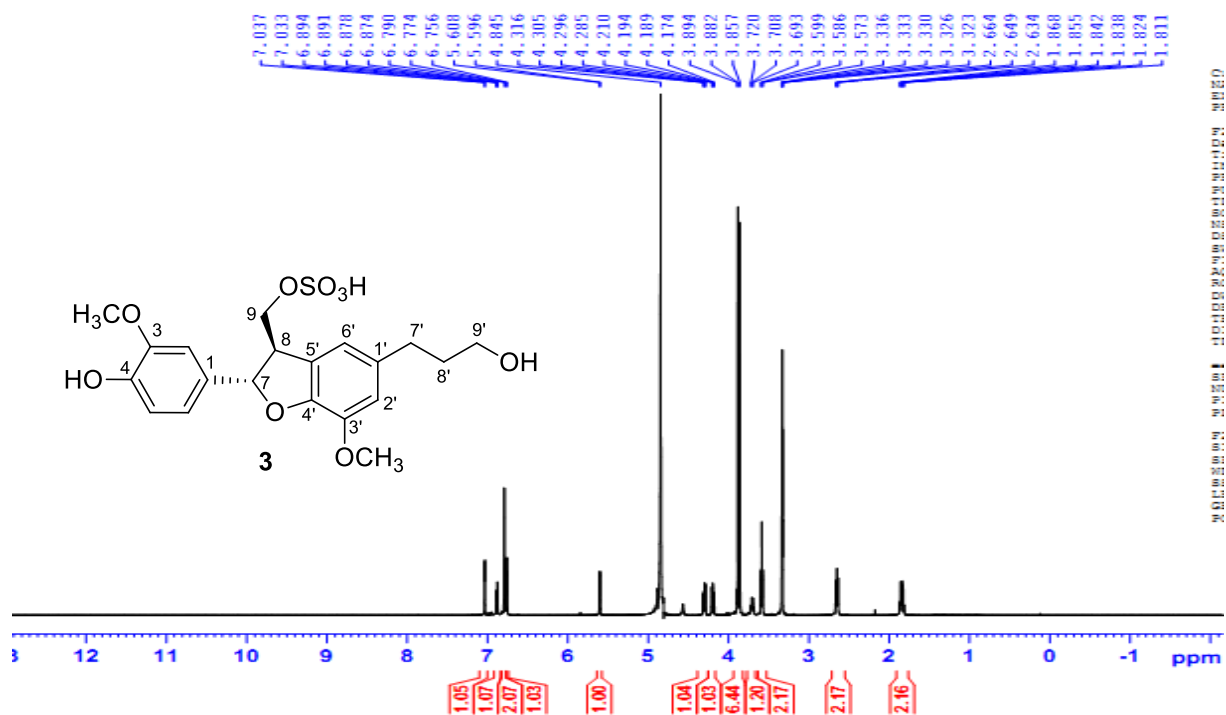


Figure S23: $^1\text{H-NMR}$ (500 MHz, CD_3OD) Spectrum of **3**

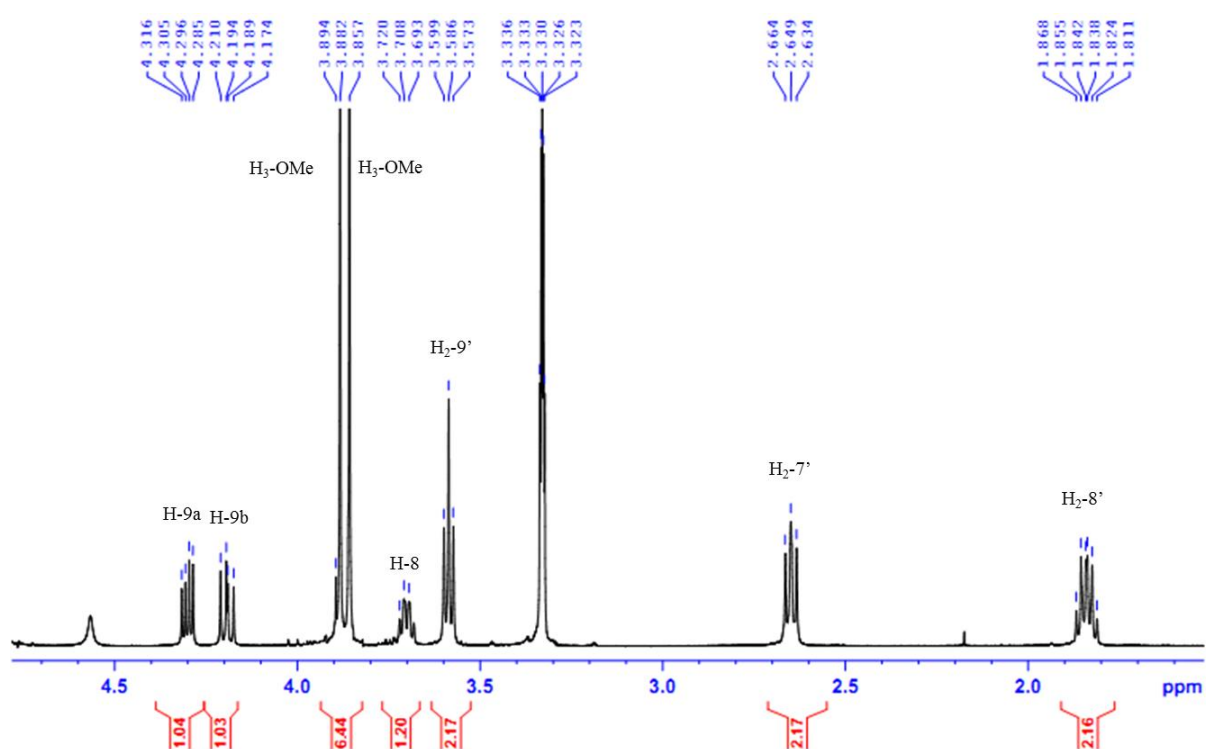


Figure S24: $^1\text{H-NMR}$ (500 MHz, CD_3OD) Spectrum of **3** (From δ_c 1.5 ppm to δ_c 4.5 ppm)

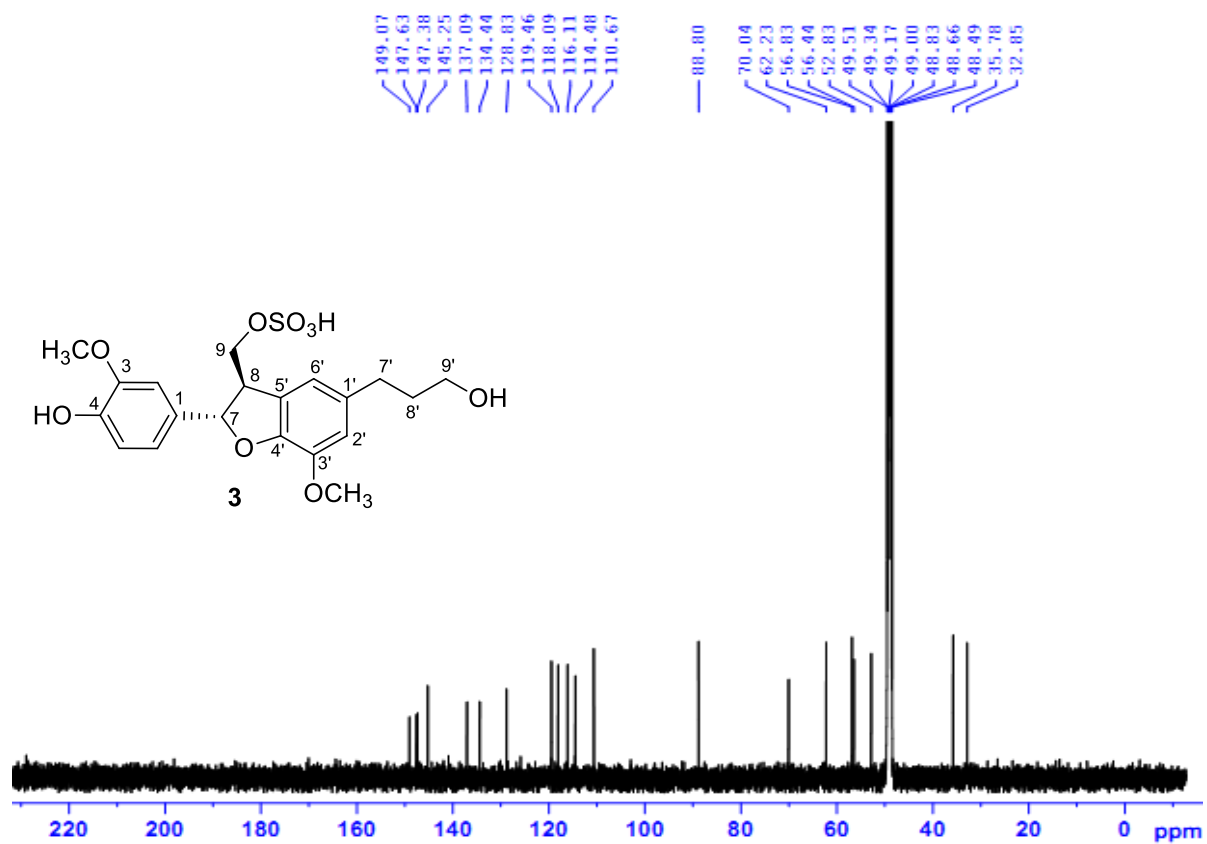


Figure S25: ¹³C-NMR (125 MHz, CD₃OD) Spectrum of **3**

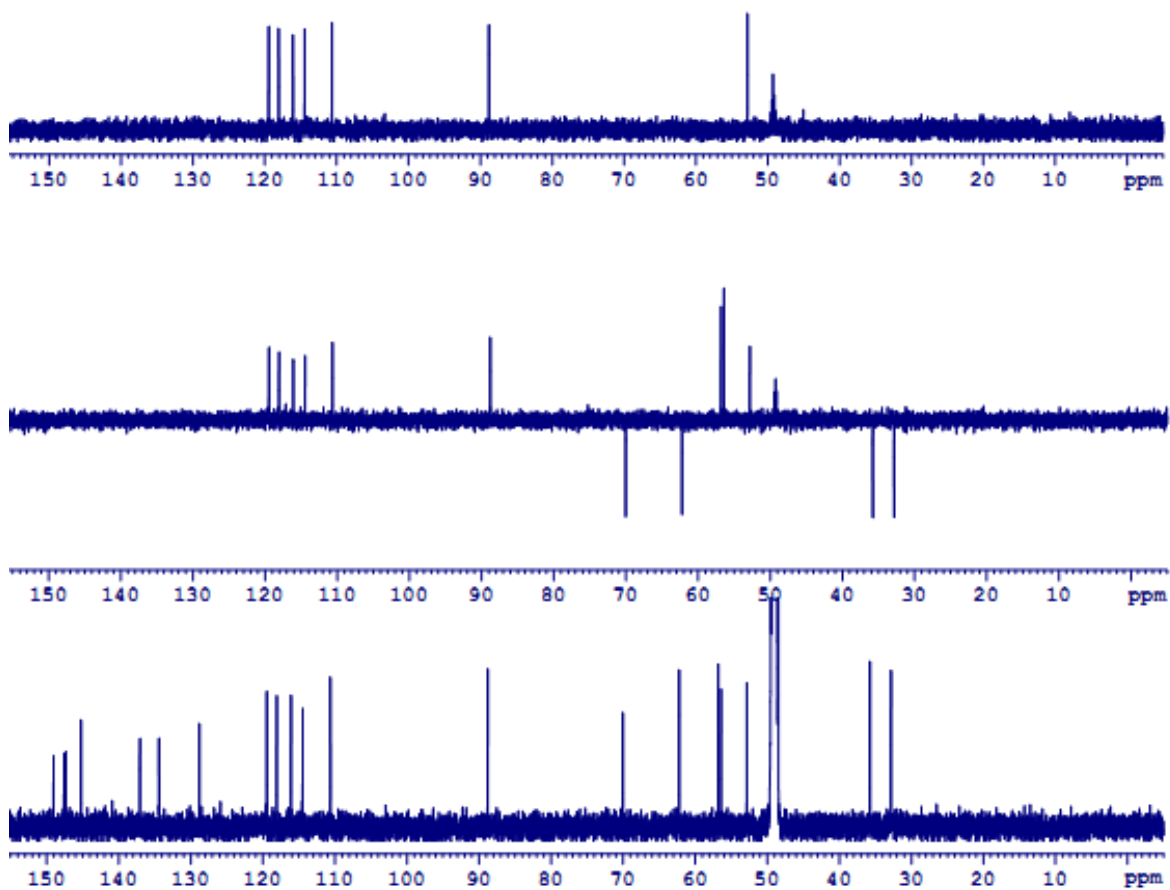


Figure S26: DEPT90 and 135 (125 MHz, CD₃OD) Spectrum of **3**

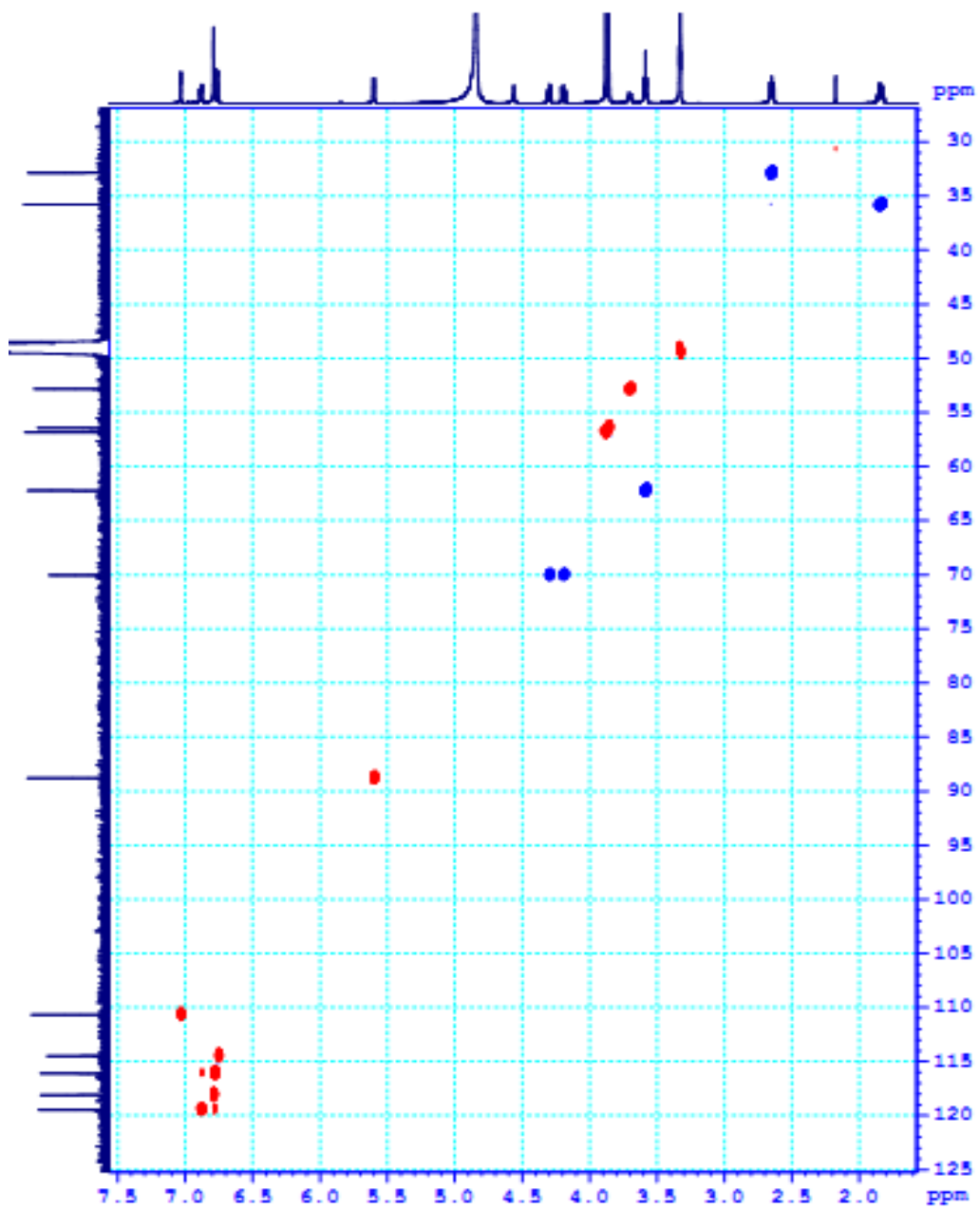


Figure S27: HSQC Spectrum of **3** (dihydrodehydrodiconiferyl alcohol-9-*O*-sulfate)

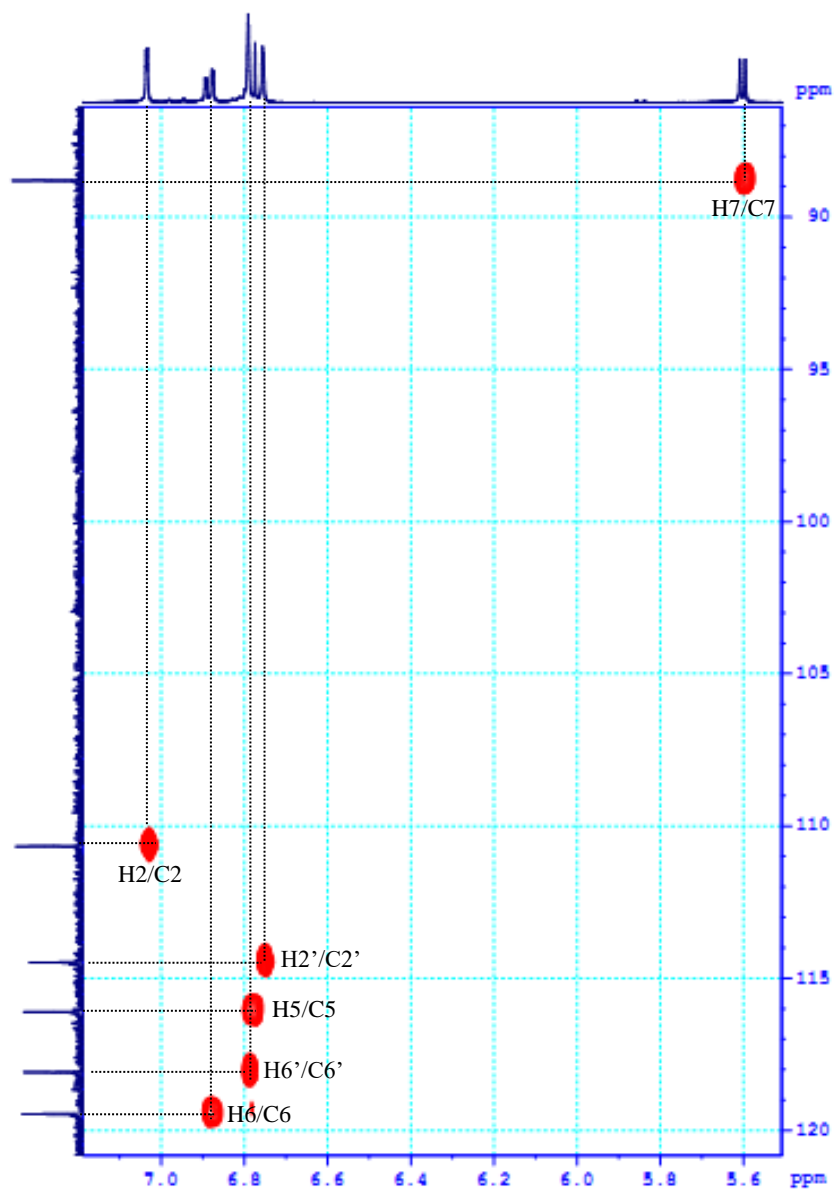


Figure S28: HSQC Spectrum of 3 (From δ_{C} 85 ppm to δ_{C} 120 ppm)

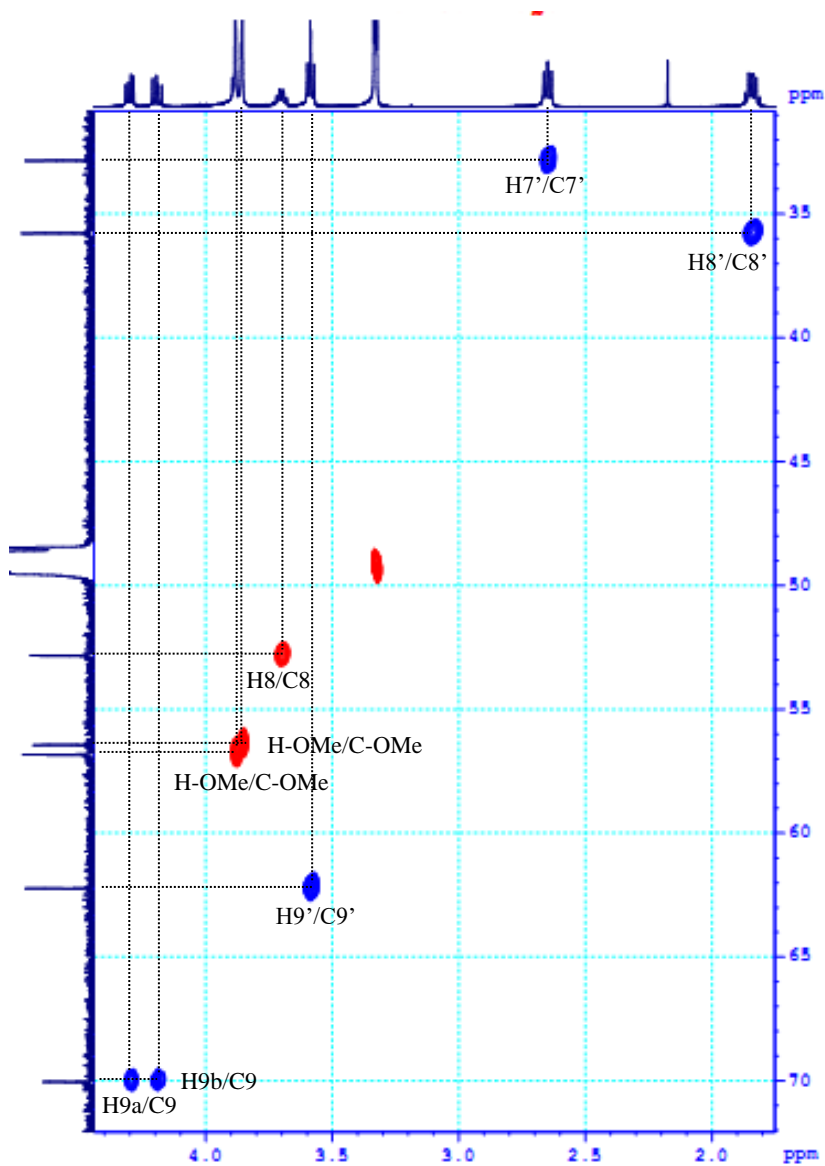


Figure S29: HSQC Spectrum of **3** (From δ_{C} 30 ppm to δ_{C} 70 ppm)

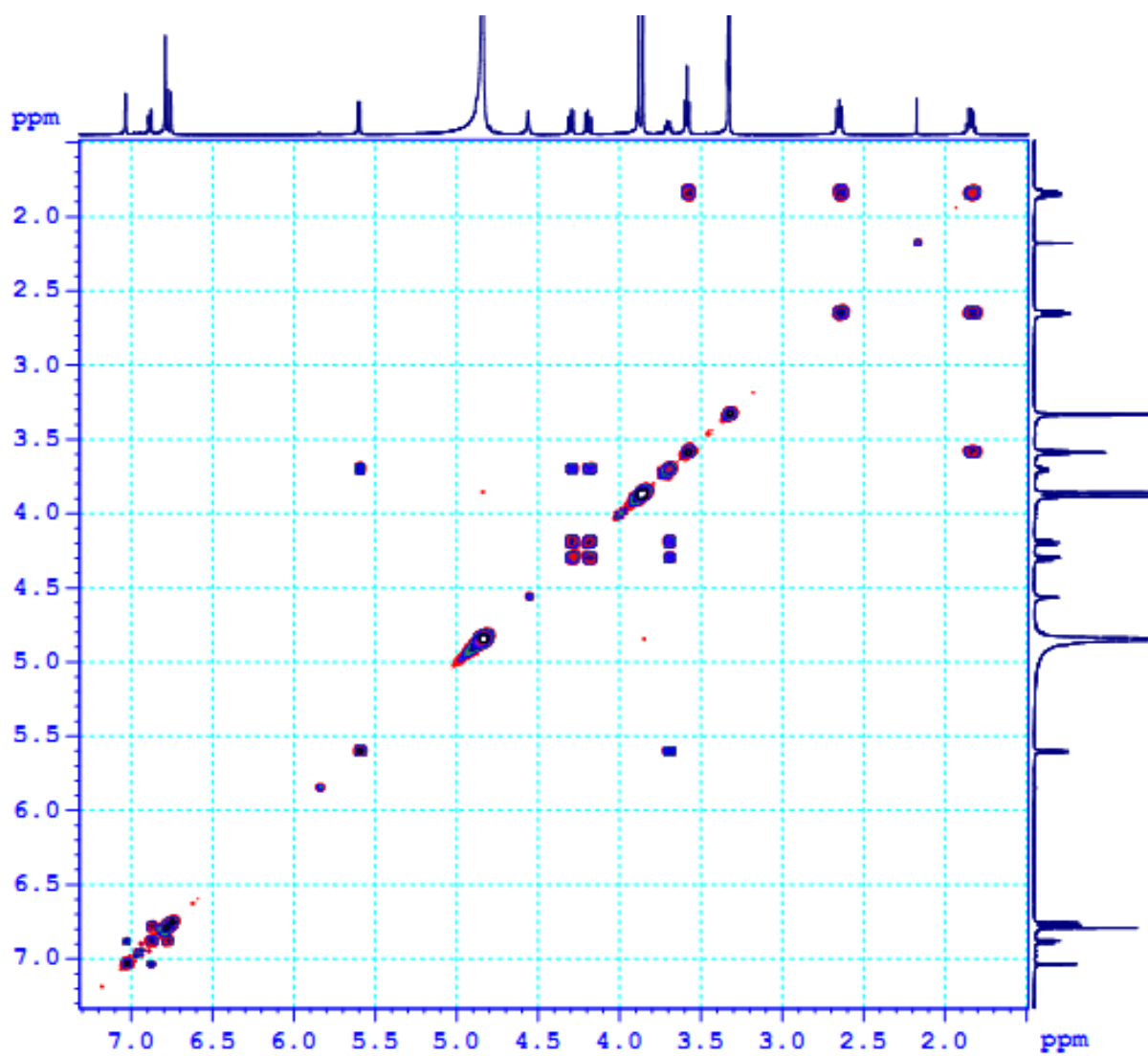


Figure S30: ^1H - ^1H COSY Spectrum of **3** (dihydrodehydrodiconiferyl alcohol-9-*O*-sulfate)

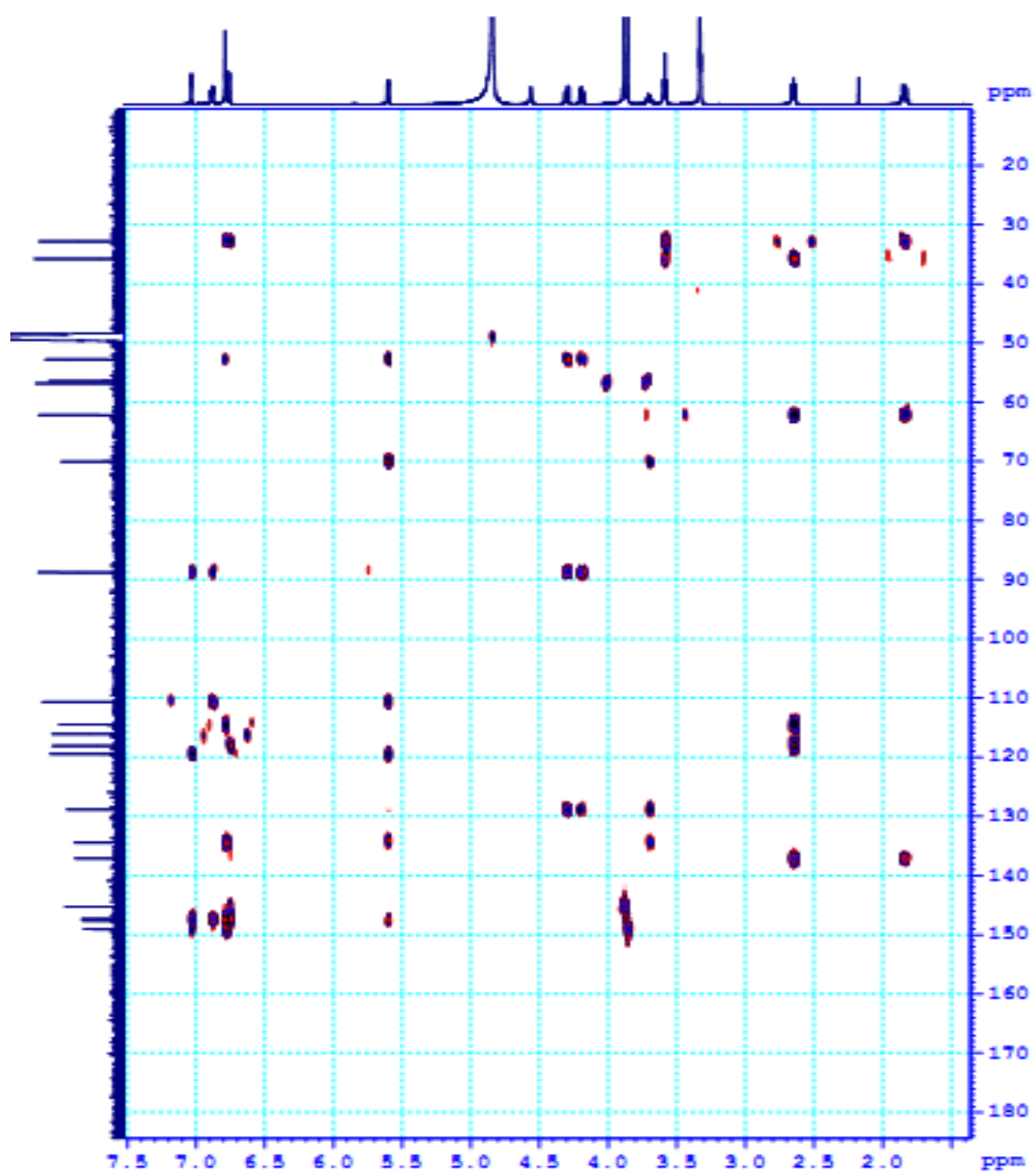


Figure S31: HMBC Spectrum of **3** (dihydrodehydrodiconiferyl alcohol-9-*O*-sulfate)

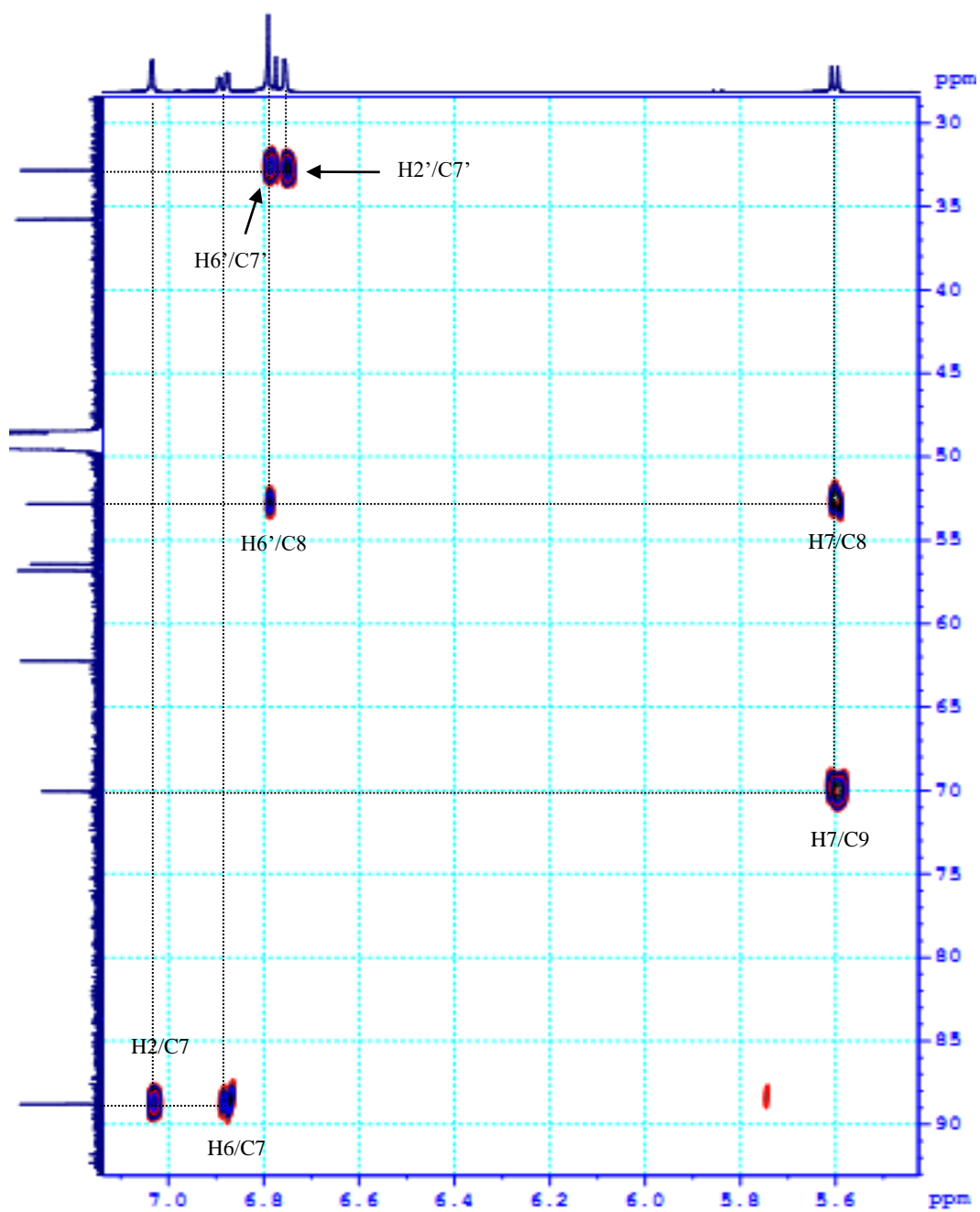


Figure S32: HMBC Spectrum of **3** (From δ_c 30 ppm to δ_c 90 ppm)

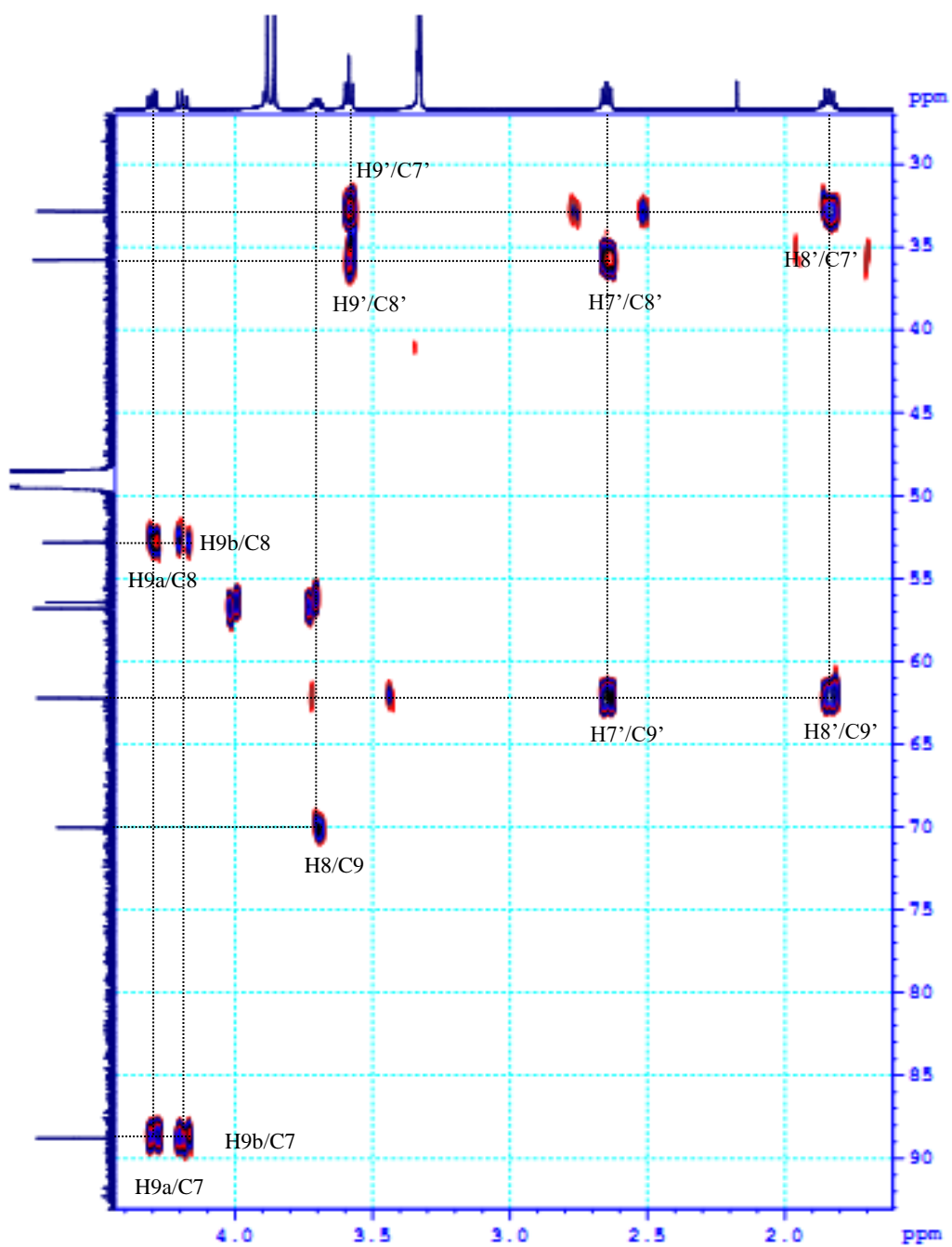


Figure S33: HMBC Spectrum of **3** (From δ_c 30 ppm to δ_c 90 ppm)

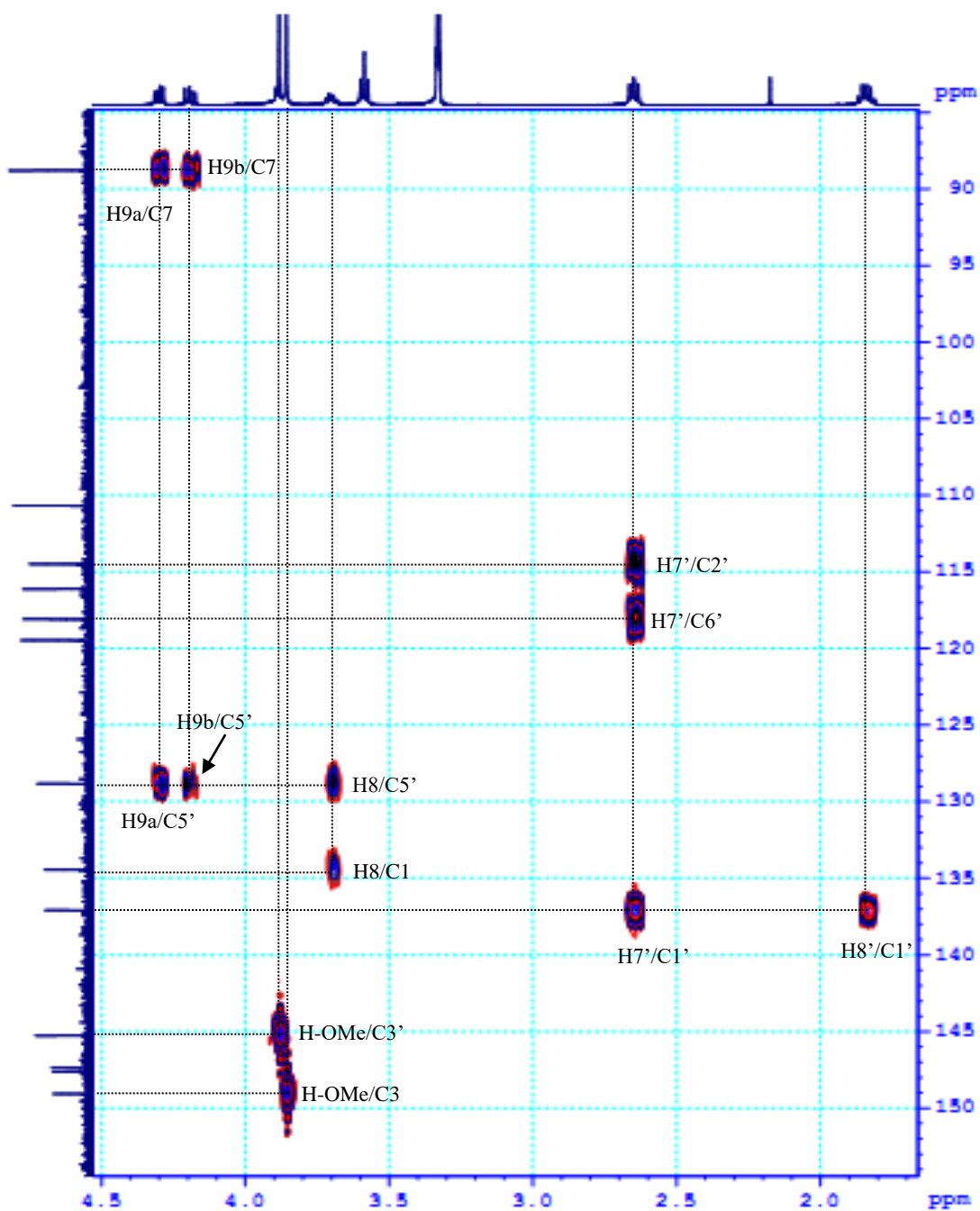


Figure S34: HMBC Spectrum of **3** (From δ_c 90 ppm to δ_c 150 ppm)

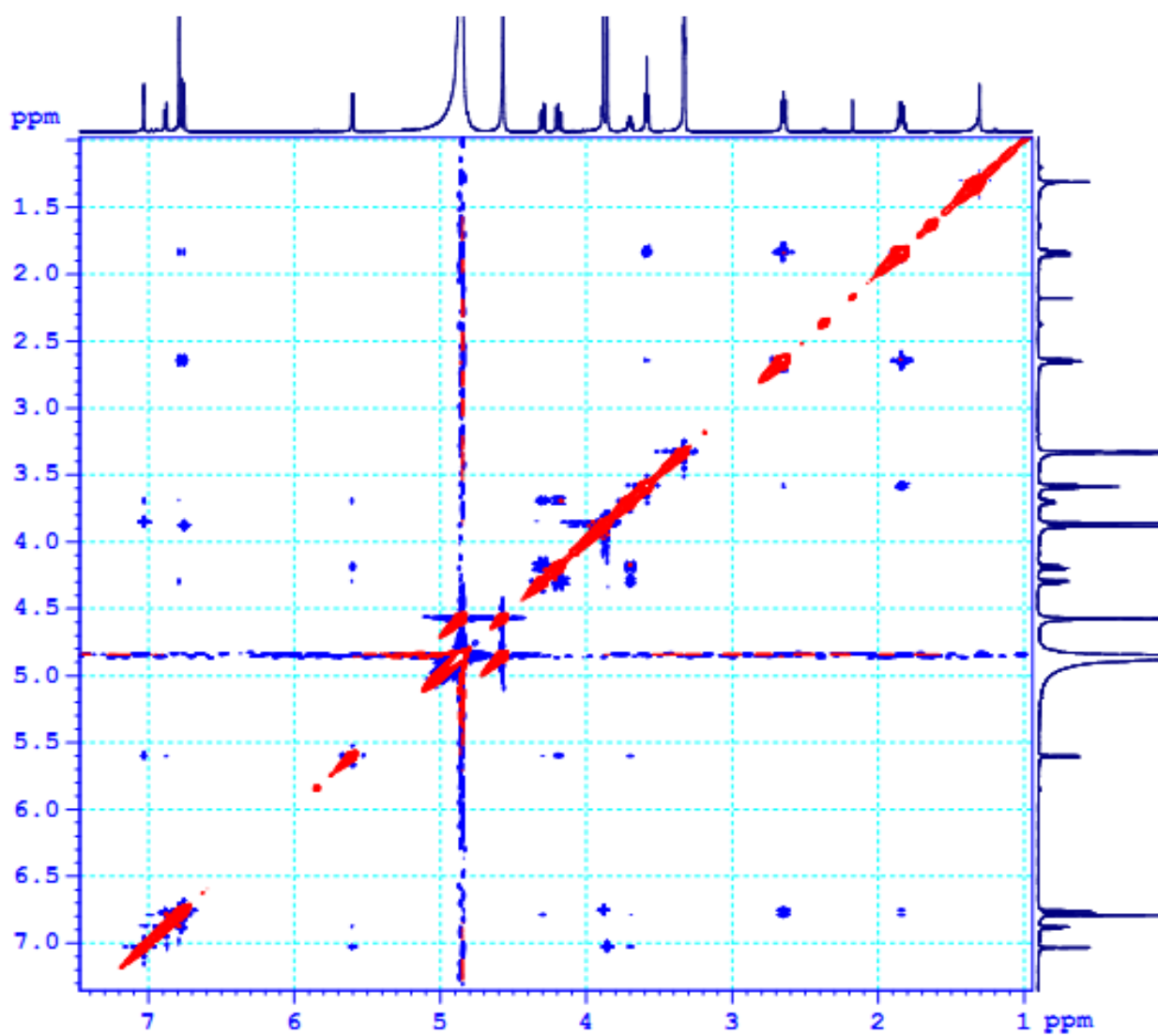


Figure S35: NOESY Spectrum of **3** (dihydrodehydrodiconiferyl alcohol-9-*O*-sulfate)

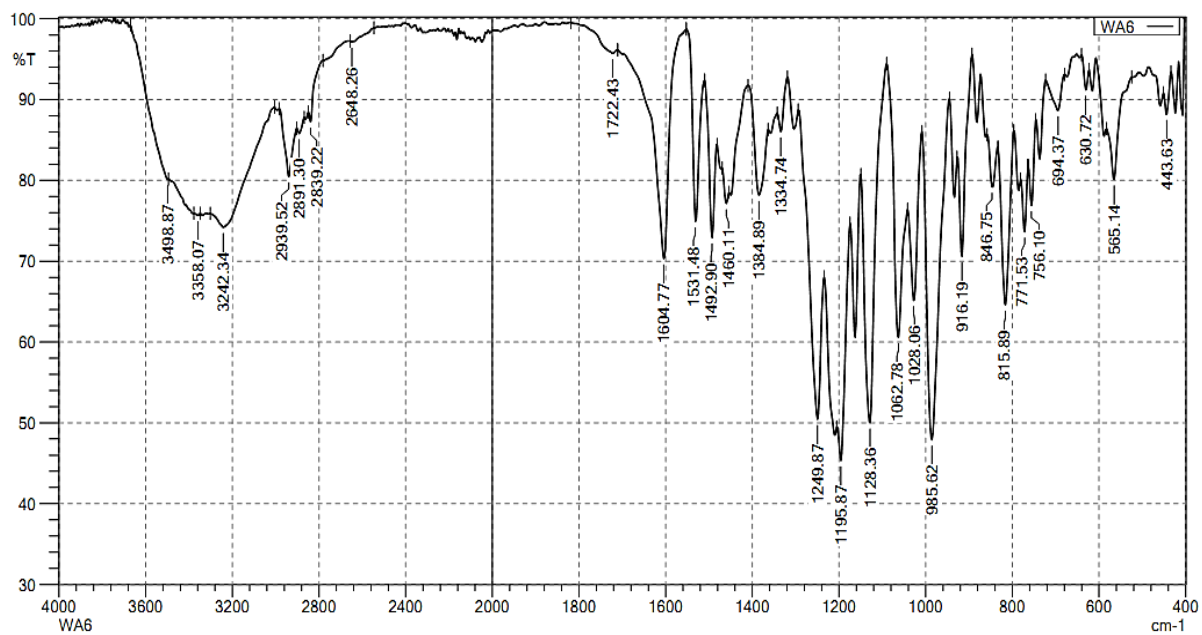


Figure S36: FT-IR Spectrum of **3** (dihydrodehydrodiconiferyl alcohol-9-*O*-sulfate)

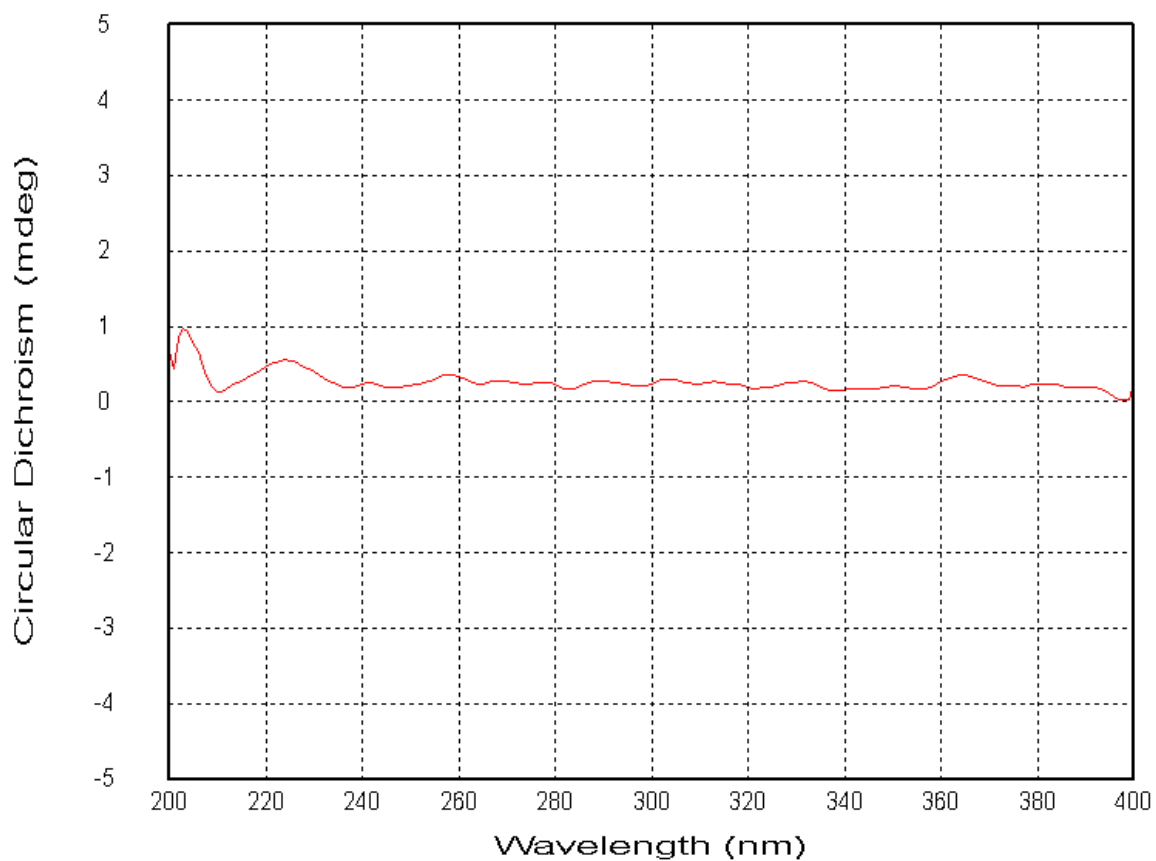


Figure S37: CD Spectrum (CH₃OH) of **3** (dihydrodehydrodiconiferyl alcohol-9-*O*-sulfate)

(+)-**pinoresinol-4-O-sulfate (4)**: ^1H NMR (500 MHz, $\text{DMSO-}d_6$) δ_{H} 8.87 (1H, *s*, 4-OH), 7.04 (1H, *d*, $J = 8.0$ Hz, H-5), 6.92 (1H, *d*, $J = 1.5$ Hz, H-2), 6.89 (1H, *d*, $J = 1.5$ Hz, H-2'), 6.82 (1H, *dd*, $J = 1.5$, 8.0 Hz, H-6), 6.76 (1H, *dd*, $J = 1.5$, 8.0 Hz, H-6'), 6.72 (1H, *d*, $J = 8.0$ Hz, H-5'), 4.67 (1H, *d*, $J = 4.5$ Hz, H-7), 4.60 (1H, *d*, $J = 4.5$ Hz, H-7'), 4.14 (2H, *m*, H-9a, H-9'a), 3.76 (3H, *s*, 3'-OCH₃), 3.75 (2H, *m*, H-9b, H-9'b), 3.74 (3H, *s*, 3-OCH₃), 3.05 (2H, *m*, H-8, H-8'). ^{13}C NMR (125 Hz, $\text{DMSO-}d_6$) data (Table S2).

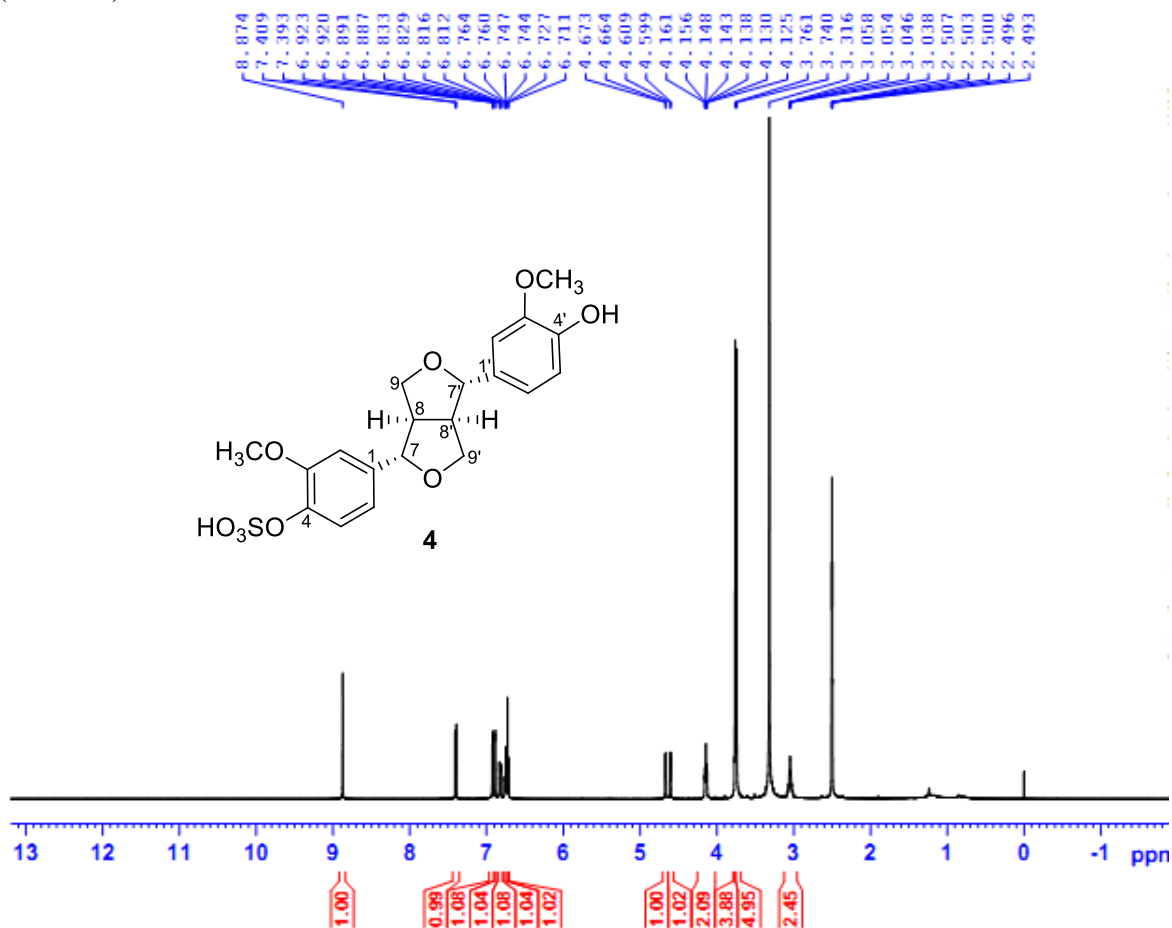


Figure S38: ^1H -NMR (500 MHz, DMSO) Spectrum of (+)-pinoresinol-4-O-sulfate (4)

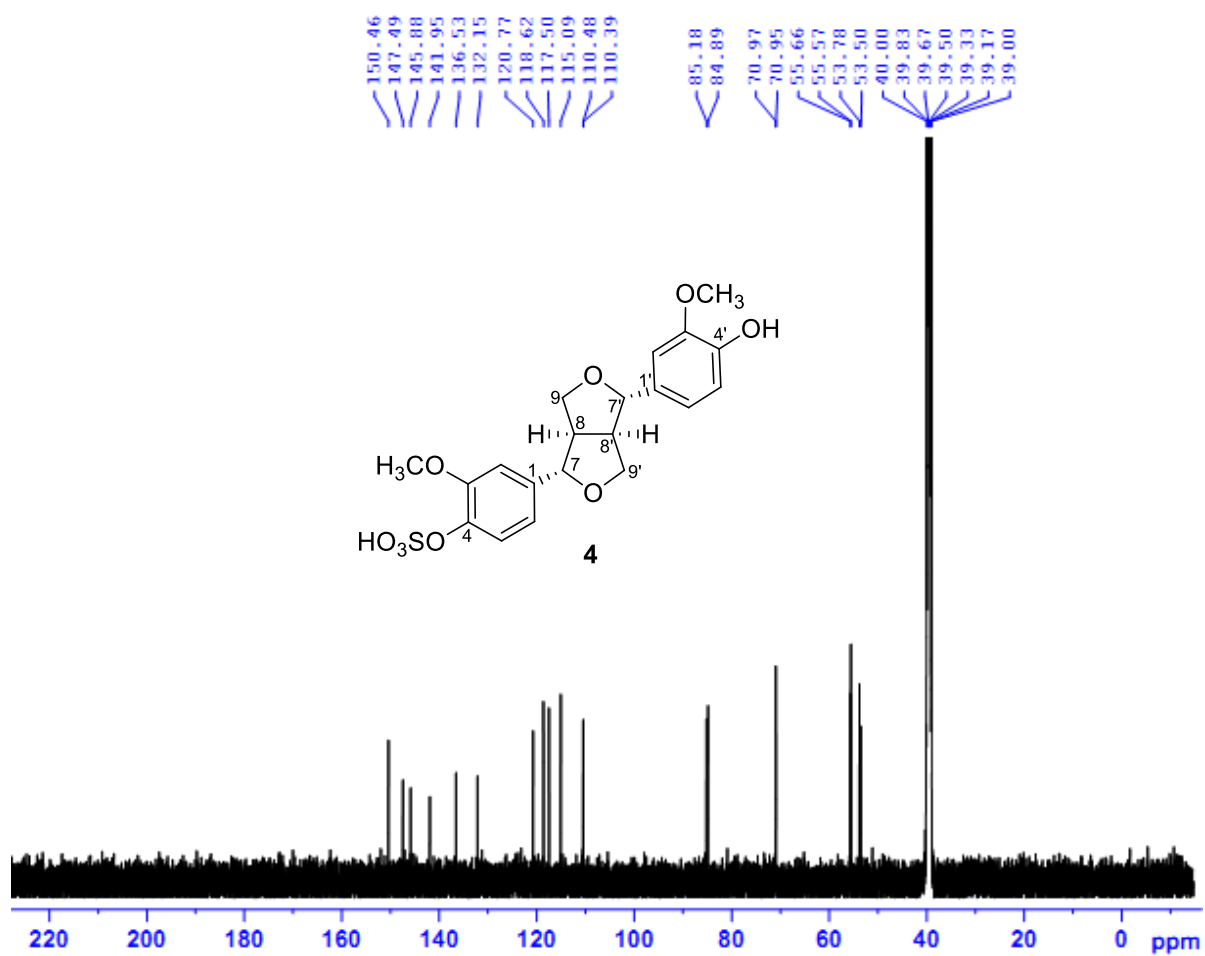


Figure S39: ¹³C-NMR (125 MHz, DMSO) Spectrum of (+)-pinoresinol-4-O-sulfate (**4**)

(+)-**pinoresinol-4-*O*-glucoside (5)**: ^1H NMR (500 MHz, CD_3OD) δ_{H} 7.17 (1H, *d*, $J = 8.0$ Hz, H-5), 7.05 (1H, *d*, $J = 2.0$ Hz, H-2), 6.97 (1H, *d*, $J = 2.0$ Hz, H-2'), 6.95 (1H, *dd*, $J = 2.0, 8.0$ Hz, H-6), 6.84 (1H, *dd*, $J = 2.0, 8.0$ Hz, H-6'), 6.79 (1H, *d*, $J = 8.0$ Hz, H-5'), 4.90 (1H, *d*, $J = 7.0$ Hz, H-1''), 4.79 (1H, *d*, $J = 4.5$ Hz, H-7'), 4.74 (1H, *d*, $J = 4.5$ Hz, H-7), 4.27 (2H, *m*, H-9a, H-9'a), 3.89 (3H, *s*, 3-OCH₃), 3.88 (3H, *s*, 3'-OCH₃), 3.88 (2H, *m*, H-9b, H-9'b), 3.16 (2H, *m*, H-8, H-8'), 3.88 (1H, *m*, H-6''a), 3.71 (1H, *m*, H-6''b), 3.40-3.55 (4H, *m*). ^{13}C NMR (125 Hz, CD_3OD) data (Table S2).

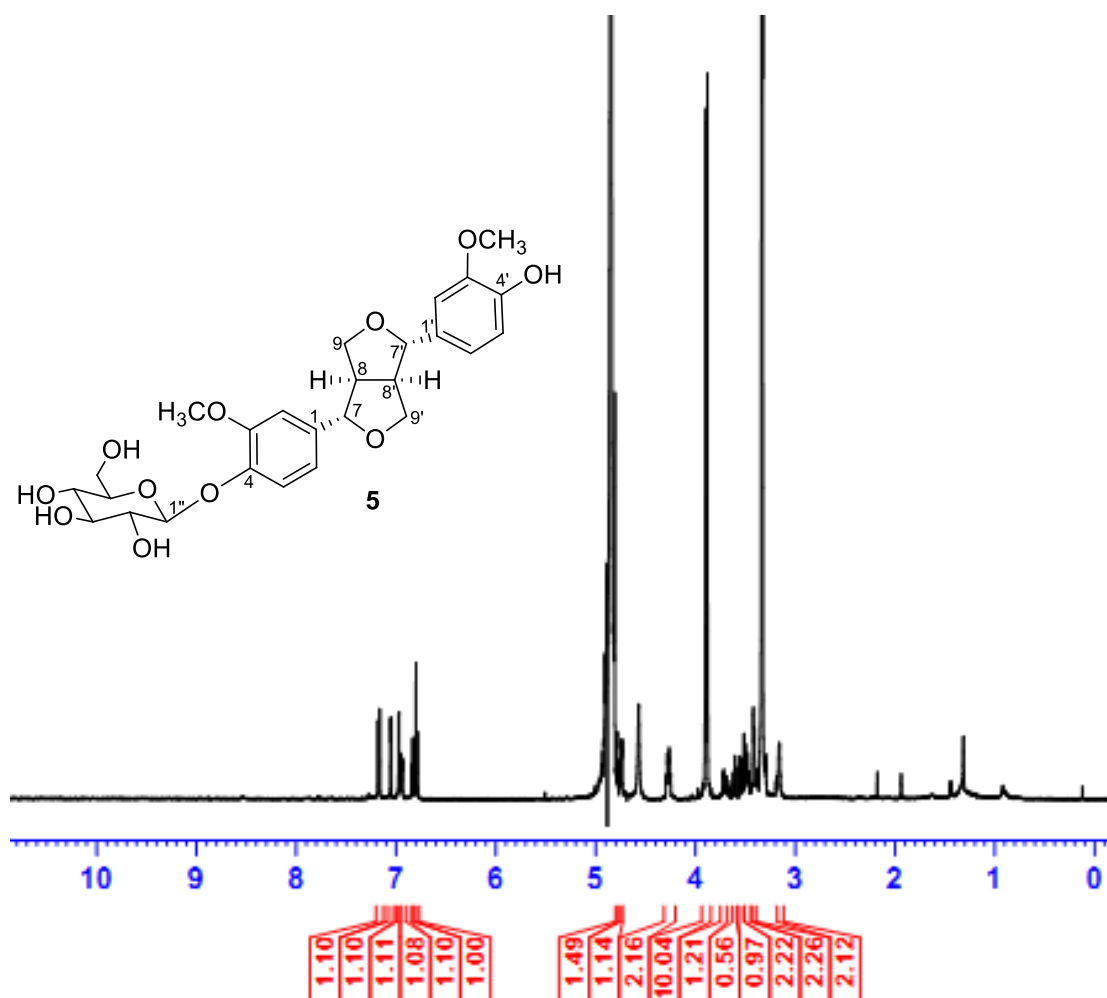


Figure S40: ^1H -NMR (500 MHz, CD_3OD) Spectrum of (+)-pinoresinol-4-*O*-glucoside (5)

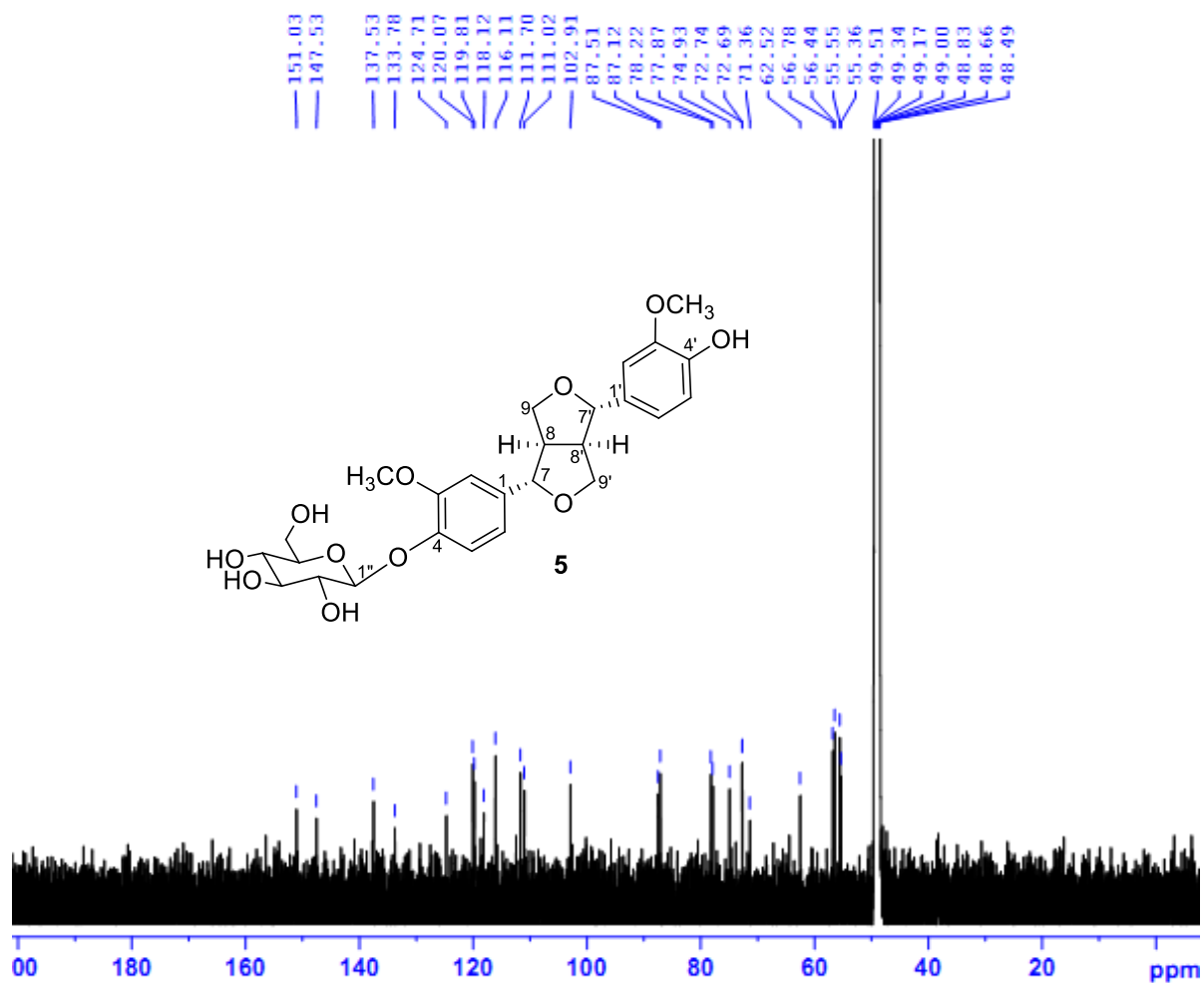


Figure S41: ¹³C-NMR (125 MHz, CD₃OD) Spectrum of (+)-pinoresinol-4-*O*-glucoside (5)

Dihydrodehydrodiconiferyl alcohol-4-*O*-glucoside (6): ^1H NMR (500 MHz, CD_3OD) δ_{H} 7.17 (1H, *d*, $J = 8.0$ Hz, H-5), 7.05 (1H, *d*, $J = 2.0$ Hz, H-2), 6.96 (1H, *dd*, $J = 2.0, 8.0$ Hz, H-6), 6.75 (1H, *s*, H-2'), 6.73 (1H, *s*, H-6'), 5.58 (1H, *d*, $J = 6.0$ Hz, H-7), 4.85 (1H, *d*, $J = 7.5$ Hz, H-1''), 3.88 (3H, *s*, 3-OCH₃), 3.86 (2H, *m*, H-6''a, H-9a), 3.85 (3H, *s*, 3'-OCH₃), 3.76 (1H, *m*, H-9b), 3.69 (1H, *m*, H-6''b), 3.60 (2H, *t*, $J = 6.5$ Hz, H₂-9'), 3.50 (1H, *m*, H-8), 3.41-3.47 (4H, *m*), 2.64 (2H, *t*, $J = 7.5$ Hz, H₂-7'), 1.83 (2H, *m*, H₂-8'). ^{13}C NMR (125 Hz, CD_3OD) data (Table S2).

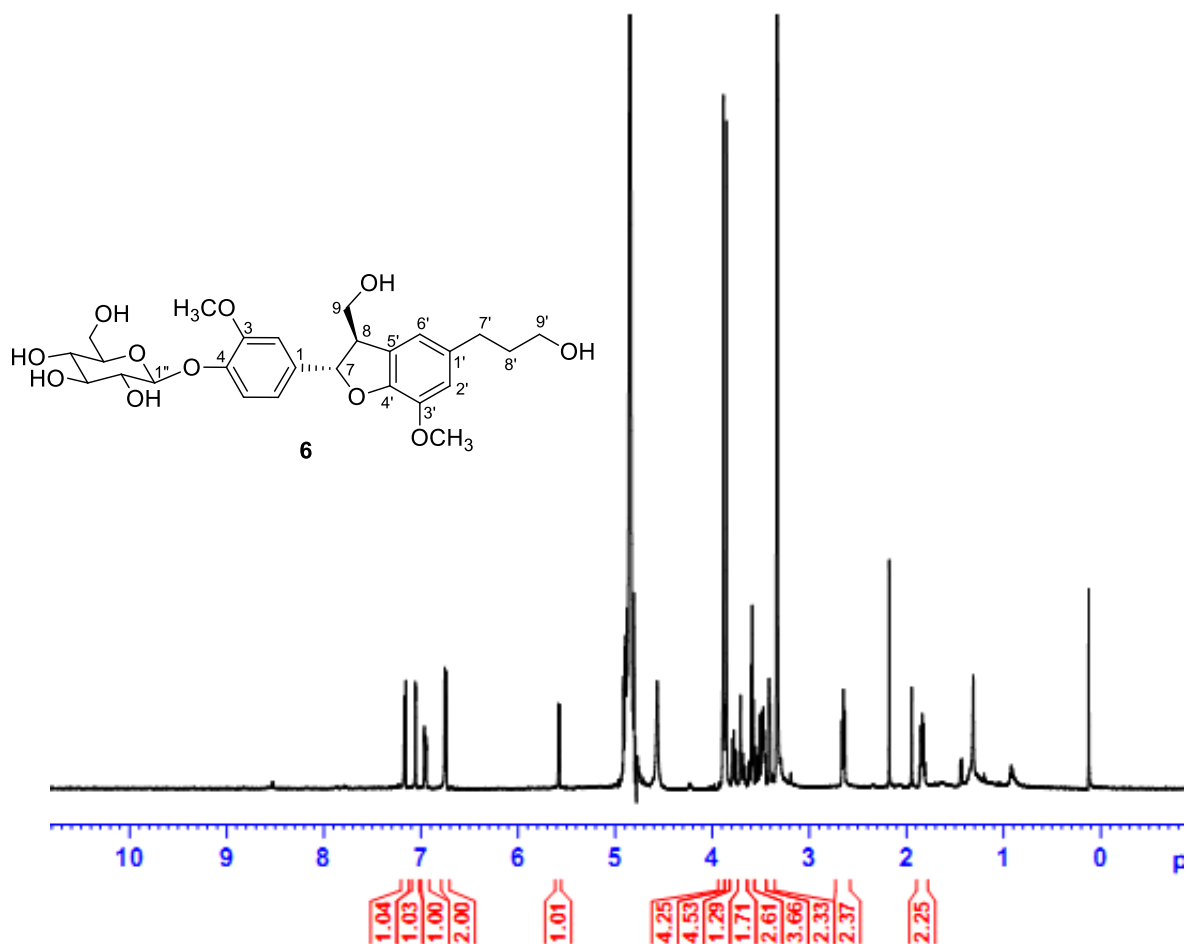


Figure S42: ^1H -NMR (500 MHz, CD_3OD) Spectrum of dihydrodehydrodiconiferyl alcohol-4-*O*-glucoside (6)

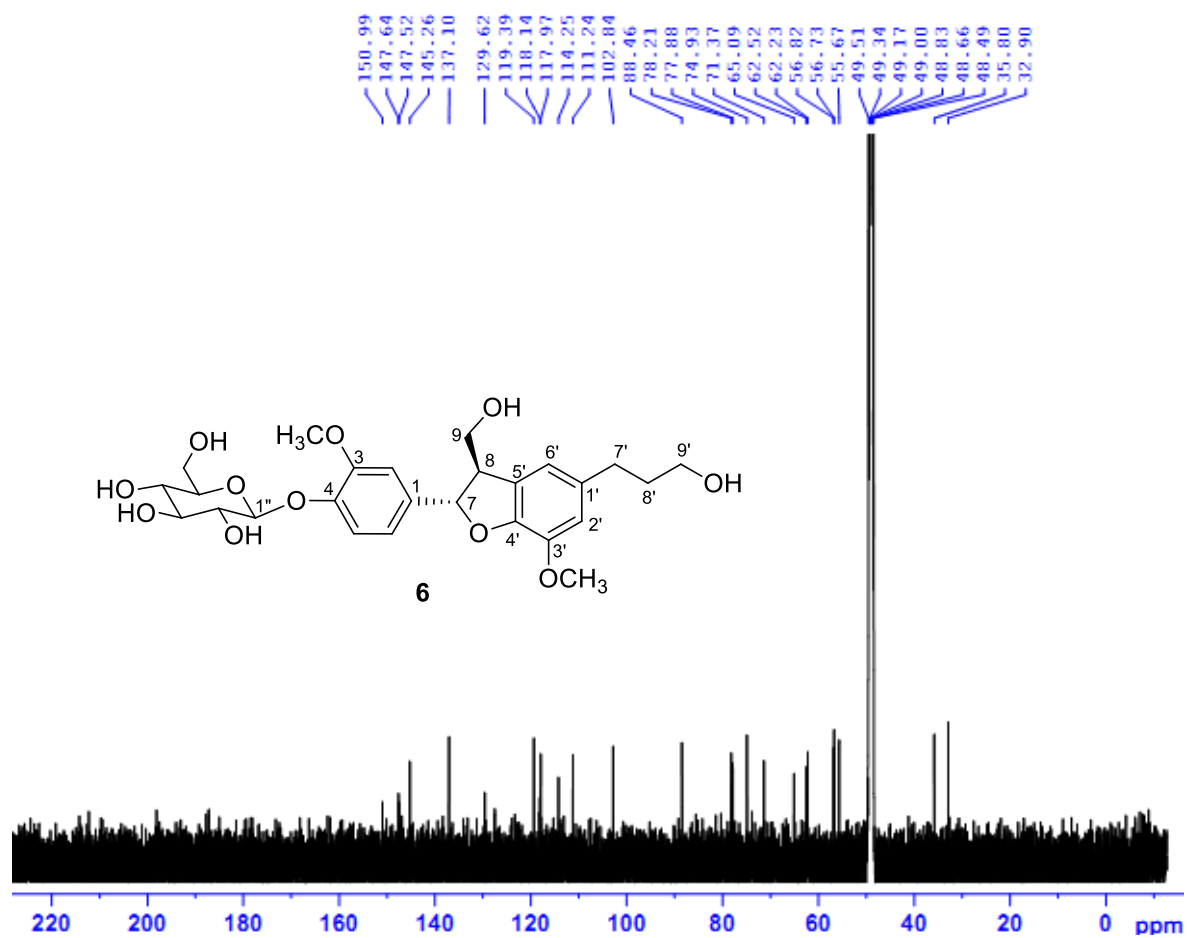


Figure S43: ¹³C-NMR (125 MHz, CD₃OD) Spectrum of dihydrodehydrodiconiferyl alcohol-4-O-glucoside (6)

(+)-isolarisiresinol-9-*O*-sulfate (**7**): ^1H NMR (500 MHz, CD_3OD) δ_{H} 6.78 (1H, *d*, $J = 1.5$ Hz, H-2), 6.75 (1H, *d*, $J = 8.0$ Hz, H-5), 6.68 (1H, *s*, H-2'), 6.62 (1H, *dd*, $J = 1.5, 8.0$ Hz, H-6), 6.22 (1H, *s*, H-5'), 4.13 (1H, *dd*, $J = 3.0, 10.0$ Hz, H-9a), 3.91 (1H, *dd*, $J = 3.0, 10.0$ Hz, H-9b), 3.96 (1H, *d*, $J = 10.5$, H-7), 3.83 (3H, *s*, 3'- OCH_3), 3.82 (3H, *s*, 3- OCH_3), 3.79 (1H, *dd*, $J = 4.0, 11.0$ Hz, H-9'a), 3.73 (1H, *dd*, $J = 6.0, 11.0$ Hz, H-9'b), 2.85 (1H, *m*, H-7'), 2.07 (1H, *m*, H-8'), 1.94 (1H, *tt*, $J = 3.0, 10.0$ Hz, H-8). ^{13}C NMR (125 Hz, CD_3OD) data (Table S2).

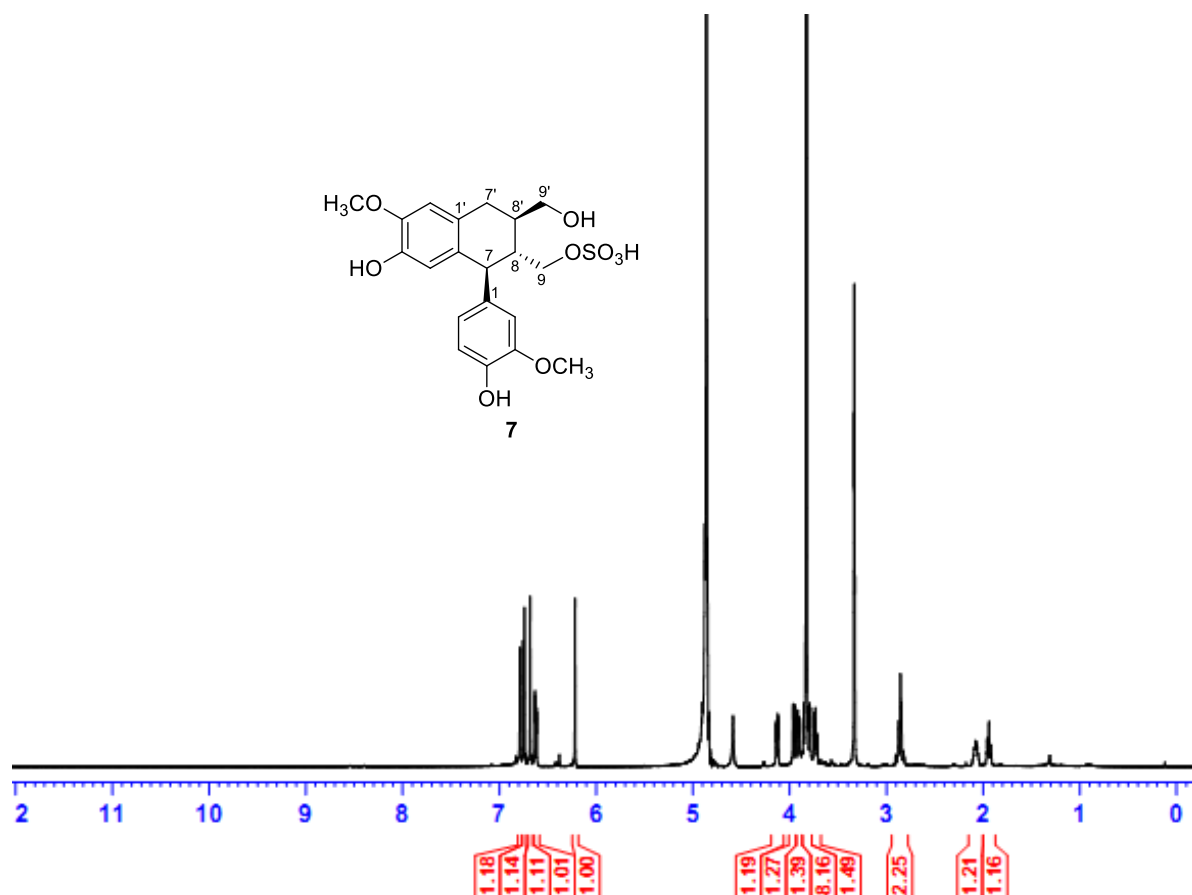


Figure S44: ^1H -NMR (500 MHz, CD_3OD) Spectrum of (+)-isolarisiresinol-9-*O*-sulfate (**7**)

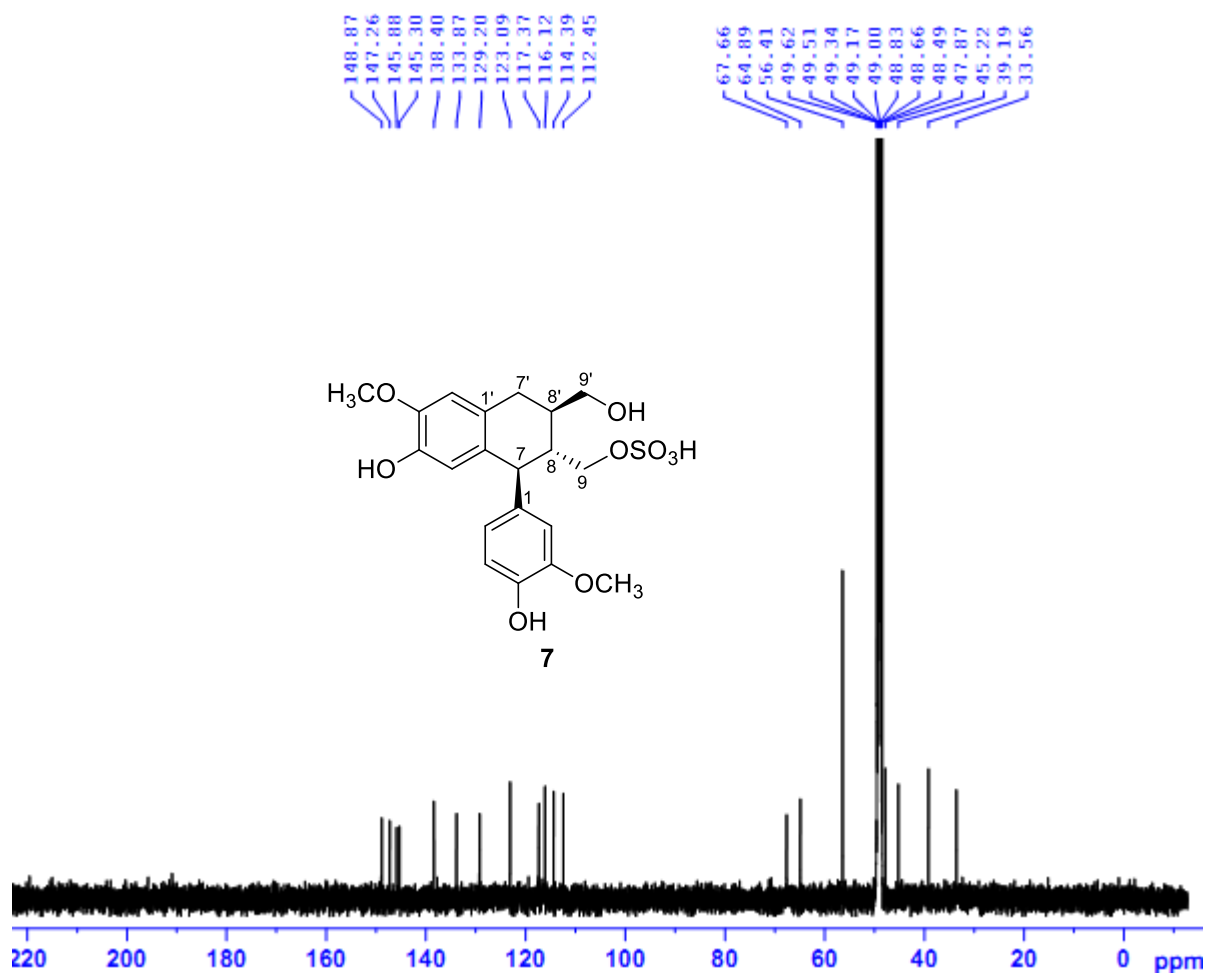


Figure S45: ¹³C-NMR (125 MHz, CD₃OD) Spectrum of (+)-isolarisiresinol-9-O-sulfate (7)

Isotachioside (8): ^1H NMR (500 MHz, CD_3OD) δ_{H} 7.03 (1H, *d*, $J = 8.5$ Hz, H-6), 6.49 (1H, *d*, $J = 2.5$ Hz, H-3), 6.32 (1H, *dd*, $J = 2.5, 8.5$ Hz, H-5), 4.71 (1H, *d*, $J = 8.5$ Hz, H-1'), 3.88 (1H, *dd*, $J = 2.5, 12.0$ Hz, H-6'a), 3.83 (3H, *s*, 2-OCH₃), 3.71 (1H, *dd*, $J = 5.5, 12.0$ Hz, H-6'b), 3.35-3.45 (4H, *m*, H-2', H-3', H-4', H-5'). ^{13}C NMR (125 MHz, CD_3OD) δ_{C} 154.9 (C-4), 152.0 (C-2), 141.0 (C-1), 120.5 (C-6), 107.6 (C-5), 104.3 (C-1'), 101.8 (C-3), 78.1 (C-3'), 77.8 (C-5'), 75.0 (C-2'), 71.4 (C-4'), 62.5 (C-6'), 56.5 (2-OCH₃).

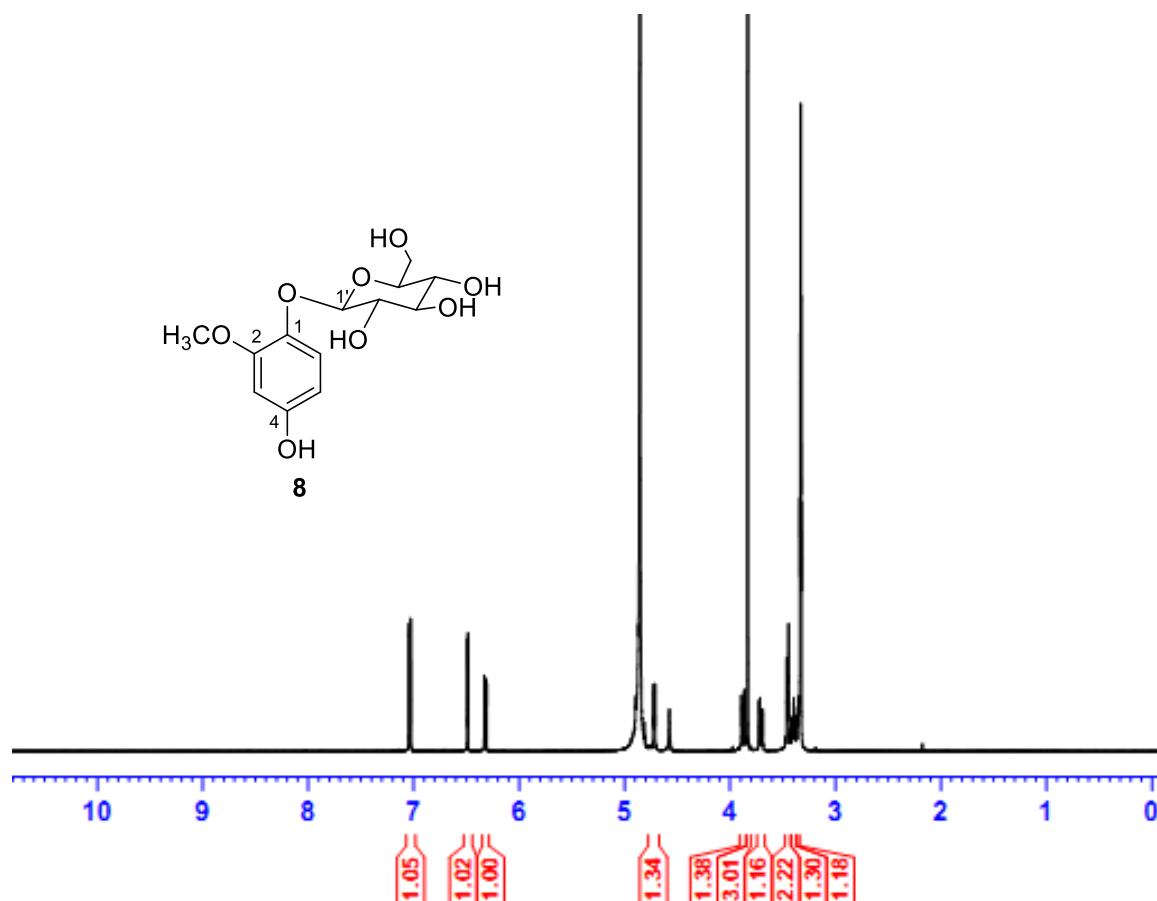


Figure S46: ^1H -NMR (500 MHz, CD_3OD) Spectrum of isotachioside (8)

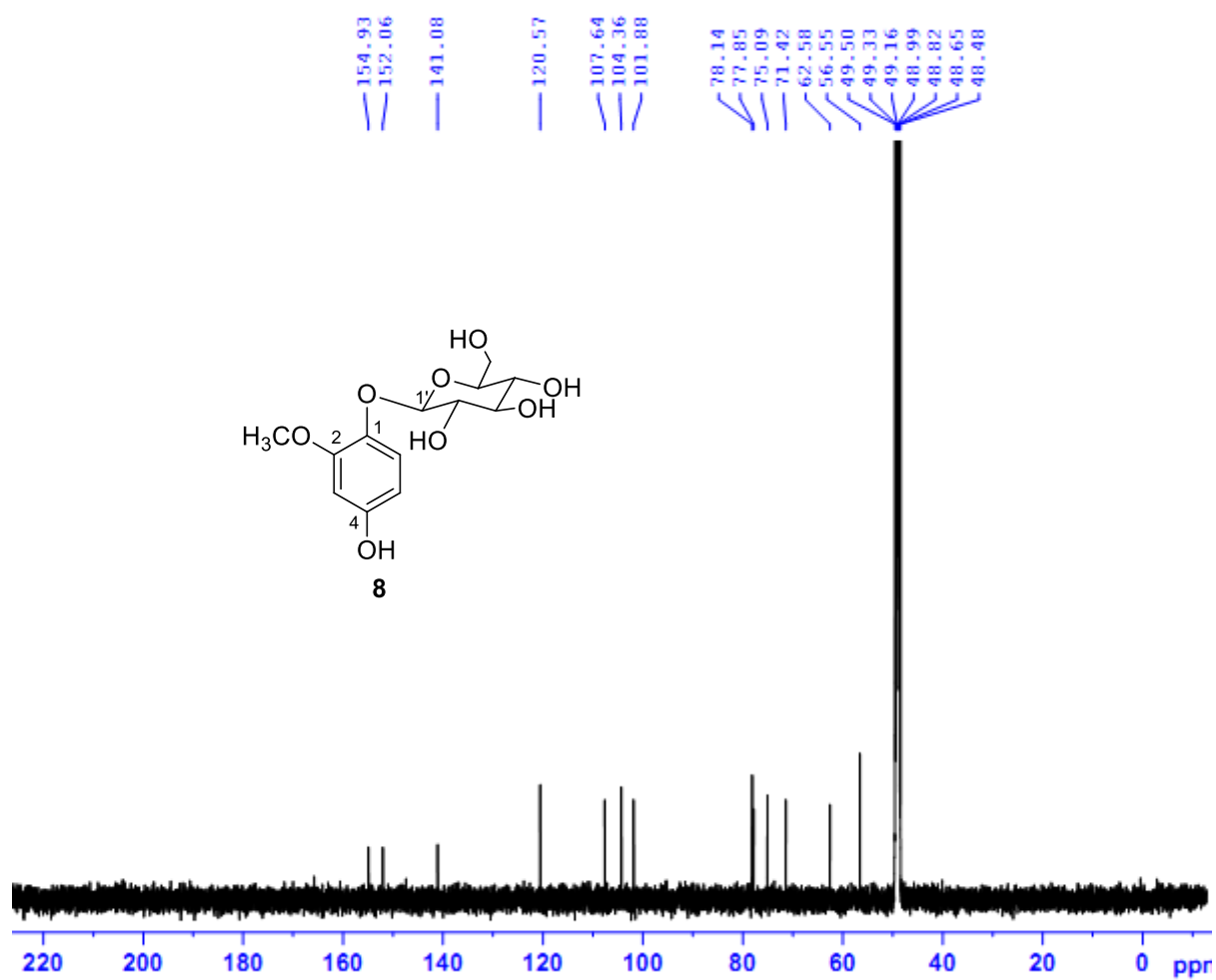
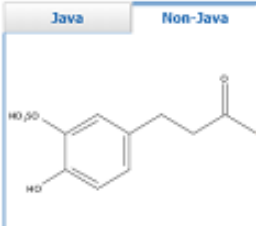


Figure S47: ¹³C-NMR (125 MHz, CD₃OD) Spectrum of isotachioside (8)

Structure Editor:

Java Non-Java




Click image to change structure or view detail.

[Import CXF](#)

Search Type:

- Exact Structure
- Substructure
- Similarity

Show precision analysis



Launch a SciFinder/SciFinder[®] substance or reaction search directly from the latest version of ChemDraw. [Learn More](#)

Select All Deselect All

1 of 6 Similarity Candidates Selected

	Substances
<input type="checkbox"/> ≥ 99 (most similar)	0
<input type="checkbox"/> 95-98	0
<input type="checkbox"/> 90-94	0
<input checked="" type="checkbox"/> 85-89	2
<input type="checkbox"/> 80-84	2
<input type="checkbox"/> 75-79	23
<input type="checkbox"/> 70-74	127
<input type="checkbox"/> 65-69	653
<input type="checkbox"/> 0-64 (least similar)	3509

[Get Substances](#)

Chemical Structure similarity > substances (2)

SUBSTANCES
Get References Get Reactions Get Commercial Sources Tools
Create Keep the Protocol Alert Send to SciFinder

Analyze Refine
Sort by: Similarity Score
0 of 2 substances selected

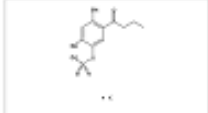
Analyze by: Substance Role

No substances available

Score: 85

1. 116936-62-6

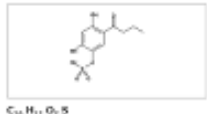
[Component: 605960-79-4]



C₁₂H₁₄O₃ · K
1-Butanone, 1-(2,4-dihydroxy-5-(sulfoxy)phenyl)-, potassium salt (1:1)

Score: 85

2. 805560-79-4

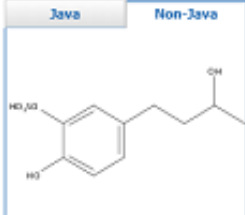


C₁₂H₁₄O₃ S
1-Butanone, 1-(2,4-dihydroxy-5-(sulfoxy)phenyl)-
[Key Physical Properties](#)

Figure S48: SciFinder Search Results of 1

Structure Editor:

Java Non-Java



Click image to change structure or view detail.

Import CXF


Search Type:

Exact Structure

Substructure

Similarity

Show precision analysis



Launch a SciFinder/SciFinder[®] substance or reaction search directly from the latest version of ChemDraw. [Learn More](#)

Select All Deselect All

0 of 5 Similarity Candidates Selected

	Substances
<input type="checkbox"/> ≥ 99 (most similar)	0
<input type="checkbox"/> 95-98	0
<input type="checkbox"/> 90-94	0
<input type="checkbox"/> 85-89	0
<input type="checkbox"/> 80-84	16
<input type="checkbox"/> 75-79	54
<input type="checkbox"/> 70-74	123
<input type="checkbox"/> 65-69	691
<input type="checkbox"/> 0-64 (least similar)	4116

[Get Substances](#)

Chemical Structure similarity > substances (16)

SUBSTANCES Get References Get Reactions Get Commercial Sources Tools

Analyze Refine Set by: Similarity Score Display Options

8 of 16 Substances Selected





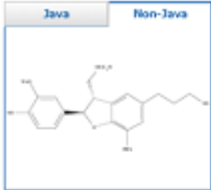
	Score: 84	Score: 84	Score: 84
Analyze by: Substance Role Biological Study: 32 Analytical Study: 11 Uses: 6 Properties: 5 Formulation: 4 Preparation: 2	1. 844626-92-5  $C_8H_{10}O_5S$ 1,2-Benzenediol, 4-(2-hydroxyethyl)-, 2-(hydrogen sulfate) > Key Physical Properties	2. 1291053-88-5 (Component: 844626-92-5)  $C_8H_{10}O_5S \cdot Na$ 1,2-Benzenediol, 4-(2-hydroxyethyl)-, 2-(hydrogen sulfate), sodium salt (1:1)	3. 2244993-32-7 (Component: 844626-92-5)  $C_8H_{10}O_5S \cdot K$ 1,2-Benzenediol, 4-(2-hydroxyethyl)-, 2-(hydrogen sulfate), potassium salt (1:1)
	4. 2415-66-7  $C_8H_{10}O_5S$ 1,2-Benzenediol, 4-(1,2-dihydroxyethyl)-, 1-(hydrogen sulfate) > Key Physical Properties		

Figure S49: SciFinder Search Results of 2

SUBSTANCES: CHEMICAL STRUCTURE

Structure Editor:




Click image to change structure or view detail.

Import CXF

[Advanced Search](#)

Search Type:
 Exact Structure
 Substructure
 Similarity

Show precision analysis

 **ChemDraw**
 Launch a SciFinder/SciFinder[®] substance or reaction search directly from the latest version of ChemDraw. [Learn More](#)

Select All Deselect All

1 of 7 Similarity Candidates Selected

Similarity Range	Substances
> 99 (most similar)	0
<input checked="" type="checkbox"/> 95-99	1
<input type="checkbox"/> 90-94	0
<input type="checkbox"/> 85-89	37
<input type="checkbox"/> 80-84	85
<input type="checkbox"/> 75-79	296
<input type="checkbox"/> 70-74	689
<input type="checkbox"/> 65-69	1349
<input type="checkbox"/> 0-64 (least similar)	6285

SUBSTANCES

Get References Get Reactions Get Commercial Sources Tools

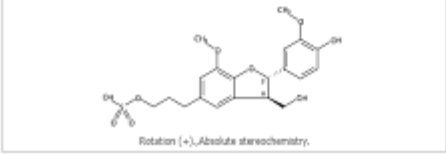
Create Keep File Printed Alert Send to SciFinder

Analyze Refine

Sort by: Similarity Score

0 of 1 Substance Selected

Score: 95
 1. [269708-17-6](#)



Rotarone (+), Absolute stereochemistry.

$C_{20}H_{24}O_5S$
 2,2-dihydro-2-(4-hydroxy-3-methoxyphenyl)-3-(hydroxymethyl)-7-methoxy-5H-benzofuran, (2S,3R)

[Key Physical Properties](#)

Figure S50: SciFinder Search Results of 3

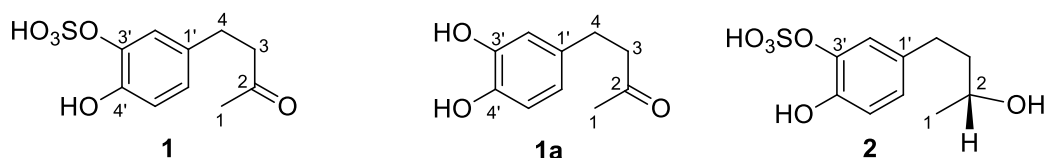


Table S1 : ^{13}C NMR (125 MHz) data for compounds **1**, **1a** and **2** in $\text{DMSO-}d_6$

Position	1	1a	2
1	29.1	30.3	23.5
2	207.7	208.4	65.2
3	44.3	45.1	41.0
4	28.1	28.9	30.6
1'	132.1	132.3	133.4
2'	122.8	115.9	122.8
3'	140.5	145.4	140.5
4'	147.2	143.7	146.9
5'	117.0	116.1	116.9
6'	124.5	119.1	124.5

1a: 4-(3',4'-dihydroxyphenyl)-2-butanone [T. T. Le, J. Yin, M. W. Lee (2017). Anti-inflammatory and anti-Oxidative activities of phenolic compounds from *Alnus sibirica* stems fermented by *Lactobacillus plantarum* subsp. *argentoratensis*, *Molecules* **22**, 1566-1574.]

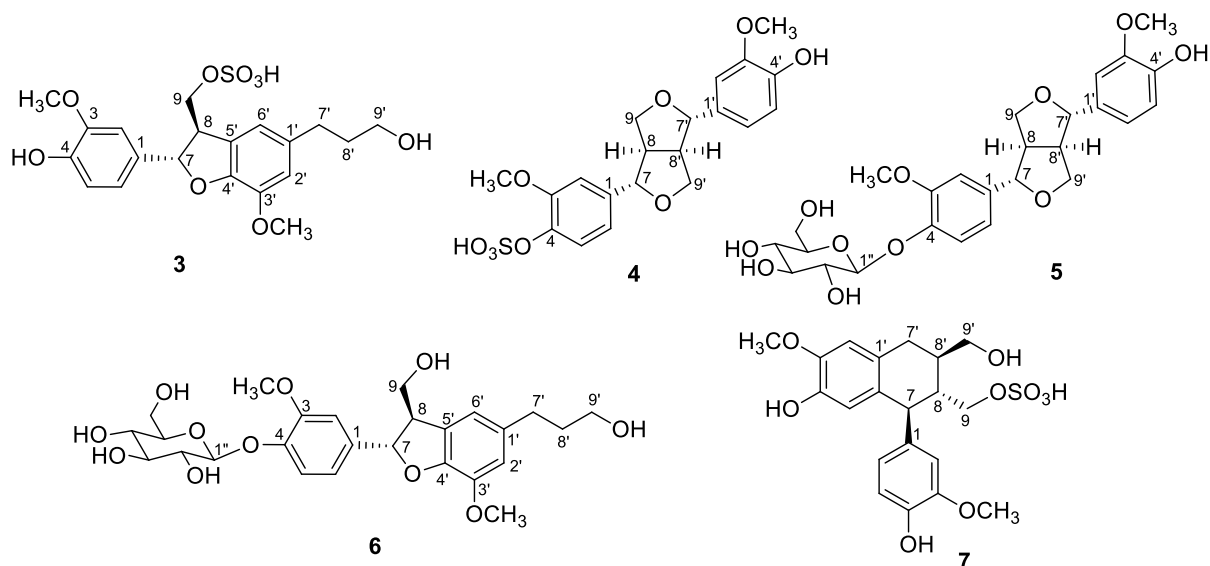


Table S2 : ^{13}C NMR (125 MHz) data for compounds **3-7**

Position	3^a	6^a	4^b	5^a	7^a
1	134.4	138.5	136.5	137.5	138.4
2	110.6	111.2	110.5	117.5	114.4
3	149.0	151.0	150.4	151.1	148.8
4	147.3	147.6	141.9	147.5	145.2
5	116.1	118.1	120.7	118.1	116.1
6	119.4	119.4	117.5	119.8	123.1
7	88.8	88.4	84.9	87.5	47.8
8	52.8	55.6	53.7	55.5	45.2
9	70.0	65.1	71.0	72.7	67.6
1'	137.1	137.1	132.1	133.7	129.2
2'	114.4	114.2	110.4	111.0	112.4
3'	145.2	145.2	147.5	148.0	147.2
4'	147.6	147.5	145.8	147.5	145.9
5'	128.8	129.6	115.1	116.1	117.4
6'	118.1	117.9	118.6	120.0	133.8
7'	32.8	32.9	85.2	87.1	33.5
8'	35.7	35.8	53.5	55.3	39.2
9'	62.2	62.2	70.9	72.6	64.9
OCH ₃	56.8	56.8	55.6	56.7	56.4
OCH ₃	56.4	56.7	55.5	56.4	56.4
1''		102.8		102.9	
2''		74.9		74.9	
3''		78.2		78.2	
4''		71.3		71.3	
5''		77.8		77.8	
6''		62.5		62.5	

^a Recorded in CD₃OD, ^b in DMSO-*d*₆

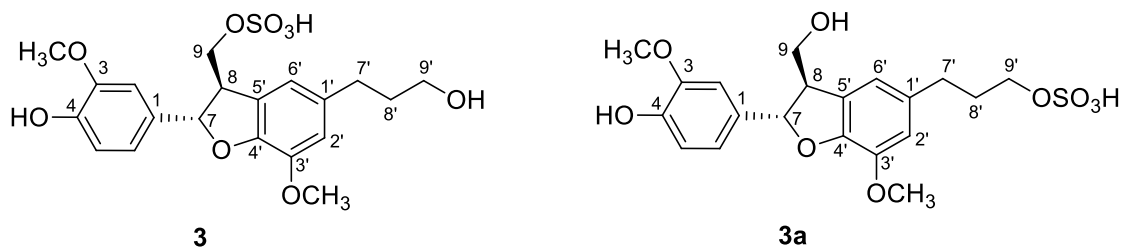


Table S3. ^1H NMR (500 MHz) and ^{13}C NMR (125 MHz) data for compounds **3** and **3a** in CD_3OD

Position	3		3a	
	δ_{C}	δ_{H} (J in Hz)	δ_{C}	δ_{H} (J in Hz)
1	134.4 (C)	-	135.0	-
2	110.6 (CH)	7.03 (1H, <i>d</i> , $J = 2.0$)	110.7	6.95 (1H, <i>d</i> , $J = 2.0$)
3	149.0 (C)	-	149.2	-
4	147.3 (C)	-	147.8	-
5	116.1 (CH)	6.77 (1H, <i>d</i> , $J = 8.0$)	116.2	6.77 (1H, <i>d</i> , $J = 8.0$)
6	119.4 (CH)	6.89 (1H, <i>dd</i> , $J = 2.0, 8.0$)	119.8	6.83 (1H, <i>dd</i> , $J = 2.0, 8.0$)
7	88.8 (CH)	5.60 (1H, <i>d</i> , $J = 6.0$)	89.1	5.50 (1H, <i>d</i> , $J = 6.0$)
8	52.8 (CH)	3.70 (1H, <i>m</i>)	55.5	3.84 (1H, <i>m</i>)
9	70.0 (CH_2)	4.30 (1H, <i>dd</i> , $J = 6.0, 10.5$) 4.19 (1H, <i>dd</i> , $J = 8.0, 10.5$)	65.0	3.47 (1H, <i>dd</i> , $J = 6.0, 11.0$) 3.76 (1H, <i>dd</i> , $J = 7.0, 11.0$)
1'	137.1 (C)	-	136.5	-
2'	114.4 (CH)	6.75 (1H, <i>s</i>)	114.9	6.68 (1H, <i>s</i>)
3'	145.2 (C)	-	145.3	-
4'	147.6 (C)	-	147.5	-
5'	128.8 (C)	-	129.9	-
6'	118.1 (CH)	6.79 (1H, <i>s</i>)	118.2	6.68 (1H, <i>s</i>)
7'	32.8 (CH_2)	2.64 (2H, <i>t</i> , $J = 7.5$)	32.7	2.68 (2H, <i>t</i> , $J = 7.0$)
8'	35.7 (CH_2)	1.84 (2H, <i>m</i>)	32.8	1.94 (2H, <i>m</i>)
9'	62.2 (CH_2)	3.58 (2H, <i>t</i> , $J = 6.5$)	68.2	4.01 (2H, <i>t</i> , $J = 6.0$)
3-OCH ₃	56.4 (CH_3)	3.85 (3H, <i>s</i>)	56.5	3.83 (3H, <i>s</i>)
3'-OCH ₃	56.8 (CH_3)	3.88 (3H, <i>s</i>)	36.9	3.87 (3H, <i>s</i>)

3a: Dihydrodehydrodiconiferyl alcohol 9'-*O*-sulfate [H. Otsuka, E. Hirata, T. Shinato, Y. Takeda (2000). Isolation of lignan glucosides and neolignan sulfate from the leaves of *Glochidion zeylanicum* (Gaertn) A. Juss, *Chem. Pharm. Bull.* **48**, 1084-1086].