

Supporting Information

Rec. Nat. Prod. X:X (2020) XX-XX

Two New Bibenzyl Compounds from *Dendrobium lindleyi*

Zhimei Shang^{1,3}, Xiaofei Li¹ and Shiji Xiao^{1,2,3*}

¹School of pharmacy, Zunyi Medical University, Zunyi, Guizhou 563000, P. R. China

²State Key Laboratory of Functions and Applications of Medicinal Plants, Guizhou Medical University, Guiyang 550014, P. R. China

³Key Laboratory of Basic Pharmacology of Ministry of Education and Joint International Research Laboratory of Ethnomedicine of Ministry of Education, Zunyi Medical University, Zunyi, Guizhou 563006, P. R. China

Table of Contents	Page
Figure S1: HR-ESI-MS Spectrum of 1	2
Figure S2: ¹ H-NMR (400 MHz, CDCl ₃) Spectrum of 1	2
Figure S3: ¹³ C-NMR (100 MHz, CDCl ₃) Spectrum of 1	3
Figure S4: HSQC Spectrum of 1	3
Figure S5: HSQC Spectrum of 1 (From δ _C 40 ppm to δ _C 90 ppm)	4
Figure S6: HSQC Spectrum of 1 (From δ _C 100 ppm to δ _C 120 ppm)	4
Figure S7: HMBC Spectrum of 1	5
Figure S8: HMBC Spectrum of 1 (From δ _C 80 ppm to δ _C 140 ppm)	5
Figure S9: ¹ H-NMR Spectrum (ABX system) (400 MHz, CDCl ₃) of 1	6
Figure S10: Scifinder Search Results of 1	6
Figure S11: HR-ESI-MS Spectrum of 2	7
Figure S12: ¹ H-NMR (400 MHz, CDCl ₃) Spectrum of 2	7
Figure S13: ¹ H-NMR Spectrum (ABX system) (400 MHz, CDCl ₃) of 2	8
Figure S14: ¹³ C-NMR (100 MHz, CDCl ₃) Spectrum of 2	8
Figure S15: ¹³ C-NMR (100 MHz, CDCl ₃) Spectrum of 2 (From δ _C 100 ppm to δ _C 140 ppm)	9
Figure S16: ¹ H- ¹ H COSY Spectrum of 2	9
Figure S17: HSQC Spectrum of 2	10
Figure S18: HSQC Spectrum of 2 (From δ _C 100 ppm to 130 ppm)	10
Figure S19: HMBC Spectrum of 2	11
Figure S20: HMBC Spectrum of 2 (From δ _C 100 ppm to 130 ppm)	11
Figure S21: Scifinder Search Results of 2	12
Table S1: ¹³ C NMR Spectral Data of Dendrophenol, Nobilin A, 1 , and 2	13
Table S2: ¹ H NMR Spectral Data of Dendrophenol, Nobilin A, 1 , and 2	14

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Monoisotopic Mass, Even Electron Ions
8476 formula(e) evaluated with 48 results within limits (up to 50 best isotopic matches for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-200 O: 0-200 S: 0-6 Cl: 0-8

Mass	Calc. Mass	mDa	PPM	DBE	Formula	C	H	N	O	S	Cl	Br
319.1164	319.1200	-3.6	-11.3	6.5	C3 H11 N16 O3	3	11	16	3			
	319.1168	-0.4	-1.3	14.5	C14 H11 N10	14	11	10				
	319.1128	3.6	11.3	10.5	C9 H11 N12 O2	9	11	12	2			
	319.1195	-3.1	-9.7	13.5	C18 H15 N4 O2	18	15	4	2			
	319.1155	0.9	2.8	9.5	C13 H15 N6 O4	13	15	6	4			
	319.1115	4.9	15.4	5.5	C8 H15 N8 O6	8	15	8	6			
	319.1187	-2.3	-7.2	1.5	C2 H15 N12 O7	2	15	12	7			
	319.1187	-1.8	-5.6	8.5	C17 H10 O6	17	10		6			



Figure S1: HR-ESI-MS Spectrum of 1

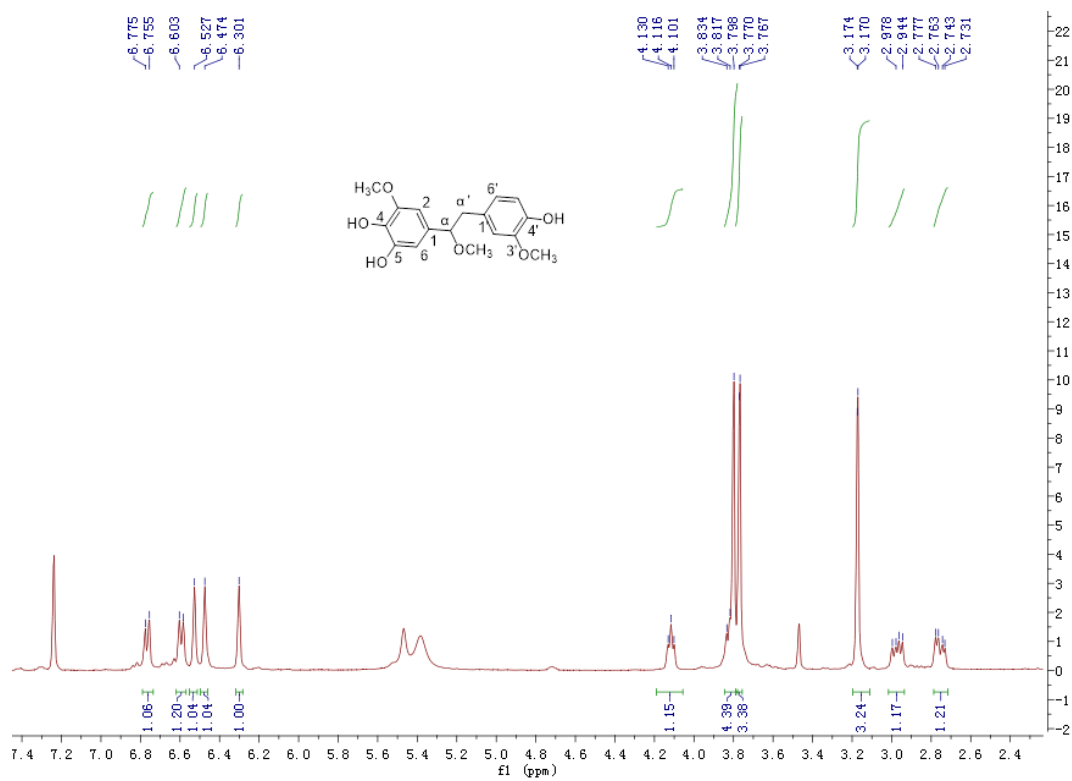


Figure S2: ¹H-NMR (400 MHz, CDCl₃) Spectrum of 1

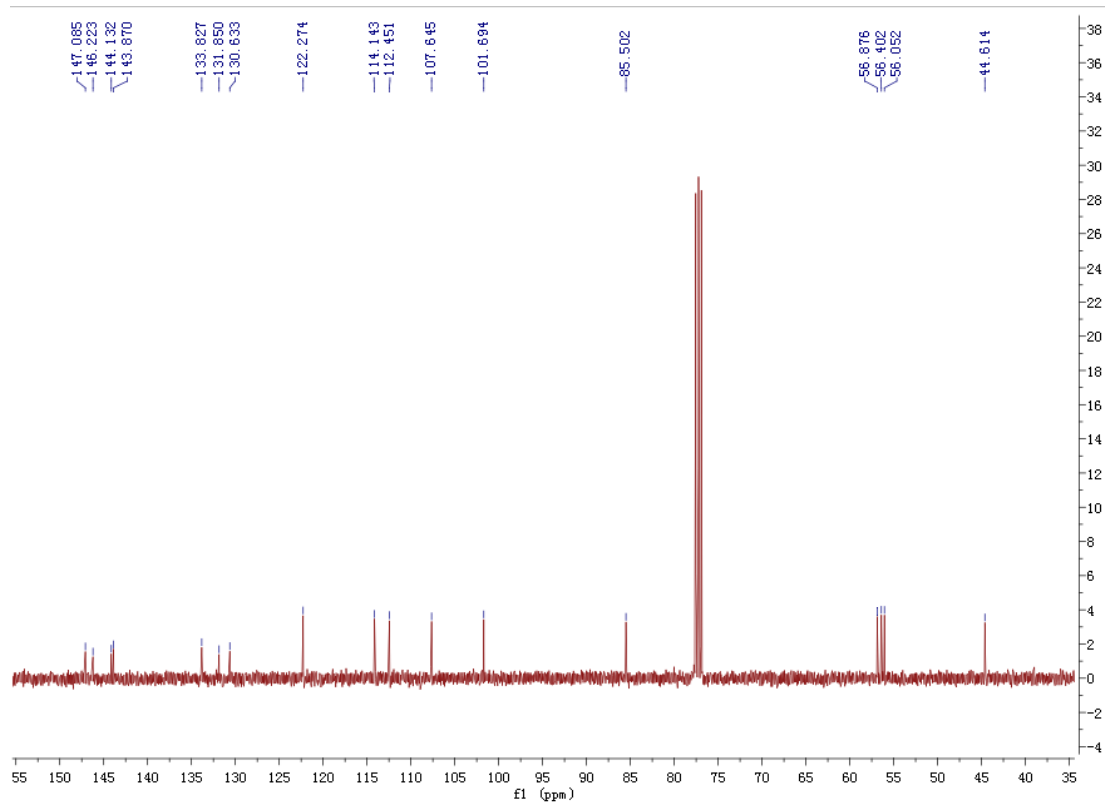


Figure S3: ^{13}C -NMR (100 MHz, CDCl_3) Spectrum of **1**

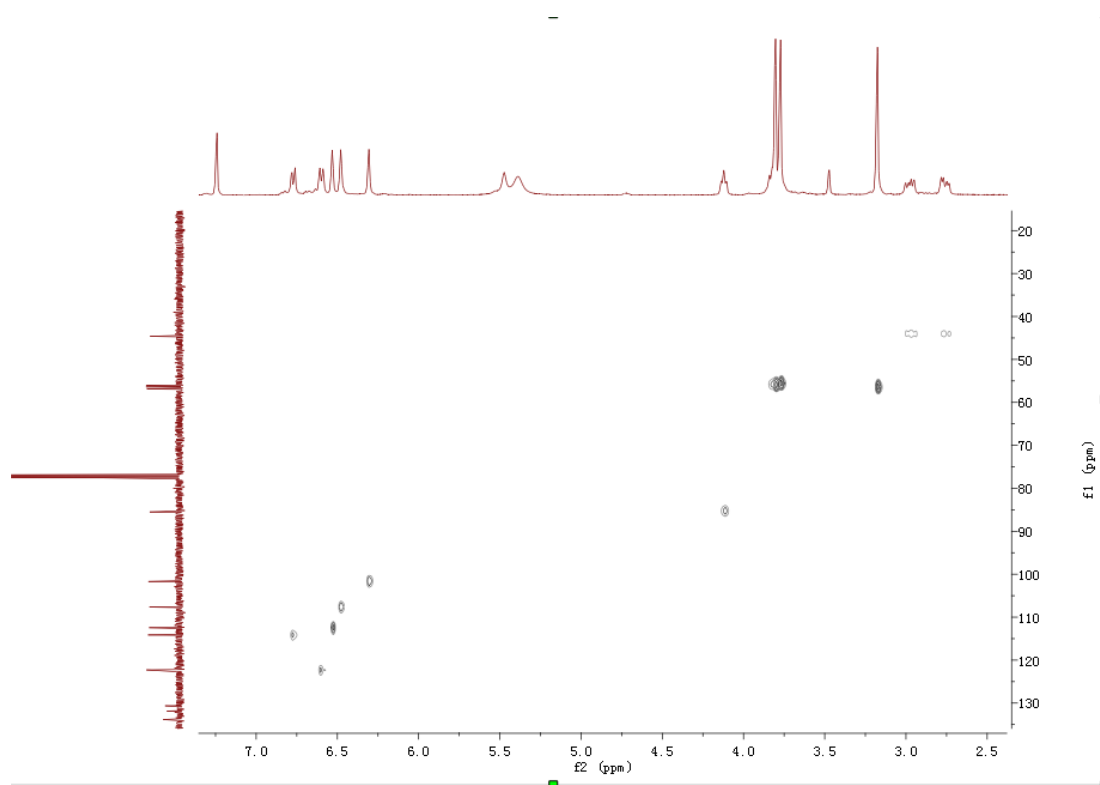


Figure S4: HSQC Spectrum of **1**

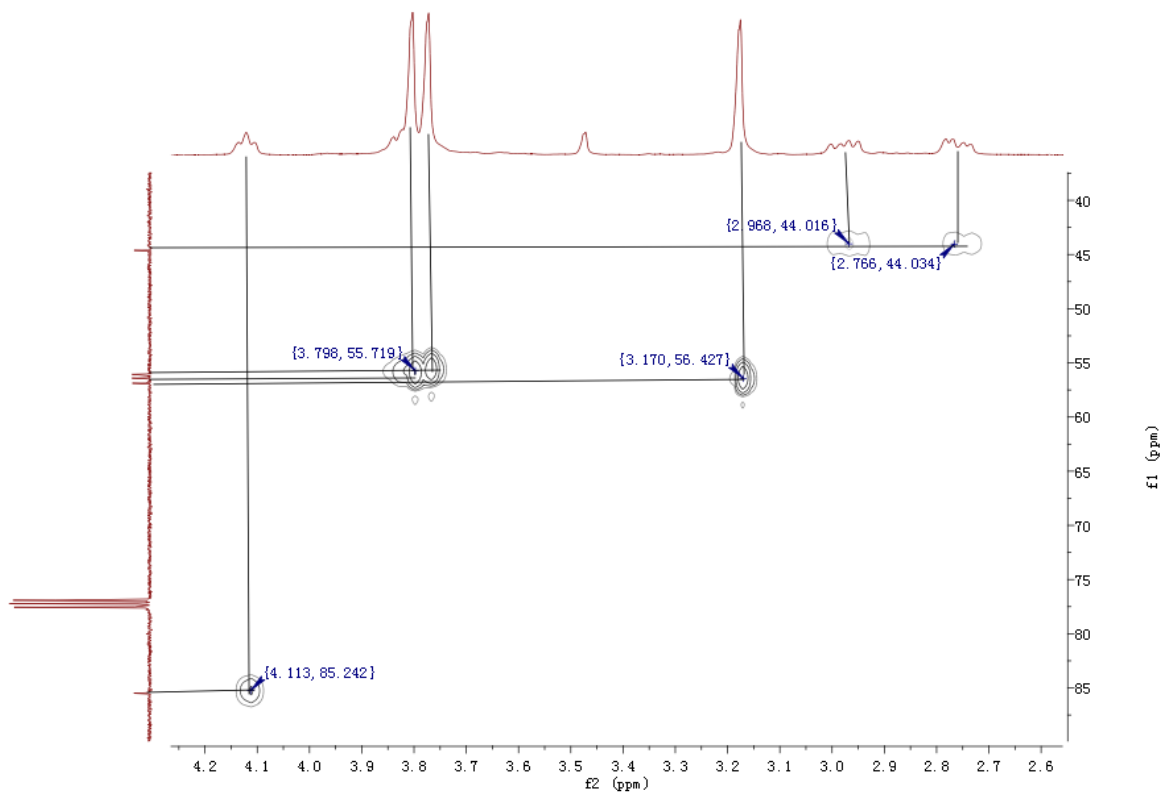


Figure S5: HSQC Spectrum of **1** (From δ_C 40 ppm to δ_C 90 ppm)

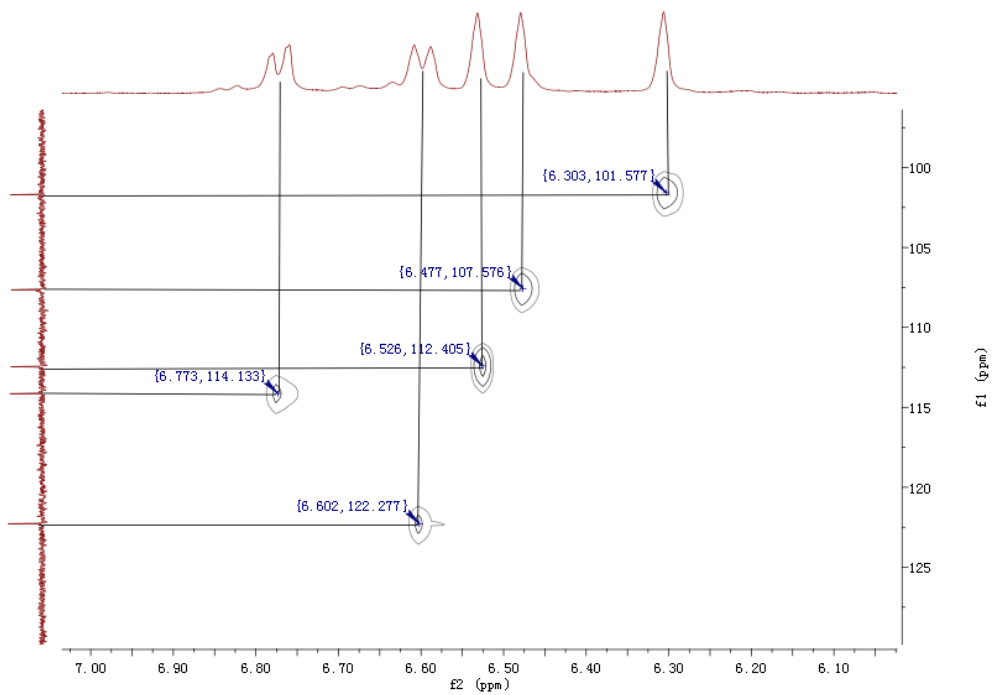


Figure S6: HSQC Spectrum of **1** (From δ_C 100 ppm to δ_C 120 ppm)

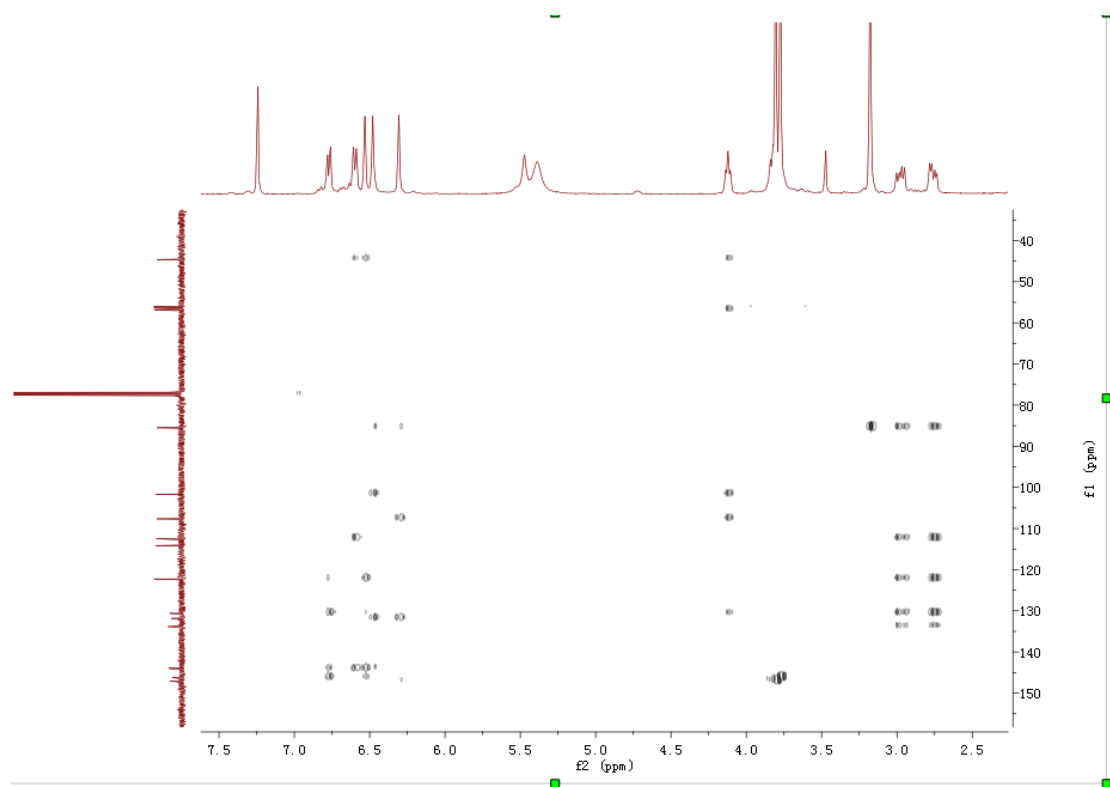
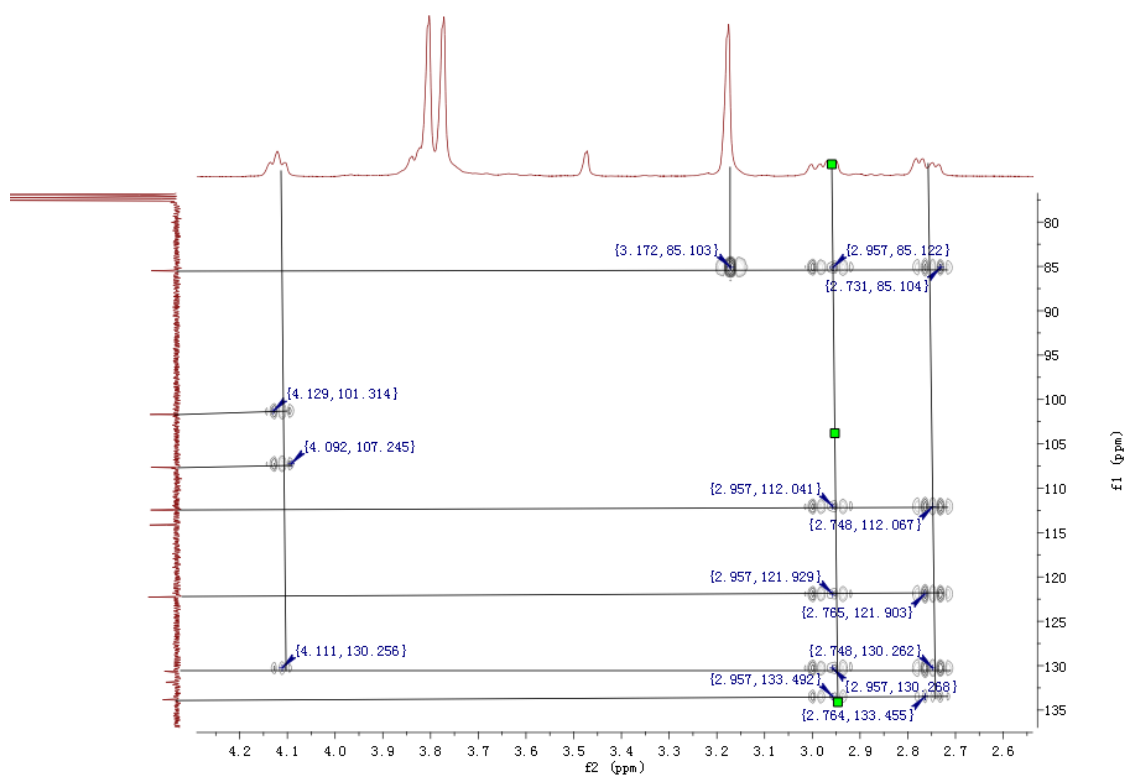


Figure S7: HMBC Spectrum of 1



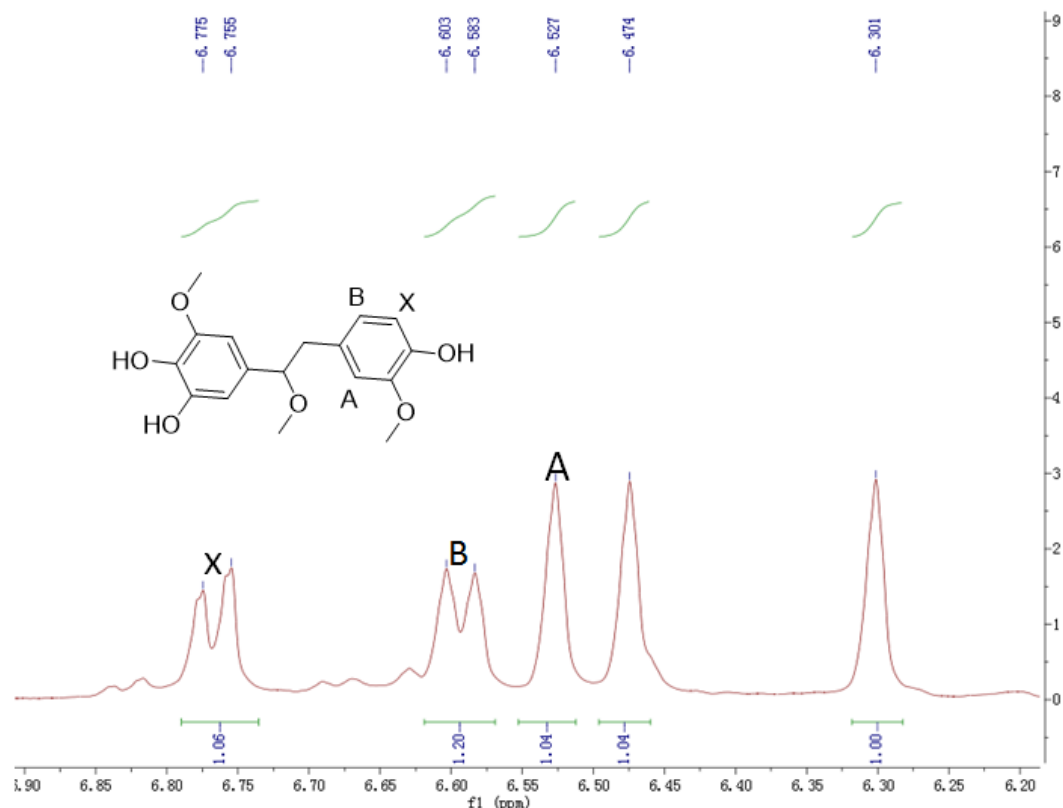


Figure S9: ¹H-NMR Spectrum (ABX system) (400 MHz, CDCl₃) of 1

SciFinder®		Page 1
<p>Score: 99</p> <p>1. 2227104-05-2</p> <p>Absolute stereochemistry.</p> <p>C₁₇H₂₀O₆ 1,2-Benzenediol, 5-[(1R)-2-(4-hydroxy-3-methoxyphenyl)-1-methoxyethyl]-3-methoxyphenyl]-1-methoxyethyl]-3-methoxyphenyl</p> <p>Key Physical Properties: Molecular Weight 320.34 Boiling Point (Predicted) Value: 486.4±45.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.282±0.06 g/cm³ Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 9.18±0.15 Condition: Most Acidic Temp: 25 °C Related Info: ~ 1 References</p>	<p>Score: 99</p> <p>3. 934266-43-0</p> <p>Currently available stereo shown., Rotation (+).</p> <p>C₁₇H₂₀O₅ 1,2-Benzenediol, 3-methoxy-5-[1-methoxy-2-(3-methoxyphenyl)ethyl]-, (+)-</p> <p>Key Physical Properties: Molecular Weight 304.34 Boiling Point (Predicted) Value: 443.2±45.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.210±0.06 g/cm³ Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 9.19±0.15 Condition: Most Acidic Temp: 25 °C Related Info: ~ 2 References</p>	<p>Score: 99</p> <p>4. 1073603-64-1</p> <p>C₁₇H₂₀O₅ Phenol, 4-[2-(3-hydroxyphenyl)-1-methoxyethyl]-2,6-dimethoxy-</p> <p>Key Physical Properties: Molecular Weight 304.34 Boiling Point (Predicted) Value: 437.1±45.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.210±0.06 g/cm³ Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 9.89±0.10 Condition: Most Acidic Temp: 25 °C Related Info: ~ 1 References</p>
<p>Score: 99</p> <p>5. 1104820-01-0</p>	<p>Score: 97</p> <p>6. 934266-44-1</p>	<p>Score: 97</p> <p>7. 1157923-80-2</p>

Figure S10: Scifinder Search Results of 1

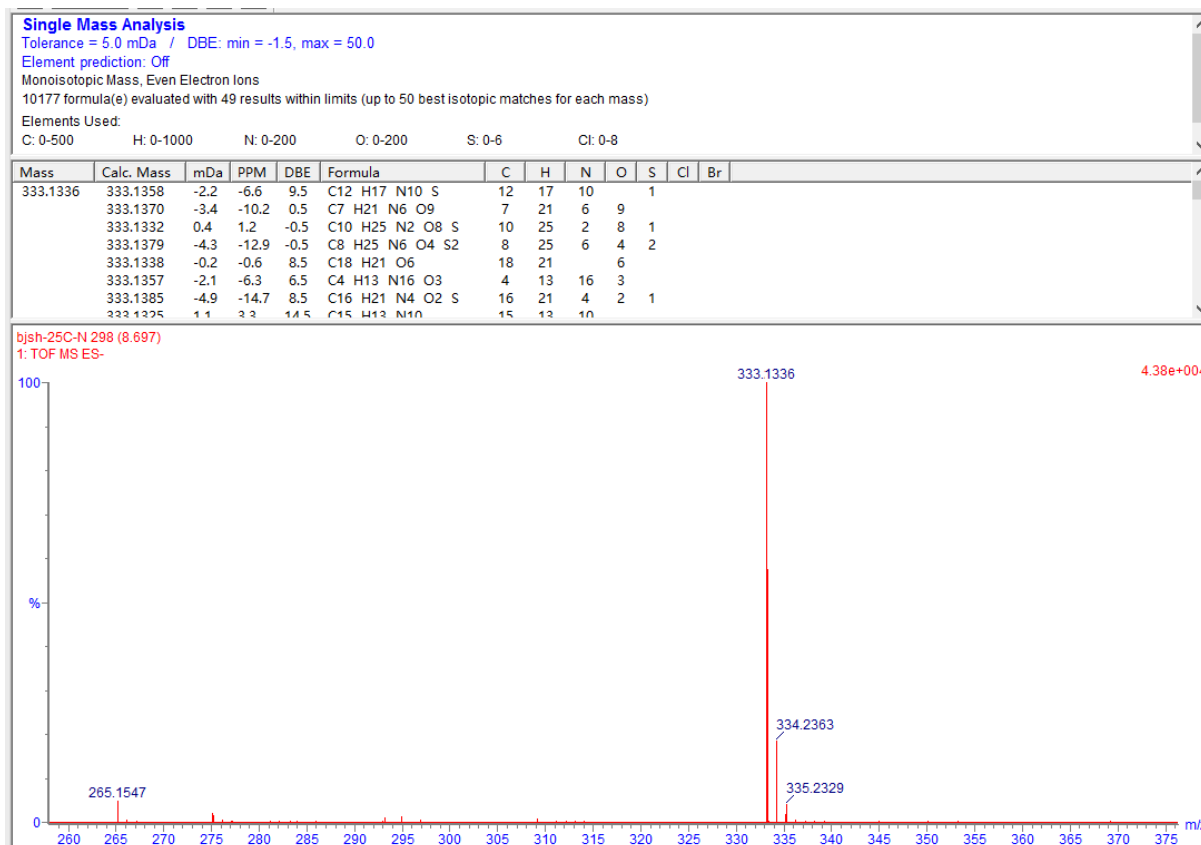


Figure S11: HR-ESI-MS Spectrum of 2

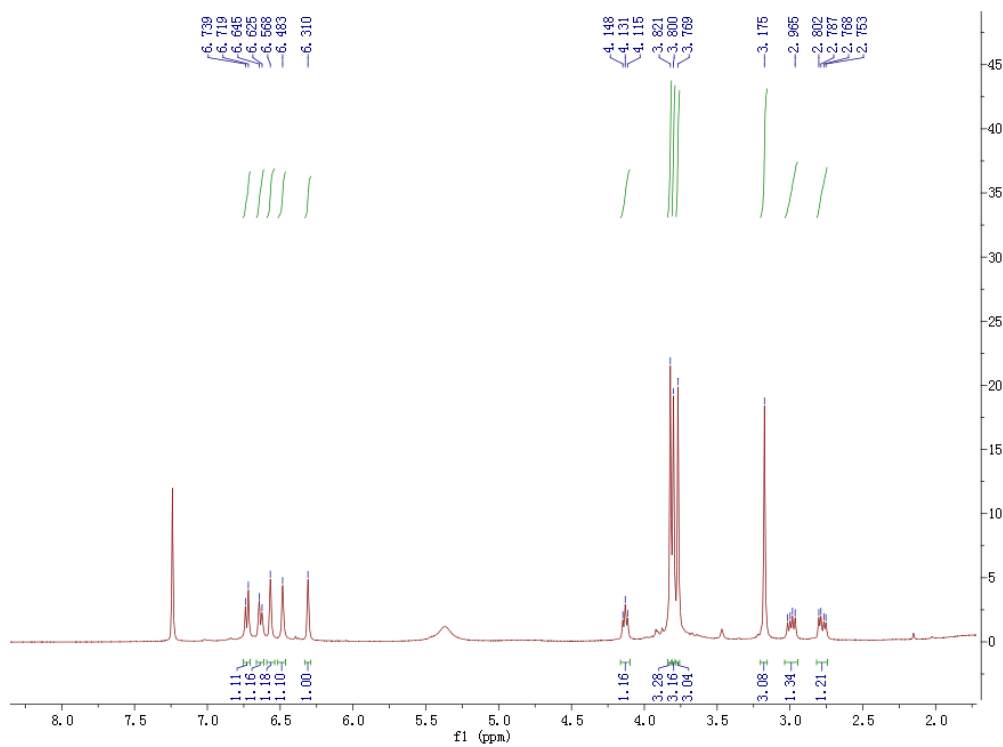


Figure S12: ¹H-NMR (400 MHz, CDCl₃) Spectrum of 2

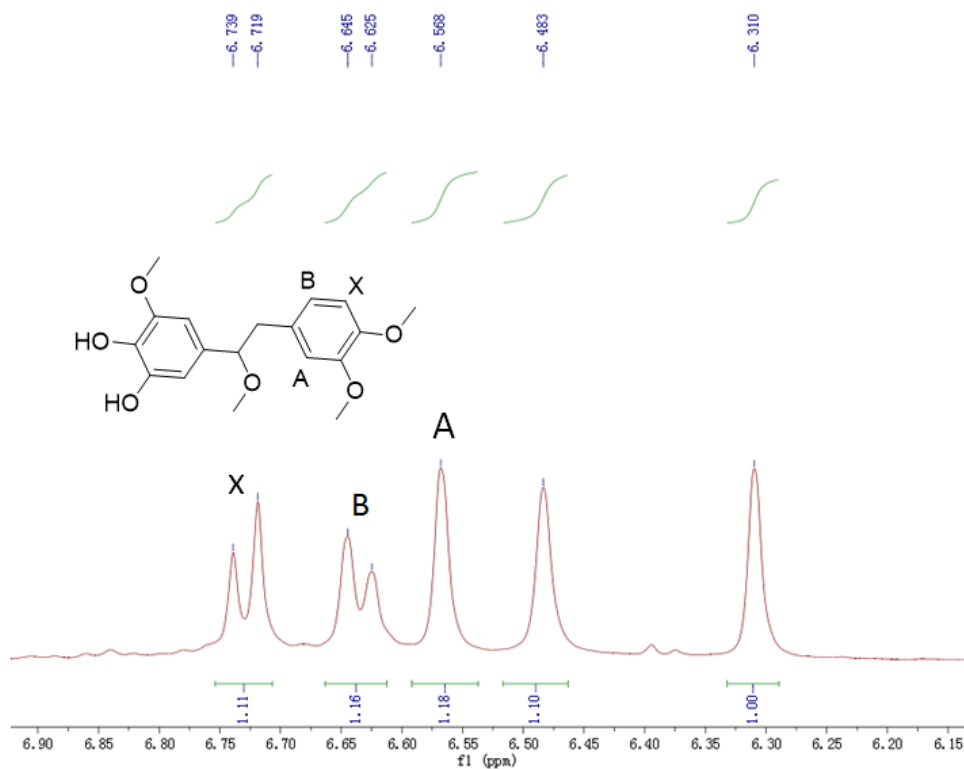


Figure S13: ¹H-NMR Spectrum (ABX system) (400 MHz, CDCl₃) of **2**

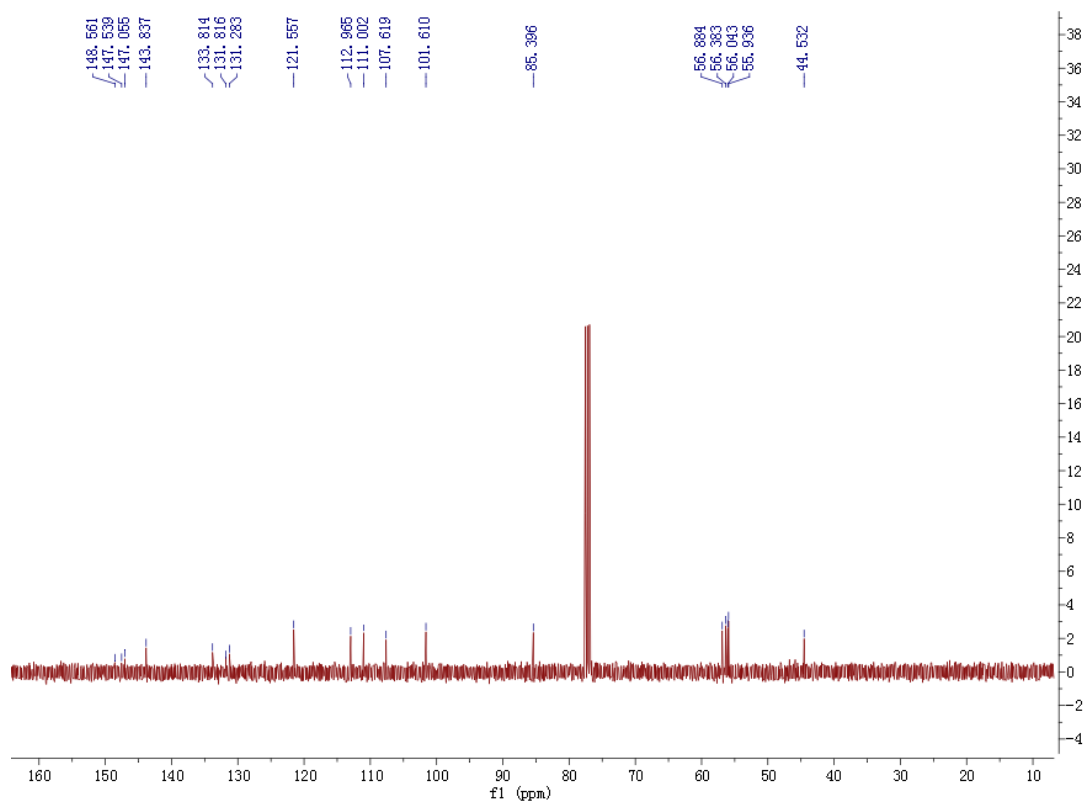


Figure S14: ¹³C-NMR (100 MHz, CDCl₃) Spectrum of **2**

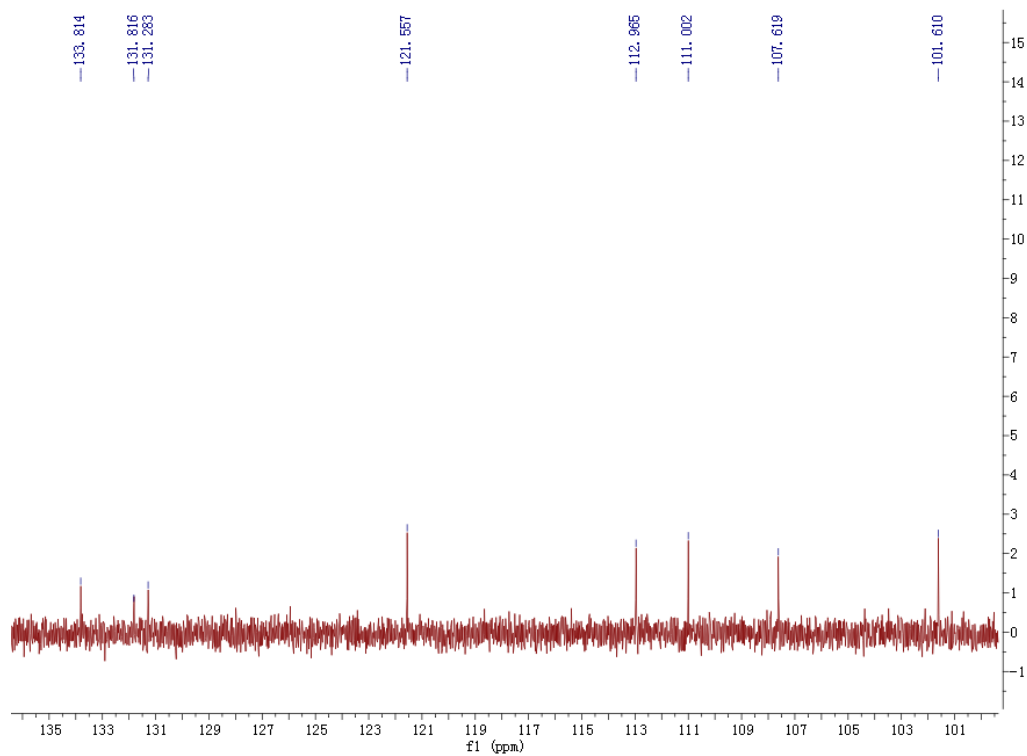


Figure S15: ^{13}C -NMR (100 MHz, CDCl_3) Spectrum of **2** (From $\delta_{\text{C}} 100$ ppm to $\delta_{\text{C}} 140$ ppm)

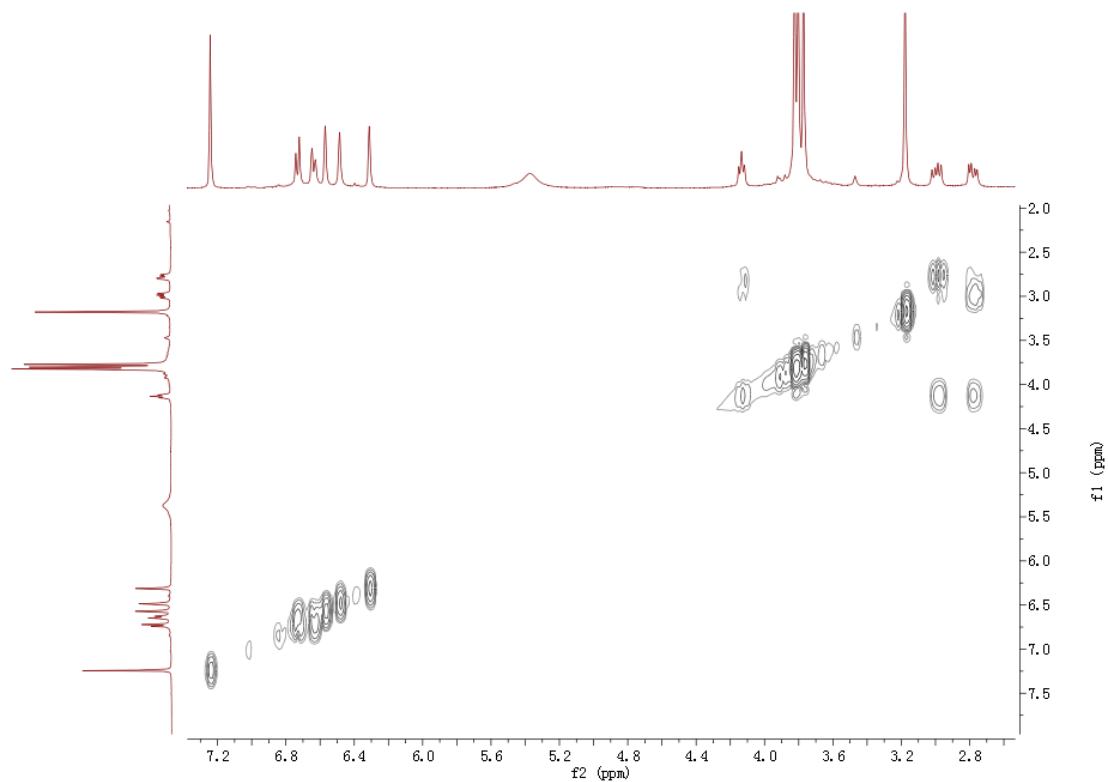


Figure S16: ^1H - ^1H COSY Spectrum of **2**

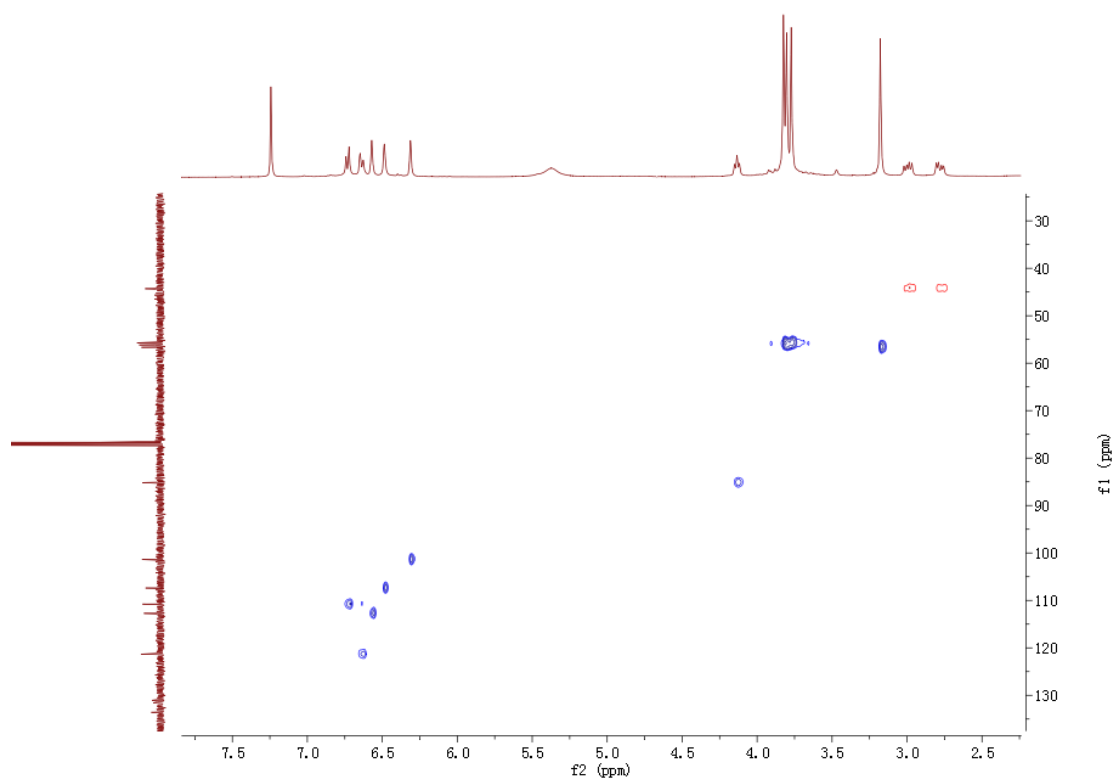


Figure S17: HSQC Spectrum of 2

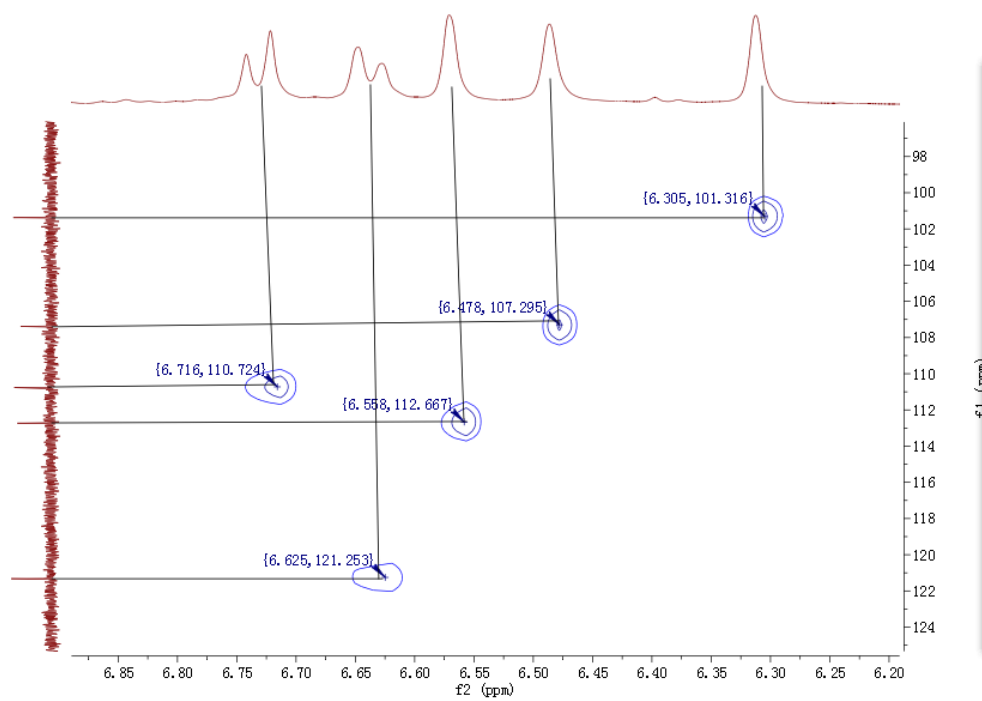


Figure S18: HSQC Spectrum of 2 (From δ_C 100 ppm to 130 ppm)

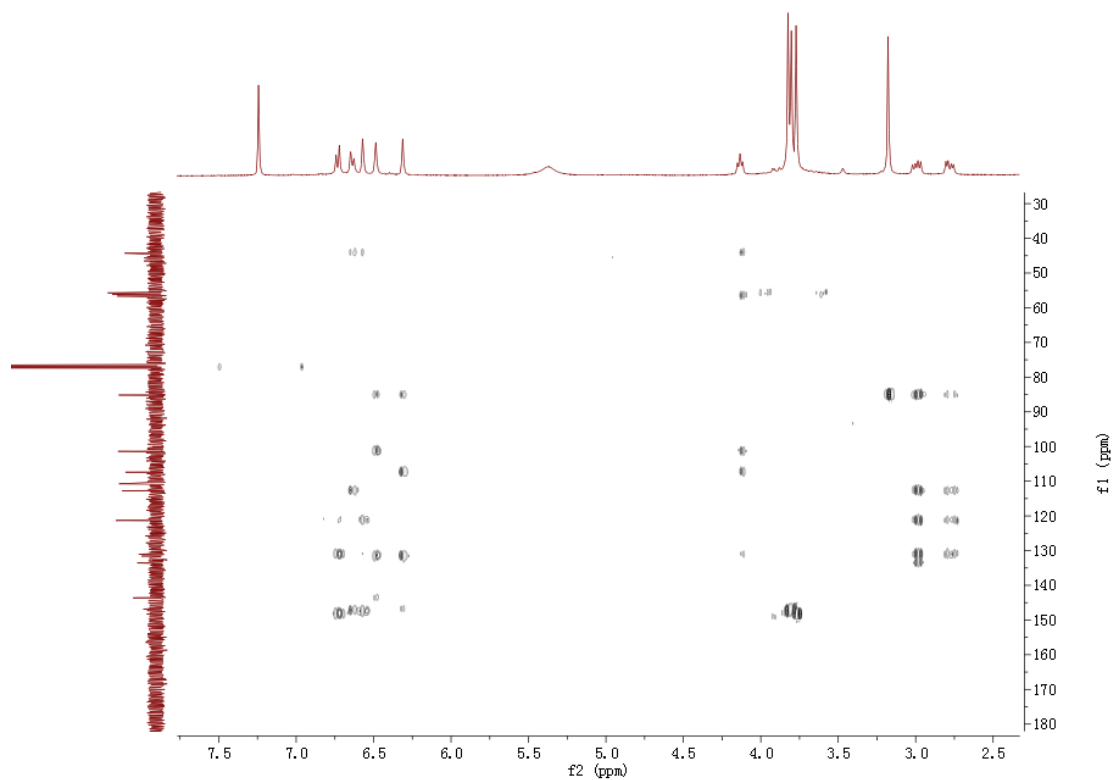


Figure S19: HMBC Spectrum of 2

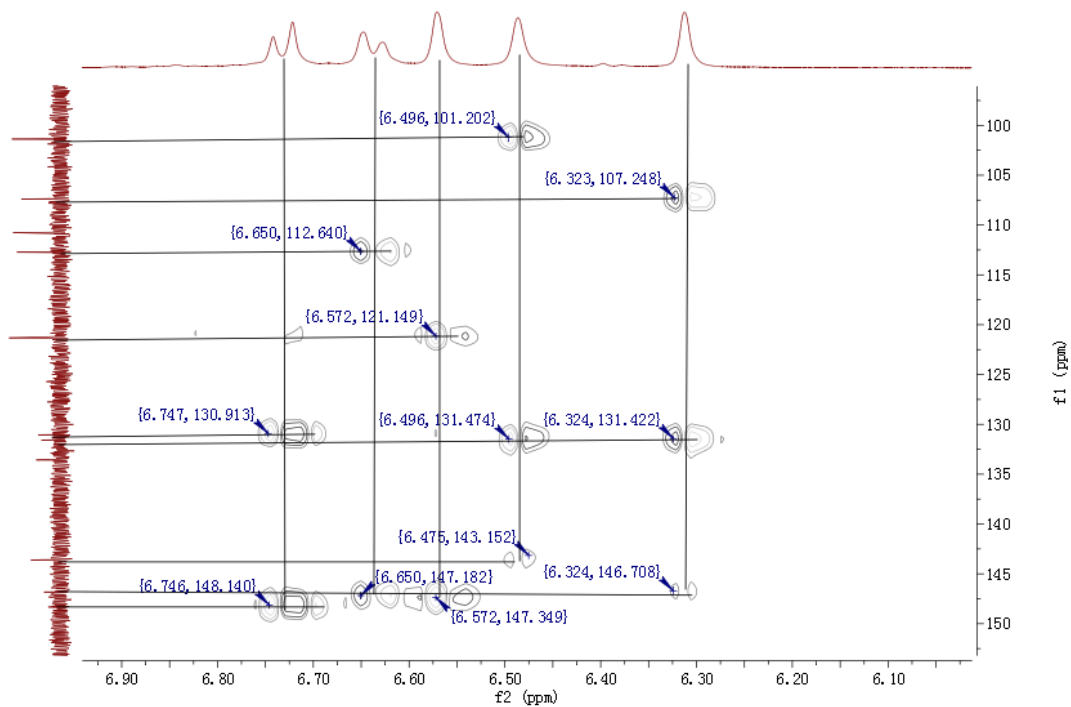
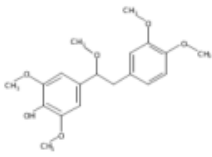
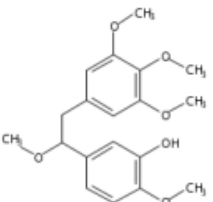
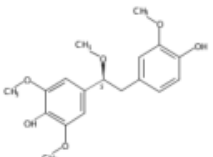
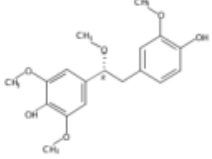
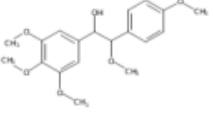
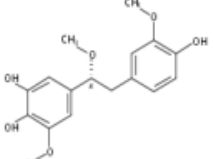
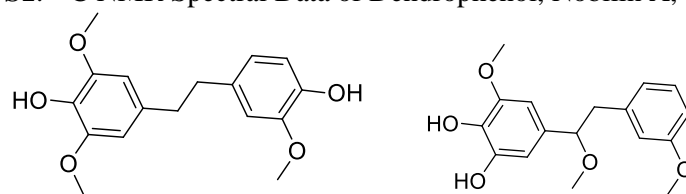


Figure S20: HMBC Spectrum of 2 (From δ_C 100 ppm to 130 ppm)

<p>Score: 99</p> <p>1.</p> <p>934266-45-2</p>  <p>Currently available stereo shown., Rotation (+).</p> <p>C₁₉ H₂₄ O₆ Phenol, 4-[2-(3,4-dimethoxyphenyl)-1-methoxyethyl]-2,6-dimethoxy-, (+)-</p> <p>Key Physical Properties: Molecular Weight 348.39 Boiling Point (Predicted) Value: 444.0±45.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.157±0.06 g/cm³ Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 9.97±0.36 Condition: Most Acidic Temp: 25 °C</p> <p>Related Info: ~ 2 References</p>	<p>Score: 99</p> <p>2.</p> <p>956699-51-7</p>  <p>C₁₉ H₂₄ O₆ Phenol, 2-methoxy-5-[1-methoxy-2-(3,4,5-trimethoxyphenyl)ethyl]-</p> <p>Key Physical Properties: Molecular Weight 348.39 Boiling Point (Predicted) Value: 453.8±45.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.157±0.06 g/cm³ Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 9.71±0.10 Condition: Most Acidic Temp: 25 °C</p> <p>Related Info: ~ 1 References Reactions</p>	<p>Score: 99</p> <p>3.</p> <p>934266-44-1</p>  <p>Rotation (+), Absolute stereochemistry.</p> <p>C₁₈ H₂₂ O₆ Phenol, 4-[(1S)-2-(4-hydroxy-3-methoxyphenyl)-1-methoxyethyl]-2,6-dimethoxy-</p> <p>Key Physical Properties: Molecular Weight 334.36 Boiling Point (Predicted) Value: 460.5±45.0 °C Condition: Press: 760 Torr Density (Predicted) Value: 1.213±0.06 g/cm³ Condition: Temp: 20 °C Press: 760 Torr pKa (Predicted) Value: 9.98±0.36 Condition: Most Acidic Temp: 25 °C</p> <p>Related Info: ~ 3 References</p>
<p>Score: 99</p> <p>4.</p> <p>1252577-64-2</p>  <p>Rotation (-), Absolute stereochemistry.</p> <p>C₁₈ H₂₂ O₆ Phenol, 4-[(1R)-2-(4-hydroxy-3-methoxyphenyl)-1-methoxyethyl]-2,6-dimethoxy-</p> <p>Key Physical Properties: Molecular Weight</p>	<p>Score: 97</p> <p>5.</p> <p>1638839-33-4</p>  <p>C₁₉ H₂₄ O₆ Benzeneethanol, β,4-dimethoxy-α-(3,4,5-trimethoxyphenyl)-</p> <p>Key Physical Properties: Molecular Weight 348.39 Boiling Point (Predicted) Value: 465.2±45.0 °C Condition: Press: 760</p>	<p>Score: 96</p> <p>6.</p> <p>2227104-05-2</p>  <p>Absolute stereochemistry.</p> <p>C₁₇ H₂₀ O₆ 1,2-Benzenediol, 5-[(1R)-2-(4-hydroxy-3-methoxyphenyl)-1-methoxyethyl]-3-methoxy-</p> <p>Key Physical Properties:</p>

SciFinder Search Results of 2

Table S1: ^{13}C NMR Spectral Data of Dendrophenol, Nobilin A, **1**, and **2**

Dendrophenol

Nobilin A

No.	Dendrophenol ^[1]	1	Nobilin A ^[2]	2
1	133.8	133.8	133.8	133.8
2	105.3	101.7	101.5	101.6
3	147.0	147.1	147.1	147.1
4	132.9	131.9	131.8	131.8
5	147.0	144.1	143.8	143.8
6	105.3	107.6	107.6	107.6
α	38.7	85.5	85.1	85.4
α'	38.1	44.6	45.0	44.5
1'	133.0	130.6	140.4	131.3
2'	114.3	112.5	115.2	113.0
3'	146.4	146.2	159.5	148.6
4'	143.9	143.9	111.8	147.5
5'	111.4	114.1	129.2	111.0
6'	121.2	122.3	122.0	121.6
3-OCH ₃	56.4	56.4	56.4	56.4
5-OCH ₃	56.4			
3'-OCH ₃	56.0	56.1	55.3	55.9
4'-OCH ₃				56.0
α -OCH ₃		56.9	56.9	56.9

Table S2: ¹H NMR Spectral Data of Dendrophenol, Nobilin A, **1**, and **2**

No.	Dendrophenol ^[1]	1	Nobilin A ^[2]	2
2	6.36 (1H, s)	6.30 (1H, br.s)	6.34 (1H, d, 1.7)	6.31 (1H, br.s)
6	6.36 (1H, s)	6.47 (1H, br.s)	6.51 (1H, d, 1.7)	6.48 (1H, br.s)
α	2.81 (2H, m)	4.12 (1H, m)	4.19 (1H, dd, 7.5, 5.7)	4.13 (1H, br.t, 6.5)
α'	2.81 (2H, m)	2.75 (1H, dd, 13.4, 5.7) 2.97 (1H, dd, 13.4, 7.3)	2.83 (1H, dd, 13.8, 5.7) 3.04 (1H, dd, 13.8, 7.5)	2.78 (1H, dd, 13.7, 5.8) 2.99 (1H, dd, 13.7, 7.3)
2'	6.61 (1H, d, 1.8)	6.53 (1H, br.s)	6.66 (1H, m)	6.57 (1H, br.s)
5'	6.84 (1H, d, 8.0)	6.76 (1H, d, 8.0)	6.73 (1H, m)	6.73 (1H, d, 8.1)
6'	6.68 (1H, dd, 8.0, 1.8)	6.59 (1H, br.d, 8.0)	6.71 (1H, m)	6.63 (1H, br.d, 8.1)
3-OCH ₃	3.84 (3H, s)	3.80 (3H, s)	3.83 (3H, s)	3.80 (3H, s)
5-OCH ₃	3.84 (3H, s)			
3'-OCH ₃	3.84 (3H, s)	3.77 (3H, s)	3.75 (3H, s)	3.77 (3H, s)
4'-OCH ₃				3.82 (3H, s)
α-OCH ₃		3.17 (3H, s)	3.19 (3H, s)	3.18 (3H, s)

References

- [1] Li MF, Hirata Y, Xu GJ, M. Niwa and H.M. Wu (1991). Studies on the chemical constituents of *Dendrobium loddogesii* Rolfe, *Acta Pharm. Sin.* (药学报). **26**, 307–310.
- [2] Zhang X, Gao H, Wang NL and X.S. Yao (2006). Three new bibenzyl derivatives from *Dendrobium nobile*, *J Asian Nat. Prod. Res.* **8**, 113–118.