Supporting Information

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Two New Bibenzyl Compounds from *Dendrobium lindleyi*

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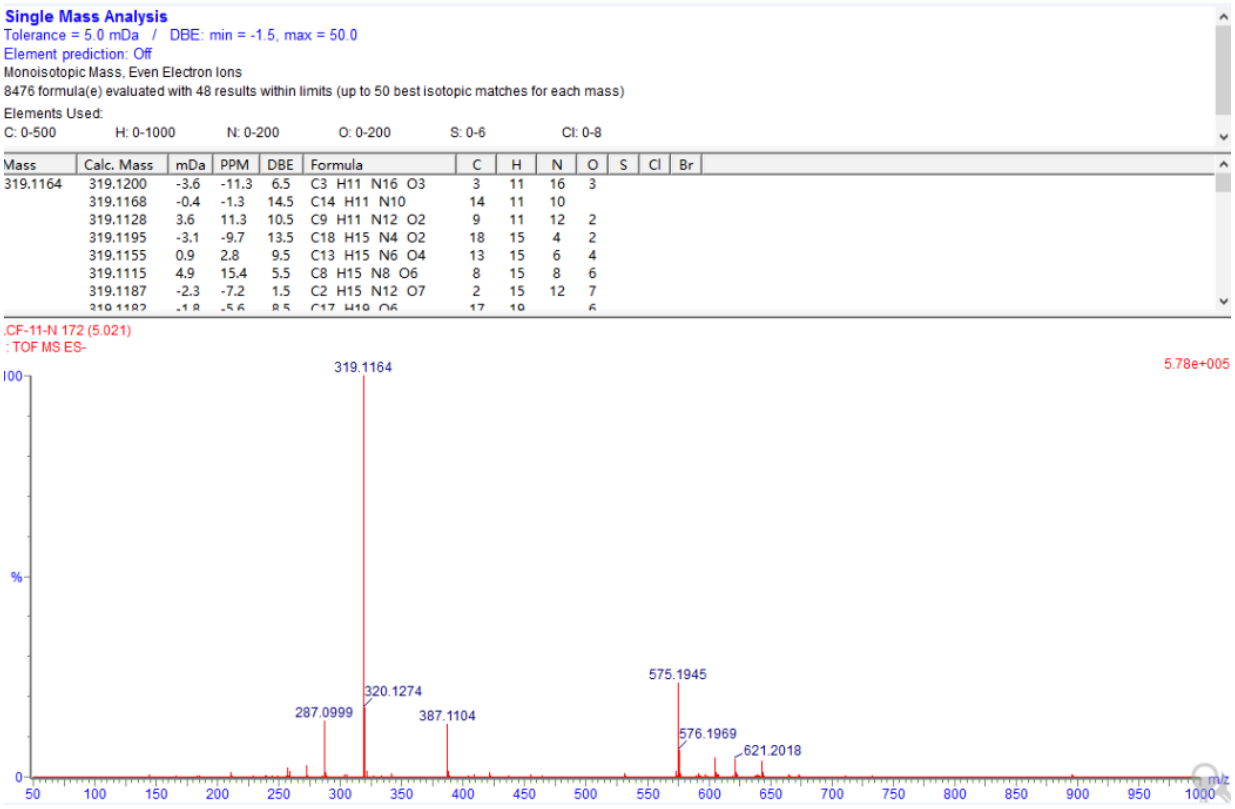


Figure S1: HR-ESI-MS Spectrum of **1**

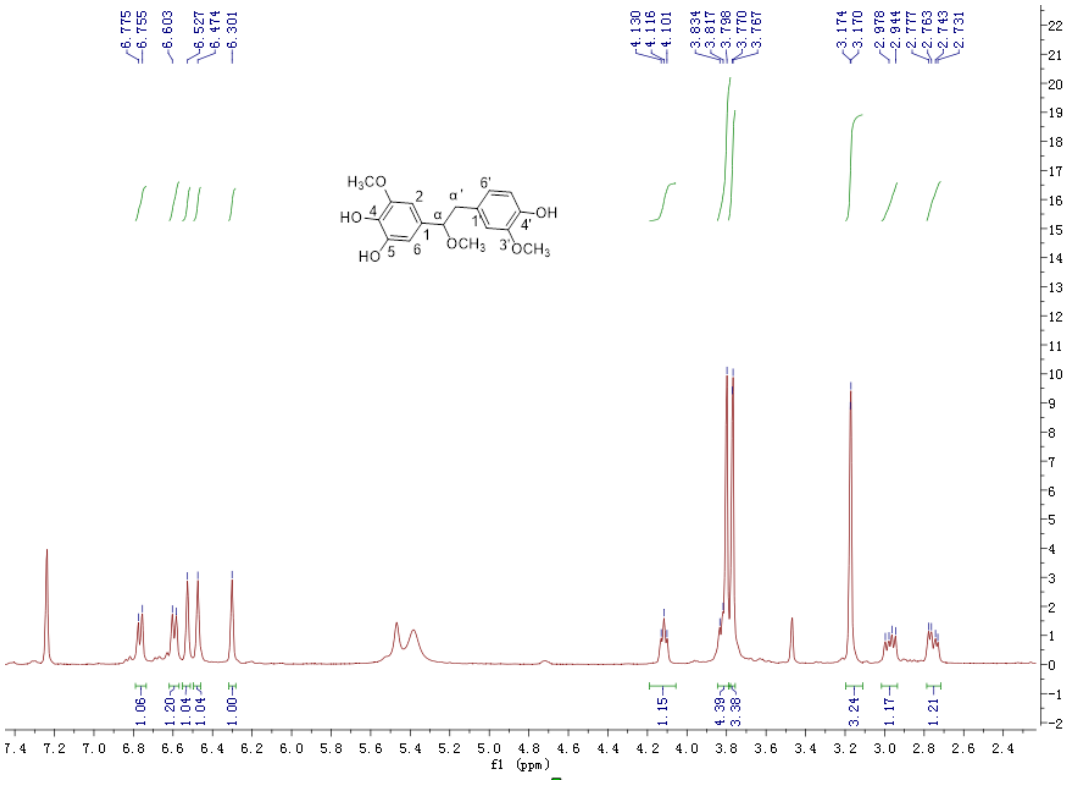


Figure S2: ^{1}H-NMR (400 MHz, $CDCl_3$) Spectrum of **1**

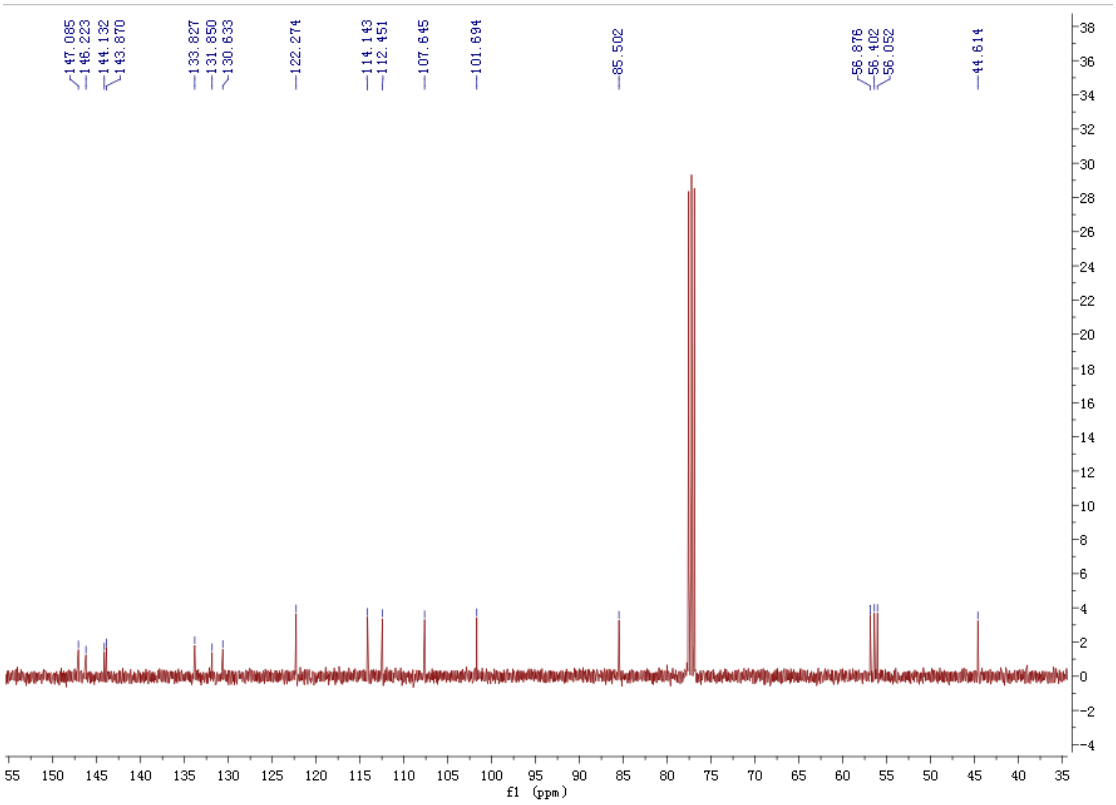


Figure S3: ^{13}C-NMR (100 MHz, $CDCl_3$) Spectrum of **1**

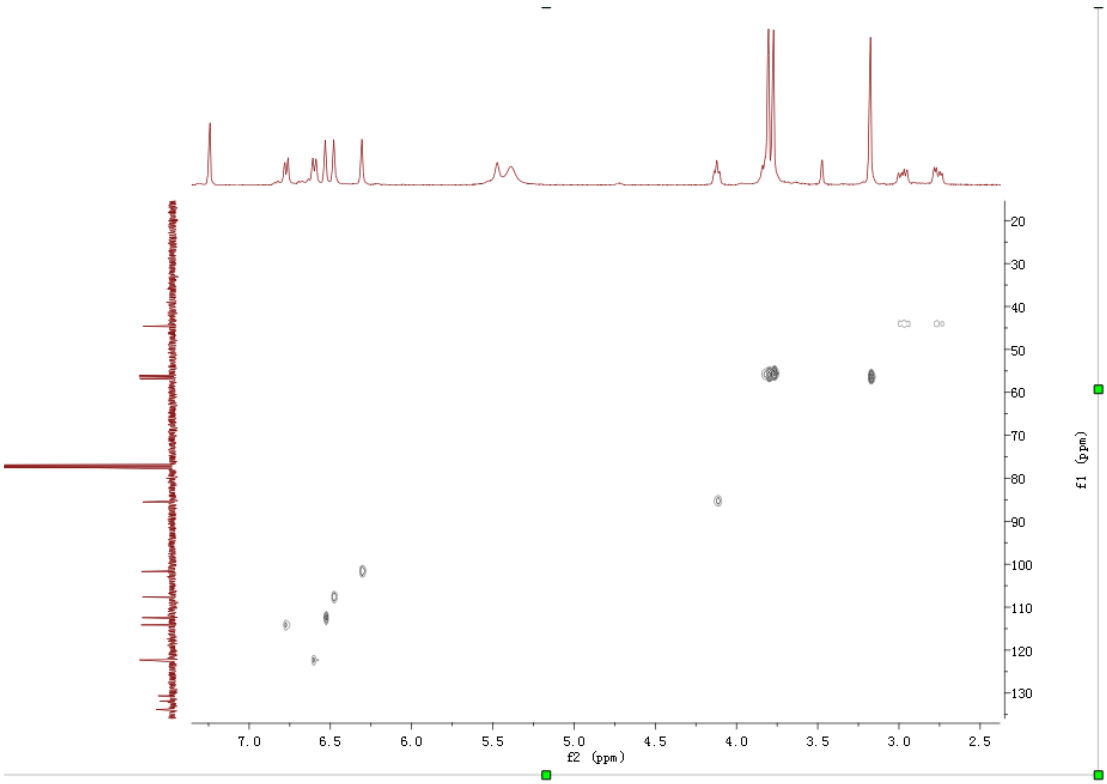


Figure S4: HSQC Spectrum of **1**

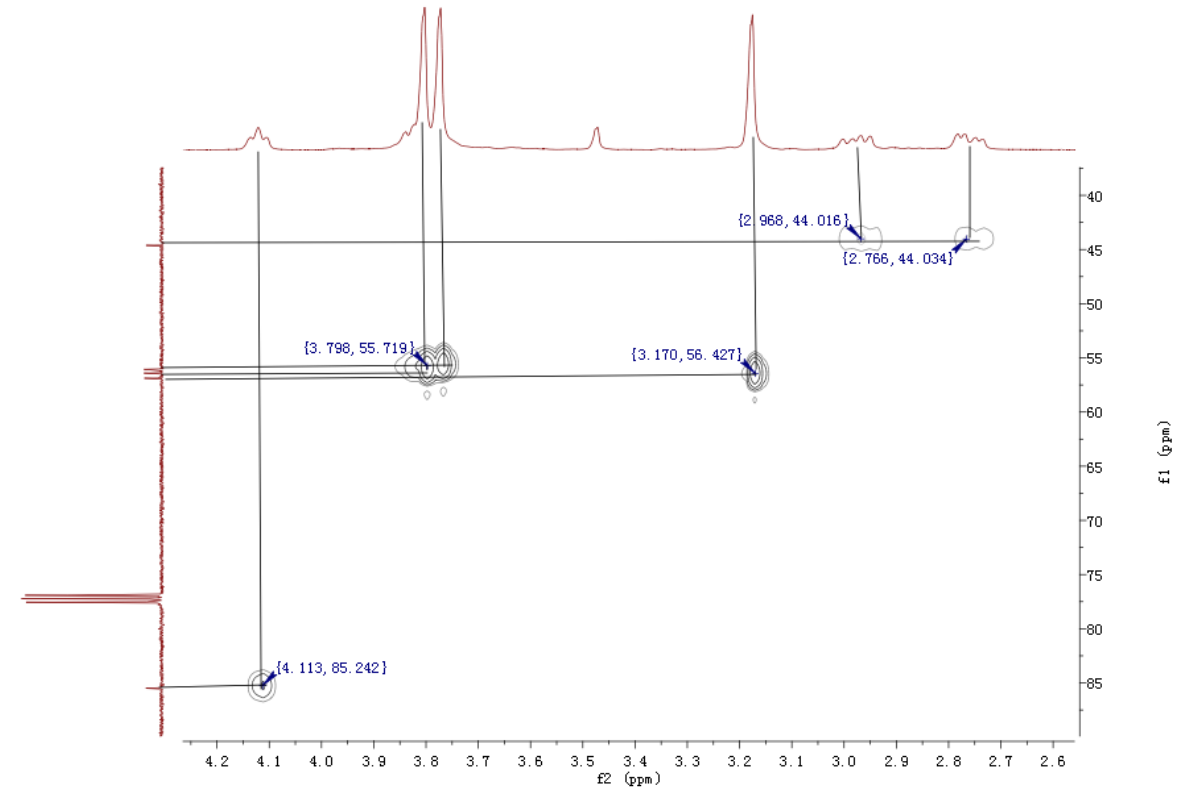


Figure S5: HSQC Spectrum of **1** (From δ_C40 ppm to δ_C 90 ppm)

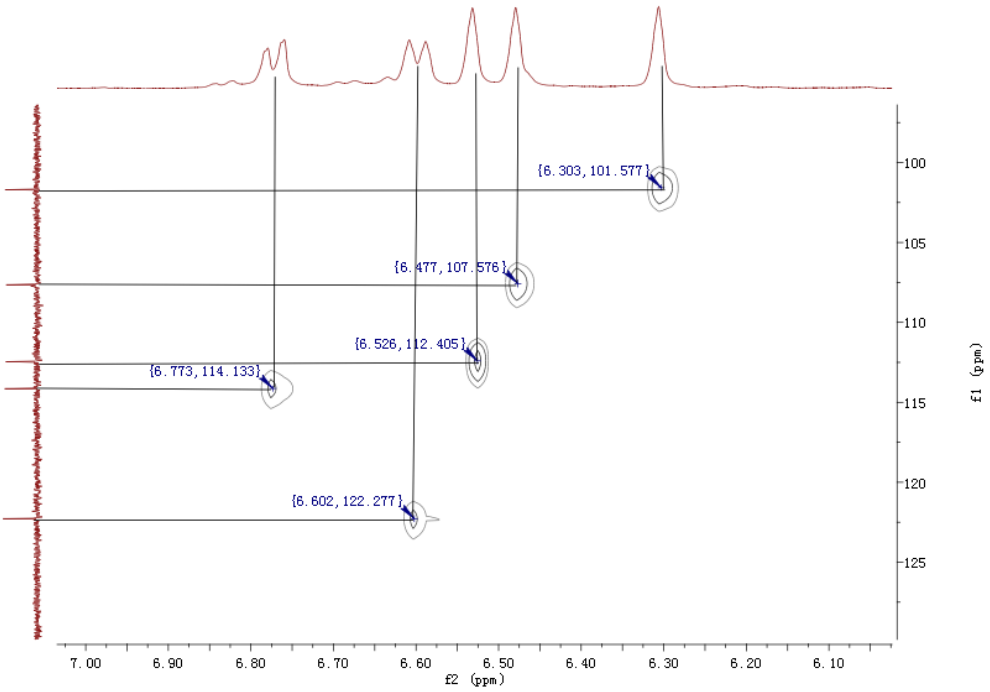


Figure S6: HSQC Spectrum of **1** (From δ_C100 ppm to δ_C 120 ppm)

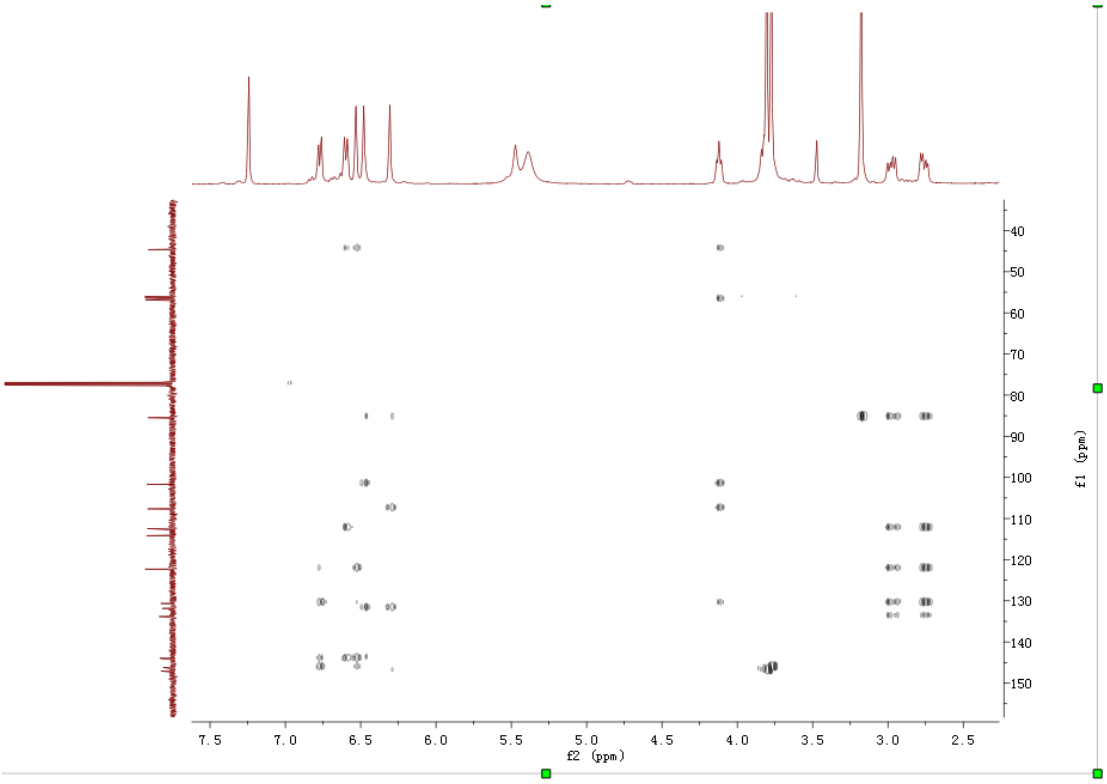
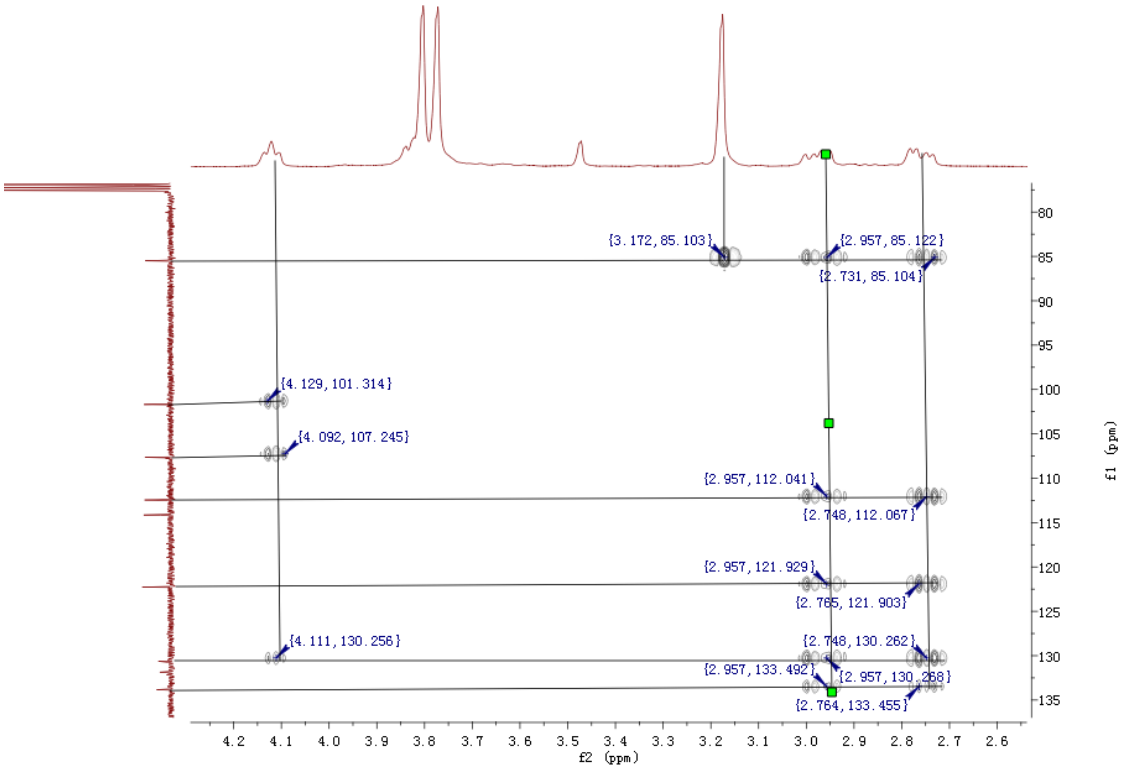


Figure S7: HMBC Spectrum of **1**



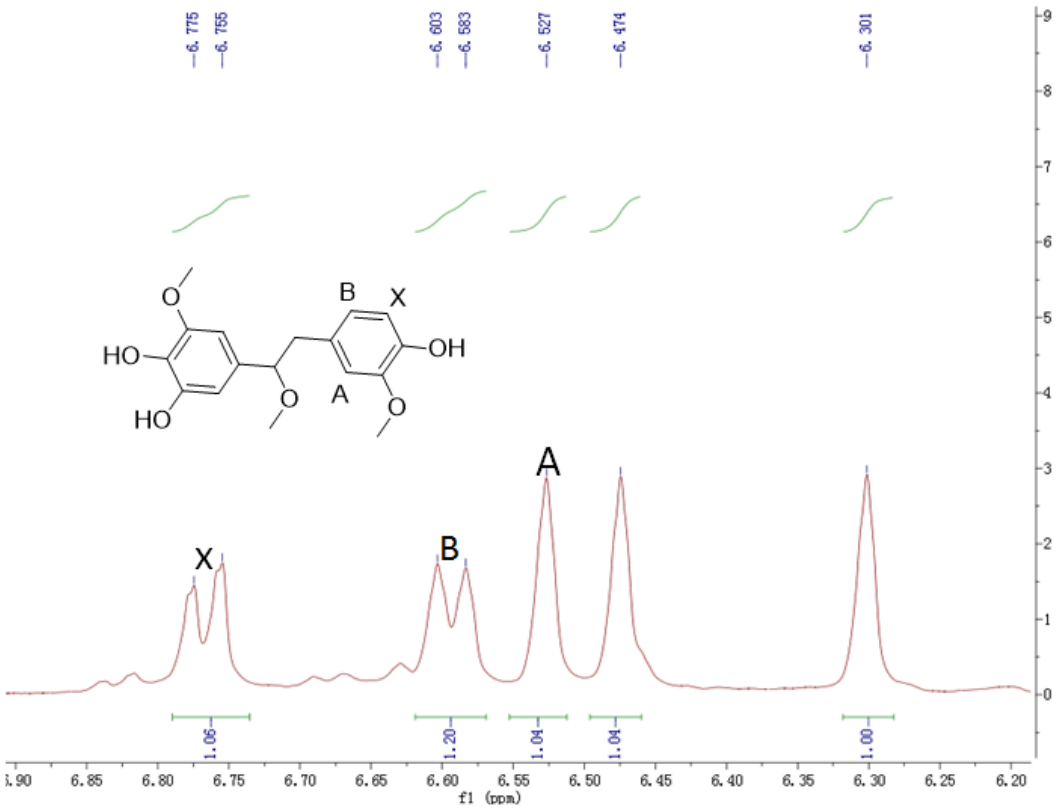


Figure S9: ^{1}H-NMR Spectrum (ABX system) (400 MHz, $CDCl_3$) of **1**

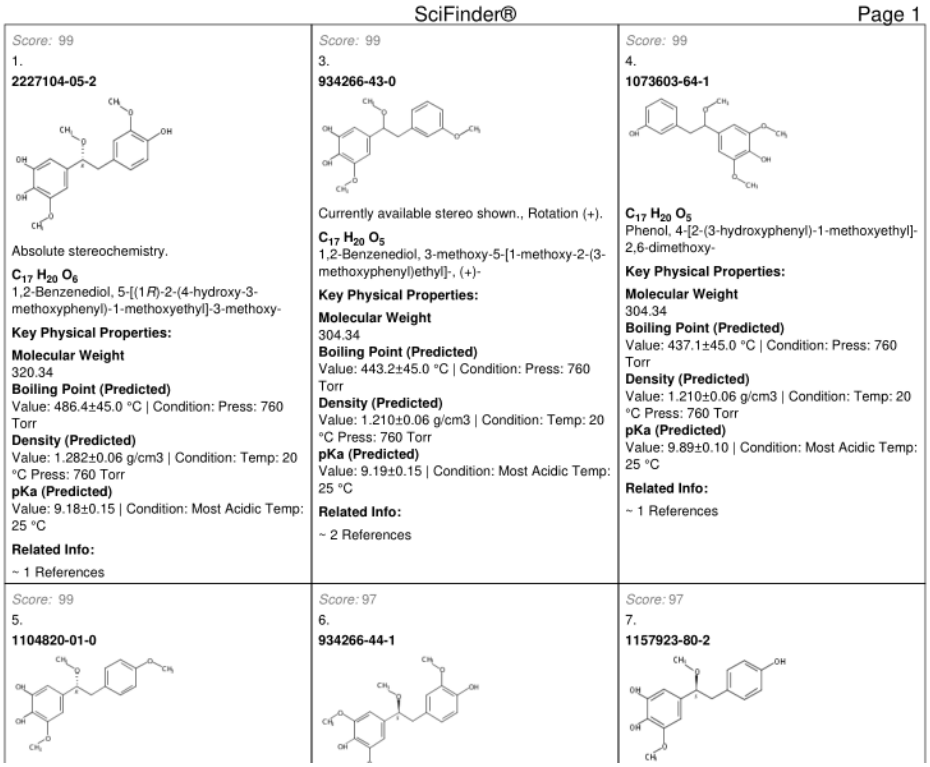


Figure S10: Scifinder Search Results of **1**

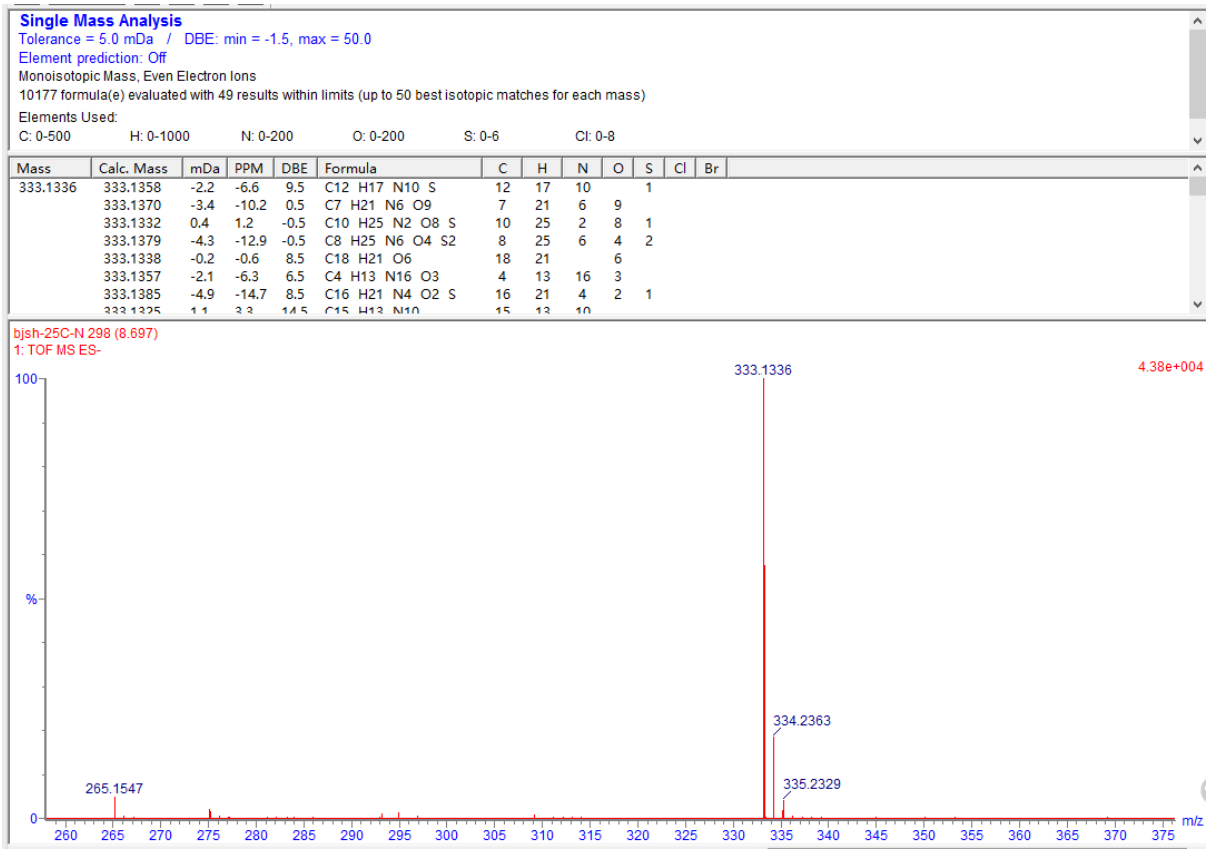


Figure S11: HR-ESI-MS Spectrum of **2**

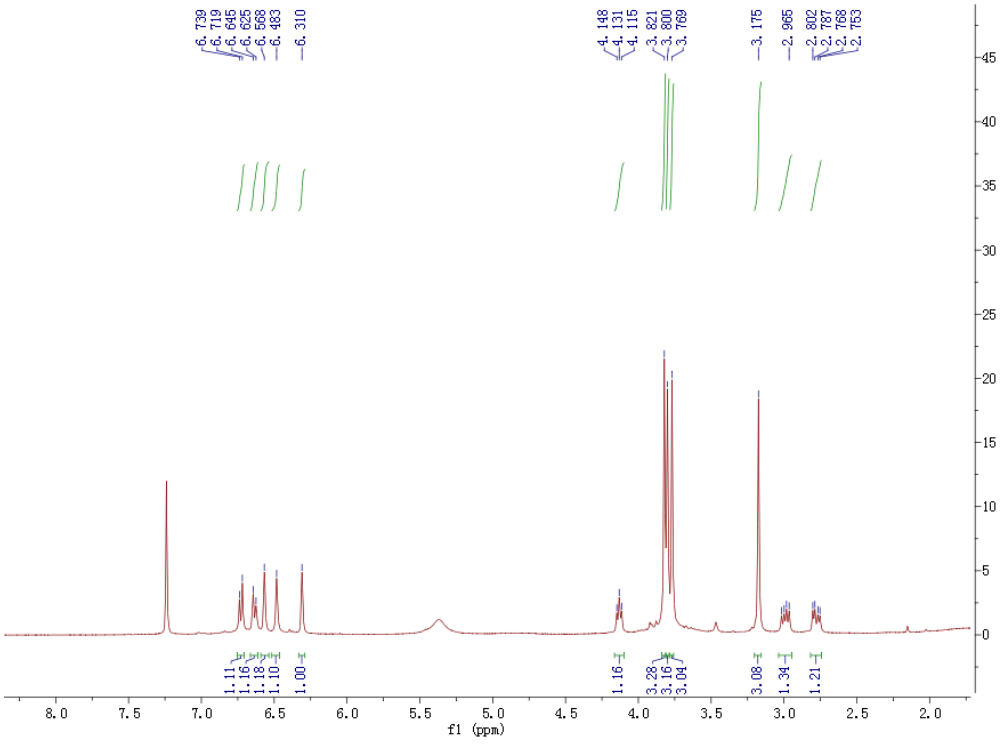


Figure S12: ^{1}H-NMR (400 MHz, $CDCl_3$) Spectrum of **2**

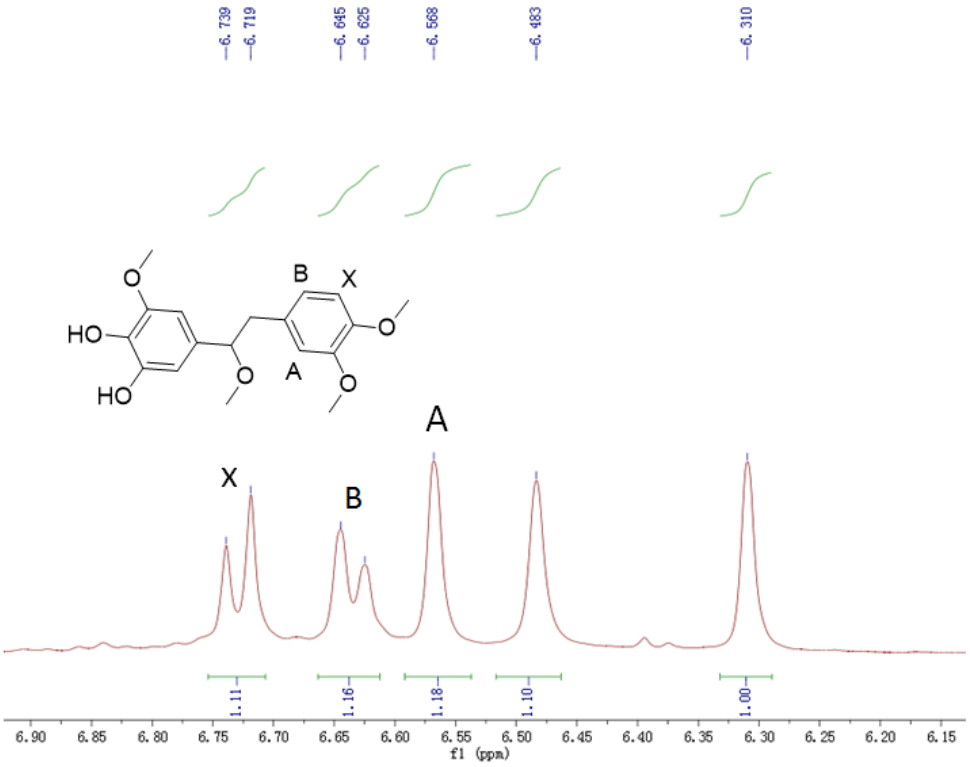


Figure S13: ^{1}H-NMR Spectrum (ABX system) (400 MHz, $CDCl_3$) of **2**

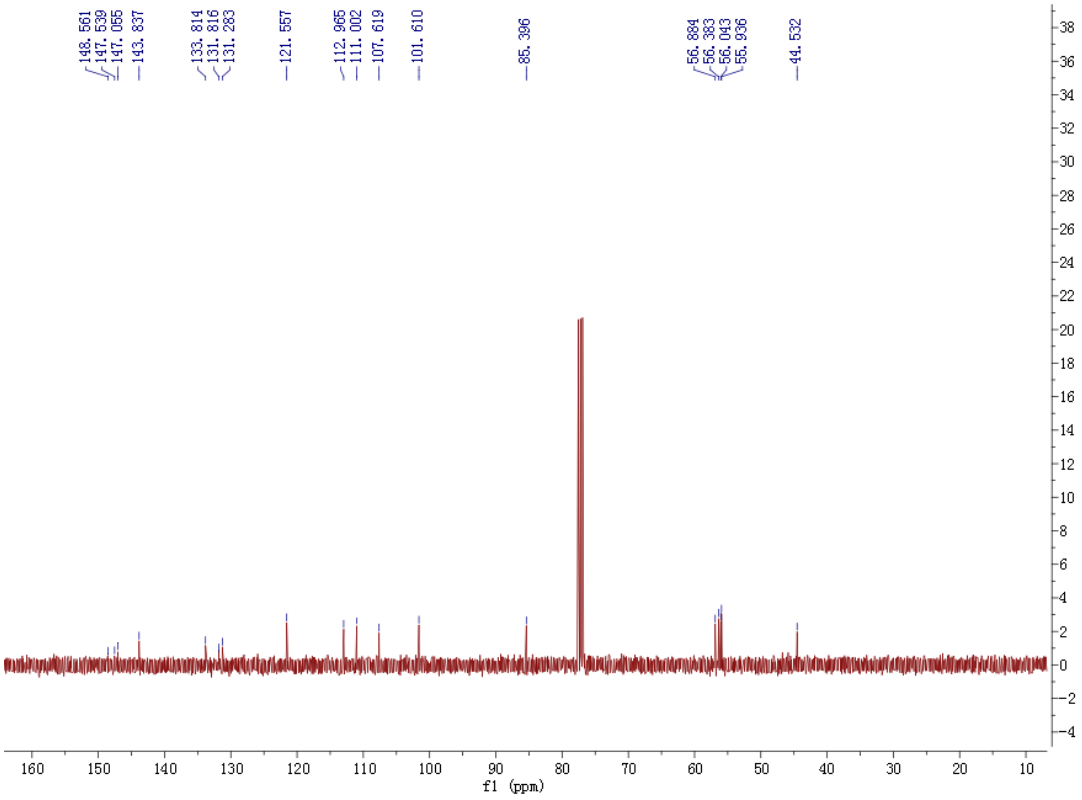


Figure S14: ^{13}C-NMR (100 MHz, $CDCl_3$) Spectrum of **2**

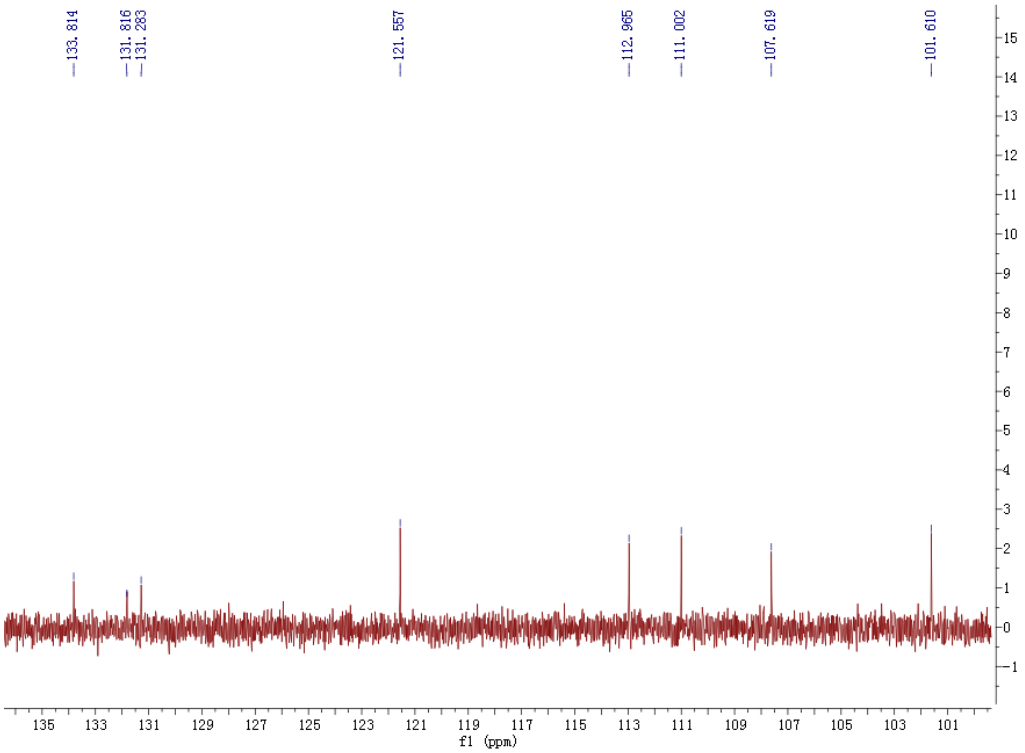


Figure S15: ^{13}C-NMR (100 MHz, $CDCl_3$) Spectrum of **2** (From δ_C100 ppm to δ_C 140 ppm)

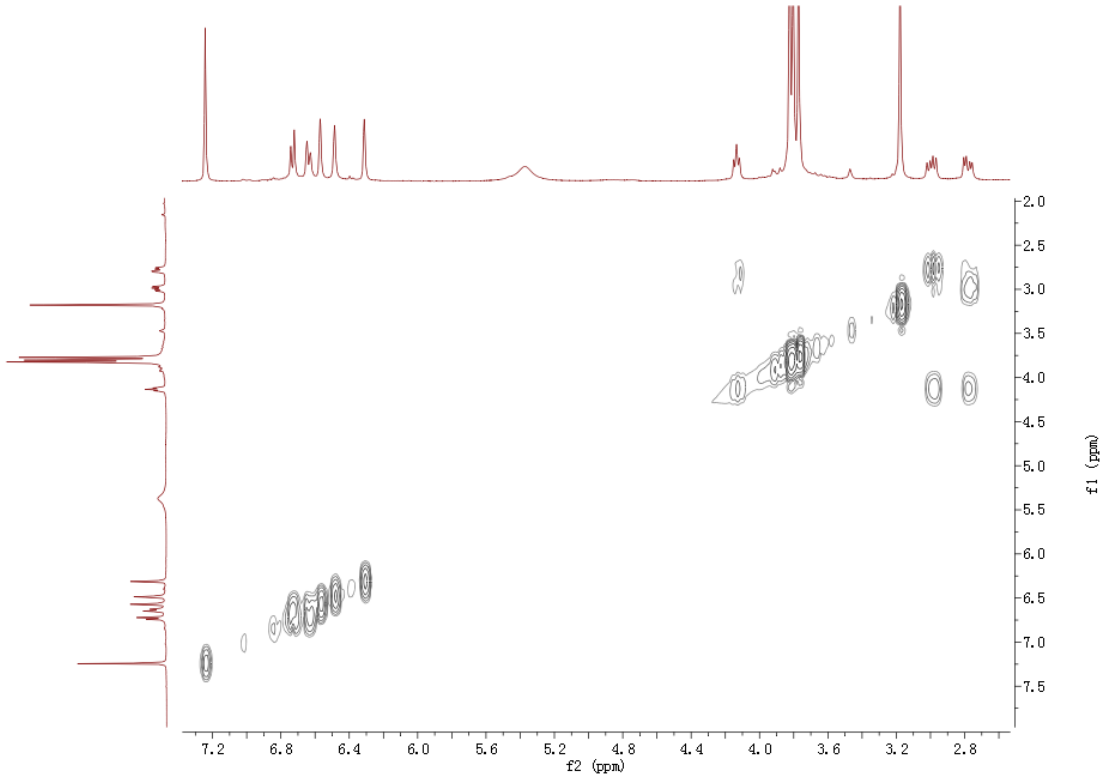


Figure S16: ^{1}H-^{1}H COSY Spectrum of **2**

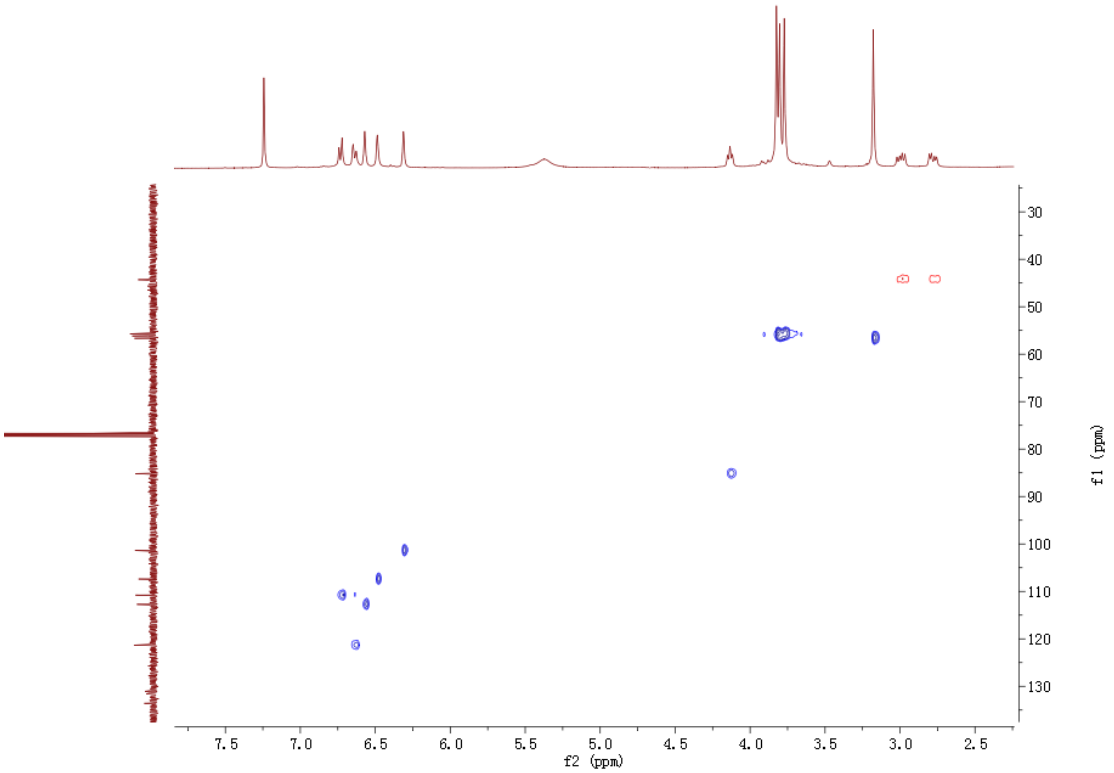


Figure S17: HSQC Spectrum of **2**

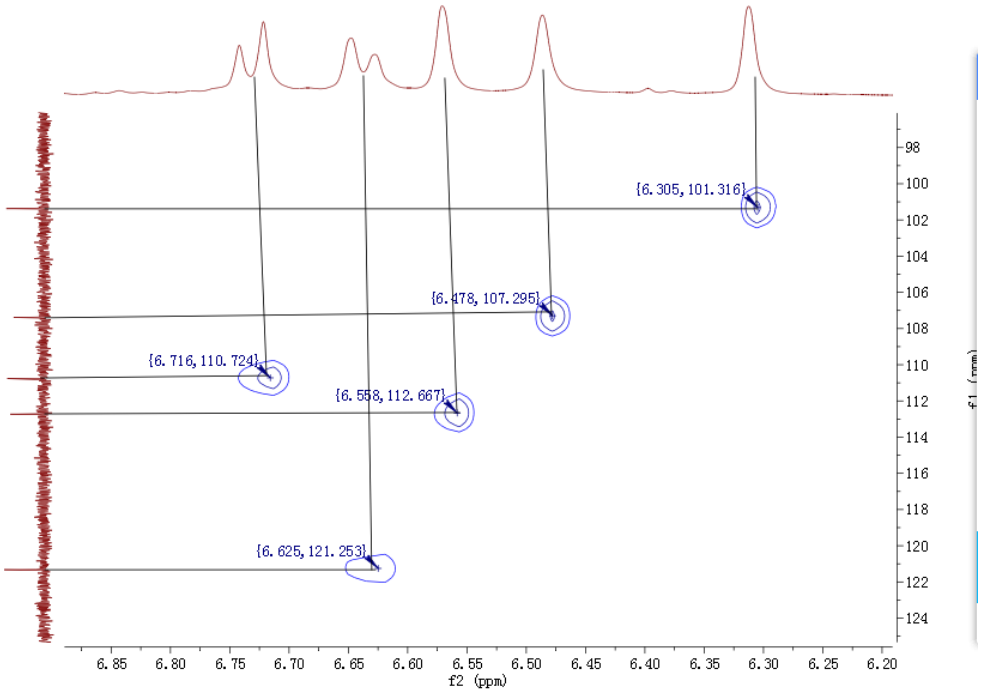


Figure S18: HSQC Spectrum of **2** (From δ_C 100 ppm to 130 ppm)

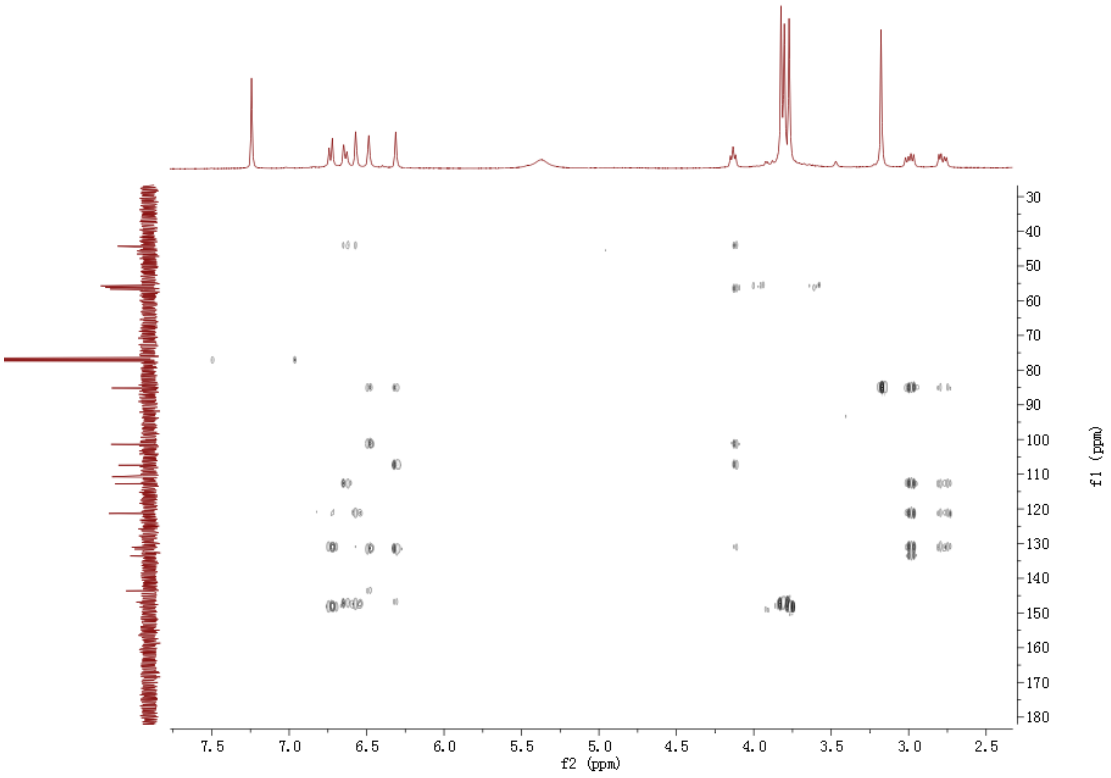


Figure S19: HMBC Spectrum of **2**

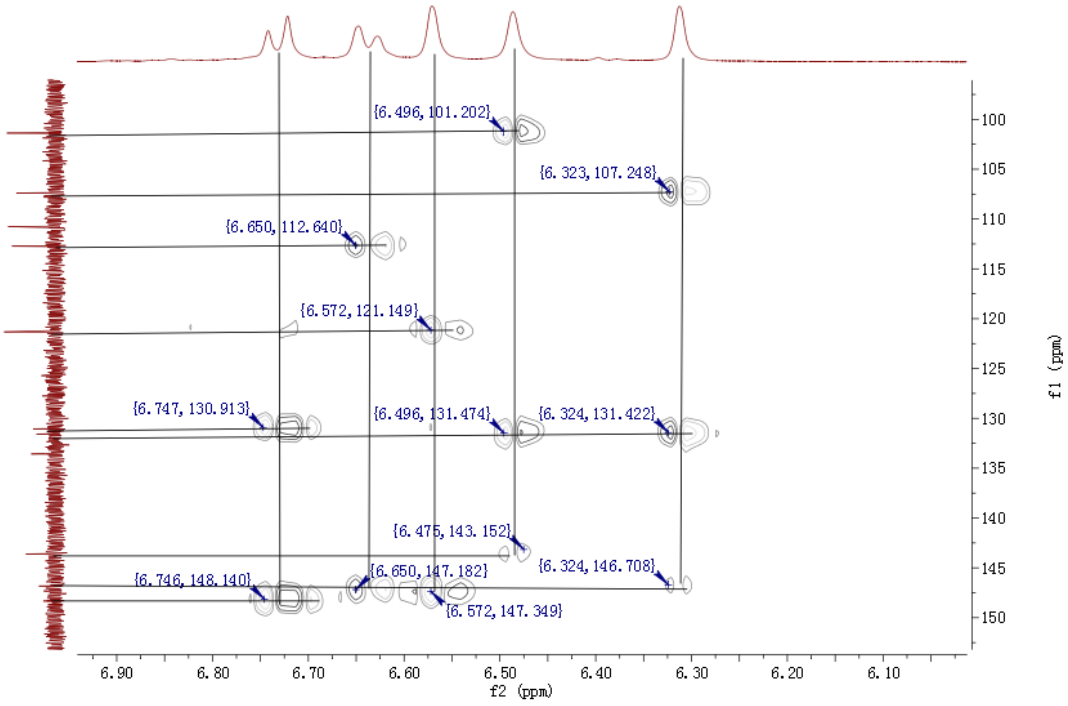
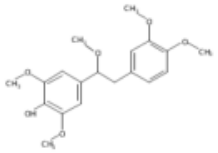


Figure S20: HMBC Spectrum of **2** (From δ_C 100 ppm to 130 ppm)

Score: 99

1.

934266-45-2



Currently available stereo shown., Rotation (+).

$C_{19}H_{24}O_6$
Phenol, 4-[2-(3,4-dimethoxyphenyl)-1-methoxyethyl]-2,6-dimethoxy-, (+)-

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

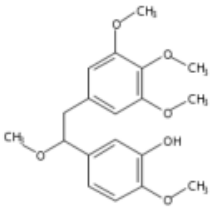
Related Info:

~ 2 References

Score: 99

2.

956699-51-7



$C_{19}H_{24}O_6$
Phenol, 2-methoxy-5-[1-methoxy-2-(3,4,5-trimethoxyphenyl)ethyl]-

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

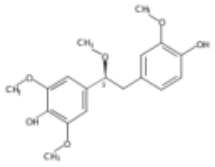
Related Info:

~ 1 References
Reactions

Score: 99

3.

934266-44-1



Rotation (+)., Absolute stereochemistry.

$C_{18}H_{22}O_6$
Phenol, 4-[(1*S*)-2-(4-hydroxy-3-methoxyphenyl)-1-methoxyethyl]-2,6-dimethoxy-

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

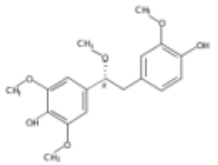
Related Info:

~ 3 References

Score: 99

4.

1252577-64-2



Rotation (-)., Absolute stereochemistry.

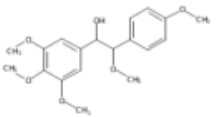
$C_{18}H_{22}O_6$
Phenol, 4-[(1*R*)-2-(4-hydroxy-3-methoxyphenyl)-1-methoxyethyl]-2,6-dimethoxy-

Key Physical Properties:

Score: 97

5.

1638839-33-4



$C_{19}H_{24}O_6$
Benzeneethanol, β,4-dimethoxy-α-(3,4,5-trimethoxyphenyl)-

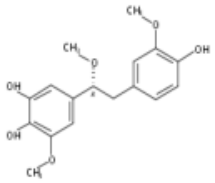
Key Physical Properties:

Molecular Weight
348.39
Boiling Point (Predicted)
Value: 465.2±45.0 °C | Condition: Press: 760

Score: 96

6.

2227104-05-2



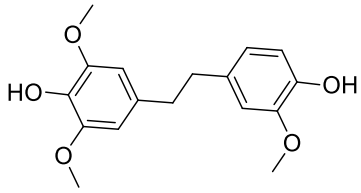
Absolute stereochemistry.

$C_{17}H_{20}O_6$
1,2-Benzenediol, 5-[(1*R*)-2-(4-hydroxy-3-methoxyphenyl)-1-methoxyethyl]-3-methoxy-

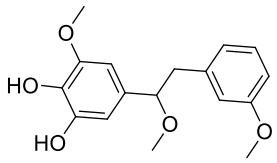
Key Physical Properties:

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: ^{1}H 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)	2.8 3(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.