

SUPPLEMENTARY MATERIAL

Two new Compounds, **Deacetylisowortmins** A and B, isolated from an Endophytic Fungus, *Talaromyces wortmannii* LGT-4

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Two new compounds, **deacetylisowortmins** A (**1**) and B (**2**), were isolated from *Talaromyces wortmannii* LGT-4. Their structures were established by 1D and 2D NMR spectra, as well as comparison of the experimental and calculated electronic circular dichroism (ECD) spectra. Monoamine oxidase and acetylcholinesterase inhibitory **activities** of **1** and **2** were also evaluated.

Keywords: Endophytic fungus; *Talaromyces wortmannii*; **Deacetylisowortmins**; Structure elucidation; Enzyme inhibition

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Table S1. ¹H NMR data of compound 1-2 (600 M)

No	1 in CDCl ₃	1 in CD ₃ OD	2 in CDCl ₃
1 α	4.31 (d, <i>J</i> = 16.0)	4.23 (d, <i>J</i> = 16.0)	4.32 (d, <i>J</i> = 16.7)
1 β	4.55 (d, <i>J</i> = 16.0)	4.42 (d, <i>J</i> = 16.0)	4.59 (d, <i>J</i> = 16.2)
3	4.07 (m)	4.08 (m)	4.08 (ddd, <i>J</i> = 10.1, 5.4, 5.0)
4 α	2.22 (dd, <i>J</i> = 18.4, 5.4)	2.33(m)	2.23 (dd, <i>J</i> = 19.1, 5.4)
4 β	2.36 (m)	2.33(m)	2.35 (dd, <i>J</i> = 18.4, 9.4)
5 α	2.60 (dd, <i>J</i> = 17.5, 6.4)	2.58(m)	2.71 (dd, <i>J</i> = 17.6, 6.1)
5 β	2.41 (dd, <i>J</i> = 17.5, 10.6)	2.58(m)	2.57(m)
6	5.09 (dd, <i>J</i> = 10.4, 6.4)	5.00 (dd, <i>J</i> = 10.1, 6.4)	6.20 (dd, <i>J</i> = 10.5, 6.2)
9	5.54 (dd, <i>J</i> = 15.0, 6.1)	5.54 (dd, <i>J</i> = 15.4, 6.2)	5.54 (dd, <i>J</i> = 15.4, 5.0)
10	5.80 (dq, <i>J</i> = 15.0, 6.9)	5.79 (dq, <i>J</i> = 15.4, 6.5)	5.81 (dq, <i>J</i> = 15.4, 6.5)
11	1.74 (d, <i>J</i> = 6.5)	1.72 (d, <i>J</i> = 6.6)	1.74 (d, <i>J</i> = 6.5)
12	1.54 (s)	1.49(s)	1.56 (s)
2''	-	-	2.07(s)
3'	6.29 (d, <i>J</i> = 2.6)	6.29 (d, <i>J</i> = 2.6)	6.30 (d, <i>J</i> = 2.4)
5'	6.29 (d, <i>J</i> = 2.6)	6.34 (d, <i>J</i> = 2.6)	6.27 (d, <i>J</i> = 2.7)
8'	2.55 (s)	2.55 (s)	2.49 (s)
-OMe	3.79 (s)	3.79 (s)	3.78 (s)
2'-OH	11.16 (s)	No observed	11.09(s)

Table S2. ¹³C NMR data of compound 1-2 (150 M)

No	1 in CD ₃ OD	2 in CDCl ₃	No	1 in CD ₃ OD	2 in CDCl ₃
1	64.1	63.6	11	18.0	18.0
3	74.8	73.6	12	16.4	17.2
4	37.2	36.5	1''	-	169.9
4a	153.6	149.3	2''	-	21.0
5	38.8	35.0	1'	107.2	105.4
6	68.7	69.7	2'	166.2	165.8
7	88.2	83.5	3'	99.8	99.0
8	195.2	191.5	4'	165.5	164.3
8a	130.1	130.3	5'	111.7	111.5
9	131.7	130.3	6'	144.6	143.2
10	129.3	129.2	-OMe	55.8	55.5

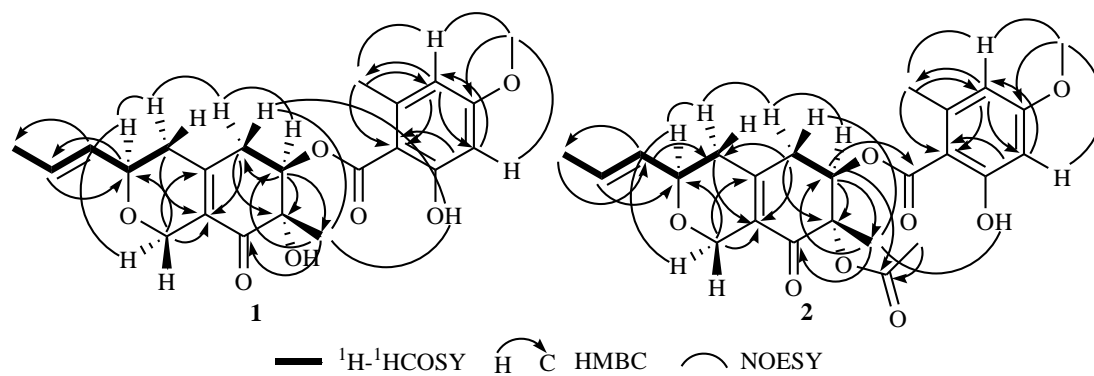


Figure S1. Key HMBC, $^1\text{H}-^1\text{H}$ COSY and NOESY correlations of **1** and **2**

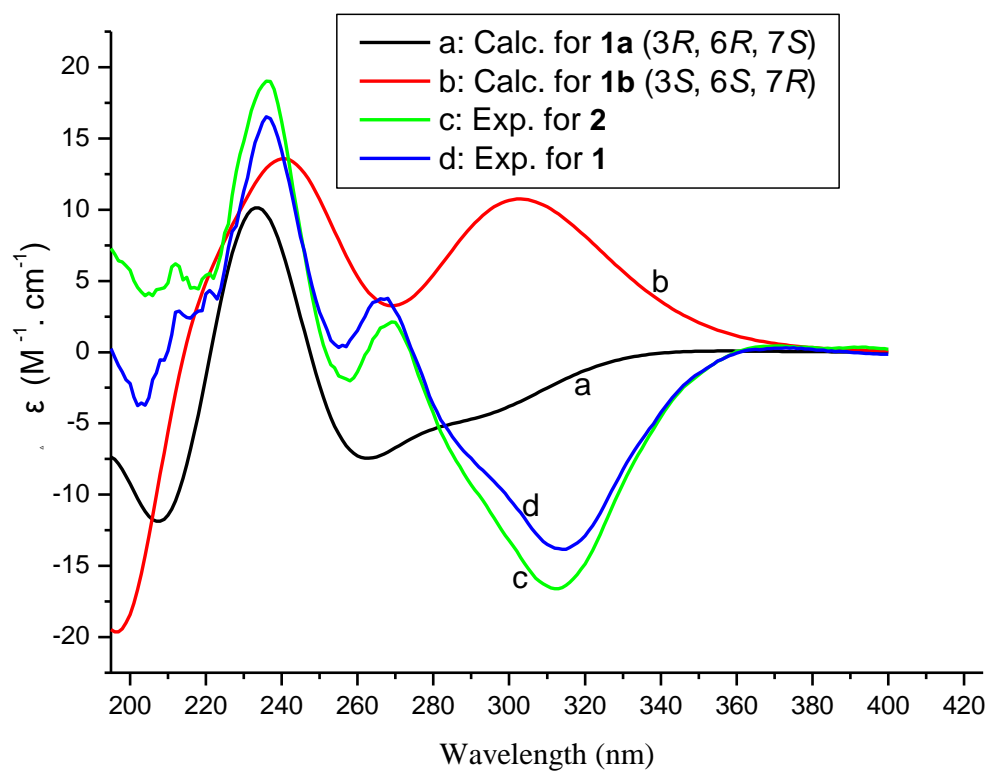


Figure S2. Calculated and experimental ECD spectra of **1** and **2**.

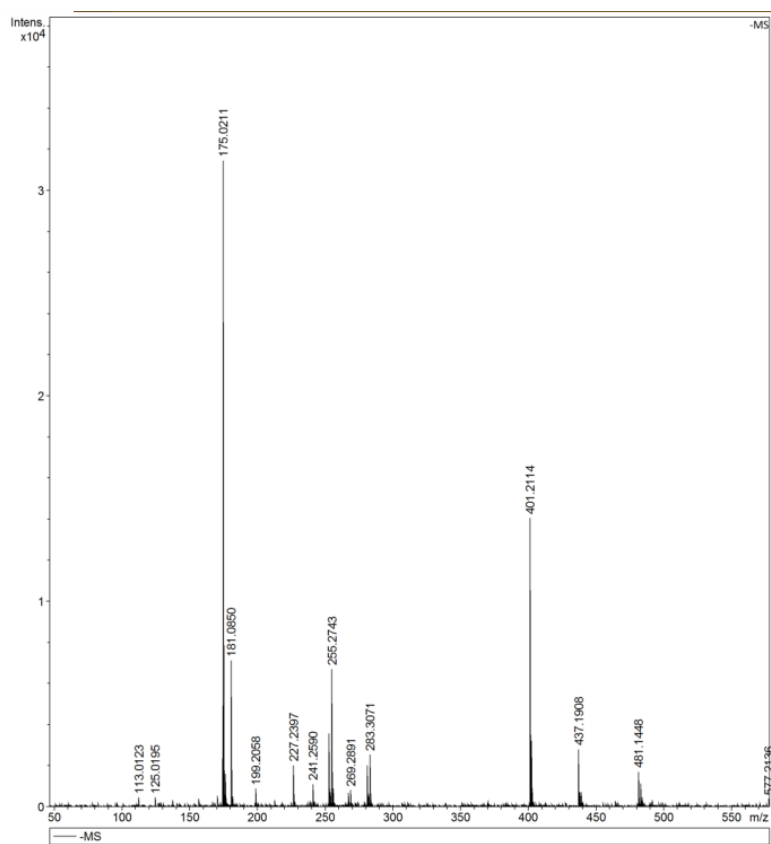
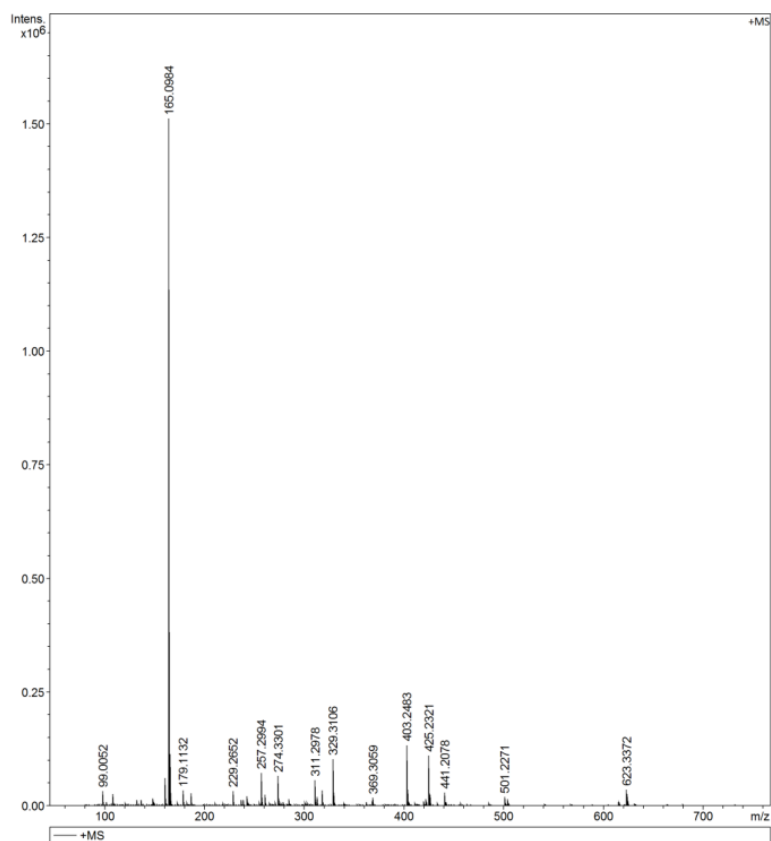


Figure S3. ESI MS spectrum of compound 1

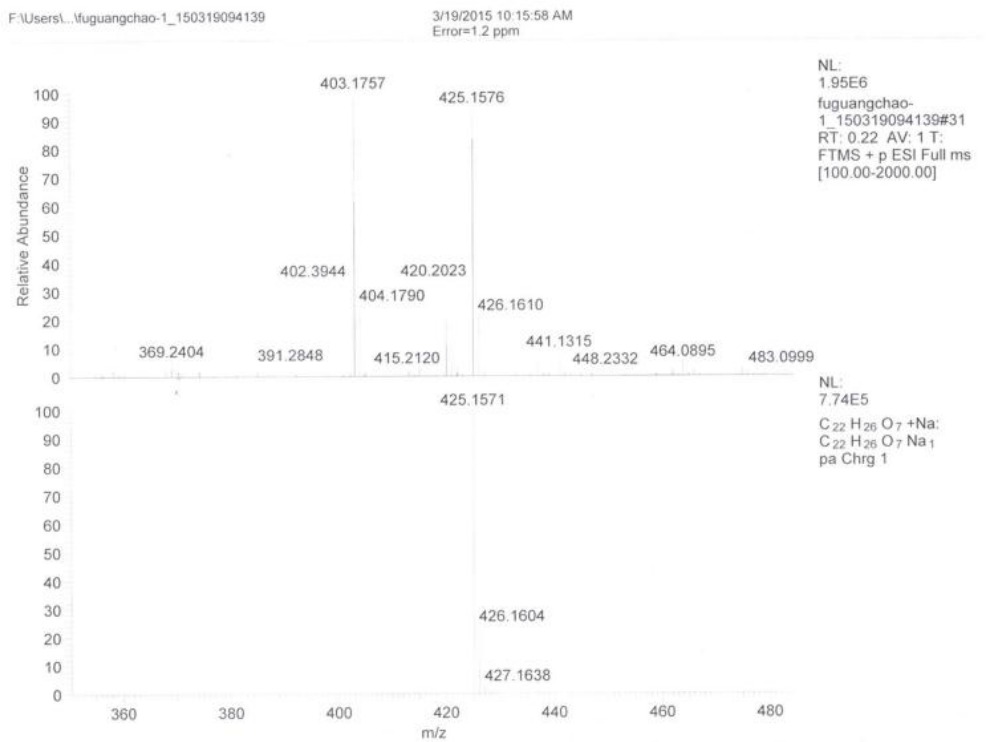


Figure S4. HRESI MS spectrum of compound **1**

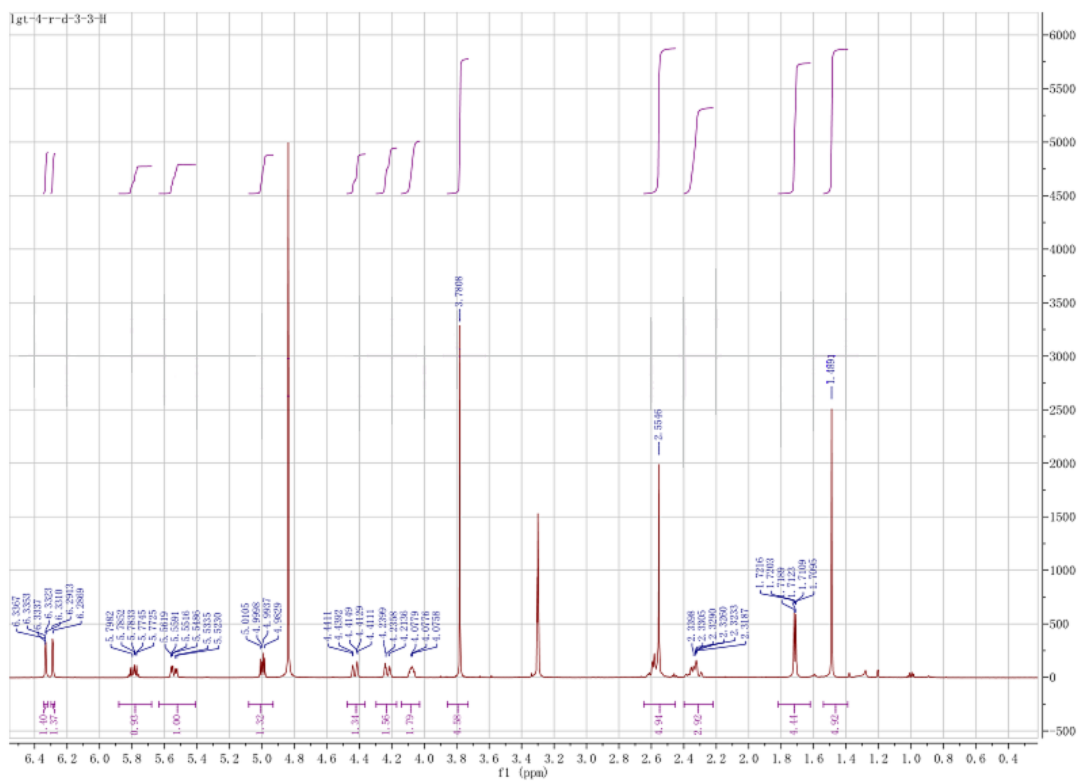


Figure S5. ¹H NMR (600 MHz, CD₃OD) spectrum of compound **1**

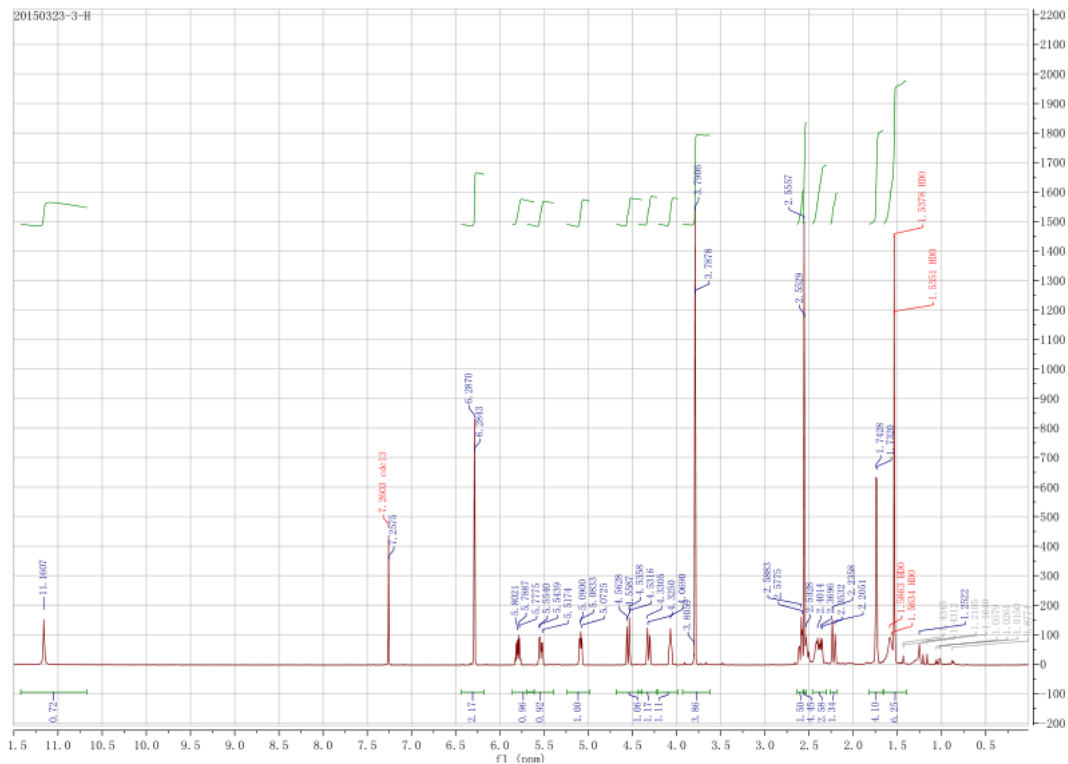


Figure S6. ^1H NMR (600 MHz, CDCl_3) spectrum of compound **1**

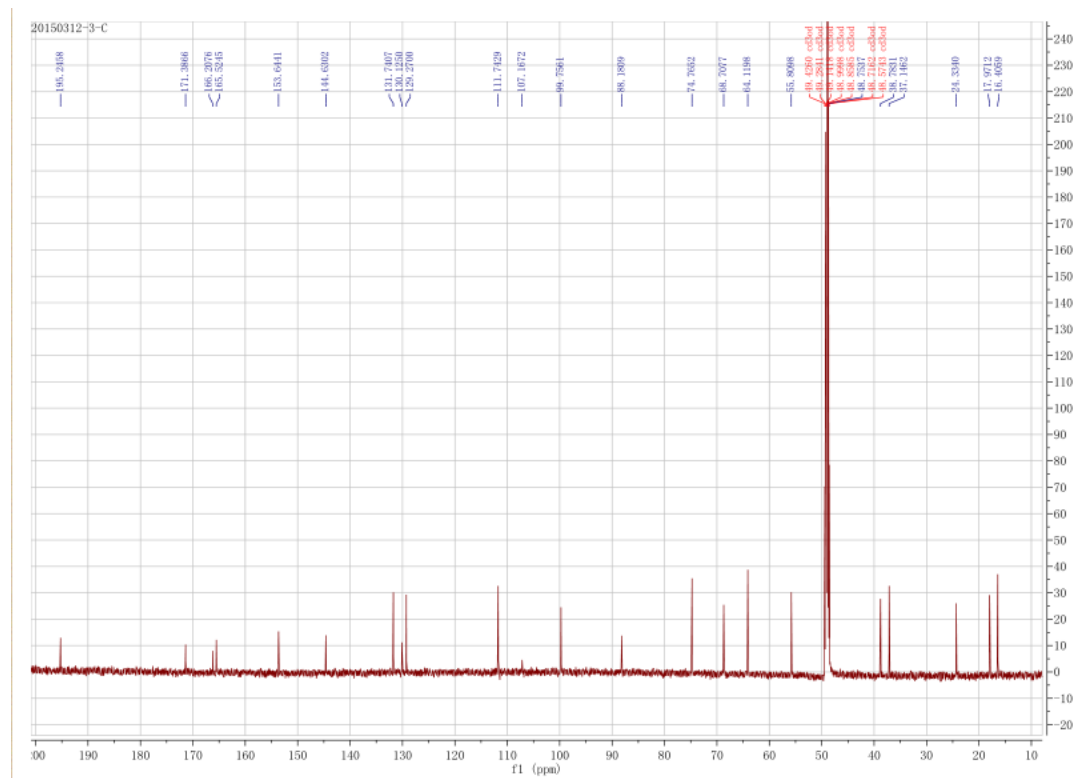


Figure S7. ^{13}C NMR (600 MHz, CD_3OD) spectrum of compound **1**

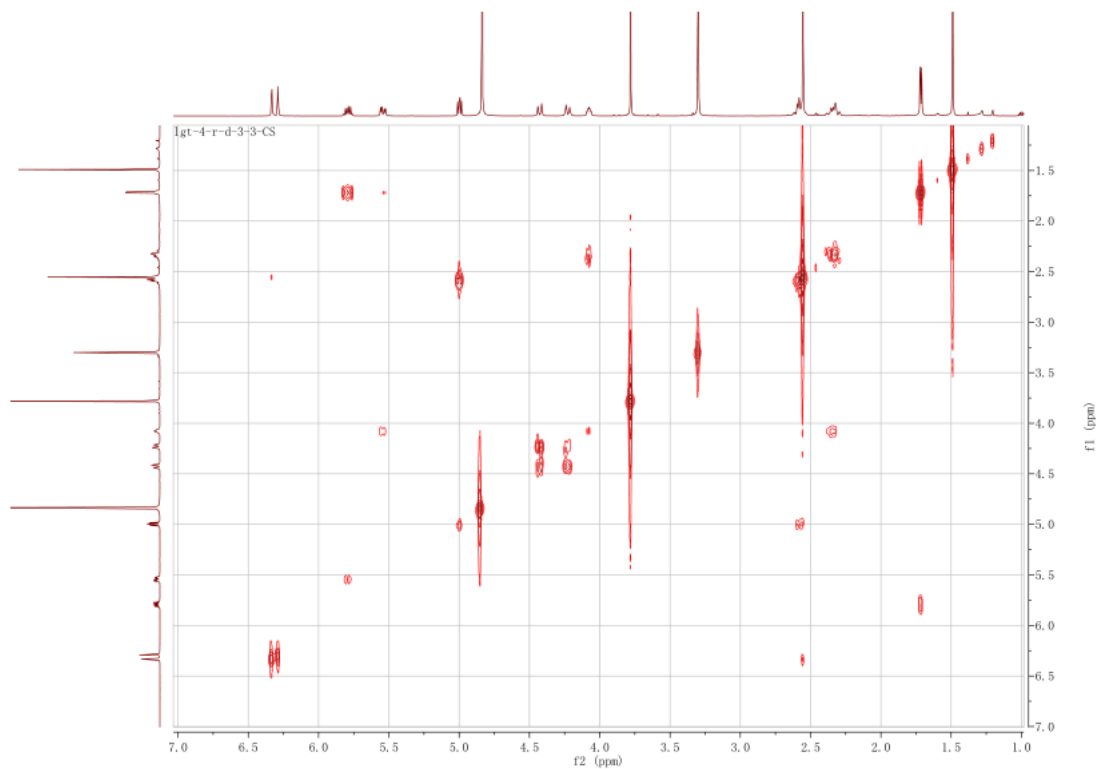


Figure S8. COSY (600 MHz, CD₃OD) spectrum of compound **1**

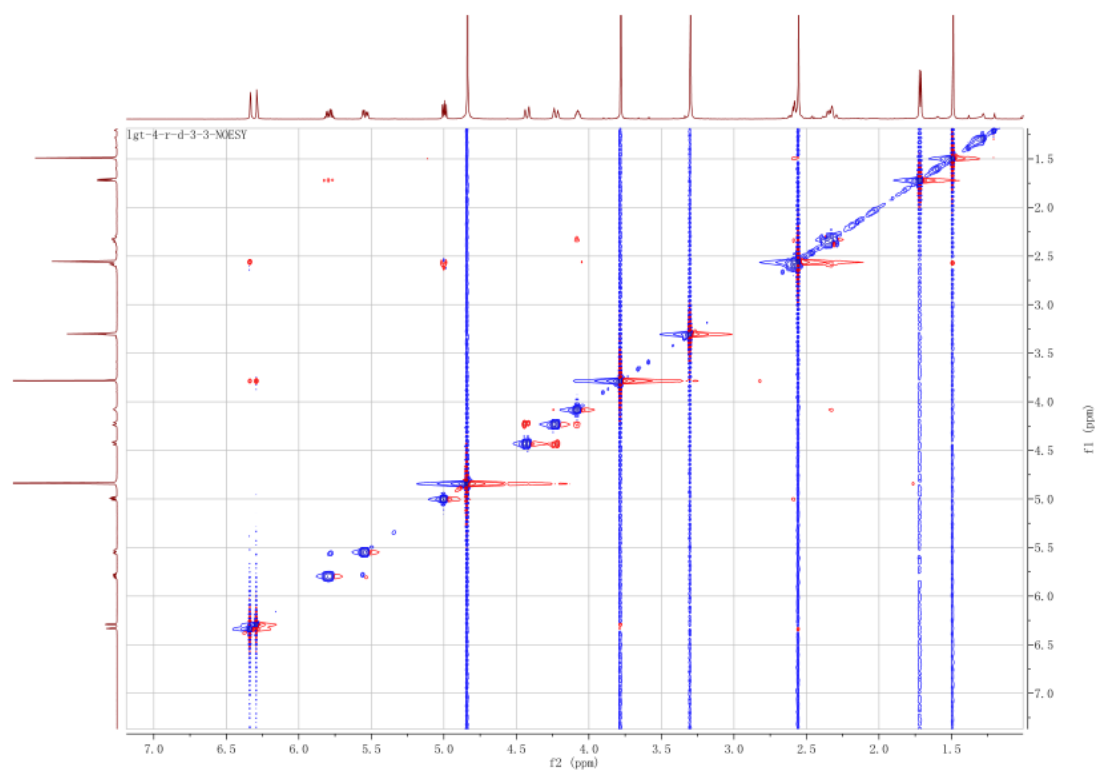


Figure S9. NOESY (600 MHz, CD₃OD) spectrum of compound **1**

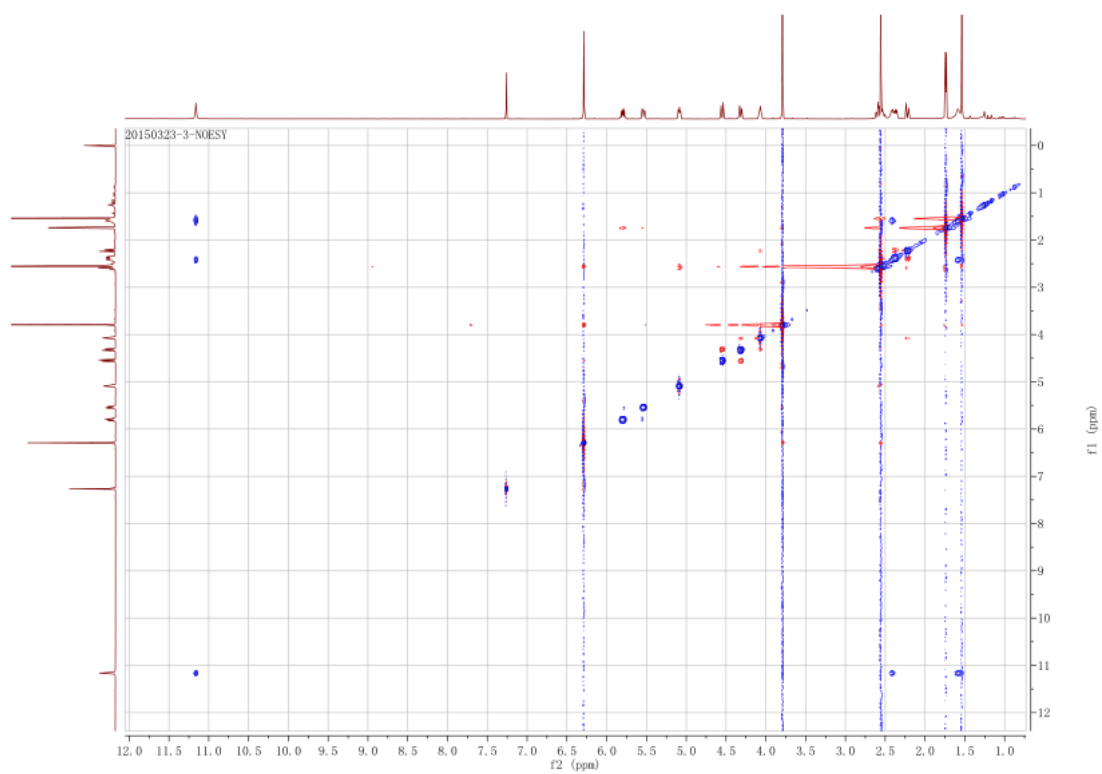


Figure S10. NOESY (600 MHz, CDCl_3) spectrum of compound **1**

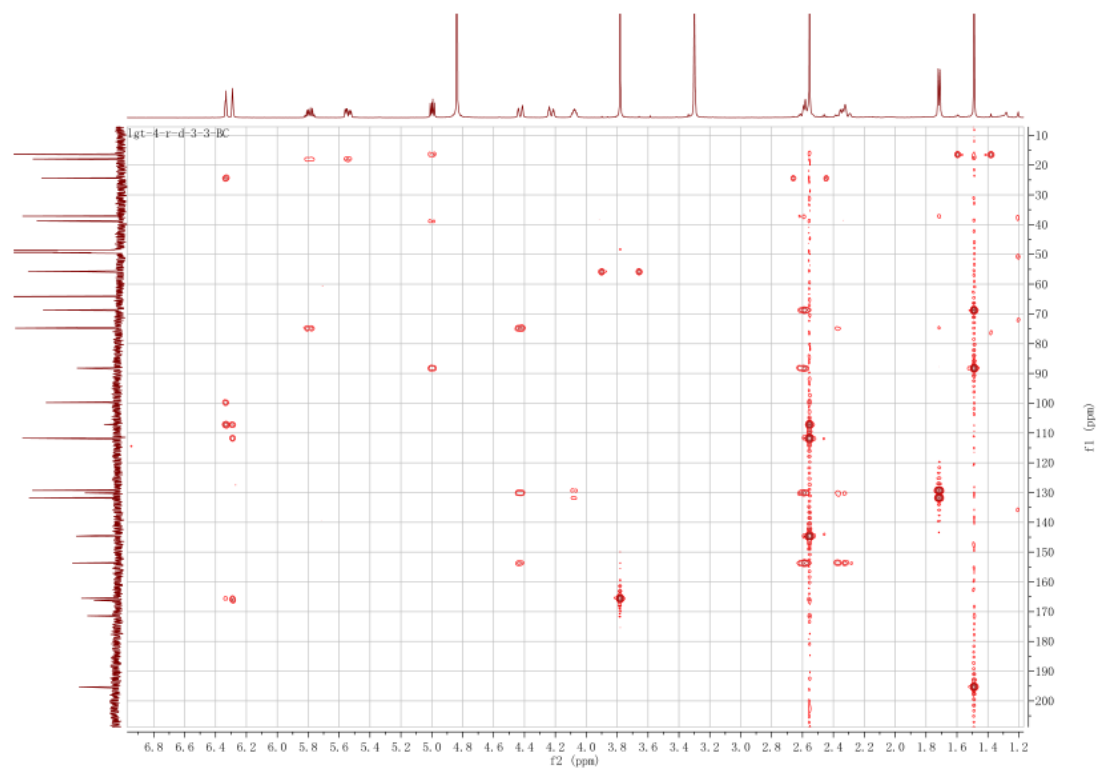


Figure S11. HMBC (600 MHz, CD_3OD) spectrum of compound **1**

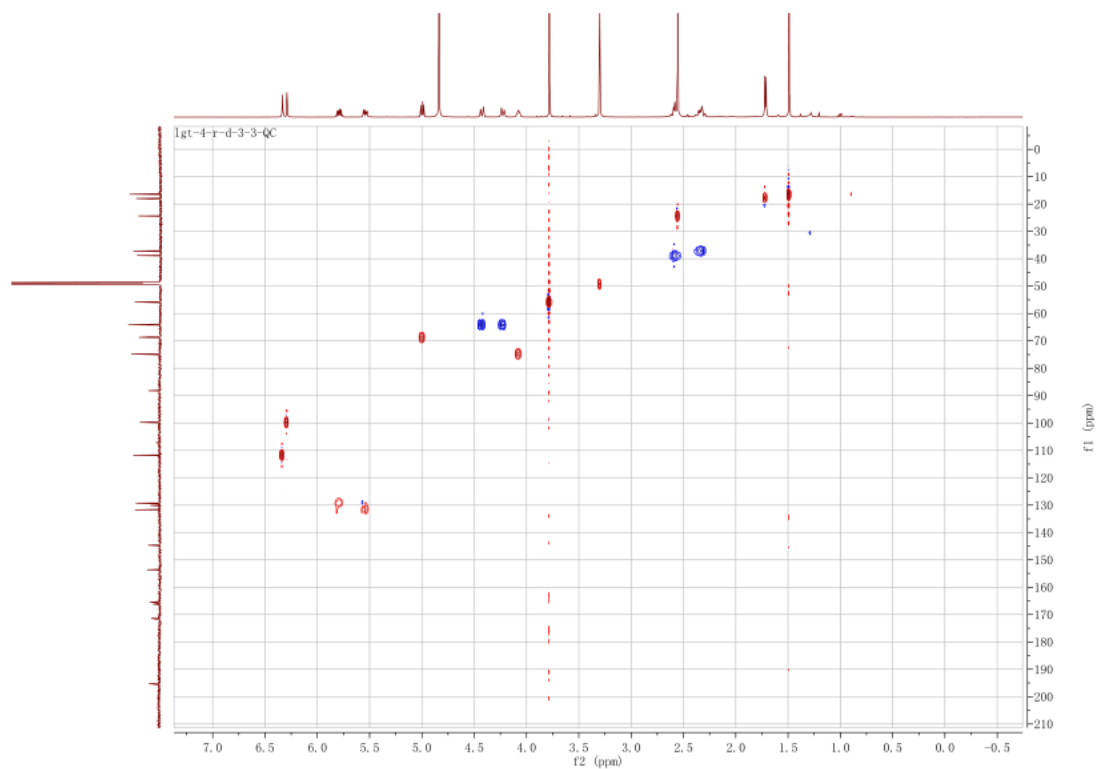


Figure S12. HMQC (600 MHz, CD₃OD) spectrum of compound **1**

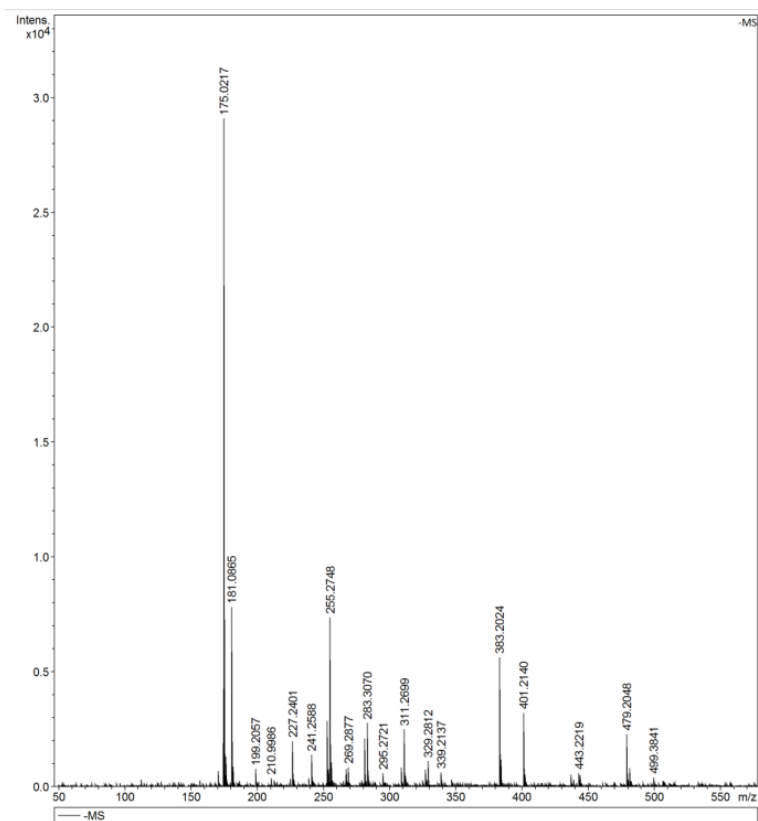
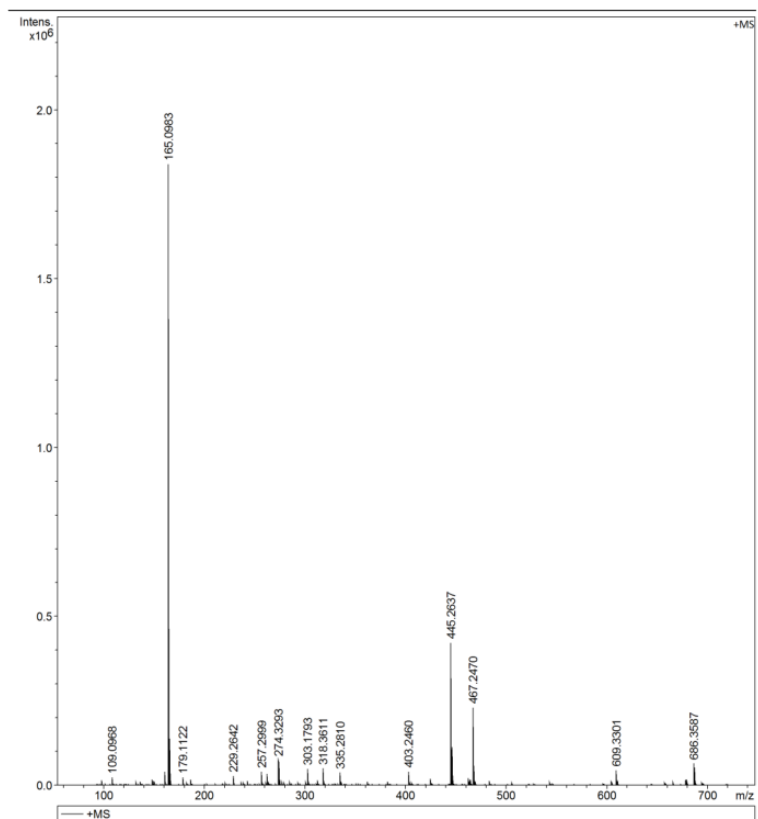


Figure S13. ESI MS spectrum of compound 2

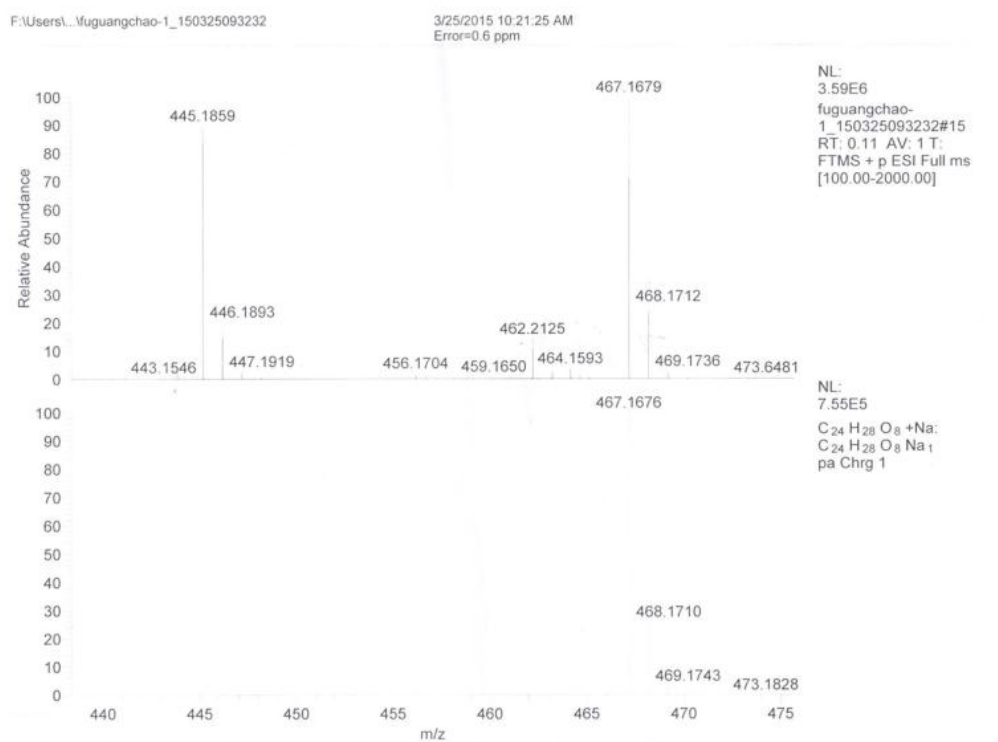


Figure S14. HRESI MS spectrum of compound **2**



Figure S15. ¹H NMR (600 MHz, CDCl₃) spectrum of compound **2**

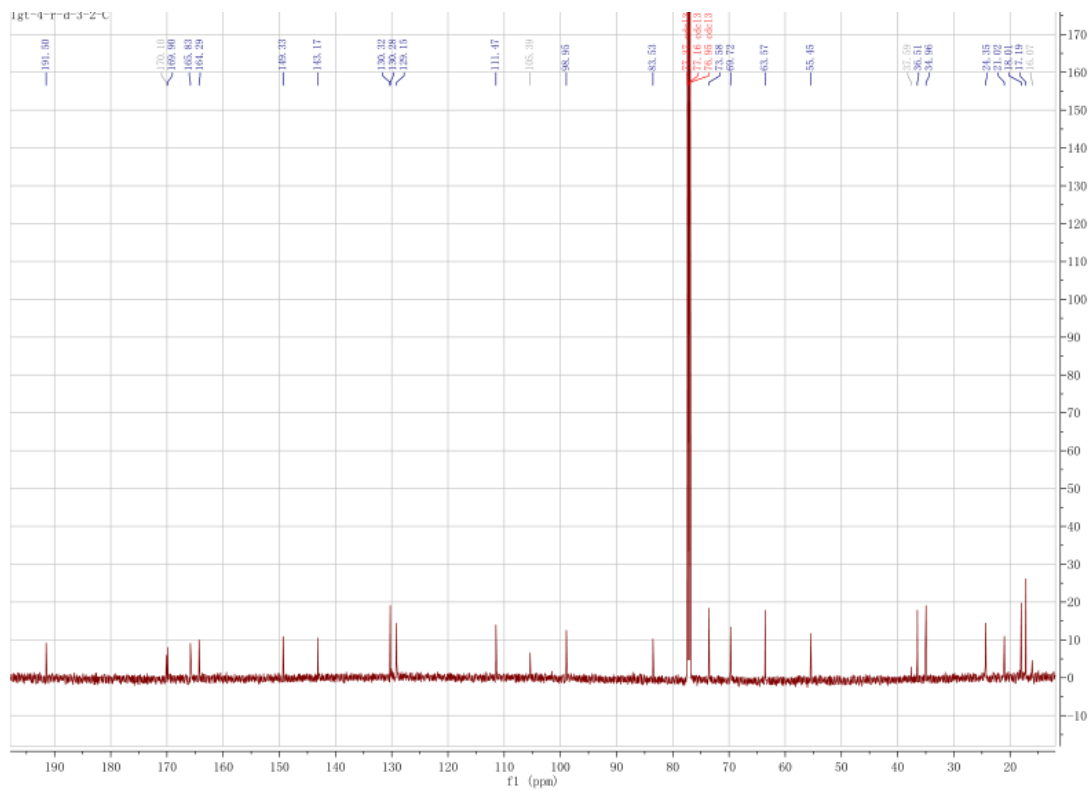


Figure S16. ^{13}C NMR (600 MHz, CDCl_3) spectrum of compound **2**

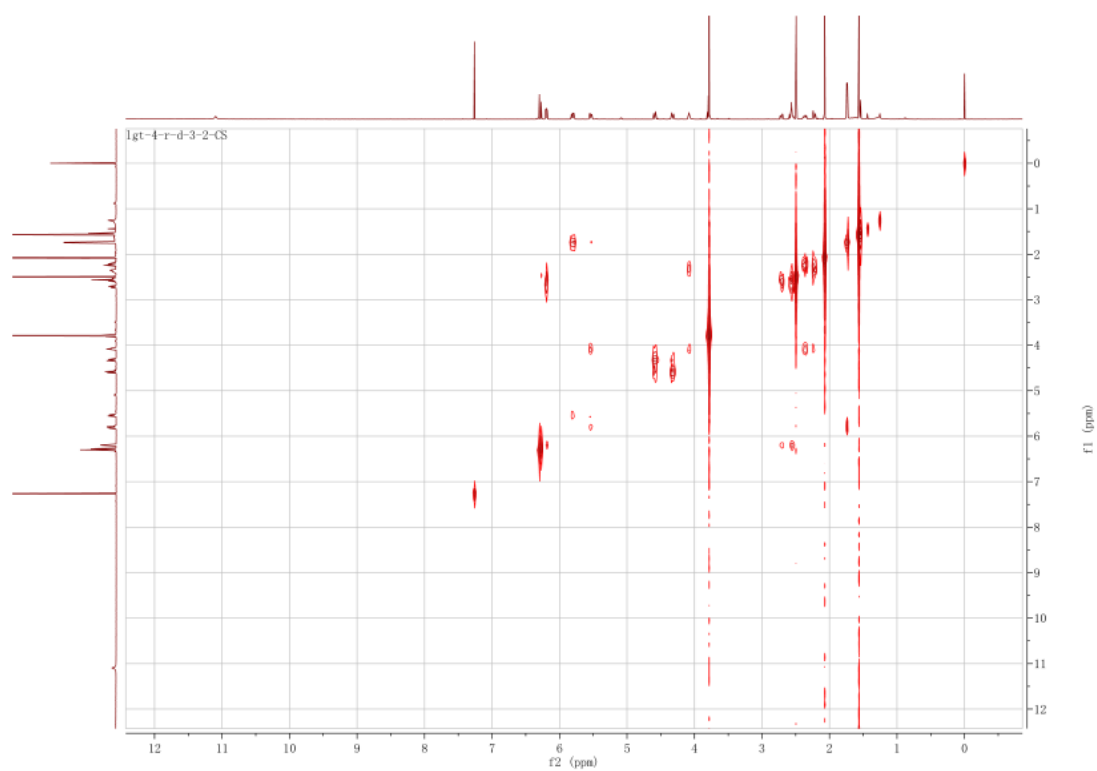


Figure S17. COSY (600 MHz, CDCl_3) spectrum of compound **2**

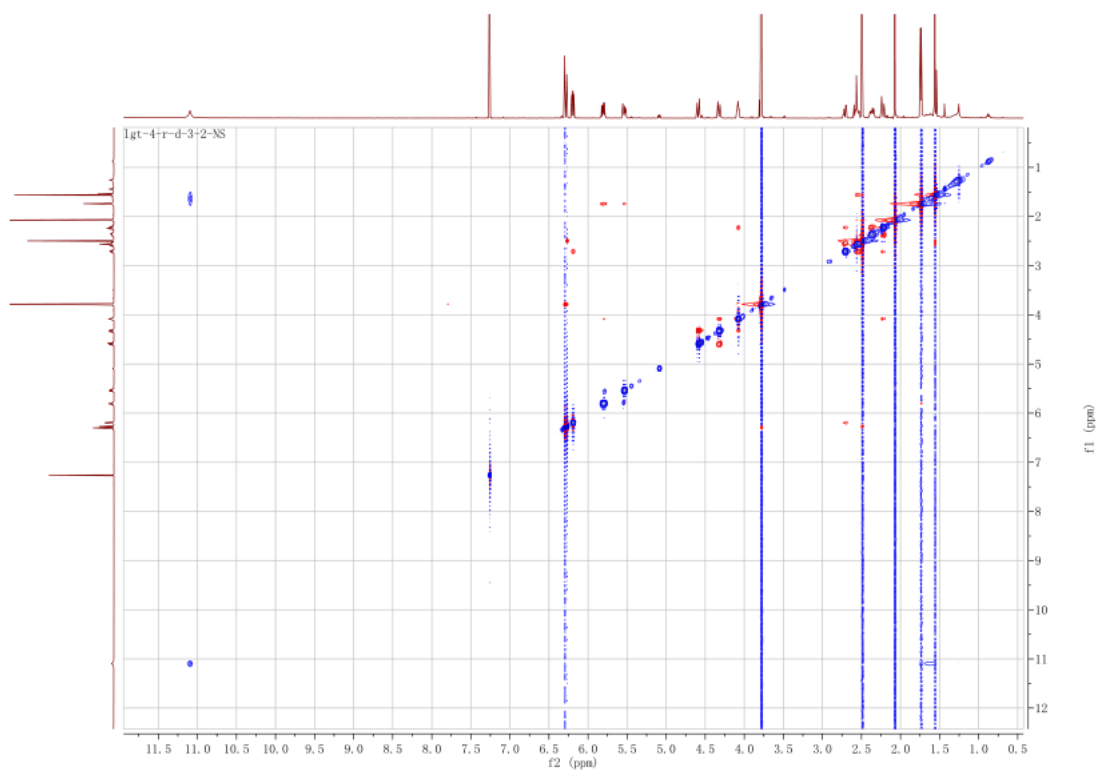


Figure S18. NOESY (600 MHz, CDCl₃) spectrum of compound **2**

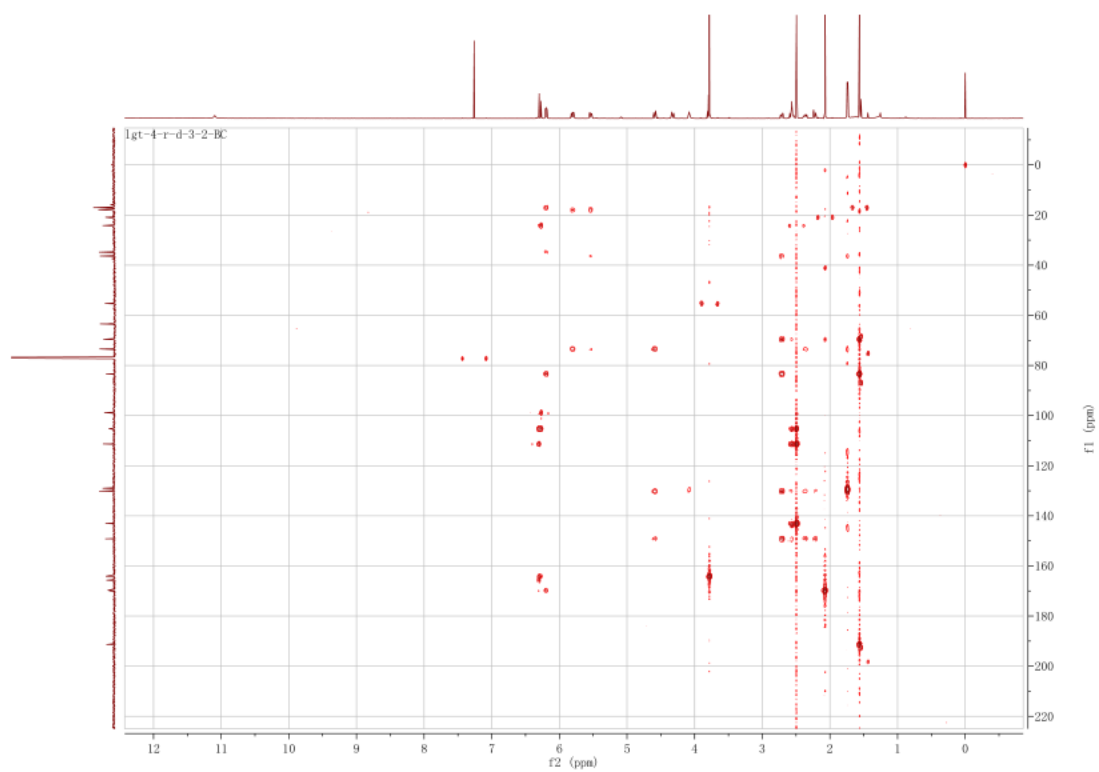


Figure S19. HMBC (600 MHz, CDCl₃) spectrum of compound **2**

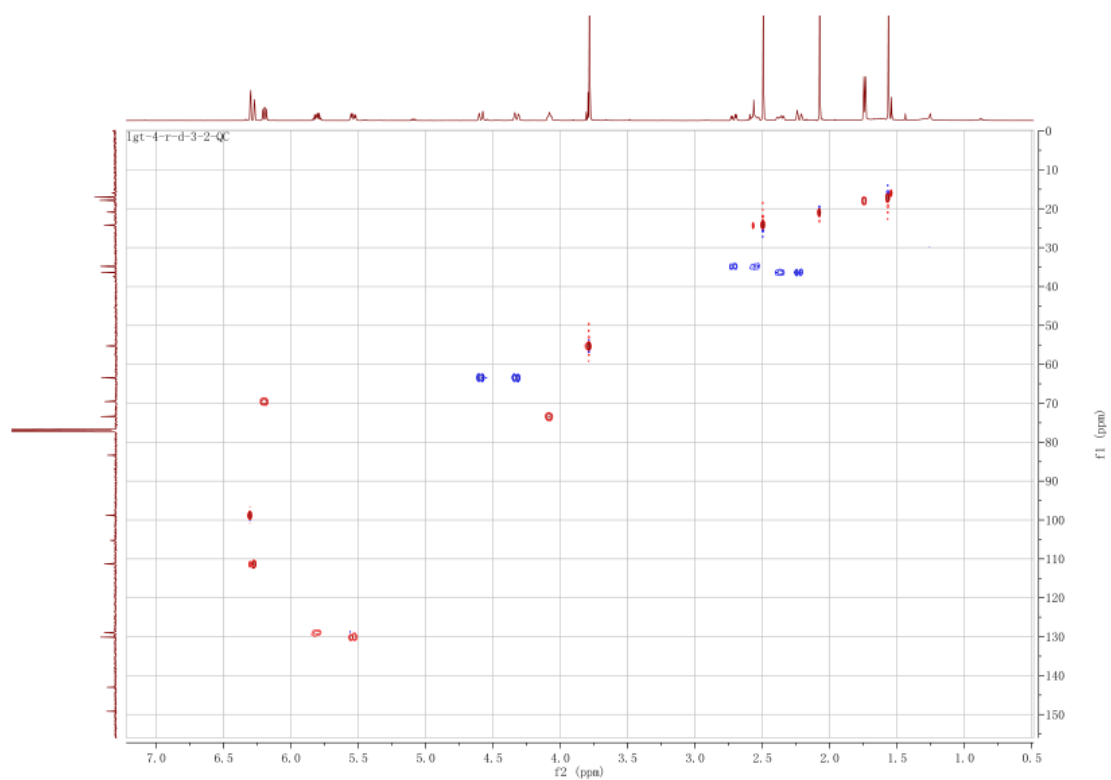


Figure S20. HMQC (600 MHz, CDCl_3) spectrum of compound **2**