

Supplementary Materials

Sesquiterpenoids from *Inula britannica* and Their Potential Effects against Triple Negative Breast Cancer Cells

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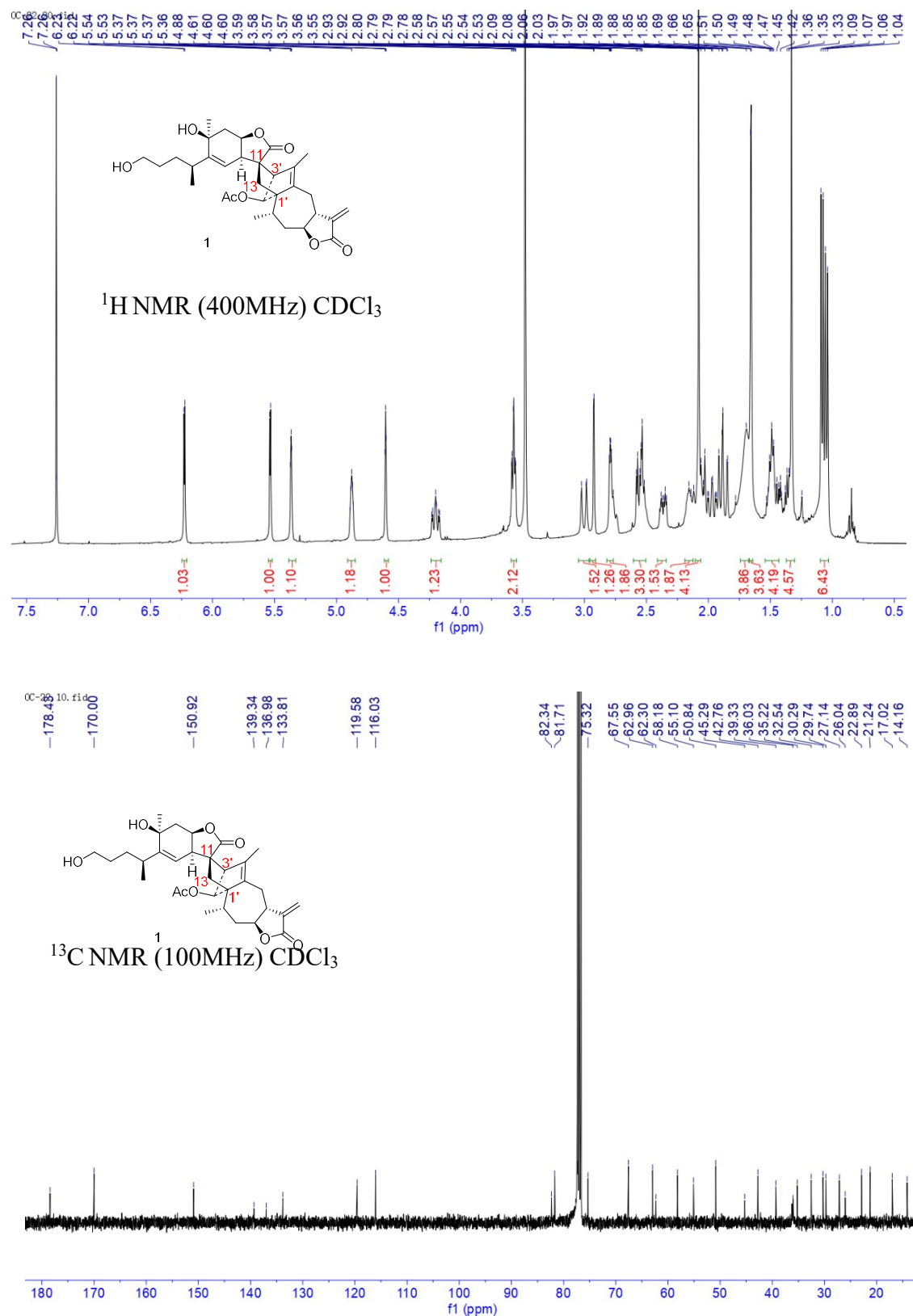
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Table S1. Crystal data and structure refinement for **4**.

Identification code	4
Empirical formula	C ₁₅ H ₂₀ O ₄
Formula weight	264.31
Temperature/K	149.96(10)
Crystal system	orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁
a/Å	9.55914(9)
b/Å	10.00802(10)
c/Å	13.83442(15)
α /°	90
β /°	90
γ /°	90
Volume/Å ³	1323.51(2)
Z	4
ρ_{calc} /cm ³	1.326
μ /mm ⁻¹	0.779
F(000)	568.0
Crystal size/mm ³	0.22 × 0.16 × 0.05
Radiation	Cu K α (λ = 1.54184)
2 Θ range for data collection/°	10.912 to 154.8
Index ranges	-9 ≤ h ≤ 11, -12 ≤ k ≤ 12, -17 ≤ l ≤ 16
Reflections collected	7356
Independent reflections	2626 [R_{int} = 0.0173, R_{sigma} = 0.0153]
Data/restraints/parameters	2626/0/183
Goodness-of-fit on F ²	1.010
Final R indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0301, wR_2 = 0.1041
Final R indexes [all data]	R_1 = 0.0303, wR_2 = 0.1044
Largest diff. peak/hole / e Å ⁻³	0.19/-0.17
Flack parameter	-0.04(5)

Spectral data for isolates 1–8:

Figure S1. ^1H , ^{13}C NMR, HSQC, HMBC and ^1H - ^1H COSY (CDCl_3) spectra of **1**.



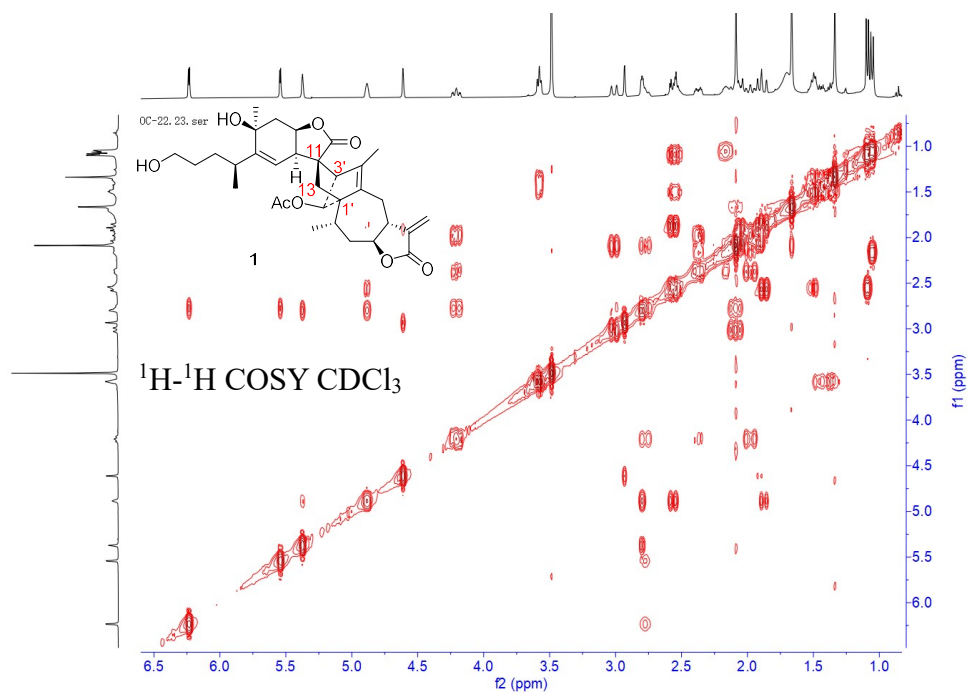
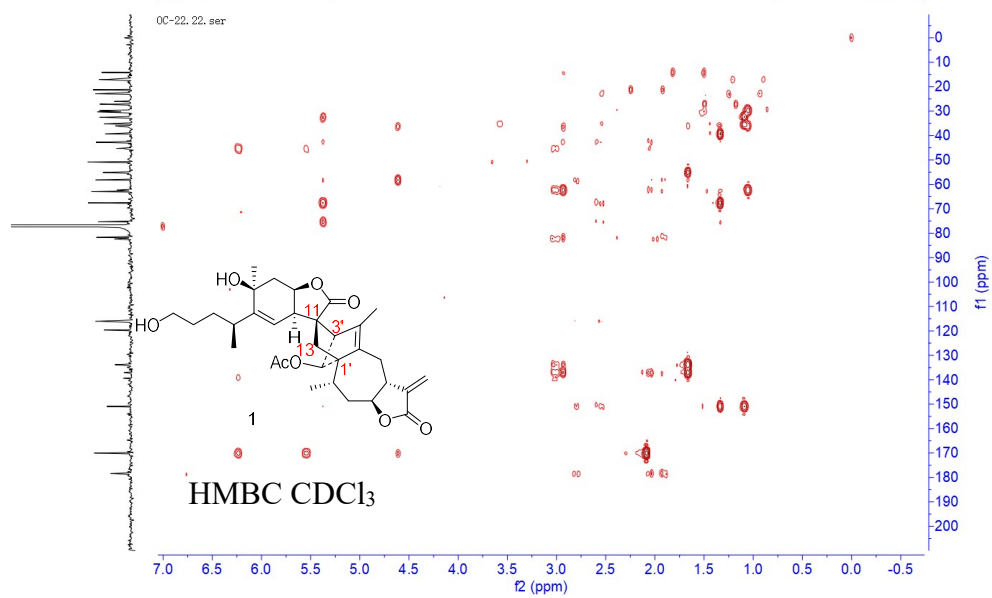
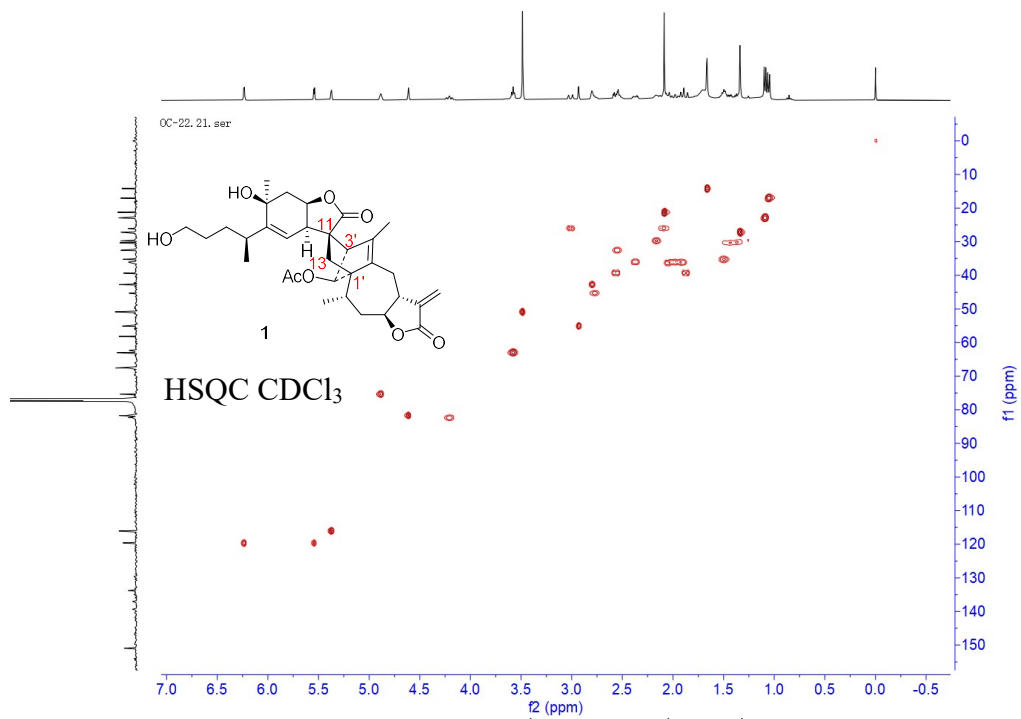
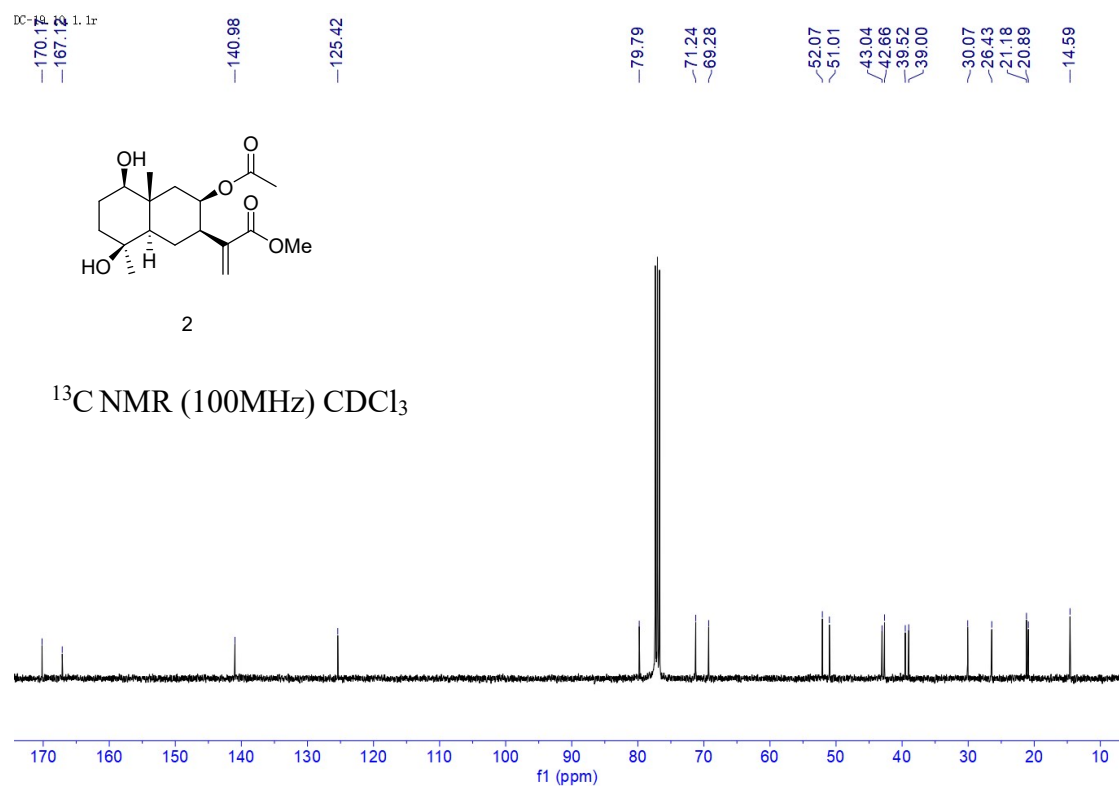
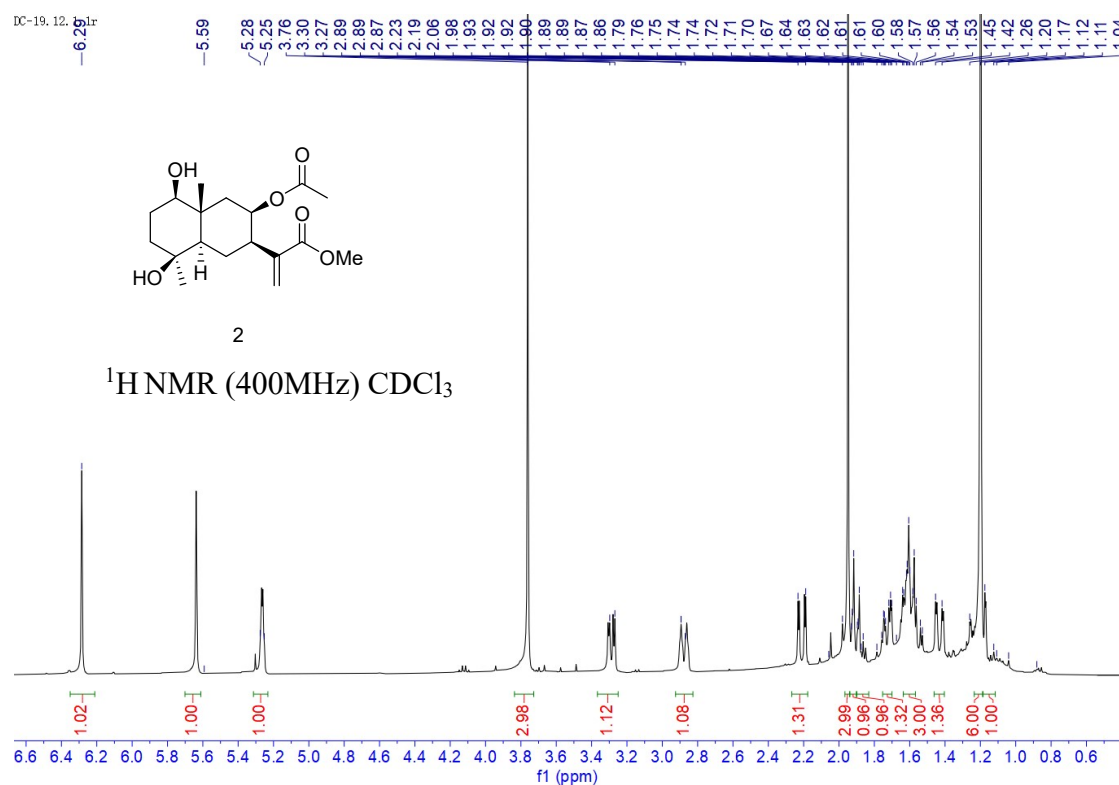
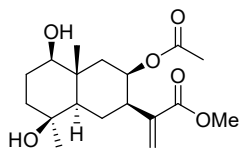
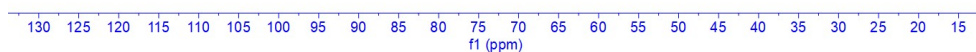
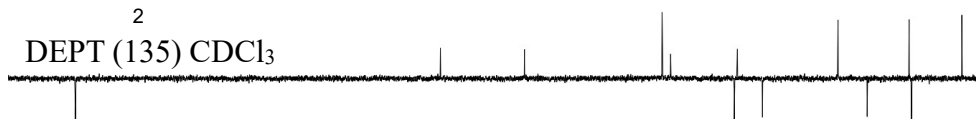


Figure S2. ^1H , ^{13}C , DEPT, HSQC and ^1H - ^1H COSY NMR (CDCl_3) spectra of **2**.

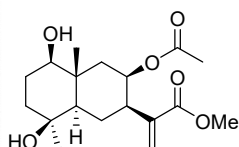




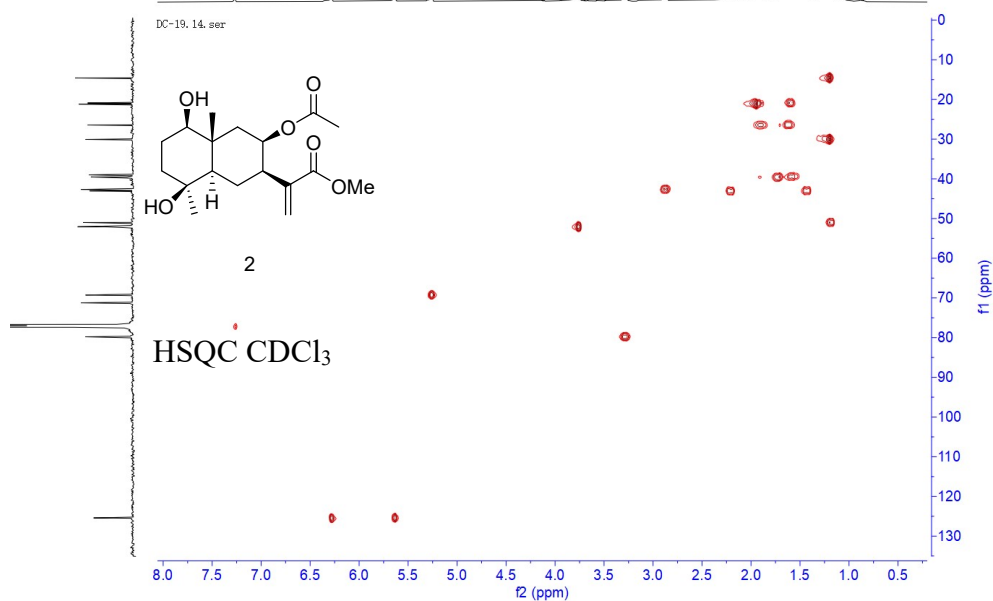
2

DEPT (135) CDCl₃

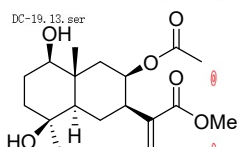
DC-19.14.ser



2

HSQC CDCl₃

DC-19.13.ser



2

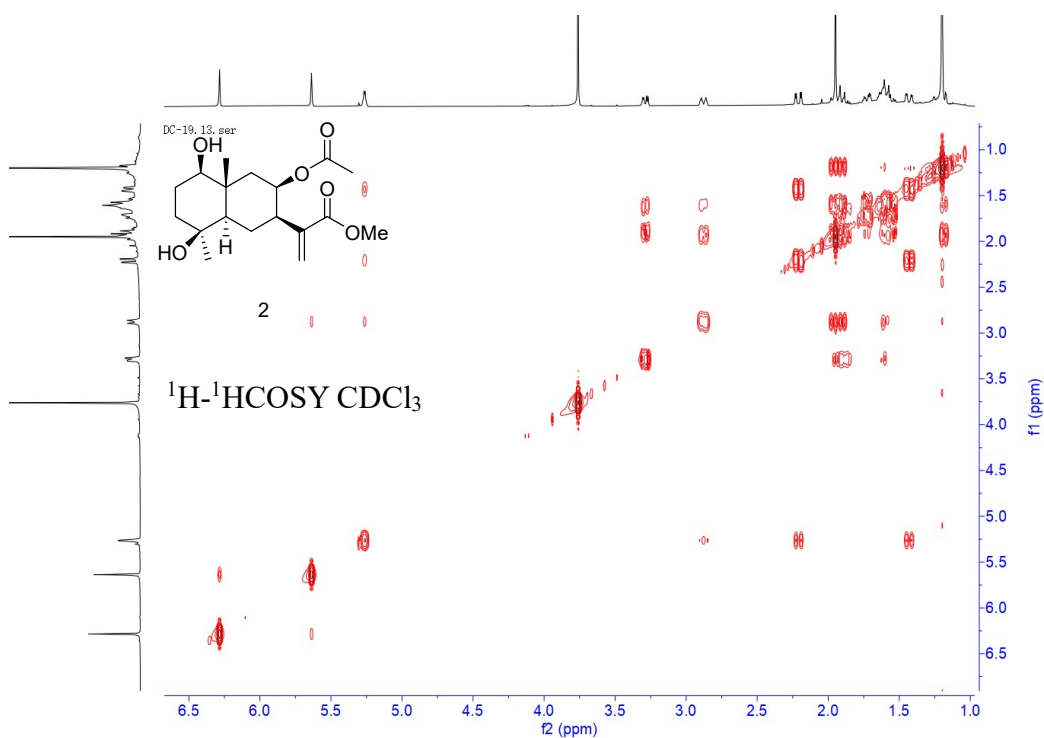
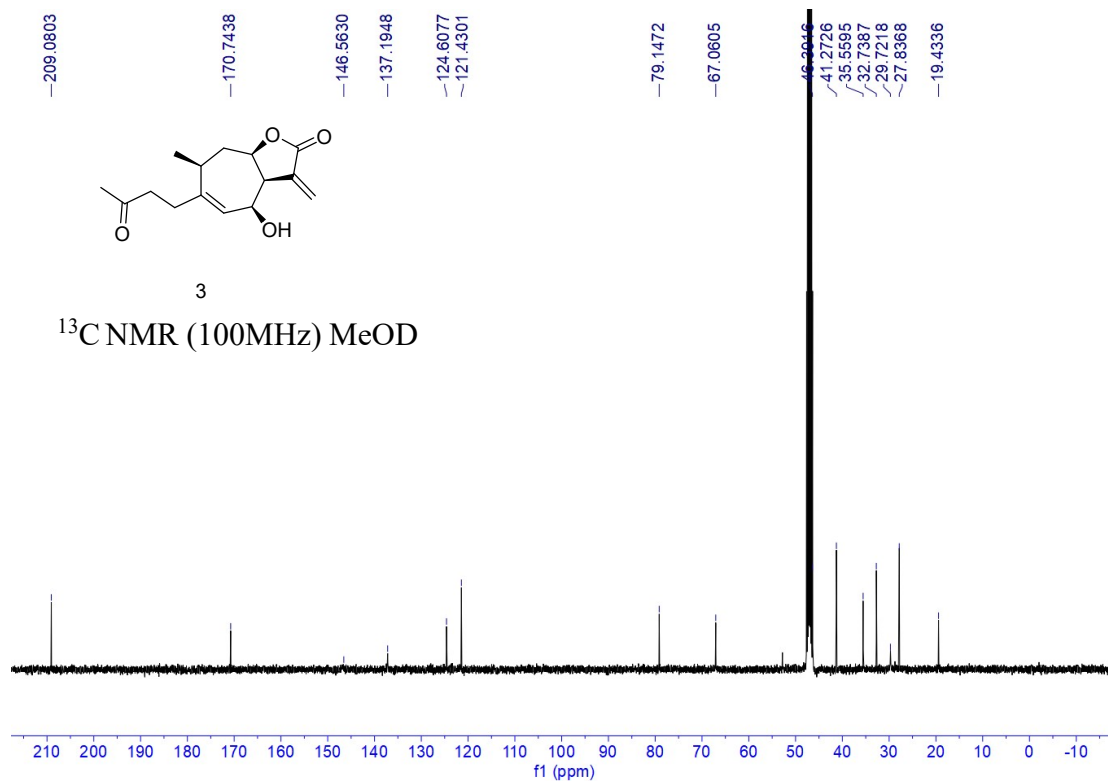
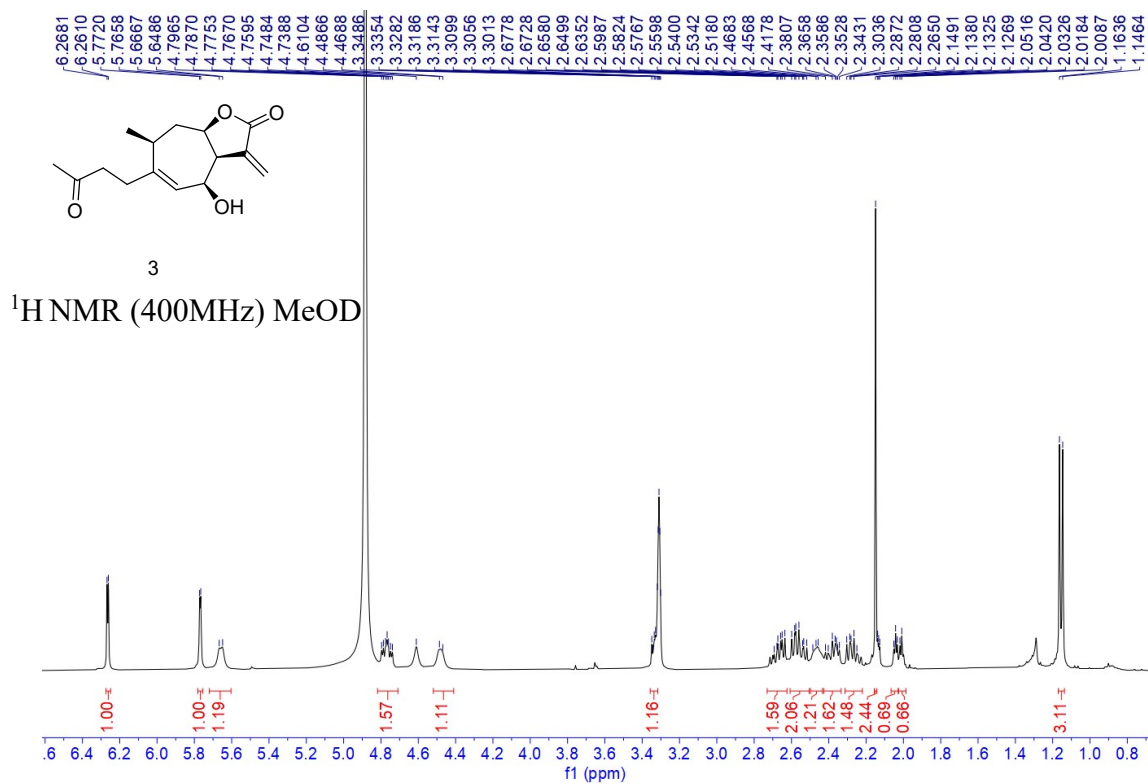
¹H-¹H COSY CDCl₃

Figure S3. ^1H , ^{13}C , DEPT, HSQC and HMBC NMR (MeOD) spectra of **3**





DEPT (135) MeOD

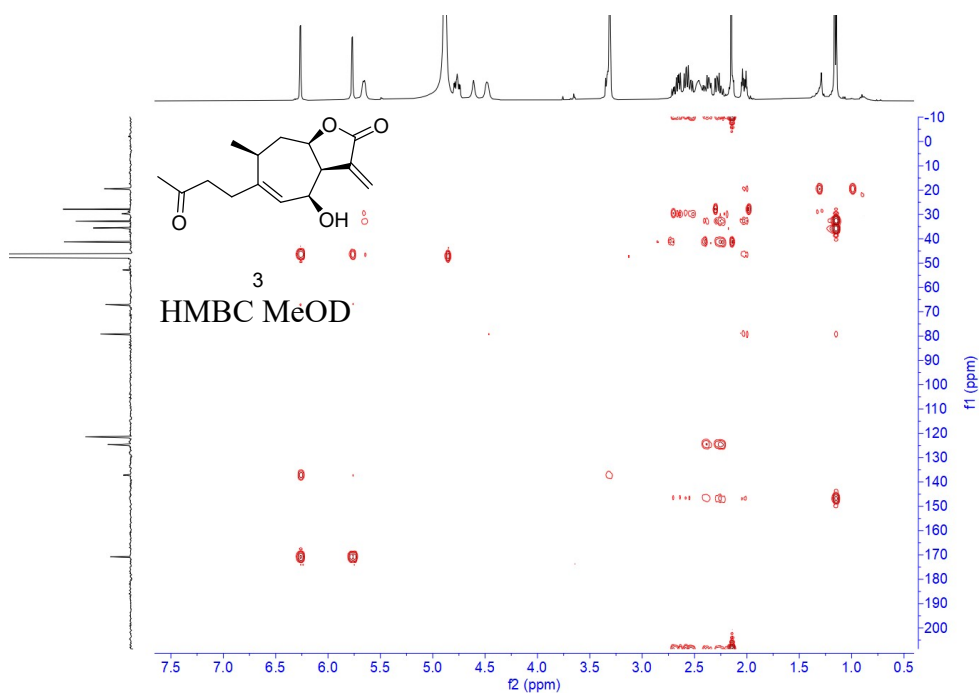
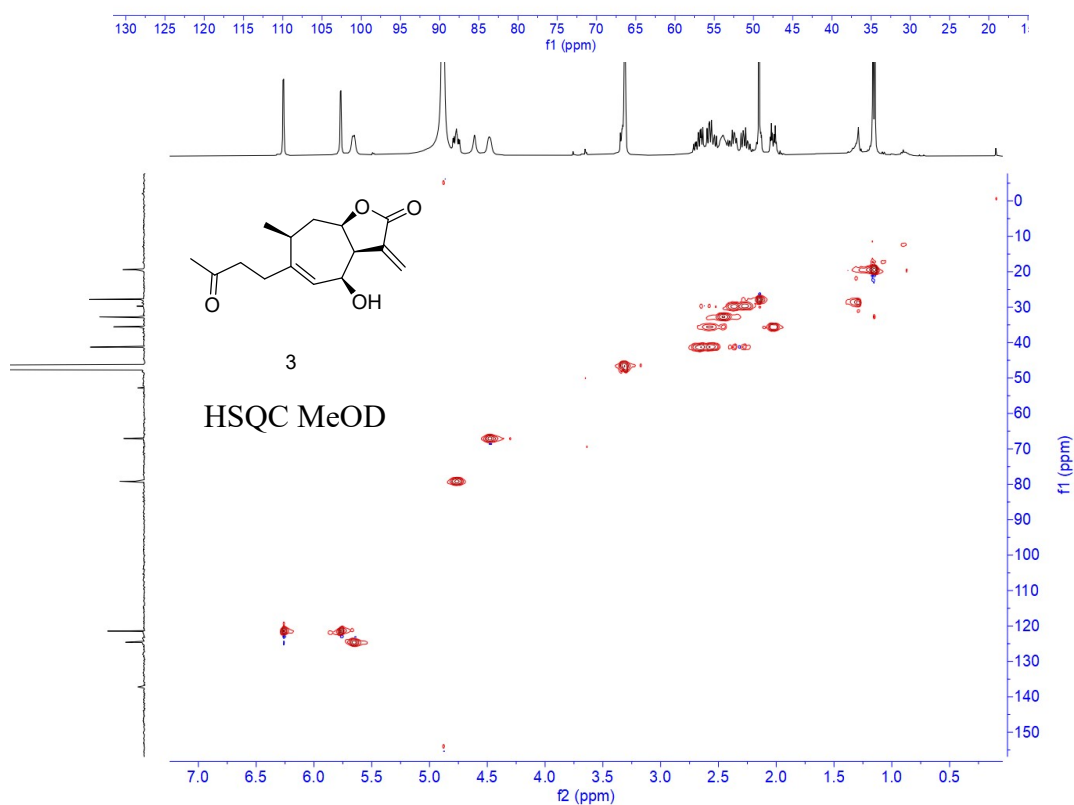
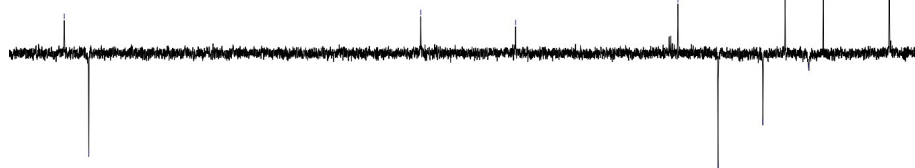
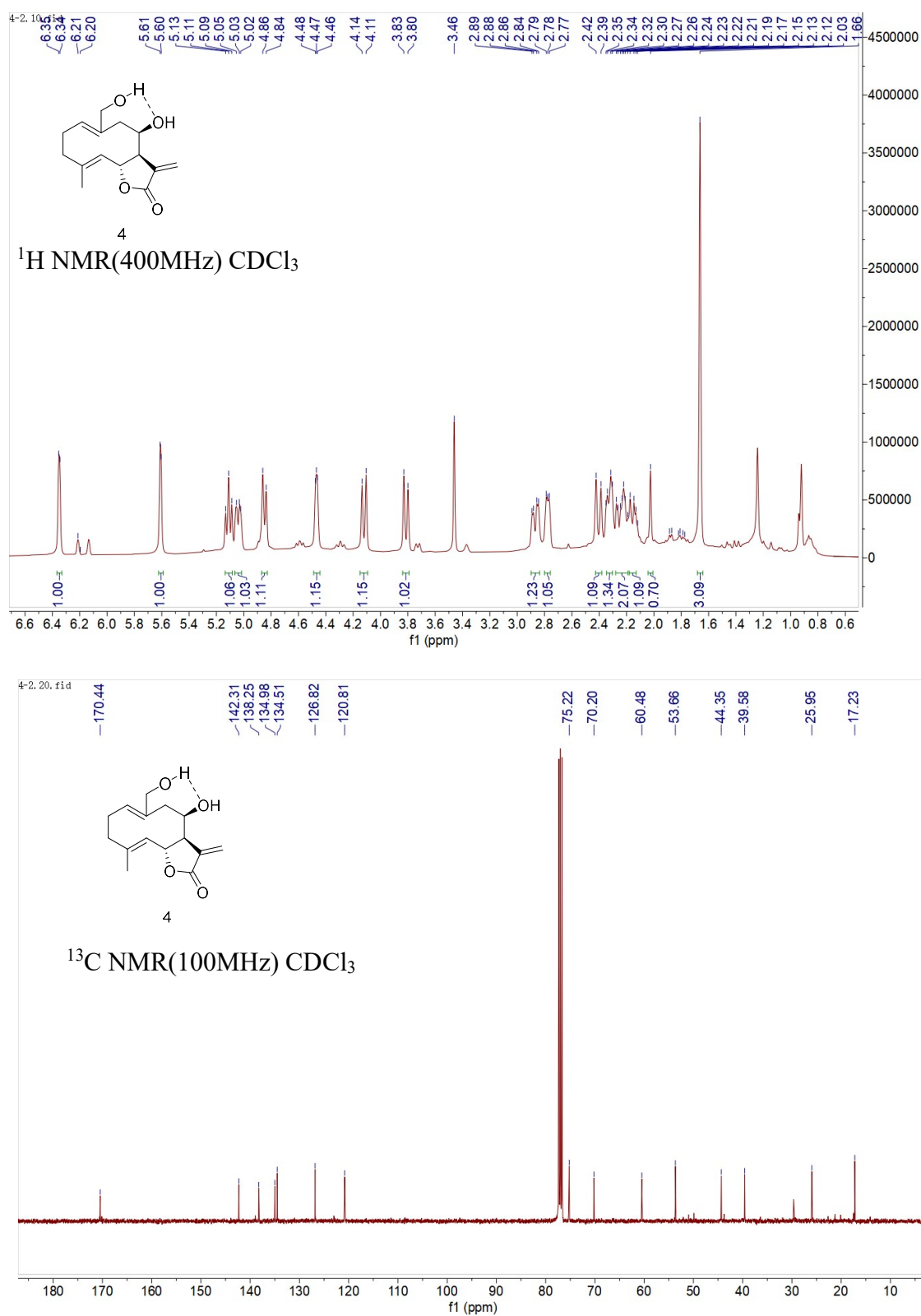
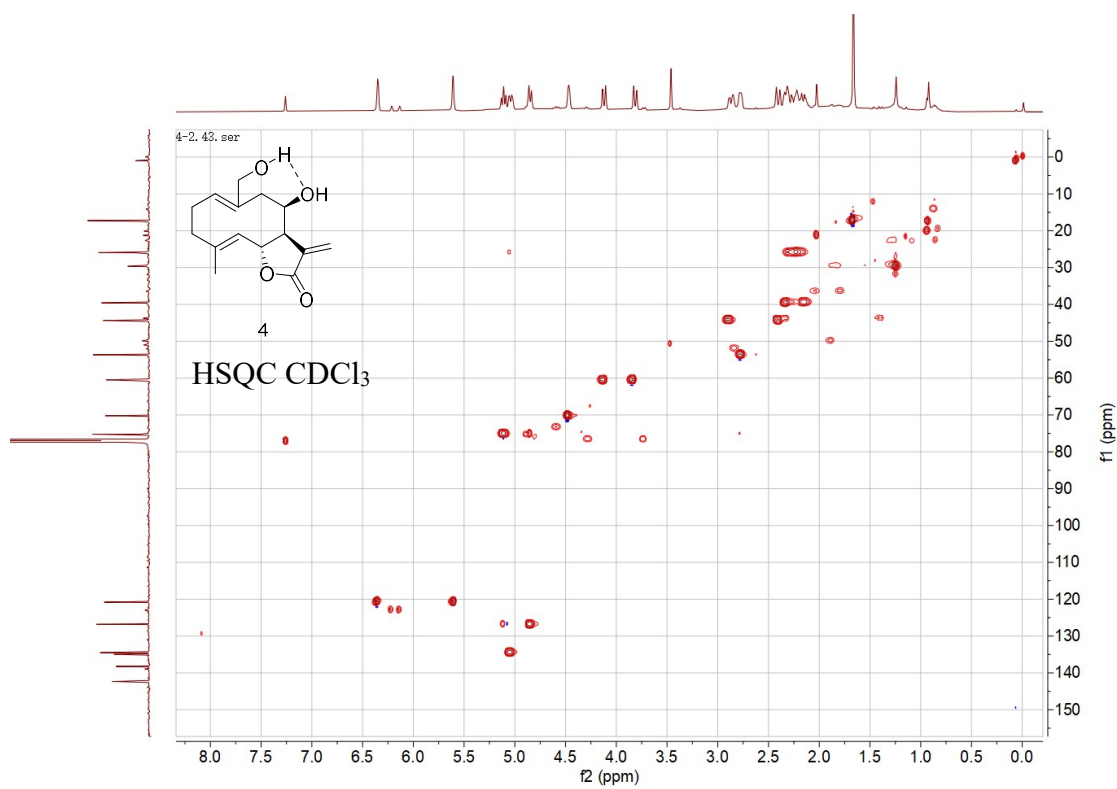
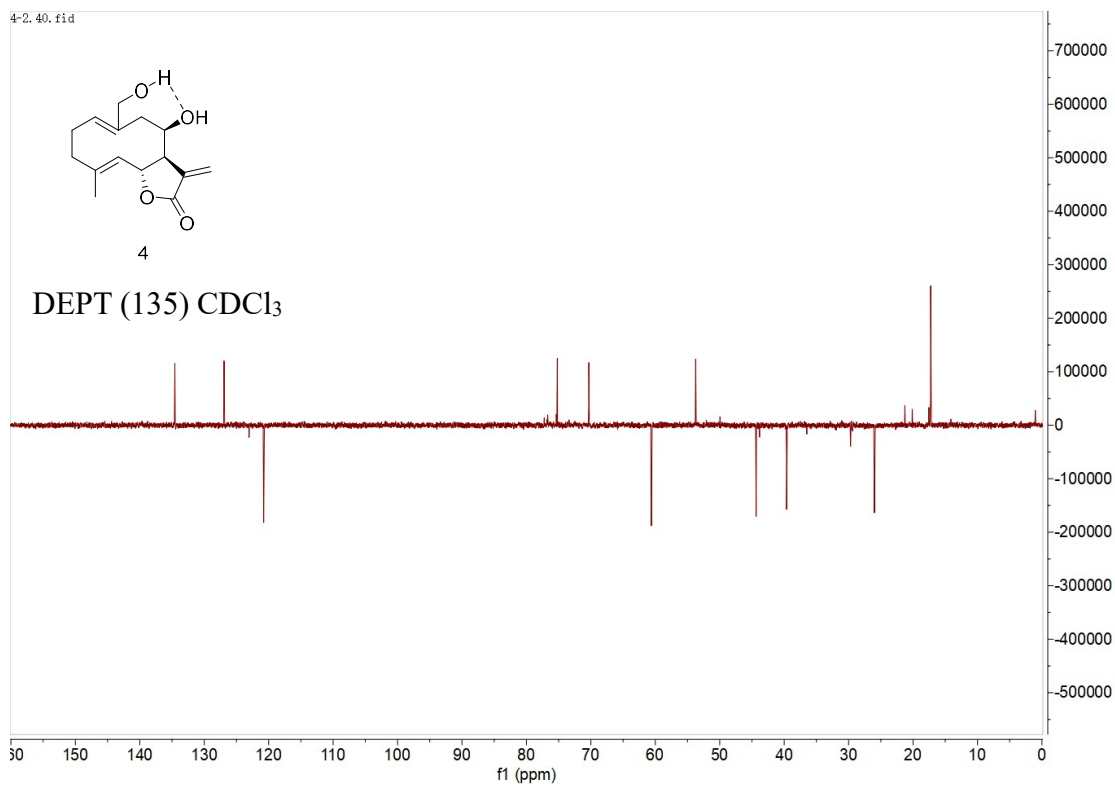


Figure S4. ^1H , ^{13}C , DEPT, HSQC, HMBC and ^1H - ^1H COSY (CDCl_3) spectra of **4**





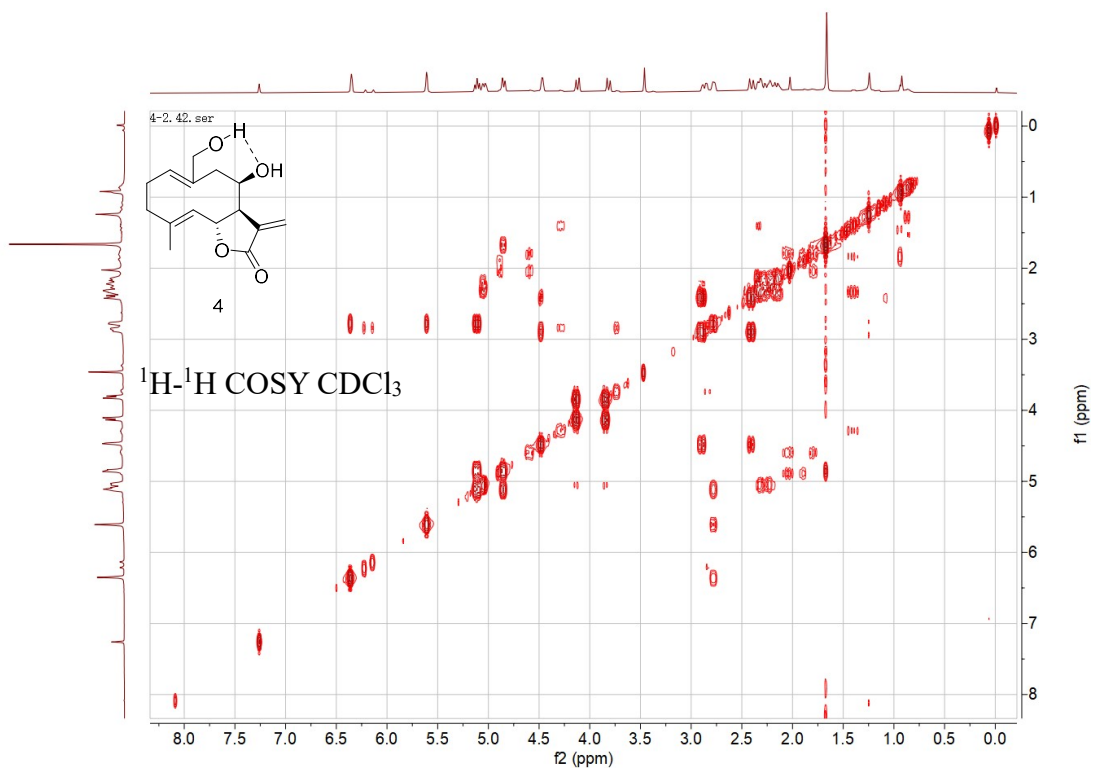
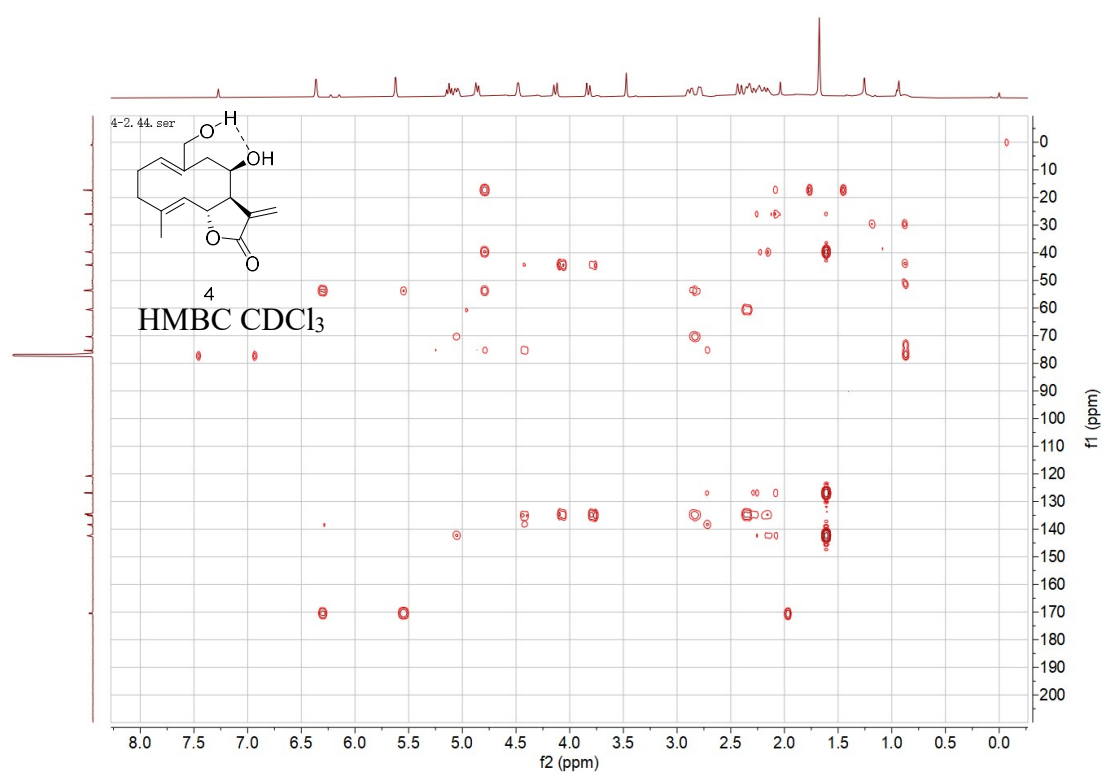
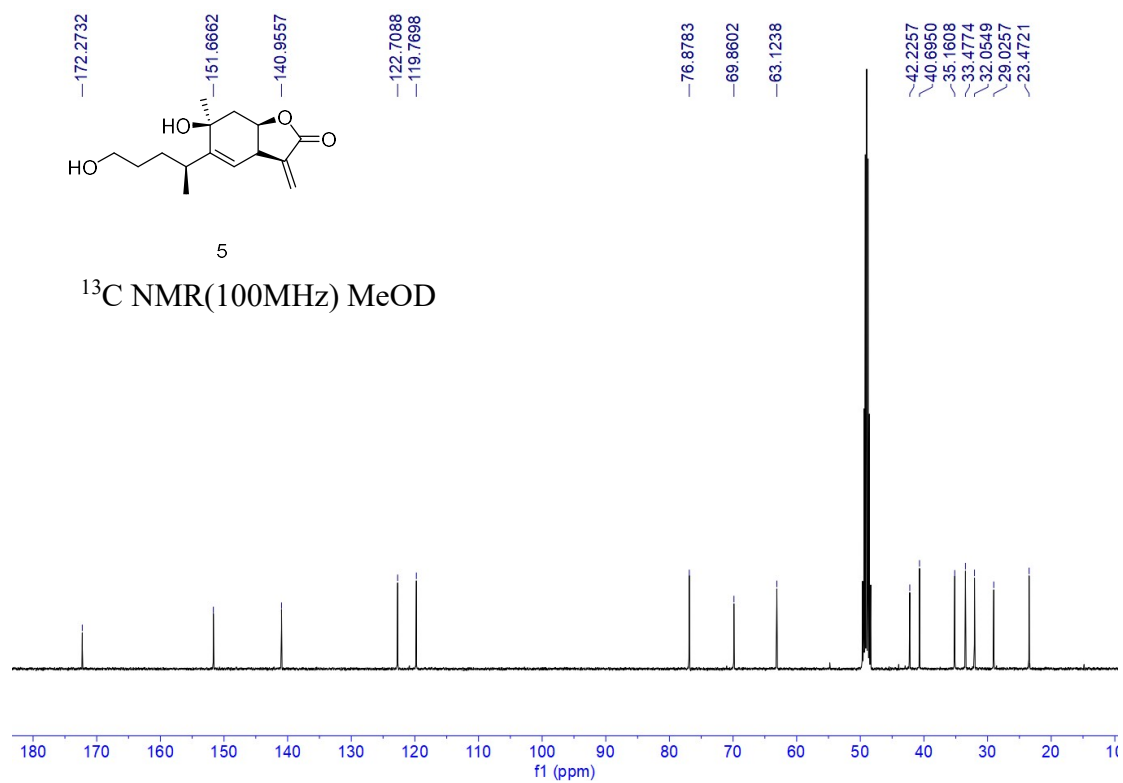
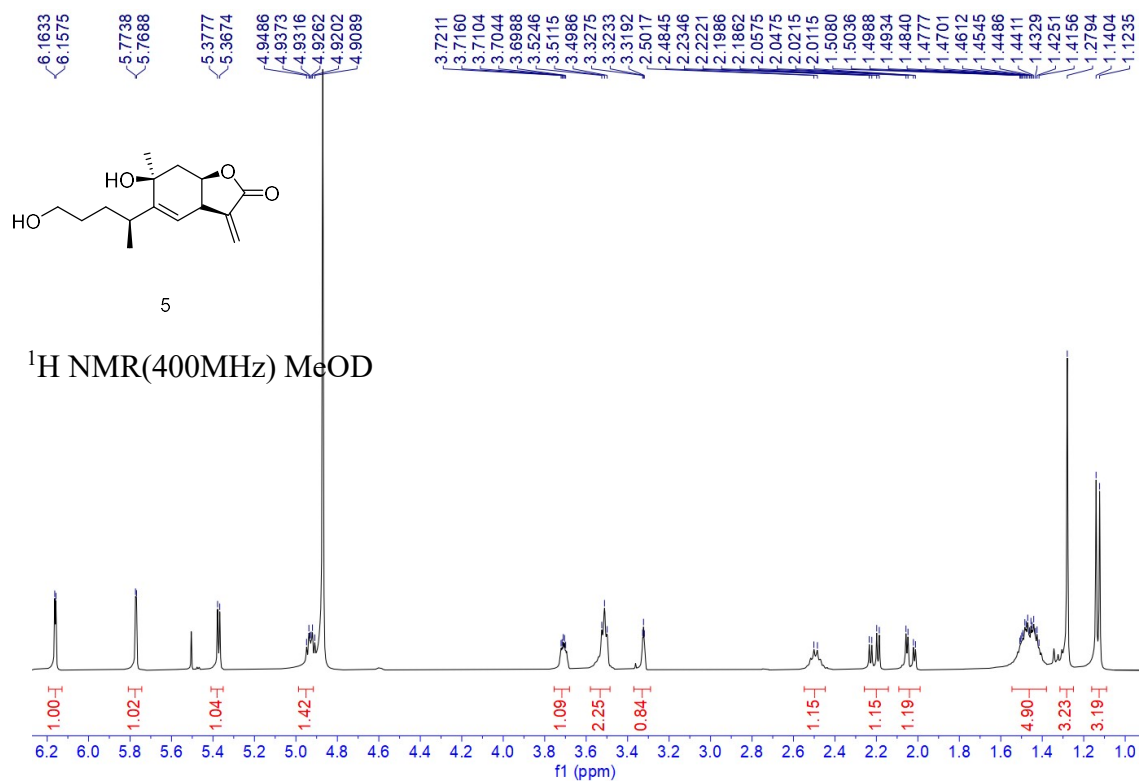


Figure S5. ^1H , ^{13}C , HSQC, HMBC and ^1H - ^1H COSY NMR (MeOD) spectra of **5**



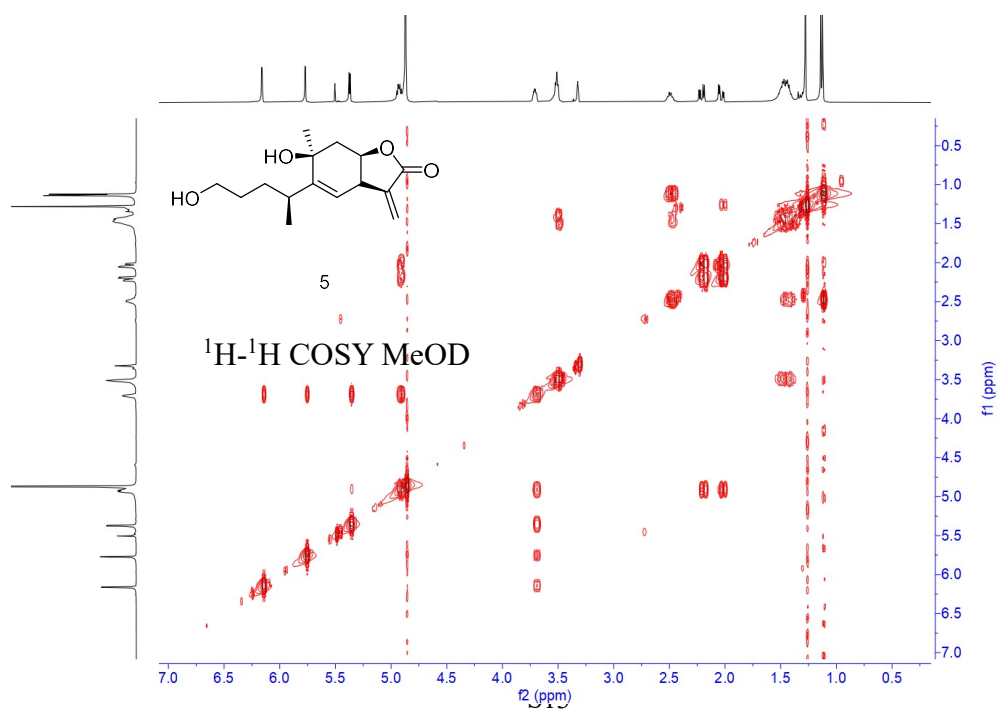
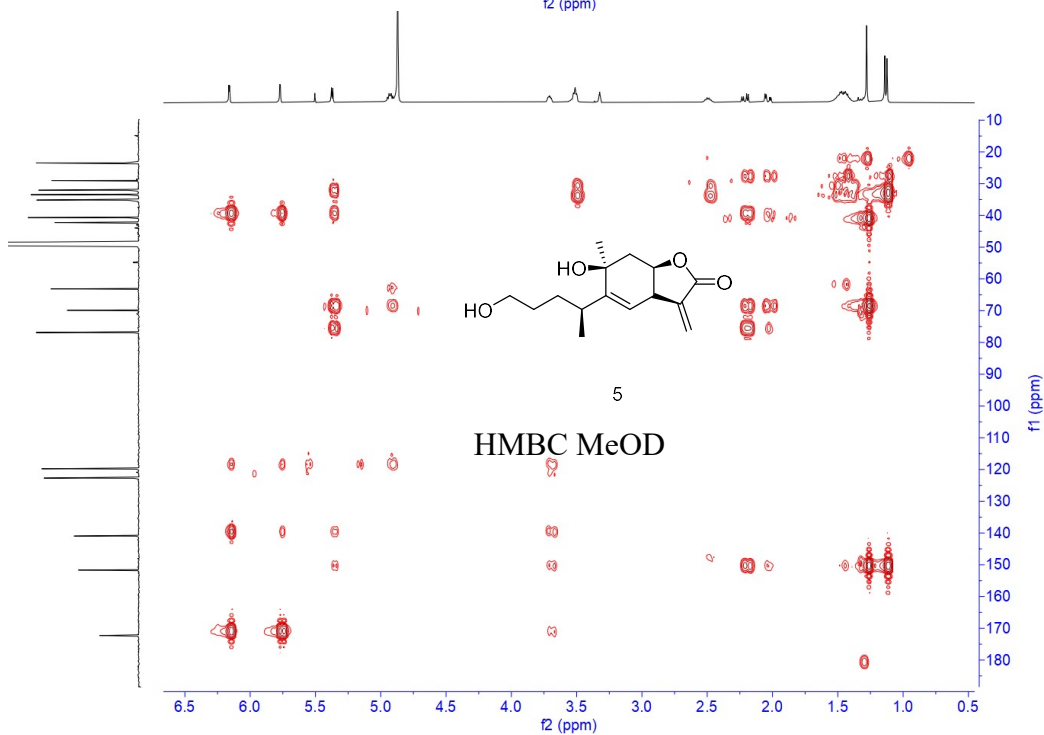
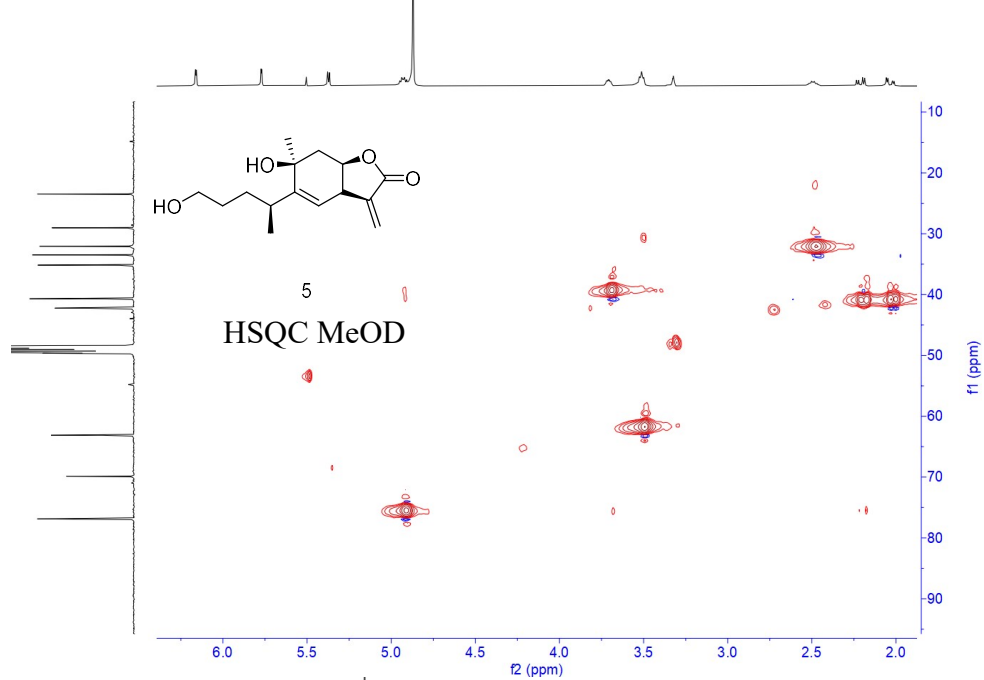
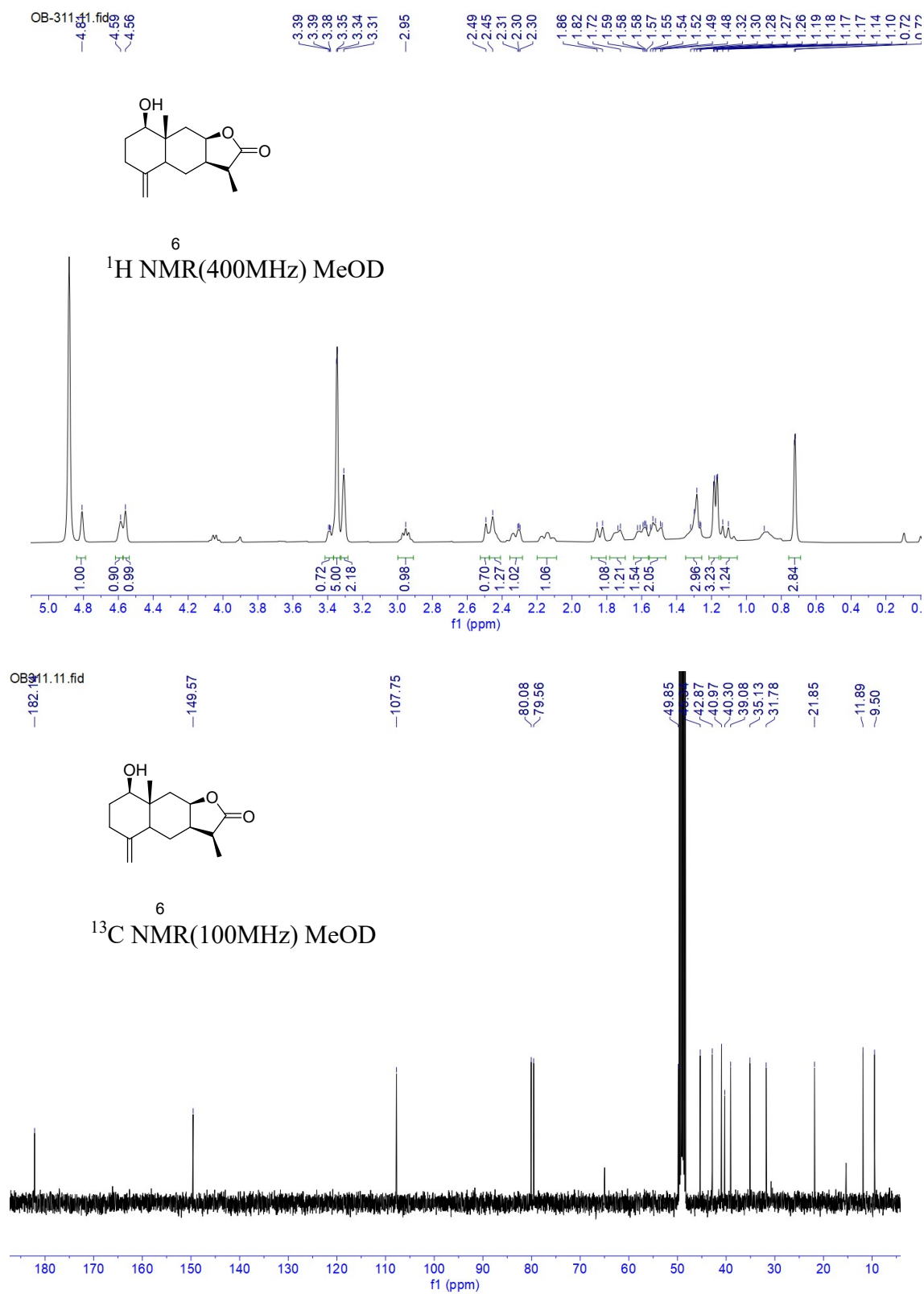
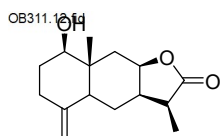


Figure S6. ^1H , ^{13}C , HSQC, HMBC, ^1H - ^1H COSY and NOE (MeOD) spectra of **6**





80.07
79.55

49.85
45.33
42.87
40.96
39.07
35.13
31.78

21.84

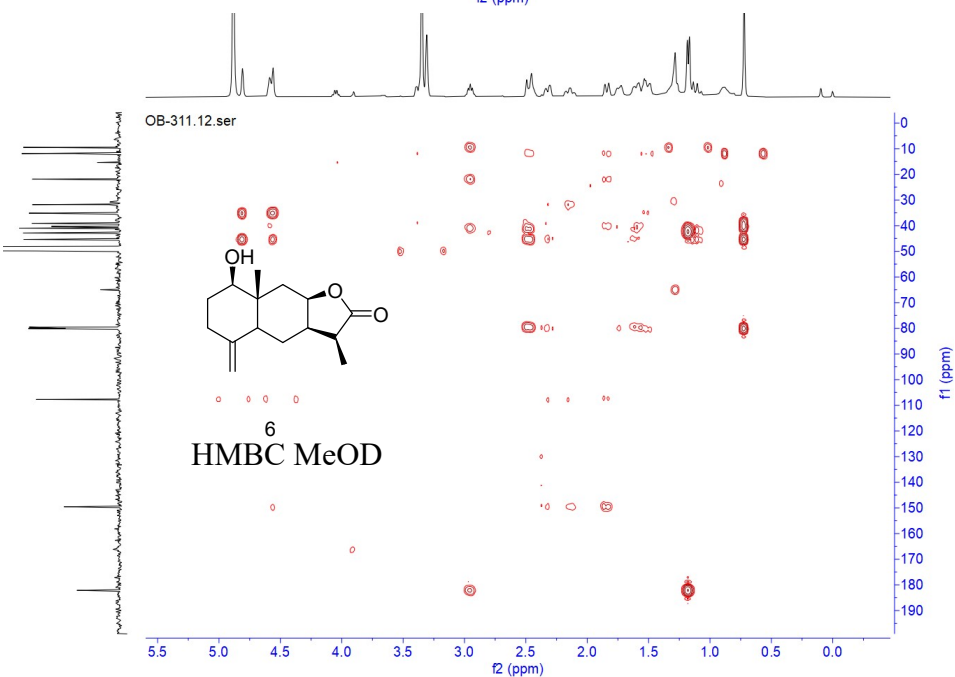
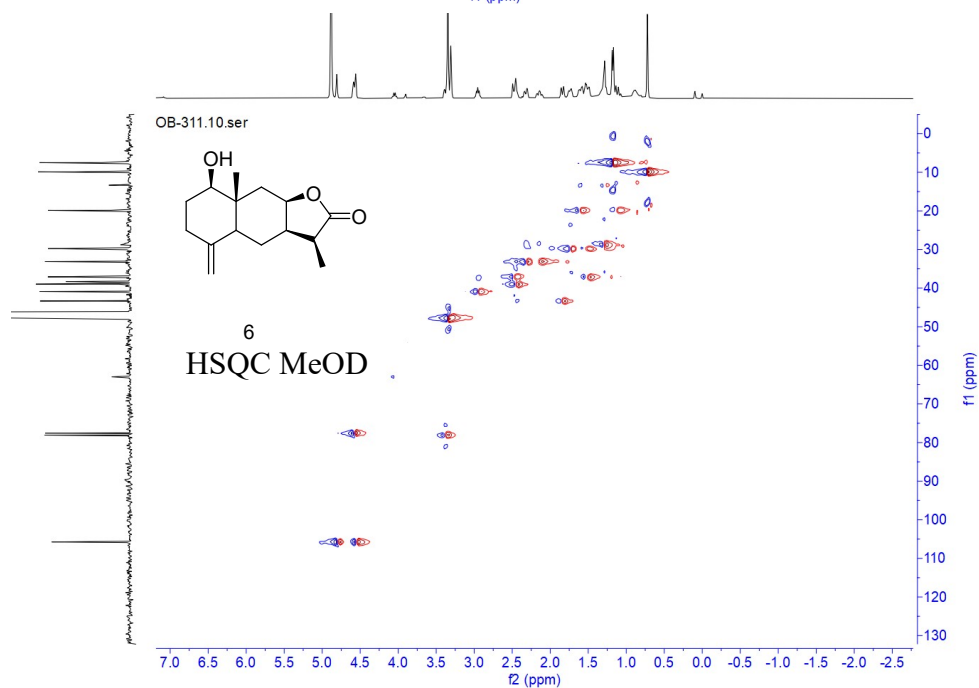
11.89
9.50

6

DEPT (135) MeOD



115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10



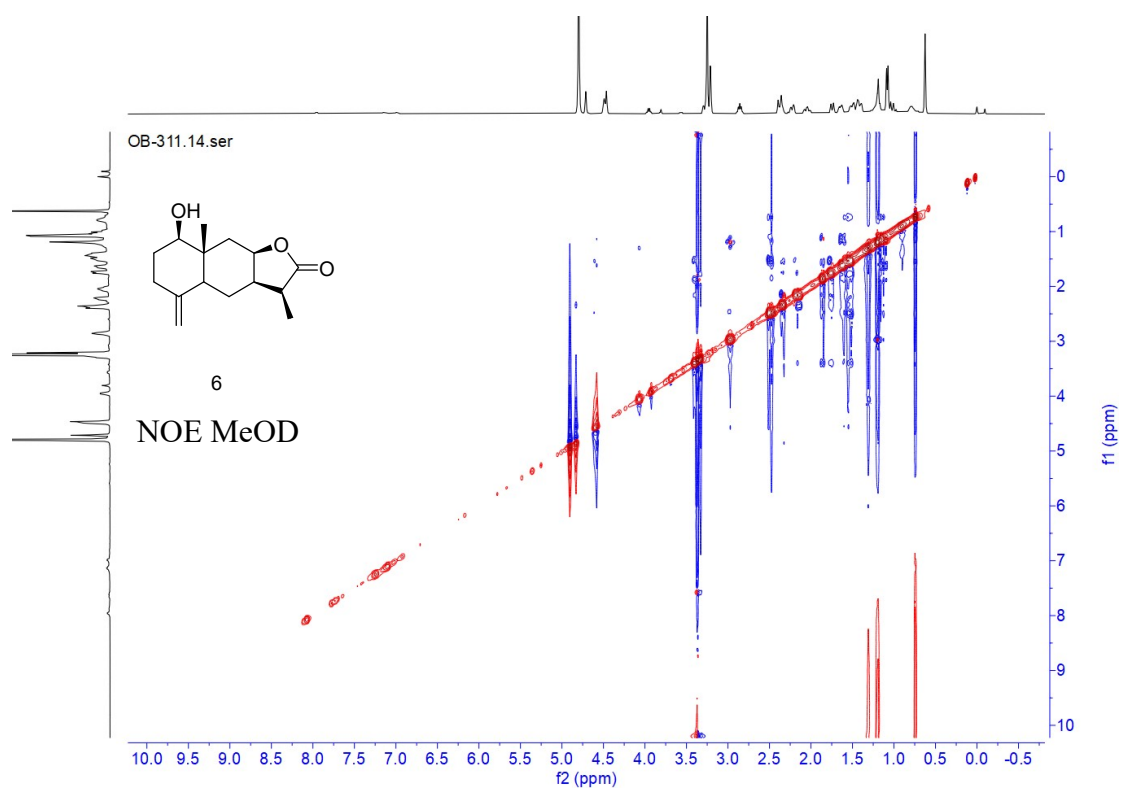
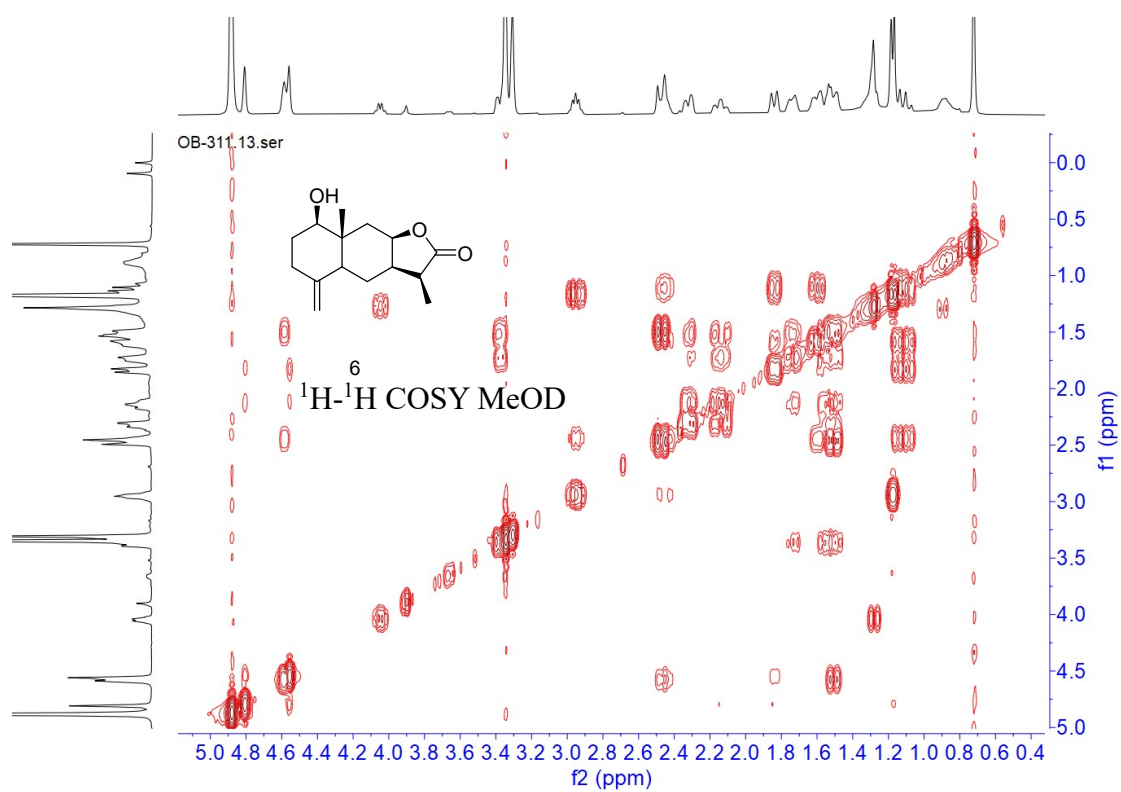
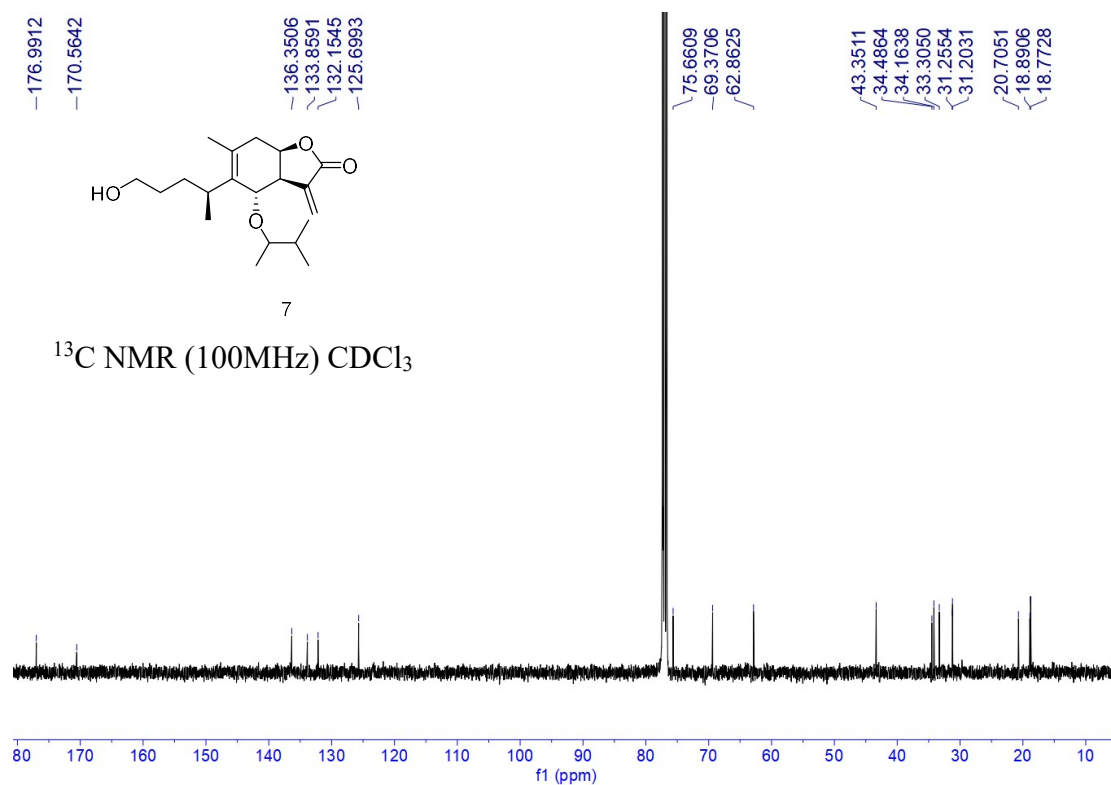
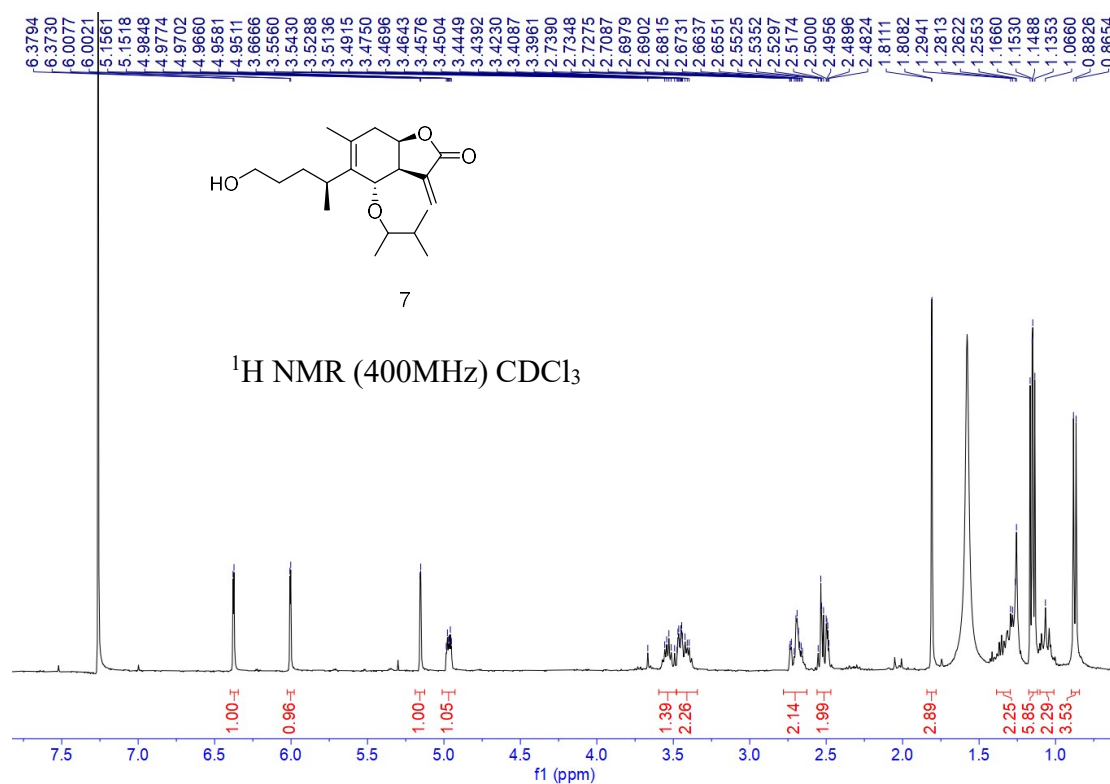
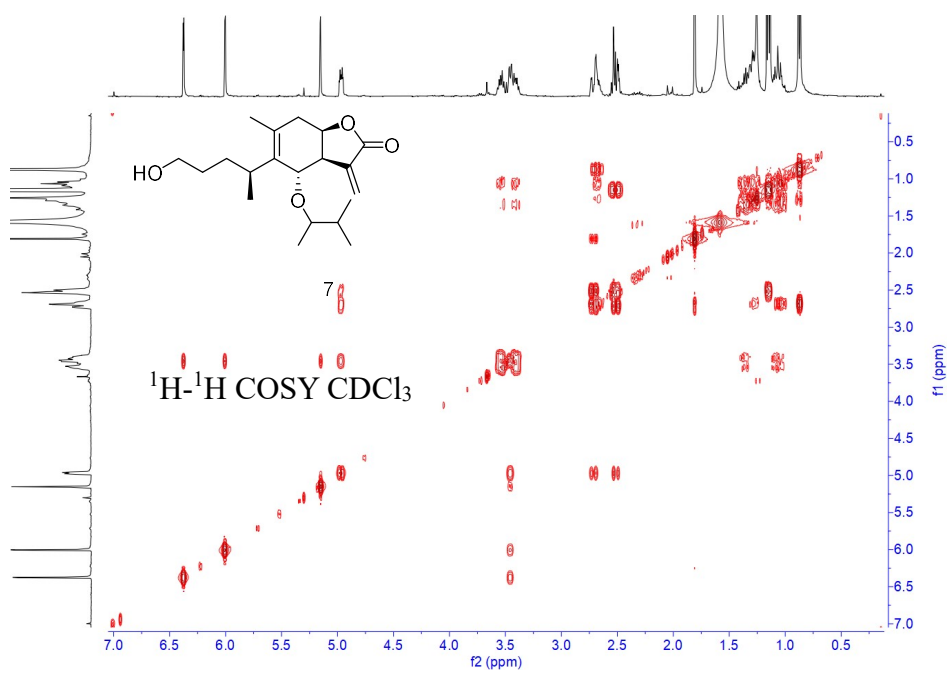
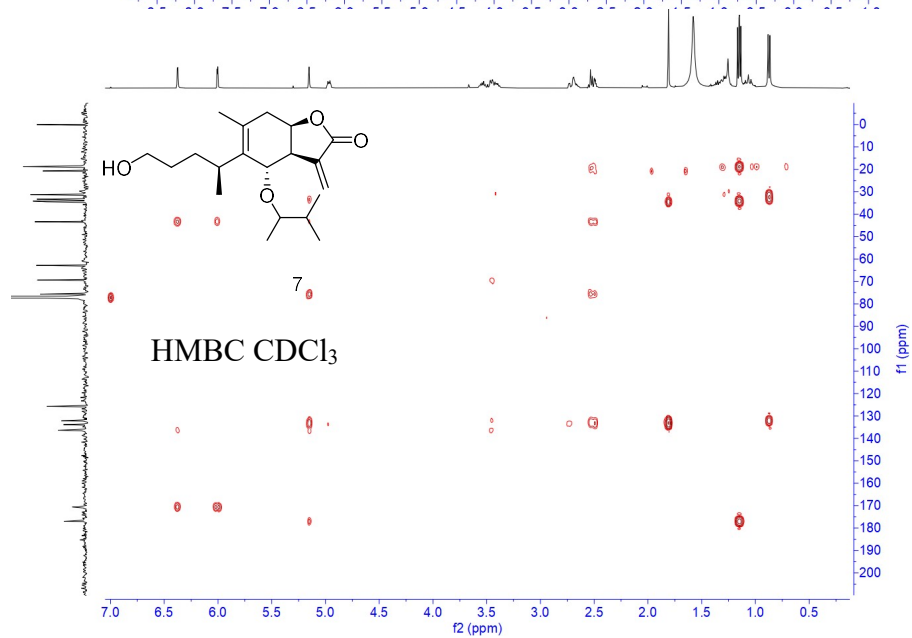
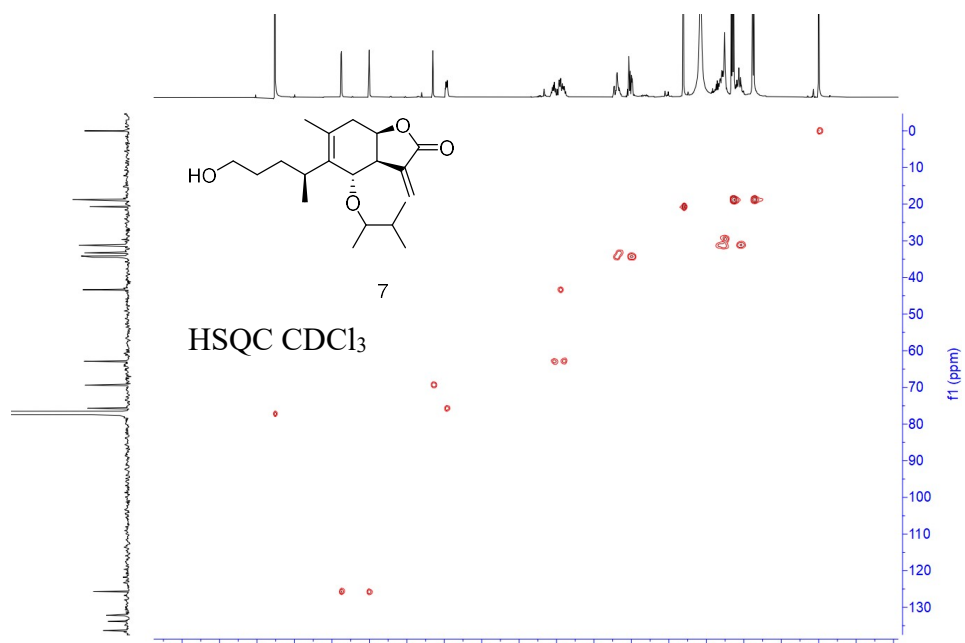
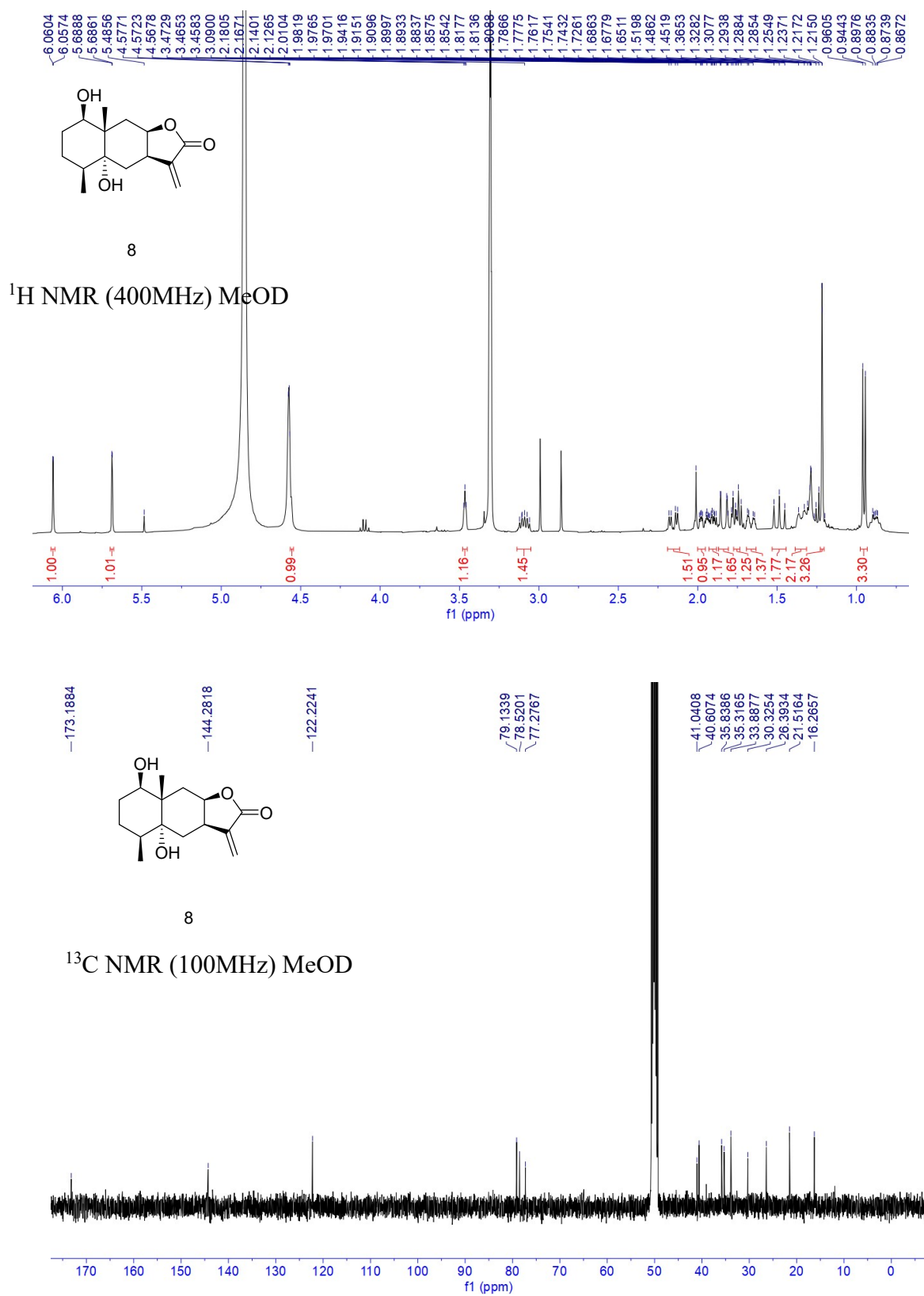


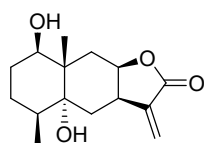
Figure S7. ^1H , ^{13}C , HSQC, HMBC and ^1H - ^1H COSY NMR (CDCl_3) spectra of **7**





FigureS8. ^1H , ^{13}C , HSQC, HMBC and ^1H - ^1H COSY NMR (MeOD) spectra of **8**





8

DEPT (135) MeOD

