

Supporting Information

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Diterpenoids from the Roots of *Clerodendrum bungei*

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Peipei Shan^{3*} and Hua Zhang^{1*}

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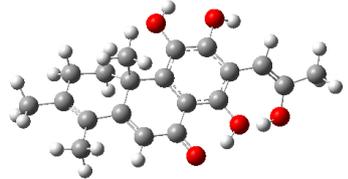
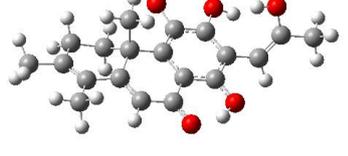
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Table of Contents	Page
Table S1: Re-optimized conformers, energies and proportions for 1 .	3
Figure S1: ¹ H NMR spectrum of 1 in CDCl ₃ .	4
Figure S2: ¹³ C and DEPT NMR spectra of 1 in CDCl ₃ .	4
Figure S3: ¹ H- ¹ H COSY spectrum of 1 in CDCl ₃ .	5
Figure S4: HSQC spectrum of 1 in CDCl ₃ .	5
Figure S5: HMBC spectrum of 1 in CDCl ₃ .	6
Figure S6: NOESY spectrum of 1 in CDCl ₃ .	6
Figure S7: (+)-HR-ESIMS spectrum of 1 .	7
Figure S8: The UV spectrum of 1 .	7
Figure S9: ¹ H NMR spectrum of 2 in CD ₃ OD.	8
Figure S10: ¹³ C NMR spectrum of 2 in CD ₃ OD.	8
Figure S11: ¹ H- ¹ H COSY spectrum of 2 in CD ₃ OD.	9
Figure S12: HSQC spectrum of 2 in CD ₃ OD.	9
Figure S13: HMBC spectrum of 2 in CD ₃ OD.	10
Figure S14: NOESY spectrum of 2 in CD ₃ OD.	10
Figure S15: (+)-HR-ESIMS spectrum of 2 .	11
Figure S16: The UV spectrum of 2 .	11
Figure S17: ¹ H NMR spectrum of 2 in CDCl ₃ .	12
Figure S18: ¹³ C and DEPT NMR spectra of 2 in CDCl ₃ .	12
Figure S19: ¹ H NMR spectrum of 2a in CDCl ₃ .	13

Figure S20: ^1H NMR spectrum of 2b in CDCl_3 .	13
Figure S21: ^1H NMR spectrum of 3 in CDCl_3 .	14
Figure S22: ^{13}C and DEPT NMR spectra of 3 in CDCl_3 .	14
Figure S23: ^1H - ^1H COSY spectrum of 3 in CDCl_3 .	15
Figure S24: HSQC spectrum of 3 in CDCl_3 .	15
Figure S25: HMBC spectrum of 3 in CDCl_3 .	16
Figure S26: NOESY spectrum of 3 in CDCl_3 .	16
Figure S27: Linear correlation between the experimental ^{13}C NMR data for 3 and the calculated data for (<i>Z</i>)- Δ^{15} (left) and (<i>E</i>)- Δ^{15} (right) isomers, respectively.	17
Figure S28: SciFinder search report for compound 1 .	17
Figure S29: SciFinder search report for compound 2 .	18
Figure S30: ^1H NMR spectrum of 4 in CDCl_3 .	19
Figure S31: ^{13}C and DEPT NMR spectra of 4 in CDCl_3 .	19
Figure S32: ^1H NMR spectrum of 5 in CDCl_3 .	20
Figure S33: ^{13}C and DEPT NMR spectra of 5 in CDCl_3 .	20
Figure S34: ^1H NMR spectrum of 6 in CD_3OD .	21
Figure S35: ^{13}C and DEPT NMR spectra of 6 in CD_3OD .	21
Figure S36: ^1H NMR spectrum of 7 in CDCl_3 .	22
Figure S37: ^{13}C and DEPT NMR spectra of 7 in CDCl_3 .	22
Figure S38: ^1H NMR spectrum of 8 in CDCl_3 .	23
Figure S39: ^{13}C and DEPT NMR spectra of 8 in CDCl_3 .	23
Figure S40: ^1H NMR spectrum of 9 in CDCl_3 .	24
Figure S41: ^{13}C and DEPT NMR spectra of 9 in CDCl_3 .	24
Figure S42: ^1H NMR spectrum of 10 in CDCl_3 .	25
Figure S43: ^{13}C and DEPT NMR spectra of 10 in CDCl_3 .	25
Figure S44: ^1H NMR spectrum of 11 in CDCl_3 .	26
Figure S45: ^{13}C and DEPT NMR spectra of 11 in CDCl_3 .	26
Figure S46: ^1H NMR spectrum of 12 in CDCl_3 .	27
Figure S47: ^{13}C and DEPT NMR spectra of 12 in CDCl_3 .	27
Figure S48: ^1H NMR spectrum of 13 in CDCl_3 .	28
Figure S49: ^{13}C and DEPT NMR spectra of 13 in CDCl_3 .	28

Table S1. Re-optimized conformers, energies and proportions for **1**.

No.	Conformer	Energy (hartree)	Energy (Kcal/mol)	Proportion (%)
1		-1151.8059374	-722769.743777874	52.57
2		-1151.8058152	-722769.667096152	46.18
3		-1151.8022875	-722767.453429125	1.10
4		-1151.7997953	-722765.889548703	0.08
5		-1151.7996883	-722765.822405133	0.07

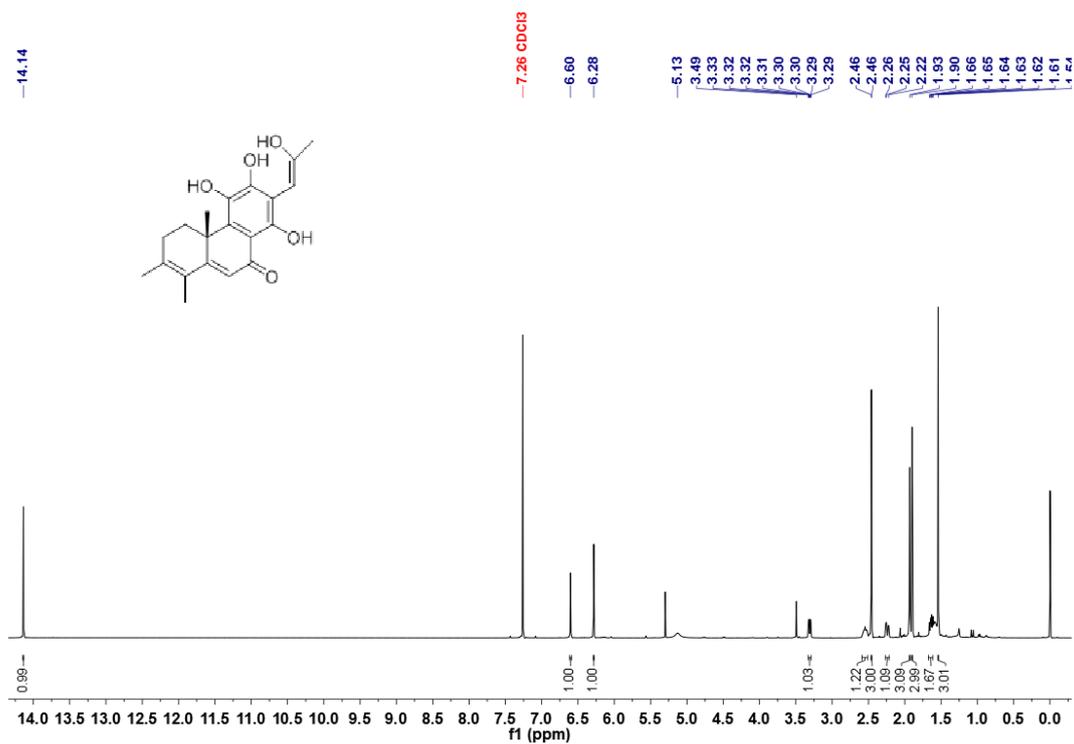


Figure S1: ¹H NMR spectrum of **1** in CDCl₃.

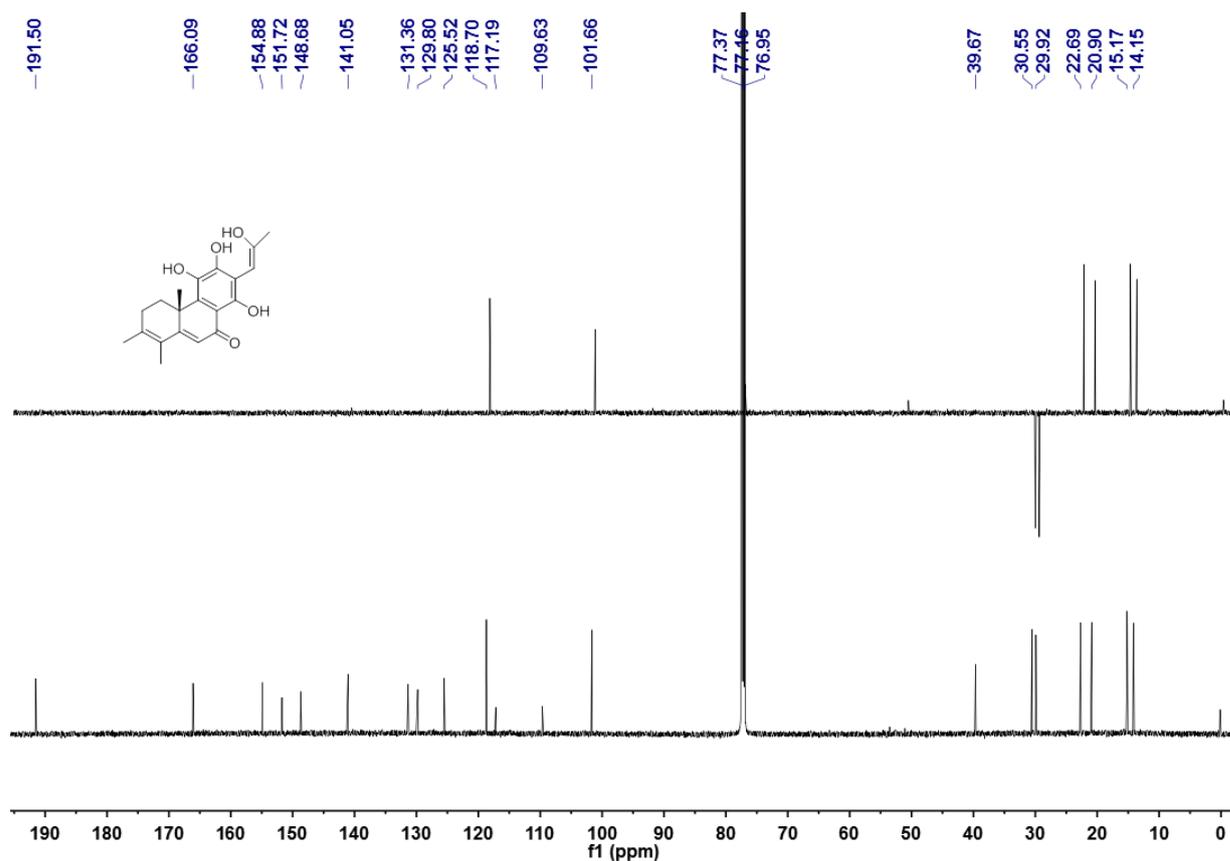


Figure S2: ¹³C and DEPT NMR spectra of **1** in CDCl₃.

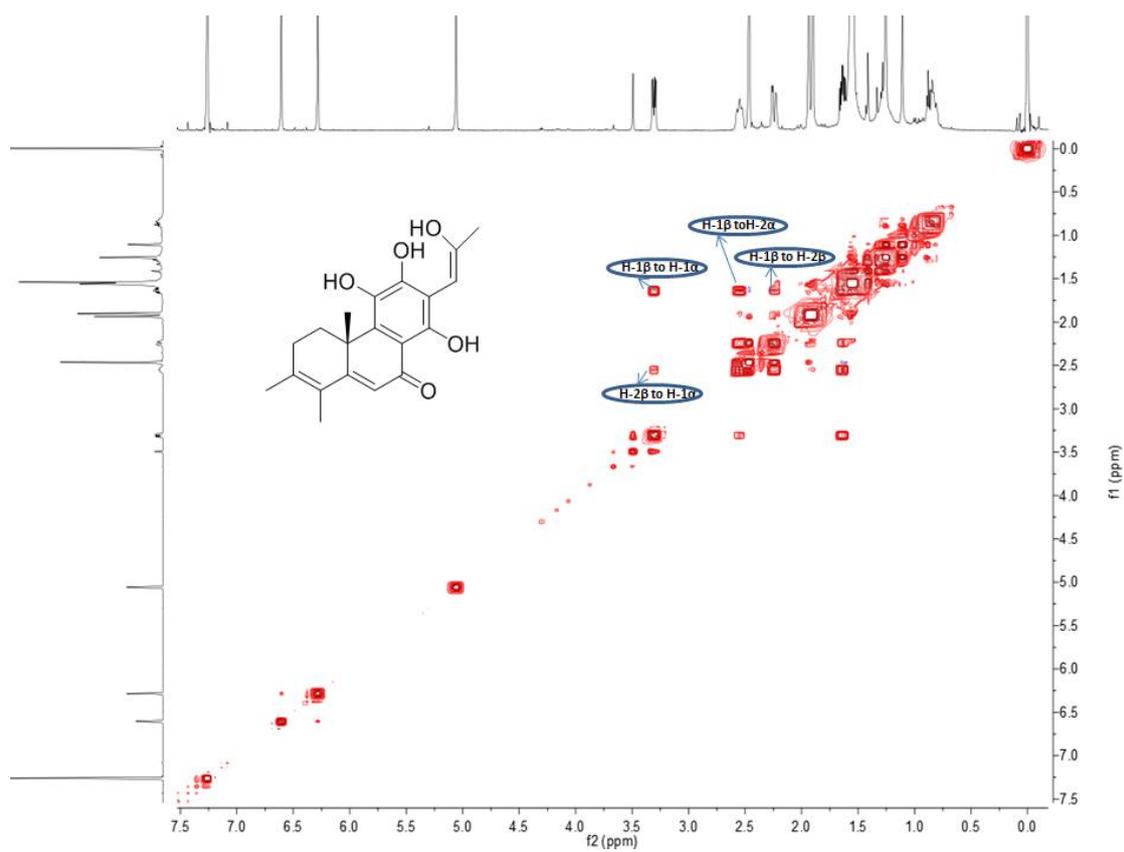


Figure S3: ^1H - ^1H COSY spectrum of **1** in CDCl_3 .

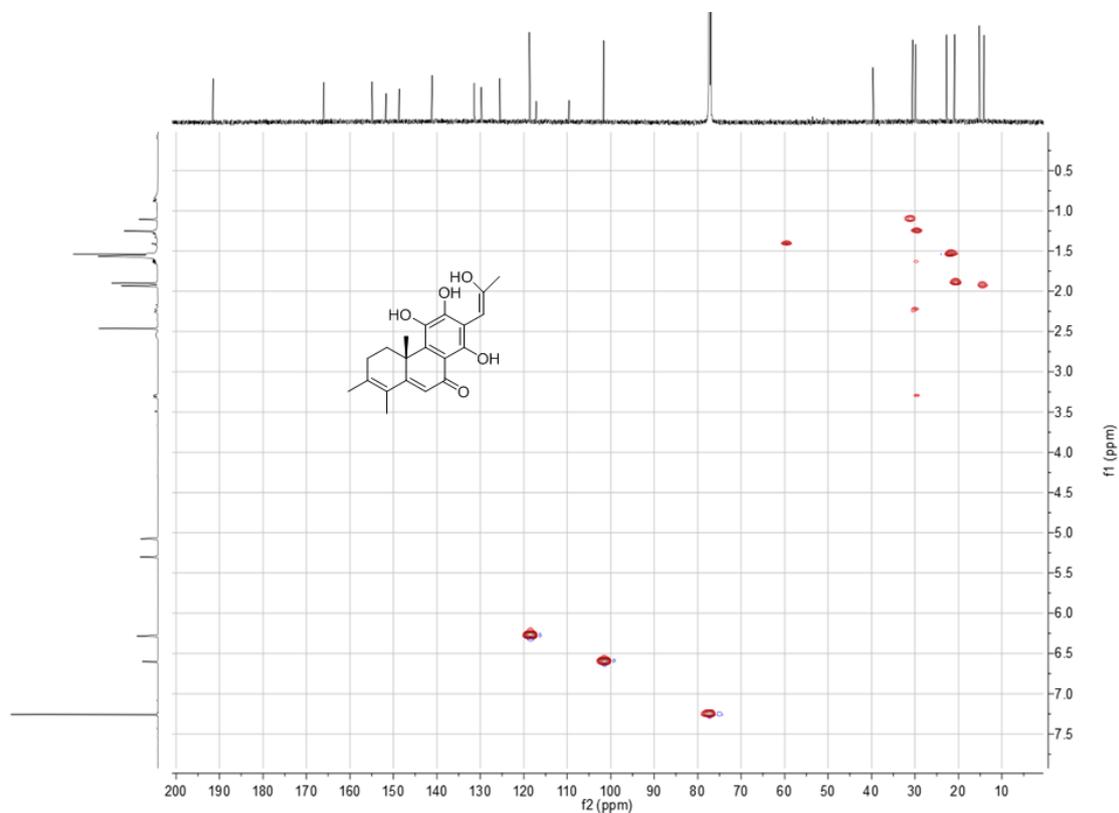


Figure S4: HSQC spectrum of **1** in CDCl_3 .

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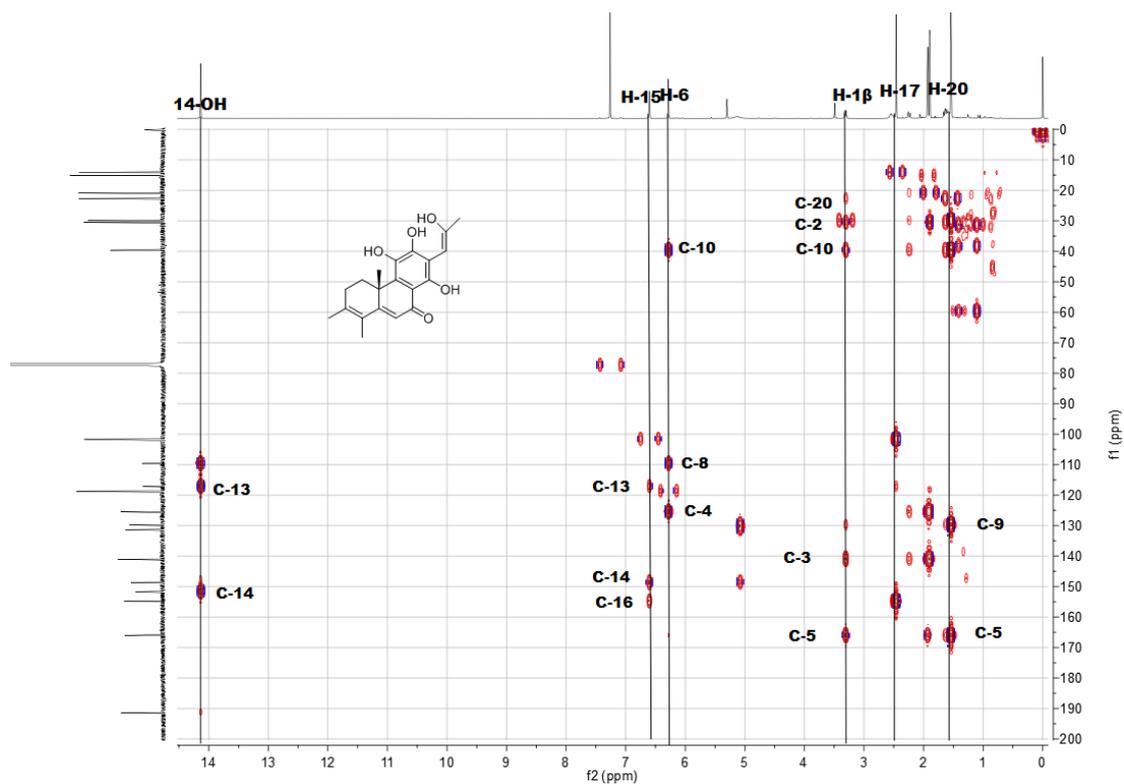


Figure S5: HMBC spectrum of **1** in CDCl_3 .

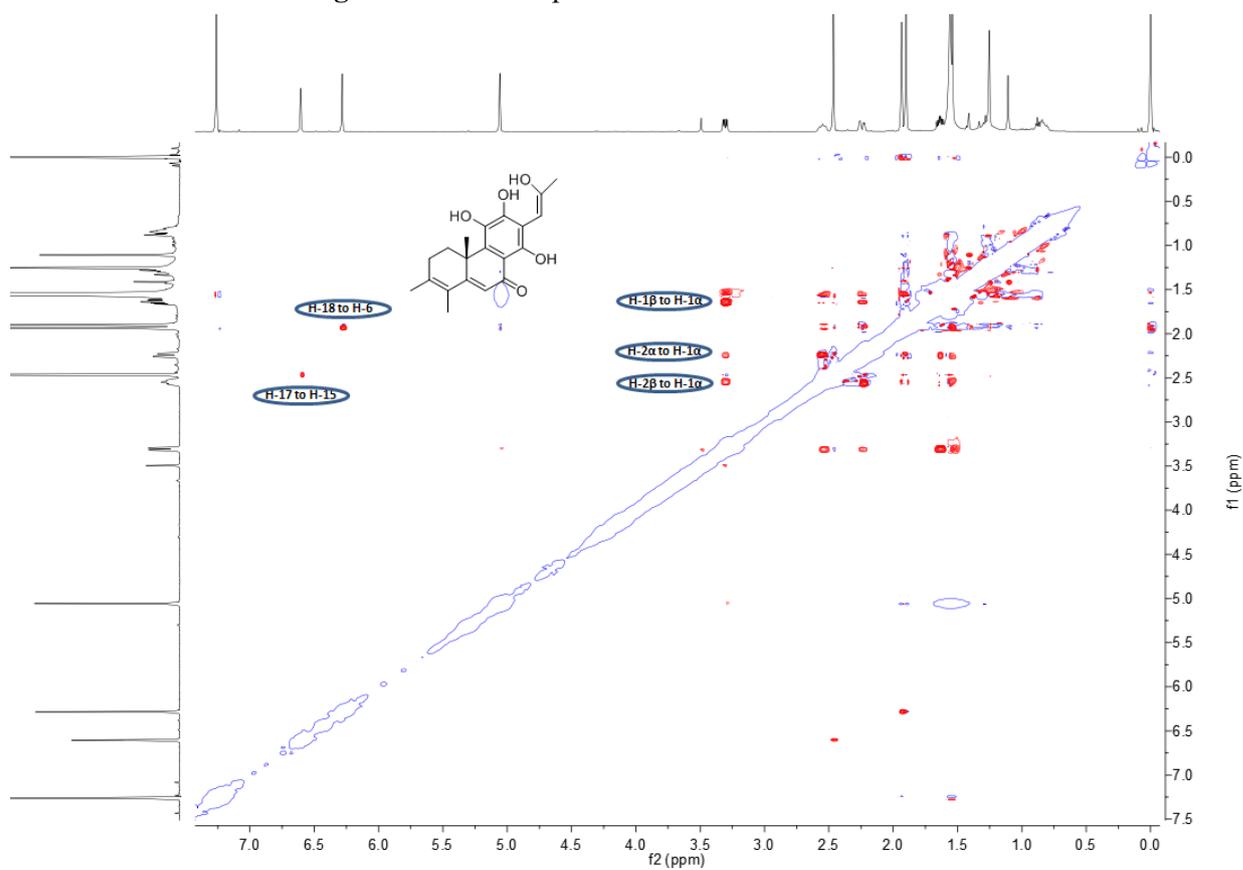


Figure S6: NOESY spectrum of **1** in CDCl_3

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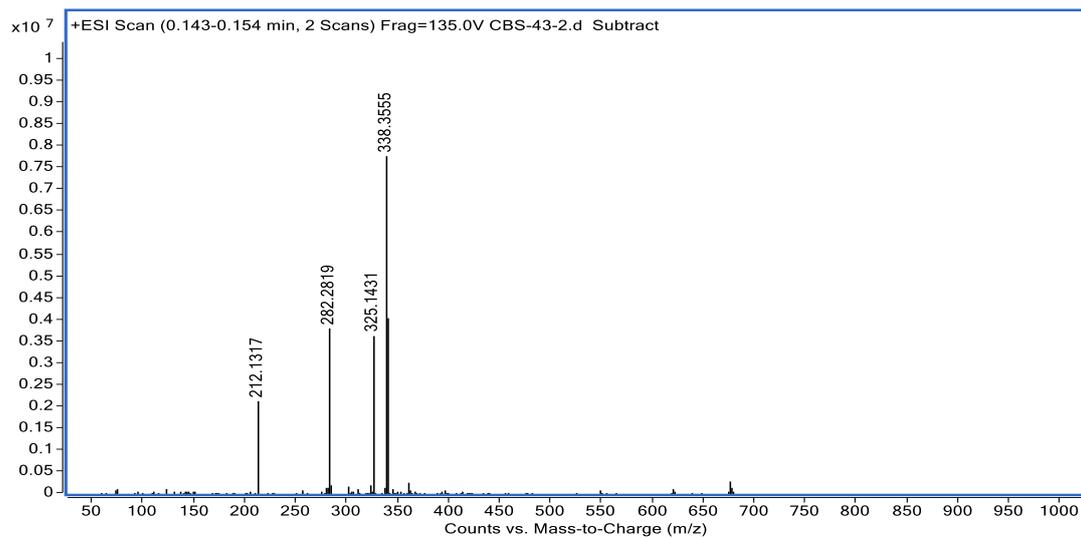


Figure S7: (+)-HR-ESIMS spectrum of 1.

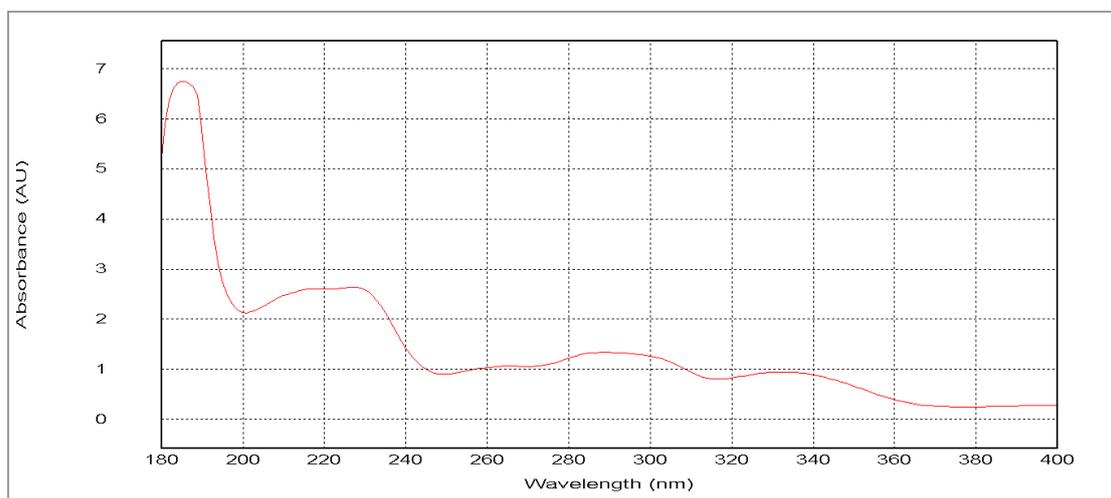


Figure S8: The UV spectrum of 1.

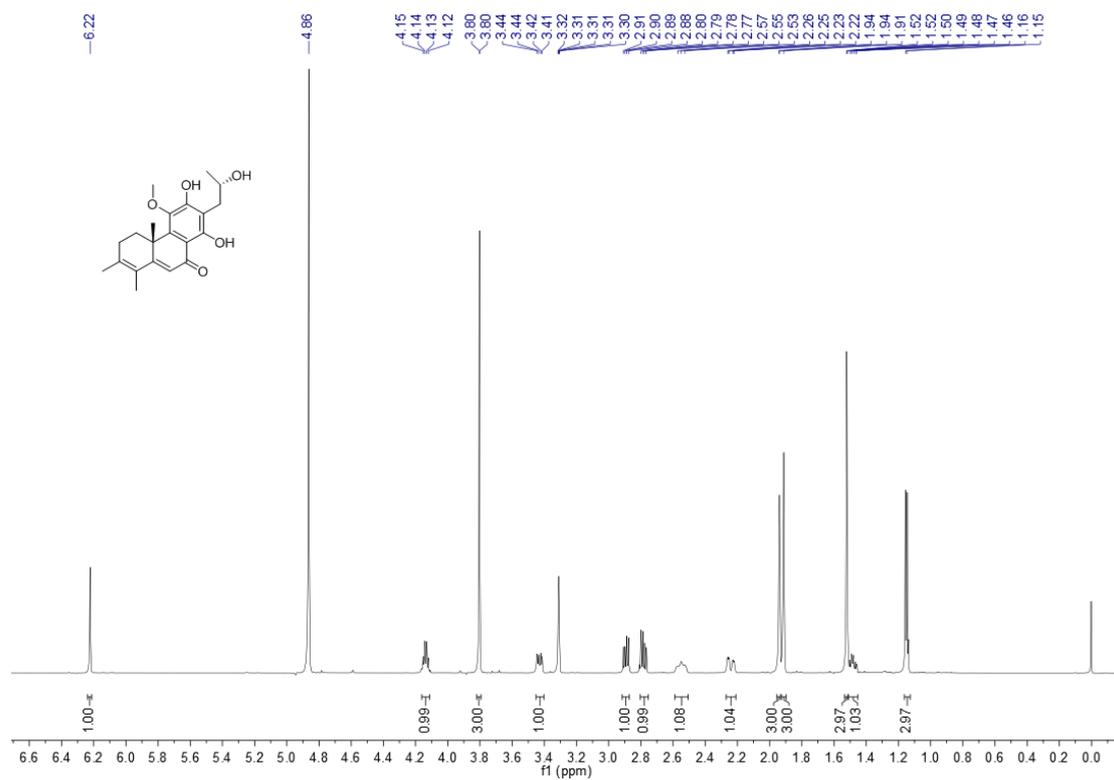


Figure S9: ^1H NMR spectrum of 2 in CD_3OD .

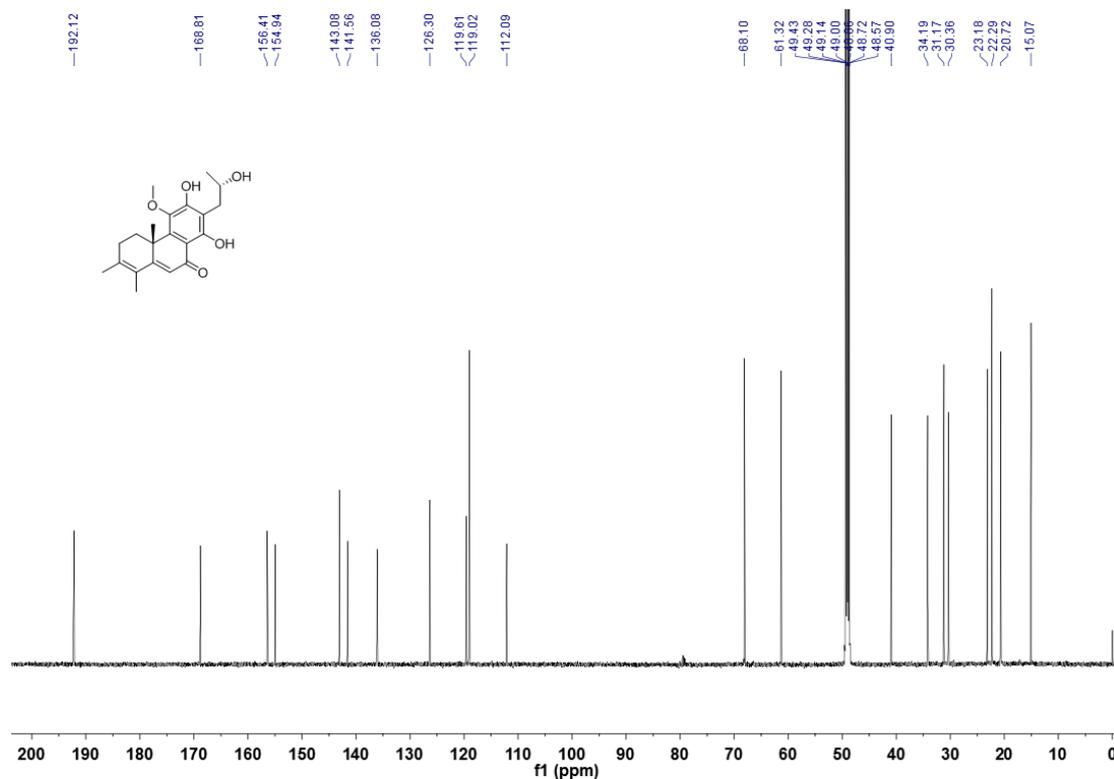


Figure S10: ^{13}C NMR spectrum of 2 in CD_3OD .

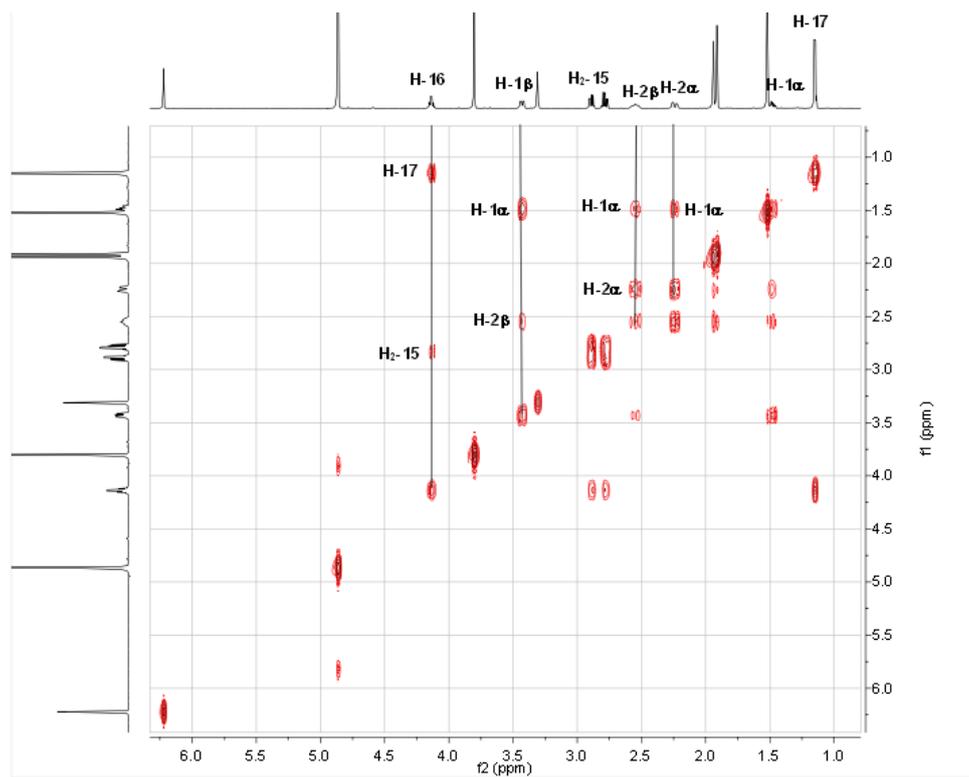


Figure S11: ^1H - ^1H COSY spectrum of **2** in CD_3OD .

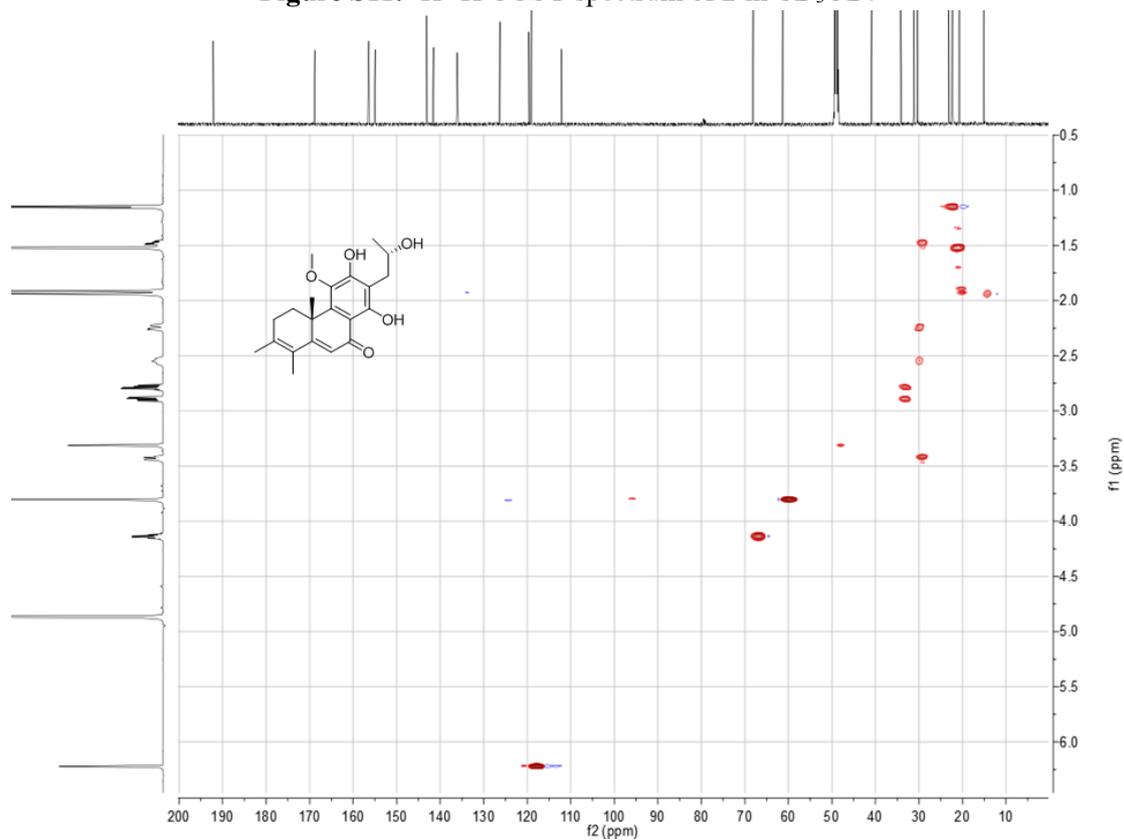


Figure S12: HSQC spectrum of **2** in CD_3OD .

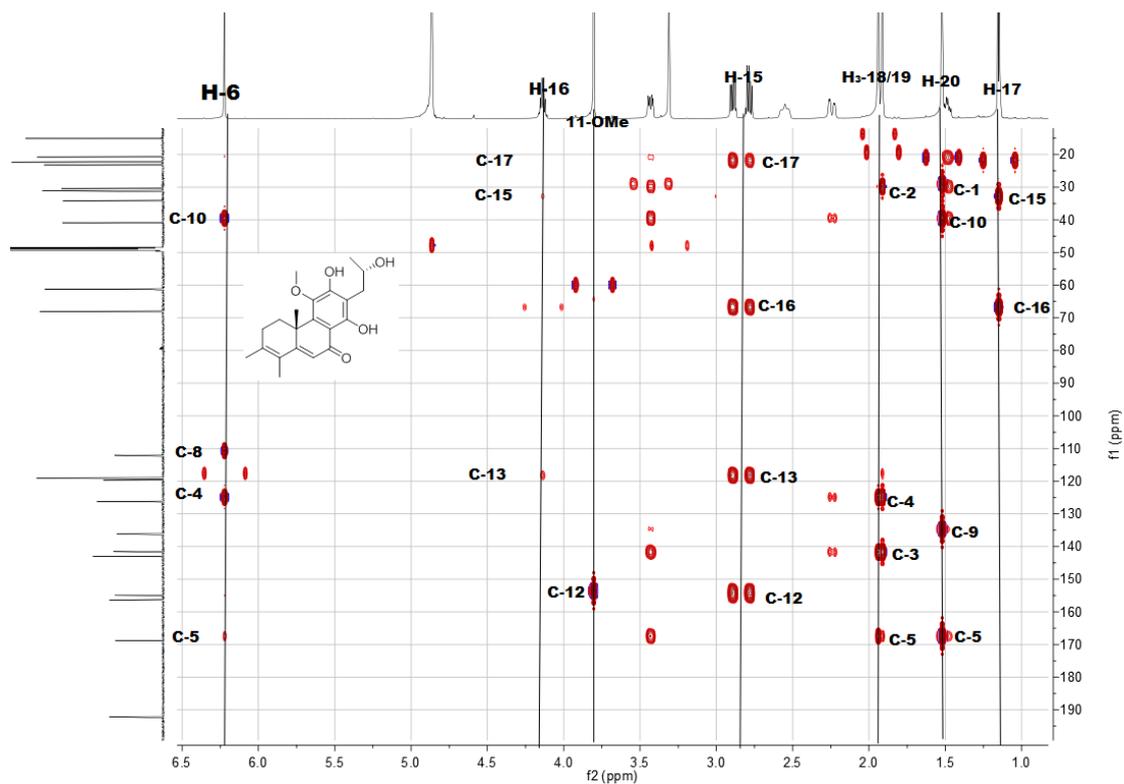


Figure S13: HMBC spectrum of **2** in CD₃OD.

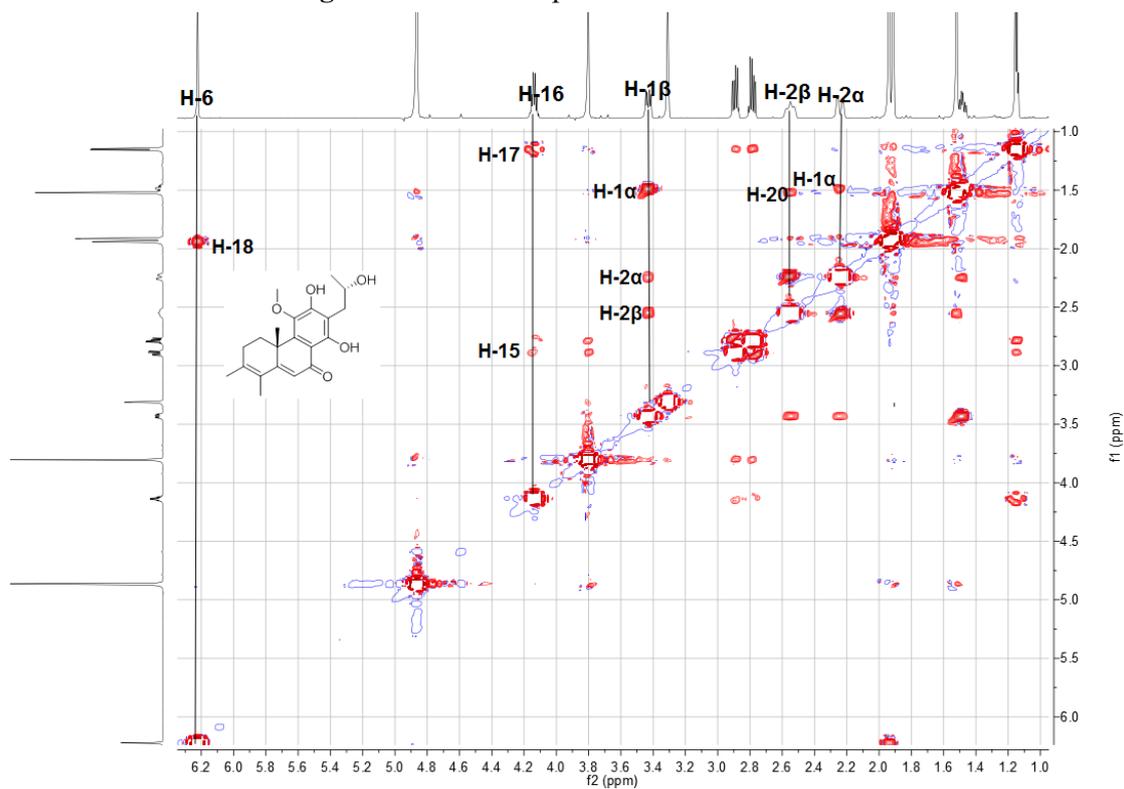


Figure S14: NOESY spectrum of **2** in CD₃OD.

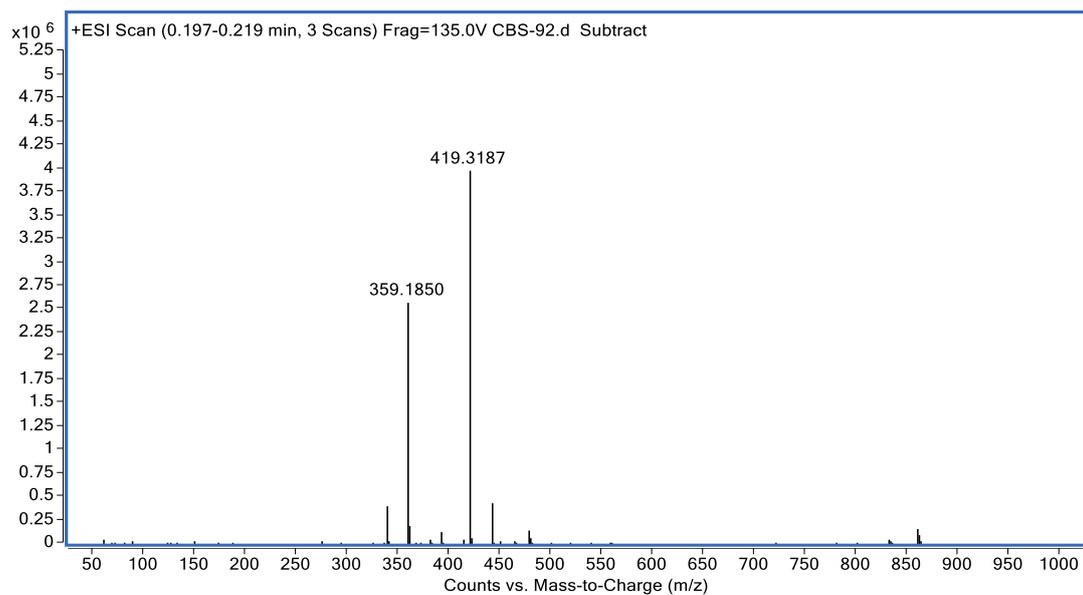


Figure S15: (+)-HR-ESIMS spectrum of **2**.

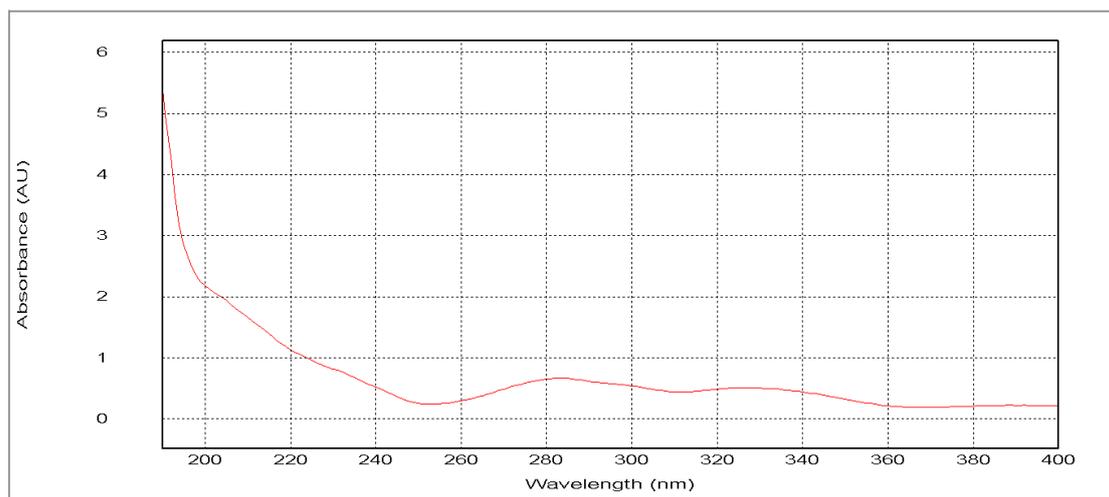


Figure S16: The UV spectrum of **2**.

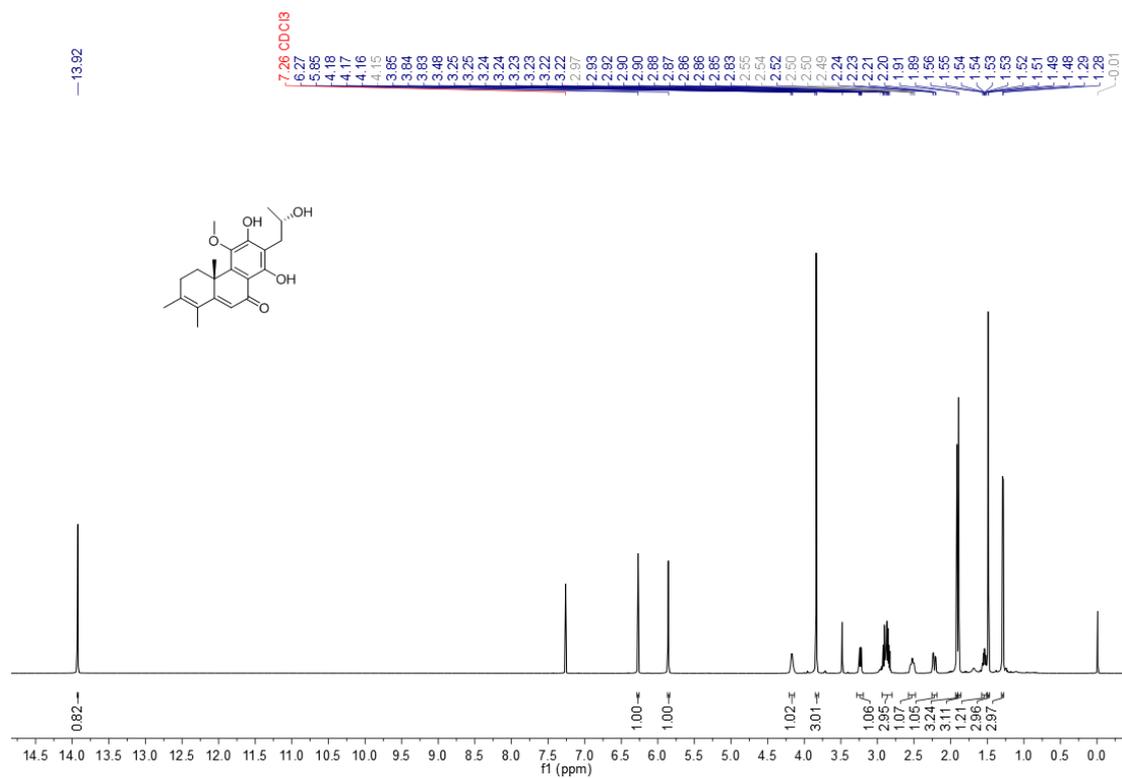


Figure S17: ¹H NMR spectrum of **2** in CDCl₃.

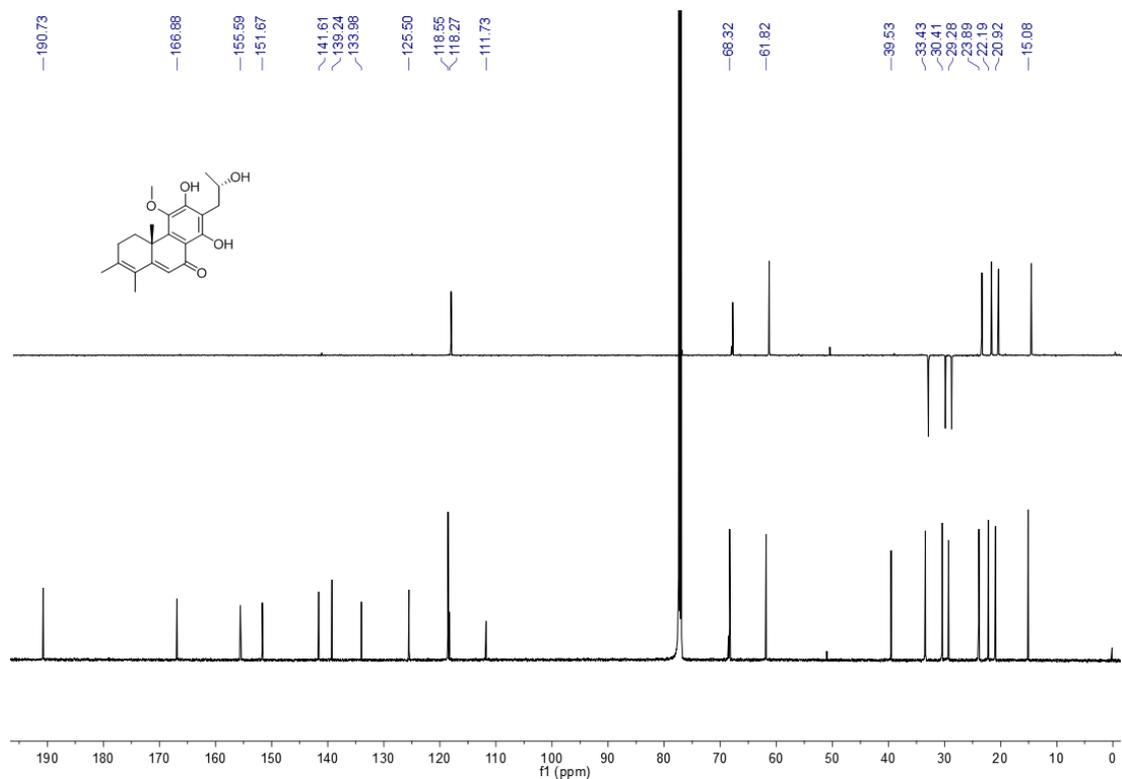


Figure S18: ¹³C and DEPT NMR spectra of **2** in CDCl₃.

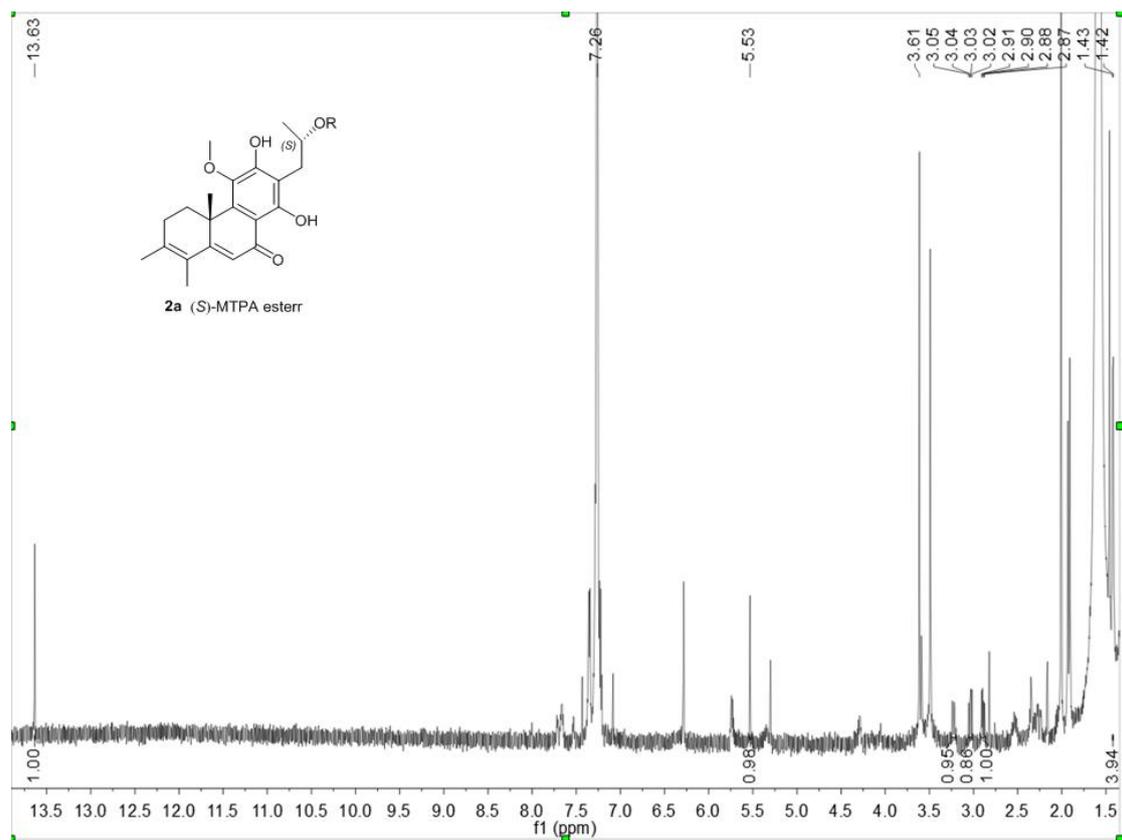


Figure S19: ^1H NMR spectrum of **2a** in CDCl_3 .

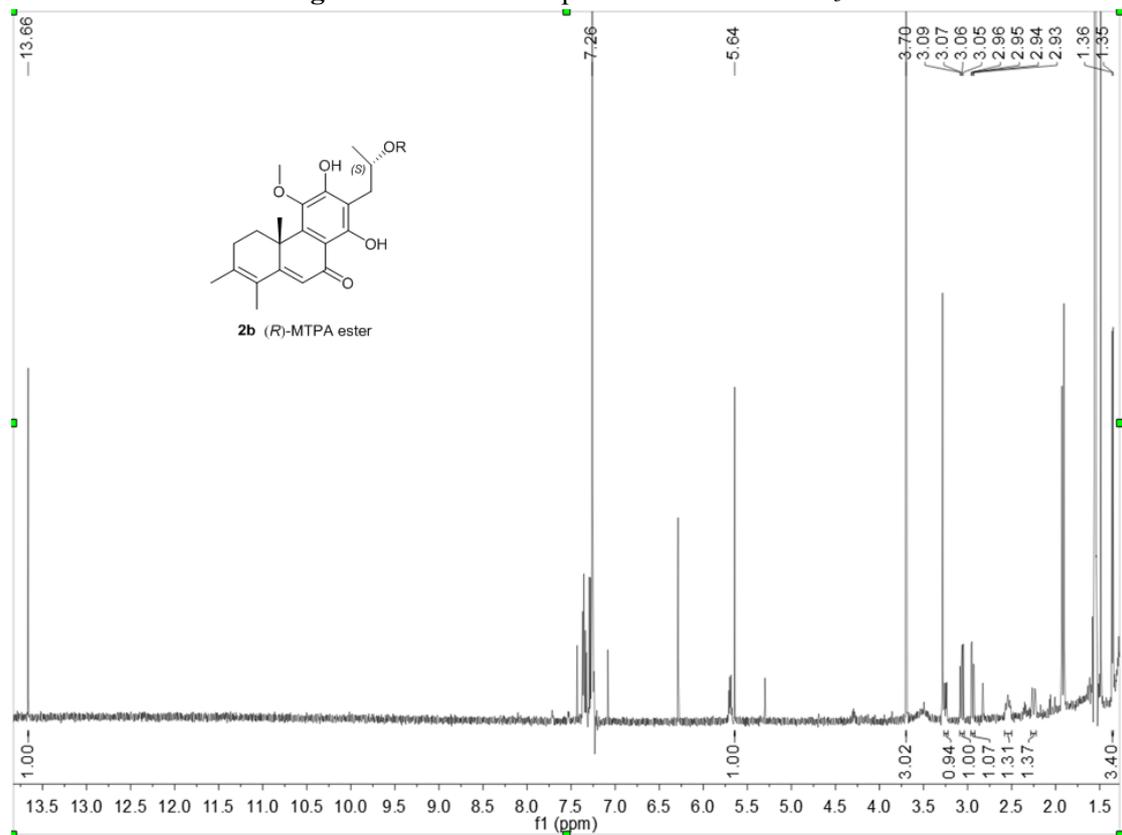
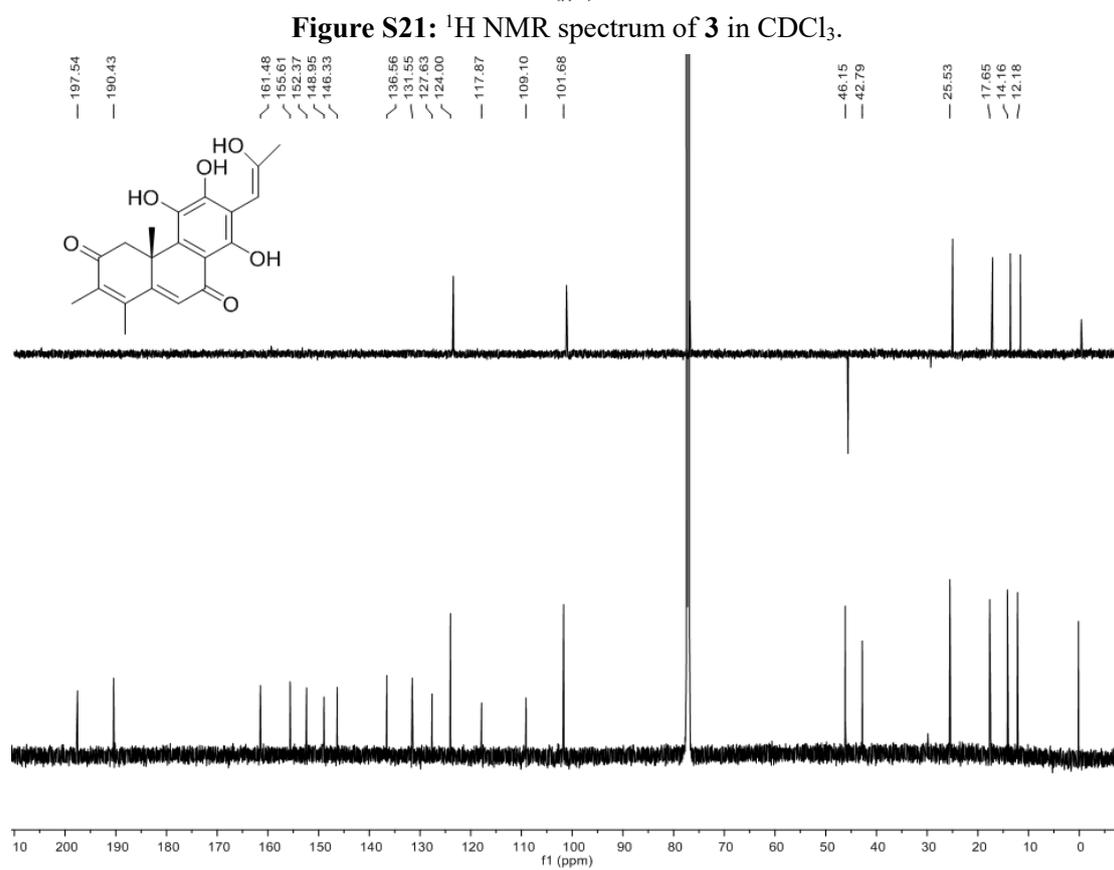
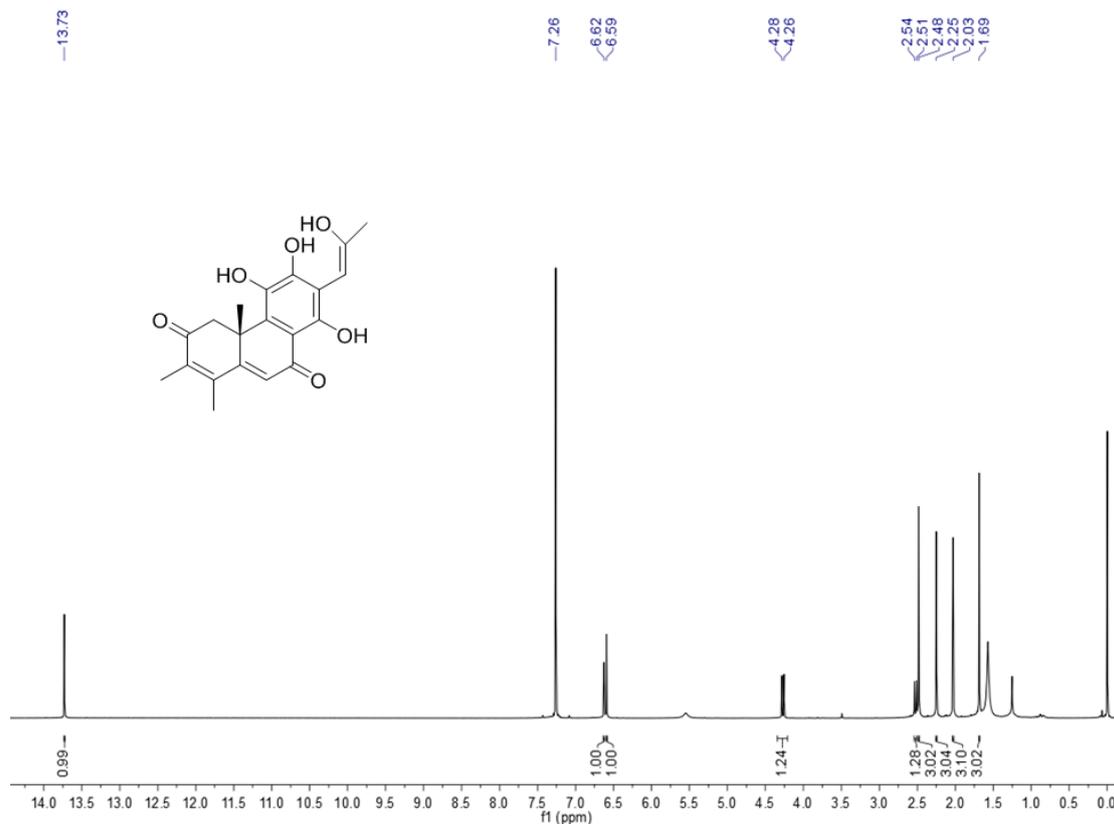


Figure S20: ^1H NMR spectrum of **2b** in CDCl_3 .



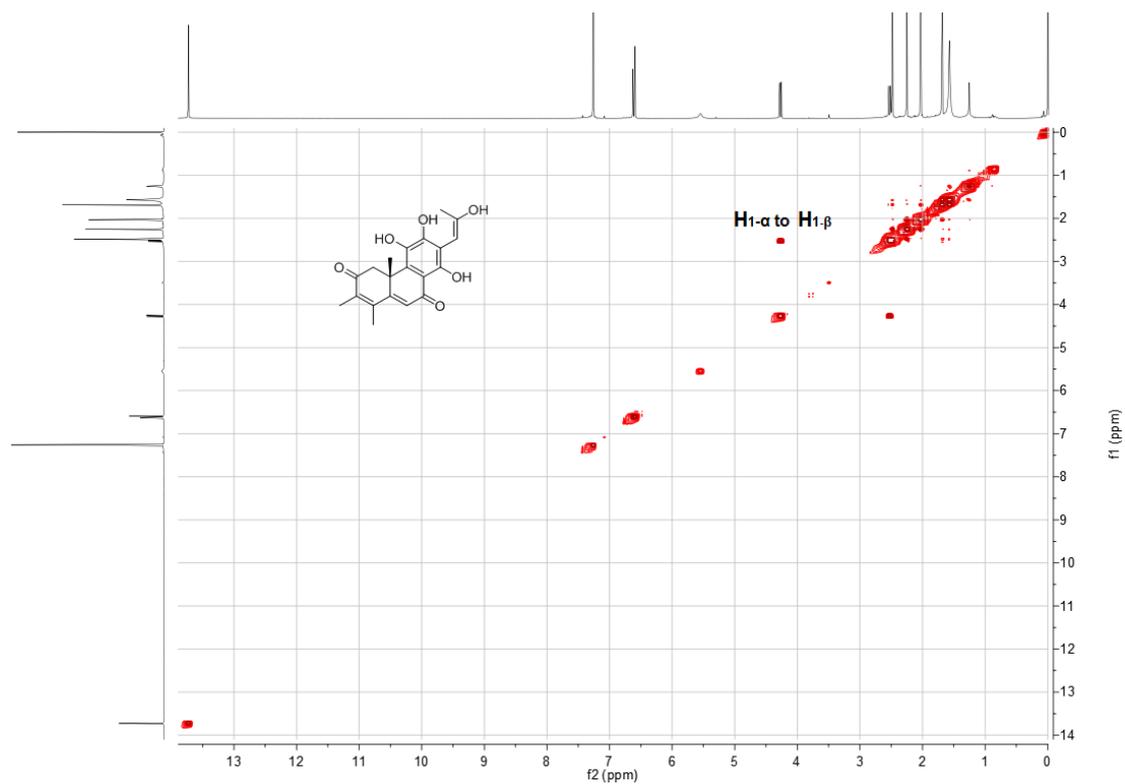


Figure S23: ^1H - ^1H COSY spectrum of **3** in CDCl_3 .

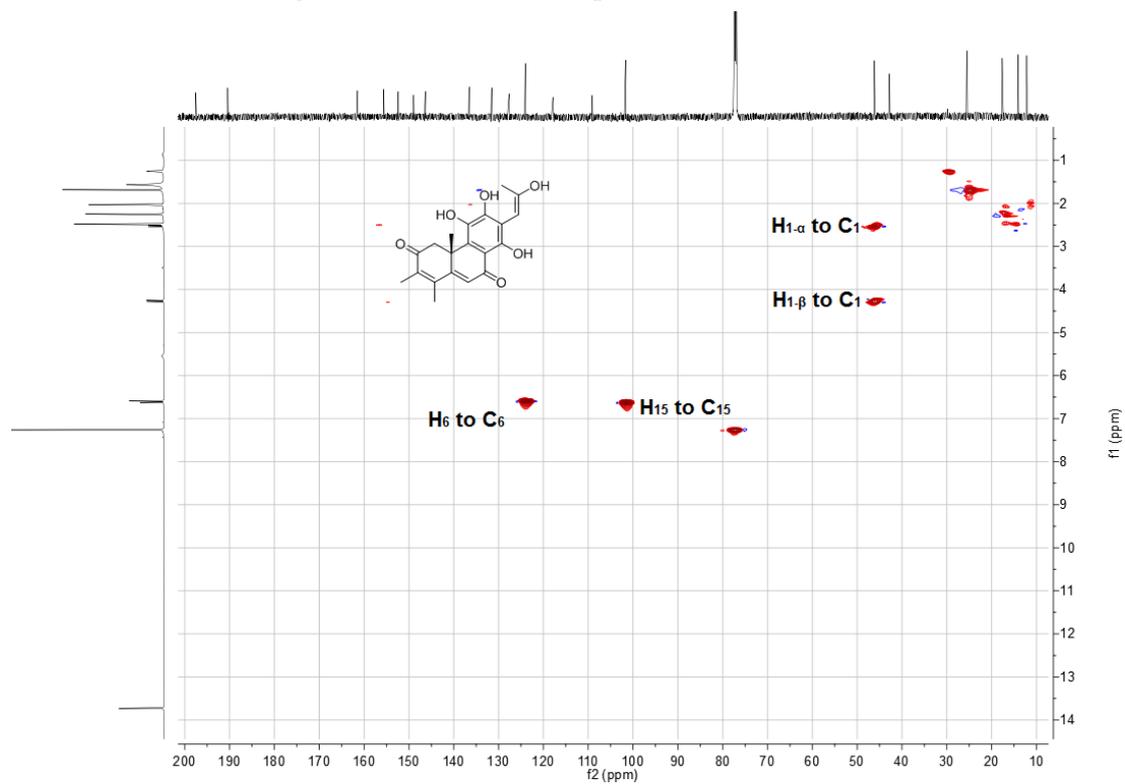


Figure S24: HSQC spectrum of **3** in CDCl_3 .

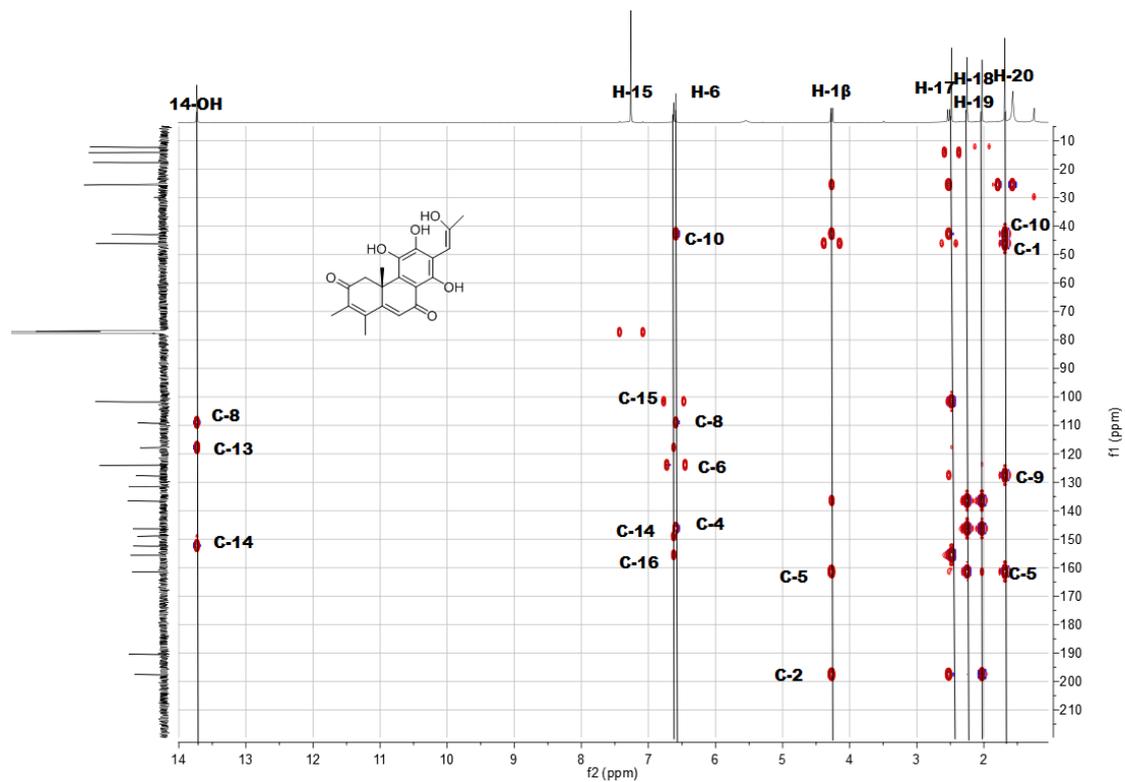


Figure S25: HMBC spectrum of **3** in CDCl₃.

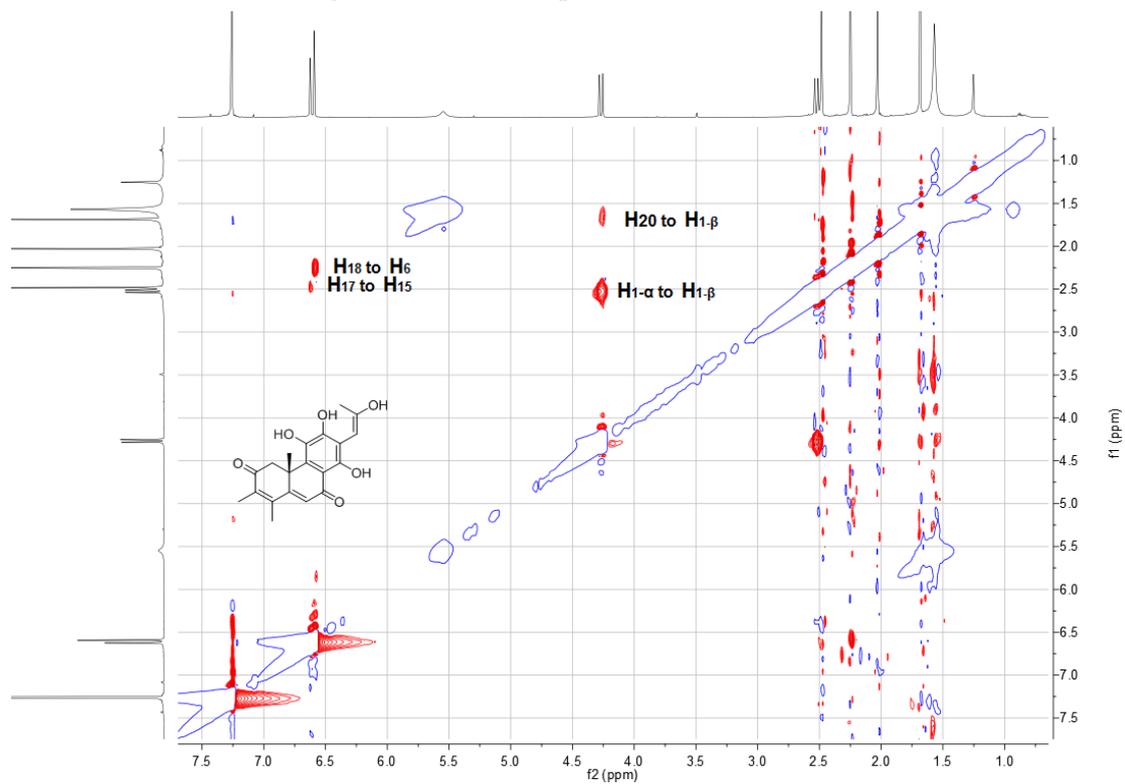


Figure S26: NOESY spectrum of **3** in CDCl₃.

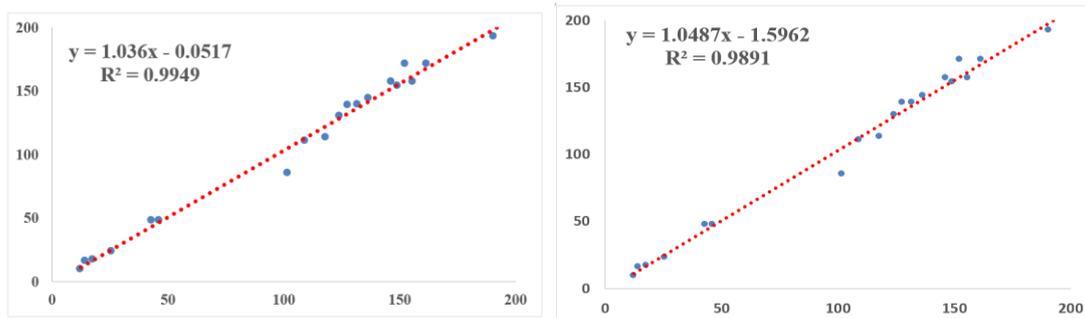


Figure S27: Linear correlation between the experimental ^{13}C NMR data for **3** and the calculated data for (*Z*)- Δ^{15} (left) and (*E*)- Δ^{15} (right) isomers, respectively.

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<input checked="" type="checkbox"/> 90-94	1
<input checked="" type="checkbox"/> 85-89	4
<input checked="" type="checkbox"/> 80-84	1
<input checked="" type="checkbox"/> 75-79	6
<input type="checkbox"/> 70-74	39
<input type="checkbox"/> 65-69	230
<input type="checkbox"/> 0-64 (least similar)	1045

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SUBSTANCES 6

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Similarity: 99-100

1 of 14 Substances Selected

Figure S28: SciFinder search report for compound **1**.

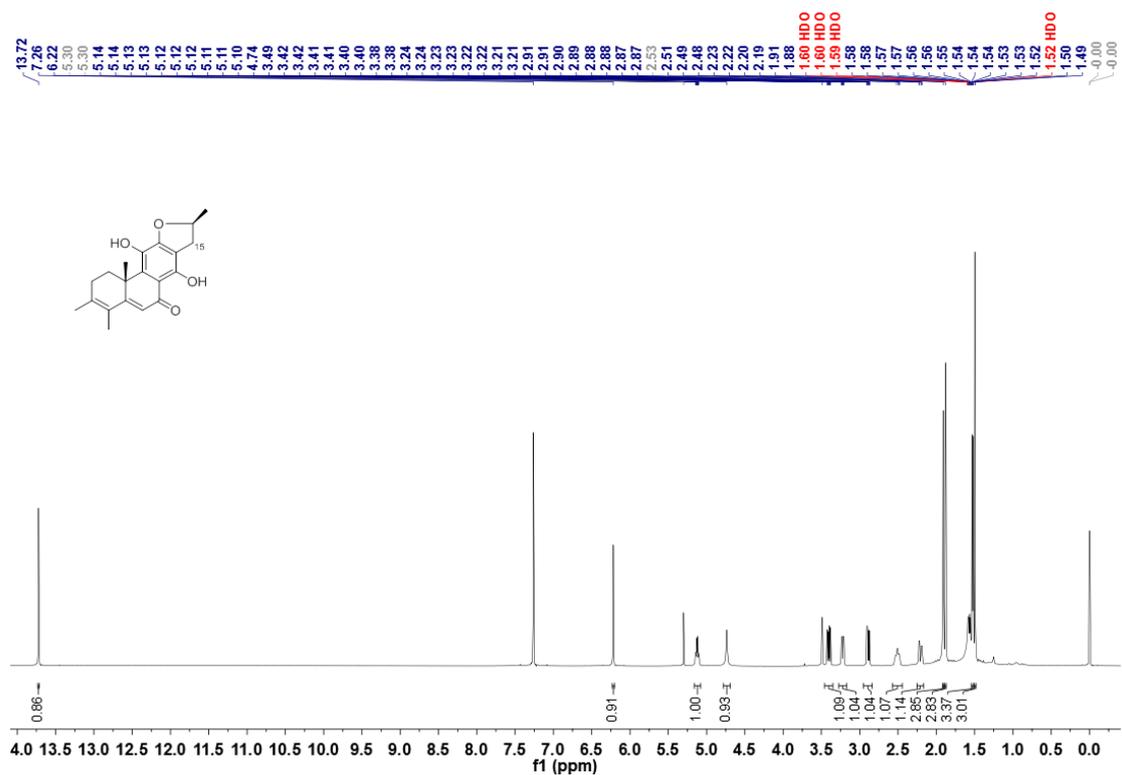


Figure S30: ^1H NMR spectrum of **4** in CDCl_3 .

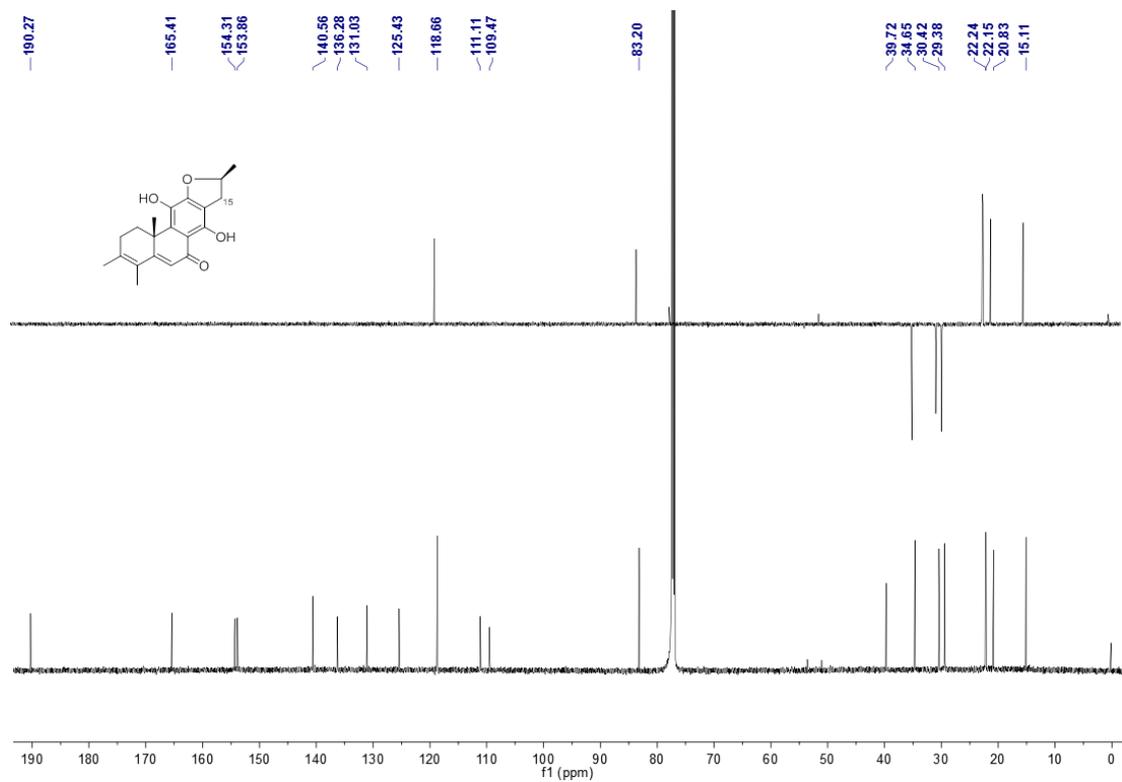


Figure S31: ^{13}C and DEPT NMR spectra of **4** in CDCl_3 .

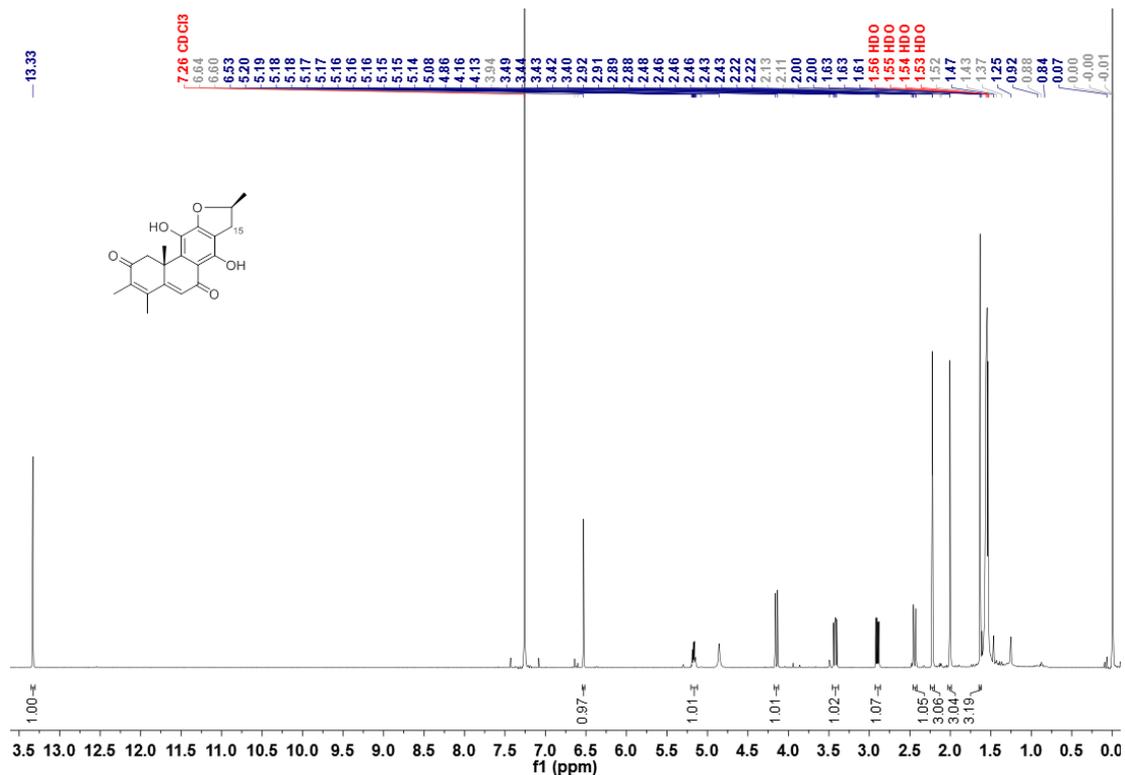


Figure S32: ¹H NMR spectrum of **5** in CDCl₃.

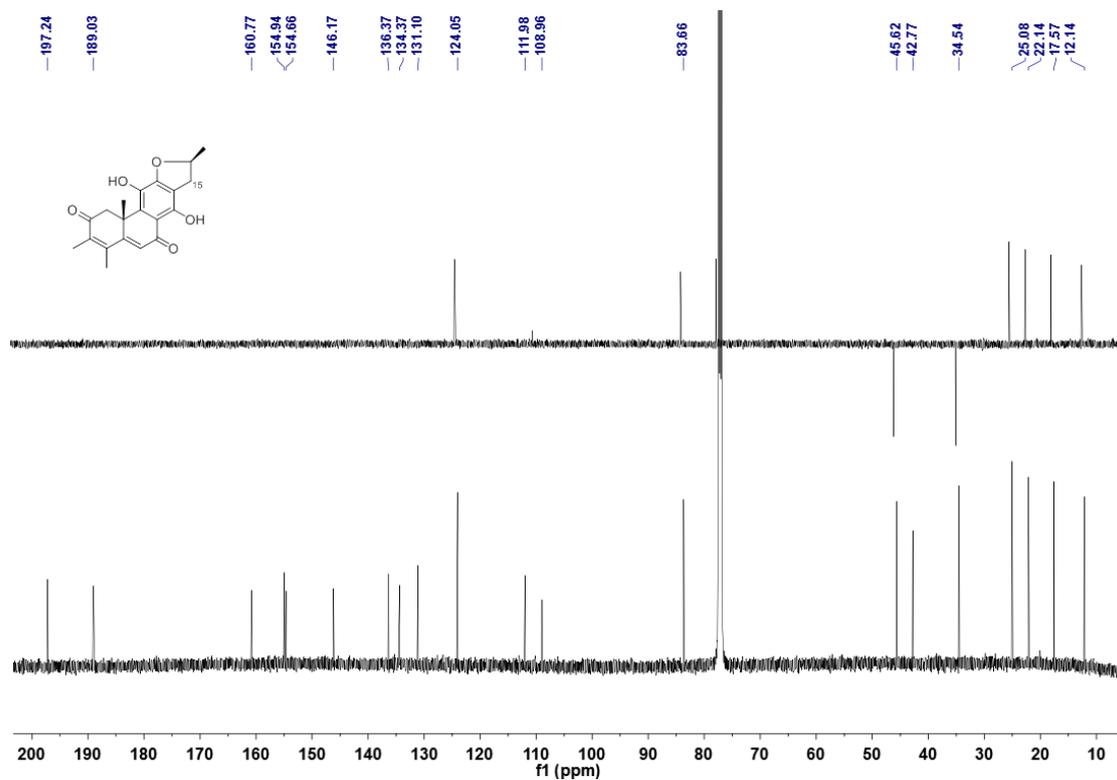


Figure S33: ¹³C and DEPT NMR spectra of **5** in CDCl₃.

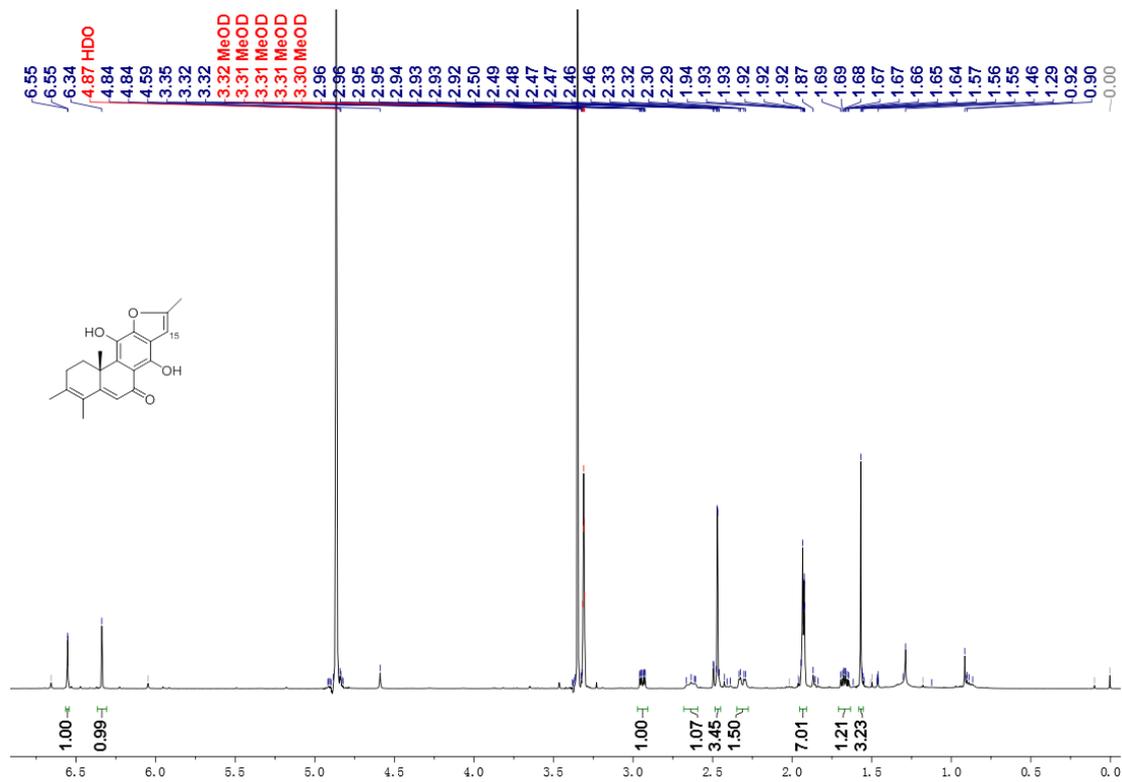


Figure S34: ¹H NMR spectrum of 6 in CD₃OD.

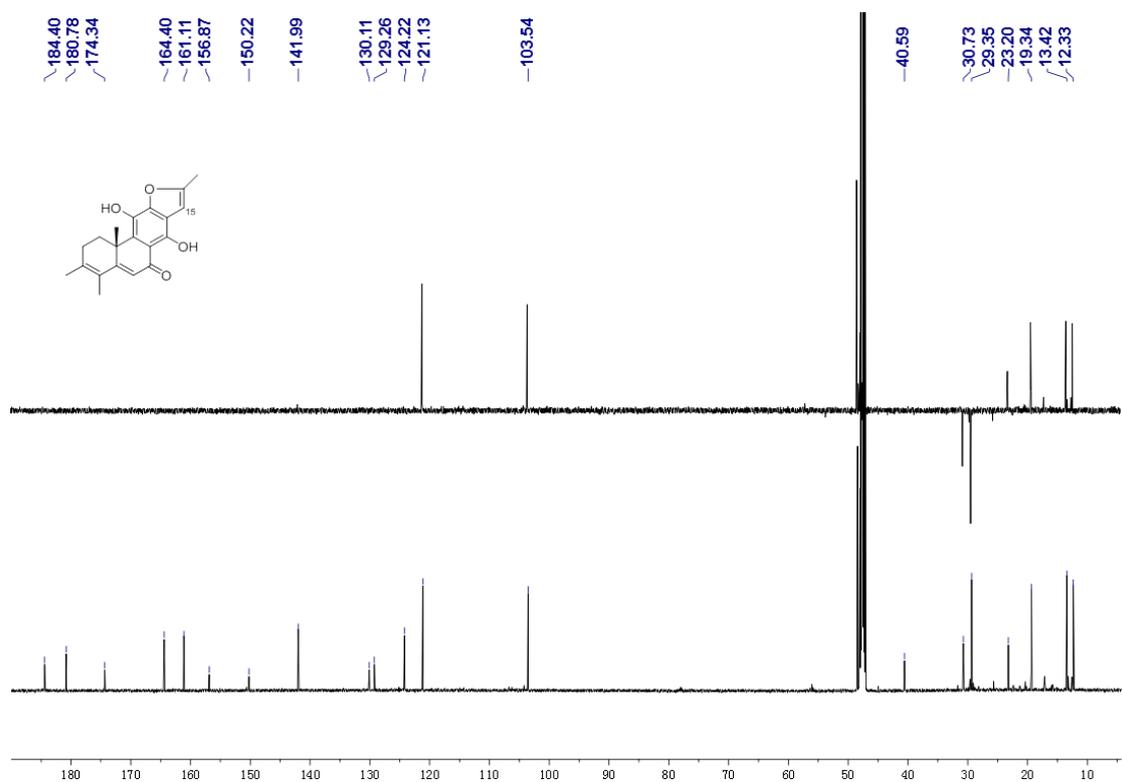


Figure S35: ¹³C and DEPT NMR spectra of 6 in CD₃OD.

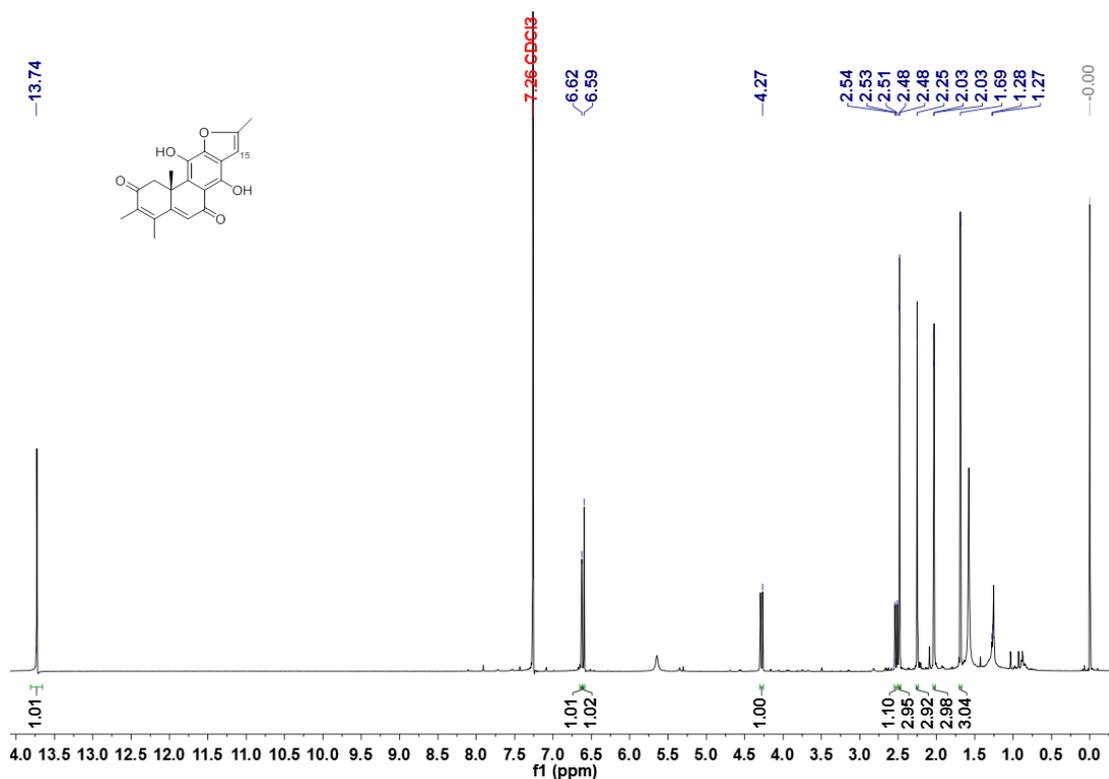


Figure S36: ¹H NMR spectrum of 7 in CDCl₃.

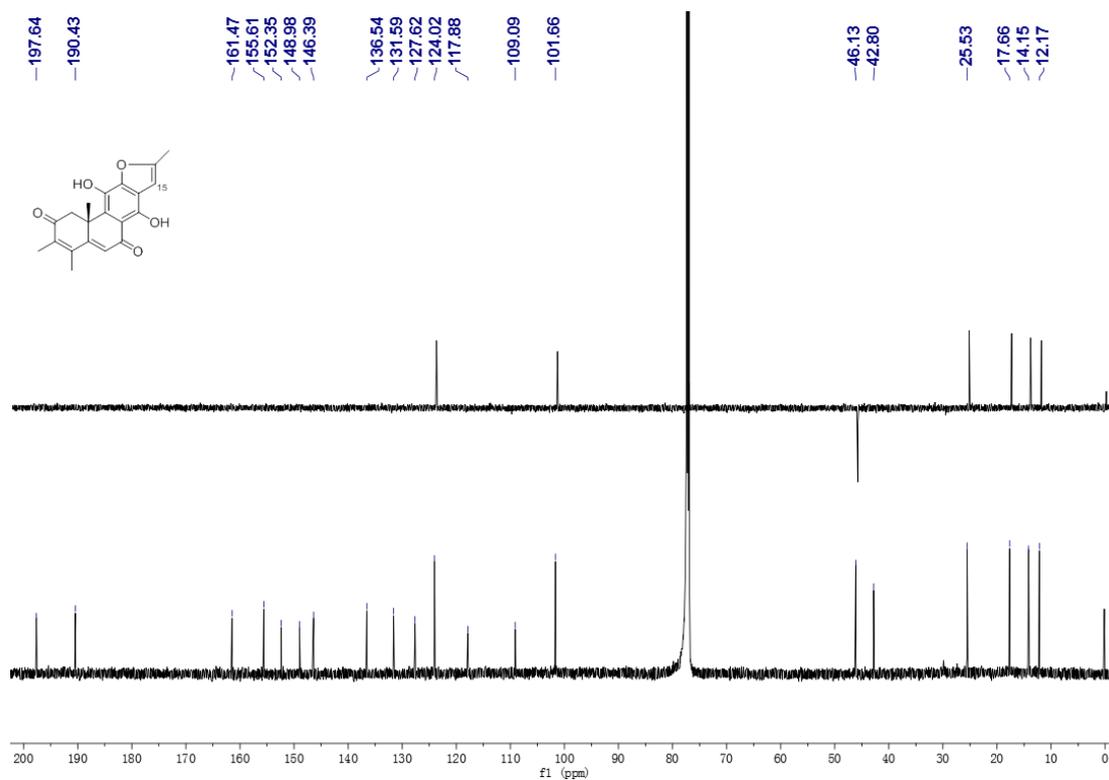


Figure S37: ¹³C and DEPT NMR spectra of 7 in CDCl₃.

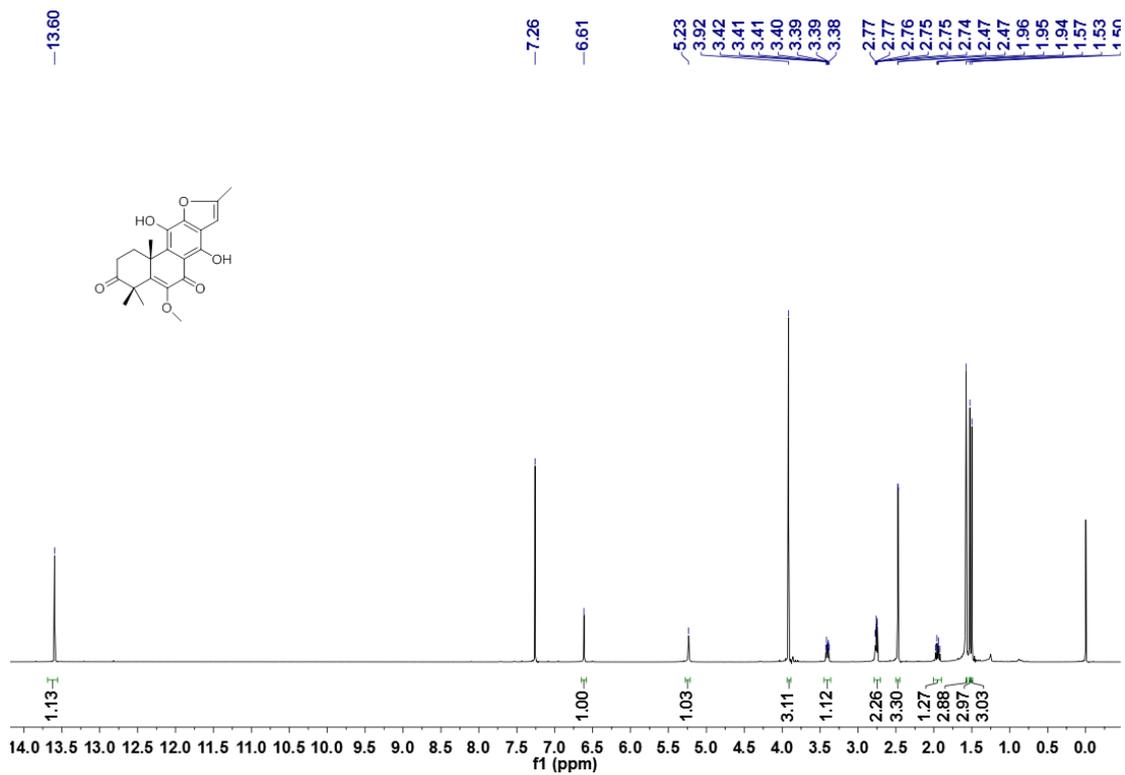


Figure S38: ^1H NMR spectrum of **8** in CDCl_3 .

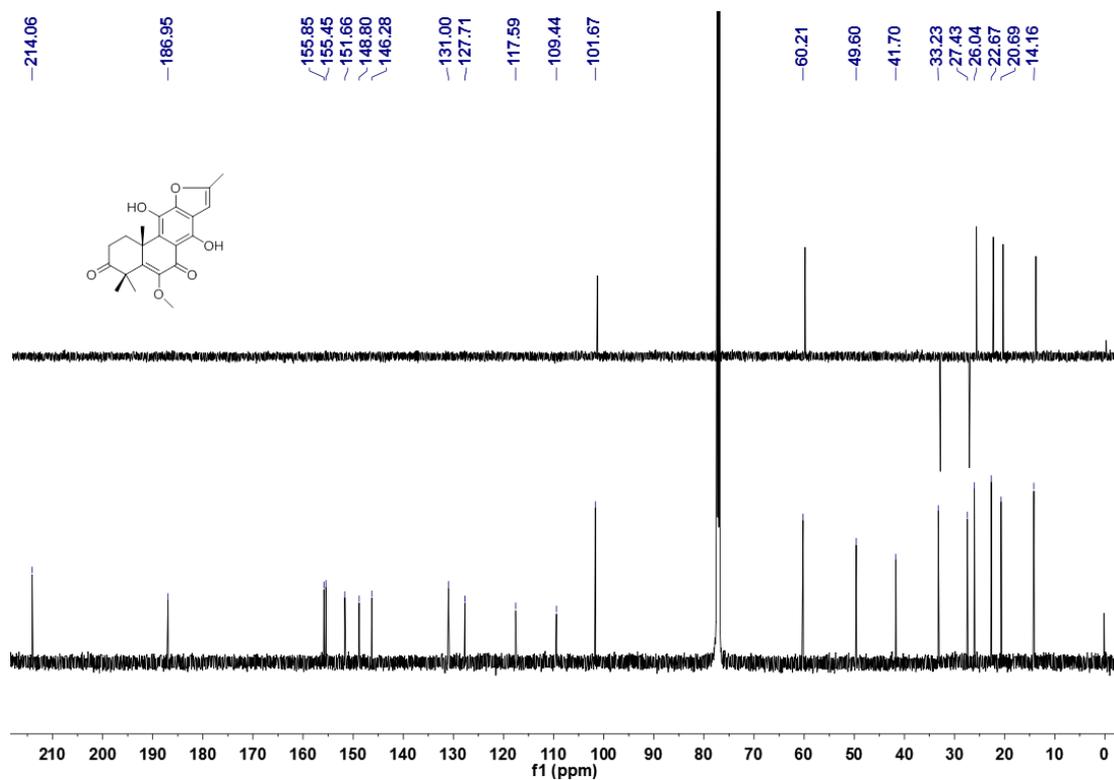


Figure S39: ^{13}C and DEPT NMR spectra of **8** in CDCl_3 .

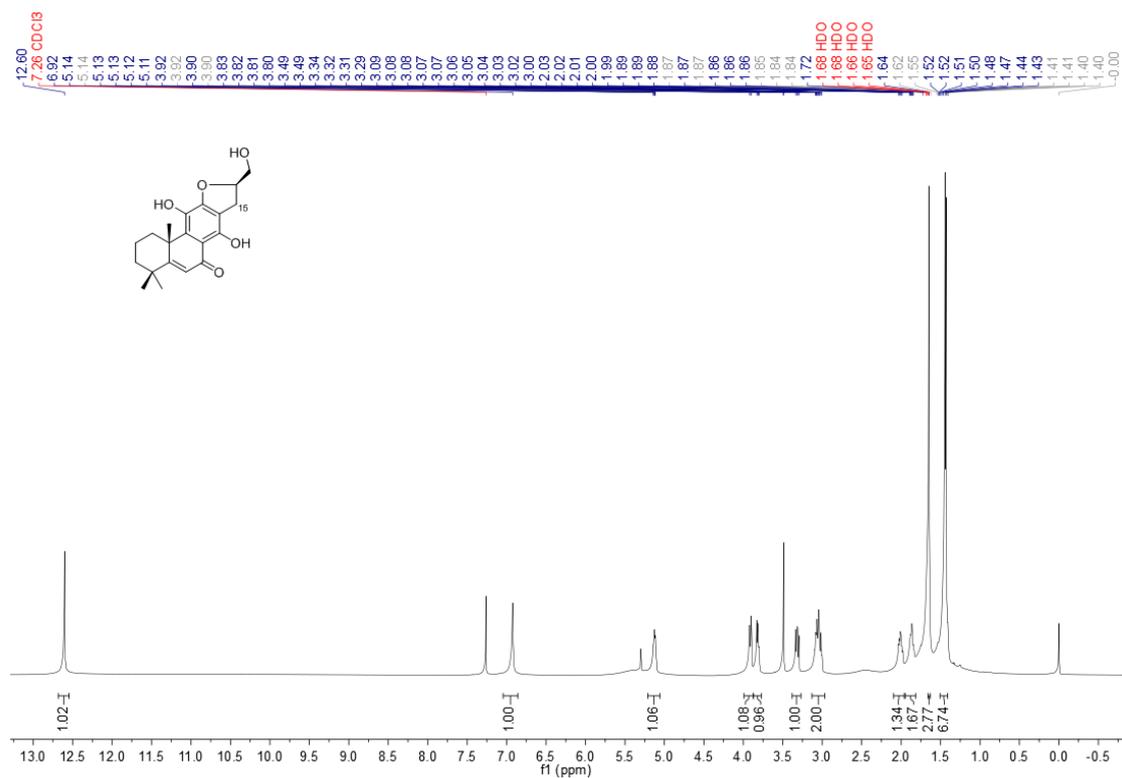


Figure S40: ¹H NMR spectrum of 9 in CDCl₃.

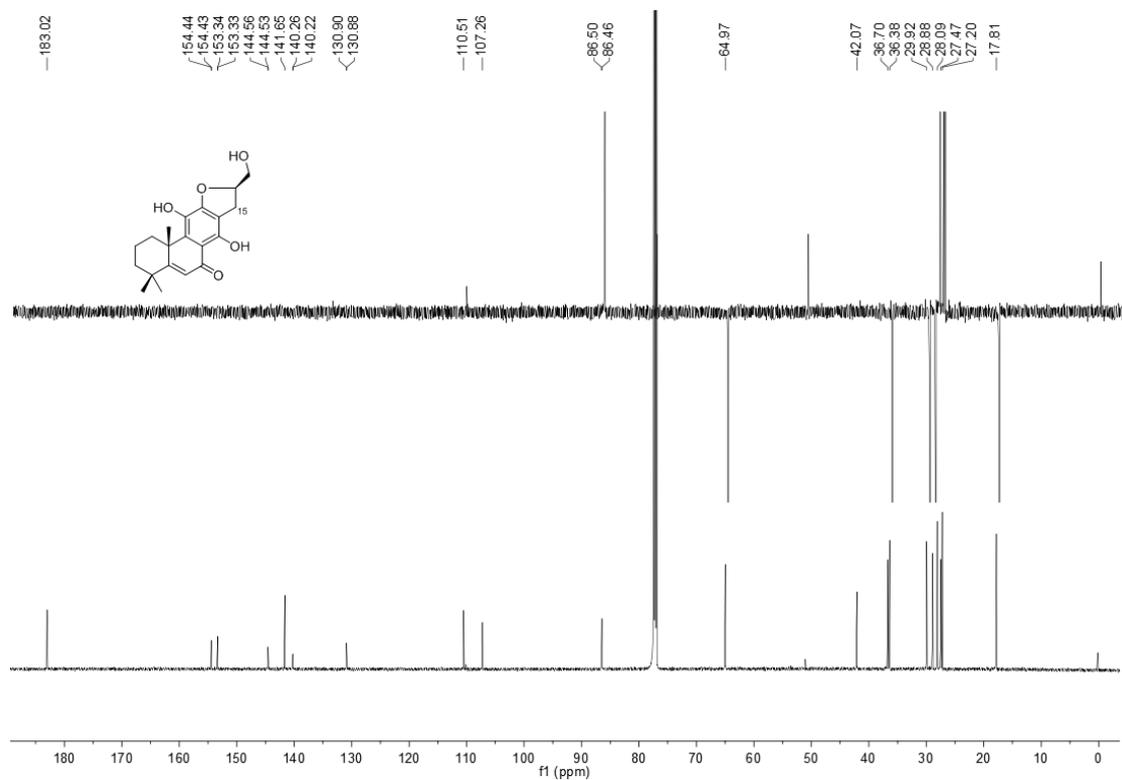


Figure S41: ¹³C and DEPT NMR spectra of 9 in CDCl₃.

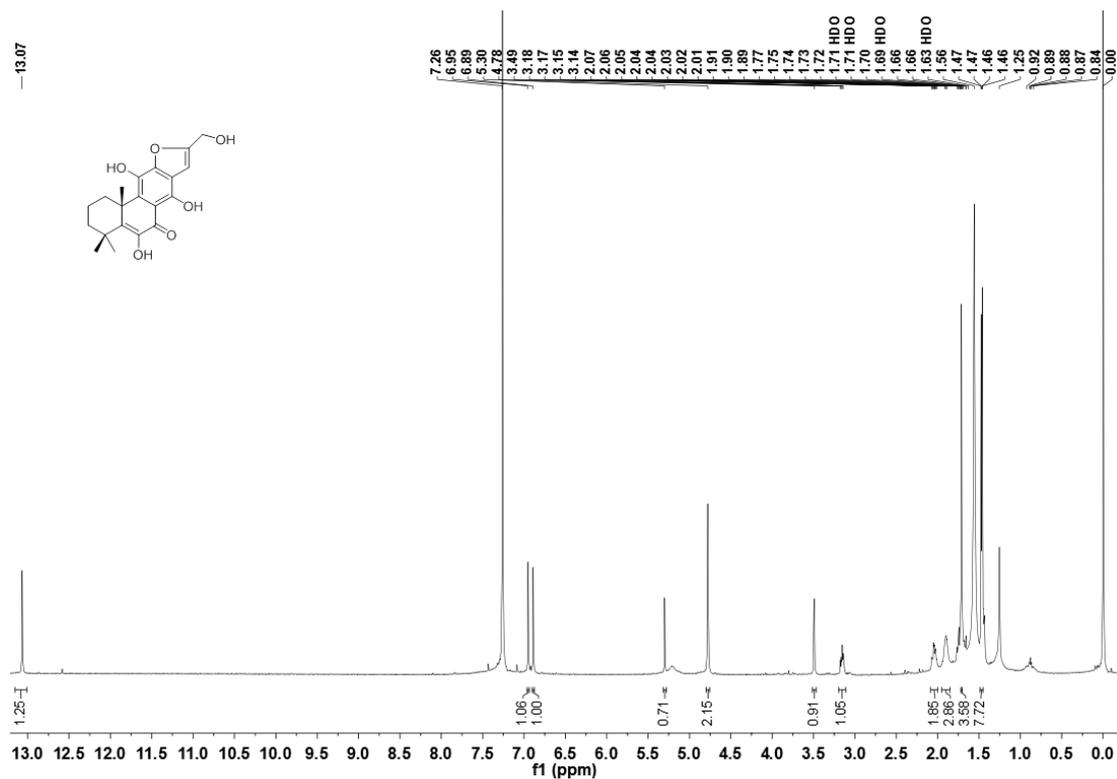


Figure S42: ^1H NMR spectrum of **10** in CDCl_3 .

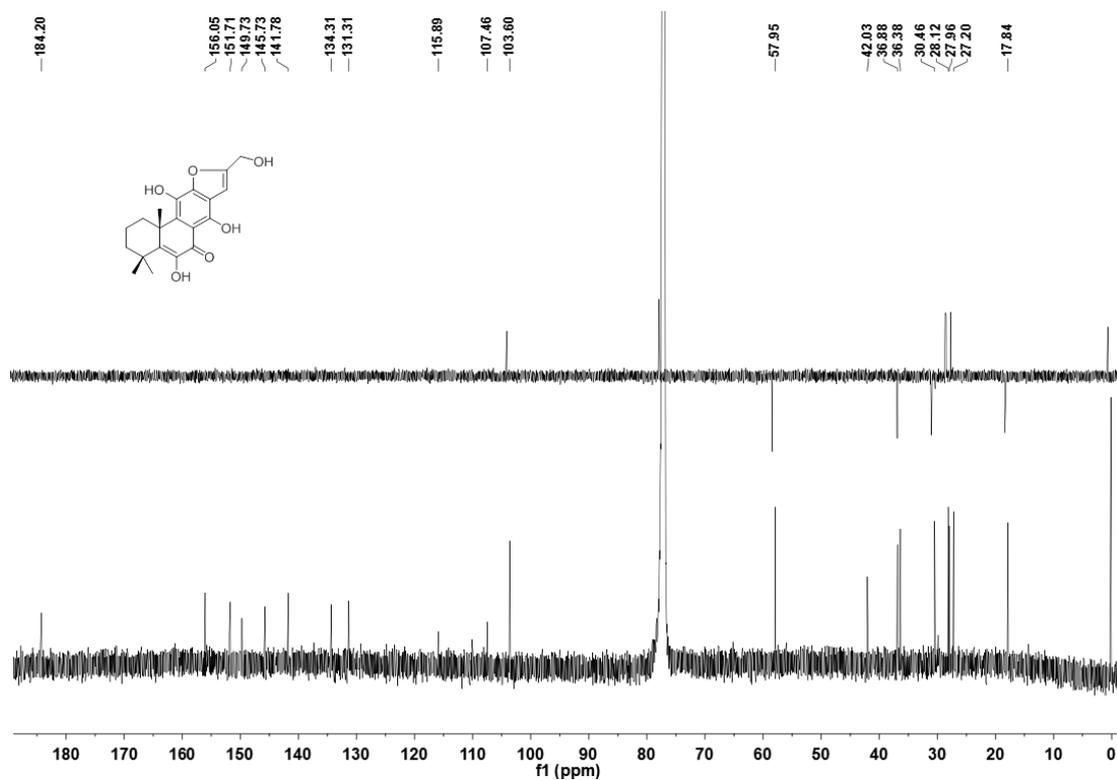


Figure S43: ^{13}C and DEPT NMR spectra of **10** in CDCl_3 .

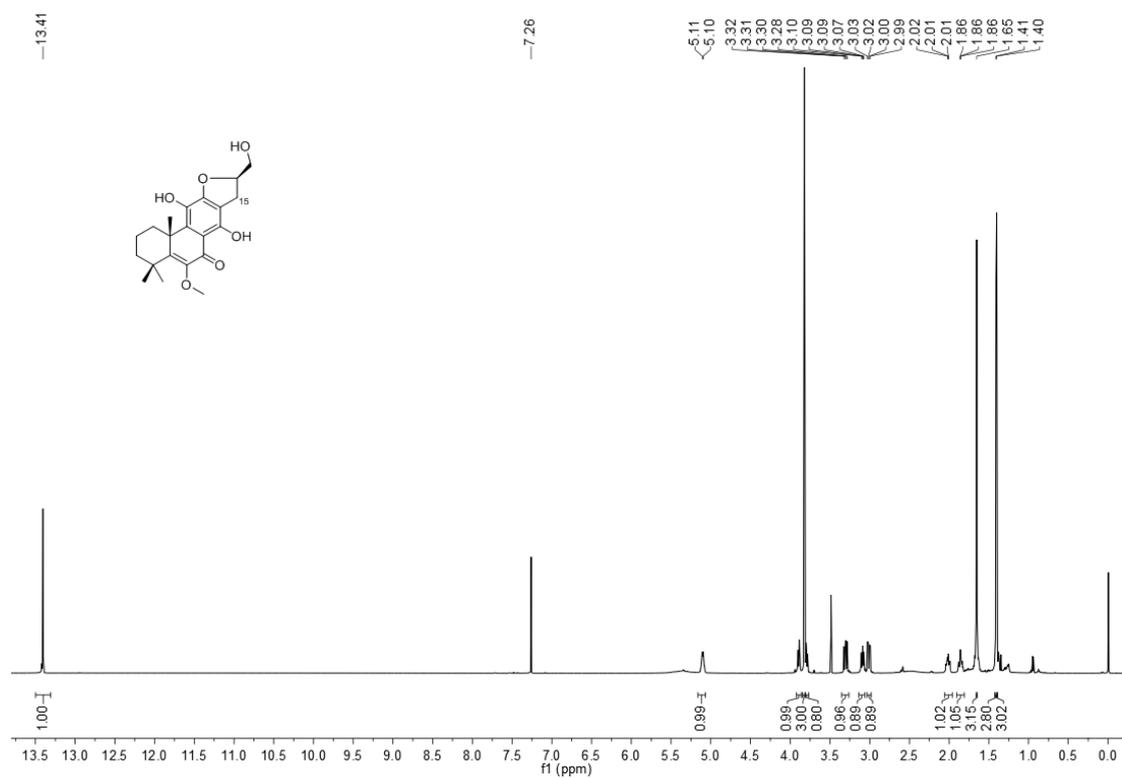


Figure S44: ^1H NMR spectrum of **11** in CDCl₃.

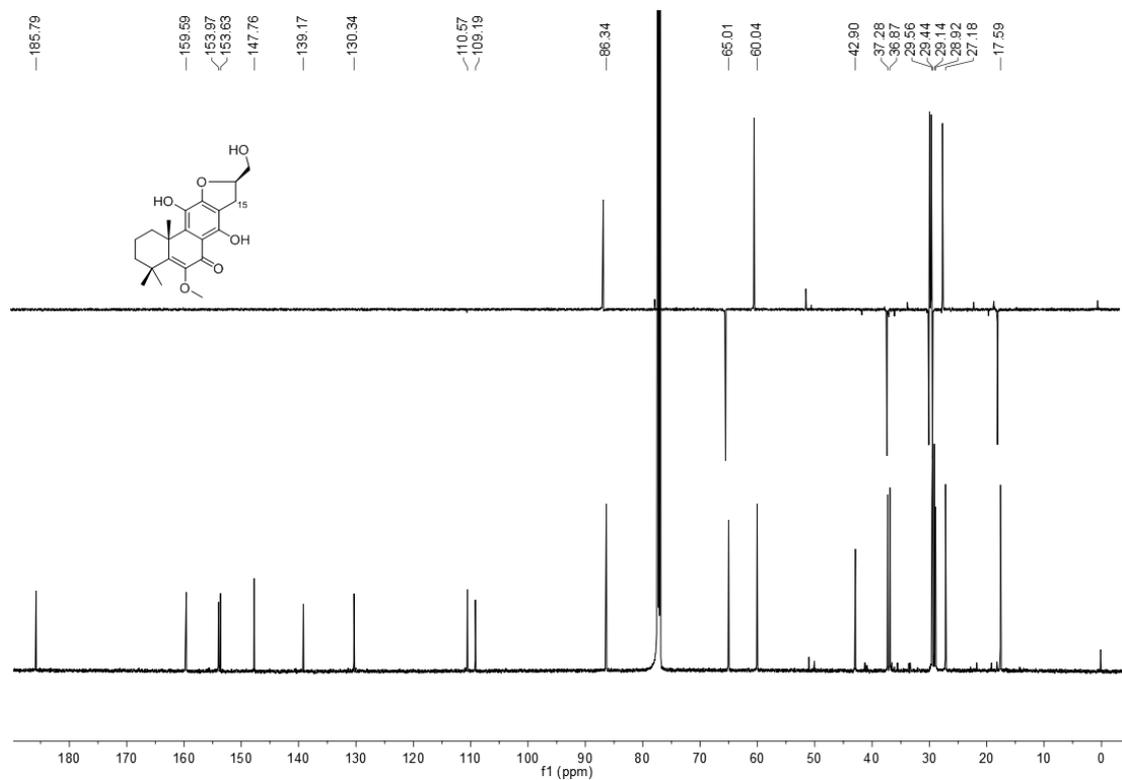


Figure S45: ^{13}C and DEPT NMR spectra of **11** in CDCl₃.

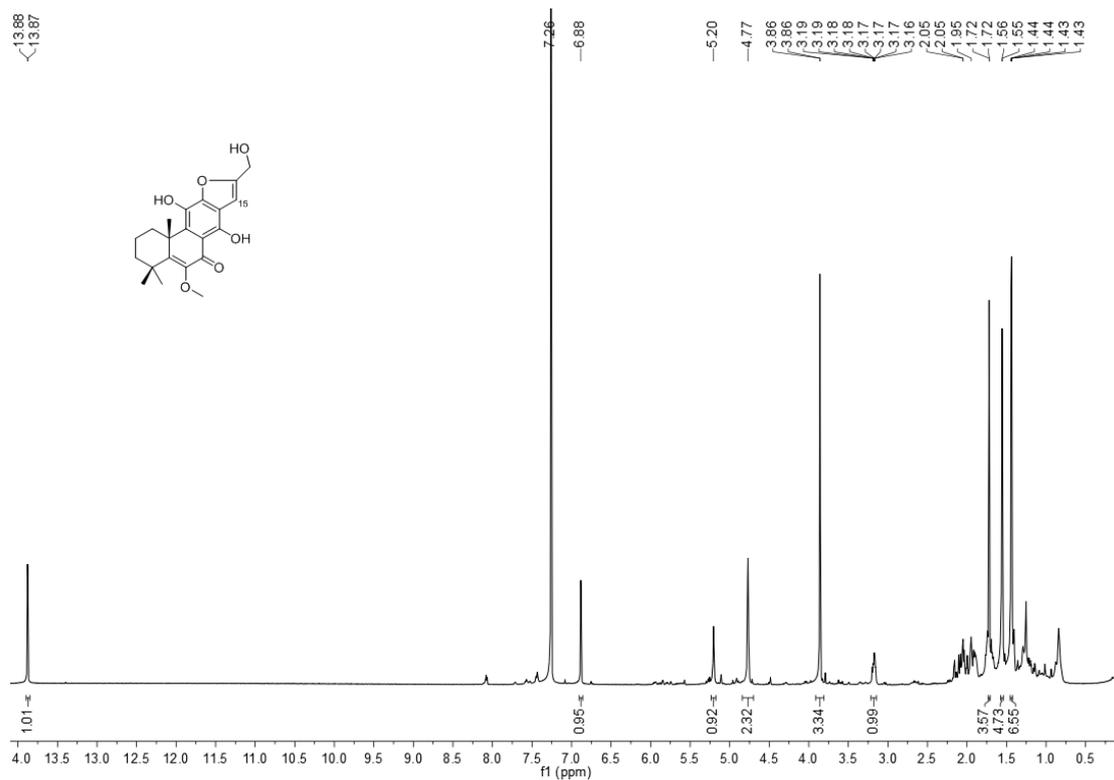


Figure S46: ^1H NMR spectrum of 12 in CDCl_3 .

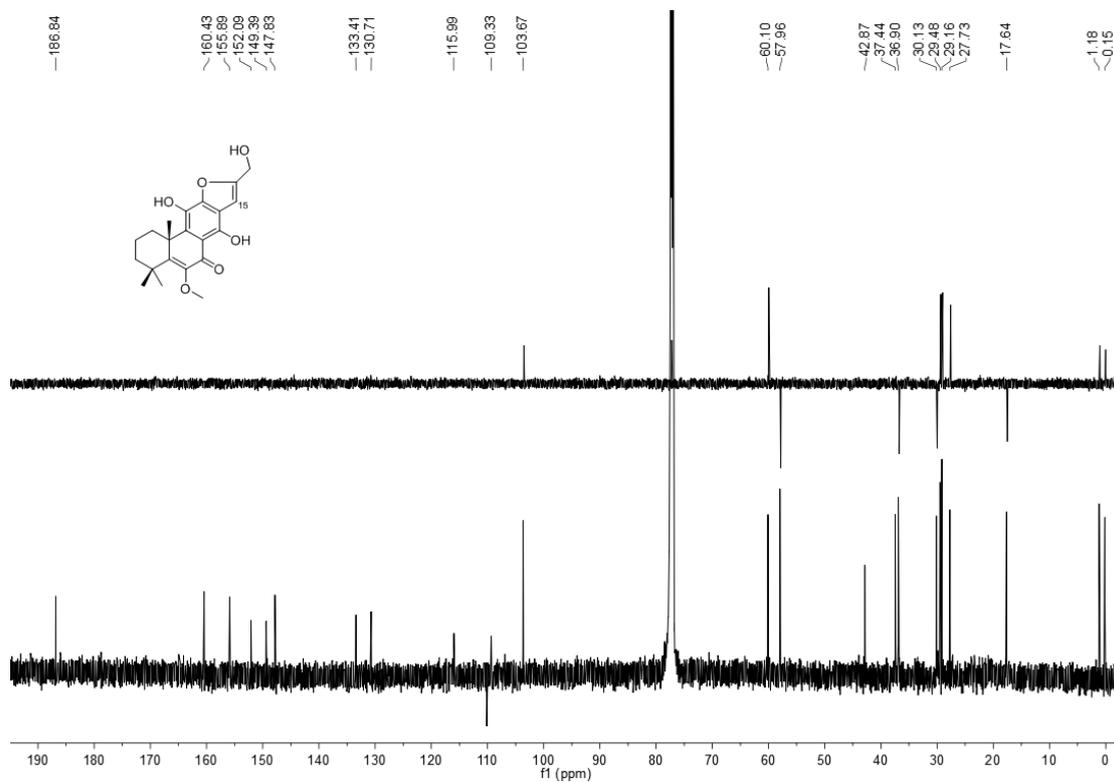


Figure S47: ^{13}C and DEPT NMR spectra of 12 in CDCl_3

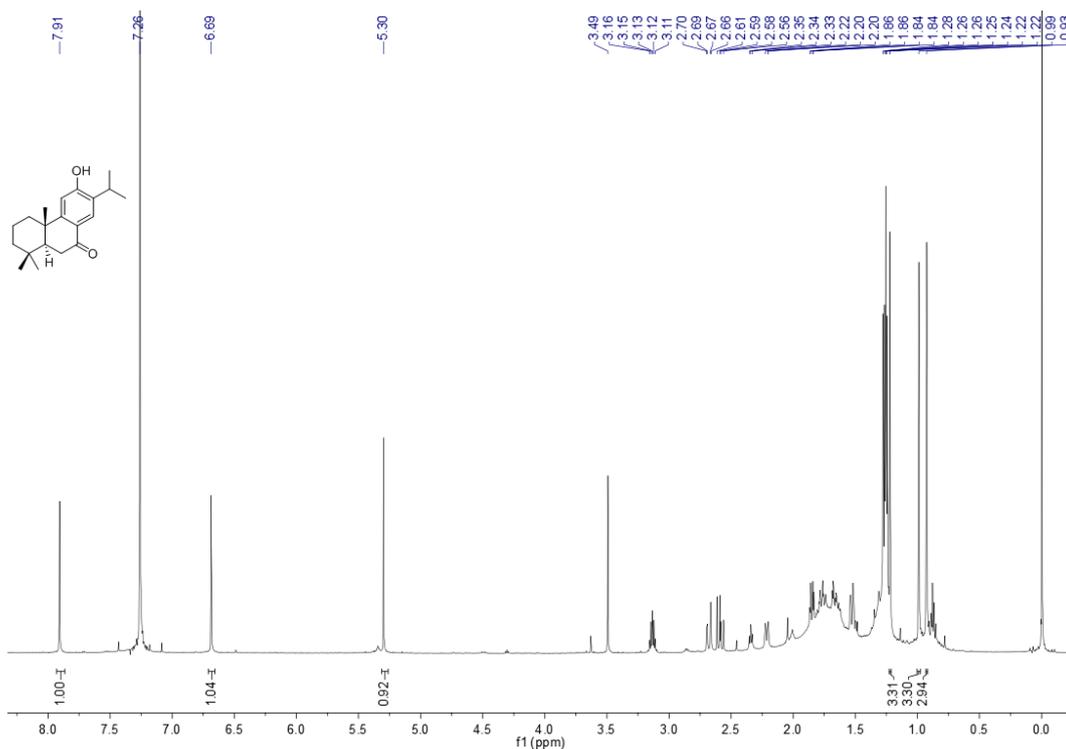


Figure S48: ^1H NMR spectrum of **13** in CDCl_3 .

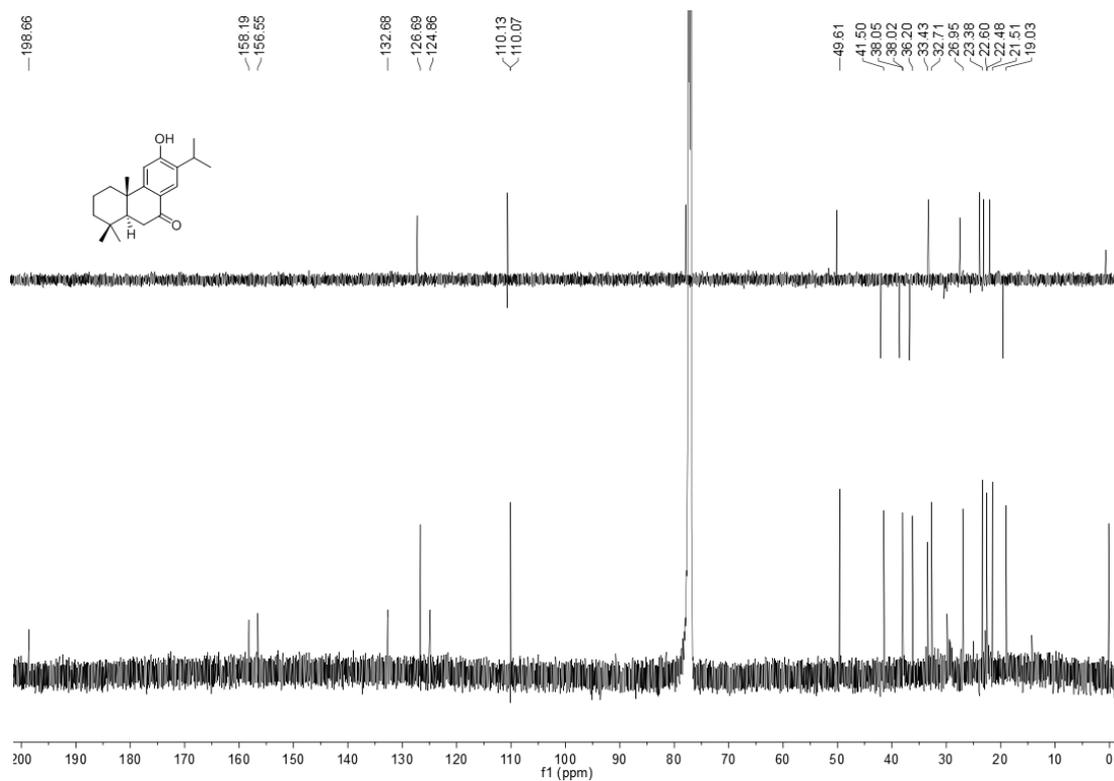


Figure S49: ^{13}C and DEPT NMR spectra of **13** in CDCl_3 .