Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Biotransformation of *α*-Terpineol by *Alternaria alternata*

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Contents

Spectroscopic information:

(–)-(*R*)-7-Hydroxy-*α*-terpineol (**2a**): [*α*]25 D –25.1 (*c* 0.020, $CHCl_3$); ^1H NMR (400 MHz, $CDCl_3$) *δ*1.19 (s, 3H, CH_3), 1.24 (s, 3H, CH_3), 1.24 (m, 1H, CH-H), 1.36 (m, 1H, CH-H), 1.52 (m, 1H, CH-H), 1.54 (m,1H, CH), 1.55 (m, 1H, CH-H), 1.76 (m, 1H, CH-H), 2.05 (m, 1H, CH-H), 4.01 (t, 2H, *J* 12.0, CH_2), 5.69 (m, 1H, CH), ^{13}C NMR (100 MHz, $CDCl_3$) *δ* 23.7, 26.5, 26.7, 26.7, 27.5, 45.2, 67.2, 72.9, 122.6, 137.6; EIMS *m/z*, observed: 170; $C_{10}H_{18}O_2$ $[M]^+$ requires: 170.

(–)-4*R*-Oleuropeic acid (**2**): [*α*]25 D -38.9 (*c* 0.020, MeOH); ^1H NMR (400 MHz, MeOD) *δ*1.17 (s, 3H, CH_3), 1.17 (s, 3H, CH_3), 1.22 (m, 1H, CH-H), 1.53 (m, 1H, CH), 2.01 (m, 1H,CH-H), 2.02 (m, 1H,CH-H), 2.08 (m, 1H,CH-H), 2.34 (br d, 1H, *J* 16.0, CH), 2.48 (br d, 1H, *J* 16.0, CH-H), 6.98 (t, 1H, *J* 2.4, CH); ^{13}C NMR (100 MHz, MeOD) *δ* 24.6, 26.4, 26.4, 27.0, 28.5, 45.6, 72.9, 131.7, 140.8, 171.1; EIMS *m/z*, observed: 184; $C_{10}H_{16}O_3$ $[M]^+$ requires: 184.

(+)-(1*S*,2*R*,4*R*)-*p*-Menthane-1,2,8-triol (**3**): [*α*]25 D +16.3 (*c* 0.020, $CHCl_3$); ^1H NMR (600 MHz, $CDCl_3$) *δ* 1.14 (s, 3H, CH_3), 1.18 (s, 3H, CH_3), 1.22 (s, 3H, CH_3), 1.34 (td, 1H, *J* 8.0, 4.0, CH-H), 1.50 (t, 1H, *J* 3.6, CH-H), 1.54 (t, 1H, *J* 8.0, CH-H), 1.63 (tt, 1H, *J* 12.0, 6.0, CH), 1.75 (t, 1H, *J* 2.0, CH-H), 1.79 (m, 2H, CH_2), 3.61 (brs, 1H, CH); ^{13}C NMR (150 MHz, $CDCl_3$) *δ* 22.2, 26.7, 27.6, 27.8, 30.0, 33.7, 41.1, 71.0, 72.8, 74.1; EIMS *m/z*, observed: 188; $C_{10}H_{20}O_3$ $[M]^+$ requires: 188.

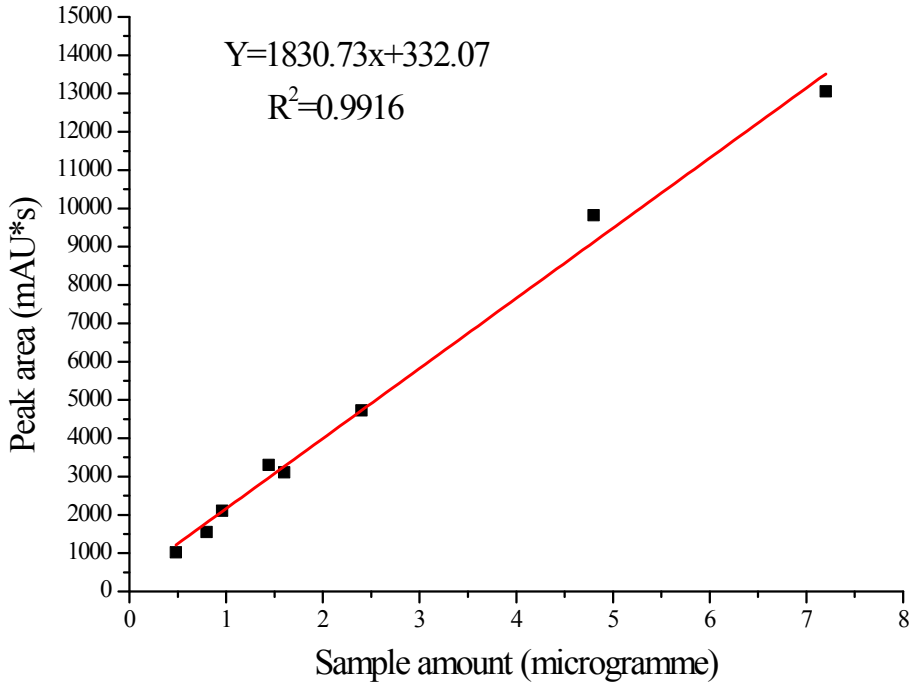

Figure S1. standard working curve for compound **2**

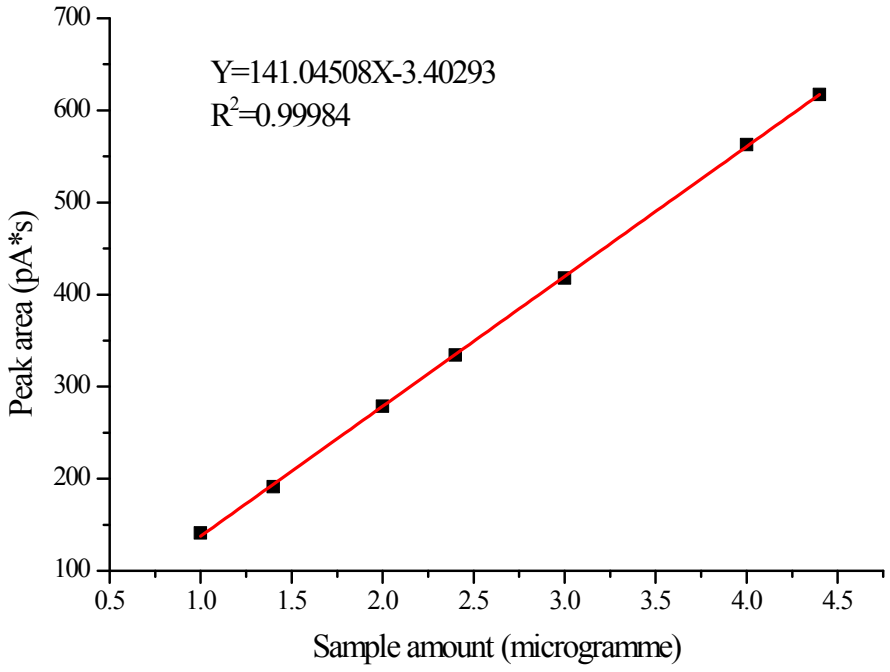

Figure S2. standard working curve for compound **3**

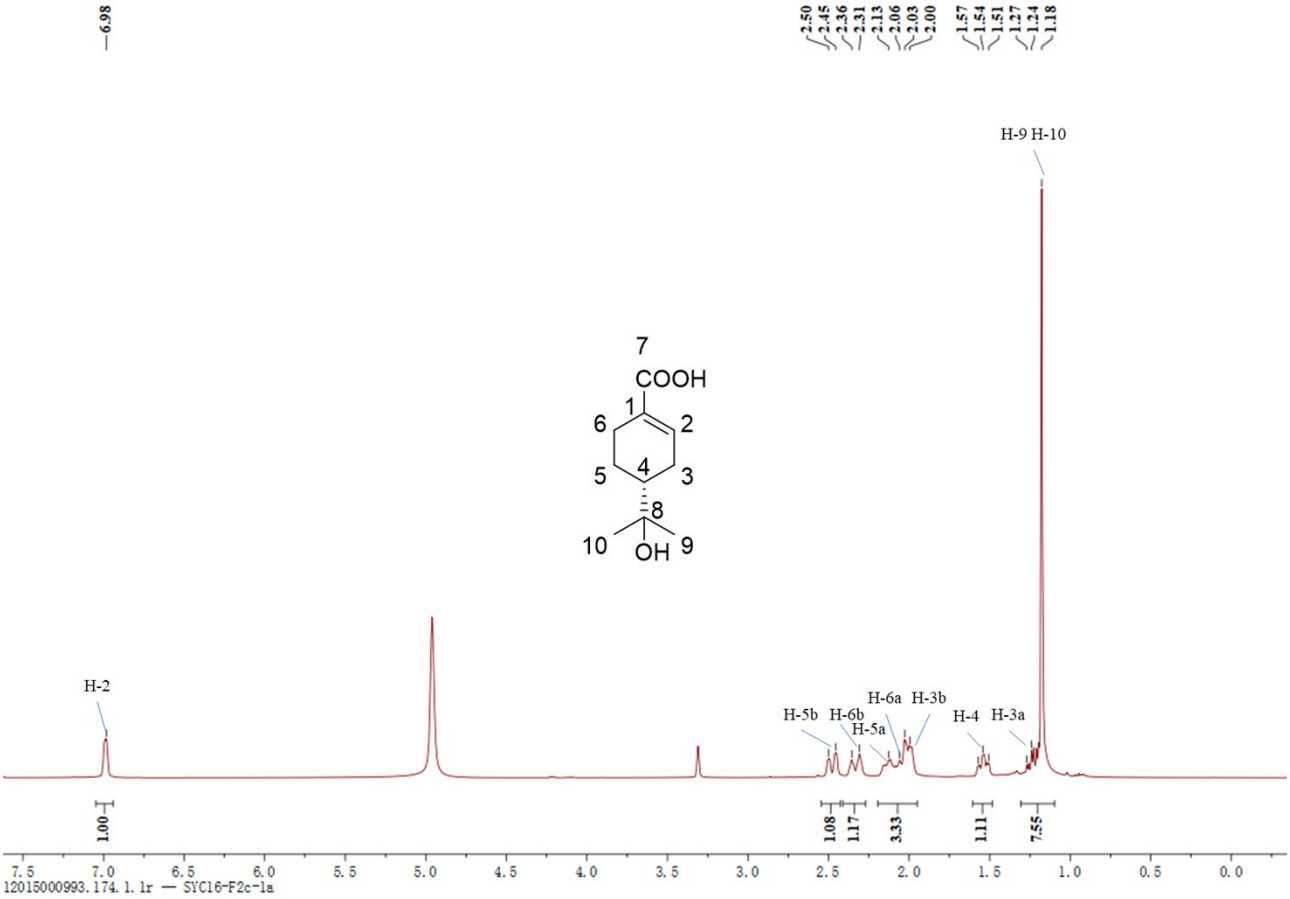

Figure S3. [1]H NMR spectrum (400 MHz, MeOD) of compound **2**

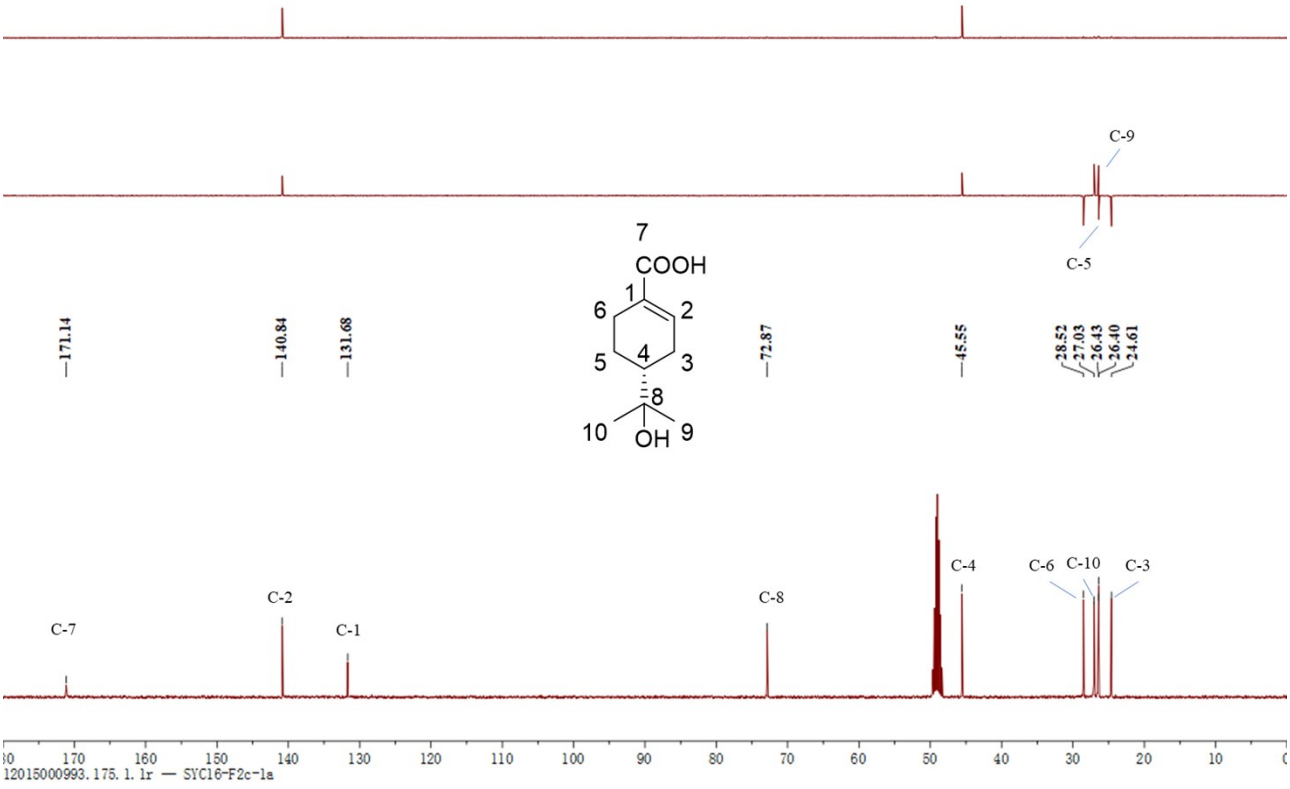

Figure S4. [13]C NMR spectrum (100 MHz, MeOD) of compound **2**

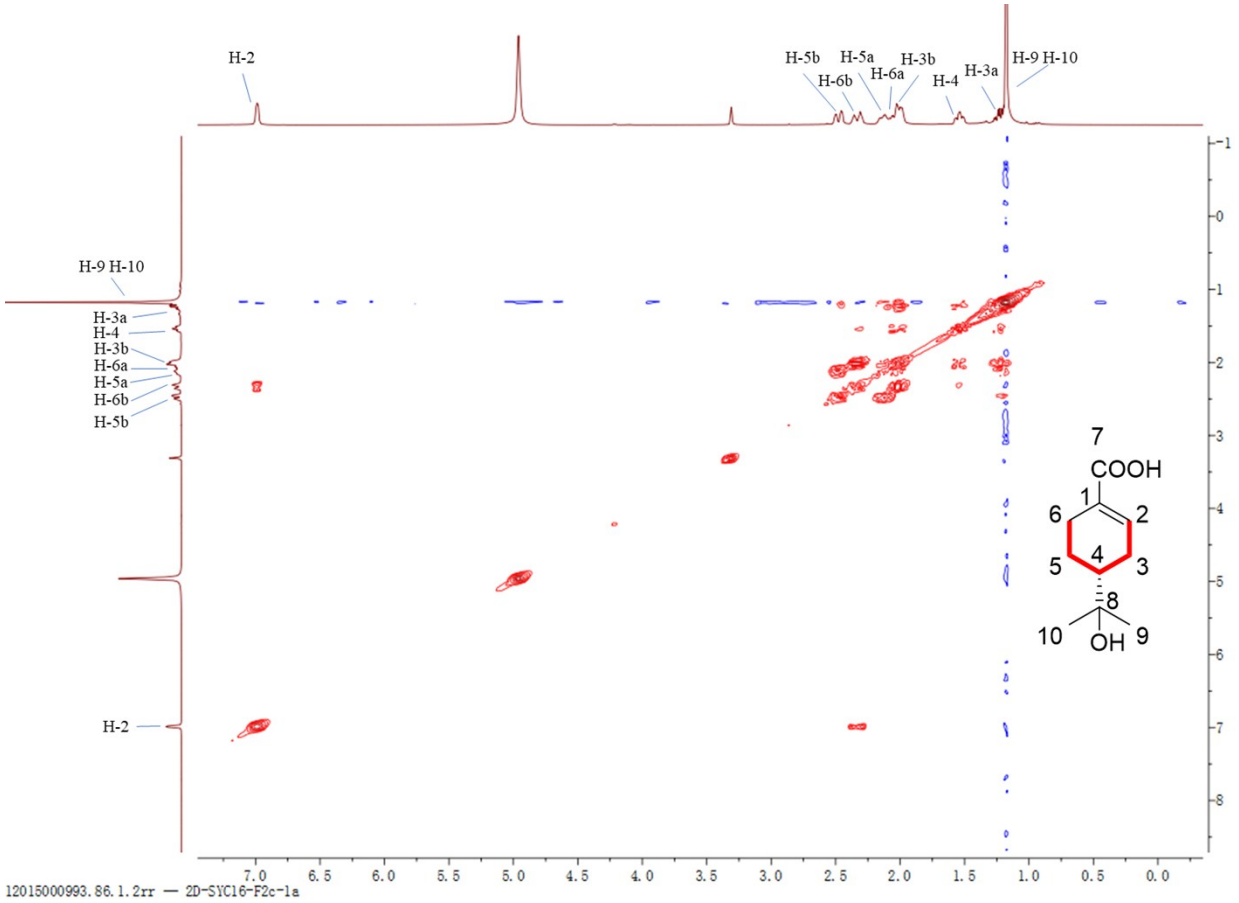

Figure S5. H-H COSY spectrum of compound **2**

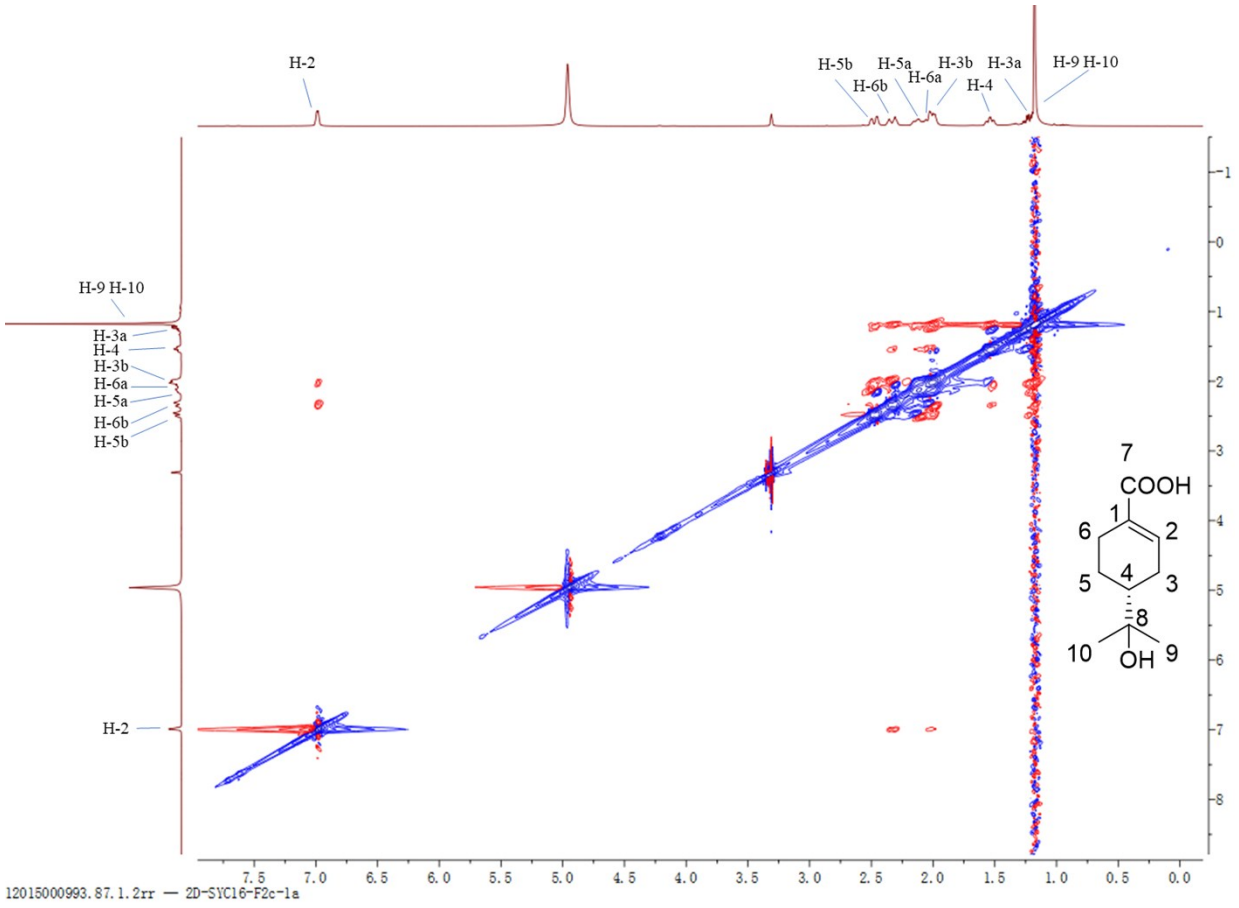

Figure S6. ROESY spectrum of compound **2**

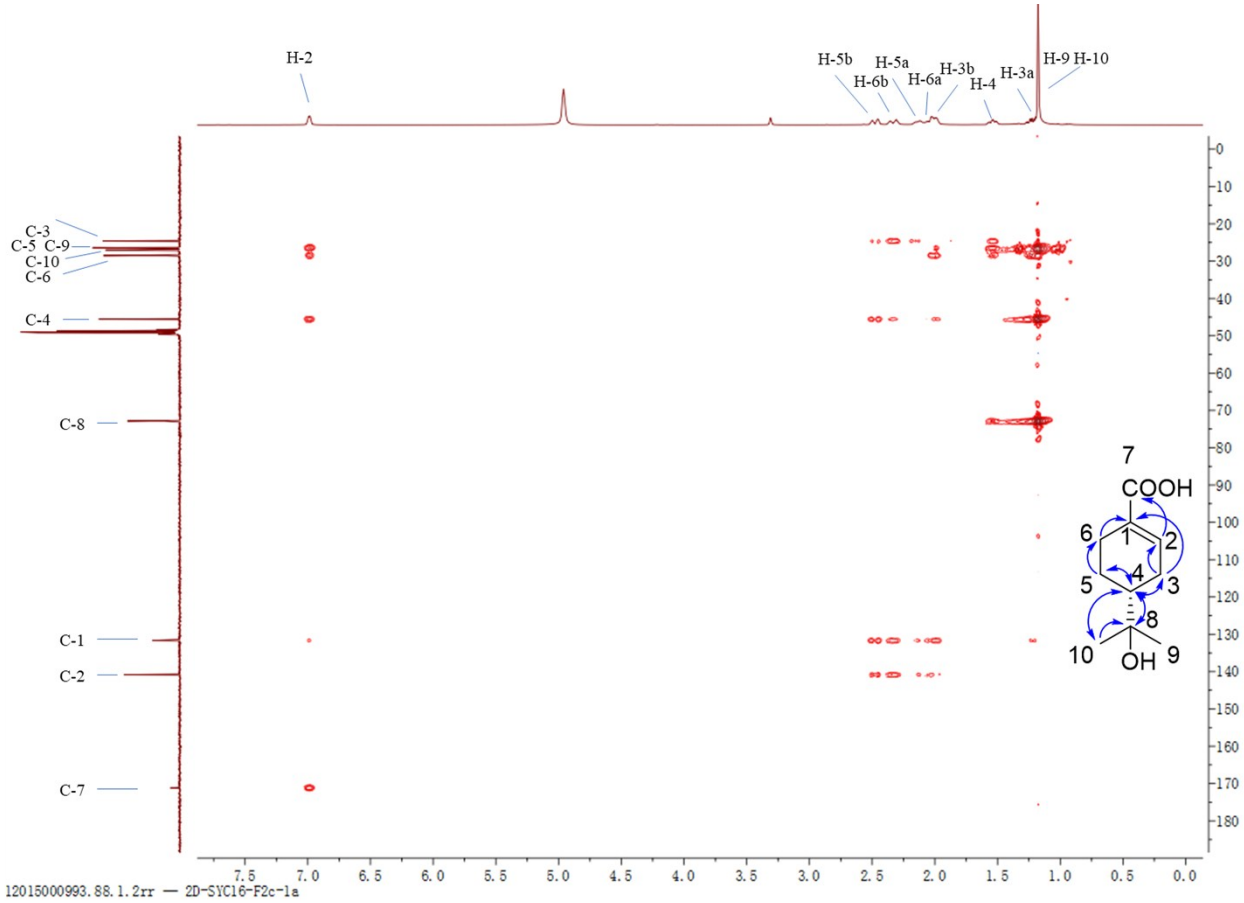

Figure S7. HMBC spectrum of compound **2**

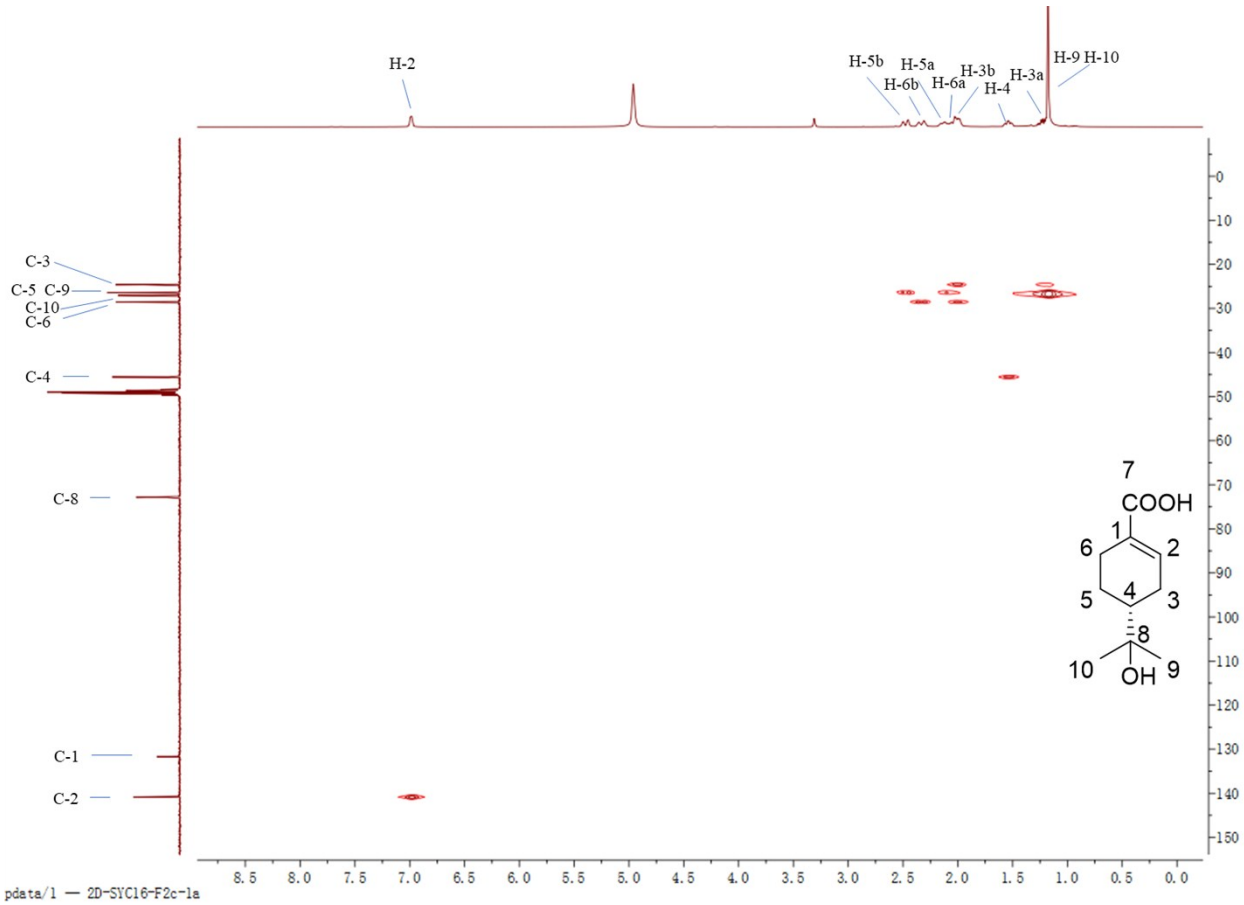

Figure S8. HSQC spectrum of compound **2**

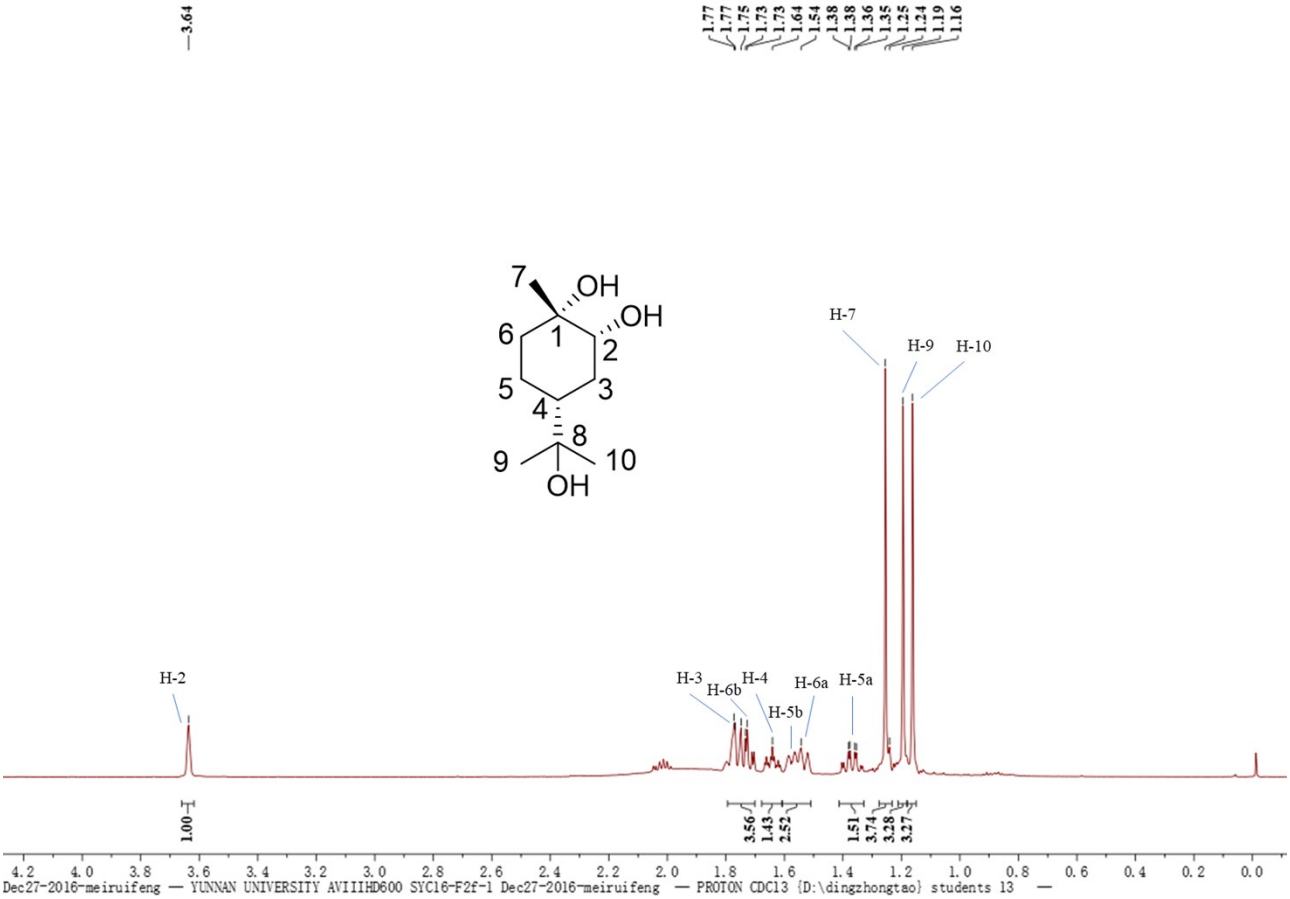

Figure S9. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of compound **3**

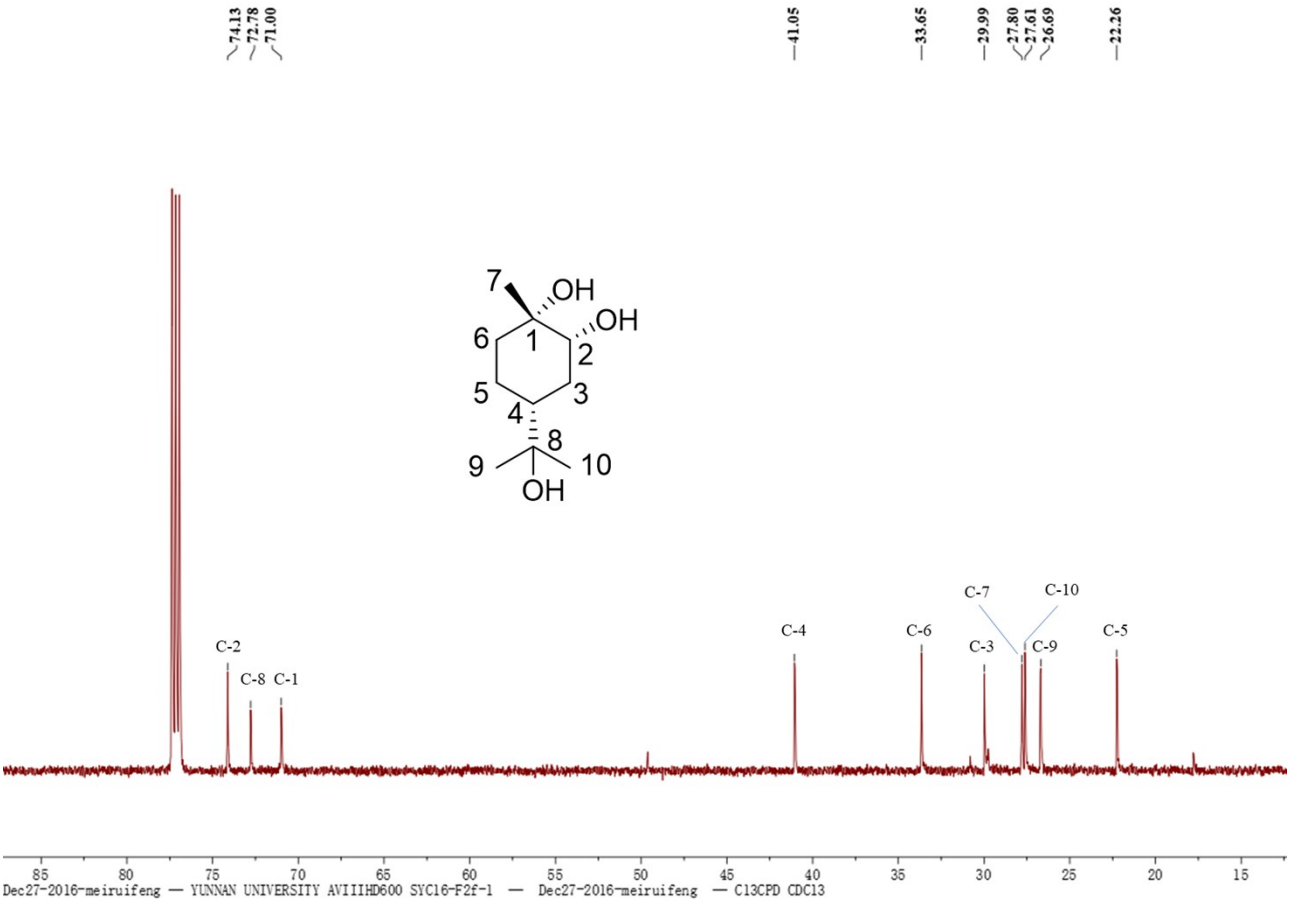

Figure S10. ^{13}C NMR spectrum (150 MHz, $CDCl_3$) of compound **3**

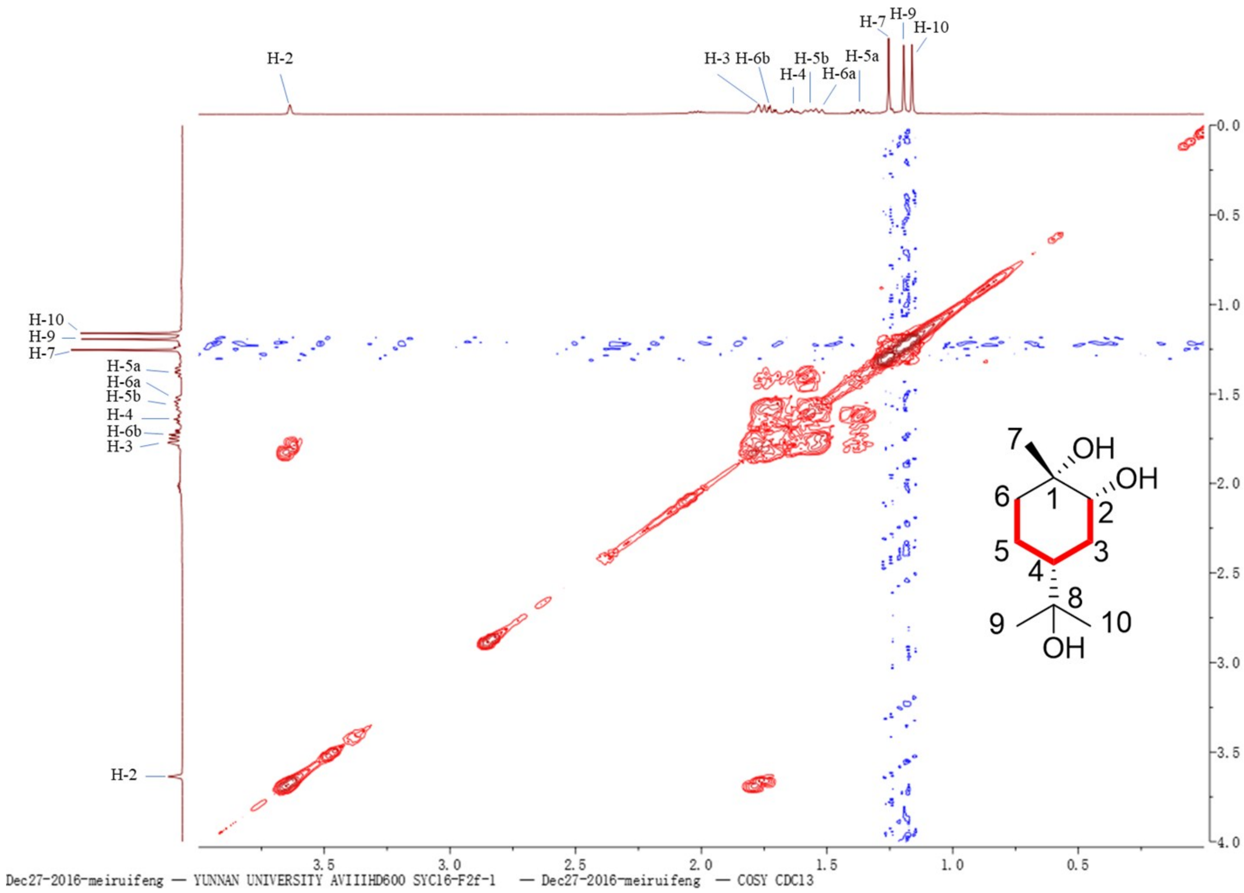

Figure S11. H-H COSY spectrum of compound **3**

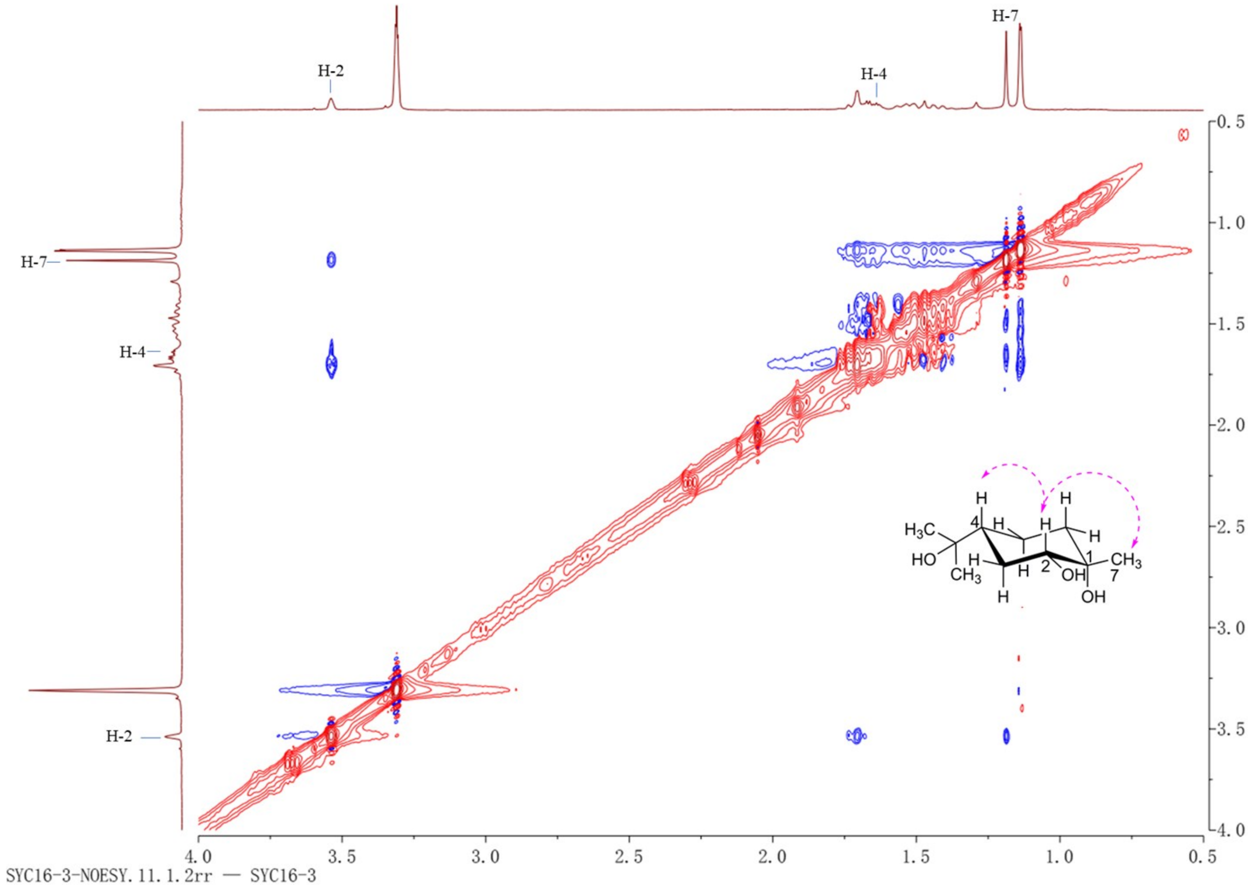

Figure S12. NOESY spectrum (400MHz, MeOD) of compound **3**

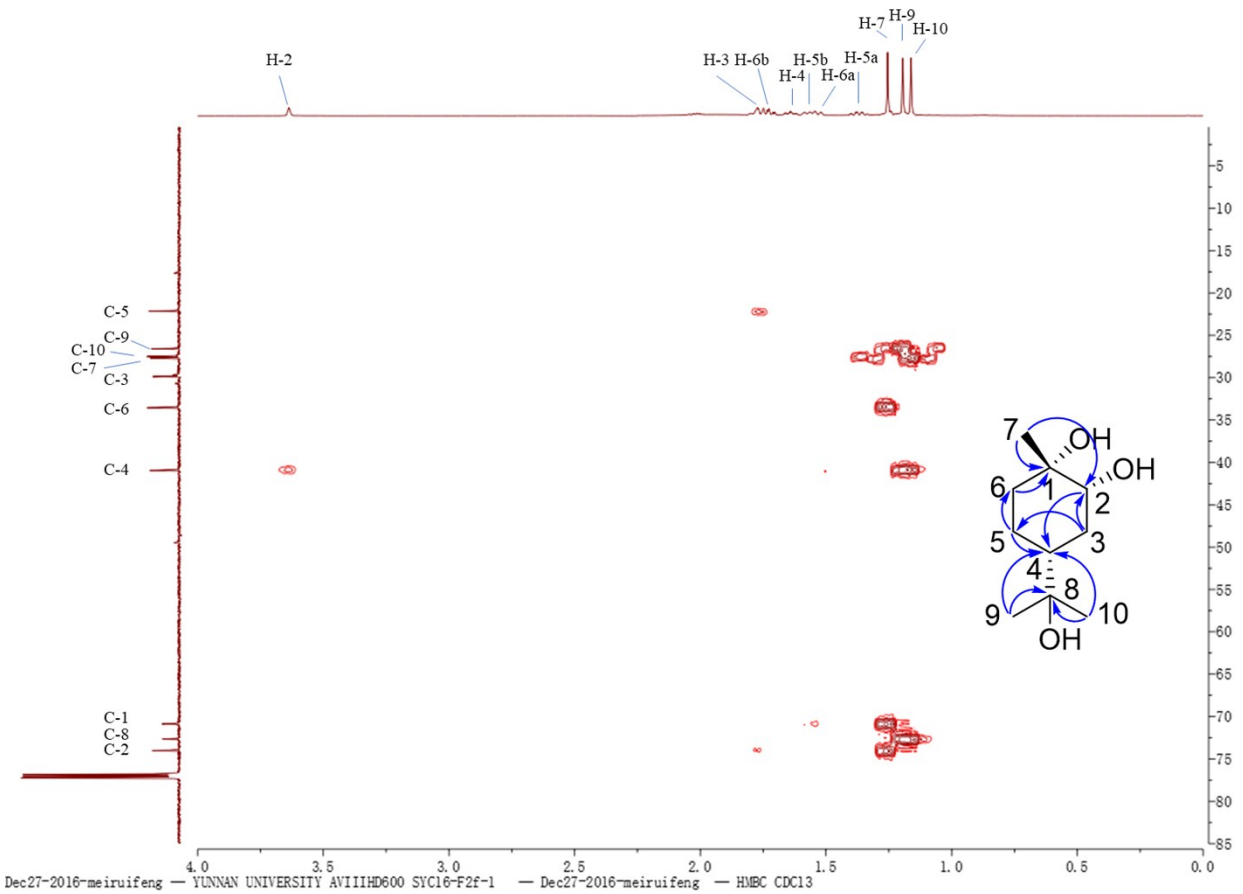

Figure S13. HMBC spectrum of compound **3**

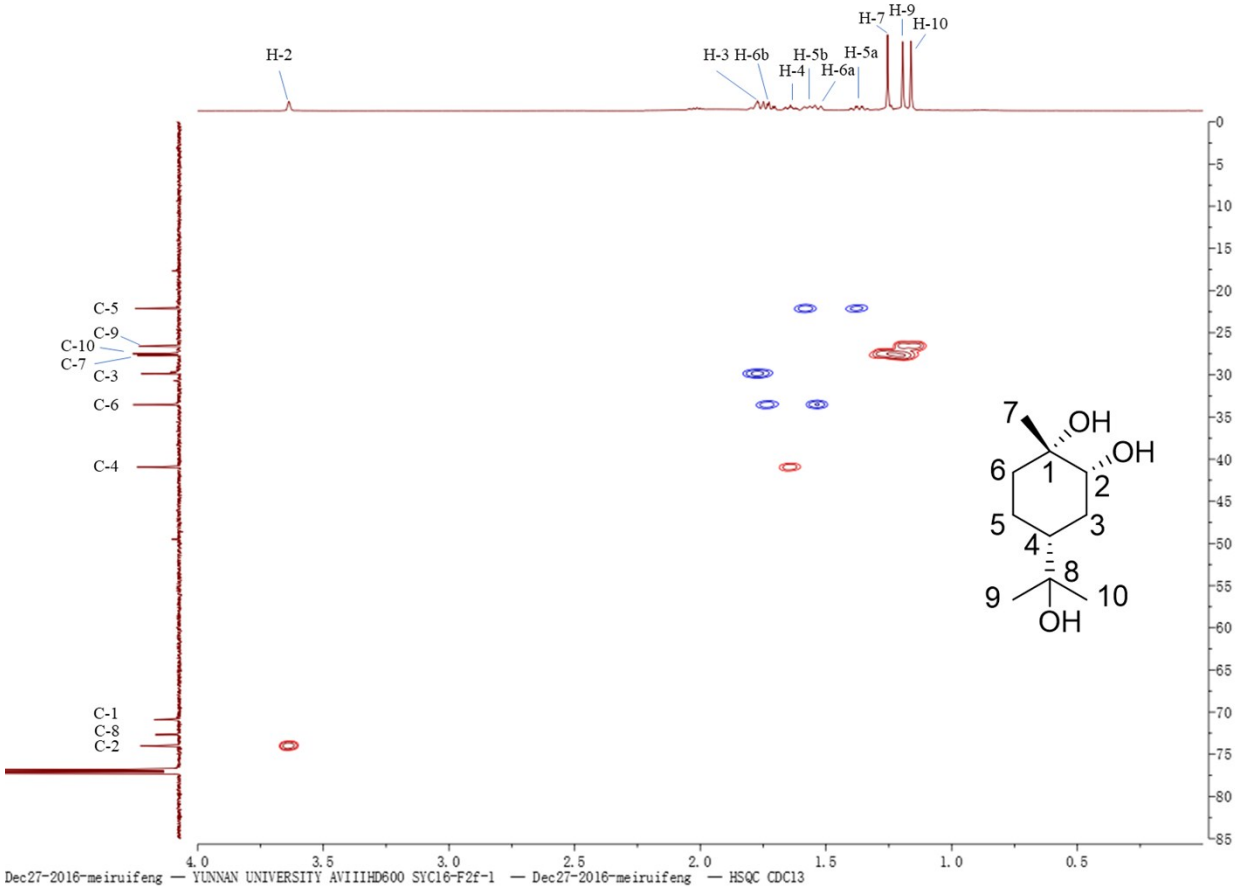

Figure S14. HSQC spectrum of compound **3**

Table S1. NMR parameters of compound **2**

□	^{1}H	^{13}C	COSY	ROESY	HMBC	HSQC
Comment	SYC16-F2c-1a	SYC16-F2c-1a	2D-SYC16-F2c-1a	2D-SYC16-F2c-1a	2D-SYC16-F2c-1a	2D-SYC16-F2c-1a
Origin	Bruker BioSpin GmbH	Bruker BioSpin GmbH	Bruker BioSpin GmbH	Bruker BioSpin GmbH	Bruker BioSpin GmbH	Bruker BioSpin GmbH
Spectrometer	spect	spect	spect	spect	spect	spect
Solvent	MeOD	MeOD	MeOD	MeOD	MeOD	MeOD
Temperature	0	0	0	0	0	0
Pulse Sequence	zg30	zgpg30	cosygpppqf	roesyphpp.2	hmbcetgpl3nd	hsqcedetgpsisp2.3
Experiment	1D	1D	COSY	ROESY	HMBC	HSQC-EDITED
Probe	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z116098/ 0088	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z116098/ 0088	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z116098/ 0088	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z116098/ 0088	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z116098/ 0088	5 mm PABBO BB/ 19F-1H/ D Z-GRD Z116098/ 0088
Number of Scans	8	512	1	4	4	8
Receiver Gain	32	196	16	16	196	196
Relaxation Delay	1	2	1.9459	2.0123	1.9386	1.5
Pulse Width	10.62	10.56	10.62	10.62	10.62	10.62
Acquisition Time	4.0895	1.2977	0.2458	0.2437	0.4874	0.0799
Spectrometer Frequency	400.15	100.62	(400.15, 400.15)	(400.15, 400.15)	(400.15, 100.62)	(400.15, 100.62)
Spectral Width	8012.8	25252.5	(4166.7, 4166.7)	(4201.7, 4201.7)	(4201.7, 22321.4)	(6410.3, 16611.3)
Lowest Frequency	-1813.3	-1922.9	(-685.0, -686.4)	(-698.0, -688.3)	(-693.2, -840.9)	(-1342.0, -989.6)
Nucleus	1H	13C	(1H, 1H)	(1H, 1H)	(1H, 13C)	(1H, 13C)
Acquired Size	32768	32768	(1024, 128)	(1024, 256)	(2048, 256)	(512, 256)
Spectral Size	65536	32768	(1024, 1024)	(1024, 1024)	(2048, 1024)	(1024, 1024)

Table S2. NMR parameters of compound **3**

□	^{1}H	^{13}C	COSY	ROESY	HMBC	HSQC
Comment	SYC16-F2f-1	SYC16-F2f-1	SYC16-F2f-1	SYC16-F2f-1	SYC16-F2f-1	SYC16-F2f-1
Origin	Bruker BioSpin GmbH	Bruker BioSpin GmbH	Bruker BioSpin GmbH	Bruker BioSpin GmbH	Bruker BioSpin GmbH	Bruker BioSpin GmbH
Spectrometer	spect	spect	spect	spect	spect	spect
Solvent	CDCl3	CDCl3	CDCl3	CDCl3	CDCl3	CDCl3
Temperature	292.1	294.5	294.3	293.5	293.9	295.2
Pulse Sequence	zg30	zgpg30	cosygpppqf	roesyphpp.2	hmbcgplpndqf	hsqcedetgpsisp2.3
Experiment	1D	1D	COSY	ROESY	HMBC	HSQC-EDITED
Probe	Z114607_0222 (PA BBO 600S3 BBF-H-D-05 Z SP)	Z114607_0222 (PA BBO 600S3 BBF-H-D-05 Z SP)	Z114607_0222 (PA BBO 600S3 BBF-H-D-05 Z SP)	Z114607_0222 (PA BBO 600S3 BBF-H-D-05 Z SP)	Z114607_0222 (PA BBO 600S3 BBF-H-D-05 Z SP)	Z114607_0222 (PA BBO 600S3 BBF-H-D-05 Z SP)
Number of Scans	1	1024	3	8	6	4
Receiver Gain	62	188	27	24	188	188
Relaxation Delay	1	2	1.9488	1.9597	1.4488	2
Pulse Width	10	12	10	10	10	10
Acquisition Time	2.7263	0.9044	0.1823	0.1823	0.1823	0.1065
Spectrometer Frequency	600.17	150.91	(600.17, 600.17)	(600.17, 600.17)	(600.17, 150.91)	(600.17, 150.91)
Spectral Width	12019.2	36231.9	(5618.0, 5618.0)	(5618.0, 5618.0)	(5618.0, 33112.6)	(9615.4, 27173.9)
Lowest Frequency	-2318.6	-3024.7	(-594.9, -594.9)	(-594.9, -594.9)	(-597.1, 44.1)	(-1998.9, -306.6)
Nucleus	1H	13C	(1H, 1H)	(1H, 1H)	(1H, 13C)	(1H, 13C)
Acquired Size	32768	32768	(1024, 256)	(1024, 256)	(1024, 256)	(1024, 256)
Spectral Size	65536	65536	(1024, 1024)	(1024, 1024)	(2048, 1024)	(1024, 1024)