

Bioactive Composition of *Reevesia formosana* Root and Stem with Cytotoxic Activity Potential

Hsun-Shuo Chang, Chu-Hung Lin, Pei-Yu Hsiao, Hung-Ti Peng, Shiow-Ju Lee, Ming-Jen Cheng, Ih-Sheng Chen*

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Figure S34. HMBC spectrum of reevesiterpenol B (**5**) in CDCl₃

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Figure S36. ¹H NMR spectrum of 3 α ,27-di-*O-trans*-caffeoylbetulinic acid (**6**) in CD₃OD at 400 MHz

Figure S37. ¹³C NMR spectrum of 3 α ,27-di-*O-trans*-caffeoylbetulinic acid (**6**) in CD₃OD at 100 MHz

Figure S38. DEPT spectrum of 3 α ,27-di-*O-trans*-caffeoylbetulinic acid (**6**) in CD₃OD at 100 MHz

Figure S39. COSY spectrum of 3 α ,27-di-*O-trans*-caffeoylbetulinic acid (**6**) in CD₃OD

Figure S40. HSQC spectrum of 3 α ,27-di-*O-trans*-caffeoylbetulinic acid (**6**) in CD₃OD

Figure S41. HMBC spectrum of 3 α ,27-di-*O-trans*-caffeoylbetulinic acid (**6**) in CD₃OD

Figure S42. NOESY spectrum of 3 α ,27-di-*O-trans*-caffeoylbetulinic acid (**6**) in CD₃OD

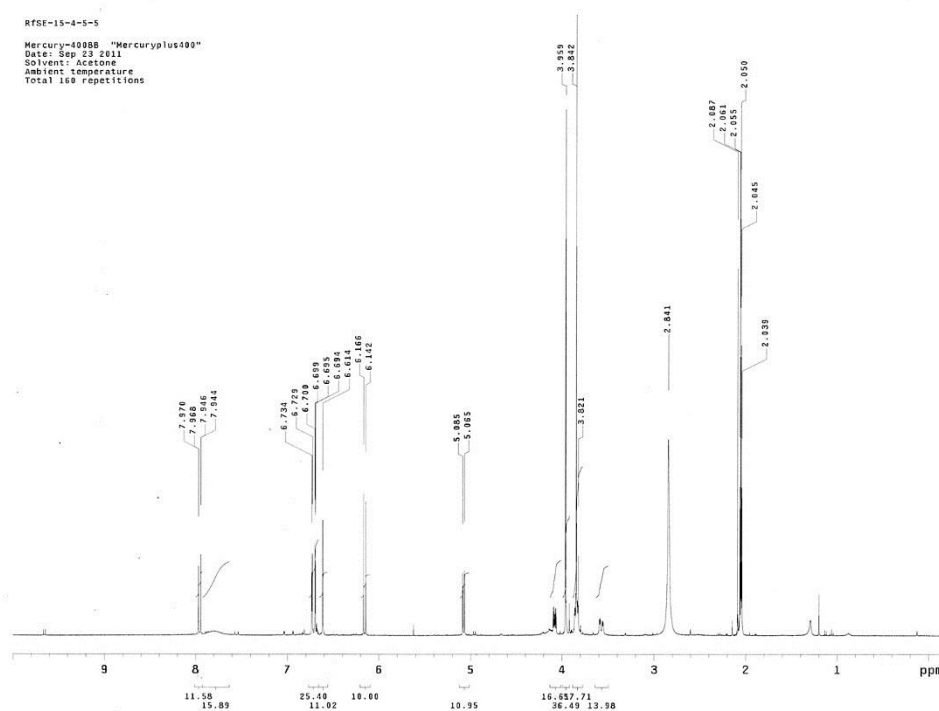


Figure S1. ^1H NMR spectrum of reevesiacoumarin (**1**) in acetone- d_6 at 400 MHz

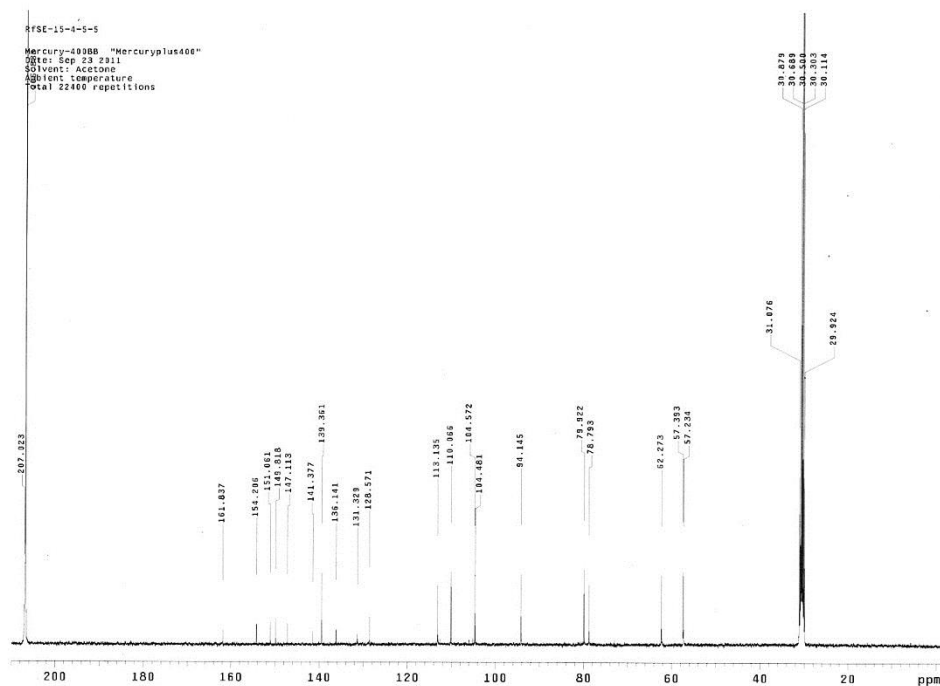


Figure S2. ^{13}C NMR spectrum of reevesiacoumarin (**1**) in acetone- d_6 at 100 MHz

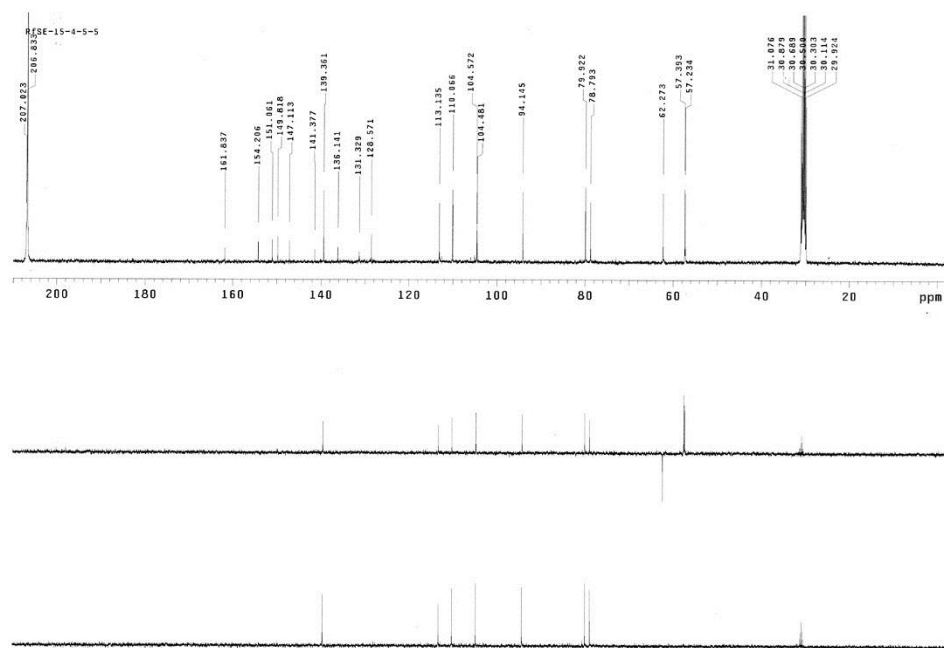


Figure S3. DEPT spectrum of reevesiacoumarin (**1**) in acetone- d_6 at 100 MHz

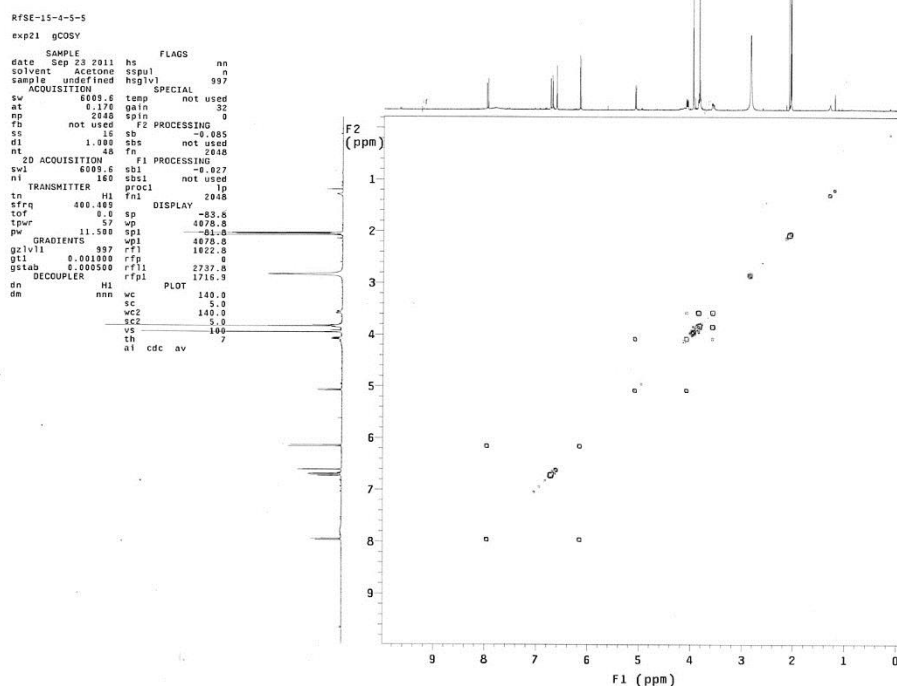


Figure S4. COSY spectrum of reevesiacoumarin (**1**) in acetone- d_6

RTSE-15-4-5-5

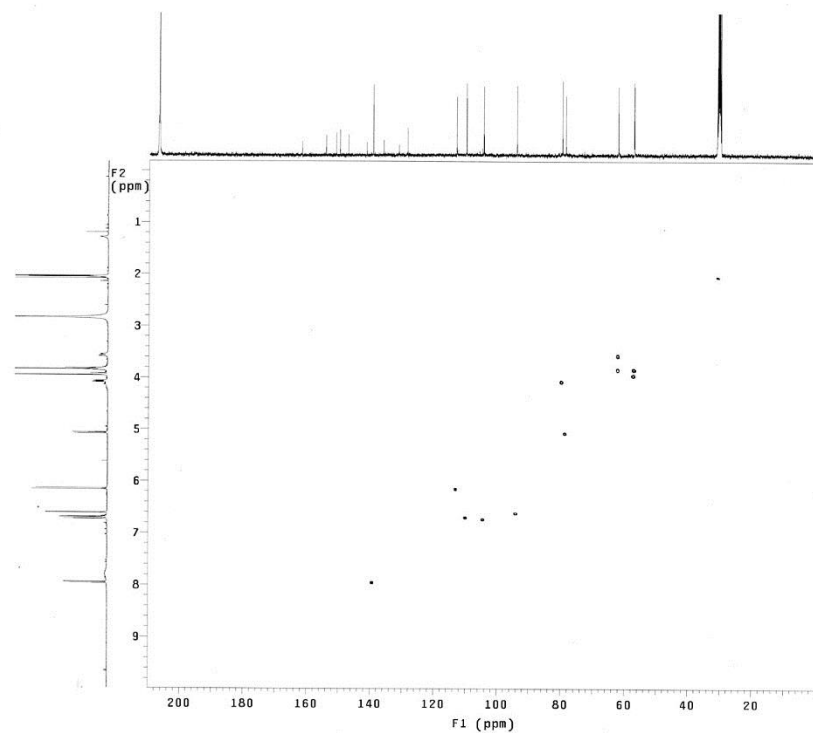


Figure S5. HSQC spectrum of reevesiacoumarin (**1**) in acetone- d_6

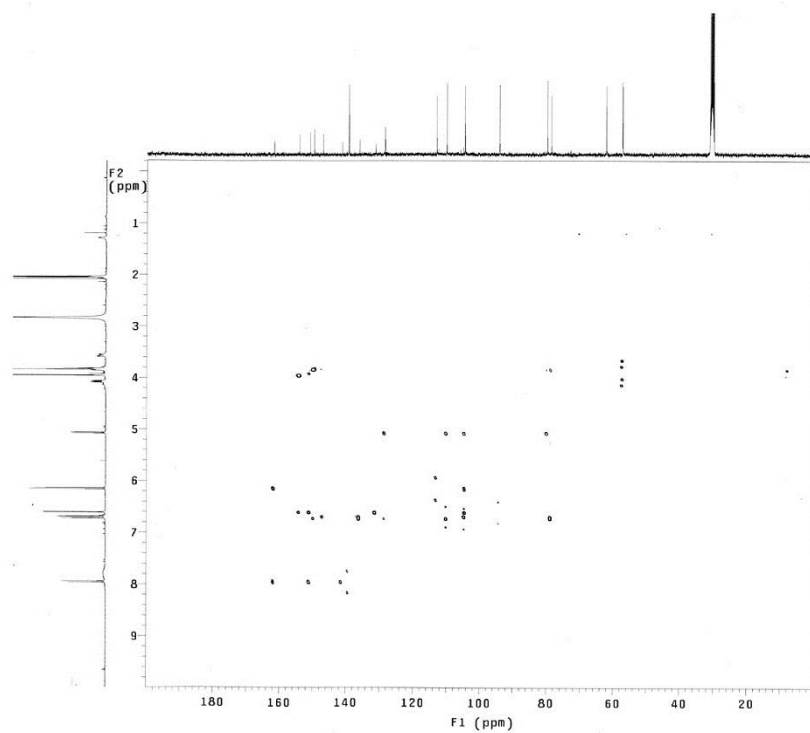


Figure S6. HMBC spectrum of reevesiacoumarin (**1**) in acetone- d_6

RFSE-15-4-5-5
exp22 NOESY

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sample undefined PFG1g y
ACQUISITION hsg1v1 397
sw 6009.6 SPECIAL
at 0.170 temp not used
mp 2048 gain 32
fd not used spin 3
ss 82 PF2 PROCESSING
d1 1.000 dt 0.079
nt 48 dts not used
2D ACQUISITION f1 PROCESSING 2048
sw1 6009.6 f1 0.022
n1 TRANSMITTER 160 gfl1 not used
tn H1 proc1 1p
rf1 400.400 fml1 2048
tot 8.0 DISPLAY
tpr 57 sp -84.0
pw 11.500 wp -84.9
mix NOESY 0.600 sp1 4078.0
PREGSATURATION rf1 1023.0
satpwr 0 rfl1 2749.8
satp1v 0 rfp1 1716.9
satfrq 0 PLOT
DECOUPLER H1 tc 146.0
dn nnn vc2 146.0
tc2 5.0
vs 100
tn al cdc ph 2

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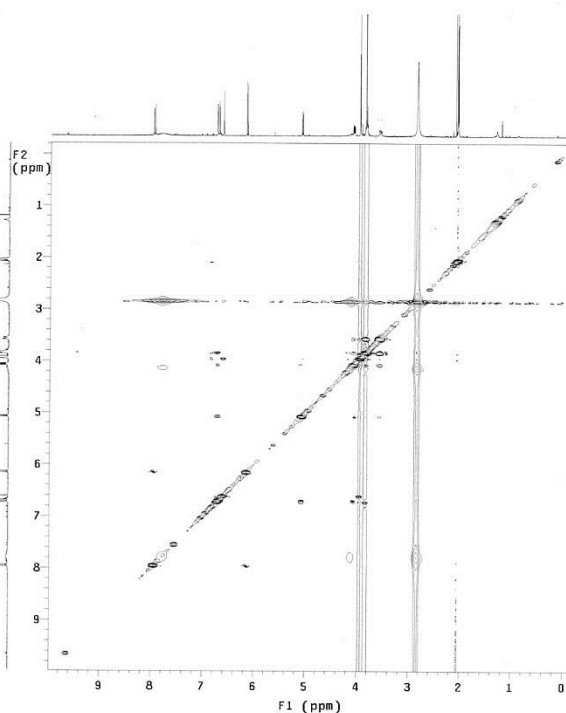


Figure S7. NOESY spectrum of reevesiacoumarin (**1**) in acetone- d_6

RFRE-10-7-4-2-A

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Pulse Sequence: s2pul
UNITYplus-600 "XNUS000"
Date: Jul 18 2012
Solvent: cd3od
Acid temperature
Total 364 repetitions

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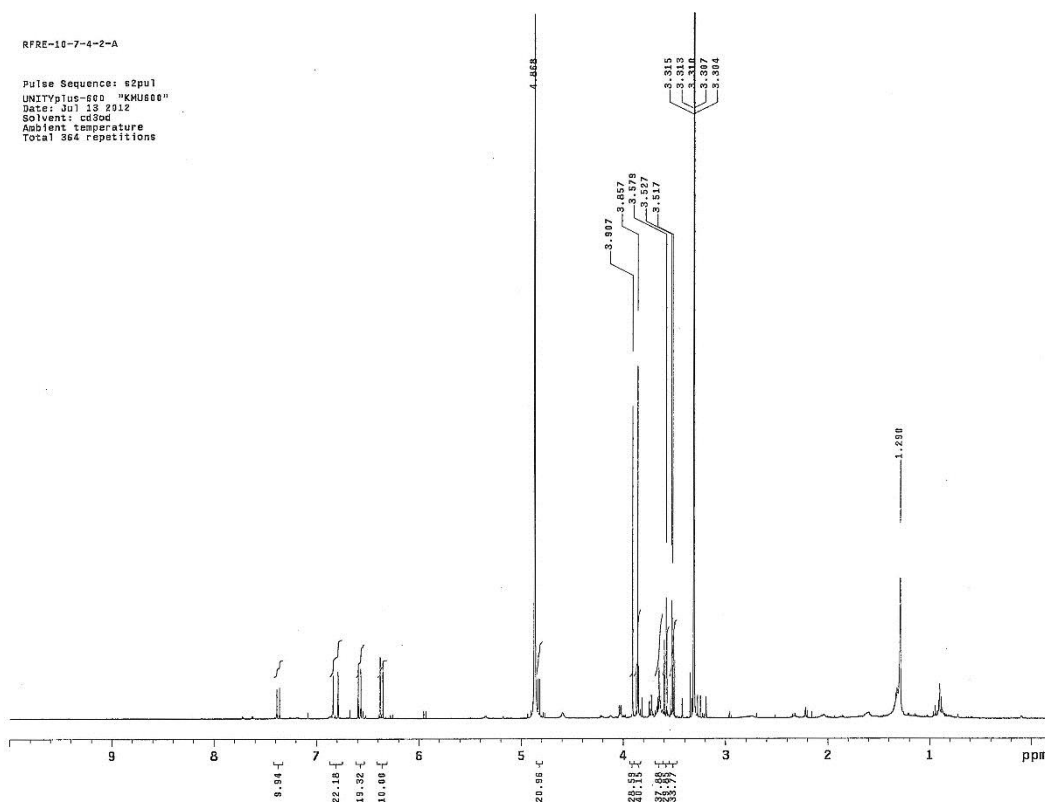


Figure S8. ^1H NMR spectrum of reevesic acid (**2**) in CD_3OD at 600 MHz

RFRE-10-7-4-2-A
exp02 0000y

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solvent	cd3od			sepi	not used				
sample	reevesic			sepi	not used				
ACQUISITION									
sv	5615.4	temp	not used						
at	1.215	spin	40						
pd	4096	spin	0						
td	4096	f2	PROCESSING	0					
ss	1.000	ss	not used						
d1	1.000	ss	not used						
nt	48	f1	PROCESSING	4096					
2D ACQUISITION									
sw1	5615.4	sb1	0.017						
ni	160	sbol	not used						
PRESATURATION									
satmode	nnn	fml	DISPLAY	4096					
satpwr	-15	wp	5000.4						
satfrq	499.0	sp	-120.1						
satpwr	-15	wp	5000.4						
TRANSMITTER									
tn	597.362	wp1	-120.1						
trfrq	597.362	wp1	5000.4						
tot	597.4	rfo	1223.5						
tpwr	59	rfl	1223.5						
pw	10.003	rfl	0						
tpwr	59	rfl	1223.5						
PLOT									
gradients	711	wc	140.0						
g1	0.001003	wc2	140.0						
g2	0.001003	wc2	140.0						
g3	0.001003	wc2	140.0						
g4	0.001003	wc2	140.0						
g5	0.001003	wc2	140.0						
g6	0.001003	wc2	140.0						
g7	0.001003	wc2	140.0						
g8	0.001003	wc2	140.0						
g9	0.001003	wc2	140.0						
g10	0.001003	wc2	140.0						
g11	0.001003	wc2	140.0						
g12	0.001003	wc2	140.0						
g13	0.001003	wc2	140.0						
g14	0.001003	wc2	140.0						
g15	0.001003	wc2	140.0						
g16	0.001003	wc2	140.0						
g17	0.001003	wc2	140.0						
g18	0.001003	wc2	140.0						
g19	0.001003	wc2	140.0						
g20	0.001003	wc2	140.0						
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g23	0.001003	wc2	140.0						
g24	0.001003	wc2	140.0						
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g28	0.001003	wc2	140.0						
g29	0.001003	wc2	140.0						
g30	0.001003	wc2	140.0						
g31	0.001003	wc2	140.0						
g32	0.001003	wc2	140.0						
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g44	0.001003	wc2	140.0						
g45	0.001003	wc2	140.0						
g46	0.001003	wc2	140.0						
g47	0.001003	wc2	140.0						
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g51	0.001003	wc2	140.0						
g52	0.001003	wc2	140.0						
g53	0.001003	wc2	140.0						
g54	0.001003	wc2	140.0						
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g60	0.001003	wc2	140.0						
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g63	0.001003	wc2	140.0						
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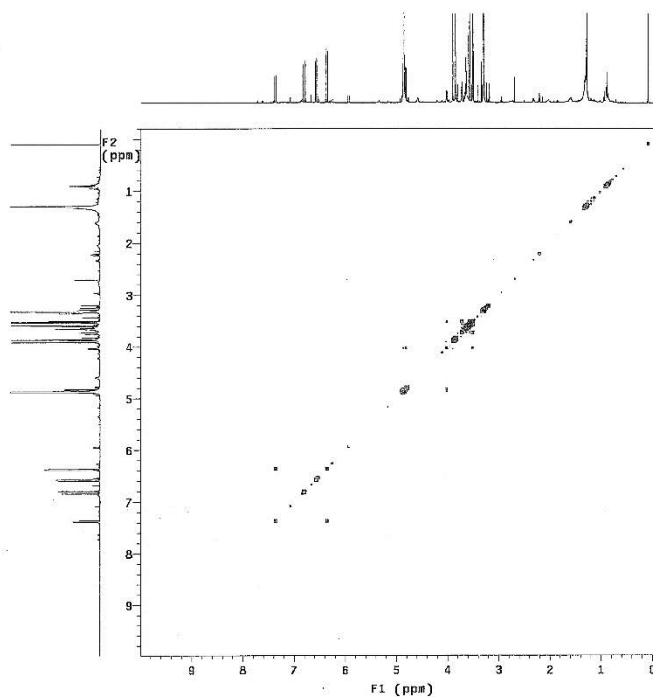


Figure S11. COSY spectrum of reevesic acid (**2**) in CD₃OD

RFRE-10-7-4-2-A

Pulse Sequence: gHSQCAD

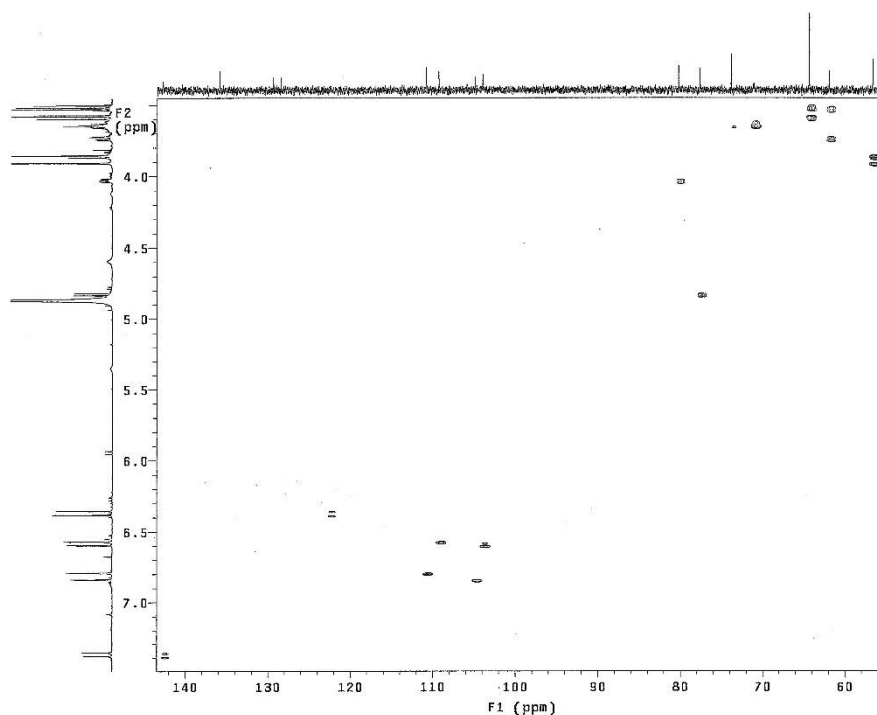


Figure S12. HSQC spectrum of reevesic acid (**2**) in CD₃OD

RFRE-10-7-4-2-A

Pulse Sequence: gHMBC

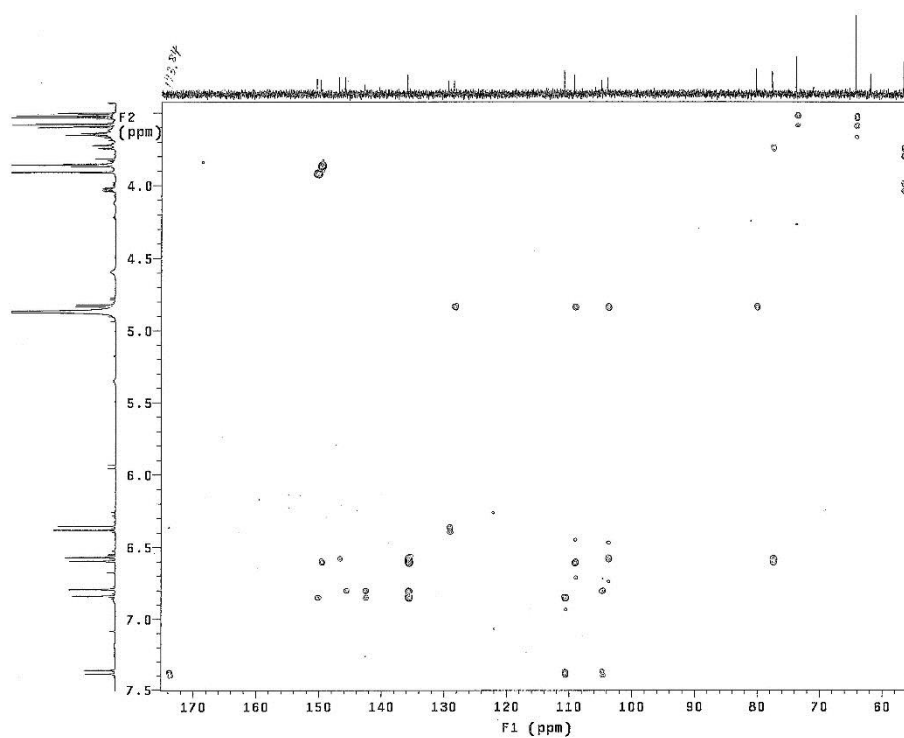


Figure S13. HMBC spectrum of reevesic acid (2) in CD₃OD

RFRE-10-7-4-2-A

exp43 Noesy

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solvent    cd3od      wp1      5089.4    arraydim  320
file
ACQUISITION    exp      ec2      140      1      phase
sfrq      587.862    rff1      1223.5    1
tn      0      H1      rfp1      0      2
at      0.213      dfrq      159.220
np      4096      dn      013
sw      9615.4      dpwr      31
fb      4050      dpr      0
hs      32      ddf      0
ss      16      dm      n
tpwr      39      dm      29412
pw      10.6      ddf      0
compht      1.0284      dseq      9.0
dl      1.010      dres      n
mix      0.930      homo      0
tof      587.4      dfrq2      0
nt      48      dn2      0
ct      40      dpwr2      1
gain      0.0025      dn2      n
gt1      711      dm2      29412
gzlv11      0.0020      dm2      1.0
hsq1      5333      dseq2      n
satnode      nnn      dres2      n
satpwr      -13      homo2      0
satdly      0      pf      0.057
scuba      n      pfs      not used
zsf1g      y      wfile      ft
alt_gnd      n      proc      4096
FLADS      n      fn      4096
il      n      math      f
ip      n      sfilter      not used
hs      nn      sorder      3
sspu1      y      sentaps      3
2D ACQUISITION
sw1      9615.4      pf1      0.013
n1      190      dres1      not used
phase      arrayed      wfile1      lp
DISPLAY      -120.1      proc1      lp
wp      5089.4      fn1      4096
vs      2671
ec      5
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fs      744.68
rff1      1223.5
rfp      0
th      2
ins      100.000
al cdc ph

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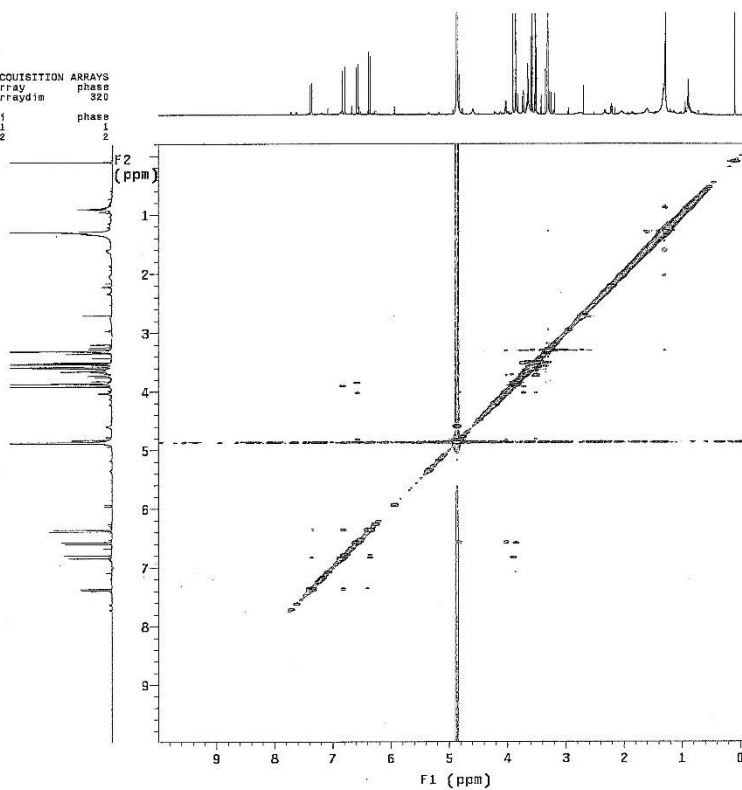


Figure S14. NOESY spectrum of reevesic acid (2) in CD₃OD

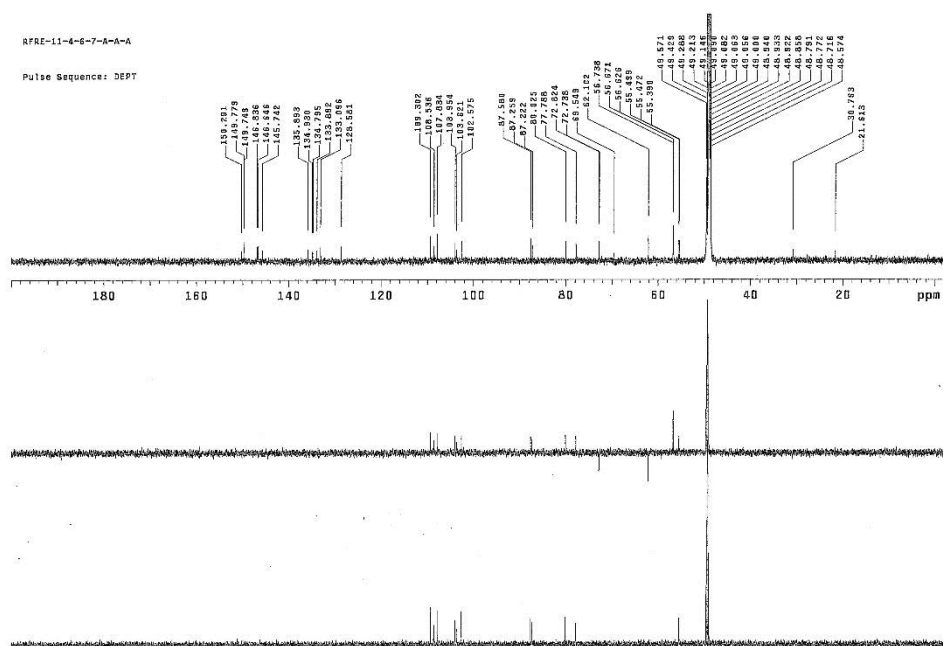


Figure S17. DEPT spectrum of reevesilignan (**3**) in CD₃OD at 150 MHz

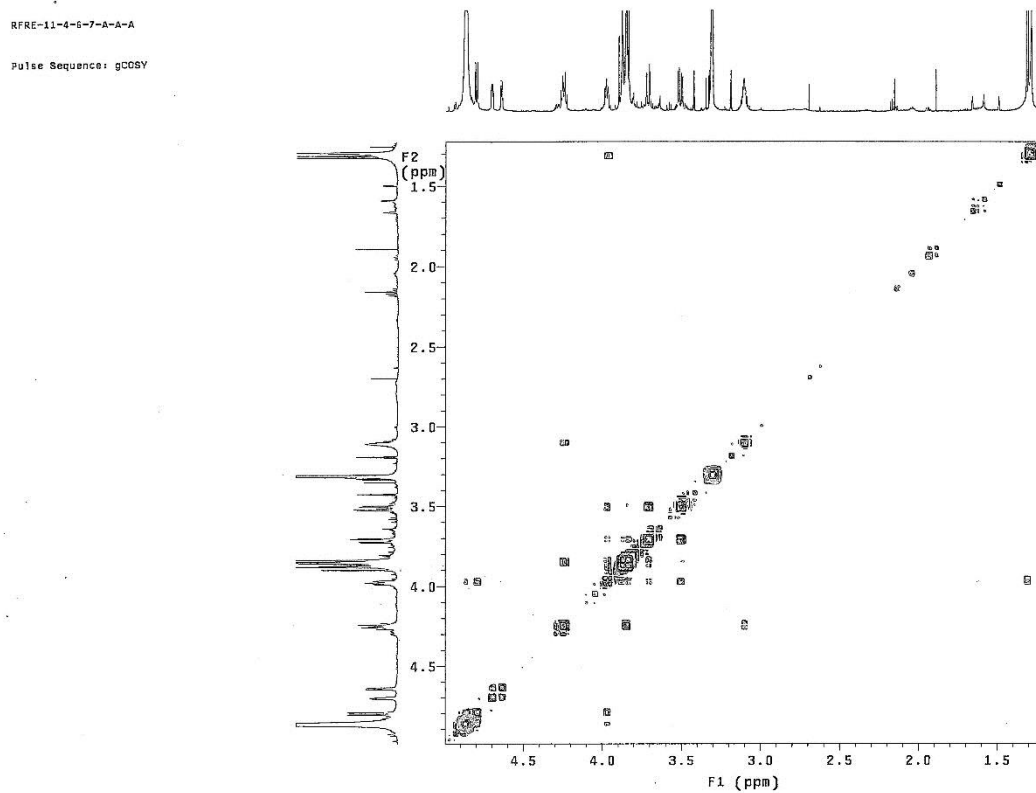


Figure S18. COSY spectrum of reevesilignan (**3**) in CD₃OD

RFRE-11-4-6-7-A-A-A
Pulse Sequence: gHSQCAD

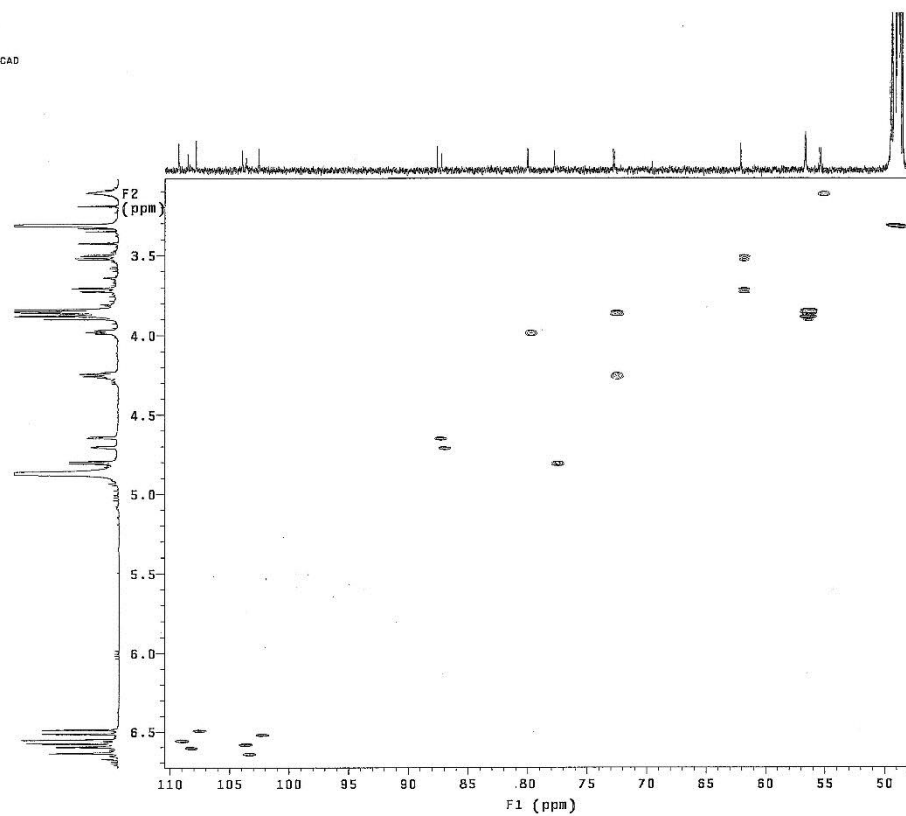


Figure S19. HSQC spectrum of reevesilignan (**3**) in CD₃OD

RFRE-11-4-6-7-A-A-A
Pulse Sequence: gHMBC

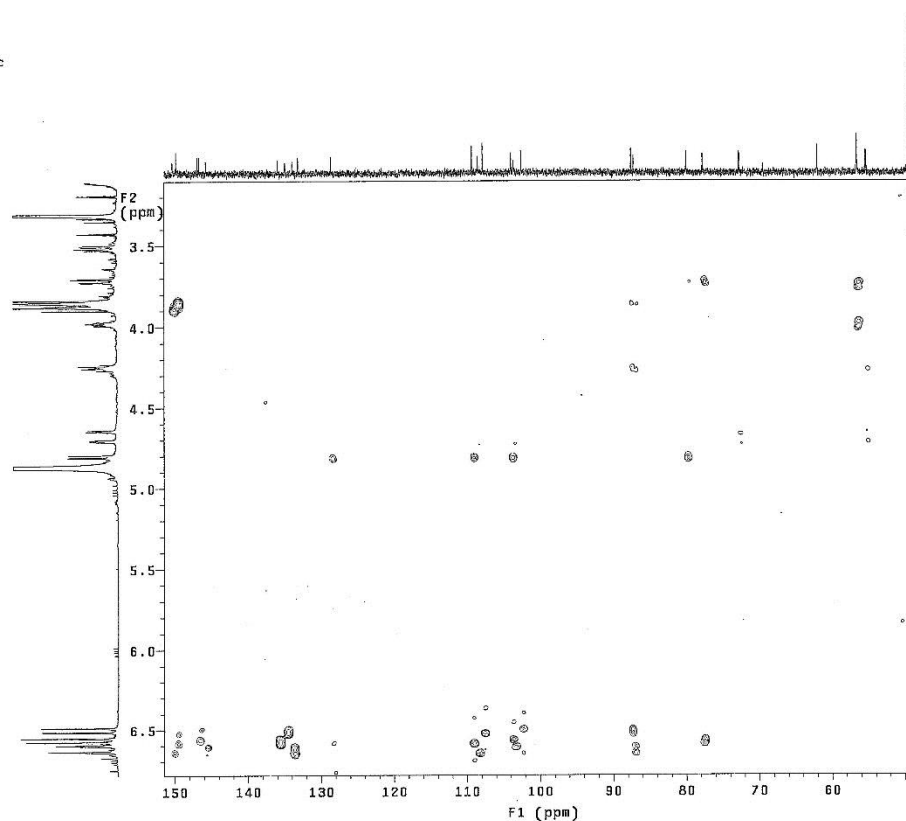


Figure S20. HMBC spectrum of reevesilignan (**3**) in CD₃OD

RFRE-11-4-6-7-A-A-A
Pulse Sequence: NOESY

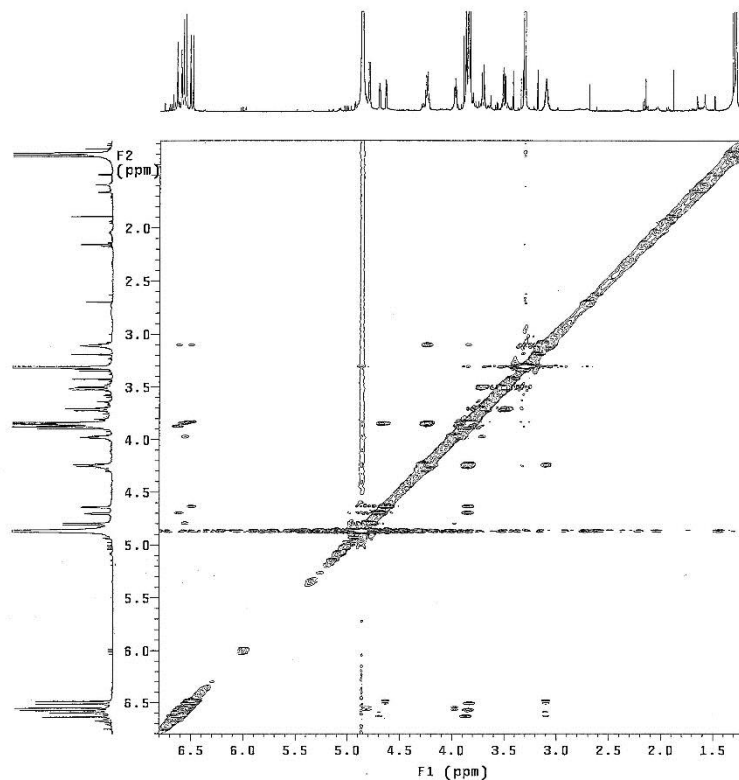


Figure S21. NOESY spectrum of reevesilignan (**3**) in CD₃OD

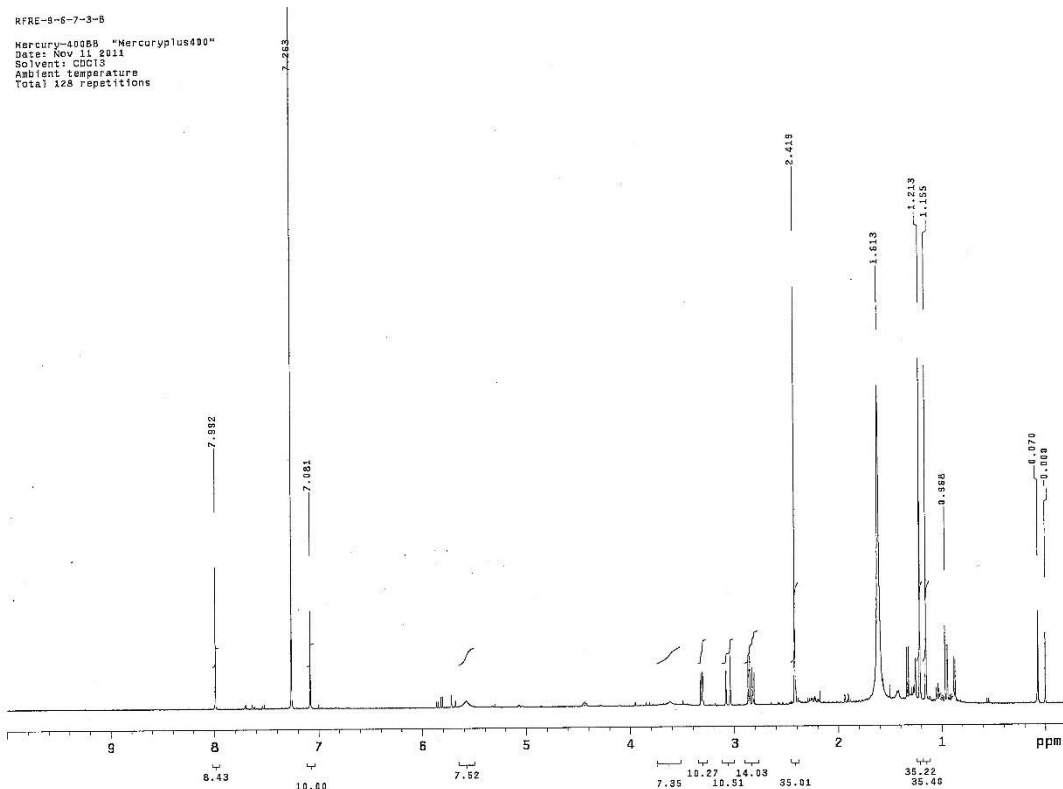


Figure S22. ¹H NMR spectrum of reevesiterpenol A (**4**) in CDCl₃ at 400 MHz

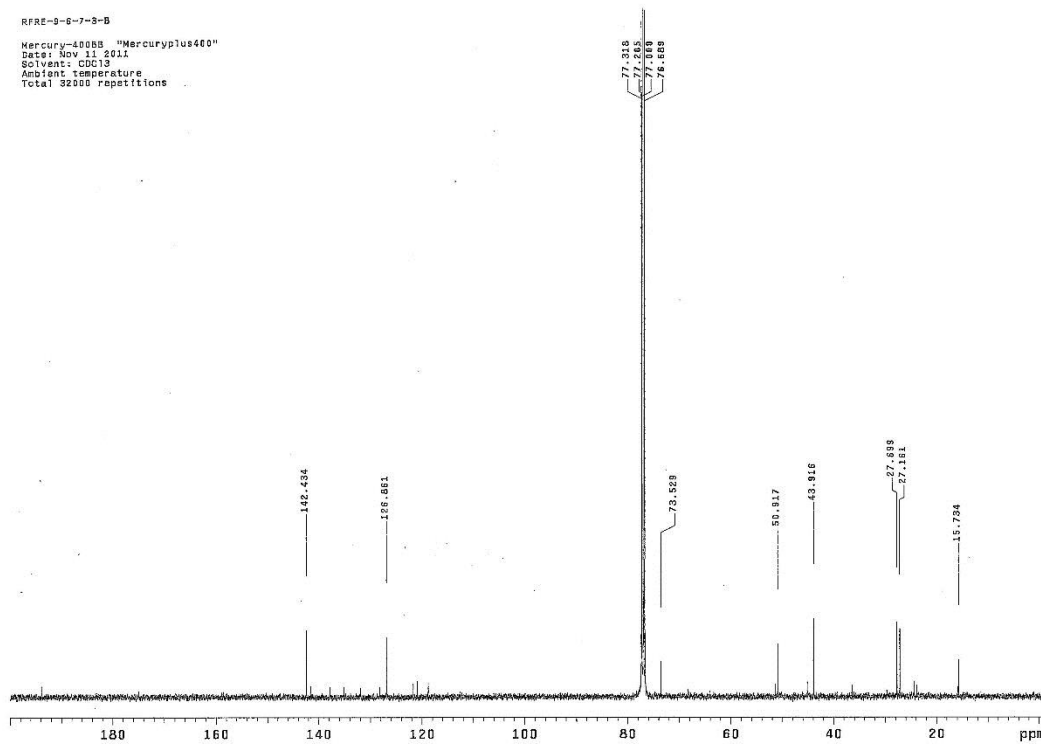


Figure S23. ^{13}C NMR spectrum of reevesiterpenol A (**4**) in CDCl_3 at 100 MHz

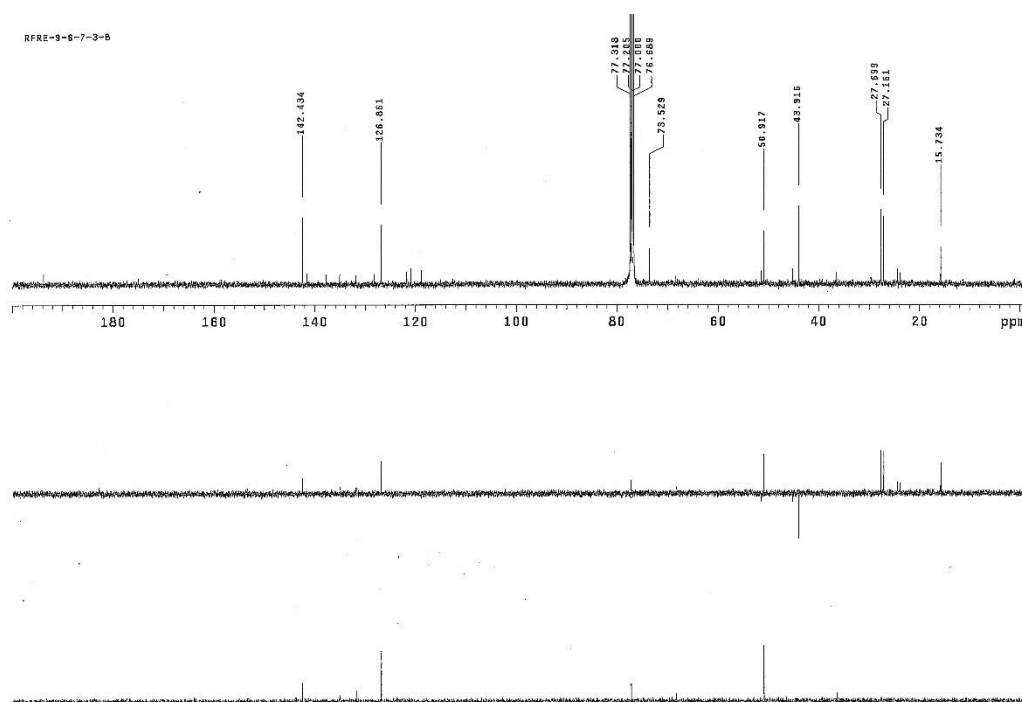


Figure S24. DEPT spectrum of reevesiterpenol A (**4**) in CDCl_3 at 100 MHz

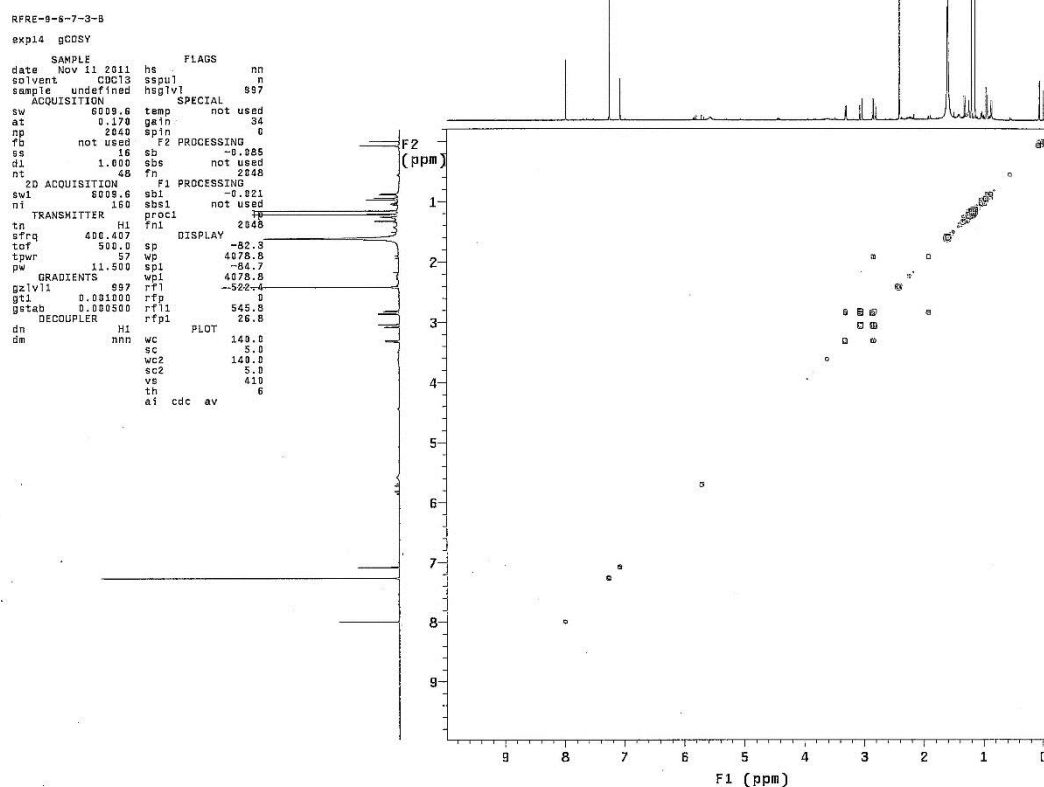


Figure S25. COSY spectrum of reevesiterpenol A (**4**) in CDCl₃

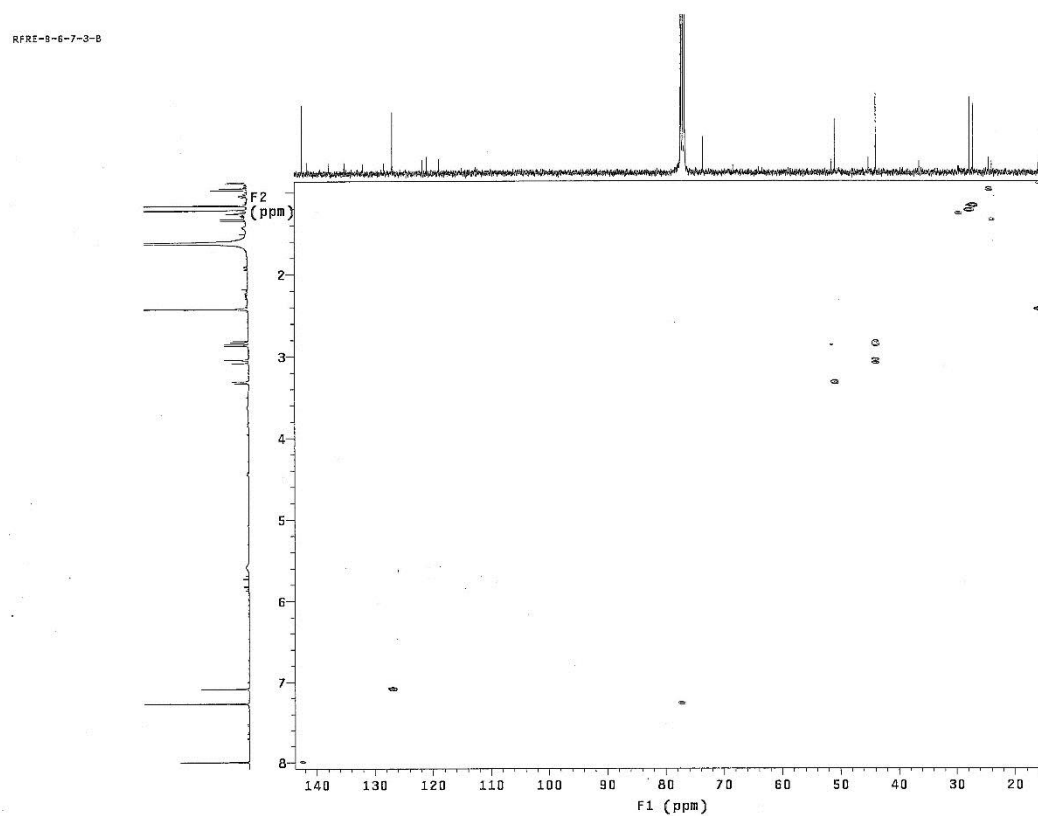


Figure S26. HSQC spectrum of reevesiterpenol A (**4**) in CDCl₃

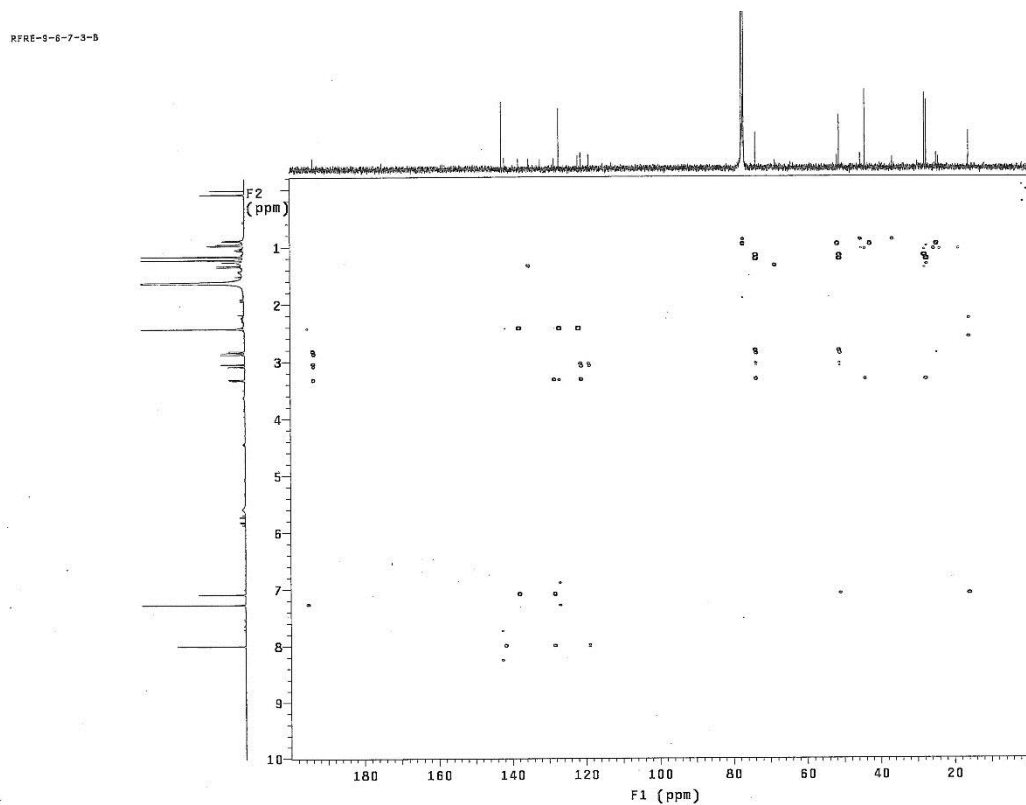


Figure S27. HMBC spectrum of reevesiterpenol A (4) in CDCl_3

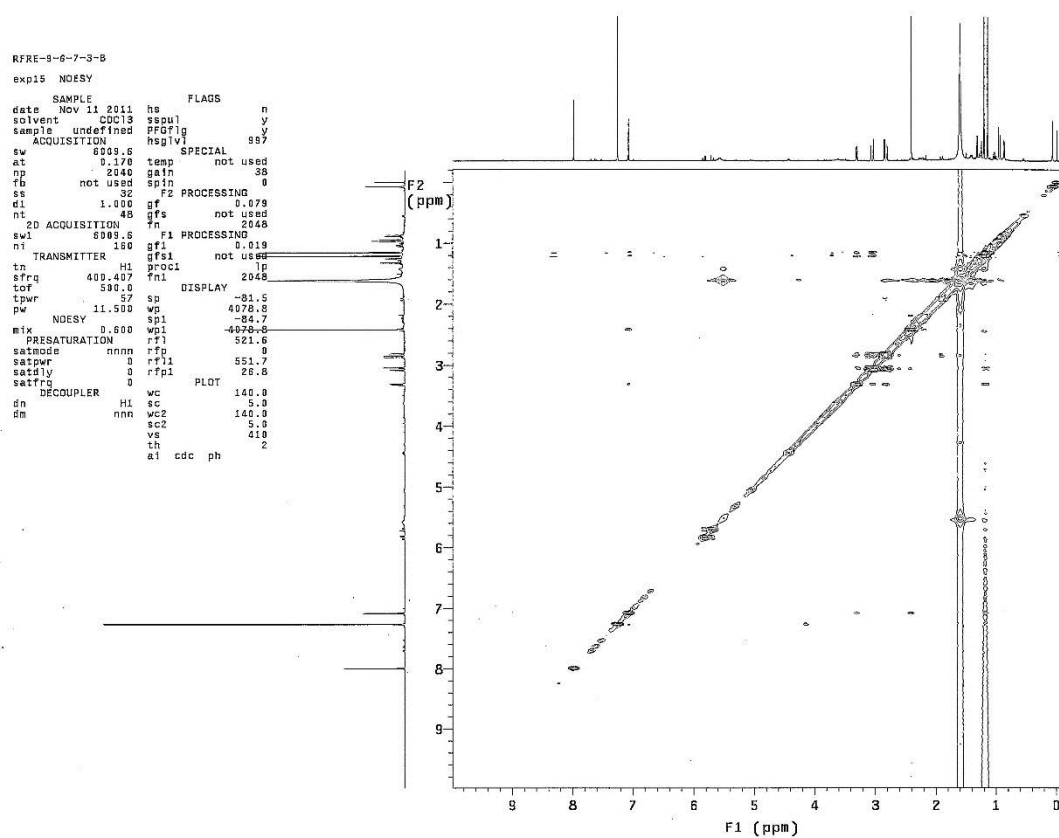


Figure S28. NOESY spectrum of reevesiterpenol A (4) in CDCl_3

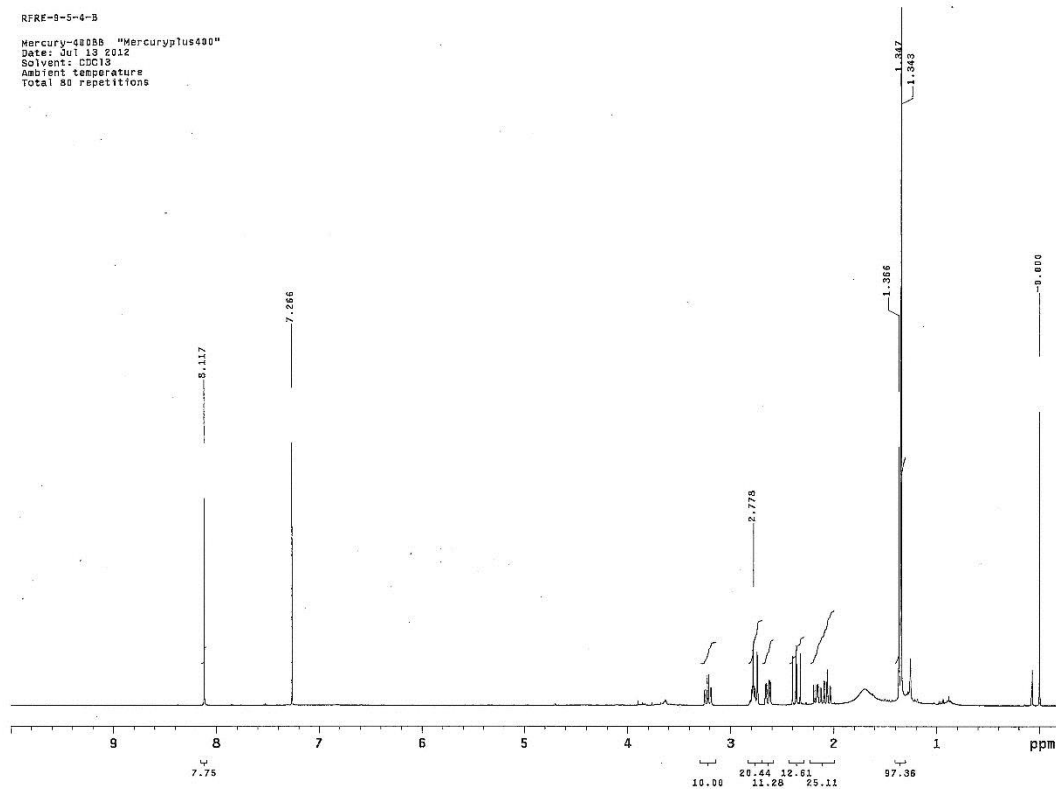


Figure S29. ^1H NMR spectrum of reevesiterpenol B (**5**) in CDCl_3 at 400 MHz

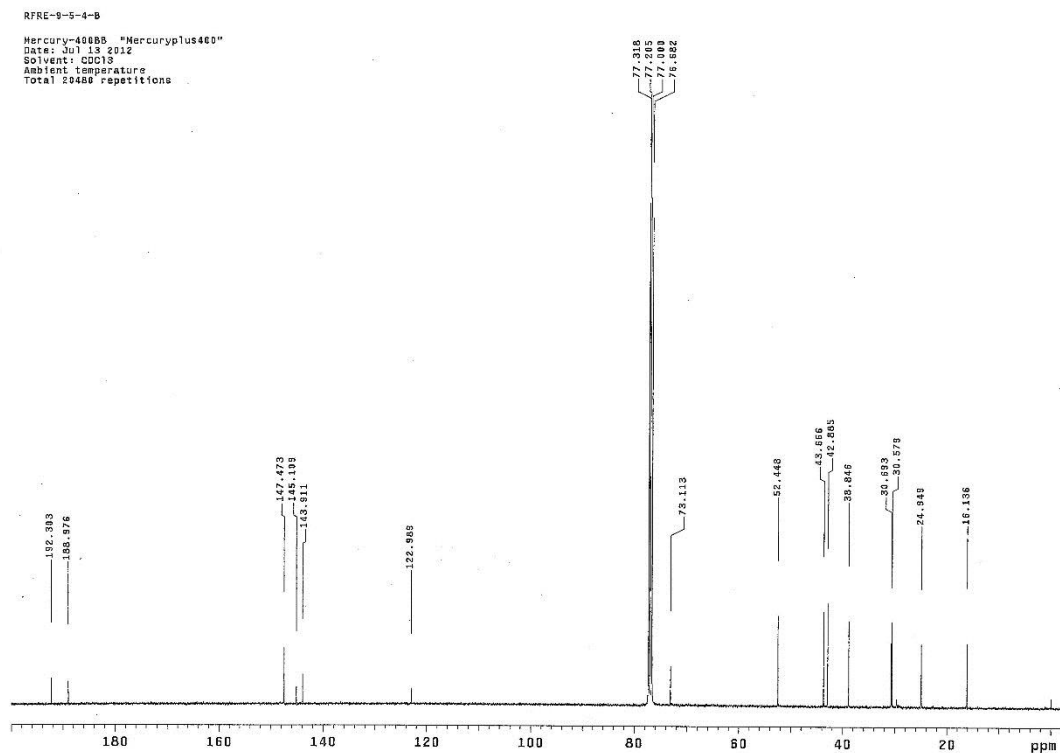


Figure S30. ^{13}C NMR spectrum of reevesiterpenol B (**5**) in CDCl_3 at 100 MHz

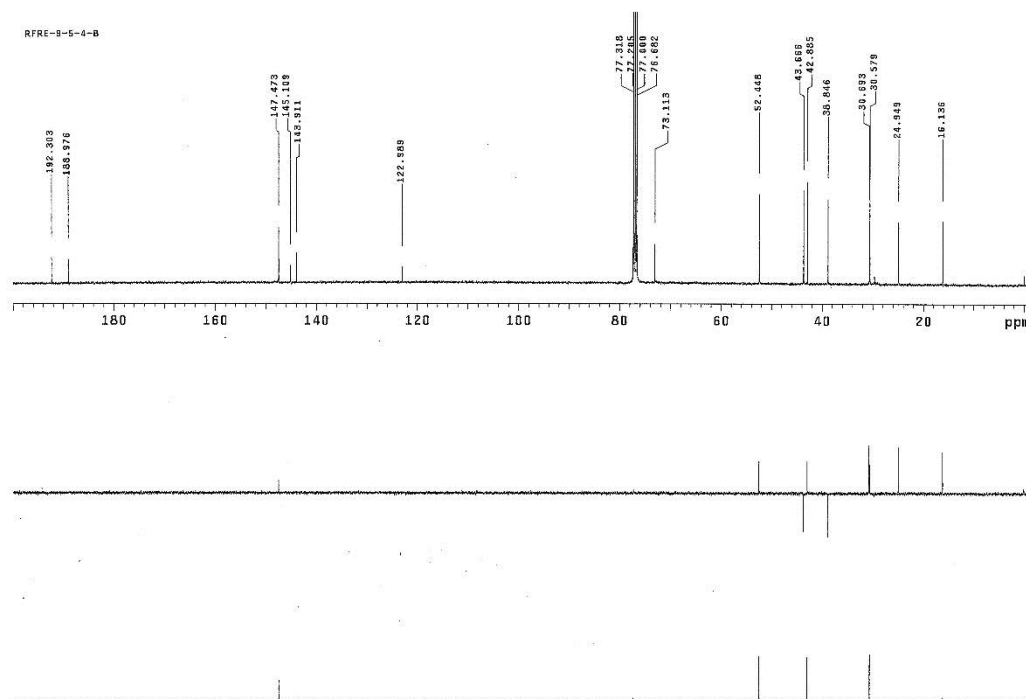


Figure S31. DEPT spectrum of reevesiterpenol B (**5**) in CDCl_3 at 100 MHz

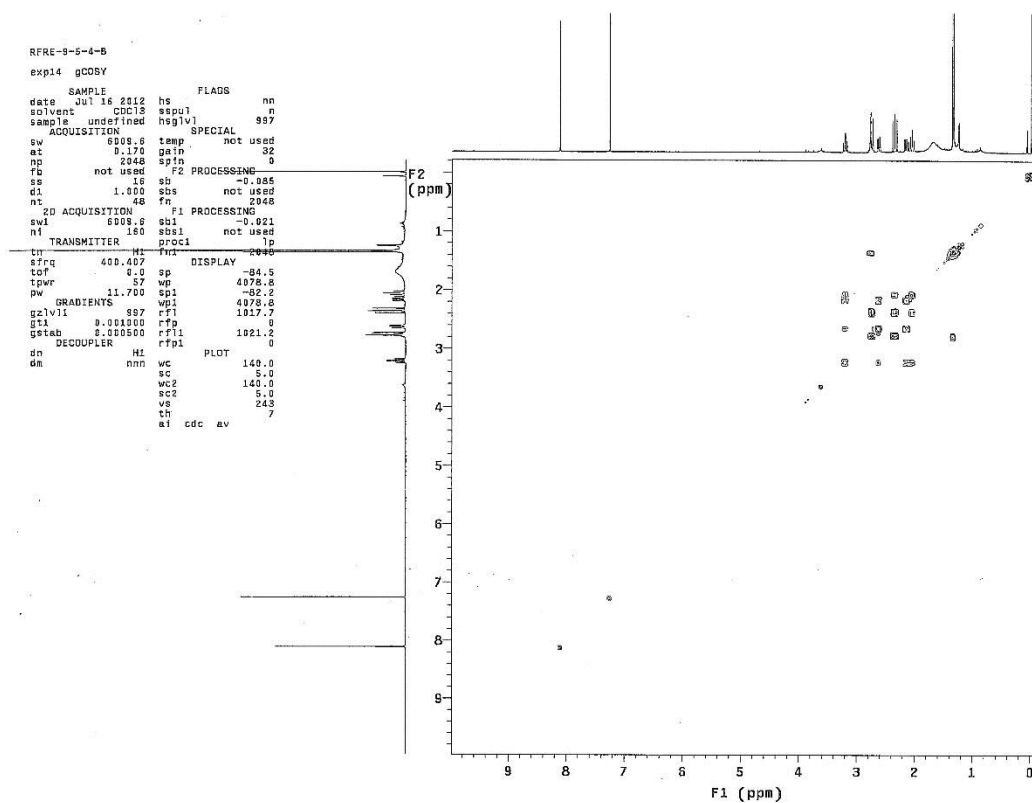


Figure S32. COSY spectrum of reevesiterpenol B (**5**) in CDCl_3

RFRE-9-5-4-B

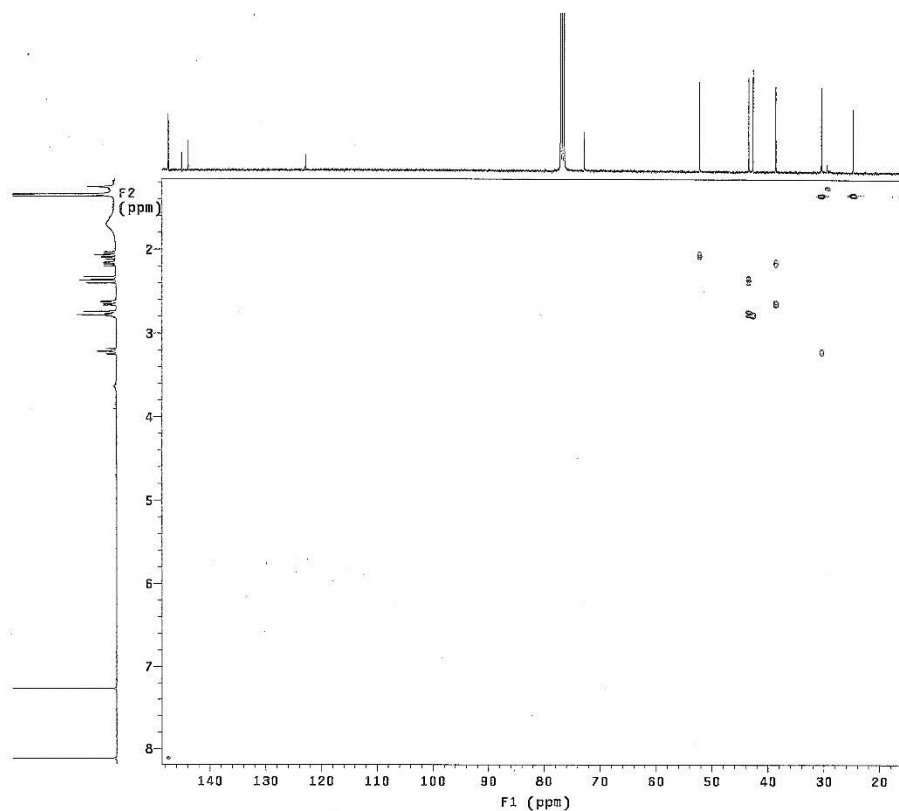


Figure S33. HSQC spectrum of reevesiterpenol B (**5**) in CDCl_3

RFRE-9-5-4-B

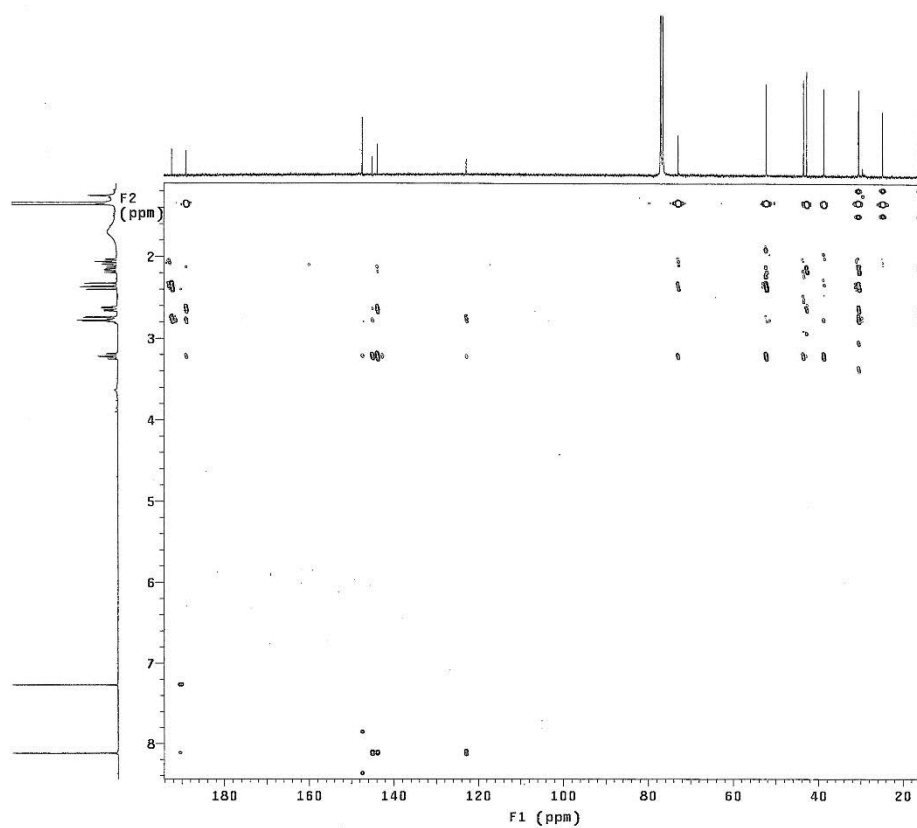


Figure S34. HMBC spectrum of reevesiterpenol B (**5**) in CDCl_3

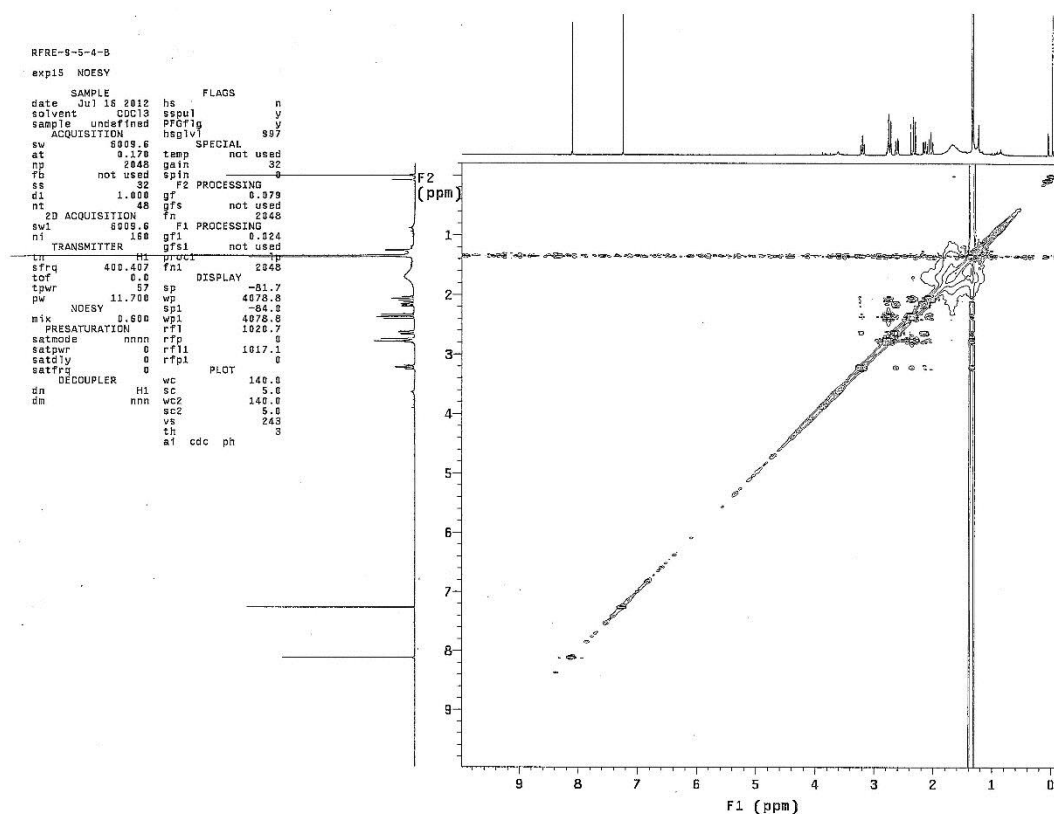


Figure S35. NOESY spectrum of reevesiterpenol B (**5**) in CDCl_3

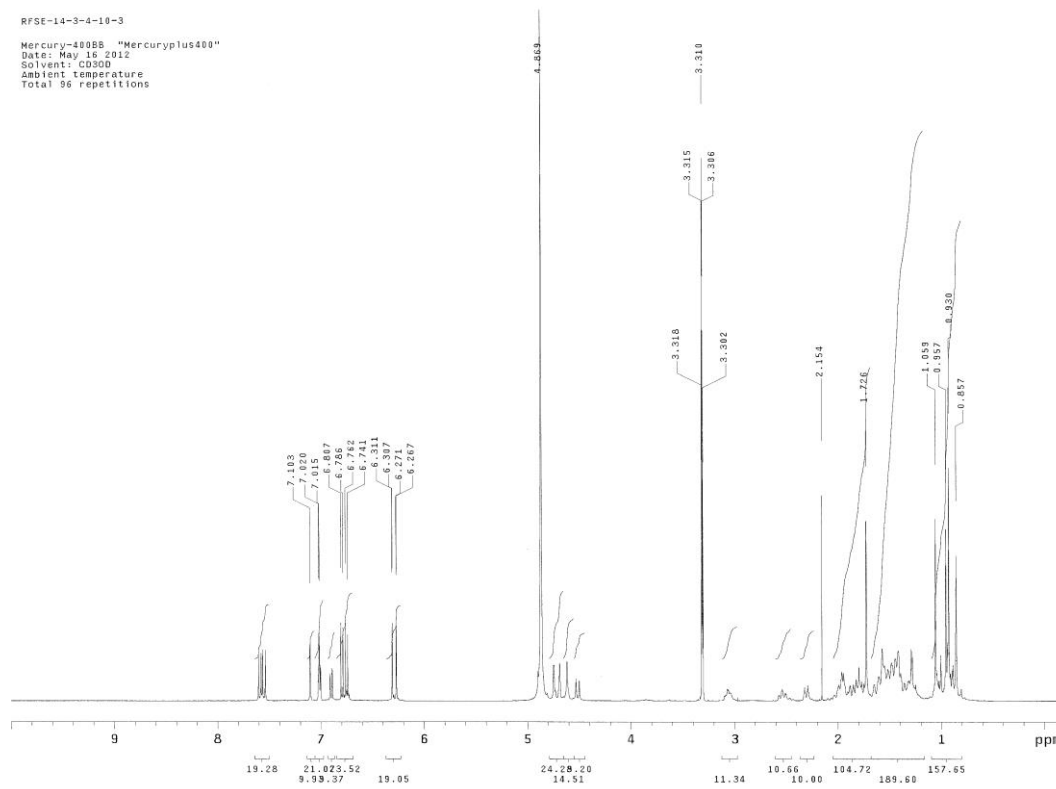


Figure S36. ^1H NMR spectrum of $3\alpha,27$ -di-*O*-*trans*-caffeoylbetulnic acid (**6**) in CD_3OD at 400 MHz

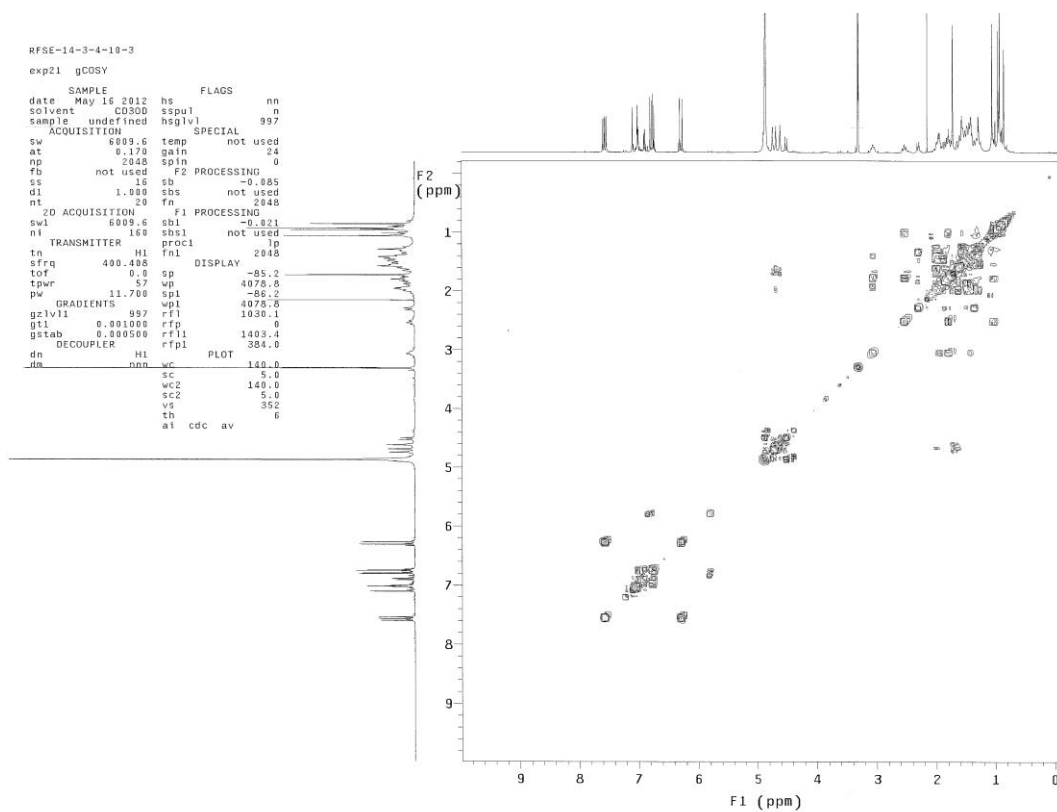


Figure S39. COSY spectrum of 3 α ,27-di-*O*-*trans*-caffeoylbetulnic acid (**6**) in CD₃OD

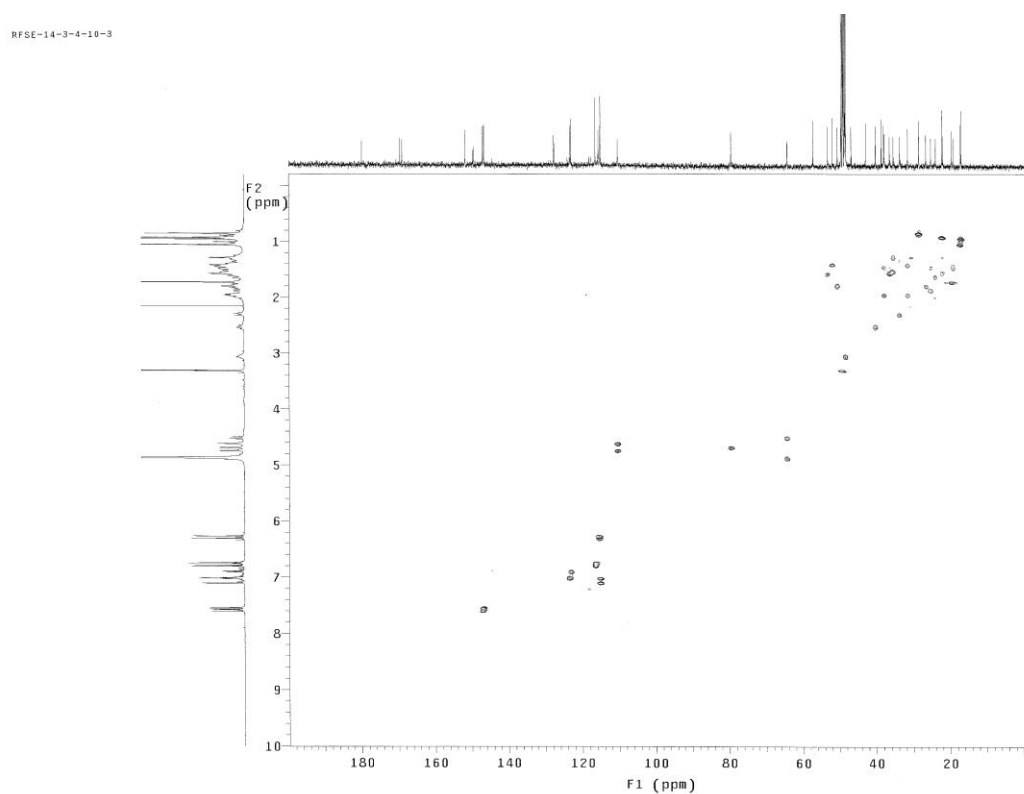


Figure S40. HSQC spectrum of 3 α ,27-di-*O*-*trans*-caffeoylbetulnic acid (**6**) in CD₃OD

RFSE-14-3-4-10-3

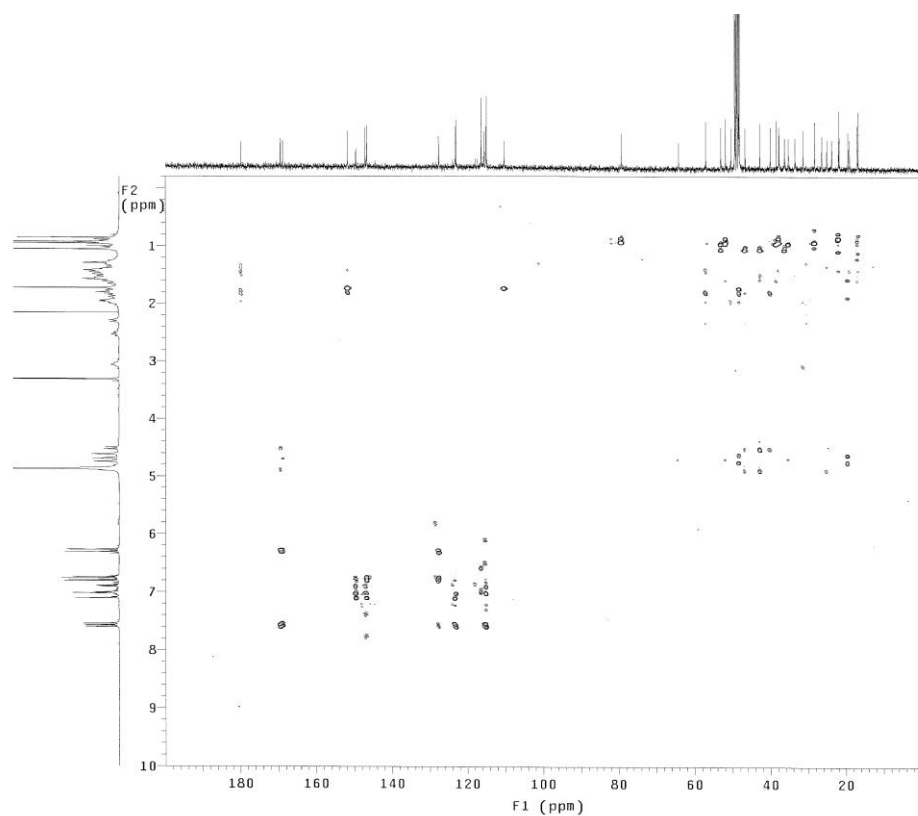


Figure S41. HMBC spectrum of 3 α ,27-di-*O*-*trans*-caffeoylbetulinic acid (**6**) in CD₃OD

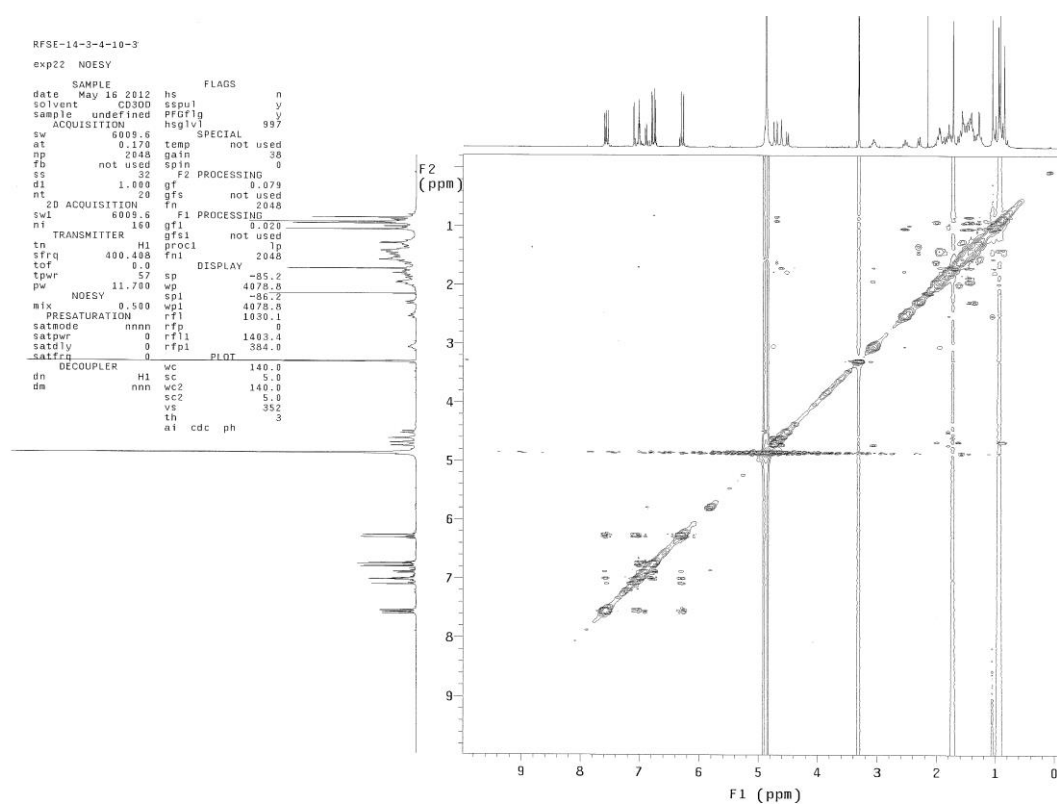


Figure S42. NOESY spectrum of 3 α ,27-di-*O*-*trans*-caffeoylbetulinic acid (**6**) in CD₃OD