

Different types of components obtained from *Monascus purpureus* with neuroprotective and anti-inflammatory potentials

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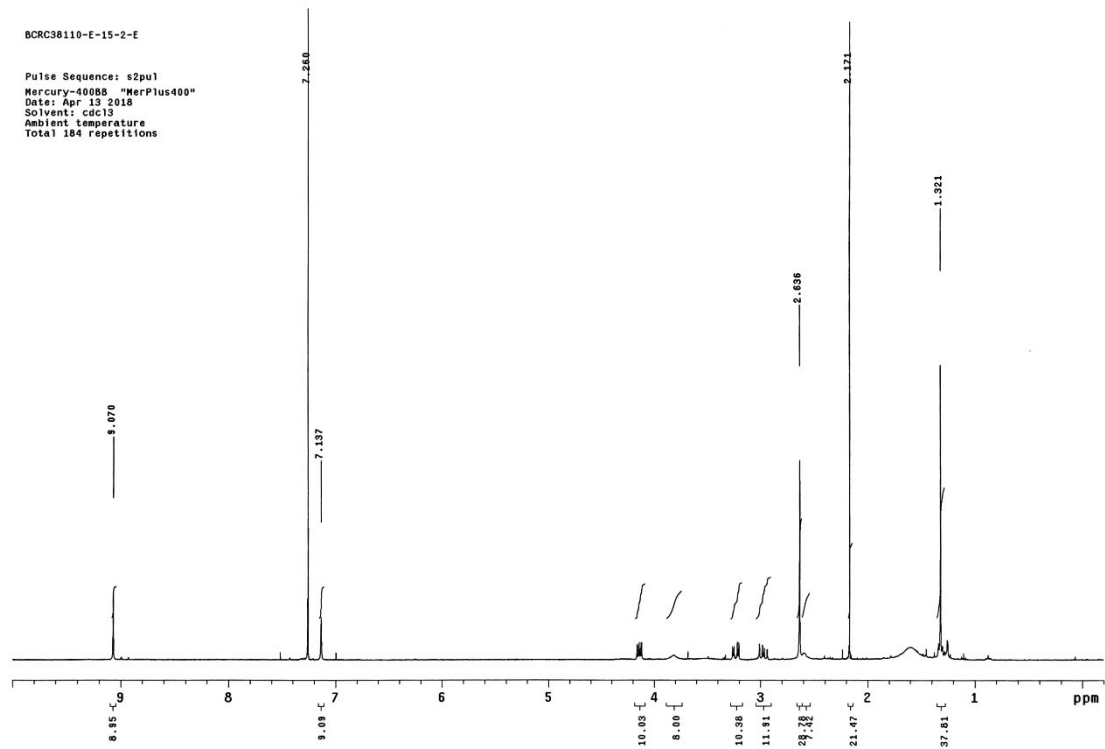


Figure S1. ^1H NMR spectrum of monapyridine A (**1**) in CDCl_3 at 400 MHz

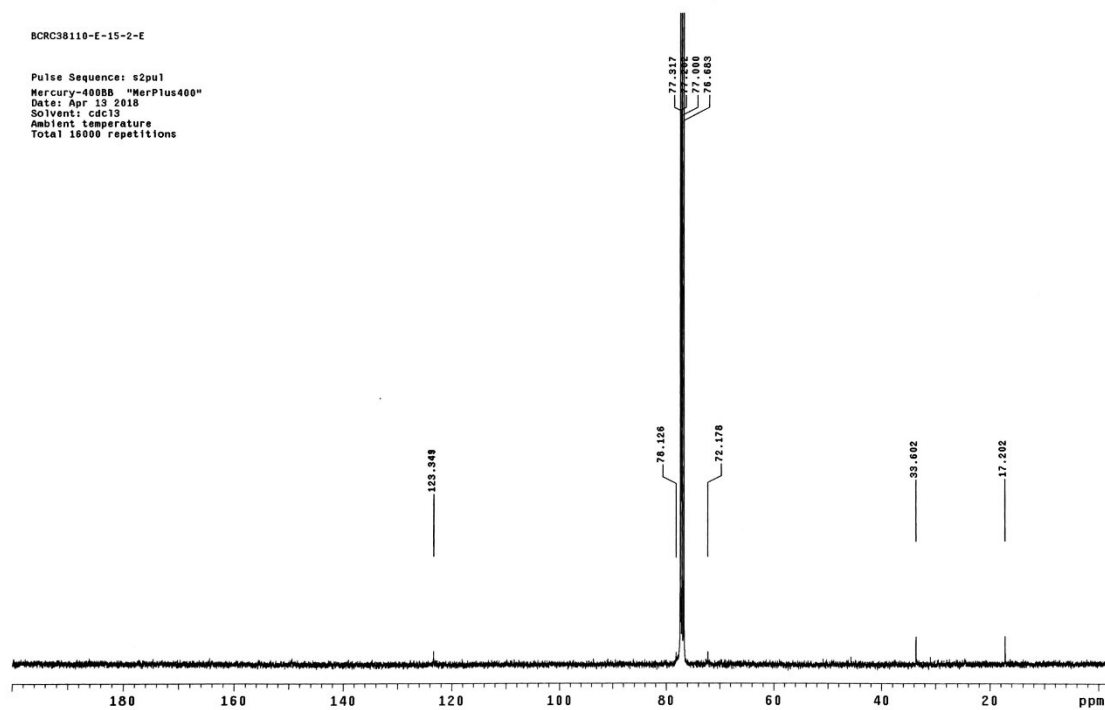


Figure S2. ^{13}C NMR spectrum of monapyridine A (**1**) in CDCl_3 at 100 MHz

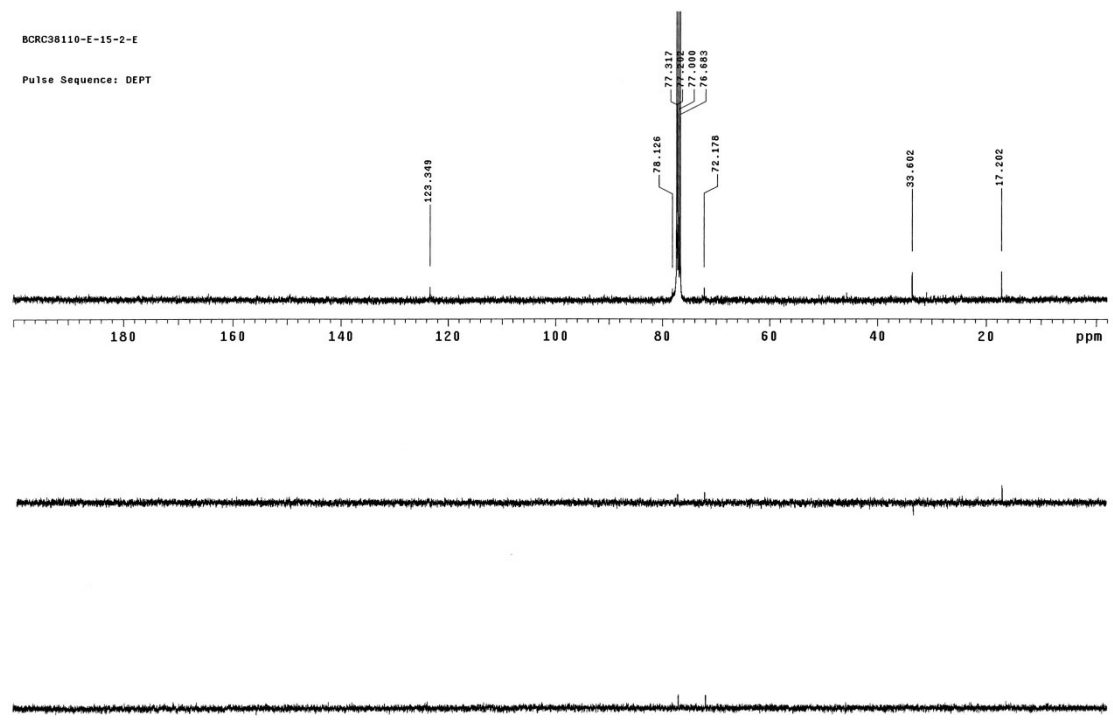


Figure S3. DEPT spectrum of monapyridine A (1)

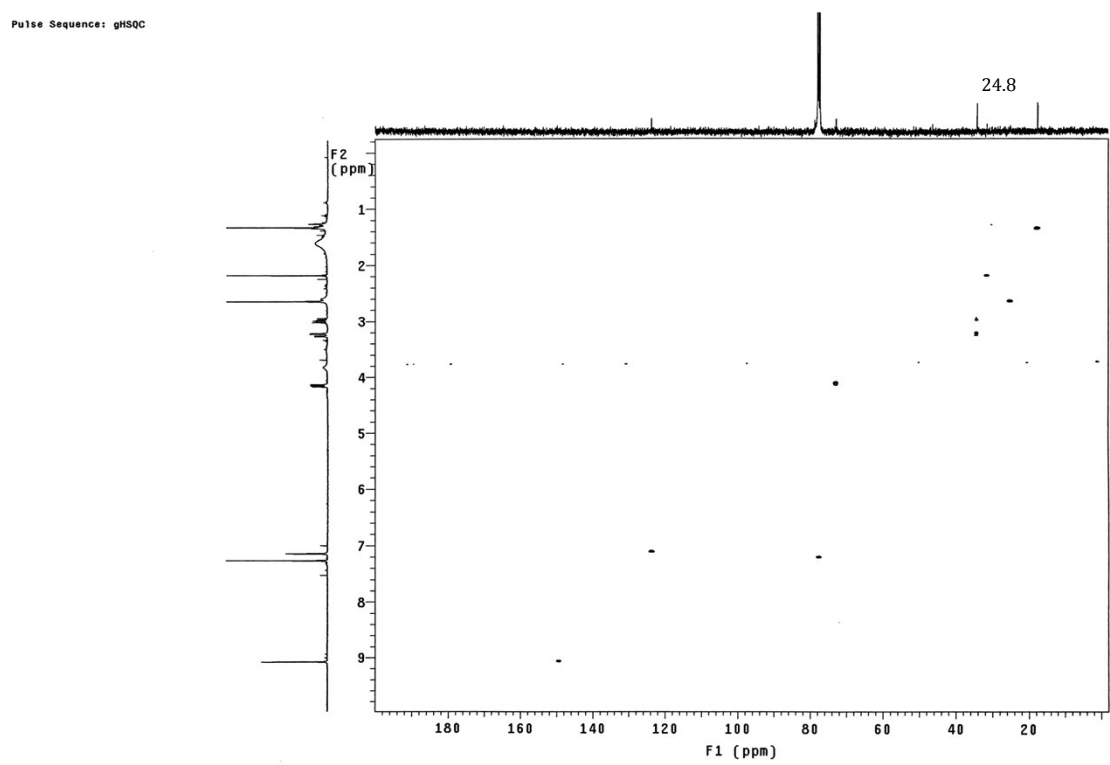


Figure S4. HSQC spectrum of monapyridine A (1)

BCRC38110-E-15-2-E

exp14 gCOSY

```
SAMPLE          FLAGS
date Apr 13 2018 hs nn
solvent cdc13 sspul y
sample          hsglv1 1224
ACQUISITION    SPECIAL
sv 840.3 temp not used
at 0.150 gain 39
np 1920 spin 0
fb not used F2 PROCESSING 0
ss 32 sb -0.075
dl 1.000 sbs not used
nt 48 fn 4096
2D ACQUISITION F1 PROCESSING
sw1 640.3 sb1 -0.020
nl 160 sbs1 not used
d2 0 proc1 1p
PRESATURATION  fn1 4096
satmode n DISPLAY -80.2
wet n sp -4081.5
TRANSMITTER n wp 4081.5
tn H1 sp1 -80.2
sfrq 400.001 wp1 4081.5
tof 600.0 rf1 568.4
tpwr 61 rfp 0
pw 11.600 rf11 568.4
GRADIENTS      rfp1 0
gz1w1e 1028 PLOT
g1e 0.001000 wc 140.0
Edratio 1.000 sc 5.0
gstab 0.000500 w2 140.0
DECOUPLER      sc2 5.0
dn C13 vs 100
dm nm tn 8
a1 cdc av 8
```

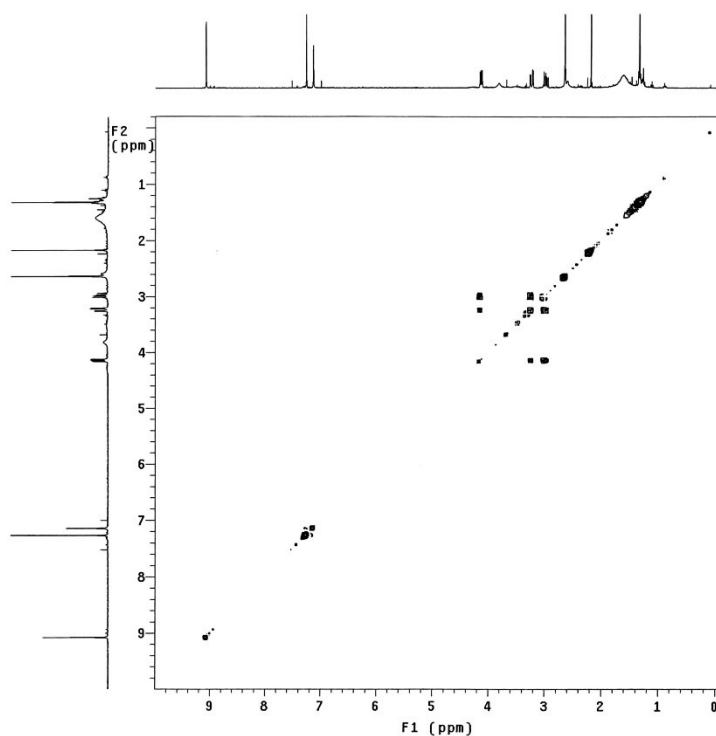


Figure S5. COSY spectrum of monapyridine A (1)

Pulse Sequence: gHMBC

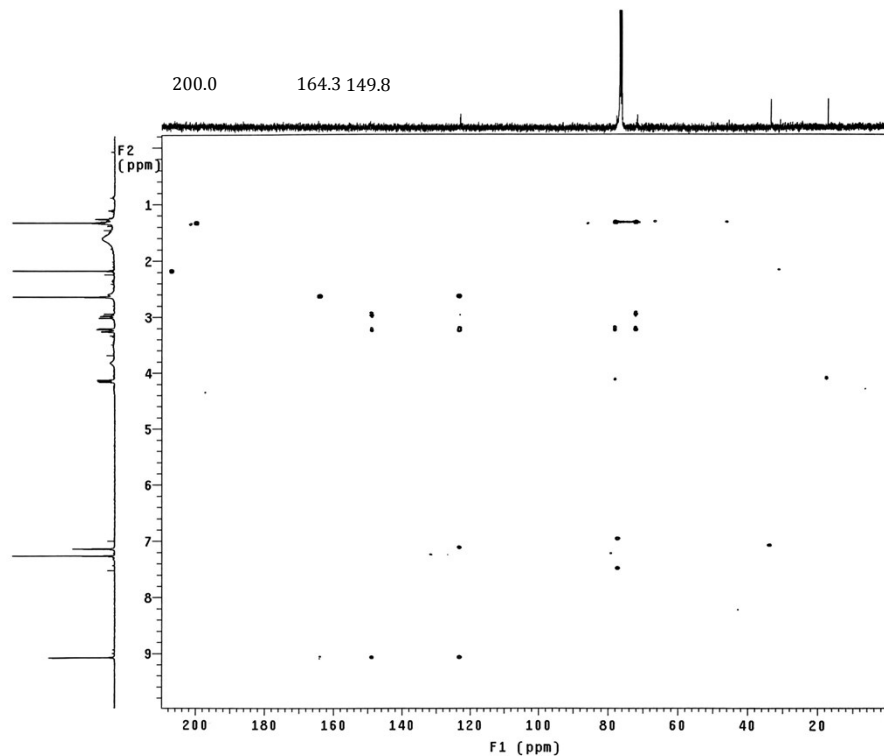


Figure S6. HMBC spectrum of monapyridine A (1)

BCRC38110-E-15-2-E

exp15 NOESY

```
SAMPLE          FLAGS
date Apr 13 2018 hs nn
solvent cdc13 sspu1 y
sample PFOFg y
ACQUISITION     SPECIAL 1224
sv 8410.3
at 0.150 temp not used
np 1920 gain 38
fb not used spin 0
ss 32 F2 PROCESSING
d1 1.000 gr 0.069
nt 48 gfs not used
2D ACQUISITION  fn 4096
sw1 8410.3 F1 PROCESSING
n1 160 gf1 0.020
TRANSMITTER     h1 not used
tn H1 proc1 1p
sfrq 400.401 fn1 4096
tof 600.0 DISPLAY
tpwr 51 sp -80.2
pw 11.600 wp 5483.8
NOESY          sp1 -80.2
mixN           wpt 5483.8
PRESATURATION  n rf1 568.4
satmode       n rfp 0
wet           n rf11 568.4
DECOUPLER     C13 rfp1 0
dn nnn
dm          wc 140.0
           sc 5.0
           wc2 140.0
           sc2 5.0
           vs 100
           th
           al cdc ph 2
```

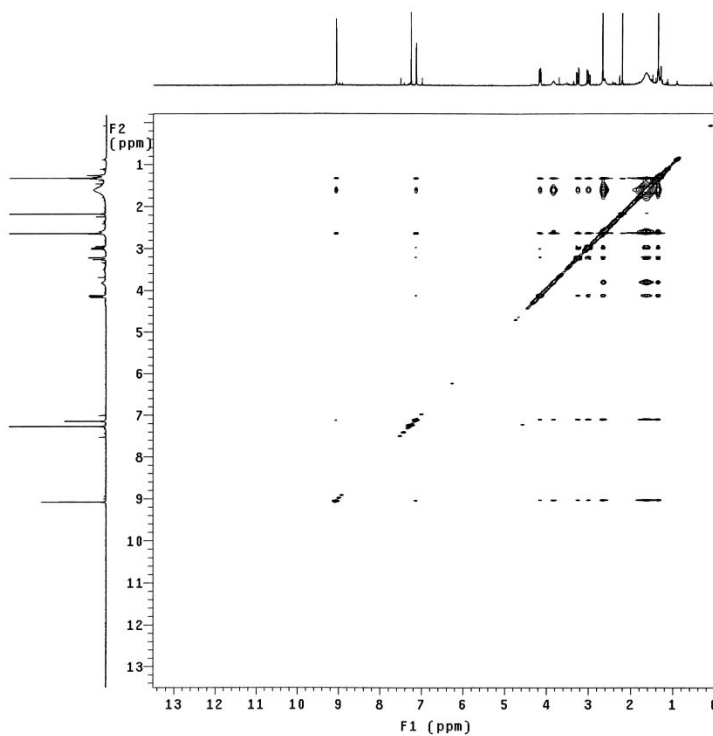


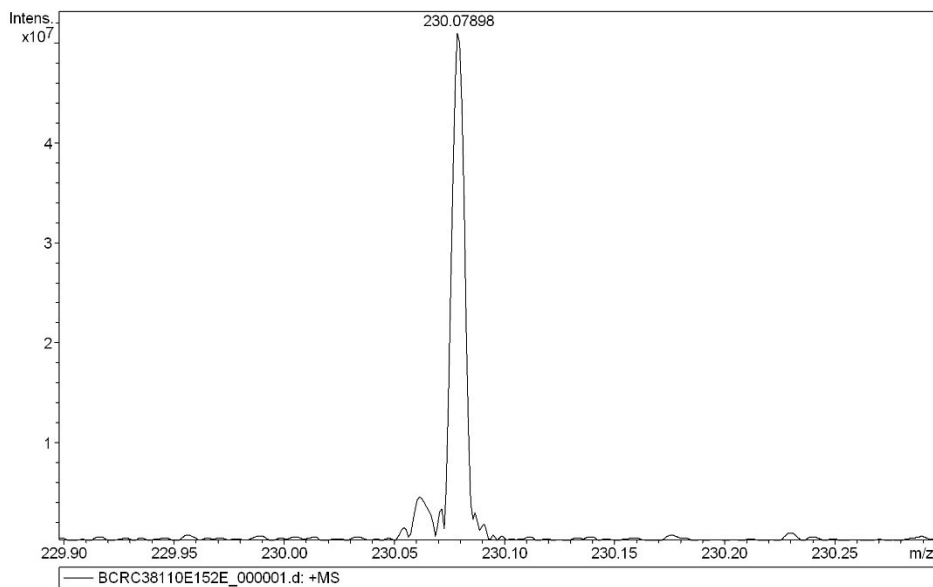
Figure S7. NOESY spectrum of monapyridine A (1)

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\7\BCRC38110E152E_000001.d
Method broadband first signal
Sample Name BCRC48110-E-15-2-E
Comment ESI Positive

3/12/2018 3:51:26 PM
Operator: YU HSIAO-CHING
Instrument: BRUKER FT-MS solarix



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
230.07898	1	C 11 H 13 N Na O 3	100.00	230.07876	-0.22	-0.94	8.4	5.5	even	ok

Figure S8. HRESIMS spectrum of monapyridine A (1)

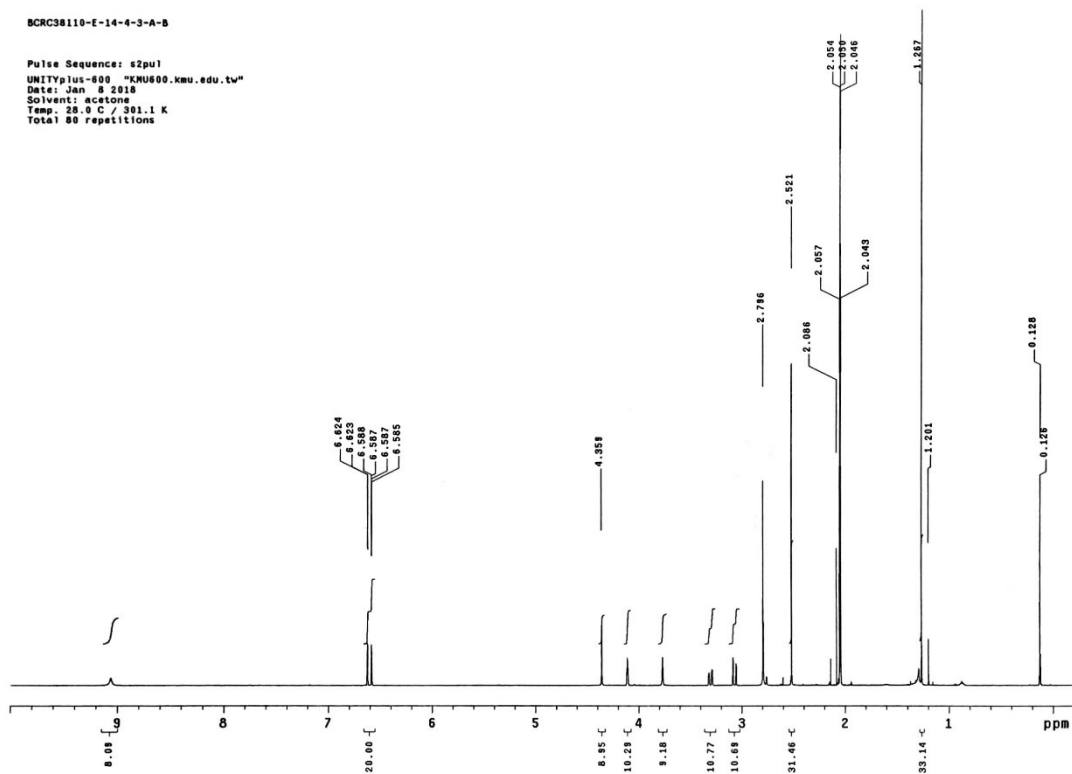


Figure S9. ^1H NMR spectrum of monatetralone A (**2**) in acetone- d_6 at 600 MHz

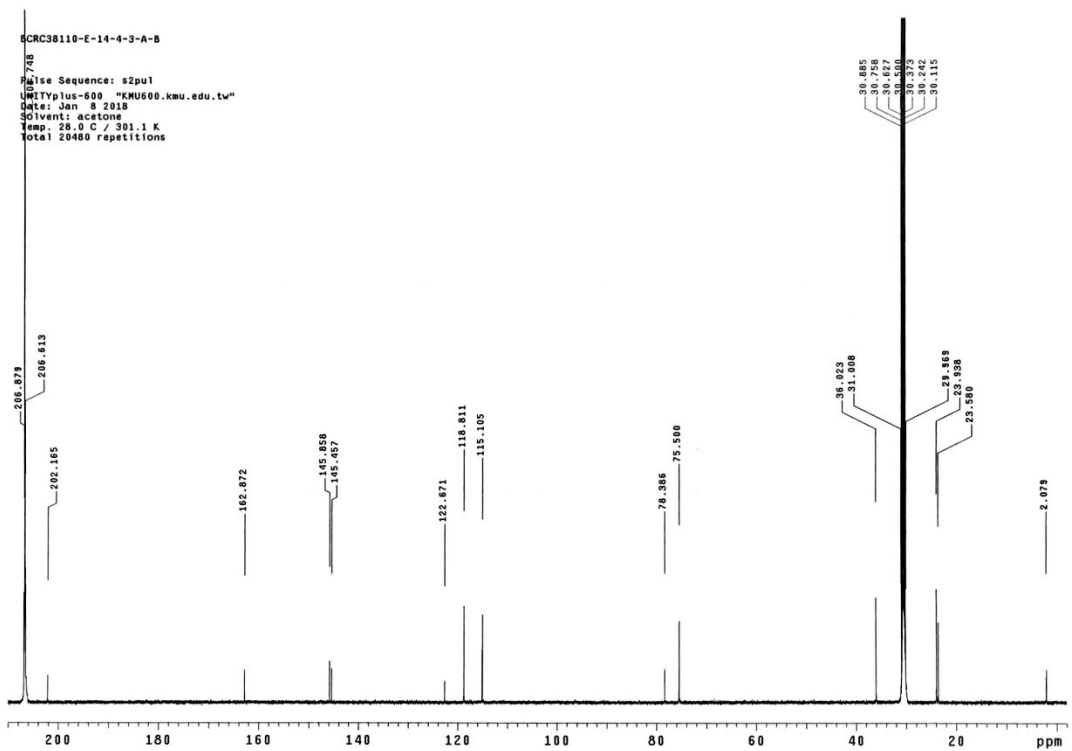


Figure S10. ^{13}C NMR spectrum of monatetralone A (**2**) in acetone- d_6 at 125 MHz

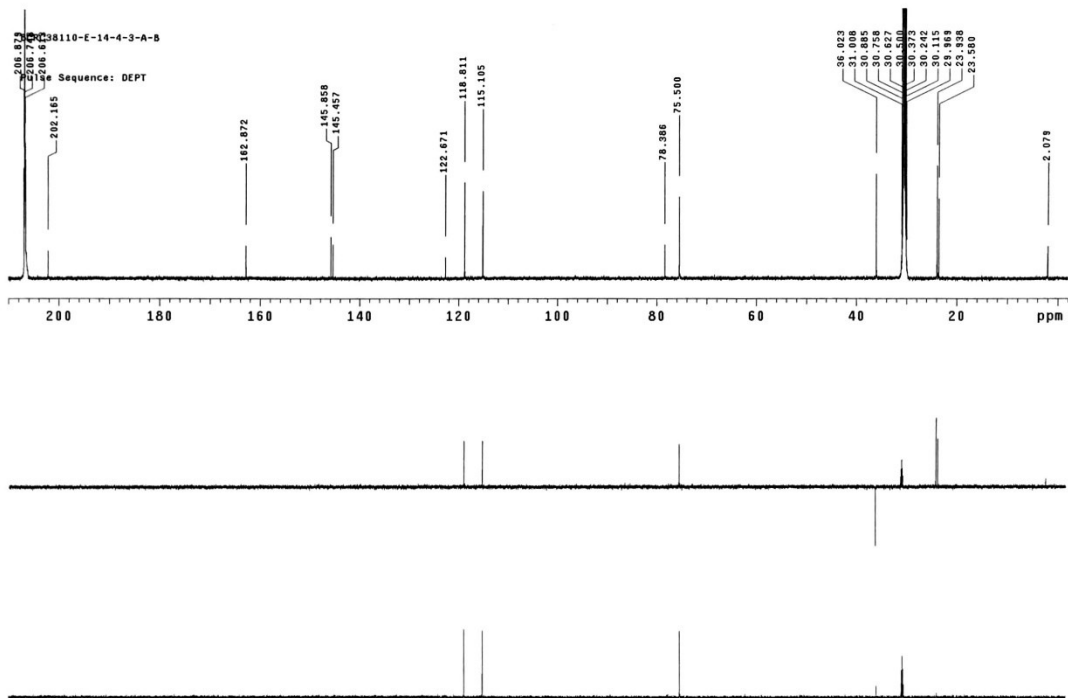


Figure S11. DEPT spectrum of monatetralone A (2)

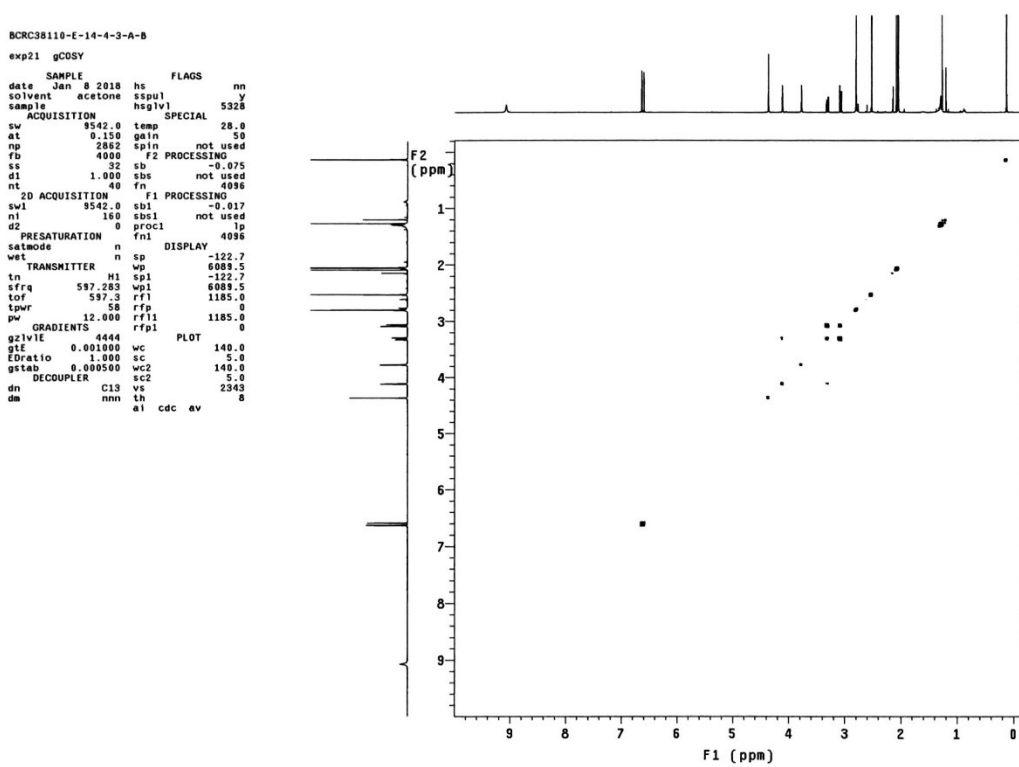


Figure S12. COSY spectrum of monatetralone A (2)

BCRC38110-E-14-4-3-A-B
Pulse Sequence: gHMBCAD

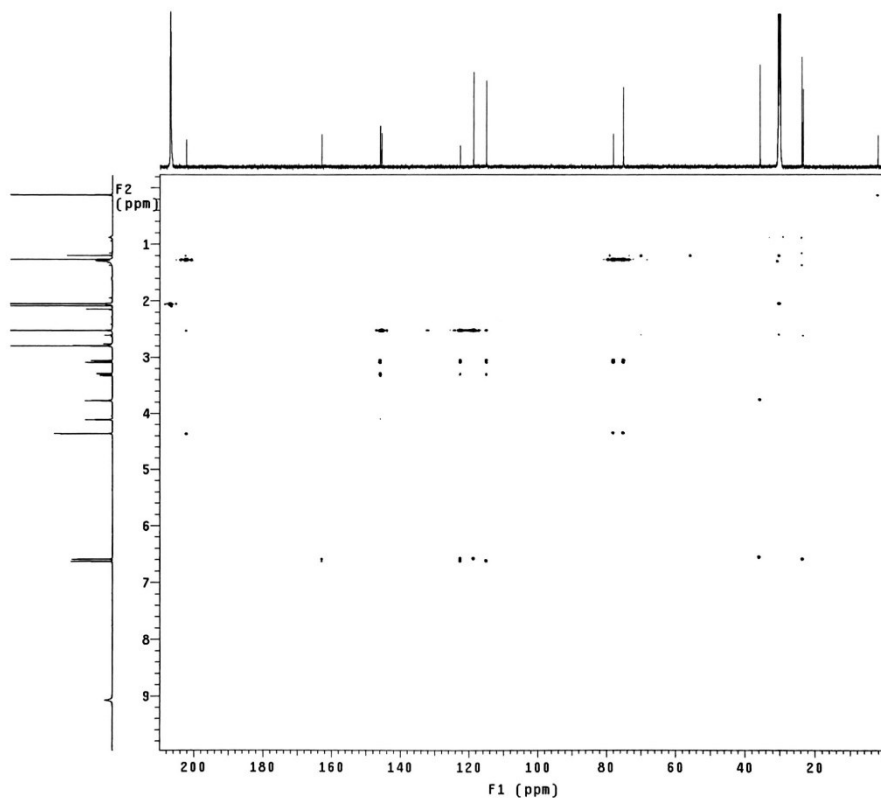


Figure S13. HMBC spectrum of monatetralone A (2)

BCRC38110-E-14-4-3-A-B
exp22 NOESY

SAMPLE		hs	FLAGS	nn
date	Jan 8 2018	hs		
solvent	acetone	sspu1	y	
sample		PFQFg	y	
ACQUISITION		hsq1v1	5328	
sw	9542.0	SPECIAL		
at	0.150	temp	28.0	
np	2882	gain	46	
rb	4000	spin	not used	
ss	32	F2	PROCESSING	
d1	1.500	gf	0.069	
nt	40	gfs	not used	
2D ACQUISITION		fn	4096	
swi	9542.0	f1	PROCESSING	
ni	160	gf1	0.015	
TRANSMITTER		gfs1	not used	
tn		h1	1p	
sfrs	597.283	fn1	4096	
tof	597.3	DISPLAY	-122.7	
tpwr	58	sp	6089.5	
pw	12.000	wp	-122.7	
NOESY		sp1	6089.5	
mixN	0.600	vp1	1185.0	
PRESATURATION		rf1	1185.0	
satmode	n	rff	0	
wet	n	rf1	1185.0	
DECOUPLER		rfp1	0	
dn	C13	PLOT		
dm	nnn	wc	140.0	
		sc	5.0	
		wc2	140.0	
		sc2	5.0	
		vs	2343	
		tn	4	
		ai	cdc ph	

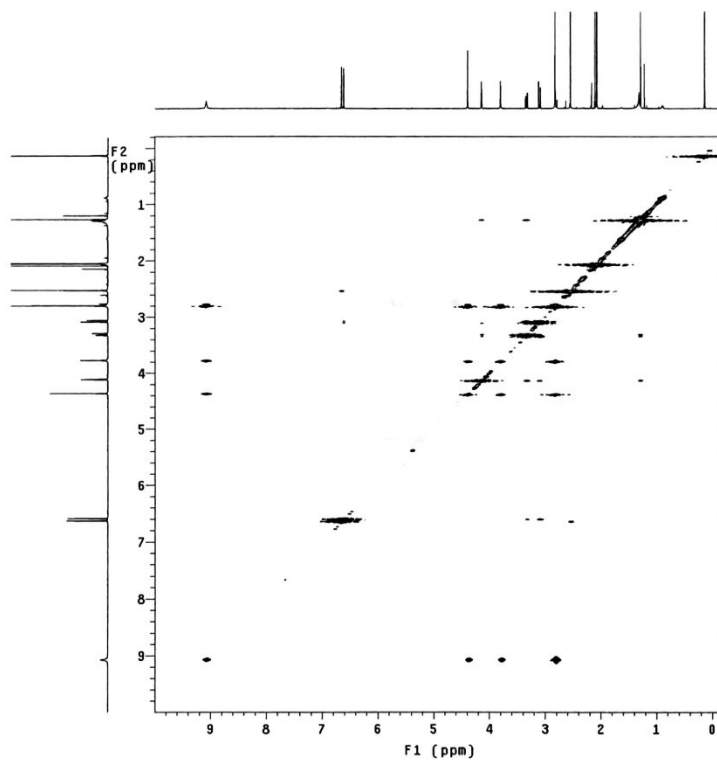


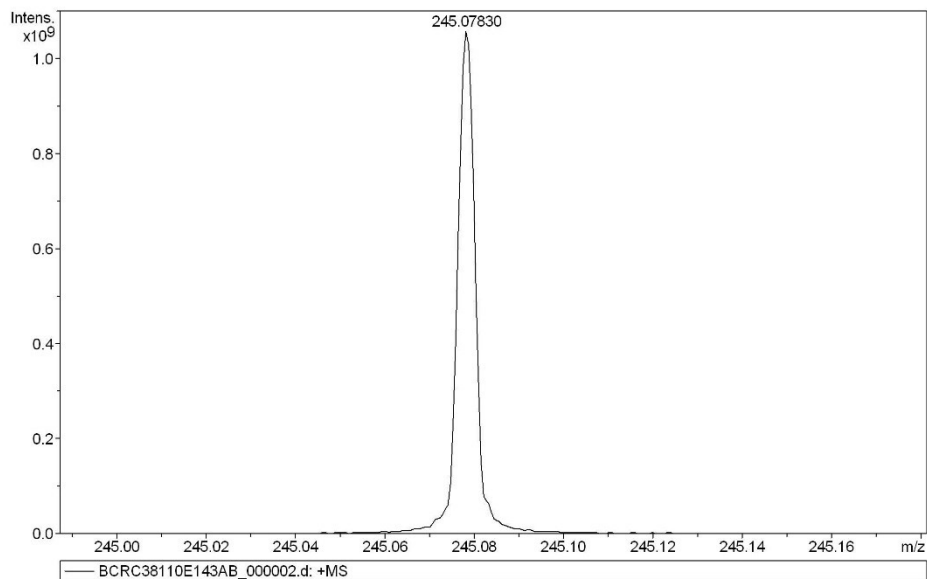
Figure S14. NOESY spectrum of monatetralone A (2)

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\7\BCRC38110E143AB_000002.d
Method broadband first signal
Sample Name BCRC38110-E-14-4-3-A-B
Comment ESI Positive

2/14/2018 1:17:13 PM
Operator: YU HSIAO-CHING
Instrument: BRUKER FT-MS solariX



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
245.07830	1	C ₁₂ H ₁₄ NaO ₄	100.00	245.07843	0.13	0.53	10.1	5.5	even	ok

Figure S15. HRESIMS spectrum of monatetralone A (2)

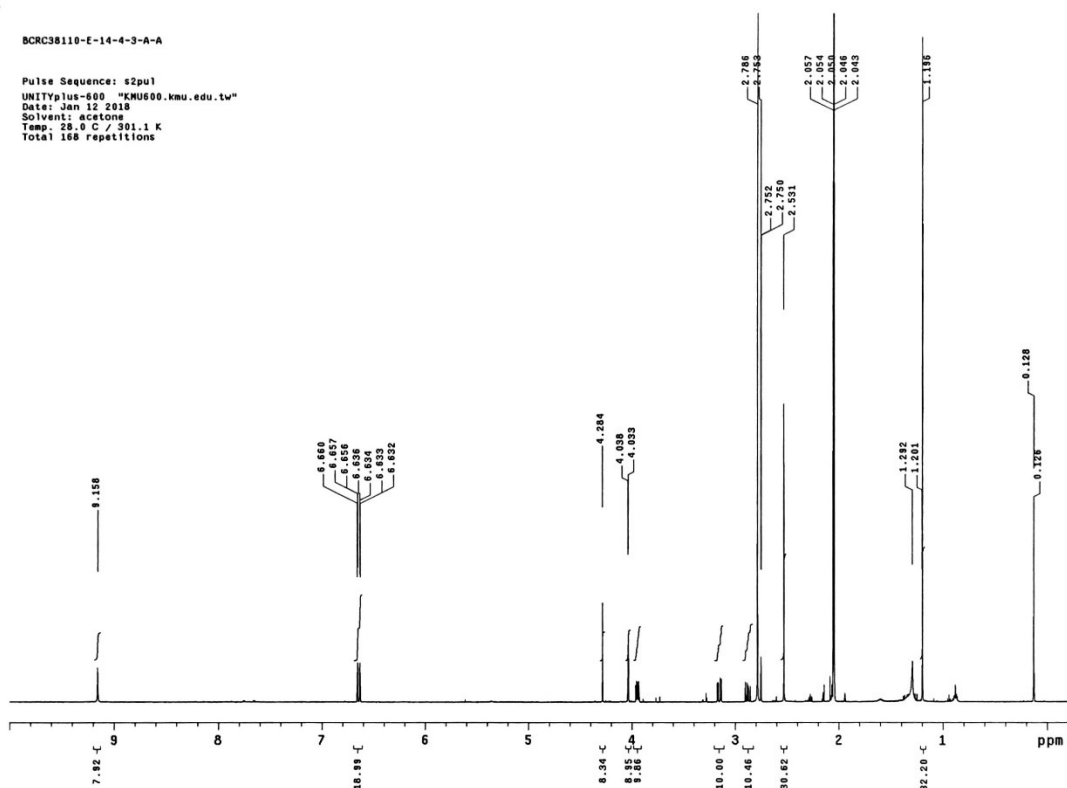


Figure S16. ¹H NMR spectrum of monatetralone B (3) in CDCl₃ at 600 MHz

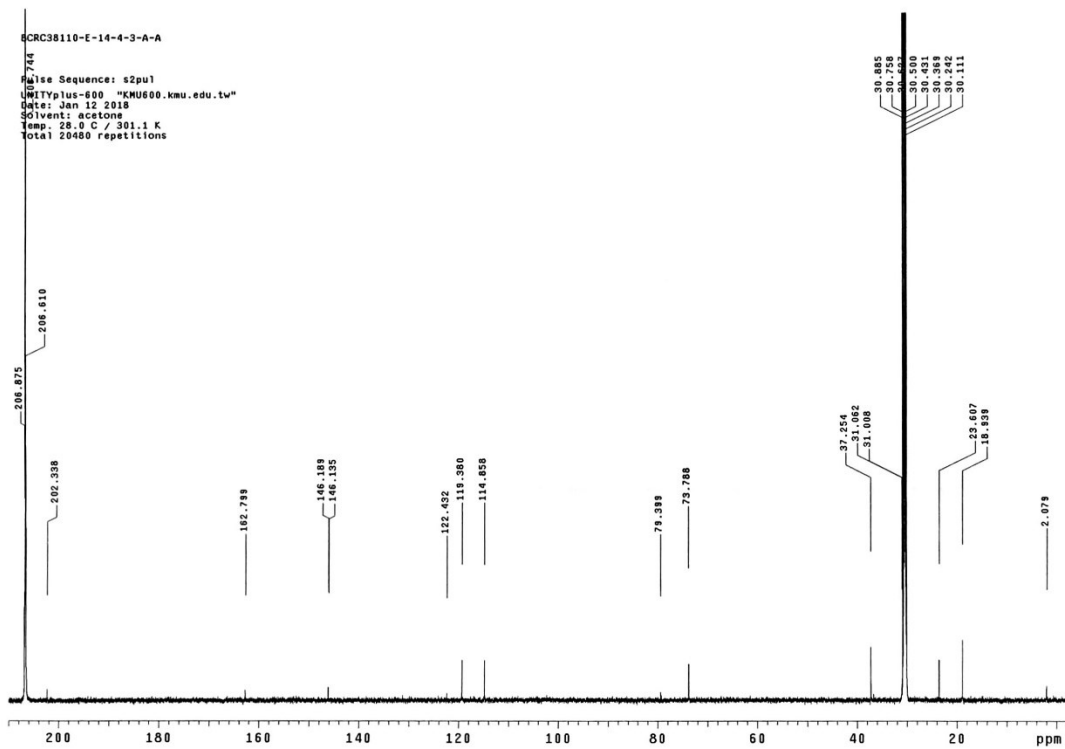


Figure S17. ^{13}C NMR spectrum of monatetralone B (**3**) in CDCl_3 at 125 MHz

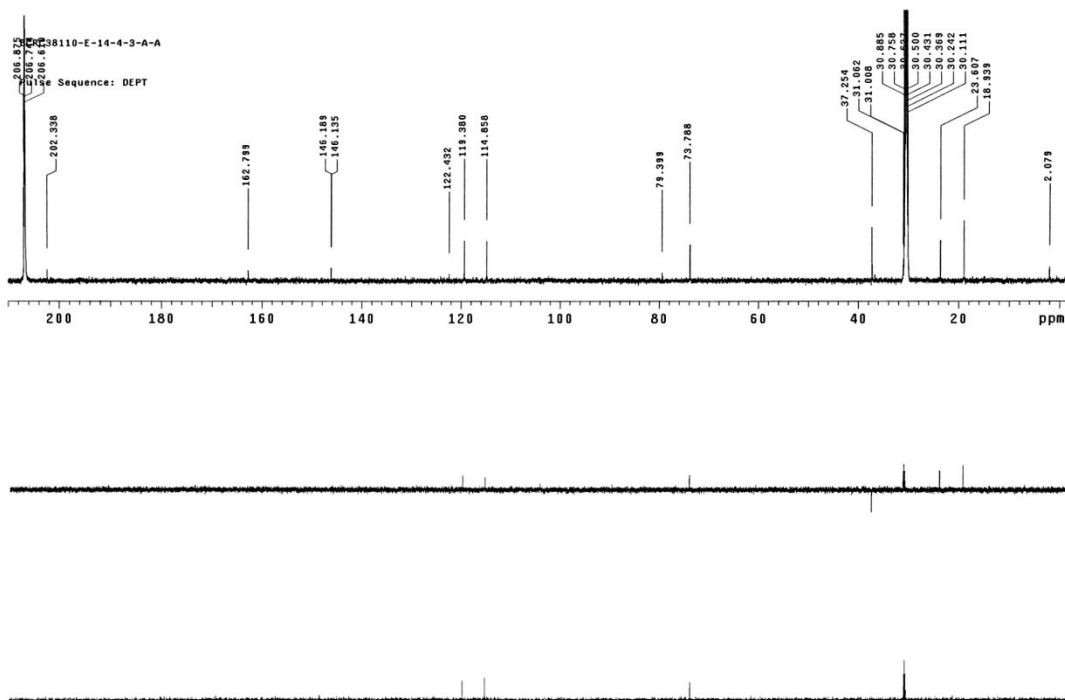


Figure S18. DEPT spectrum of monatetralone B (**3**)

BCRC38110-E-14-4-3-A-A

exp21 gCOSY

SAMPLE		FLAGS	
date	Jan 12 2018	hs	nn
solvent	acetone	ssp1	y
sample		hs1v1	5328
ACQUISITION		SPECIAL	
sw	9542.0	temp	28.0
at	0.150	gain	54
np	2862	spin	not used
fb	4000	F2	PROCESSING
ss	32	sb	-0.075
d1	1.000	sbs	not used
nt	32	fn	4096
2D ACQUISITION		F1 PROCESSING	
sw1	9542.0	sb1	-0.017
nt1	160	sbs1	not used
d2	PRESATURATION	procl	1p
		fn1	4096
satmode	n	DISPLAY	
wet	n	sp	-122.7
TRANSMITTER		wp	
tn	H1	sp1	-122.7
sfrq	597.283	wp1	6088.5
tof	597.3	rf1	1185.0
tpwr	58	rfp	0
pw	12.000	rf11	1185.0
GRADIENTS		rfp1	
g2iv1E	4444	PLOT	
g1E	0.001900	wc	140.0
Edratio	1.000	sc	5.0
gstab	0.000500	wc2	140.0
DECOUPLER		sc2	5.0
dn	C13	vs	2343
dm	nm	th	8
	al	cdc	av

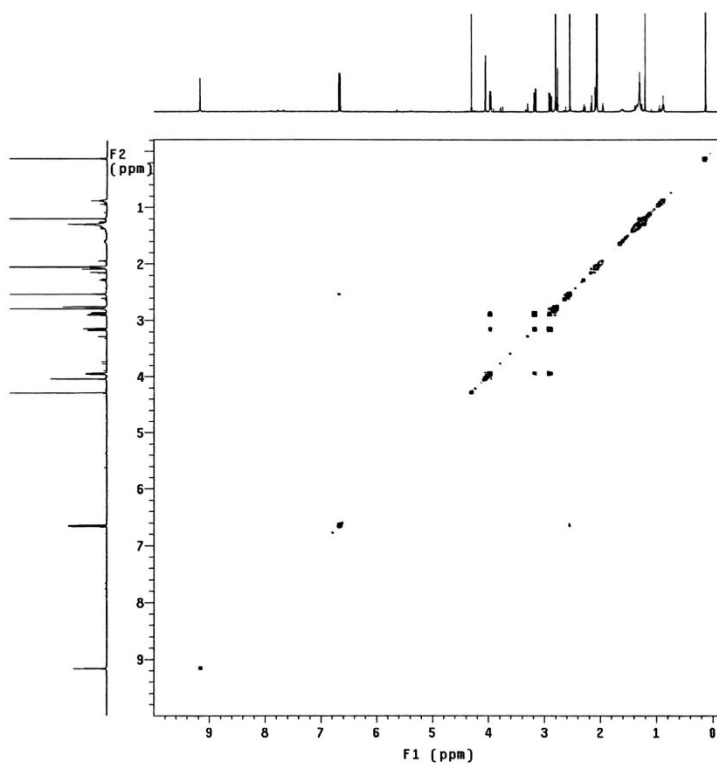


Figure S19. COSY spectrum of monatetralone B (3)

BCRC38110-E-14-4-3-A-A

Pulse Sequence: gHMBCAD

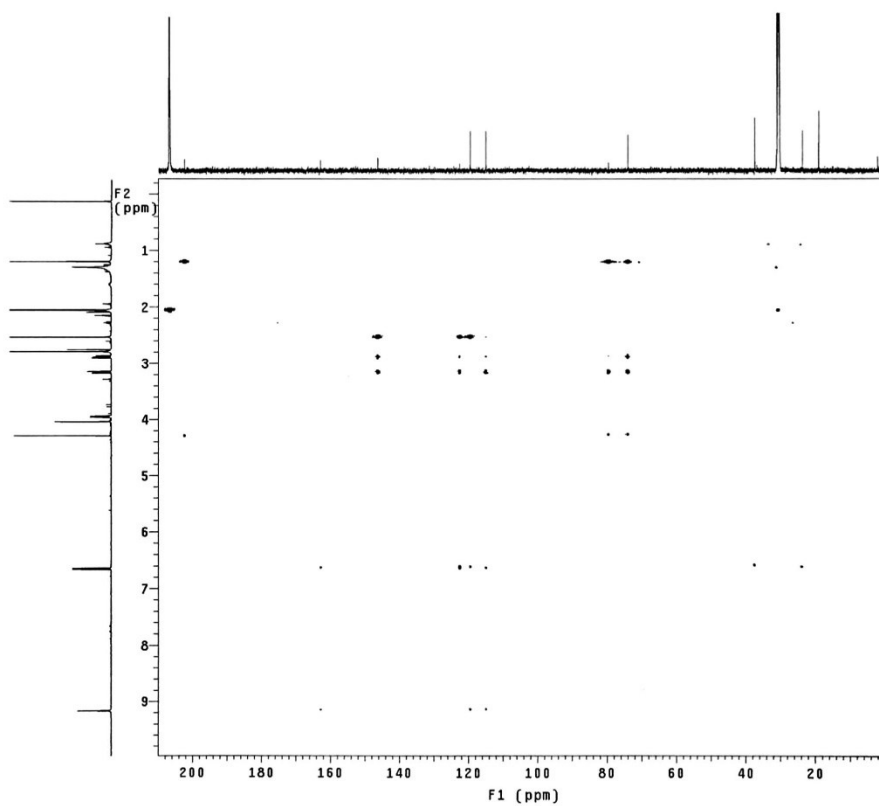


Figure S20. HMBC spectrum of monatetralone B (3)

BCRC38110-E-14-4-3-A-A

exp22 NOESY

```
SAMPLE          FLAGS
date Jan 12 2018 hs nn
solvent acetone sspu1 y
sample          PFG1g y
ACQUISITION    hsg1v1 5328
sv 9542.0      SPECIAL 28.0
at 0.150 temp 28.0
np 2862 gain 50
fb 4000 spin not used
ss 32 F2 PROCESSING
dl 1.000 gf 0.069
nt 32 gfs not used
2D ACQUISITION fn F1 PROCESSING 4096
sv1 9542.0      F1 0.015
nl 160 gf1 not used
TRANSMITTER H1 procl 1p
tn 597.283 fn1 4096
tof 597.3 sp DISPLAY -122.7
tpwr 38 wp 6089.5
pw 12.000 wp1 -122.7
mixN NOESY 0.600 wp1 6089.5
PRESATURATION rff1 1185.0
satmode n rfp 0
wet n rff1 1185.0
DECOUPLER n rfp1 0
dn C13 PLOT 140.0
dm nnn wc 5.0
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wc2 5.0
sc2 5.0
vs 2343
th 4
at cdc ph
```

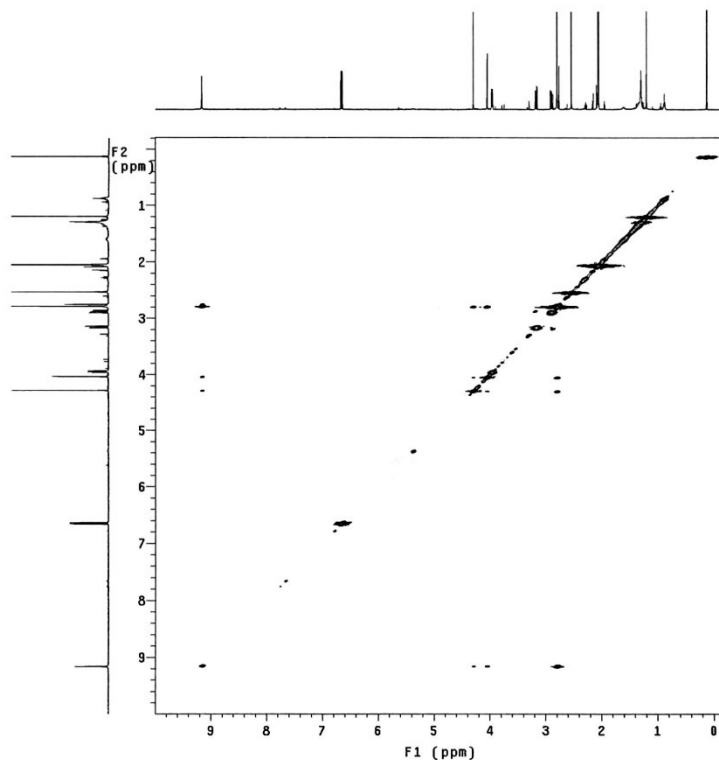


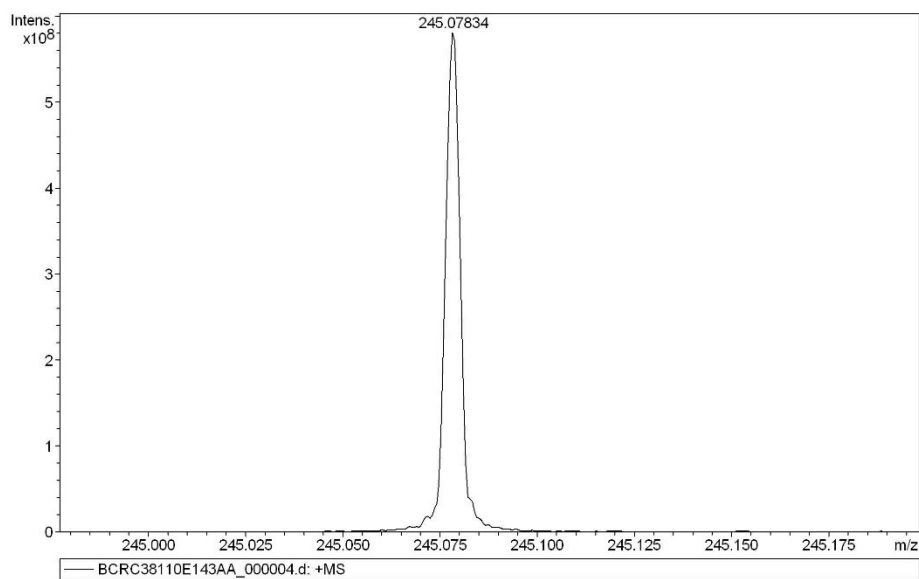
Figure S21. NOESY spectrum of monatetralone B (3)

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\7\BCRC38110E143AA_000004.d
Method broadband first signal
Sample Name BCRC38110-E-14-4-3-A-A
Comment ESI Positive

2/14/2018 1:13:26 PM
Operator: YU HSIAO-CHING
Instrument: BRUKER FT-MS solarix



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
245.07834	1	C ₁₂ H ₁₄ NaO ₄	100.00	245.07843	0.09	0.37	9.1	5.5	even	ok

Figure S22. HRESIMS spectrum of monatetralone B (3)

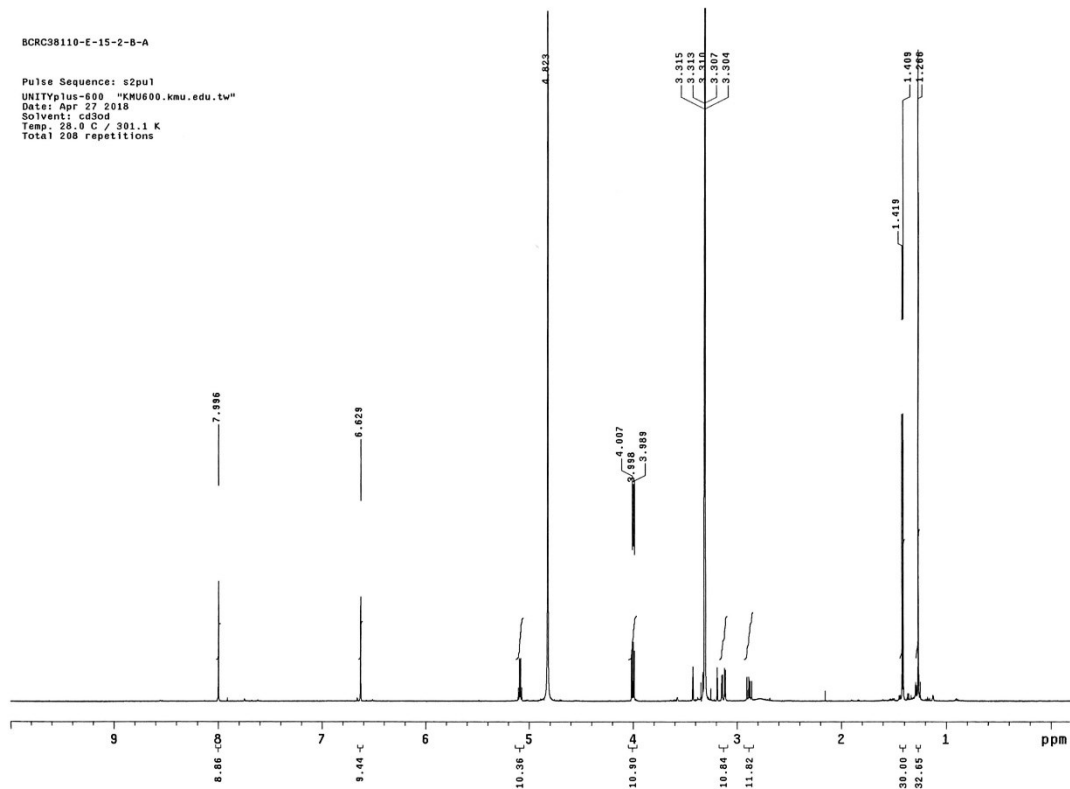


Figure S23. ^1H NMR spectrum of monatetralone C (**4**) in CD_3OD at 600 MHz

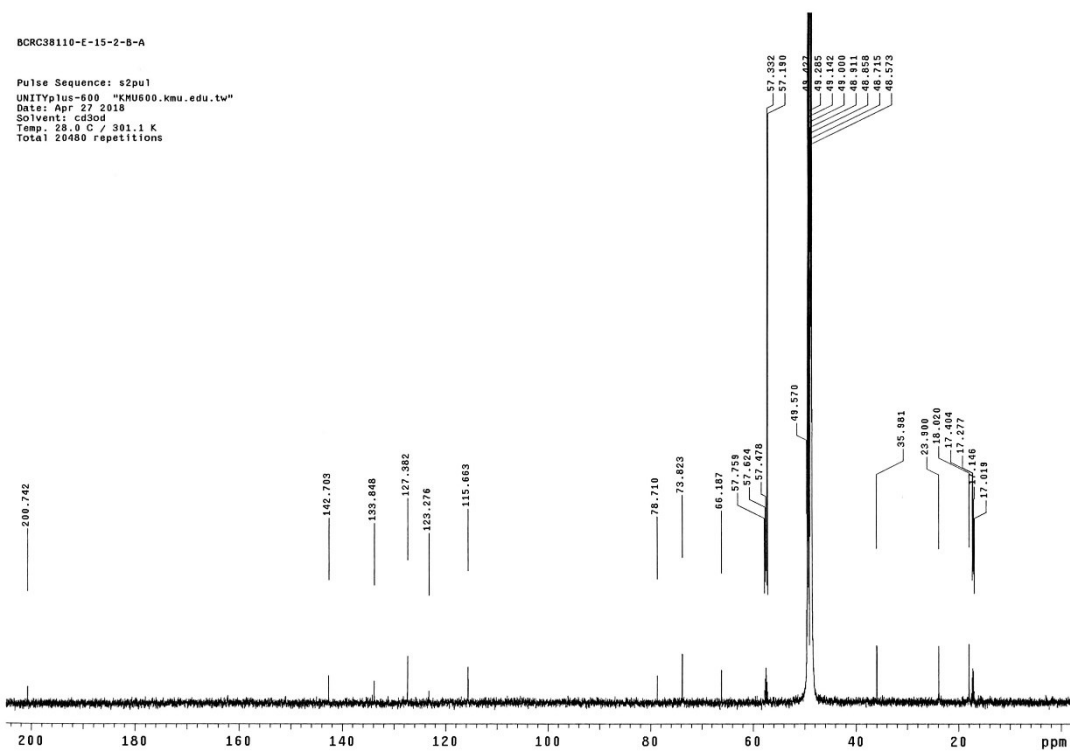


Figure S24. ^{13}C NMR spectrum of monatetralone C (**4**) in CD_3OD at 125 MHz

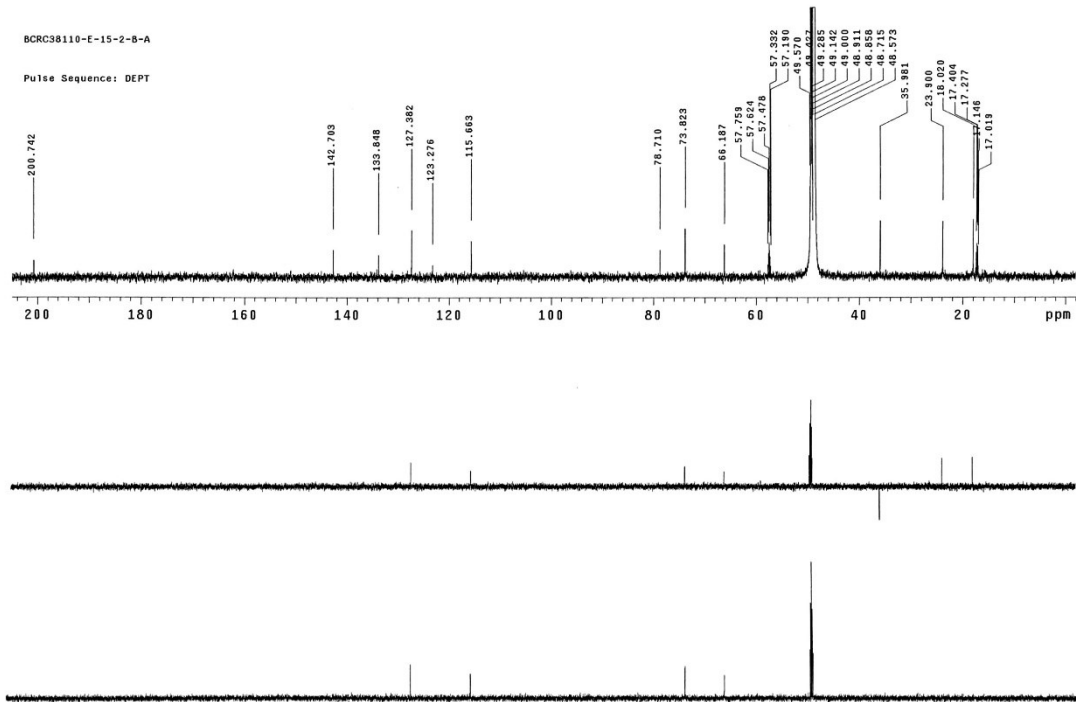


Figure S25. DEPT spectrum of monatetralone C (4)

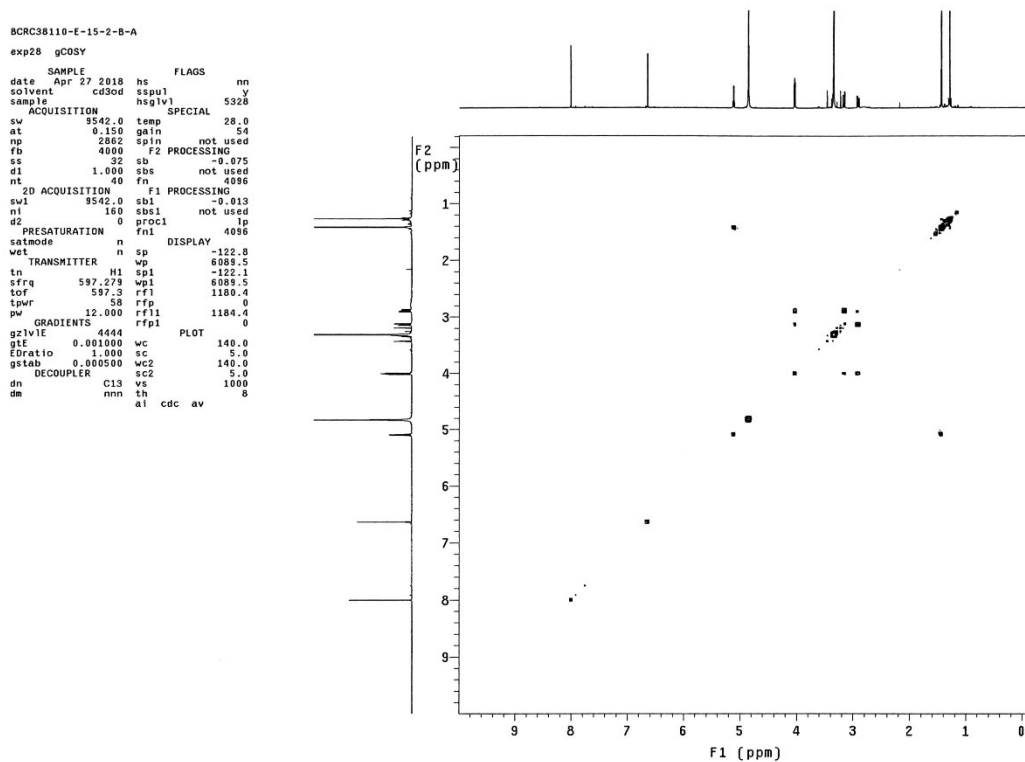


Figure S26. COSY spectrum of monatetralone C (4)

BCRC38110-E-15-2-B-A
Pulse Sequence: gHMBCAD

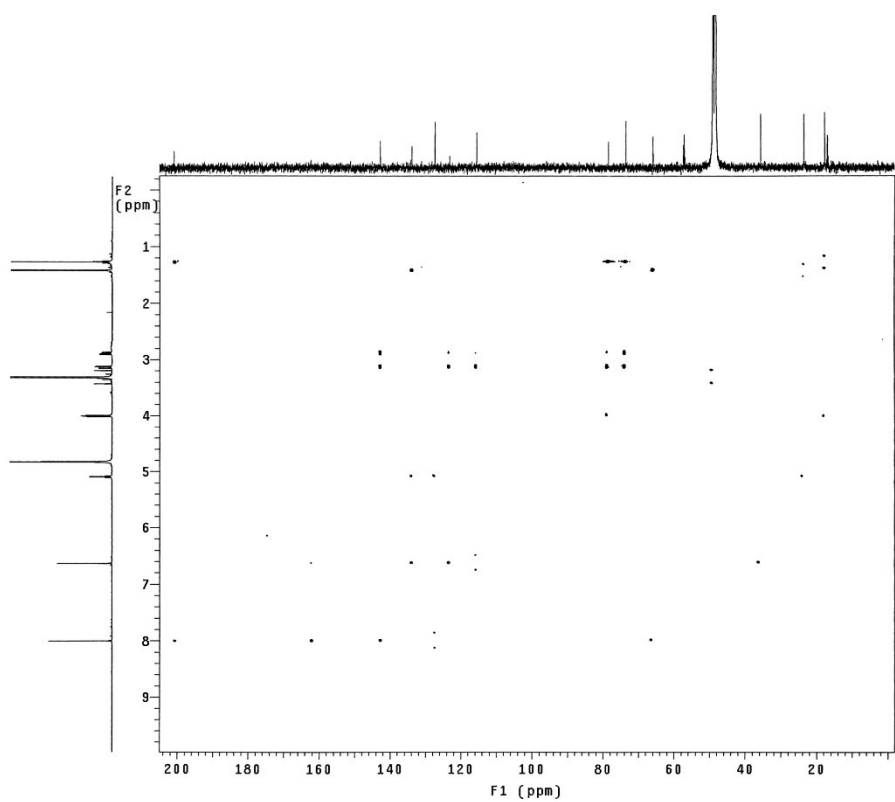


Figure S27. HMBC spectrum of monatetralone C (4)

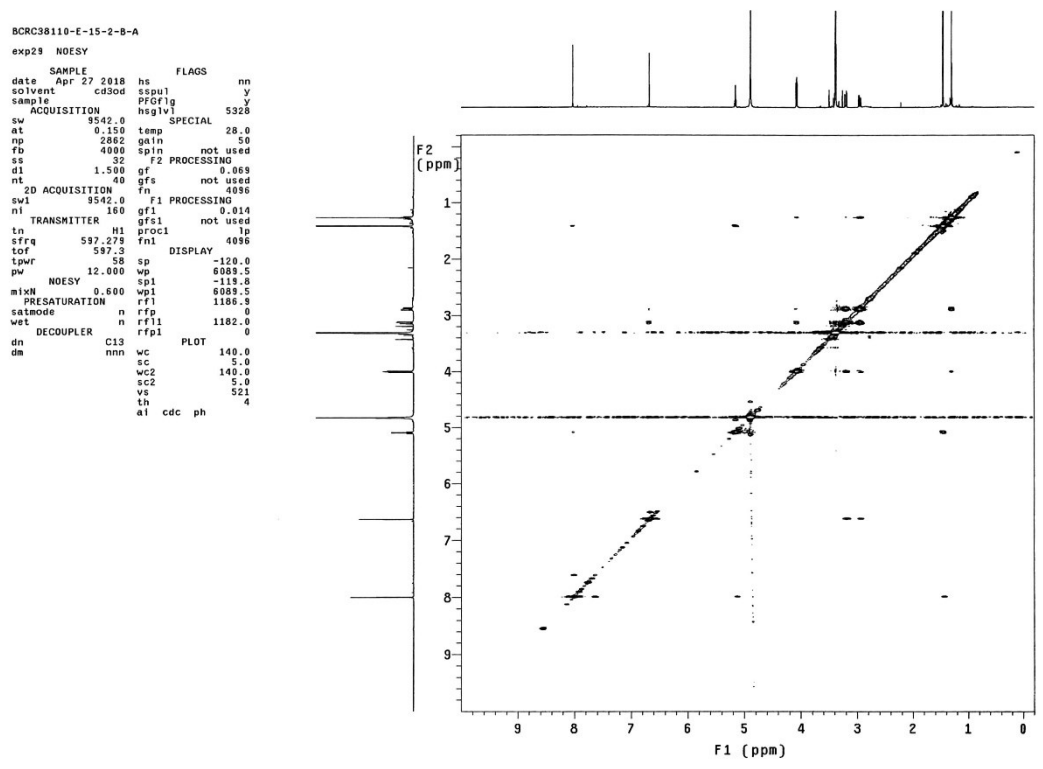


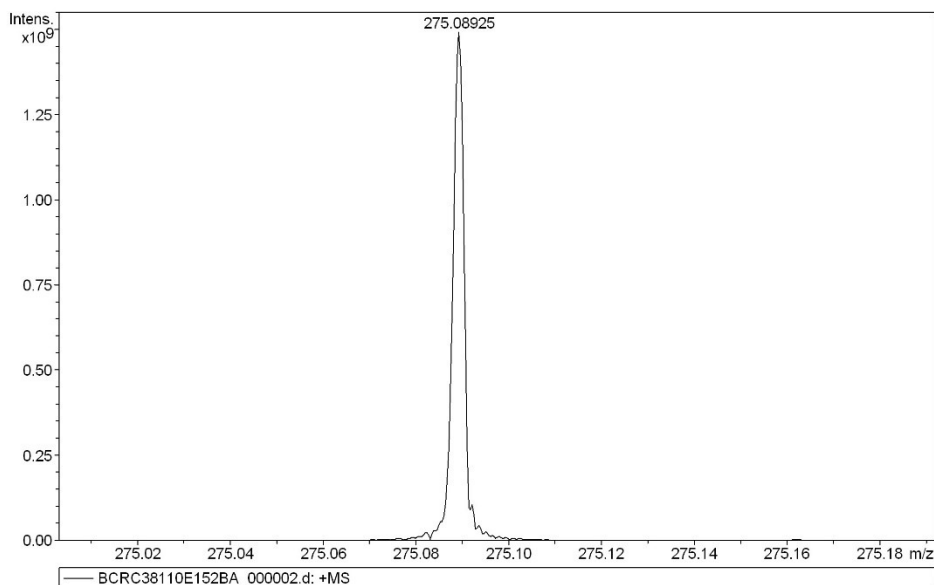
Figure S28. NOESY spectrum of monatetralone C (4)

Mass Spectrum SmartFormula Report

Analysis Info

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Method broadband first signal
Sample Name BCRC38110-E-15-2-B-A
Comment ESI Positive

5/11/2018 3:20:47 PM
Operator: YU HSIAO-CHING
Instrument: BRUKER FT-MS solariX



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻	Conf	N-Rule
275.08925	1	C ₁₃ H ₁₆ NaO ₅	100.00	275.08899	-0.26	-0.94	8.0	5.5	even		ok

Figure S29. HRESIMS spectrum of monatetralone C (4)

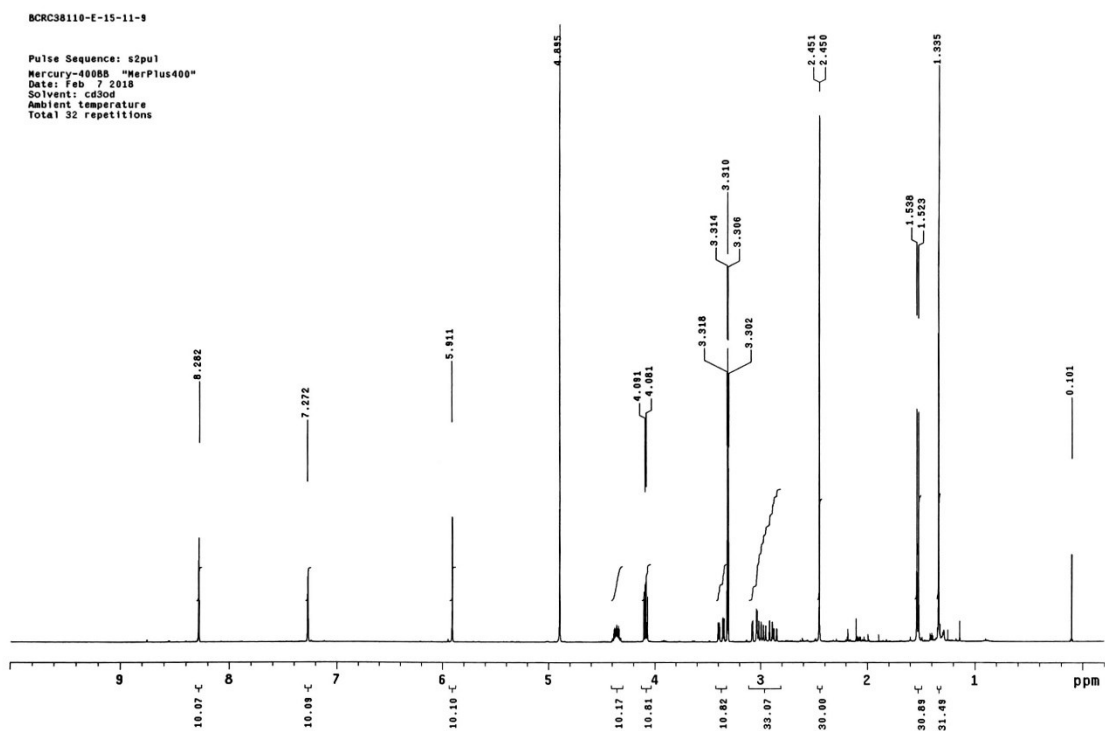


Figure S30. ¹H NMR spectrum of monatetralone D (5) in CD₃OD at 400 MHz

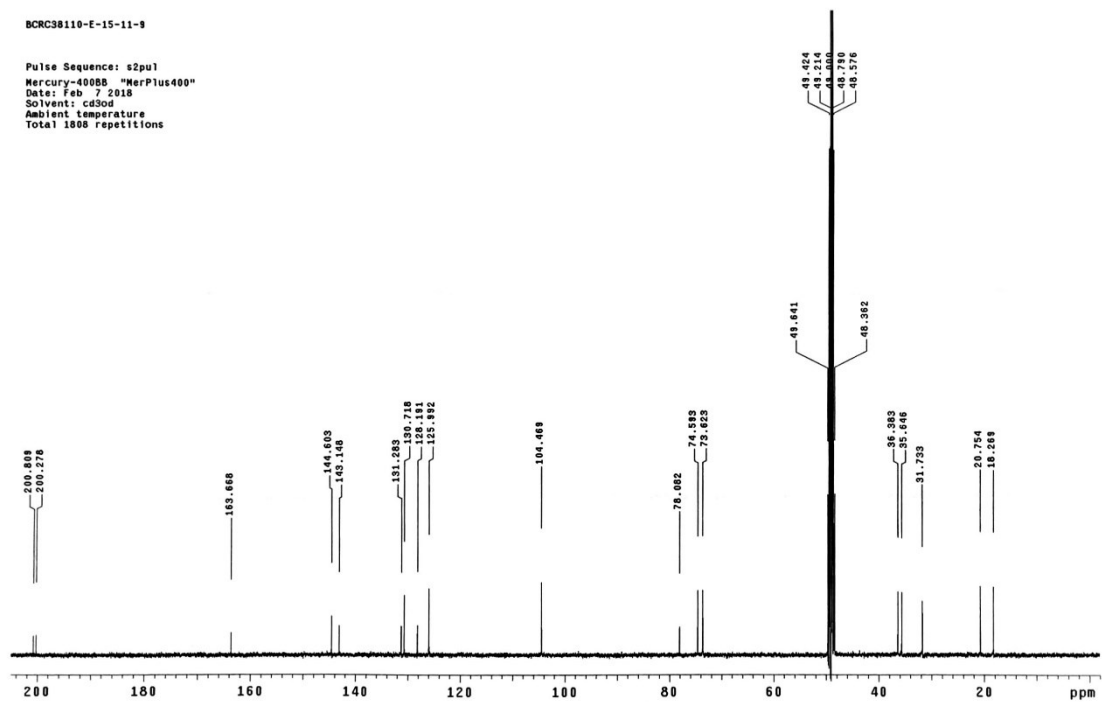


Figure S31. ^{13}C NMR spectrum of monatetralone D (5) in CD_3OD at 100 MHz

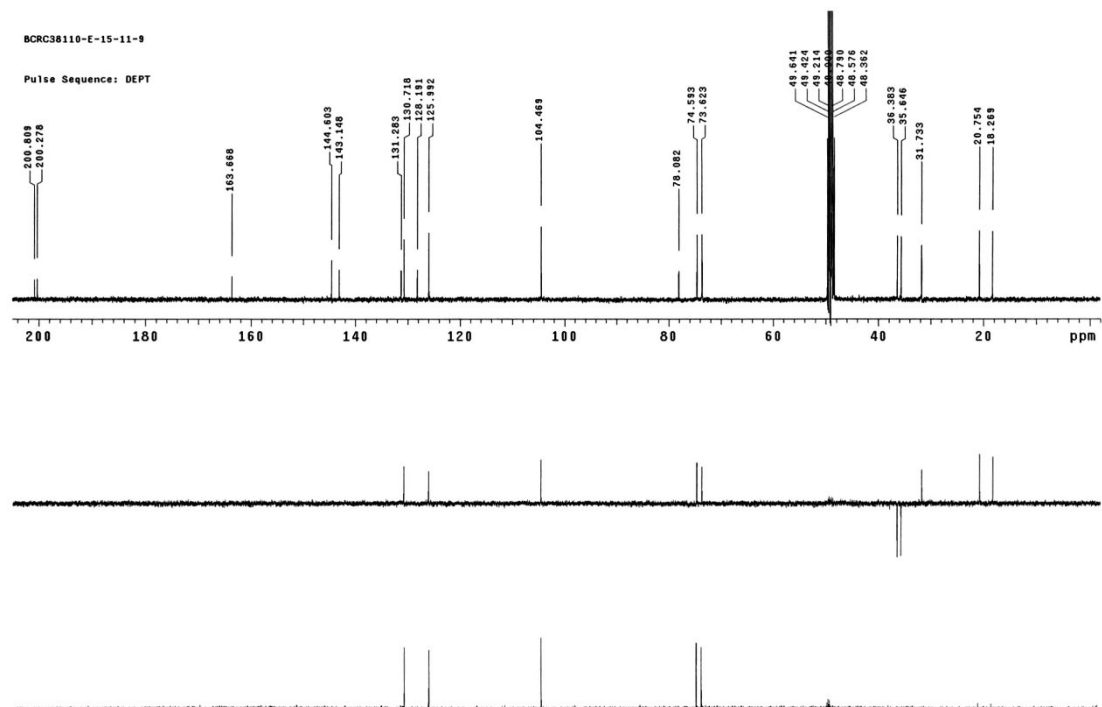


Figure S32. DEPT spectrum of monatetralone D (5)

BCRC38110-E-15-11-9
exp28 gCOSY

SAMPLE		FLAGS	
date	Feb 7 2018	hs	nn
solvent	cd3od	ssu1	y
sample		hsglv1	1224
ACQUISITION			
sw	640.3	temp	not used
at	0.150	gain	30
np	1320	sp1n	not used
fb	not used	F2	PROCESSING
ss	32	sb	-0.075
d1	1.000	sbs	not used
nt	20	fn	4086
2D ACQUISITION			
sw1	640.3	sb1	-0.020
nl	160	sbs1	not used
d2	0	procl	1p
PRESATURATION			
	fn1		4086
TRANSMITTER			
satmode	n	sp	DISPLAY -80.4
wet		wp	4081.5
tn	H1	sp1	-80.4
sfrq	400.402	wp1	4081.5
tof	366.0	rf1	800.3
tpwr	61	rpp	0
pw	11.600	rf11	800.3
GRADIENTS			
gz1w1e	1028		PLOT 0
g1e	0.001000	wc	140.0
EDratio	1.000	sc	5.0
gstab	0.000500	wc2	140.0
DECOUPLER		sc2	5.0
dn	C13	vs	100
dm	nmn	th	8
		al	av

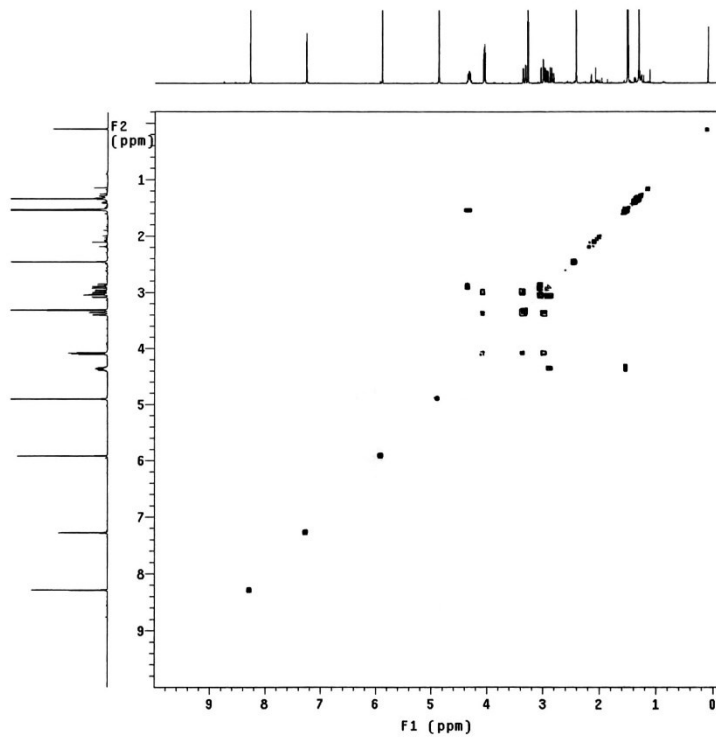


Figure S33. COSY spectrum of monatetralone D (5)

Pulse Sequence: gHMBC

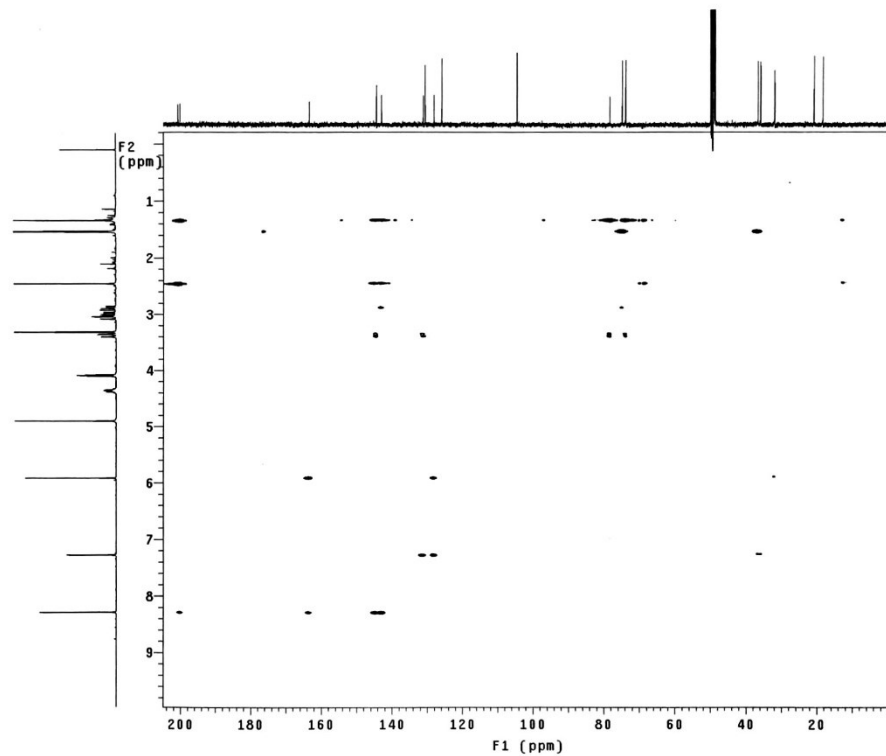


Figure S34. HMBC spectrum of monatetralone D (5)

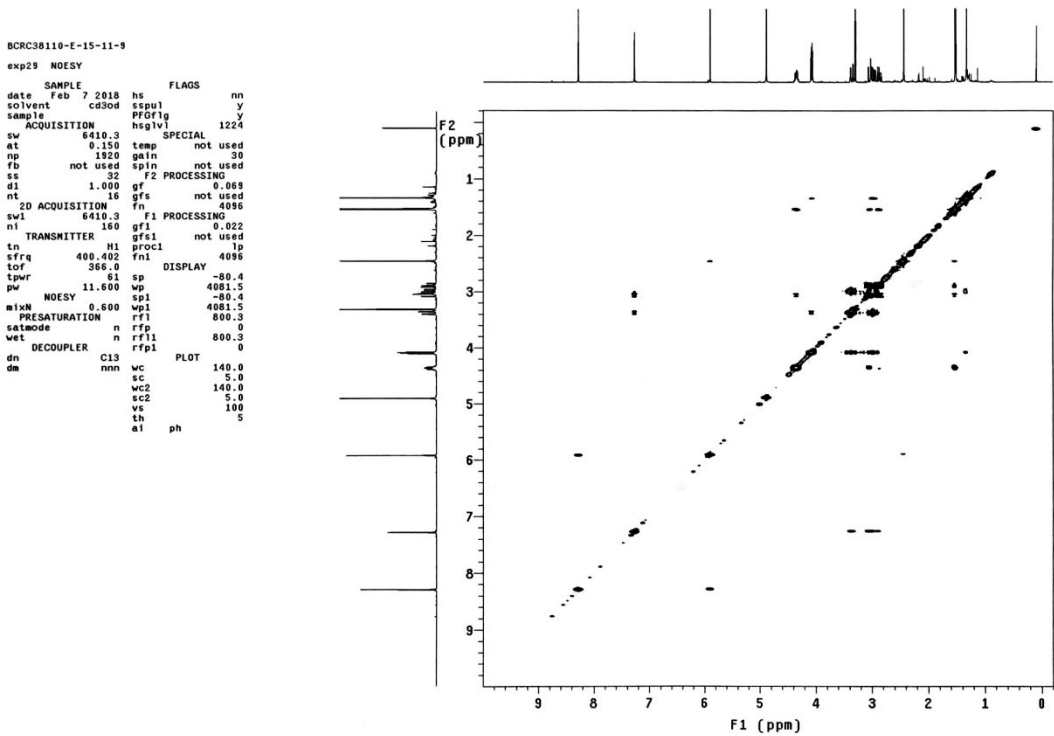
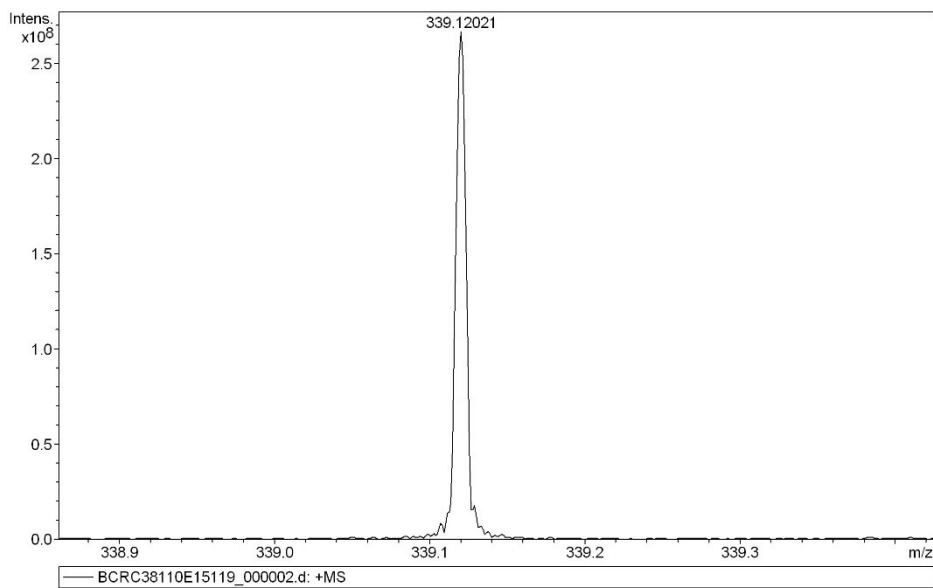


Figure S35. NOESY spectrum of monatetralone D (5)

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name	D:\Data\7\BCRC38110E15119_000002.d	3/12/2018 2:45:16 PM
Method	broadband first signal	Operator: YU HSIAO-CHING
Sample Name	BCRC48110-E-15-11-9	Instrument: BRUKER FT-MS solariX
Comment	ESI Positive	



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
339.12021	1	C ₁₈ H ₂₀ NaO ₅	100.00	339.12029	0.08	0.25	6.0	8.5	even	ok

Figure S36. HRESIMS spectrum of monatetralone D (5)

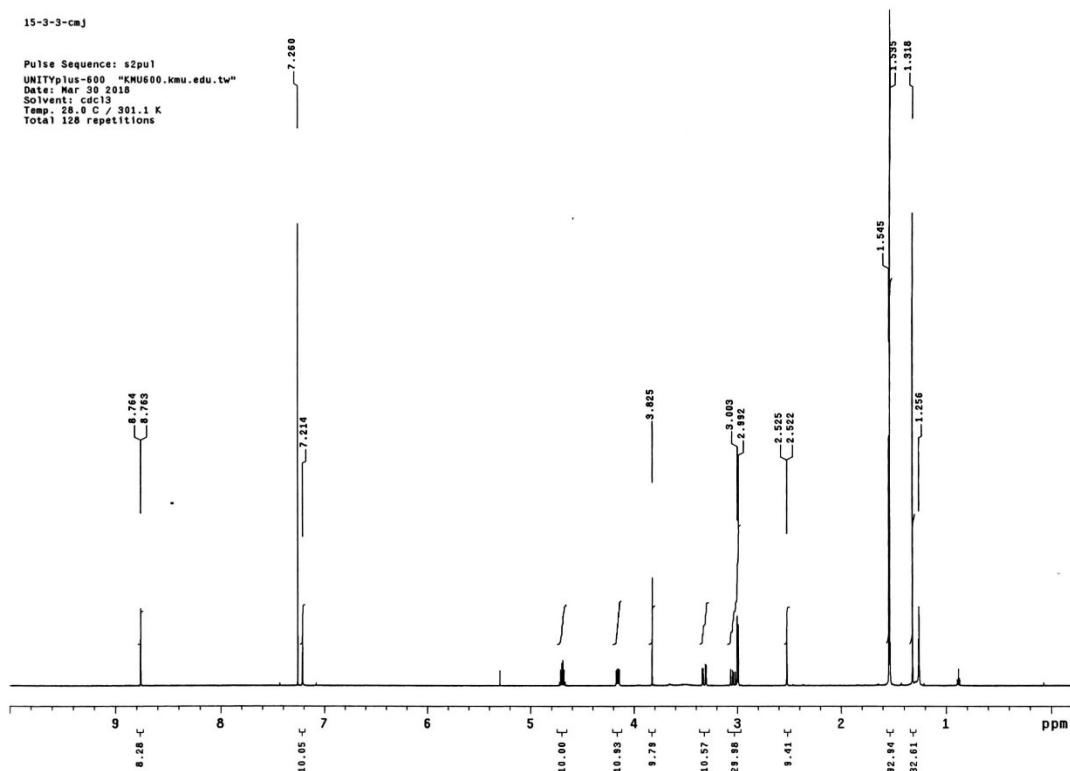


Figure S37. ^1H NMR spectrum of monatetralone E (**6**) in CDCl_3 at 600 MHz

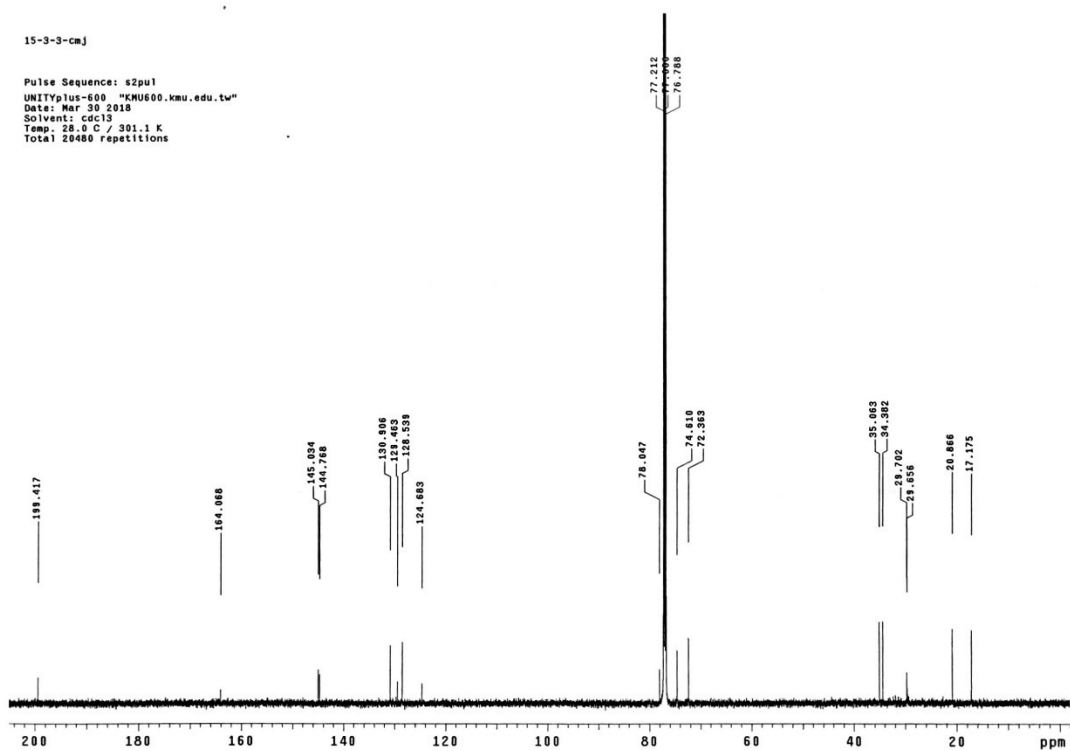


Figure S38. ^{13}C NMR spectrum of monatetralone E (**6**) in CDCl_3 at 125 MHz

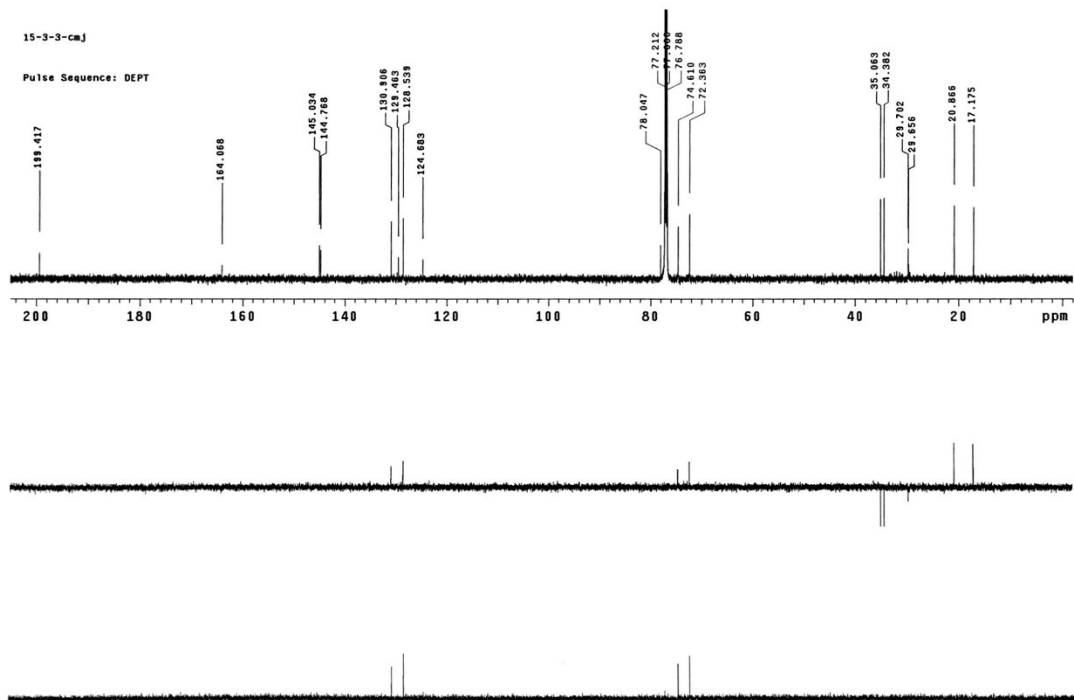


Figure S39. DEPT spectrum of monatetralone E (6)

15-3-3-cmJ

exp14 gCOSY

SAMPLE		FLAGS	
date	Mar 30 2018	hs	nm
solvent	cdc13	sspu	y
sample	hsjw1		5328
ACQUISITION		SPECIAL	
sv	9542.0	temp	25.0
at	0.150	gain	60
np	2862	spin	0
fb	4000	F2	PROCESSING
ss	32	sb	-0.075
d1	1.000	sbs	not used
nt	40	fn	4096
2D ACQUISITION		F1 PROCESSING	
sw1	9542.0	sb1	-0.013
nt1	160	sb1	not used
d2	0	procl	1p
PRESATURATION		n	
satmode	n	fn1	4096
wt	TRANSMITTER	n	sp
tn	M1	wp	6089.5
sfrq	597.277	sp1	-121.1
tof	597.3	rf1	1187.5
tpwr	58	rff	0
pw	12.000	rf1	1187.4
GRADIENTS		PLOT	
g2lvie	4444	wc	140.0
gc	0.001000	sc	5.0
Edratio	1.000	wc2	140.0
gsfab	0.000500	sc2	5.0
DECOUPLER		vs	
dn	C13	th	165
dm	nnn	ai	cdc av
			7

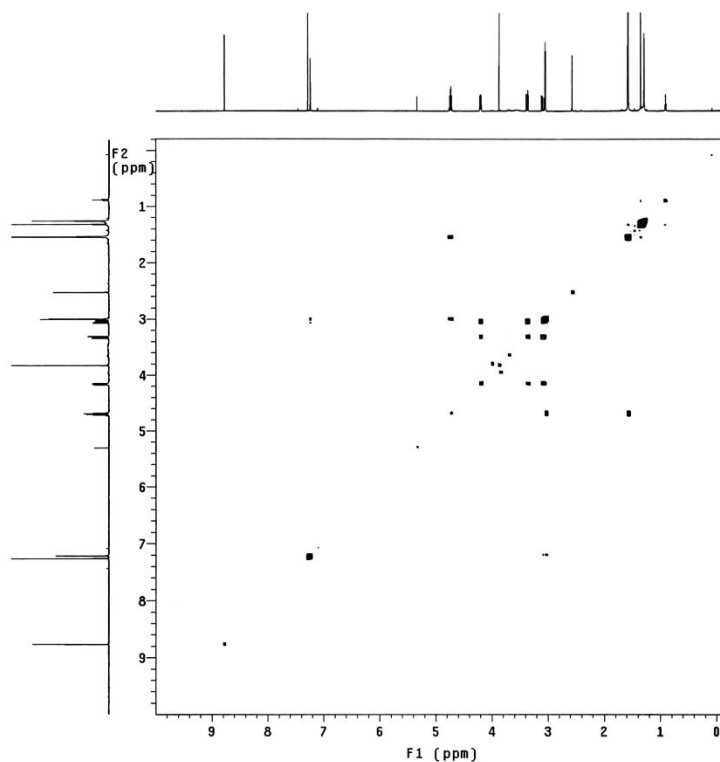


Figure S40. COSY spectrum of monatetralone E (6)

15-3-3-cmj
Pulse Sequence: gHMBCAD

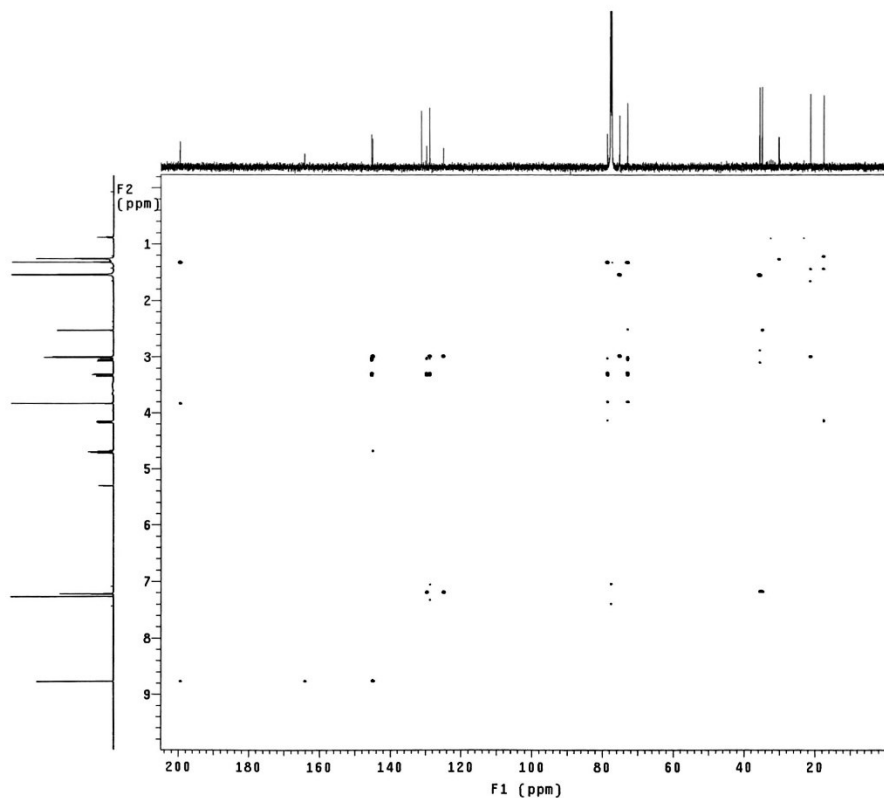


Figure S41. HMBC spectrum of monatetralone E (6)

```

15-3-3-cmj
exp15 NOESY
SAMPLE FLAGS
date Mar 30 2018 hs nn
solvent cdc13 sspu1 y
sample PFGlg y
ACQUISITION hsglv1 5328
sv 9542.0 SPECIAL
at 0.150 temp 28.0
np 2862 gain 52
fs 4000 spin 0
ss 32 F2 PROCESSING
dl 1.500 gf 0.969
nt 40 gfs not used
2D ACQUISITION fn 4096
sv1 9542.0 F1 PROCESSING
n1 160 gf1 0.015
tn TRANSMITTER H1 gfs1 not used
sfrq 597.277 fn1 1p
tof 597.3 DISPLAY -122.0
tpwr 58 sp 6089.5
pw 12.000 wp -121.1
mixN NOESY wp1 6089.5
PRESATURATION rf1 1193.6
satmode n rfp 0
wet n rf11 1192.7
dn DECOUPLER rfp1 0
dm C13 PLOT 140.0
nnn wc 5.0
sc 140.0
sc2 5.0
vs 1172
th 4
a1 cdc ph

```

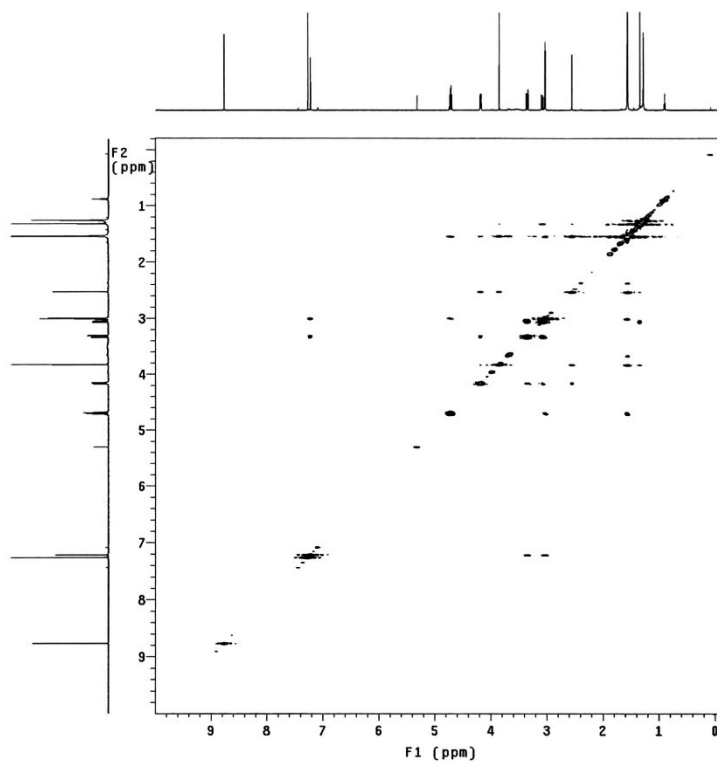


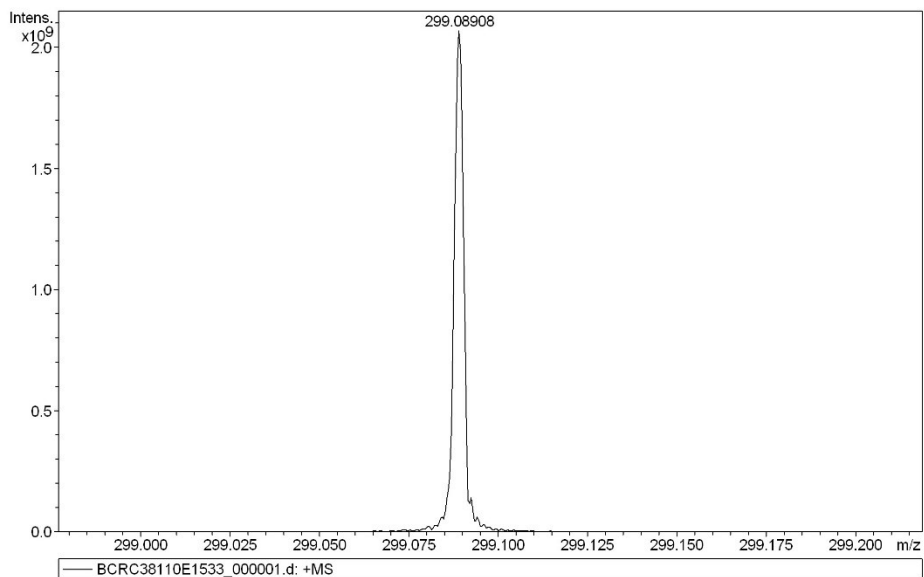
Figure S42. NOESY spectrum of monatetralone E (6)

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\7\BCRC38110E1533_000001.d
Method broadband first signal
Sample Name BCRC38110-E-15-3-3
Comment ESI Positive

5/11/2018 4:18:05 PM
Operator: YU HSIAO-CHING
Instrument: BRUKER FT-MS solariX



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
299.08908	1	C 15 H 16 Na O 5	100.00	299.08899	-0.09	-0.30	5.8	7.5	even	ok

Figure S43. HRESIMS spectrum of monatetralone E (6)

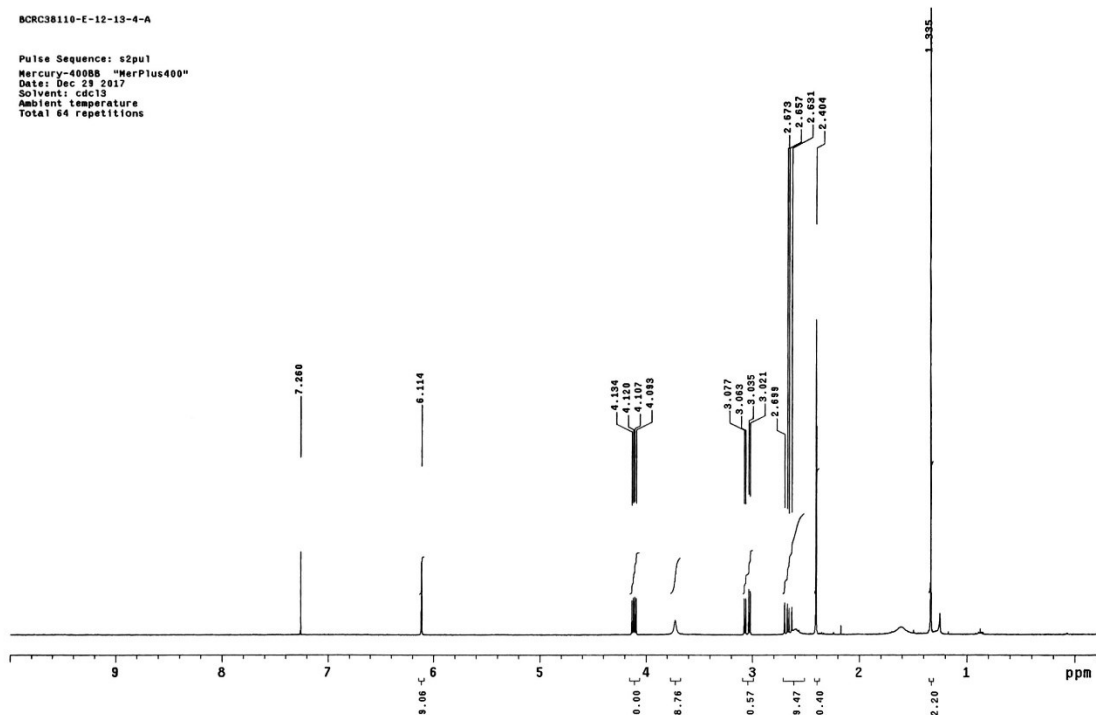


Figure S44. ¹H NMR spectrum of monabenzofuranone (7) in CDCl₃ at 400 MHz

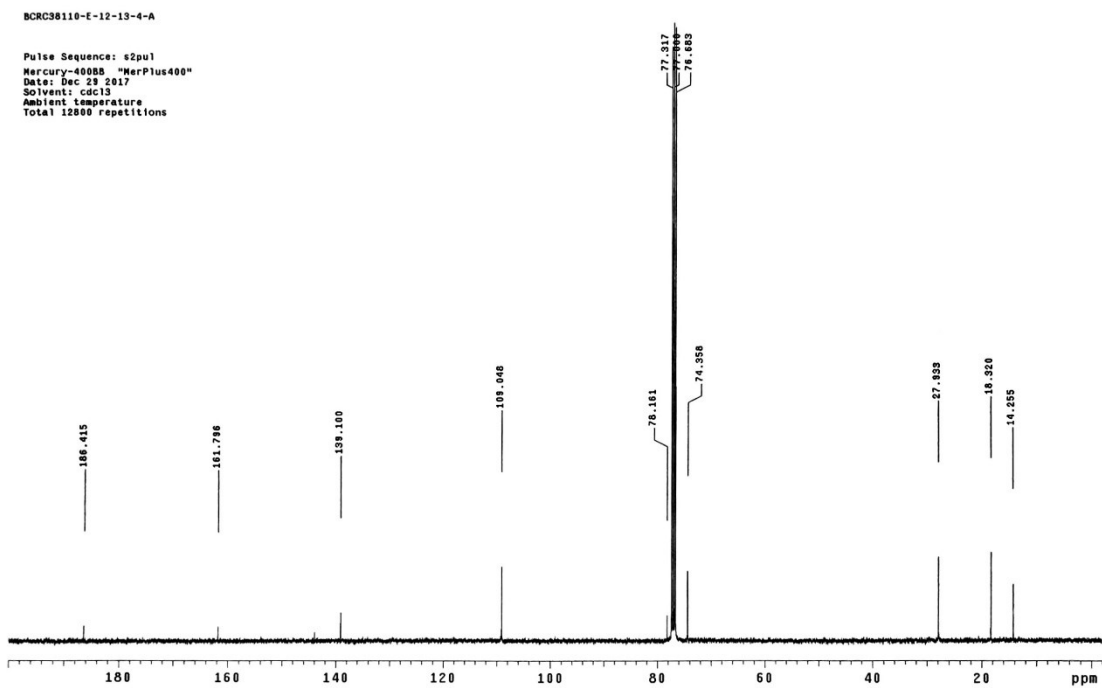


Figure S45. ^{13}C NMR spectrum of monabenzofuranone (**7**) in CDCl_3 at 100 MHz

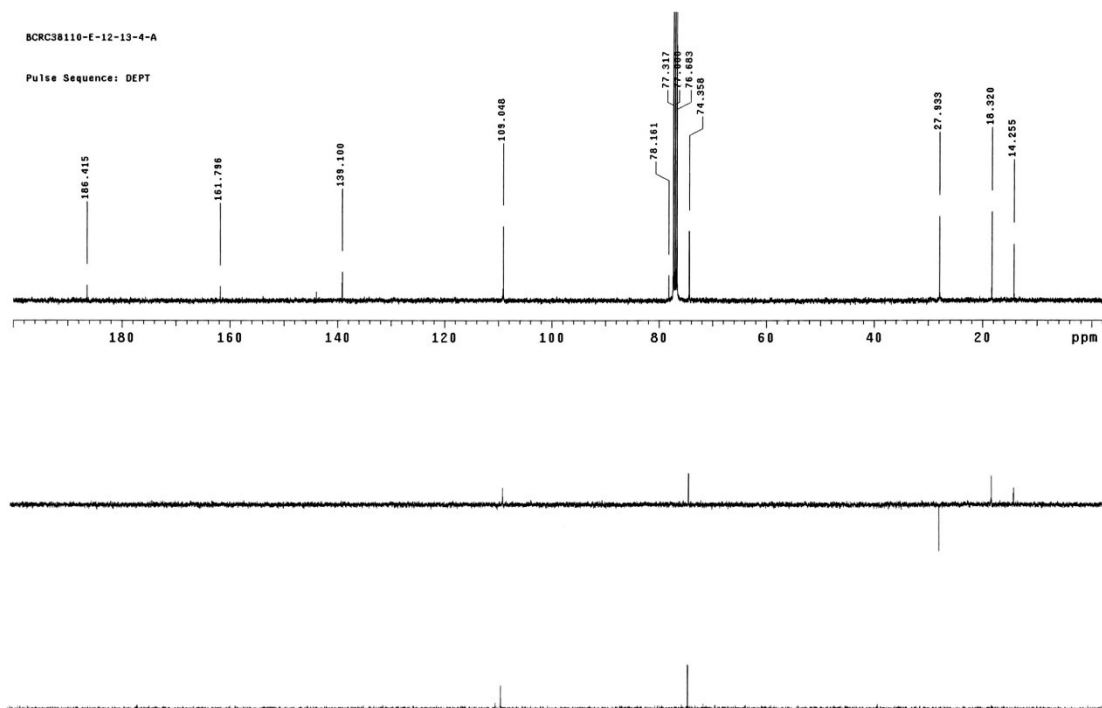


Figure S46. DEPT spectrum of monabenzofuranone (**7**)

BCRC38110-E-12-13-4-A
exp14 gCOSY

```
SAMPLE          FLAGS
date   Dec 28 2017   hs      nn
solvent cdc13       spul    y
sample  hg1v1       1224

ACQUISITION     SPECIAL
sw       5410.3    temp    not used
at       0.150    gain    36
np       1920     spin    not used
fb       not used  f2     PROCESSING
ss       32       sb      -0.075
d1       1.000    sb1    not used
nt       32       fr      4936

2D ACQUISITION  F1 PROCESSING
sw1      5410.3    sb1    -0.025
n1       160     sb1    not used
d2       0       procl  lp
PRESATURATION  fn1    DISPLAY 4936
ratmode   n       sp      -82.6
wet       n       wp      4081.5
TRANSMITTER H1    sp1    -82.6
sfreq     400.401  wp1    4081.5
tof       366.0    rf1    802.5
tpwr     61       rfp    0
pw       11.600   rfp1   0
GRADIENTS
gzlvie    1028    PL0T
gtf       0.001000  wc     140.0
EDratio   1.000    sc     5.0
gstab     0.000500  wc2    140.0
DECOUPLER C13   vs     150
dm        nm    th     8
          a1    av     0
```

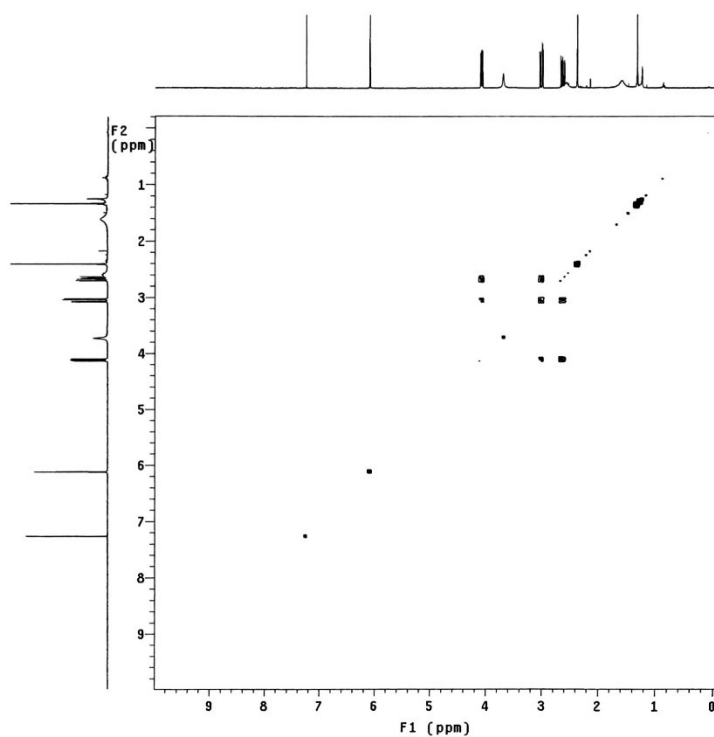


Figure S47. COSY spectrum of monabenzofuranone (7)

Pulse Sequence: gHMBC

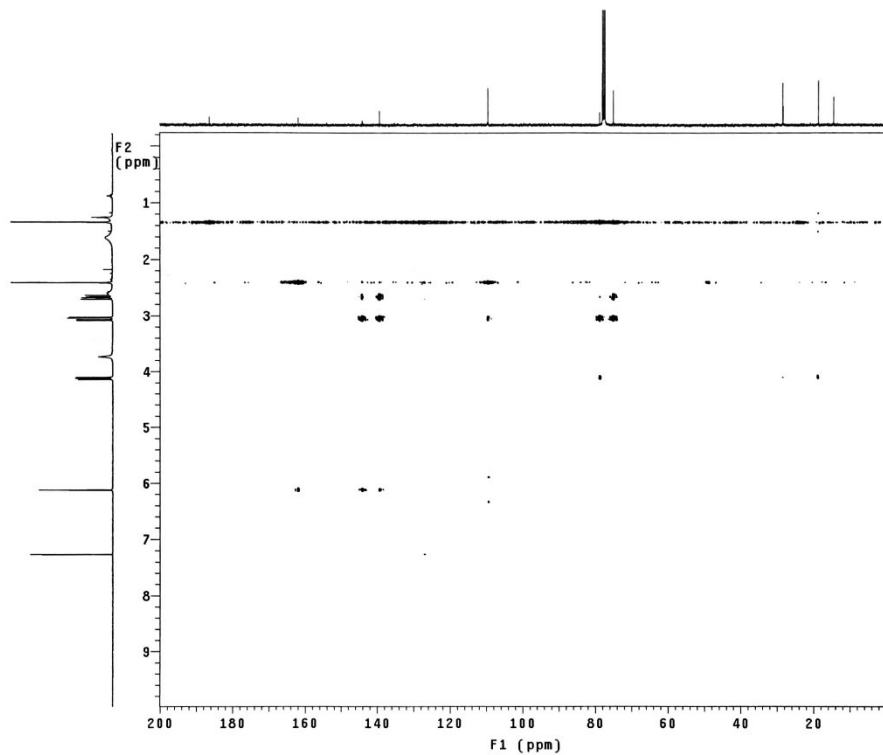


Figure S48. HMBC spectrum of monabenzofuranone (7)

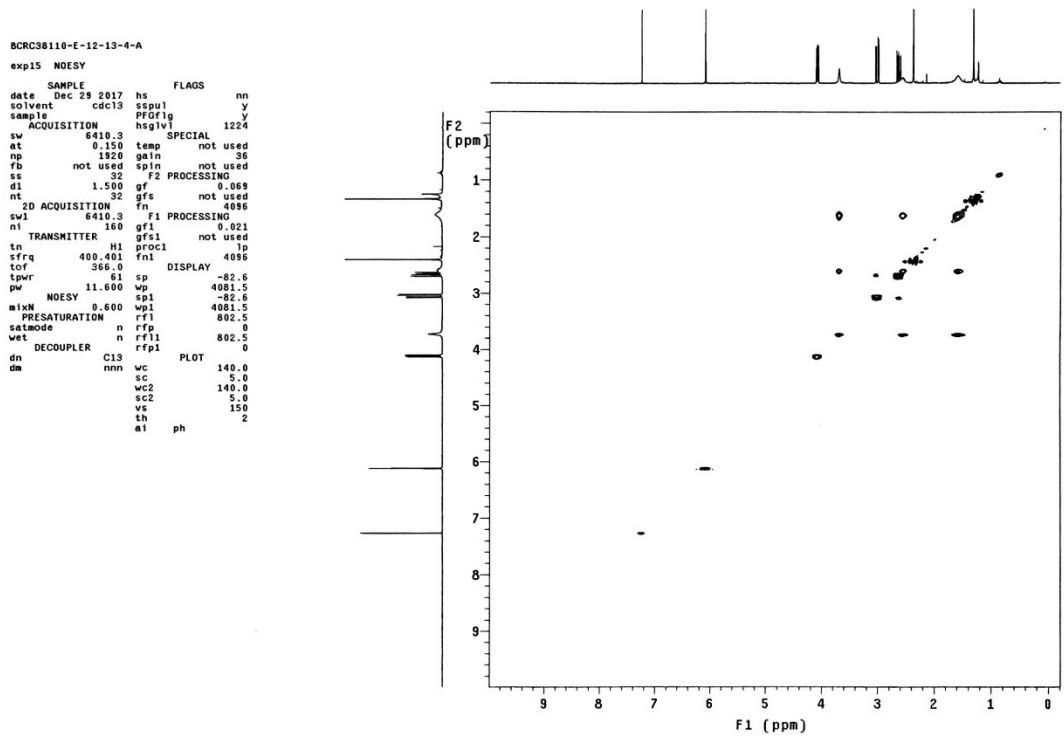


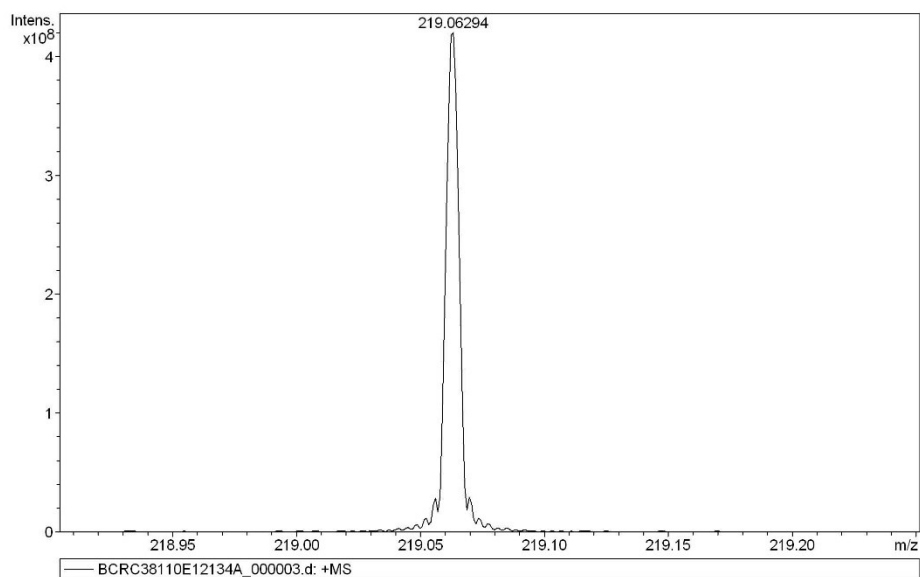
Figure S49. NOESY spectrum of monabenzofuranone (7)

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\7\BCRC38110E12134A_000003.d
Method broadband first signal
Sample Name BCRC38110-E-12-13-4-A
Comment ESI Positive

2/14/2018 12:51:53 PM
Operator: YU HSIAO-CHING
Instrument: BRUKER FT-MS solarix



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
219.06294	1	C ₁₀ H ₁₂ NaO ₄	100.00	219.06278	-0.16	-0.73	13.1	4.5	even	ok

Figure S50. HRMS spectrum of monabenzofuranone (7)

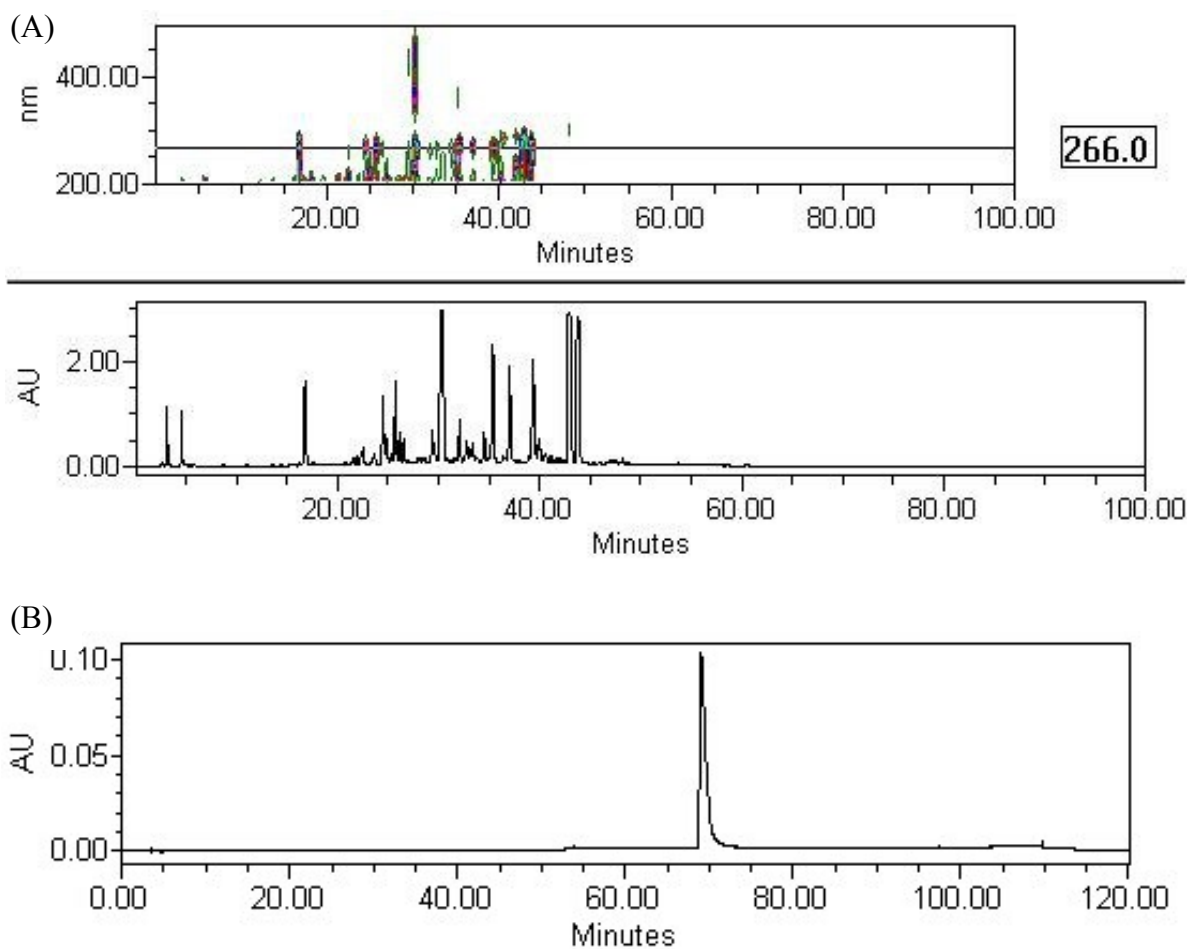


Figure S51. (A) HPLC chromatographic profile of red mold rice from *Monascus purpureus* BCRC 38110. (B) HPLC chromatographic profile of citrinin

The dried red yeast rice of *Monascus purpureus* BCRC 38110 (1.5 kg)

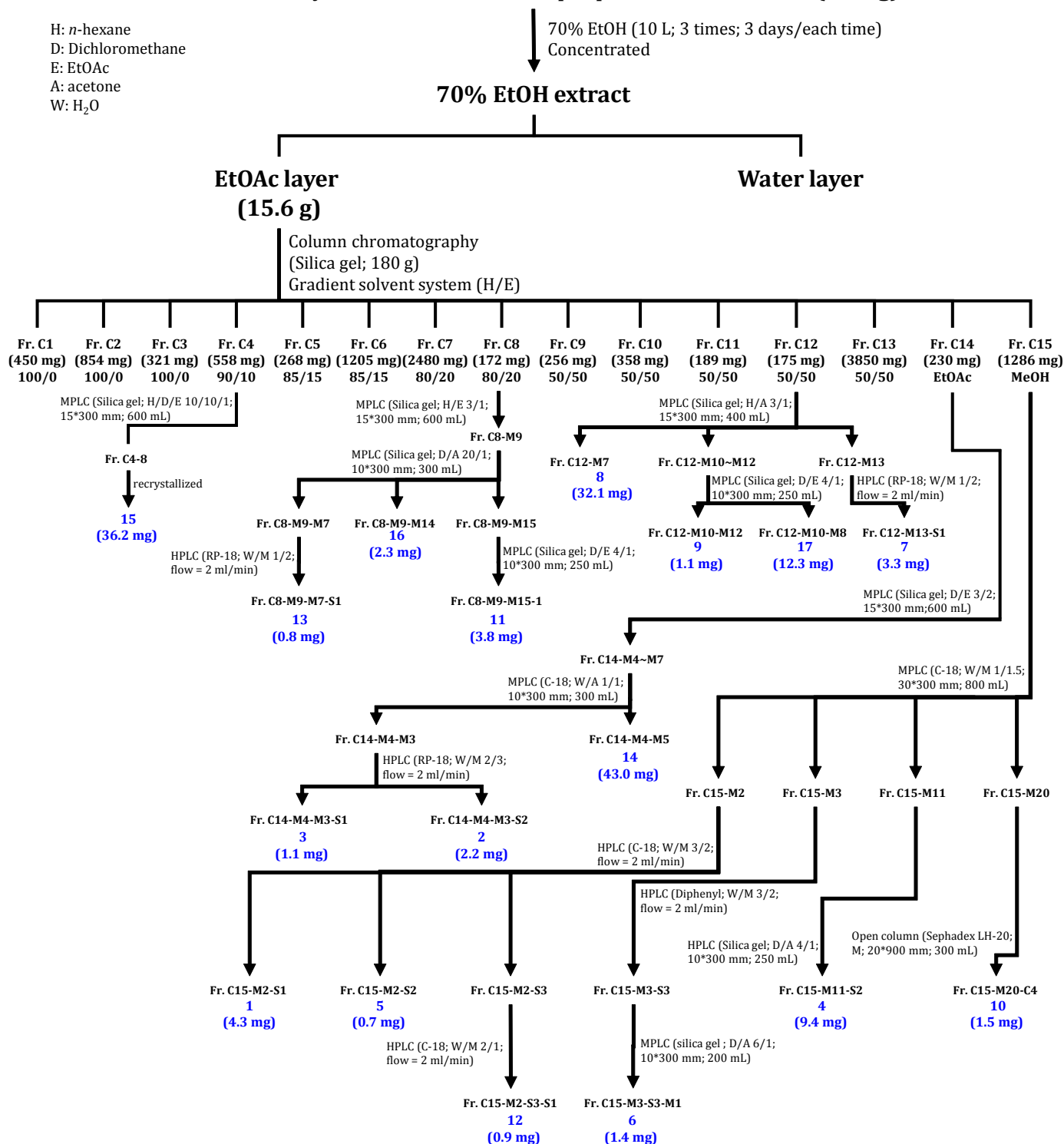


Figure S52. The isolation flowchart of *M. purpureus* BCRC 38110