

Investigations into chemical components from *Monascus purpureus* with photoprotective and anti-melanogenic activities

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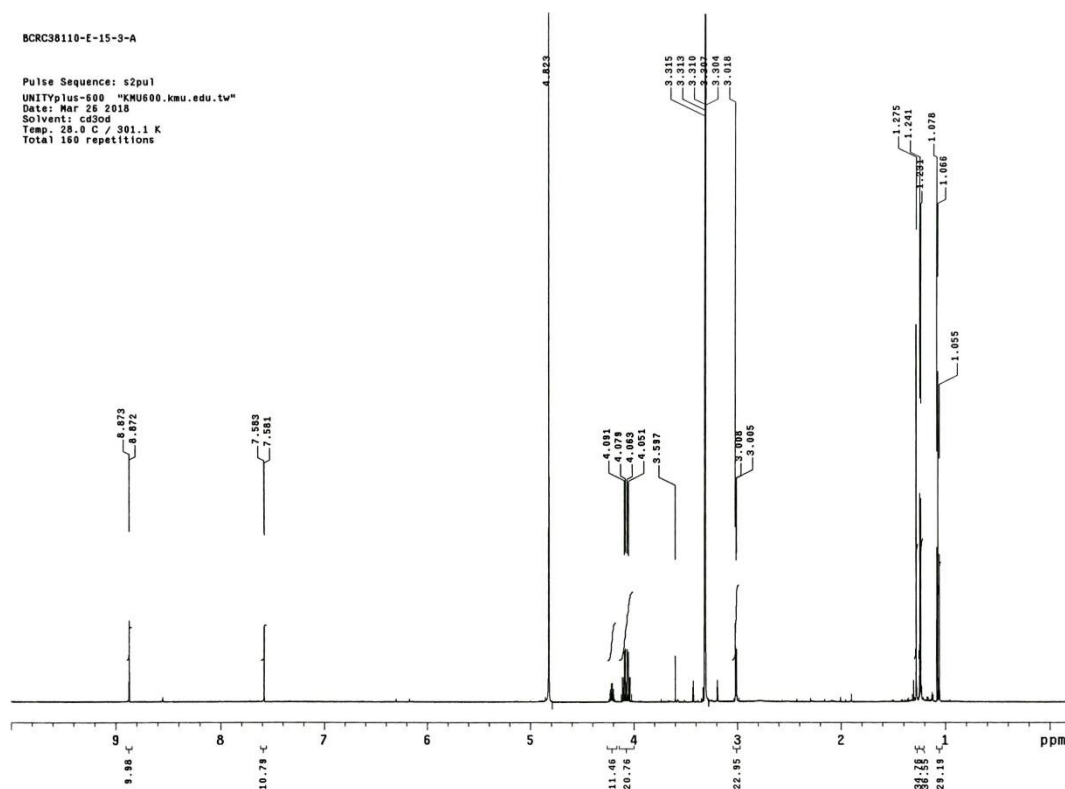


Figure S1. ^1H NMR spectrum of 5S,6S-monaspurpyridine A (**1**) in CD_3OD at 600 MHz

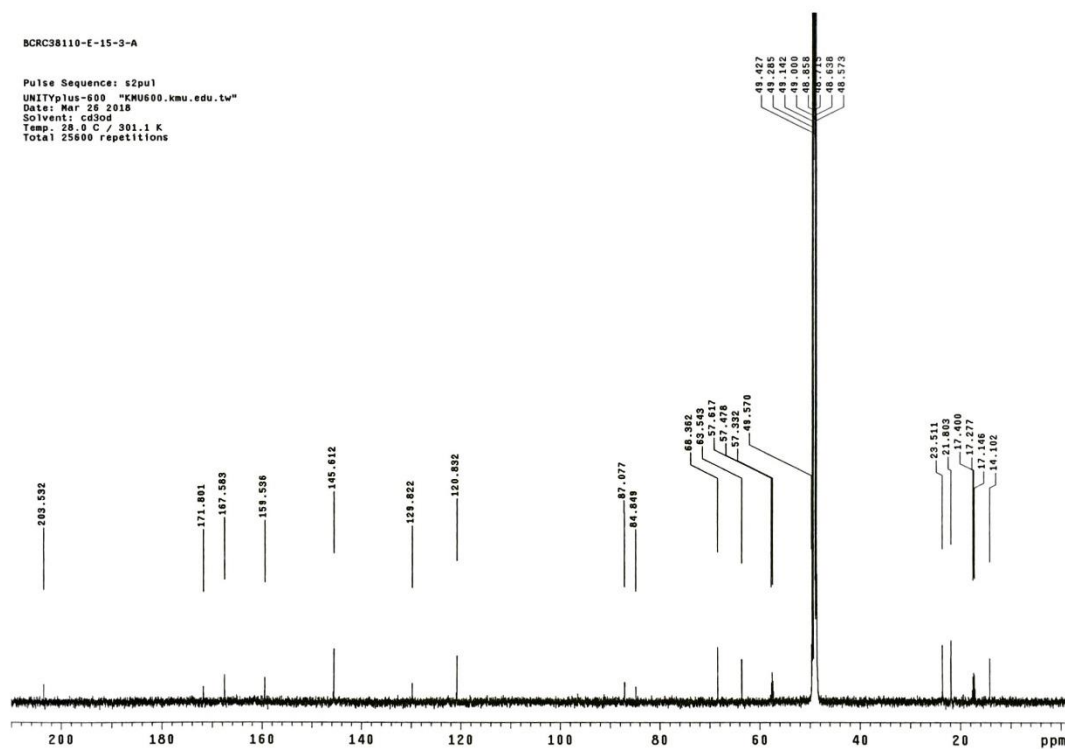


Figure S2. ^{13}C NMR spectrum of 5S,6S-monaspurpyridine A (**1**) in CD_3OD at 125 MHz

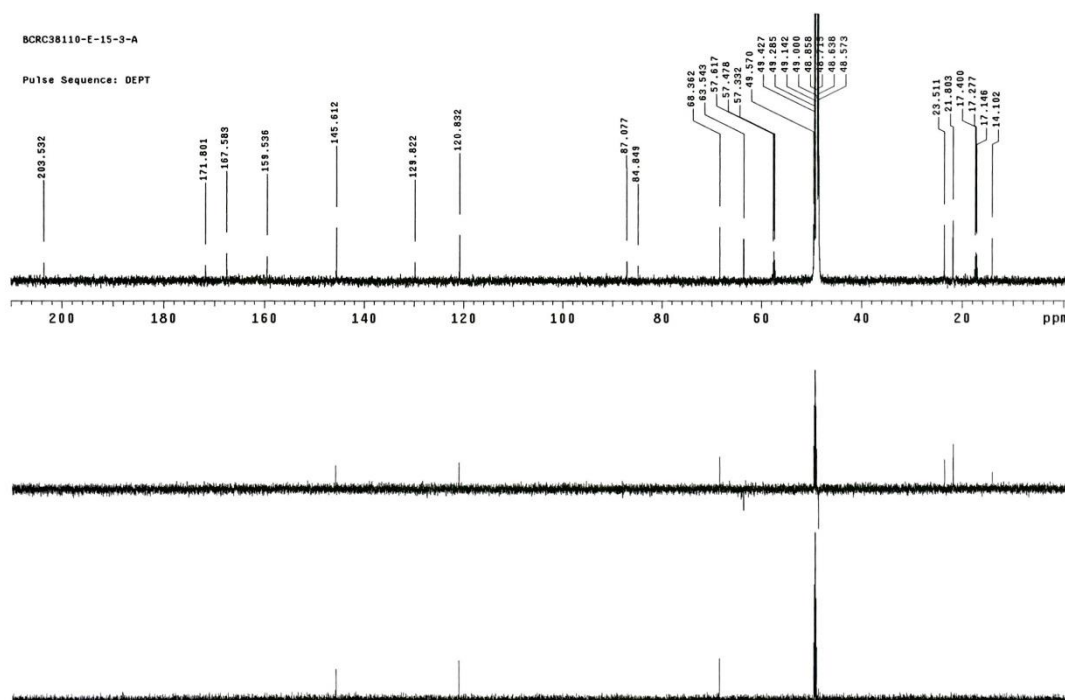


Figure S3. DEPT spectrum of 5S,6S-monaspurpyridine A (1)

BCRC38110-E-15-3-A

exp28 gCOSY

date Mar 26 2018 hs flags nn

solvent cd3od sspul y

sample hsglv 5323

ACQUISITION SPECIAL

sw 9542.0 temp 28.0

at 0.150 gain 53

np 2862 spin not used

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

nt 160 sb1 not used

d2 PRESATURATION 0 proci lp

satmode n fnl DISPLAY 4096

wet TRANSMITTER n sp -122.8

tn H1 ep1 8089.5

sfrq 597.279 wp1 -122.1

torf 597.3 rfp 8089.5

tpwr 58 rfp 1180.4

pv 12.000 rfp1 0

GRADIENTS rfp1 0

gzlvie 4444 PLOT

giz 0.001000 wc 140.0

Edratio 1.000 sc 5.0

gstab 0.000500 wc2 140.0

DECOUPLER sc2 5.0

dn C13 vs 1000

da nn al cdc av 8

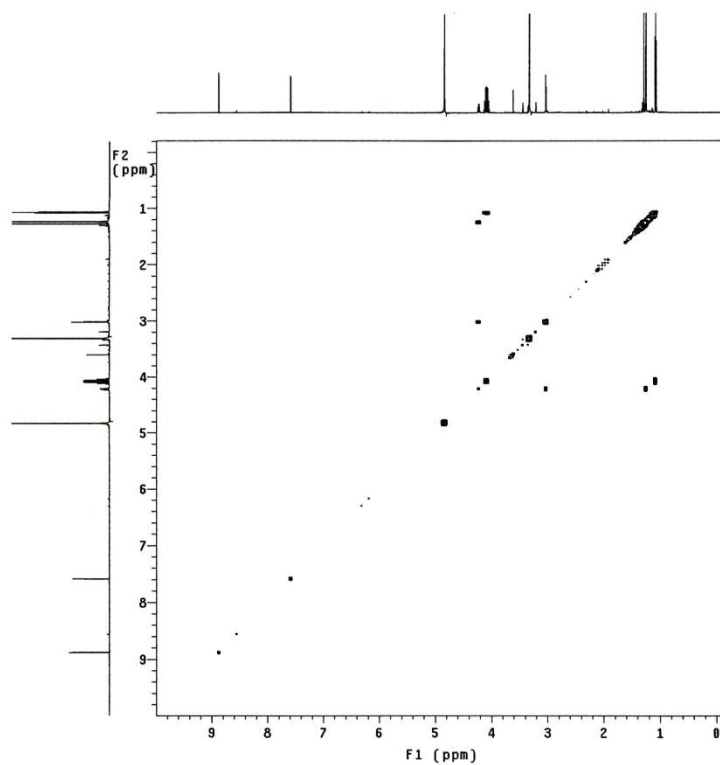


Figure S4. COSY spectrum of 5S,6S-monaspurpyridine A (1)

BCRC38110-E-15-3-A

Pulse Sequence: gHMBCAD

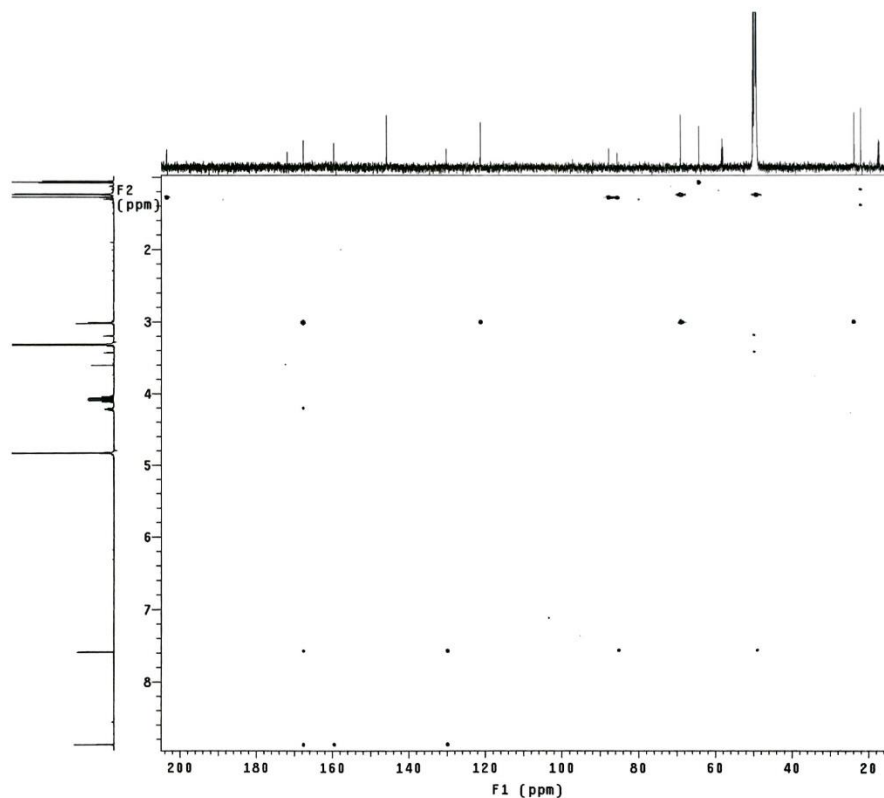


Figure S5. HMBC spectrum of 5S,6S-monapurpyridine A (1)

BCRC38110-E-15-3-A

exp29 NOESY

SAMPLE		FLAGS	
date	Mar 26 2018	hs	nn
solvent	cd3od	sspul	y
sample	PF01g	y	
ACQUISITION			
sw	9542.0	hsglv1	5328
at	0.150	temp	SPECIAL 28.0
np	2862	gain	48
fb	4000	spin	not used
ss	32	f2	PROCESSING
dl	1.500	gf	0.069
nt	40	dfs	not used
2D ACQUISITION			
sw1	9542.0	gf1	PROCESSING
nt1	160	gf1	0.014
TRANSMITTER			
tn	H1	gfsl	not used
sfrq	597.279	fn1	1p
tof	597.3	fn1	4096
tpwr	58	sp	DISPLAY -120.0
pw	12.000	wp	6089.5
NOESY			
mixN	0.600	wp1	6089.5
PRESATURATION			
satmode	n	rf1	1186.9
wet	n	rf11	0
DECOUPLER			
dn	C13	rfp1	1182.0
da	nnn	rfp1	0
PLOT			
wc	140.0		
sc	5.0		
vc2	140.0		
sc2	5.0		
vs	321		
th	4		
al	cdc	ph	

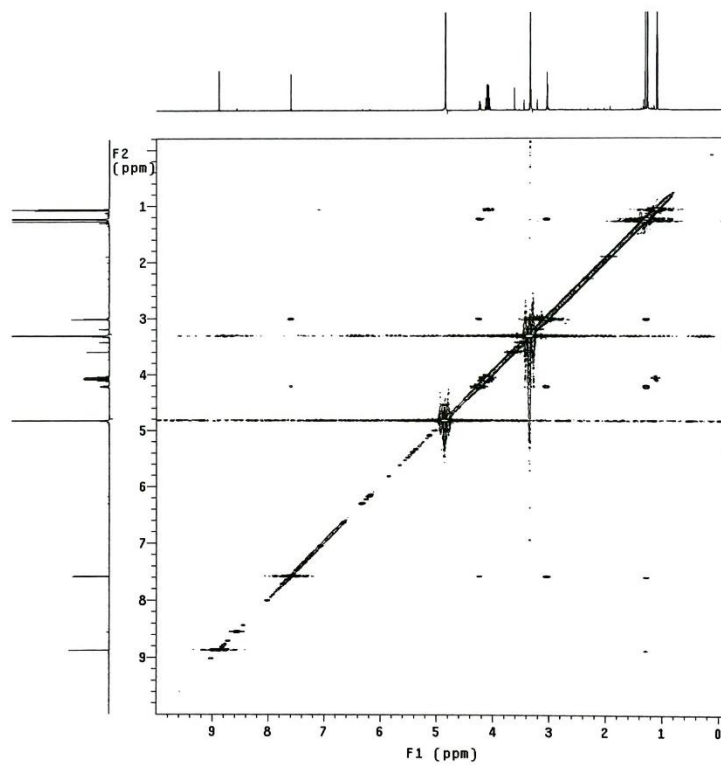


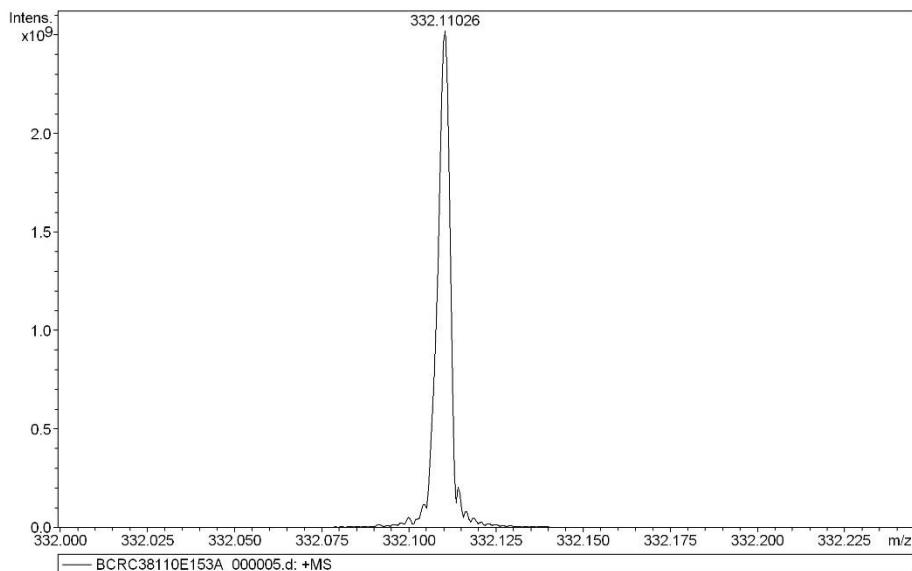
Figure S6. NOESY spectrum of 5S,6S-monapurpyridine A (1)

Mass Spectrum SmartFormula Report

Analysis Info

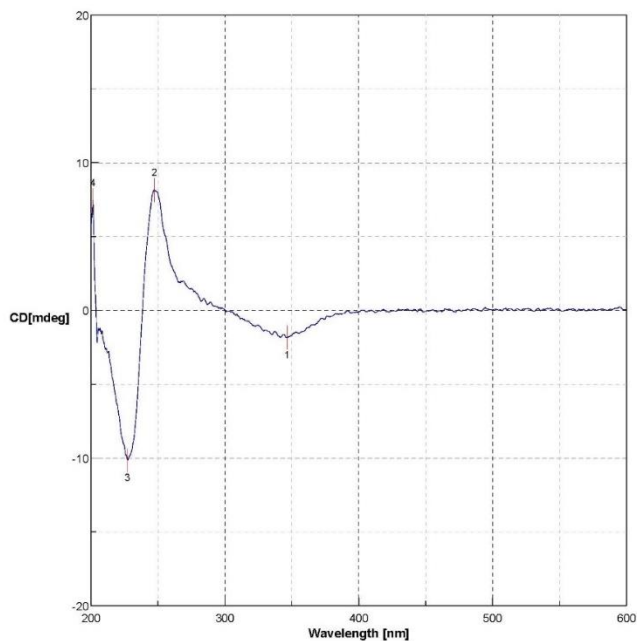
Analysis Name D:\Data\7\BCRC38110E153A_000005.d
 Method broadband first signal
 Sample Name BCRC38110-E-15-3-A
 Comment ESI Positive

5/11/2018 3:36:13 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
332.11026	1	C 15 H 19 N Na O 6	100.00	332.11046	0.20	0.59	10.1	6.5	even	ok

Figure S7. HRESIMS spectrum of 5S,6S-monapurpyridine A (1)



Date/Time 2018/7/4 9:53 下午
 Operator User
 File Name BCRC38110-E-15-3-A(smooth).jws
 Sample Name
 Comment

No.	nm	CD[mdeg]	No.	nm	CD[mdeg]	No.	nm	CD[mdeg]
1	346.6	-1.84031	2	247.2	8.1544	3	227.4	-10.1339
4	201.4	7.45978						

Figure S8. CD spectrum of 5S,6S-monapurpyridine A (1)

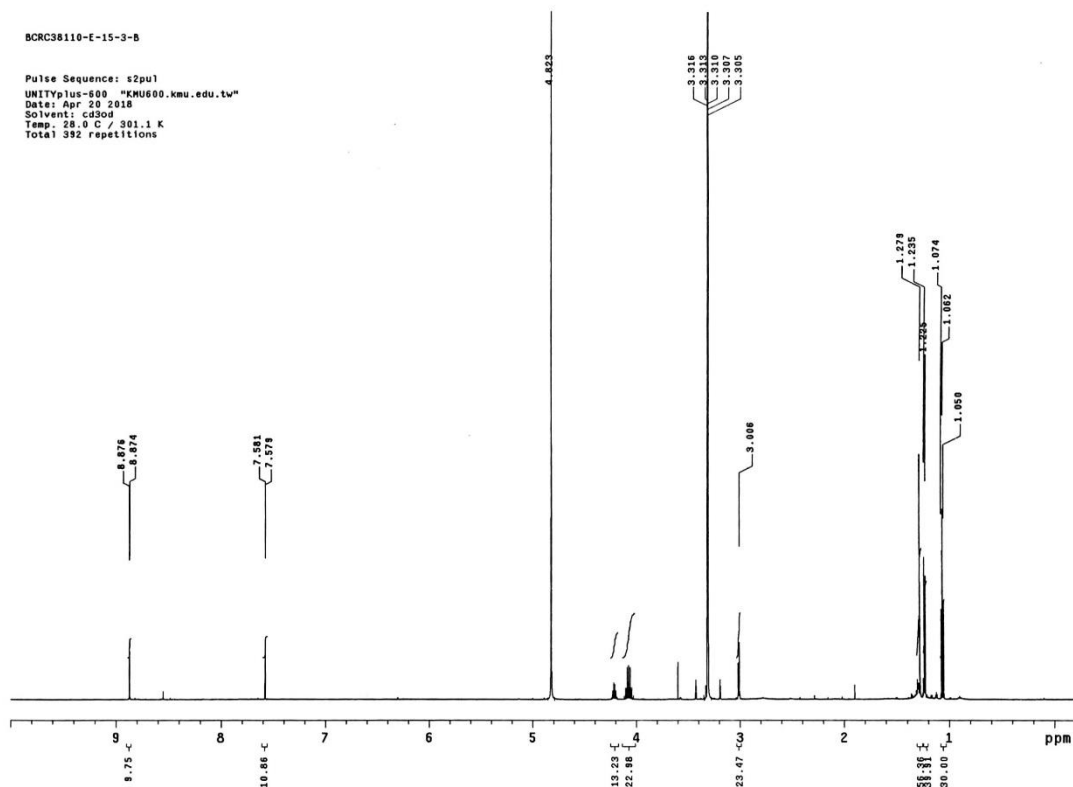


Figure S9. ^1H NMR spectrum of 5R,6R-monaspurpyridine A (**2**) in CD_3OD at 600 MHz

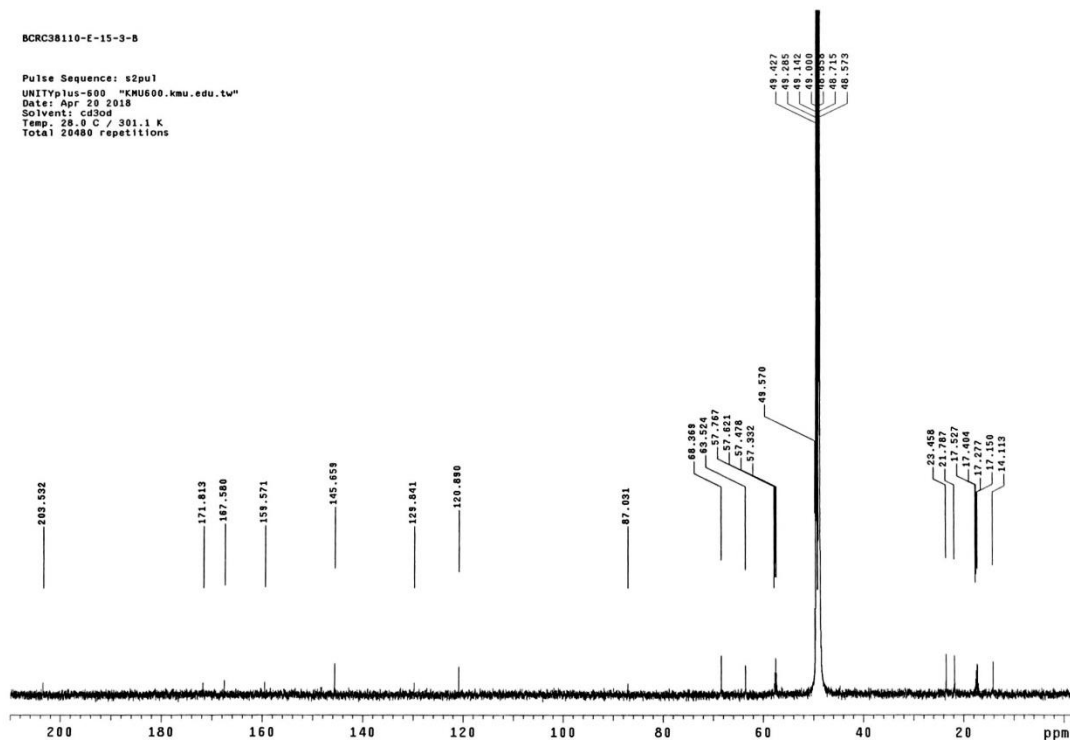


Figure S10. ^{13}C NMR spectrum of 5R,6R-monaspurpyridine A (**2**) in CD_3OD at 125 MHz

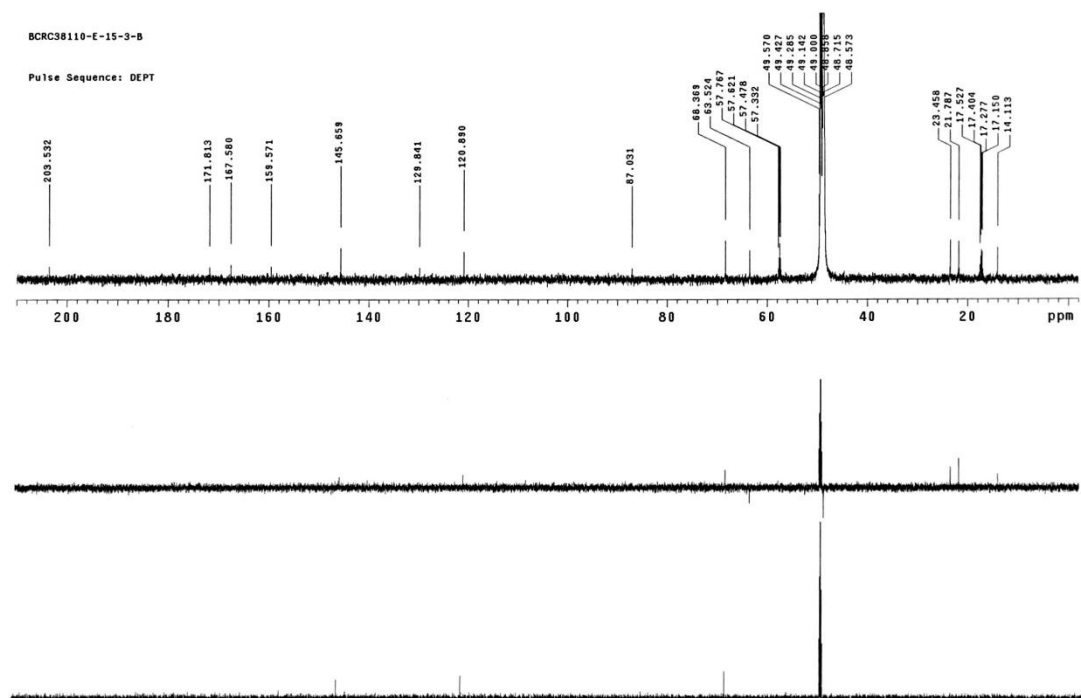


Figure S11. DEPT spectrum of 5R,6R-monaspurpyridine A (2)

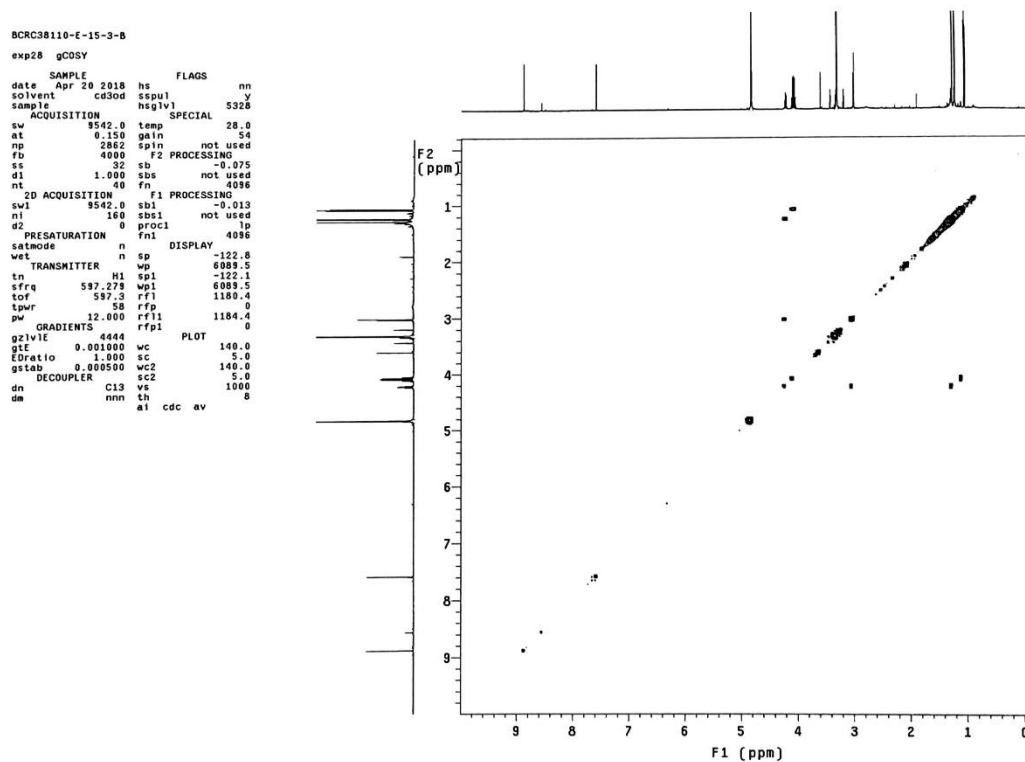


Figure S12. COSY spectrum of 5R,6R-monaspurpyridine A (2)

BCRC38110-E-15-3-B

Pulse Sequence: gHMBCAD

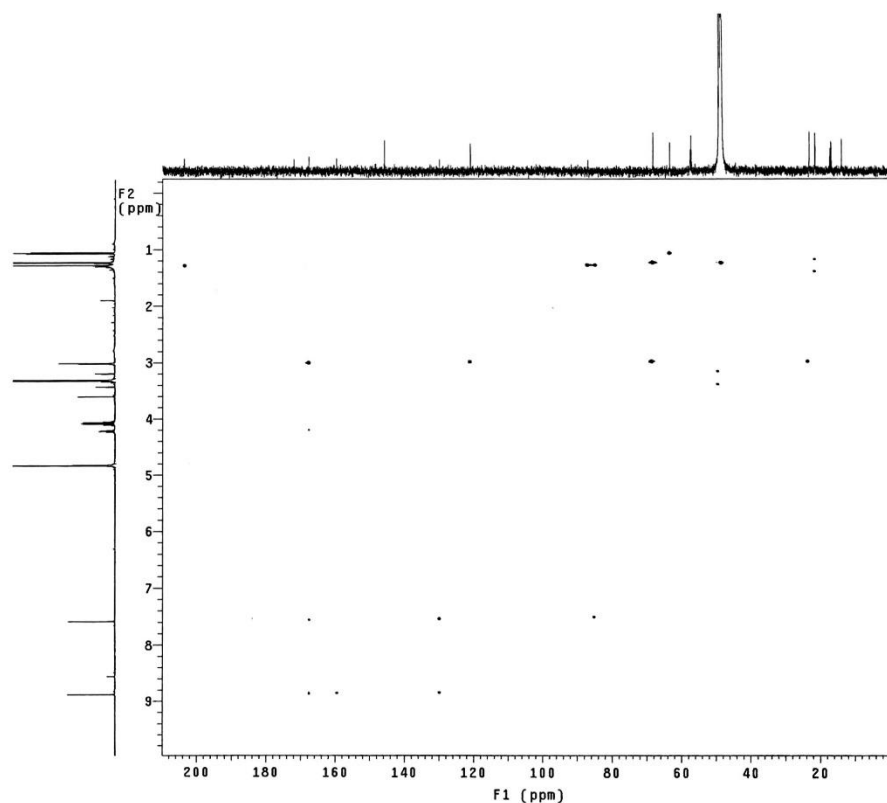


Figure S13. HMBC spectrum of 5R,6R-monaspurpyridine A (2)

BCRC38110-E-15-3-B

exp29 NOESY

SAMPLE		FLAGS	
date	Apr 20 2018	hs	nn
solvent	cd3od	sspul	y
sample		PF01g	y
ACQUISITION		hsglv1	5328
sv	9542.0	SPECIAL	
at	0.150	temp	28.0
np	2862	gain	50
fb	4000	spin	not used
ss	32	F2 PROCESSING	
d1	1.500	gf	0.069
nt	40	gfs	not used
2D ACQUISITION		fn	9096
sw1	9542.0	gf1	0.014
nl	160	gfs1	not used
tn		PROC1	lp
sfrq	597.279	fn1	4096
tof	597.3	sp	DISPLAY
tpwr	58	vp	-120.0
pw	12.000	vp1	6089.5
mixN	NOESY	sp1	-119.8
	0.600	vp1	6089.5
PRESATURATION		rf1	1186.9
satmode	n	rfp	0
wet	n	rf11	1182.0
DECOUPLER		rfp1	0
dn	C13	PLOT	
dm	nnn	vc	140.0
		sc	5.0
		vc2	140.0
		sc2	5.0
		vs	321
		th	4
		a1	cdc ph

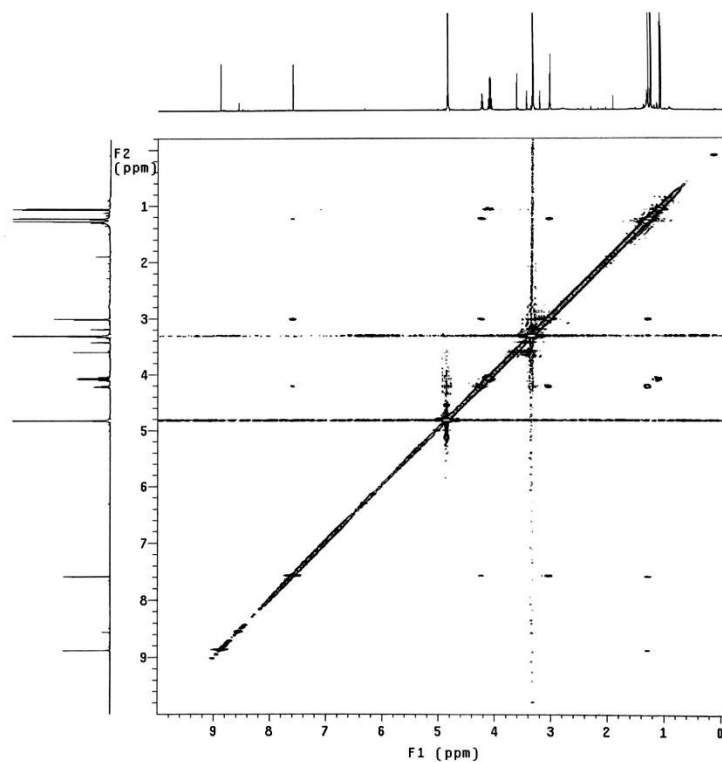


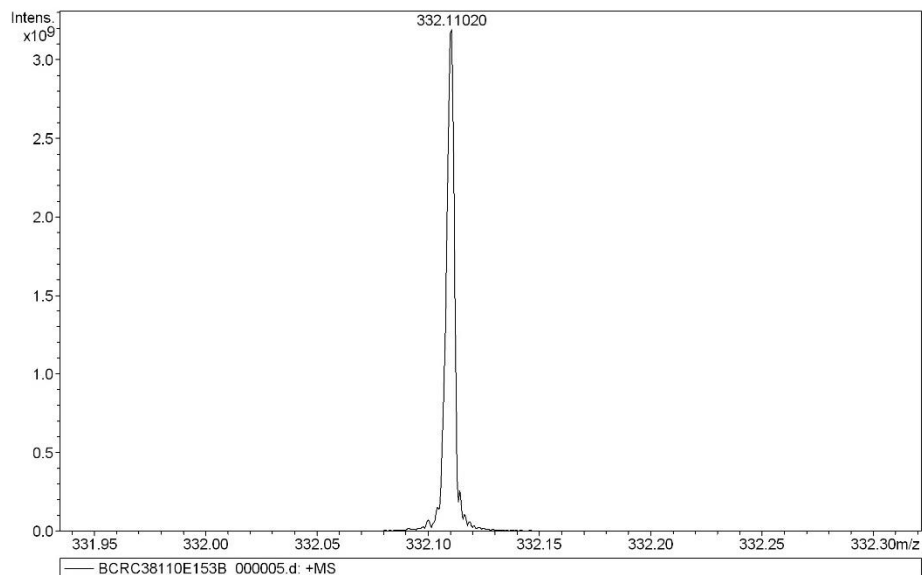
Figure S14. NOESY spectrum of 5R,6R-monaspurpyridine A (2)

Mass Spectrum SmartFormula Report

Analysis Info

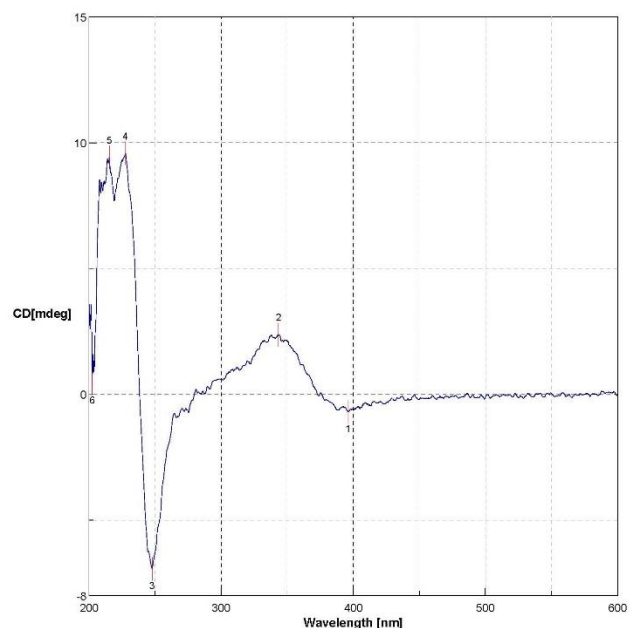
Analysis Name D:\Data\7\BCRC38110E153B_000005.d
 Method broadband first signal
 Sample Name BCRC38110-E-15-3-B
 Comment ESI Positive

5/11/2018 4:08:05 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
332.11020	1	C ₁₅ H ₁₉ N ₃ NaO ₆	100.00	332.11046	0.26	0.78	14.0	6.5	even		ok

Figure S15. HRESIMS spectrum of 5*R*,6*R*-monaspurpyridine A (2)



Date/Time 2018/7/4 10:01
 Operator User
 File Name BCRC38110-E-15-3-B(smooth).jws
 Sample Name
 Comment

No.	nm	CD[mdeg]	No.	nm	CD[mdeg]	No.	nm	CD[mdeg]
1	396.1	-0.683127	2	343.4	2.37172	3	247.7	-6.92546
4	227.6	9.57412	5	215.4	9.41946	6	202.5	0.443001

Figure S16. CD spectrum of 5*R*,6*R*-monaspurpyridine A (2)

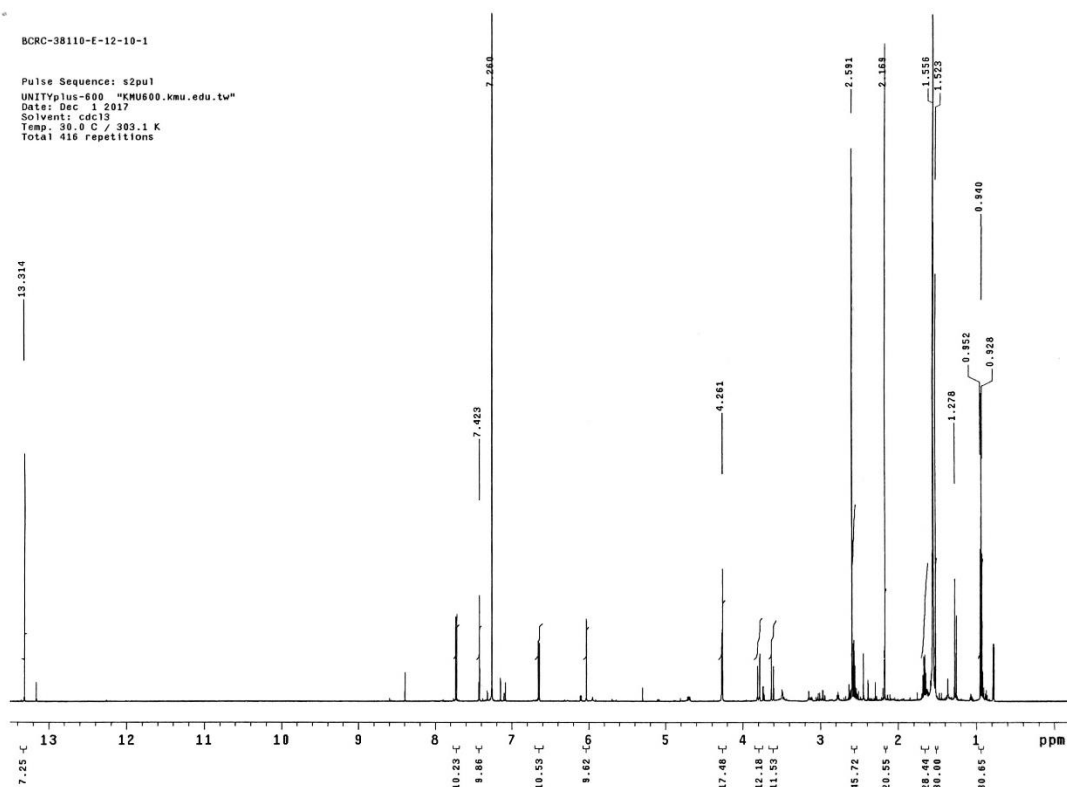


Figure S17. ^1H NMR spectrum of monasxanthone A (**3**) in CDCl_3 at 600 MHz

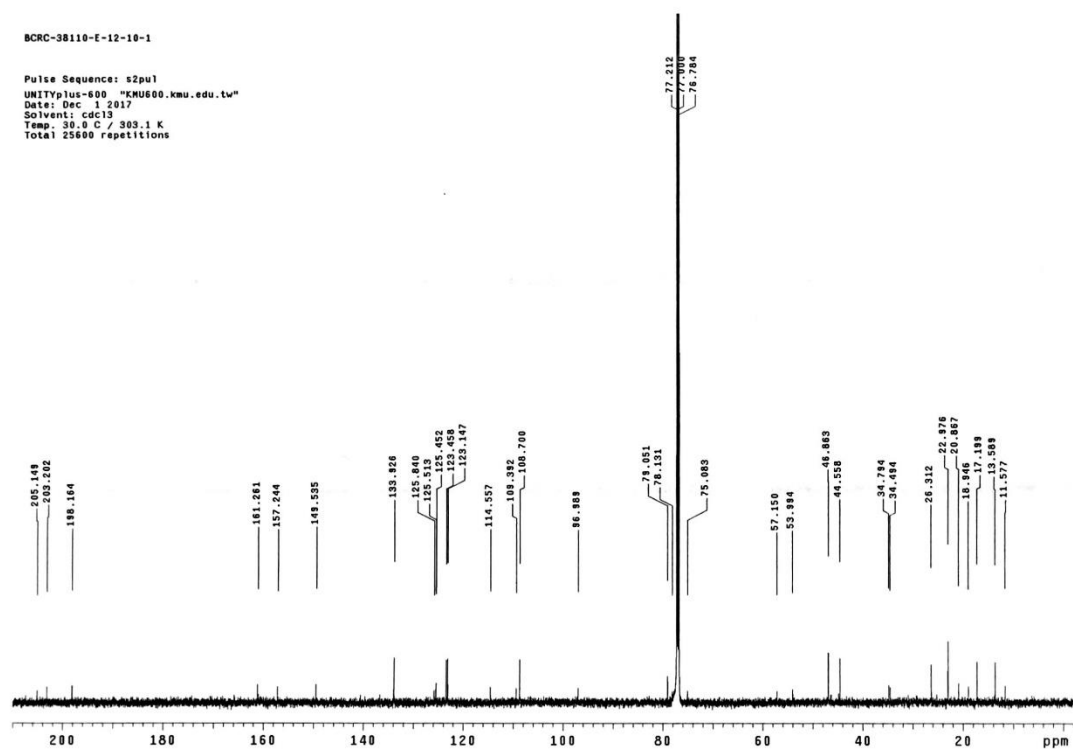


Figure S18. ^{13}C NMR spectrum of monasxanthone A (**3**) in CDCl_3 at 125 MHz

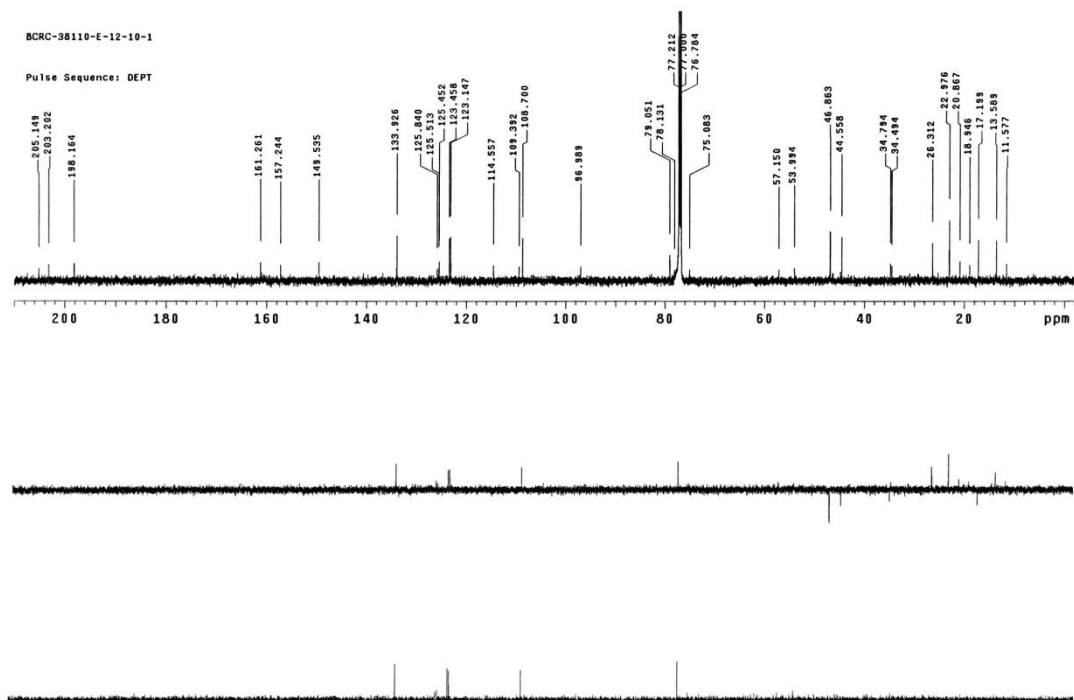


Figure S19. DEPT spectrum of monasxanthone A (3)

BCRC-38110-E-12-10-1

exp49 gCOSY

SAMPLE

date Dec 1 2017 hs

solvent cdc13

sample hsg1v1

ACQUISITION

sv 9542.0 temp

at 0.150 gain

rp 2882 spin

fb 4000 f2 PROCESSING

ss 32 sb

d1 1.000 sbs

nt 40 fn

2D ACQUISITION

sv1 9542.0 sb1

nt 160 sb1

d2 PRESATURATION

satmode n

wet TRANSMITTER

tn H1

sfrq 597.287

tofr 597.2

tpwr 58

GRADIENTS

g2lvie 4024

g2 0.001000

EDratio 1.000

gstab 0.000500

DECOUPLER

dn C13

dm nnn

nnn

th

av

8

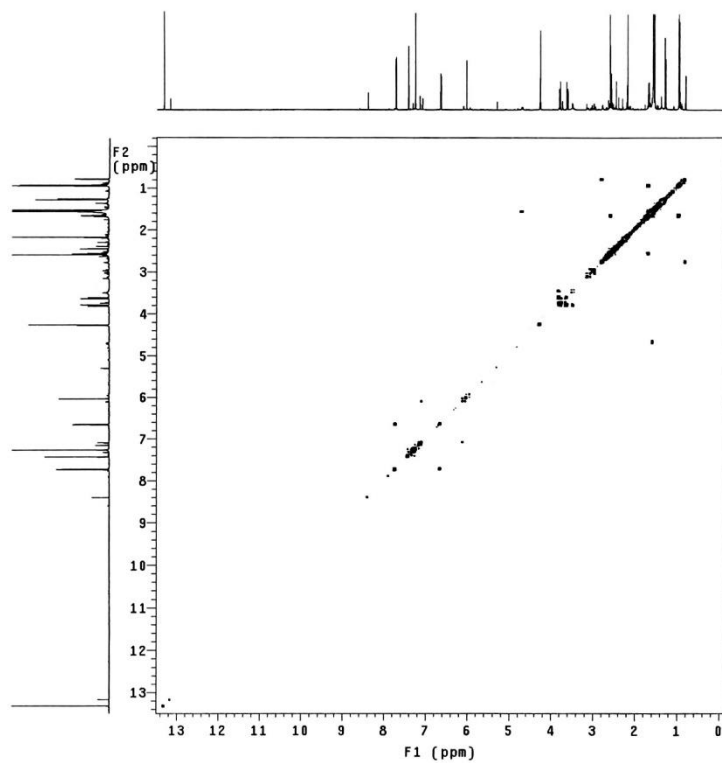


Figure S20. COSY spectrum of monasxanthone A (3)

BCRC-38110-E-12-10-1

Pulse Sequence: gHMBCAD

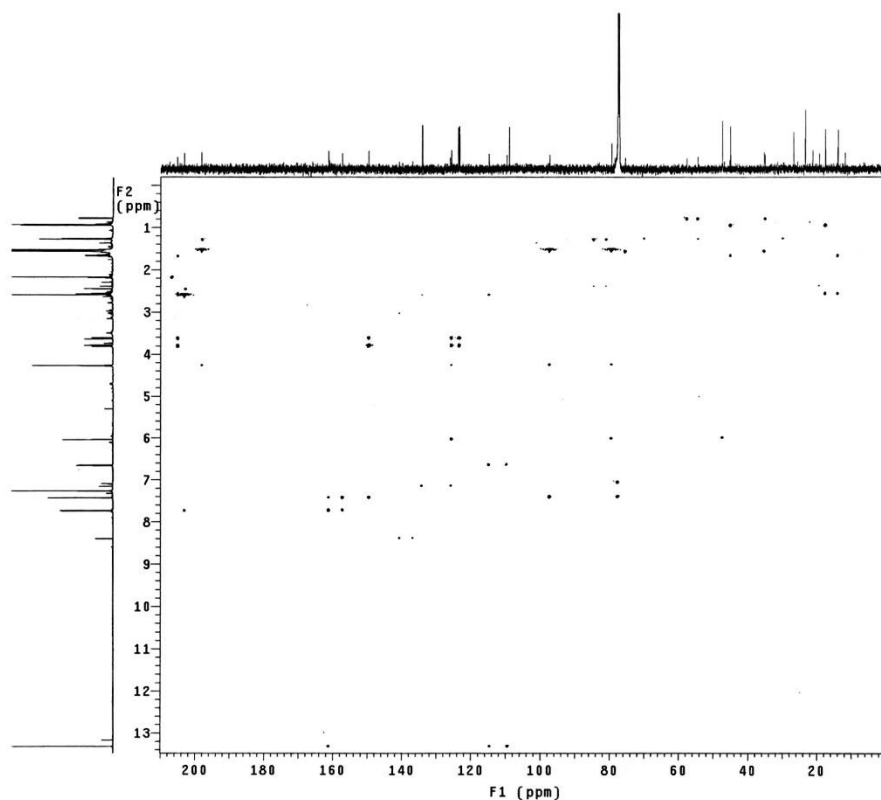


Figure S21. HMBC spectrum of monasxanthone A (3)

BCRC-38110-E-12-10-1

exp50 NOESY

SAMPLE		FLAGS	
date	Dec 1 2017	hs	nn
solvent	cdc13	sspul	y
sample		PF01g	y
ACQUISITION		hsglv1	5304
sv	9542.0	SPECIAL	30.0
at	0.150	temp	50
np	2862	gain	not used
fb	4000	spin	not used
ss	32	F2 PROCESSING	
d1	1.500	qf	0.059
nt	40	qfs	not used
2D ACQUISITION		fn	4096
sw1	9542.0	gf1	0.019
nt	160	gfsl	not used
tn		H1	lp
sfreq	597.287	fn1	4096
tof	597.2	sp	-124.0
tpwr	58	wp	8181.5
pw	12.500	ep1	-124.0
mixN	0.600	wp1	8181.5
PRESATURATION		rf1	1195.7
satmode	n	rfp	0
wet	n	rf11	1195.7
DECOUPLER		rfp1	0
dn	C13	PLOT	
da	nnn	vc	140.0
		sc	5.0
		vc2	140.0
		sc2	5.0
		vs	975
		th	2
		al	cdc ph

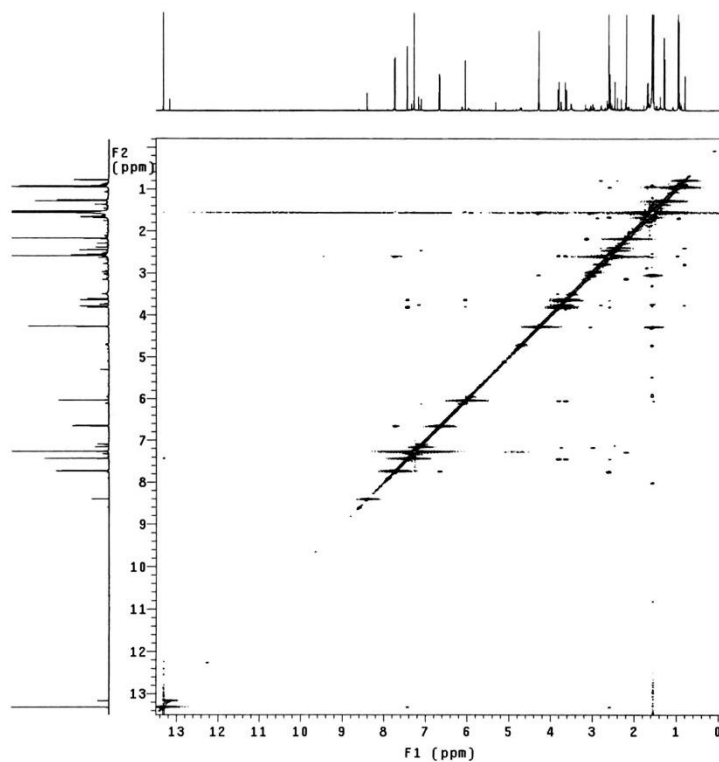


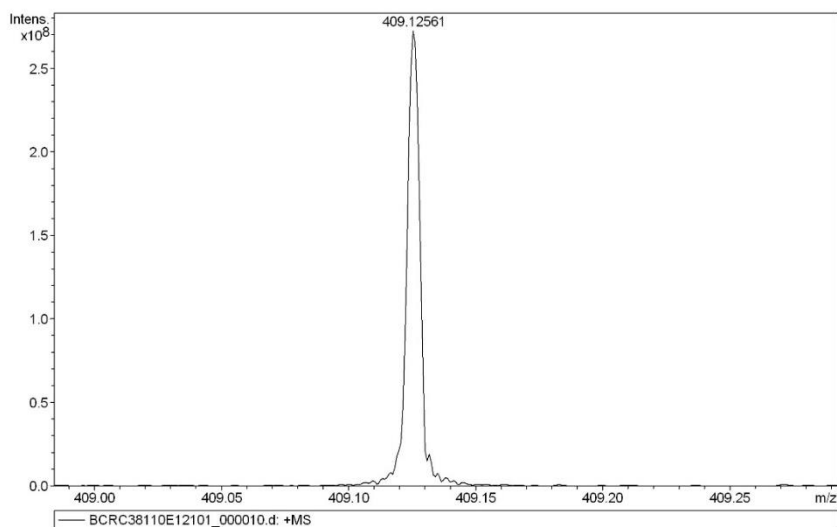
Figure S22. NOESY spectrum of monasxanthone A (3)

Mass Spectrum SmartFormula Report

Analysis Info

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Method broadband first signal
Sample Name BCRC38110-E-12-10-1
Comment ESI Positive

1/12/2018 4:53:40 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
409.12561	1	C ₂₁ H ₂₂ NaO ₇	100.00	409.12577	0.17	0.41	15.9	10.5	even	ok

Figure S23. HRESIMS spectrum of monasxanthone A (3)

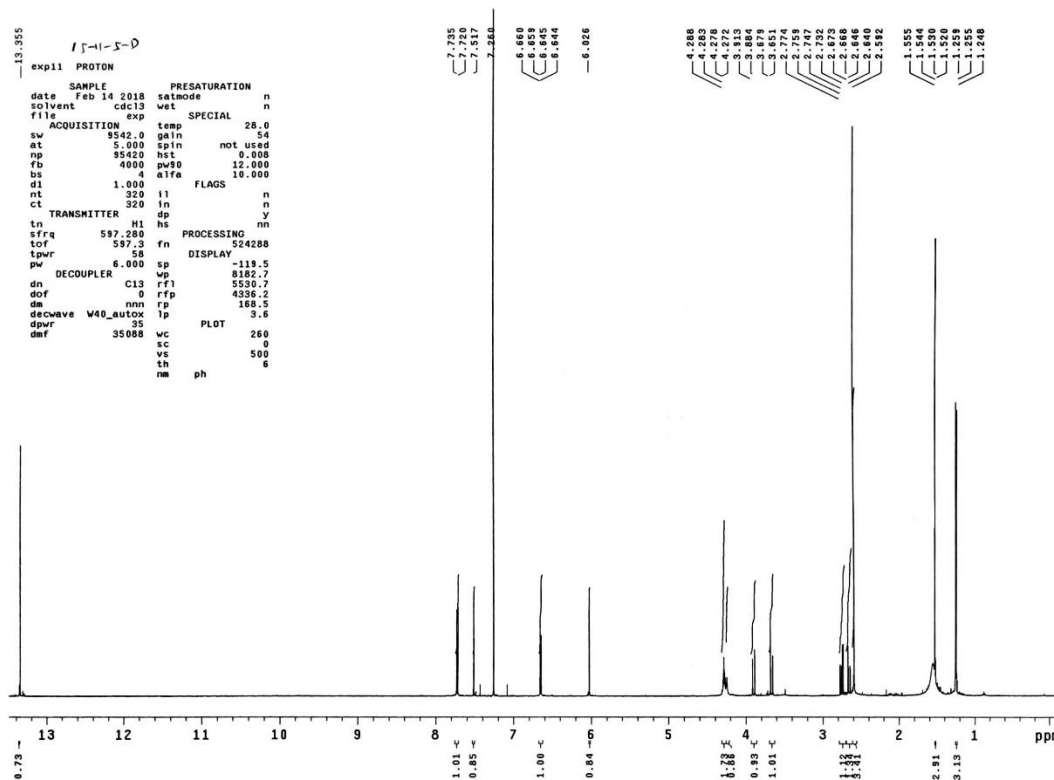


Figure S24. ¹H NMR spectrum of monasxanthone B (4) in CDCl₃ at 600 MHz

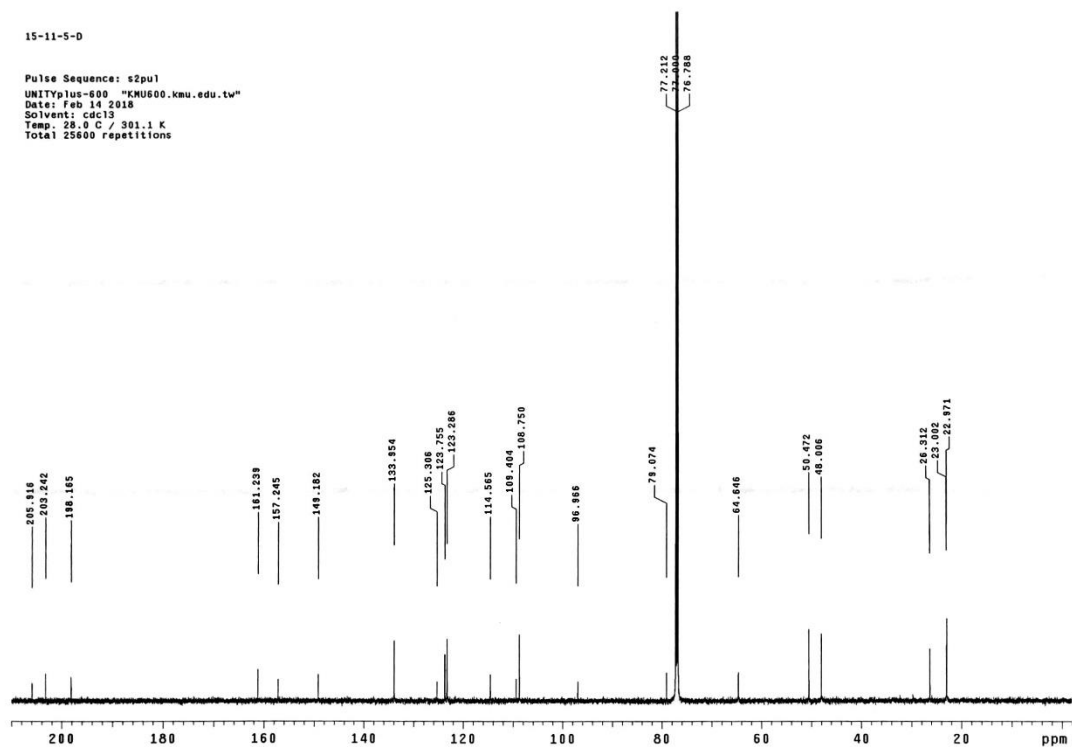


Figure S25. ^{13}C NMR spectrum of monasxanthone B (**4**) in CDCl_3 at 125 MHz

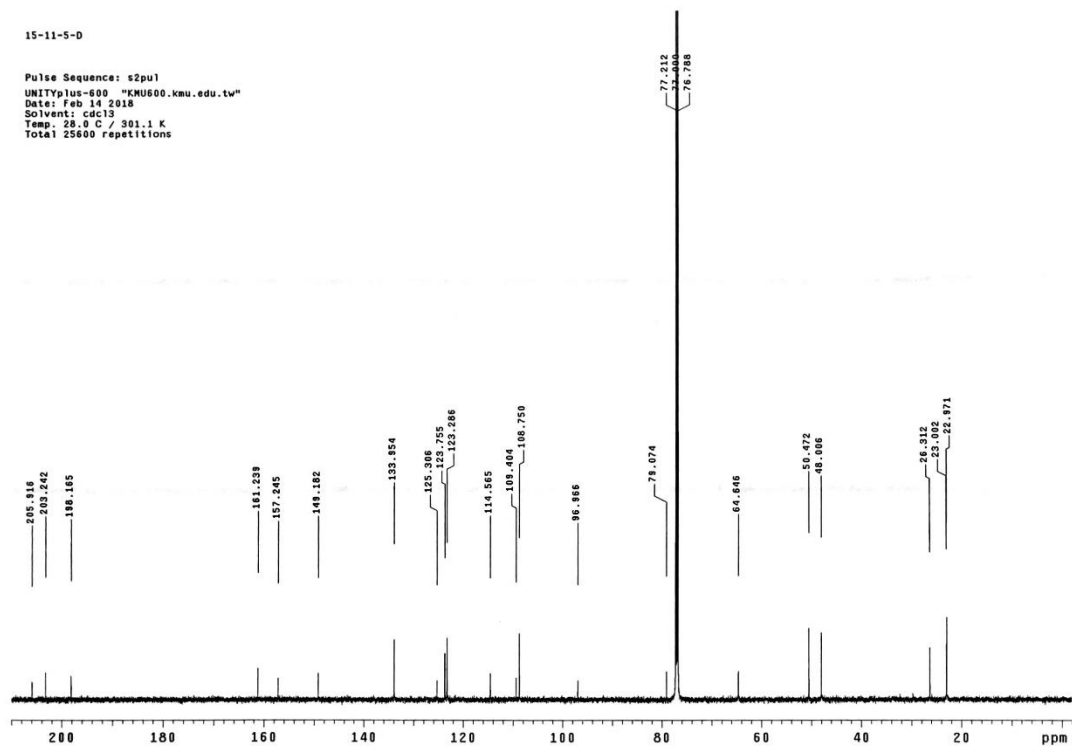


Figure S26. DEPT spectrum of monasxanthone B (**4**)

exp14 gCOSY

date	Feb 14 2018	hs	flags	nm
solvent	cdcl3	sspul		y
sample	hsglv1	5328		
ACQUISITION				
sw	9542.0	temp	28.0	
at	0.150	gain	54	
np	2882	spin	not used	
fb	4000	f2 PROCESSING		
ss	32	sb	-0.075	
d1	1.000	sbs	not used	
nt	40	fn	4095	
2D ACQUISITION				
sw1	9542.0	sb1	-0.013	
nl	180	sbs1	not used	
d2	0	procl	lp	
PRESATURATION				
satmode	n	fn1	4095	
wet	n	sp	-1.7	
TRANSMITTER				
tn	H1	sp1	-1.7	
sfrq	597.280	wp1	8242.1	
tor	597.3	rf1	1194.5	
tpwr	58	rffp	0	
pw	12.000	rff1	1194.5	
GRADIENTS				
g2lv1E	4444	PL0T		
g1E	0.001000	vc	140.0	
Edratio	1.000	sc	5.0	
gstab	0.000500	vc2	140.0	
DECOUPLER				
dn	C13	vs	165	
dm	nnn	th	cdc av	7

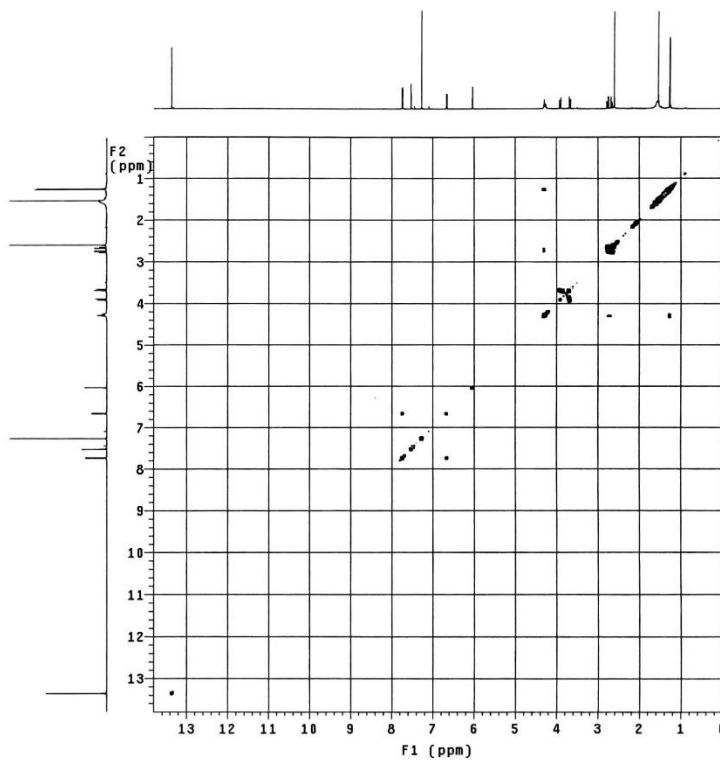


Figure S27. COSY spectrum of monasxanthone B (4)

Pulse Sequence: gHMBCAD

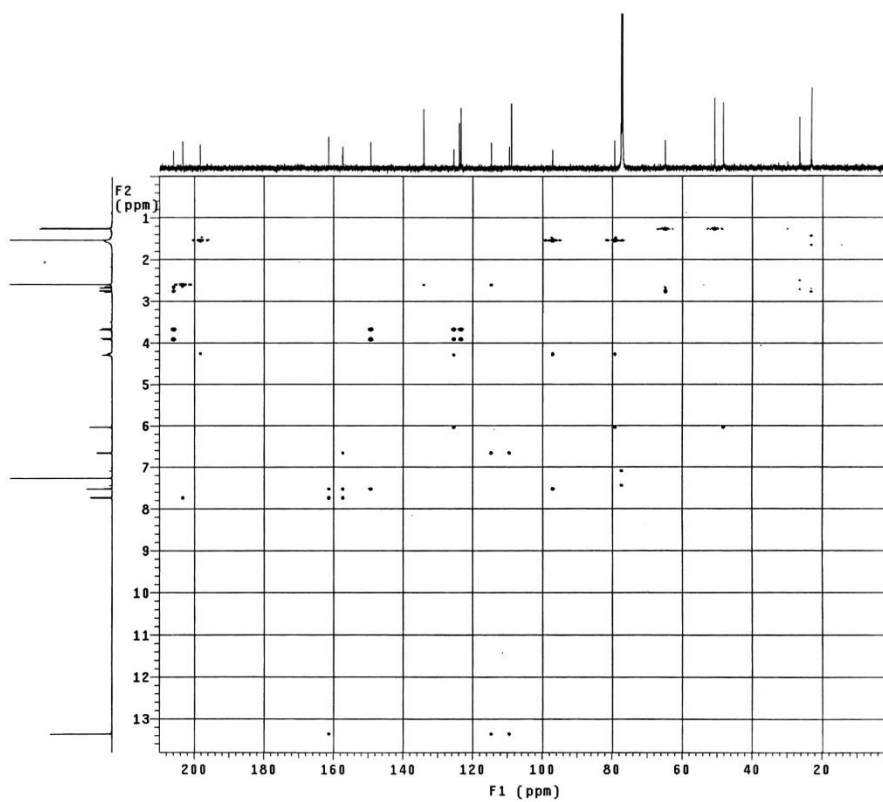


Figure S28. HMBC spectrum of monasxanthone B (4)

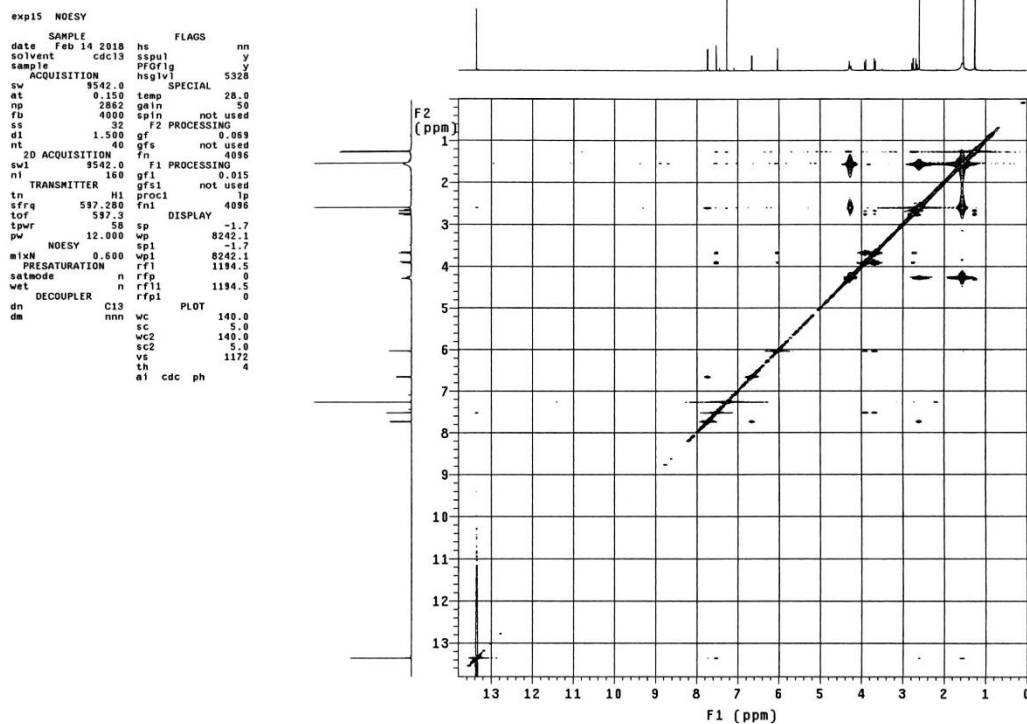


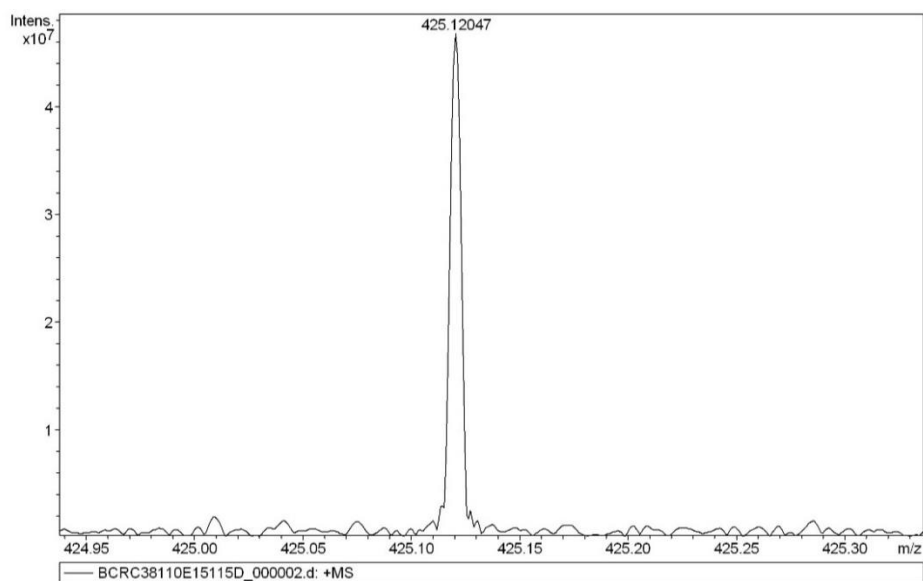
Figure S29. NOESY spectrum of monasxanthone B (4)

Mass Spectrum SmartFormula Report

Analysis Info

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 Sample Name BCRC48110-E-15-11-5-D
 Comment ESI Positive

3/12/2018 2:54:25 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
425.12047	1	C 21 H 22 Na O 8	100.00	425.12069	0.22	0.52	20.6	10.5	even	ok

Figure S30. HRESIMS spectrum of monasxanthone B (4)

15-3-C_COSY
exp21 gCOSY

SAMPLE		FLAGS	nn
date	Mar 22 2018	hs	nn
solvent	acetone	sspl	Y
sample		hsglv	5328
ACQUISITION		SPECIAL	
sw	9542.0	temp	28.0
at	0.150	goin	54
np	2862	spin	0
fb	4000	F2 PROCESSING	
ss	32	sb	-0.075
d1	1.000	sbs	not used
nt	64	fn	4096
2D ACQUISITION		F1 PROCESSING	
sw1	9542.0	sb1	-0.017
n1	160	sbs1	not used
d2	0	procl	1p
PRESATURATION		fn1	4096
satmode	n	sp	-1.5
wet	TRANSMITTER	vp	6089.5
tn	H1	sp1	-1.5
sfrq	597.280	vp1	6089.5
tof	597.3	rf1	1184.9
tpwr	58	rfp	0
pw	12.000	rf11	1184.9
GRADIENTS		rfp1	0
g2lv1e	4444	PLOT	
g1e	0.001000	vc	140.0
Edratio	1.000	sc	5.0
gsteb	0.000500	wc2	140.0
DECOUPLER	sc2	vc2	5.0
dn	C13	vs	2343
dm	nnn	th	8
	et	cdc	av

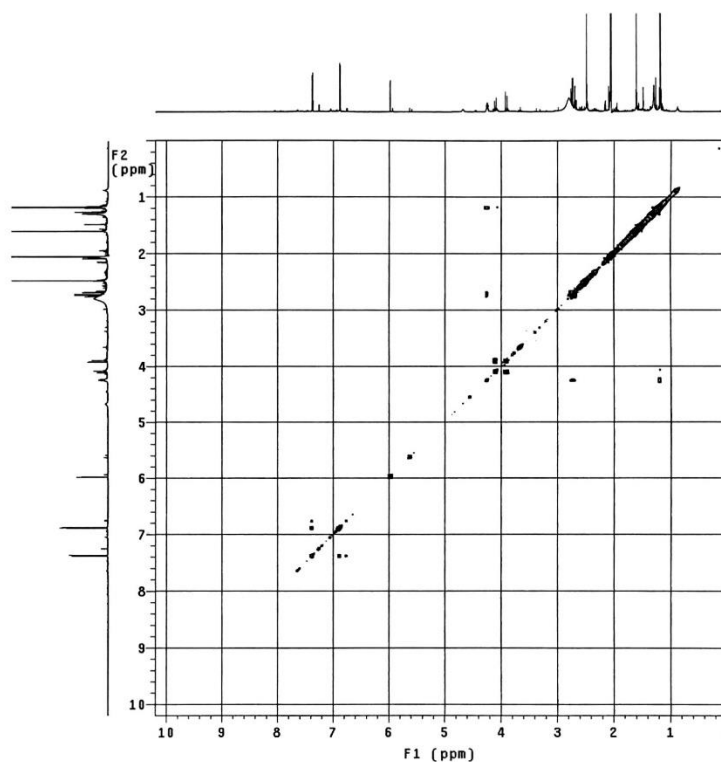


Figure S33. COSY spectrum of monasnaphthalenone (5)

BCRC38110-E-15-3-C

Pulse Sequence: gHMBC

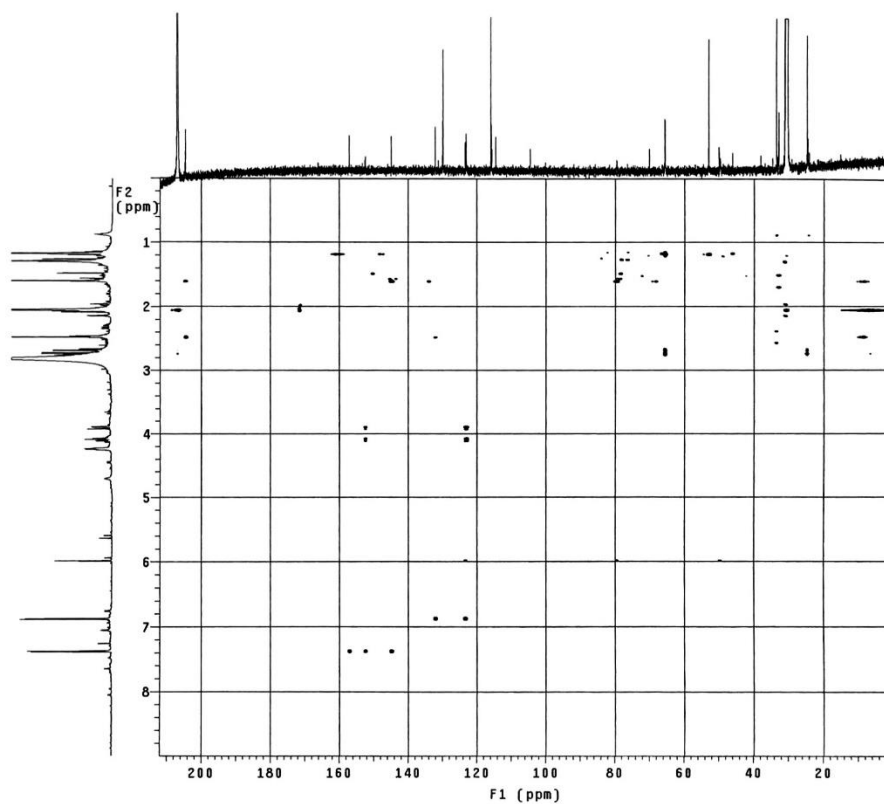


Figure S34. HMBC spectrum of monasnaphthalenone (5)

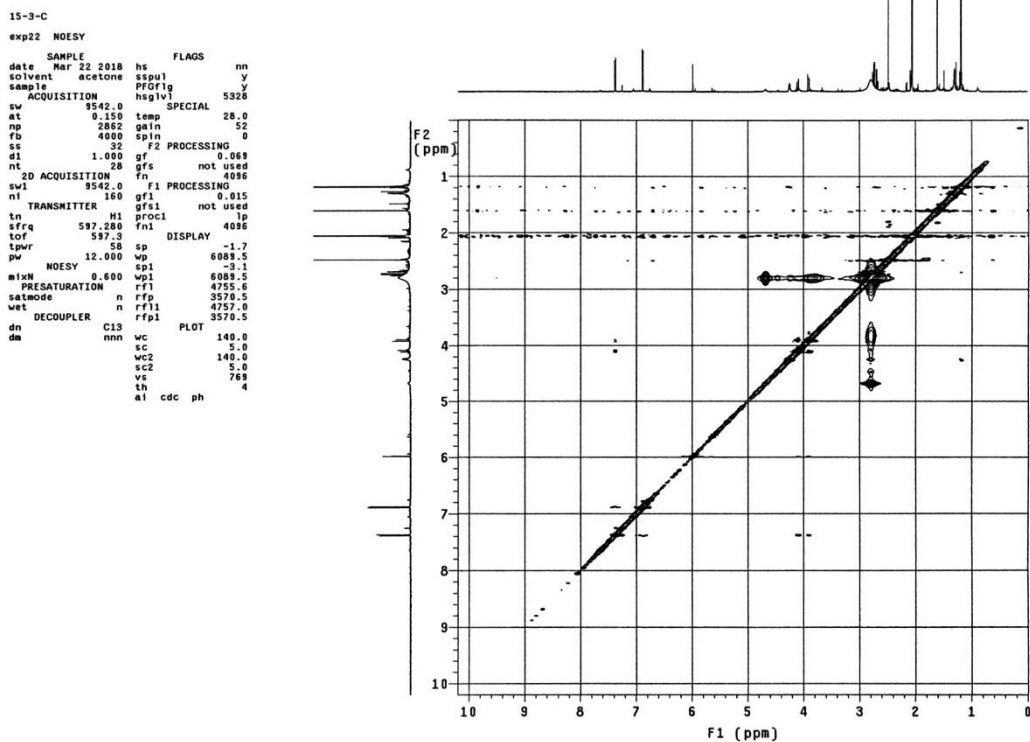
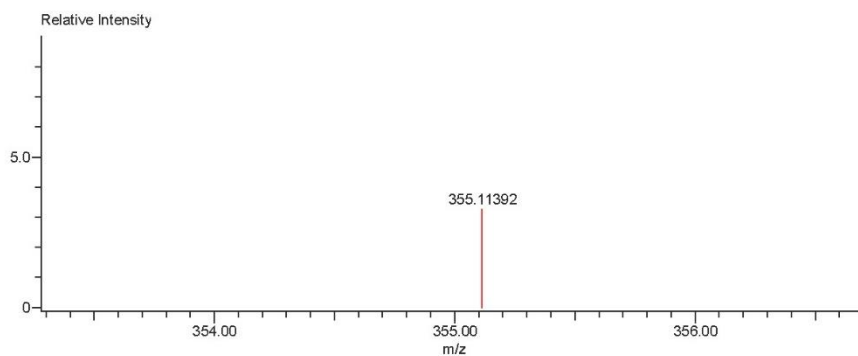


Figure S35. NOESY spectrum of monasnaphthalenone (5)

Data:BCRC38110-E-15-3-C
Comment:
Description:
Ionization Mode:ESI+
History:Average(MS[1] 0.37..0.43)

Acquired:5/2/2018 11:18:35 AM
Operator:AccuTOF
m/z Calibration File:20180418-1TFANA...
Created:5/2/2018 12:03:17 PM
Created by:

Charge number:1 Tolerance:100.00[ppm], 5.00 .. 15.00[... Unsaturation Number:-200.0 .. 500.0 (...
Element:¹²C:18 .. 18, ¹H:0 .. 21, ¹⁰B:0 .. 0, ⁷⁹Br:0 .. 0, ³⁵Cl:0 .. 0, ¹⁹F:0 .. 0, ¹²⁷I:0 .. 0, ¹⁴N:0 .. 0, ²³Na:0 .. 1, ¹⁶O:6 .. 6, ...



Mass	Intensity	Calc. Mass	Mass Difference [mDa]	Mass Difference [ppm]	Possible Formula
355.11392	1183.60	355.11576	-1.84	-5.17	¹² C ₁₈ ¹ H ₂₀ ²³ Na ₁ ¹⁶ O ₆

Figure S36. HRESIMS spectrum of monasnaphthalenone (5)

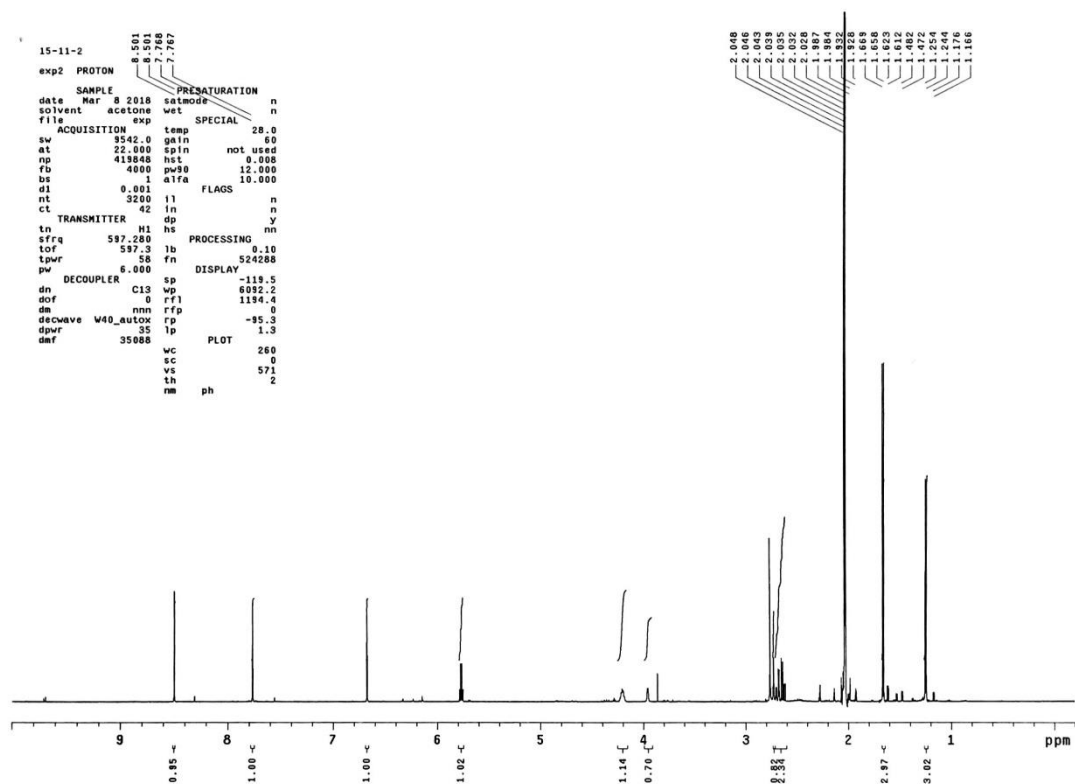


Figure S37. ^1H NMR spectrum of monapurpurin (6) in acetone- d_6 at 600 MHz

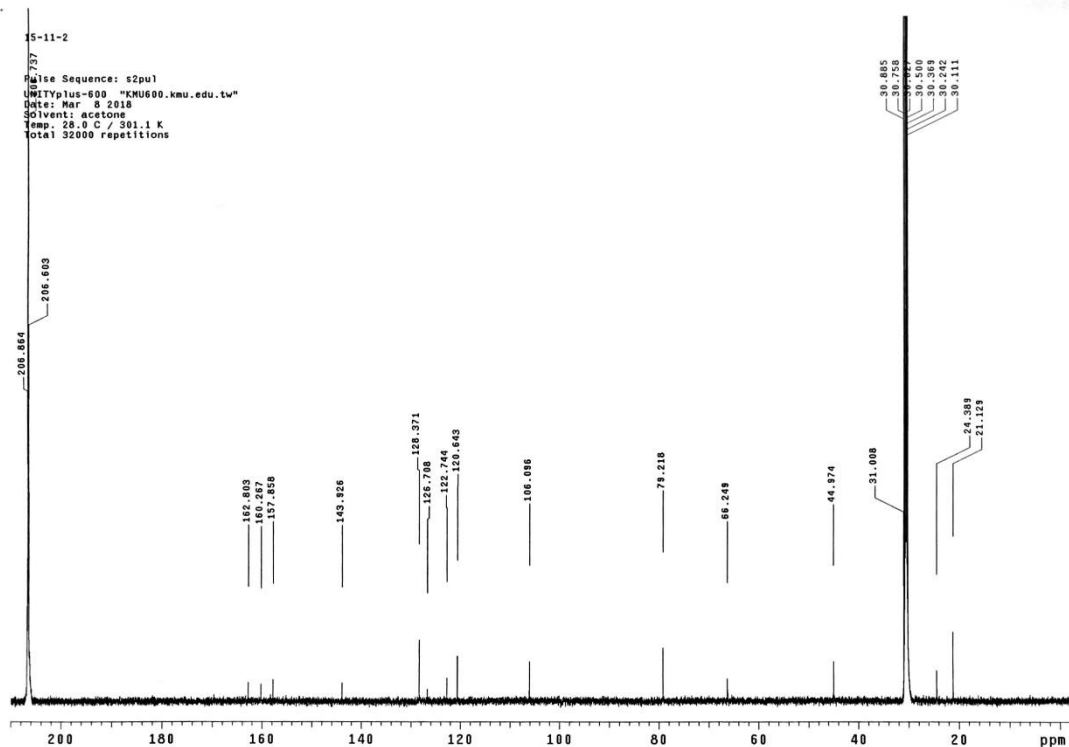


Figure S38. ^{13}C NMR spectrum of monapurpurin (6) in acetone- d_6 at 125 MHz

15-11-2_COSY_acetone-d6

exp21 gCOSY

```

SAMPLE      FLAOS      nm
date May 24 2018 hs
solvent acetone sspul y
sample hsglv1 5328
ACQUISITION SPECIAL
sw 9542.0 temp 28.0
at 0.150 gain 58
np 2862 spin 0
fb 4000 F2 PROCESSING
ss 32 sb sb -0.075
d1 1.000 sbs not used
nt 18 fn 4096
2D ACQUISITION F1 PROCESSING
sw1 9542.0 sb1 -0.017
ni 160 sbs1 not used
d2 0 proc1 lp
PRESATURATION fml 4096
satmode n DISPLAY
wet n sp -1.5
TRANSMITTER H1 wp 6089.5
tn H1 sp1 -1.5
sfrq 597.280 wp1 6089.5
tof 597.3 rff 1184.9
tpwr 58 rfp 0
pw 12.000 rff1 1184.9
GRADIENTS rfp1 0
gzlvie 1444 PLOT
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 2343
dm nnn th 8
ai cdc av

```

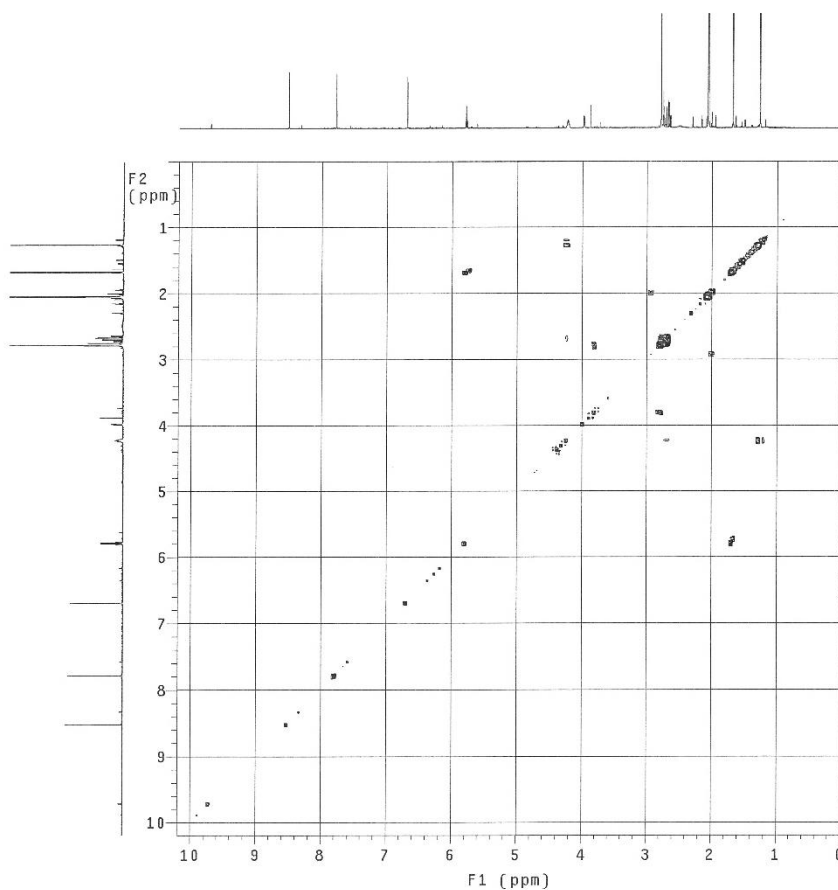


Figure S39. COSY spectrum of monapurpurin (6)

15-11-2

Pulse Sequence: gHMBCAD

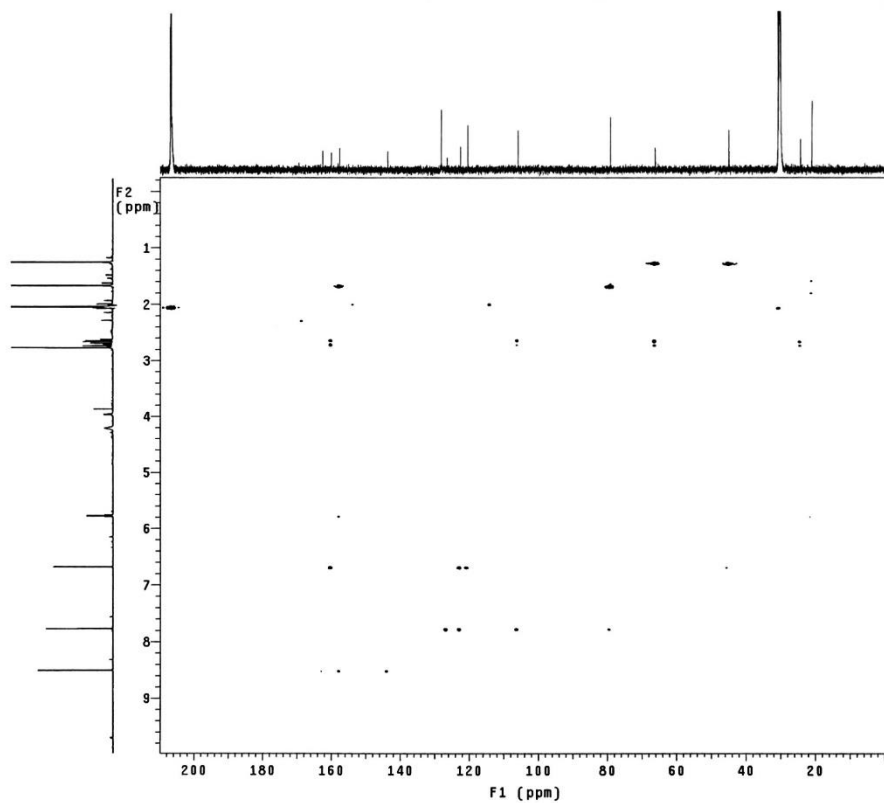


Figure S40. HMBC spectrum of monapurpurin (6)

15-11-2_NOESY_acetone-d6

exp22 NOESY

SAMPLE hs nn
date May 24 2018 sspul y
solvent acetone PFG1g
sample Y 5328
ACQUISITION SPECIAL
sw 9542.0
at 0.150 temp 28.0
np 2862 gain 54
fb 4000 spin 0
ss 32 F2 PROCESSING
d1 1.500 gf 0.069
nt 48 gfs not used
2D ACQUISITION fn 4096
sw1 9542.0 F1 PROCESSING
nt 160 gf1 0.014
TRANSMITTER H1 gfs1 not used
tn H1 procl lp
sfreq 597.280 fnl 4096
tof 597.3
tpwr 58 sp -2.6
pw NOESY 12.000 wp 5988.4
mixN 0.600 wp1 5988.4
PRESATURATION rf1 1186.0
satmode n rfp 0
wet n rfp1 1187.5
dn DECOUPLER C13 rfp1 0
dm nnn wc PLOT 140.0
sc 5.0
wc2 140.0
sc2 5.0
vs 769
th 4
al ph

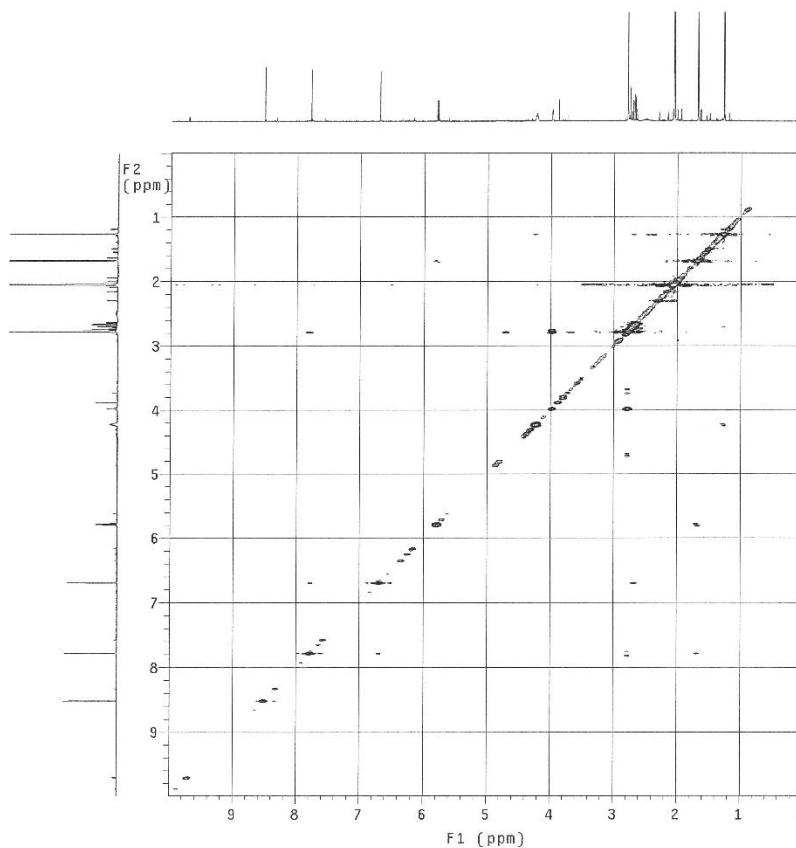


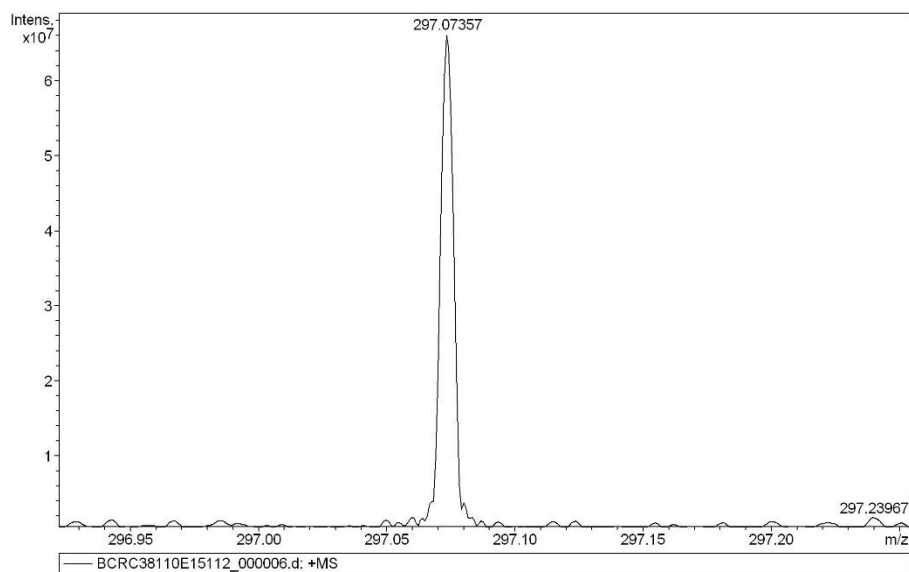
Figure S41. NOESY spectrum of monapurpurin (6)

Mass Spectrum SmartFormula Report

Analysis Info

Analysis Name D:\Data\7\BCRC38110E15112_000006.d
Method broadband first signal
Sample Name BCRC48110-E-15-11-2
Comment ESI Positive

3/12/2018 3:04:04 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
297.07357	1	C 15 H 14 Na O 5	100.00	297.07334	-0.23	-0.76	16.0	8.5	even	ok

Figure S42. HRESIMS spectrum of monapurpurin (6)