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

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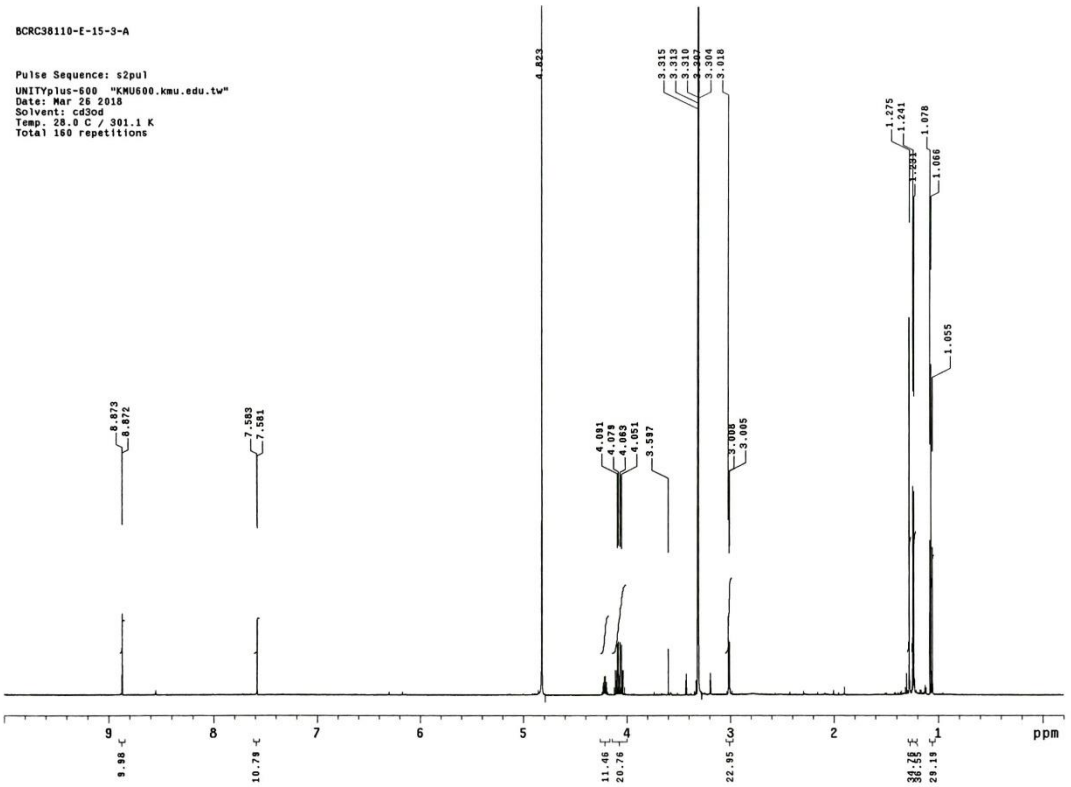

Figure S1. ^{1}H NMR spectrum of 5*S*,6*S*-monaspurpyridine A (**1**) in CD_3OD at 600 MHz

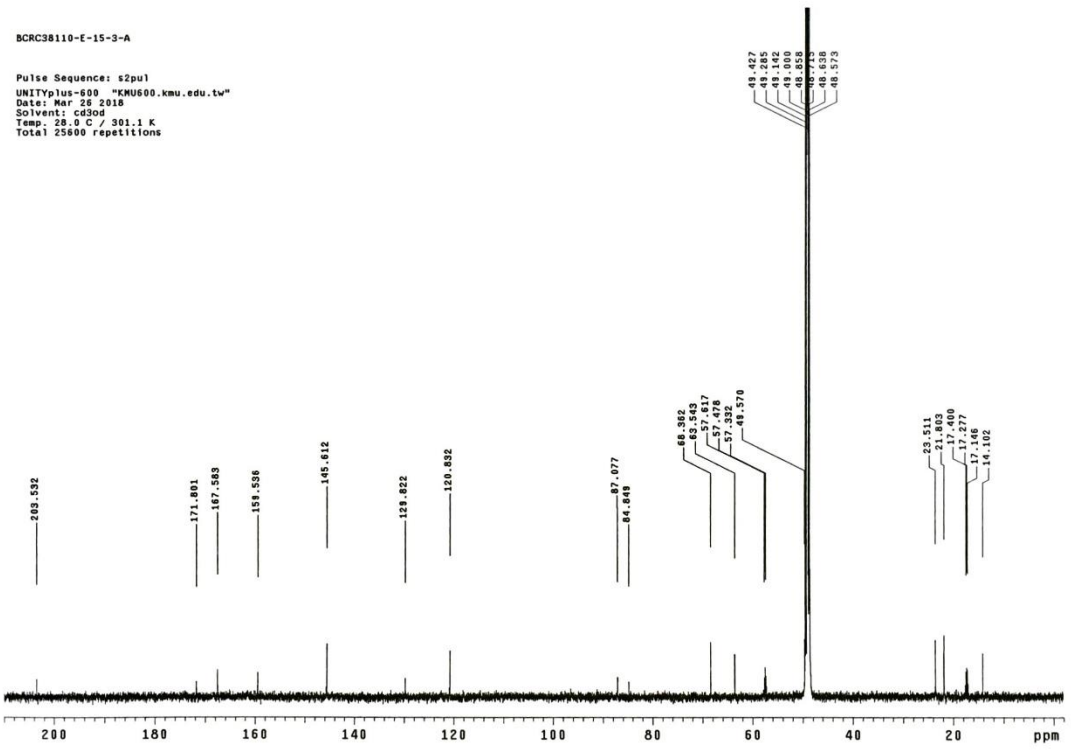

Figure S2. ^{13}C NMR spectrum of 5*S*,6*S*-monaspurpyridine A (**1**) in CD_3OD at 125 MHz

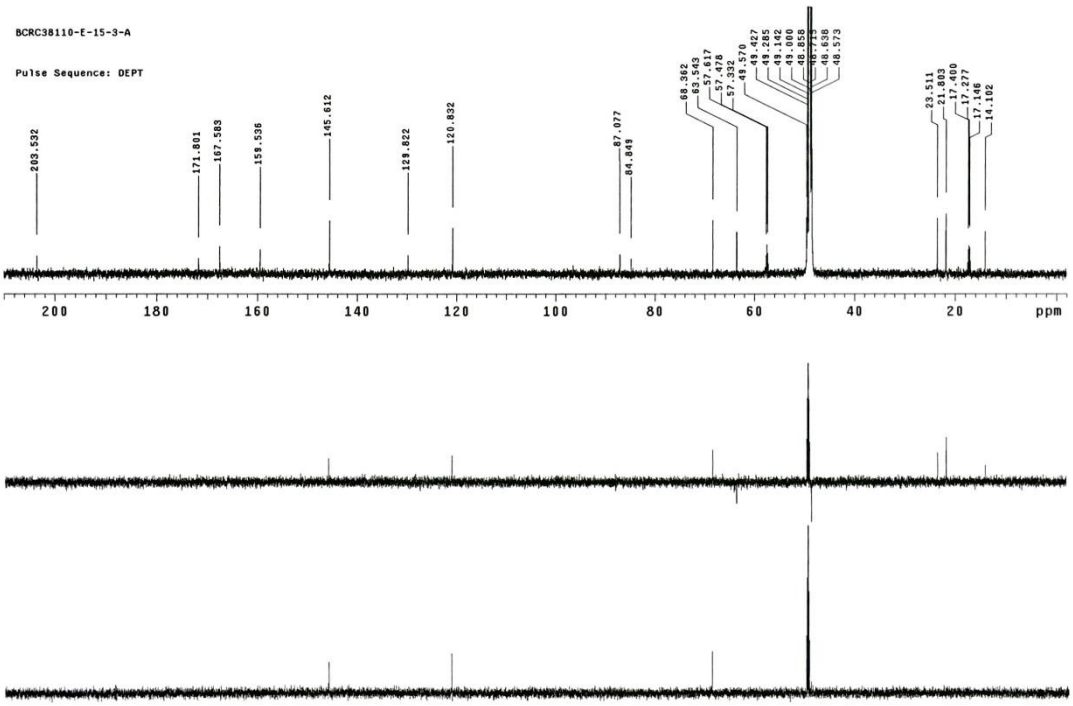

Figure S3. DEPT spectrum of 5*S*,6*S*-monaspurpyridine A (**1**)

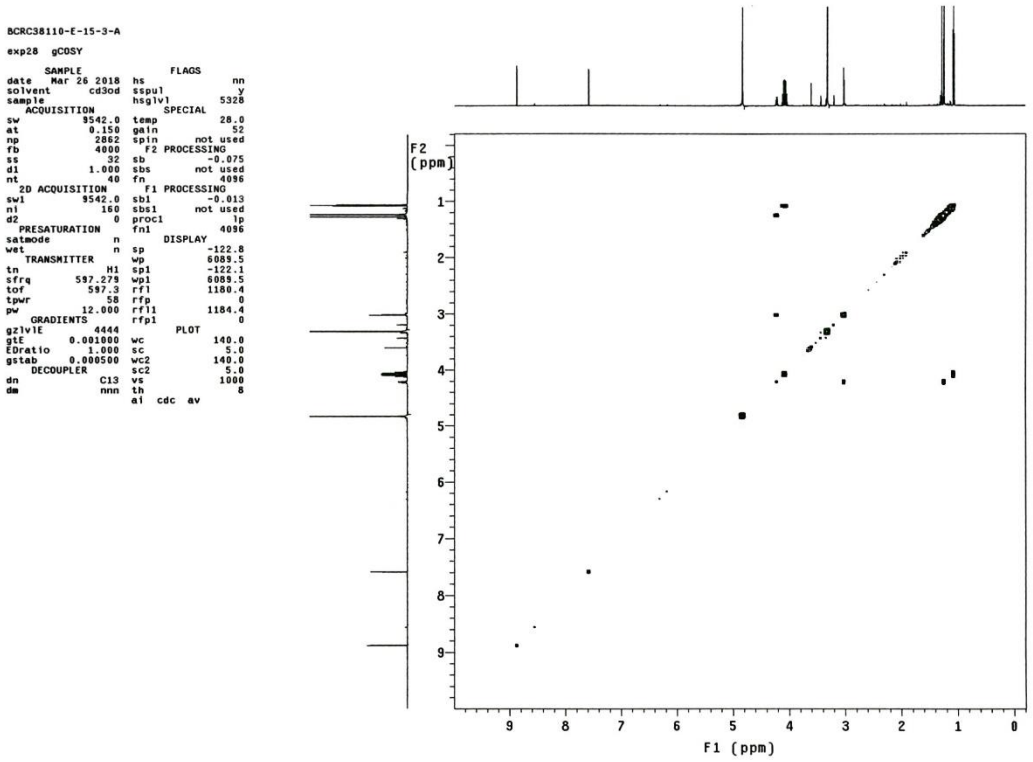

Figure S4. COSY spectrum of 5*S*,6*S*-monaspurpyridine A (**1**)

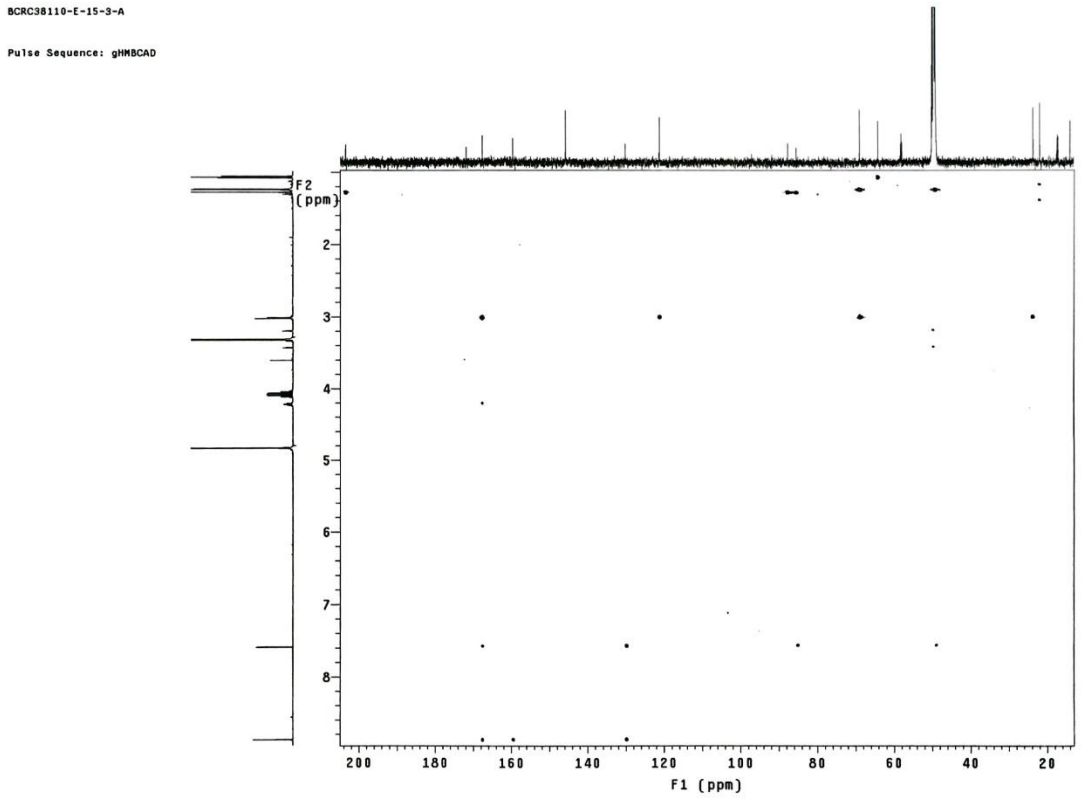

Figure S5. HMBC spectrum of 5*S*,6*S*-monapurpyridine A (**1**)

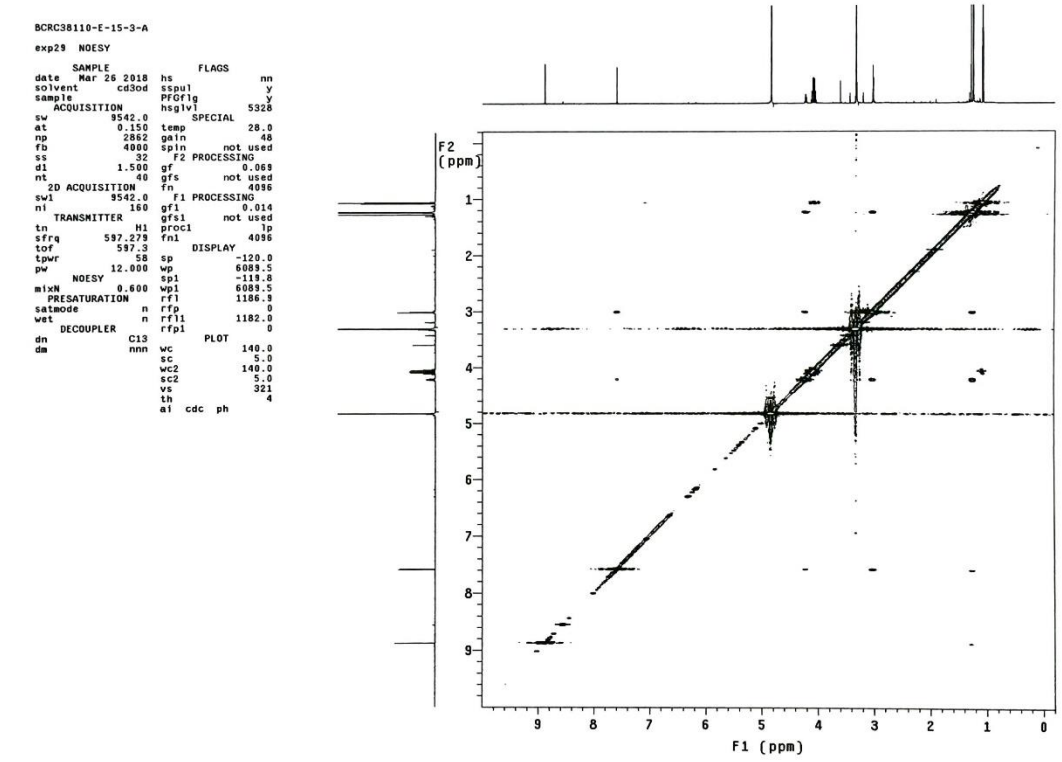

Figure S6. NOESY spectrum of 5*S*,6*S*-monaspurpyridine A (**1**)

Mass Spectrum SmartFormula Report

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Comment	ESI Positive		

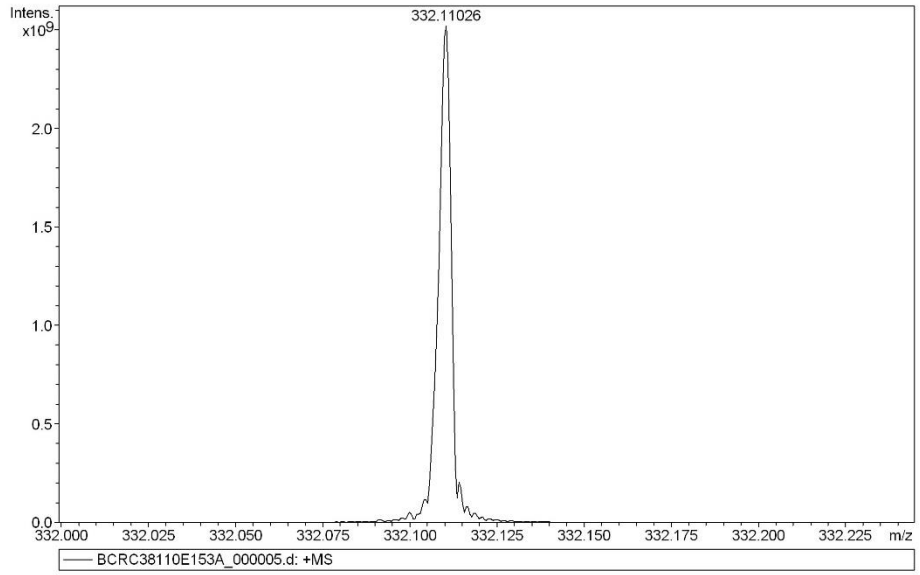

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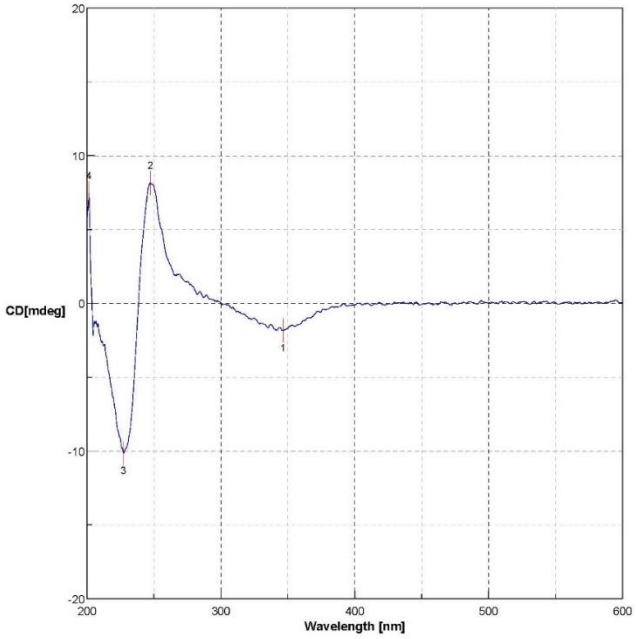
Figure S7. HRESIMS spectrum of 5*S*,6*S*-monapurpyridine A (**1**)



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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 5*S*,6*S*-monaspurpyridine A (**1**)

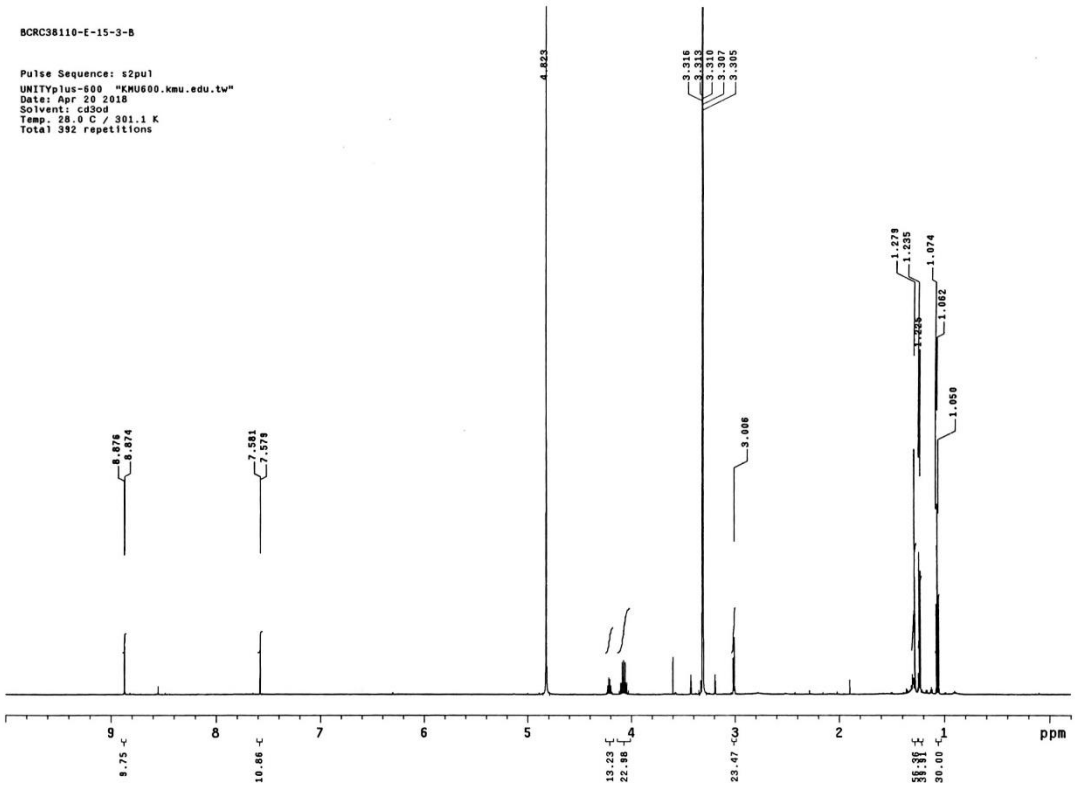

Figure S9. ^{1}H NMR spectrum of 5*R*,6*R*-monaspurpyridine A (**2**) in CD_3OD at 600 MHz

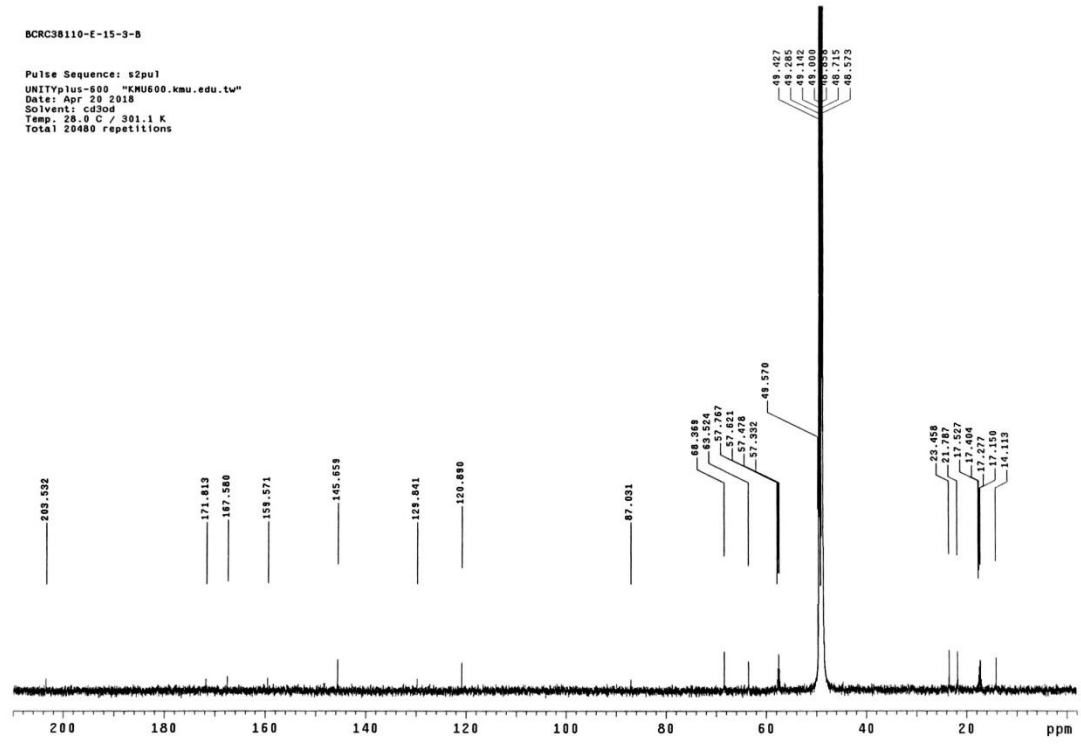

Figure S10. ^{13}C NMR spectrum of 5*R*,6*R*-monaspurpyridine A (**2**) in CD_3OD at 125 MHz

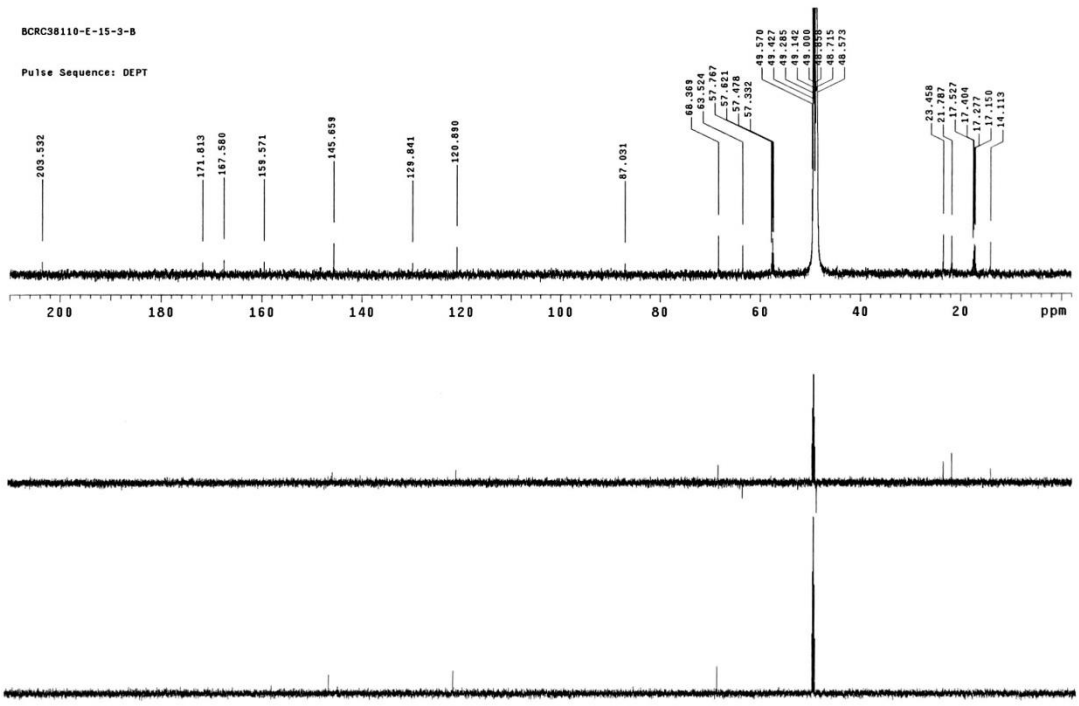

Figure S11. DEPT spectrum of 5*R*,6*R*-monaspurpyridine A (**2**)

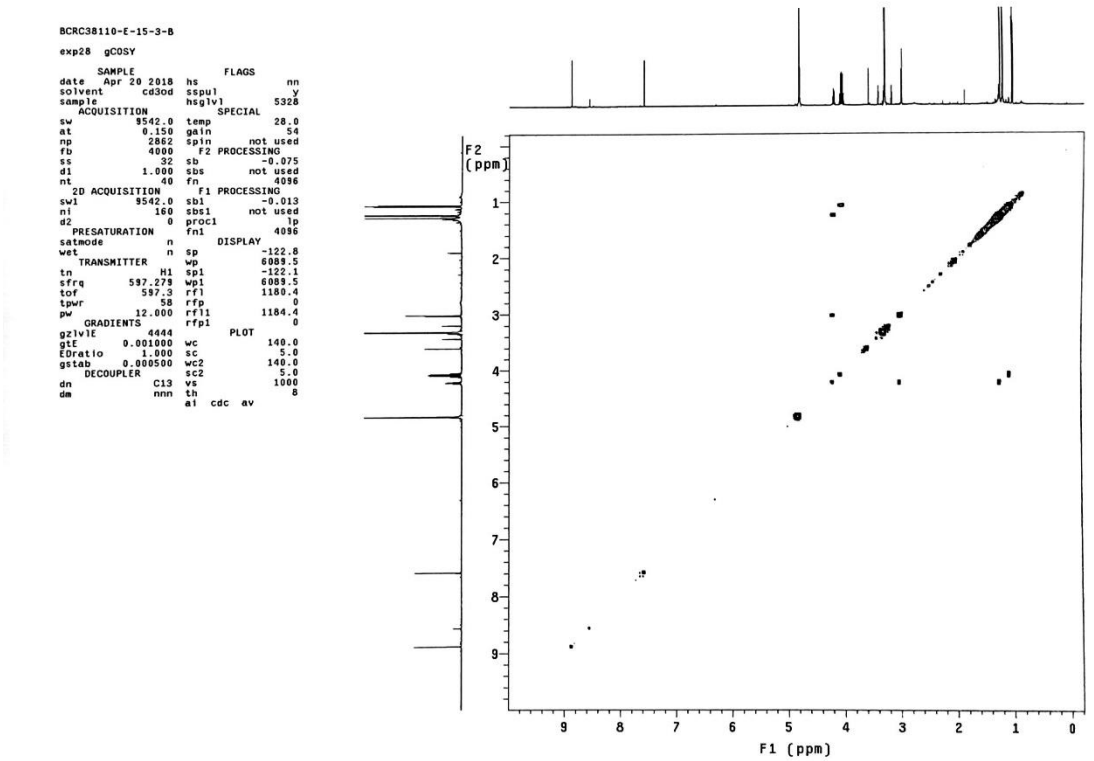

Figure S12. COSY spectrum of 5*R*,6*R*-monaspurpyridine A (**2**)

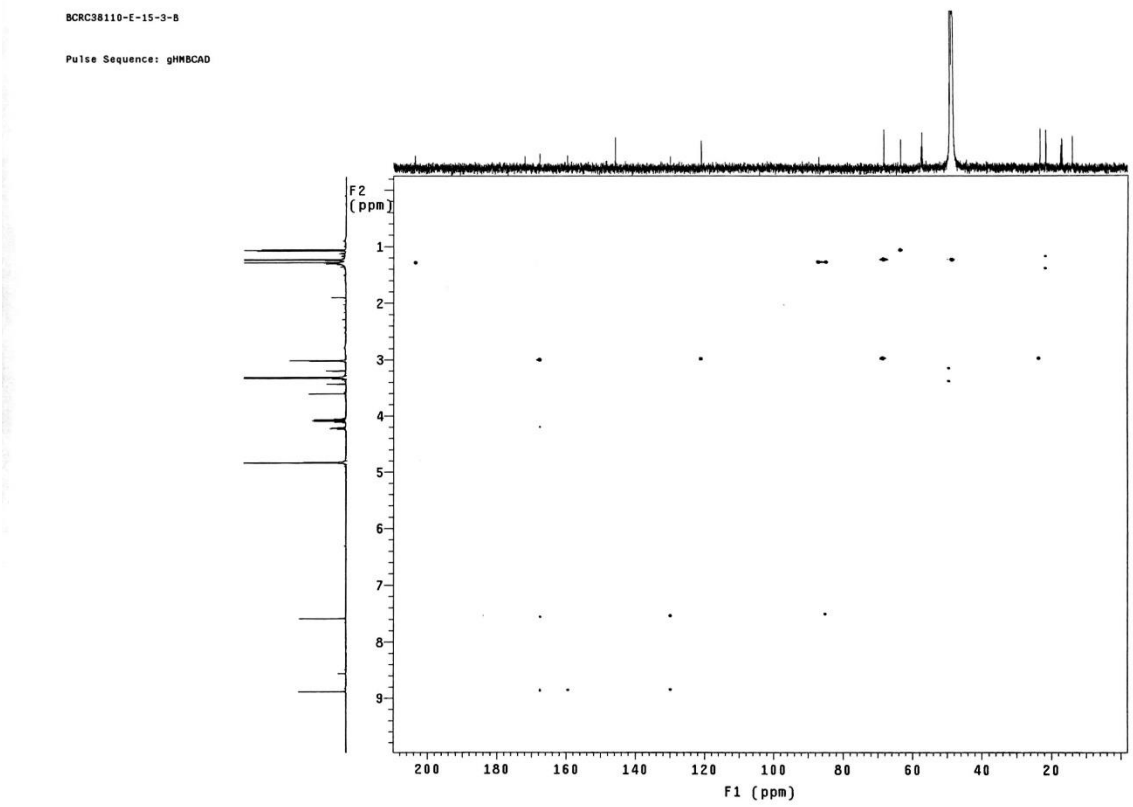

Figure S13. HMBC spectrum of 5*R*,6*R*-monaspurpyridine A (**2**)

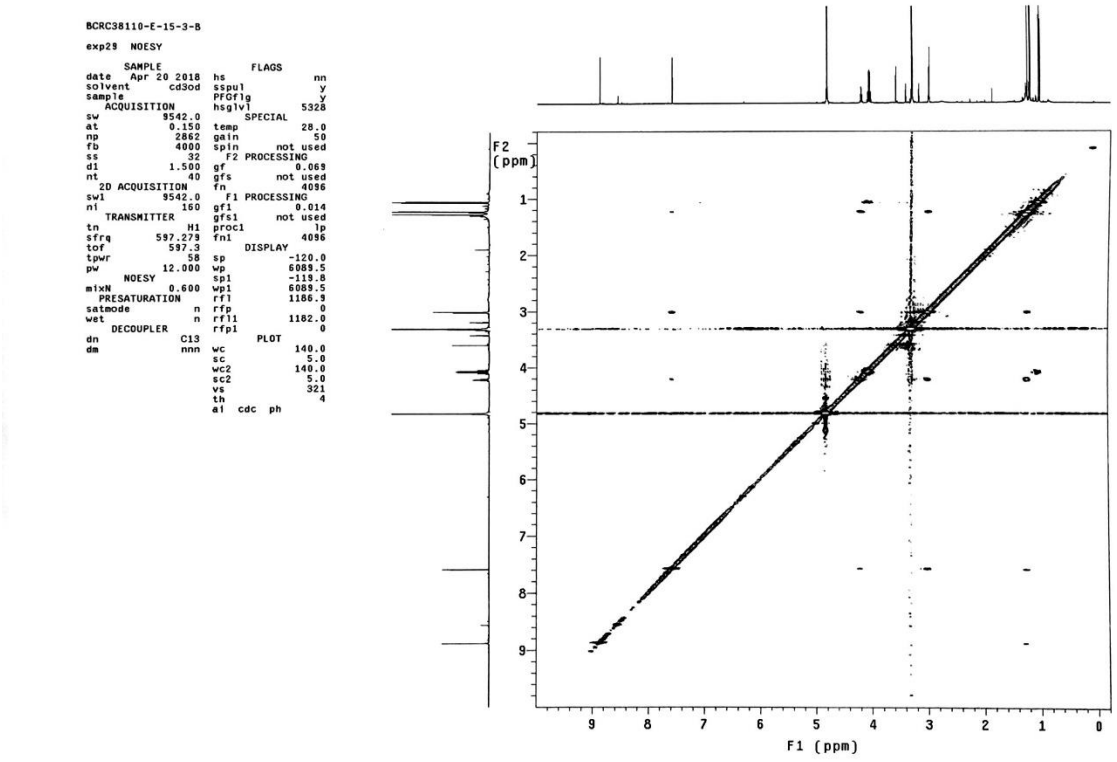

Figure S14. NOESY spectrum of 5*R*,6*R*- monaspurpyridine A (**2**)

Mass Spectrum SmartFormula Report

Analysis Info

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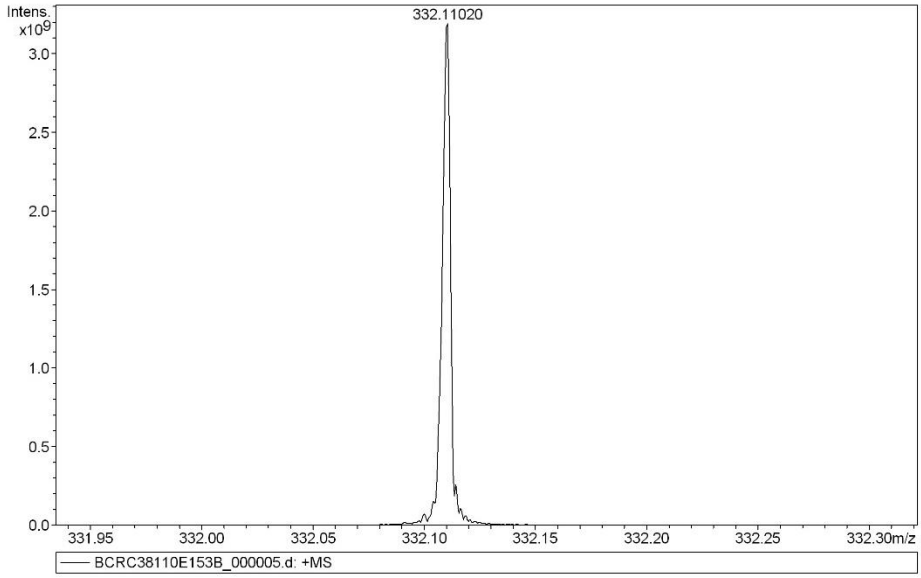
Comment	ESI Positive	



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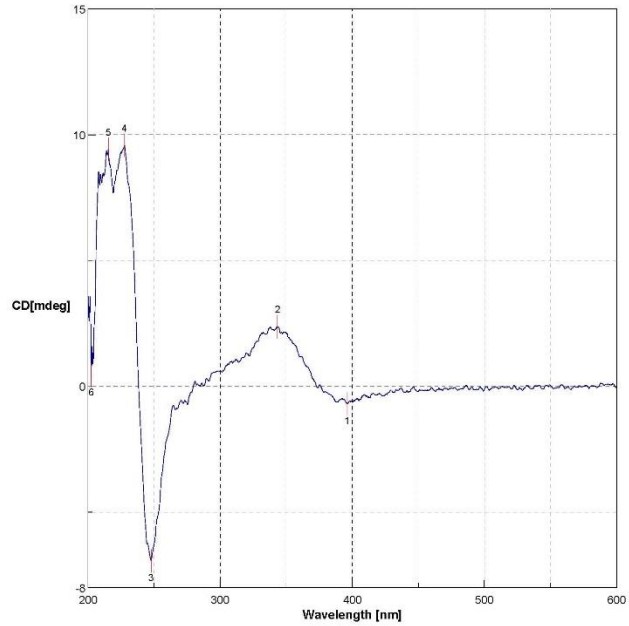
332.11020	1	C 15 H 19 N Na O 6	100.00	332.11046	0.26	0.78	14.0	6.5	even	ok

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



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Operator	User
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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	-6.92545
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**)

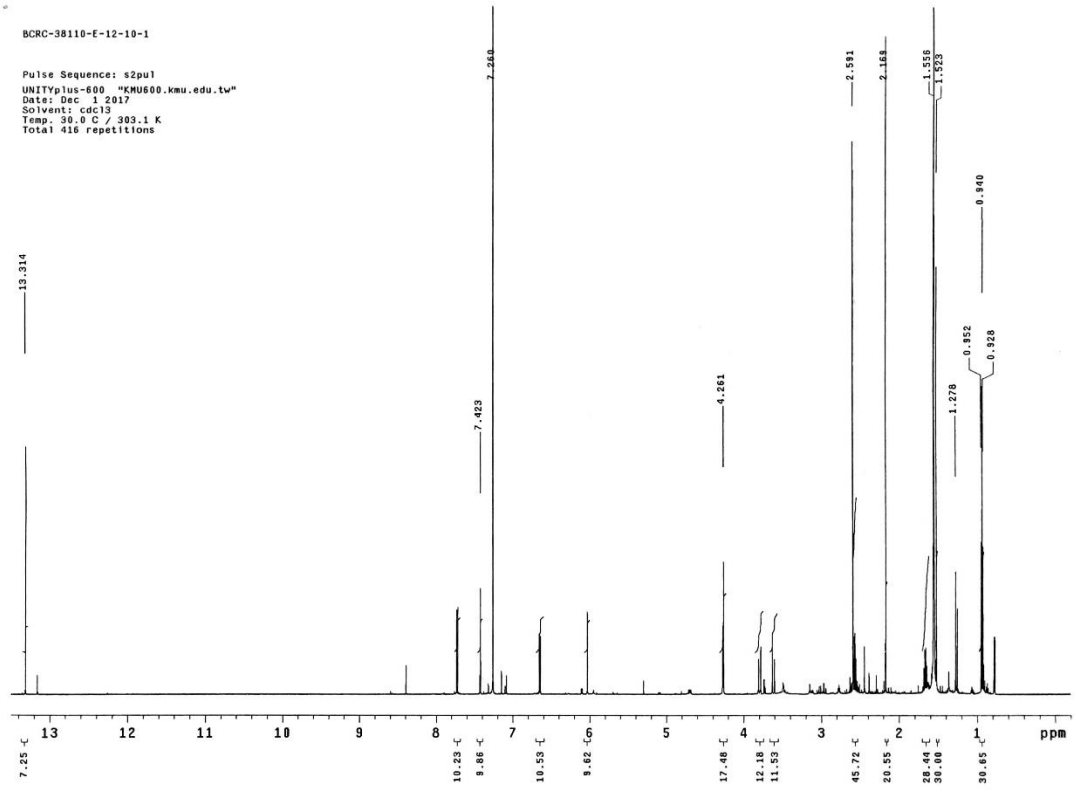


Figure S17. ^{1}H NMR spectrum of monasxanthone A (**3**) in $CDCl_3$ at 600 MHz

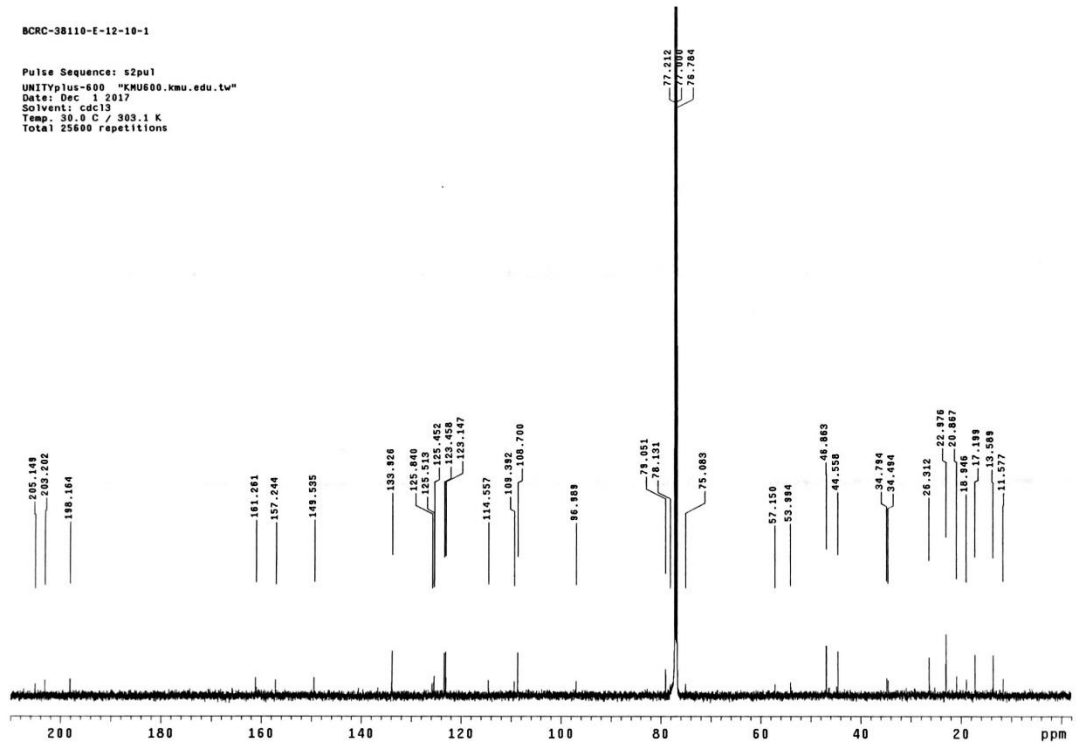


Figure S18. ^{13}C NMR spectrum of monasxanthone A (**3**) in $CDCl_3$ at 125 MHz

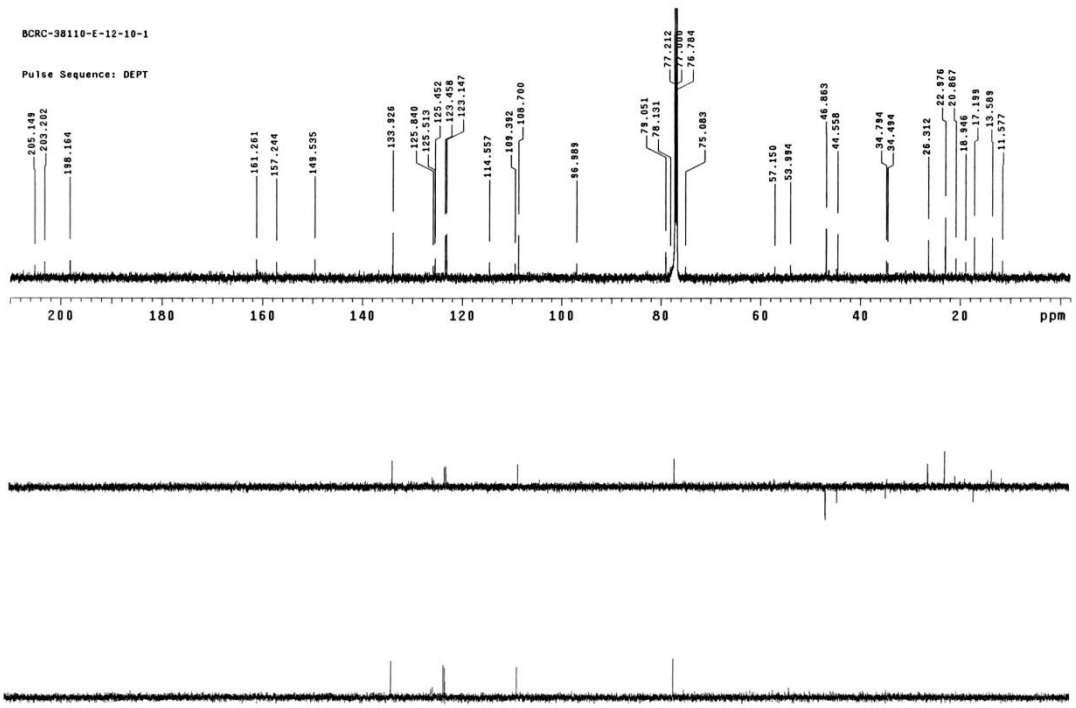


Figure S19. DEPT spectrum of monasxanthone A (**3**)

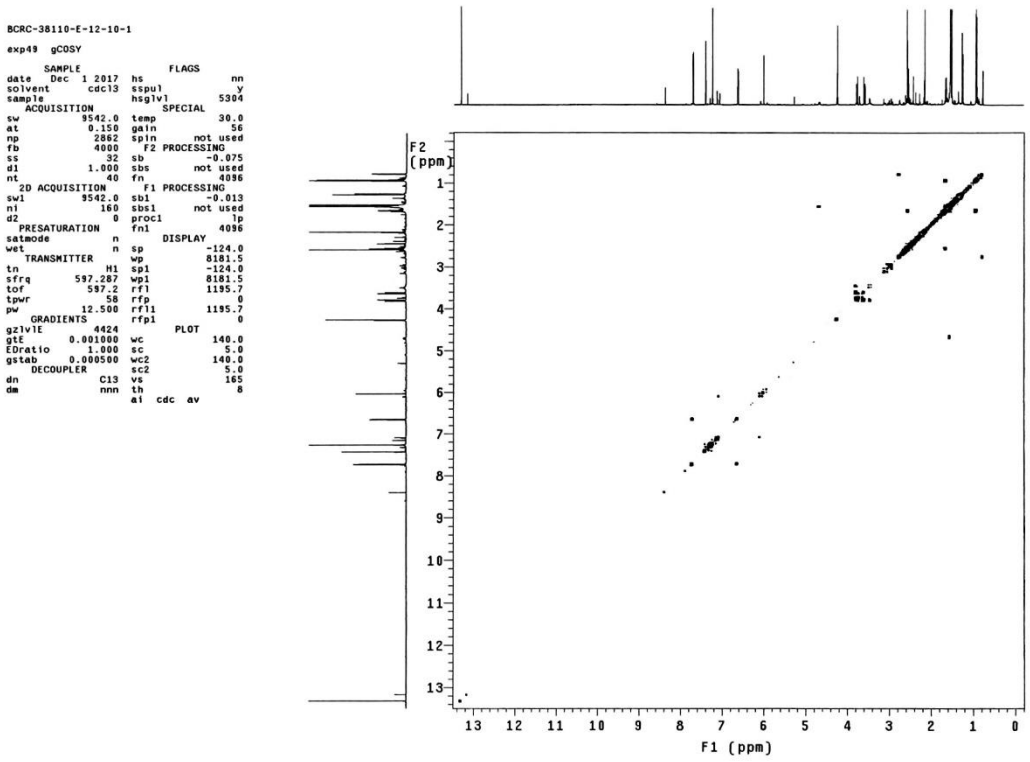


Figure S20. COSY spectrum of monasxanthone A (**3**)

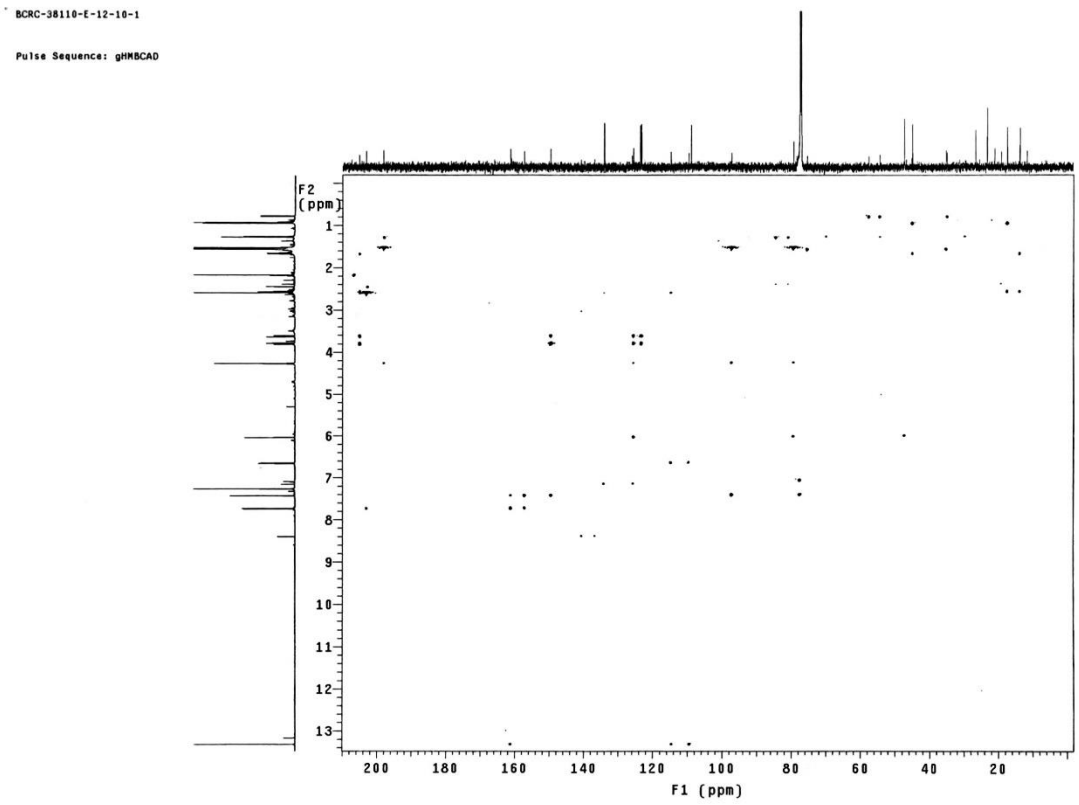


Figure S21. HMBC spectrum of monasxanthone A (**3**)

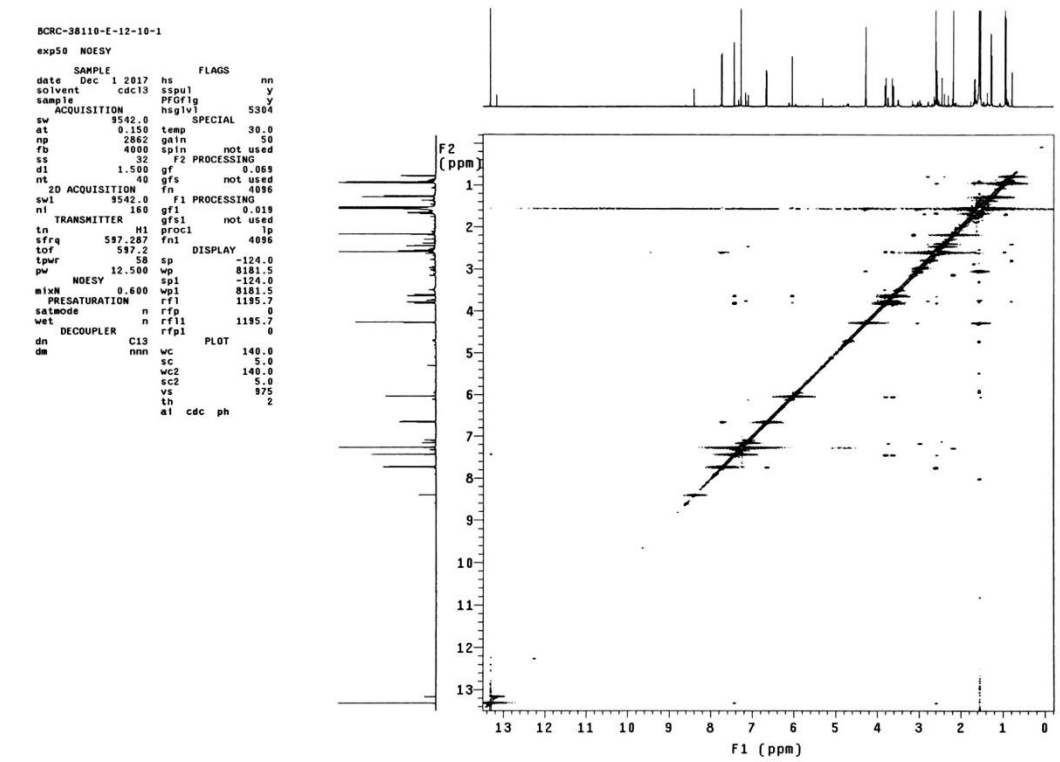


Figure S22. NOESY spectrum of monasxanthone A (**3**)

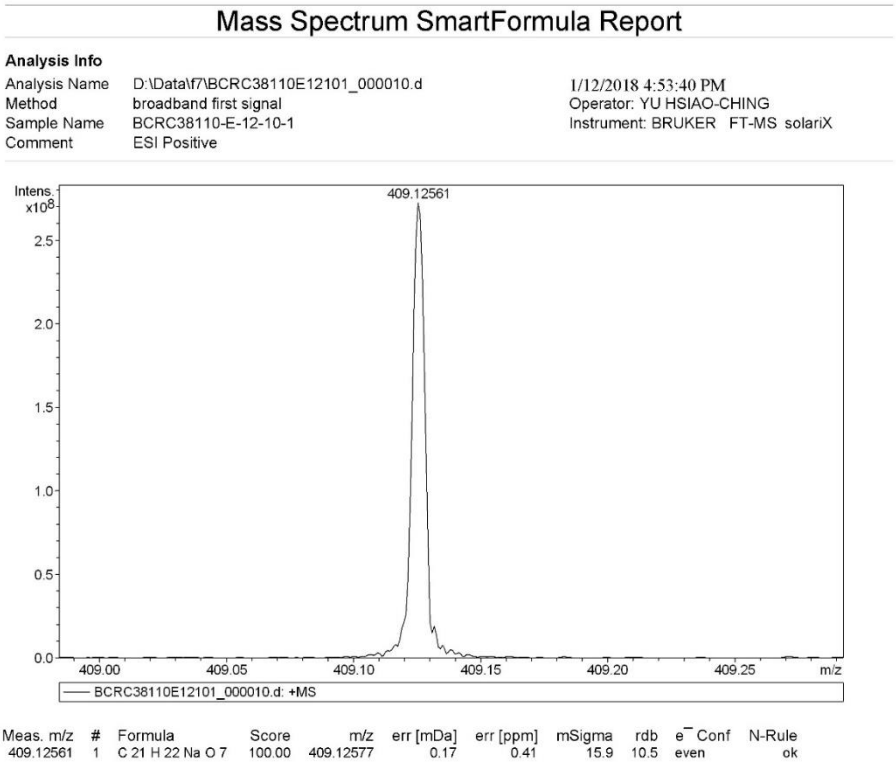


Figure S23. HRESIMS spectrum of monasxanthone A (**3**)

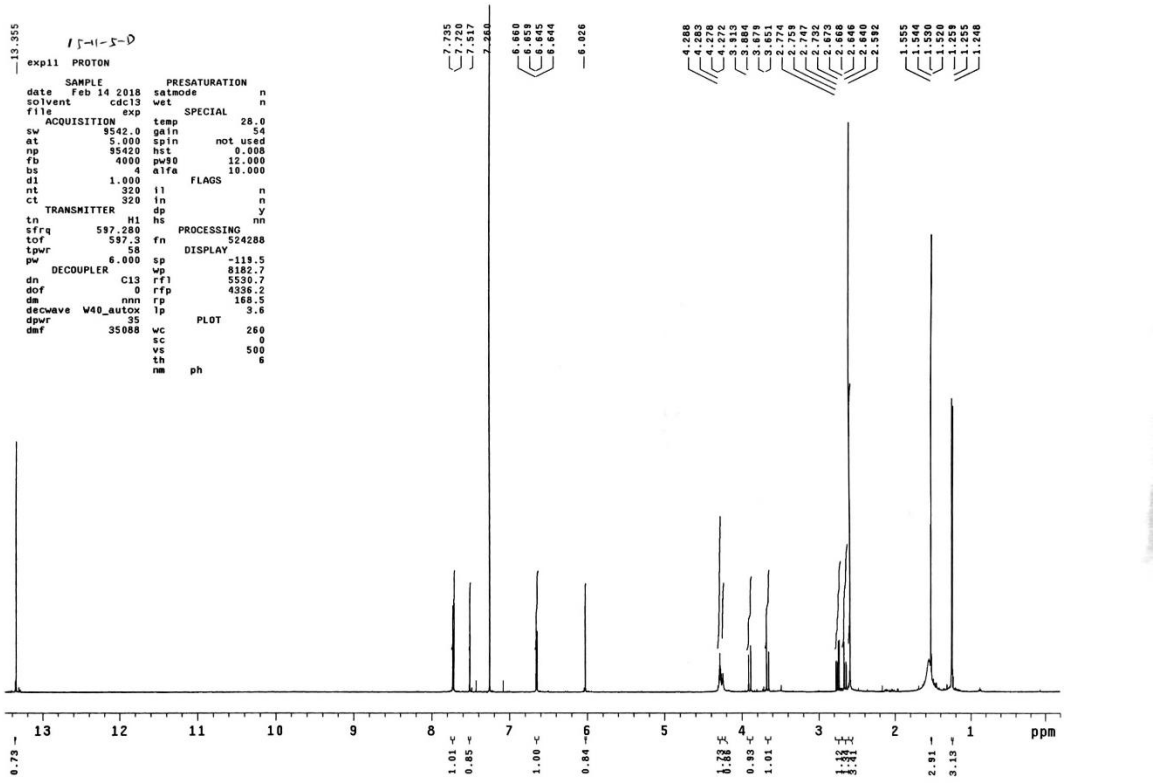


Figure S24. ^{1}H NMR spectrum of monasxanthone B (**4**) in $CDCl_3$ at 600 MHz

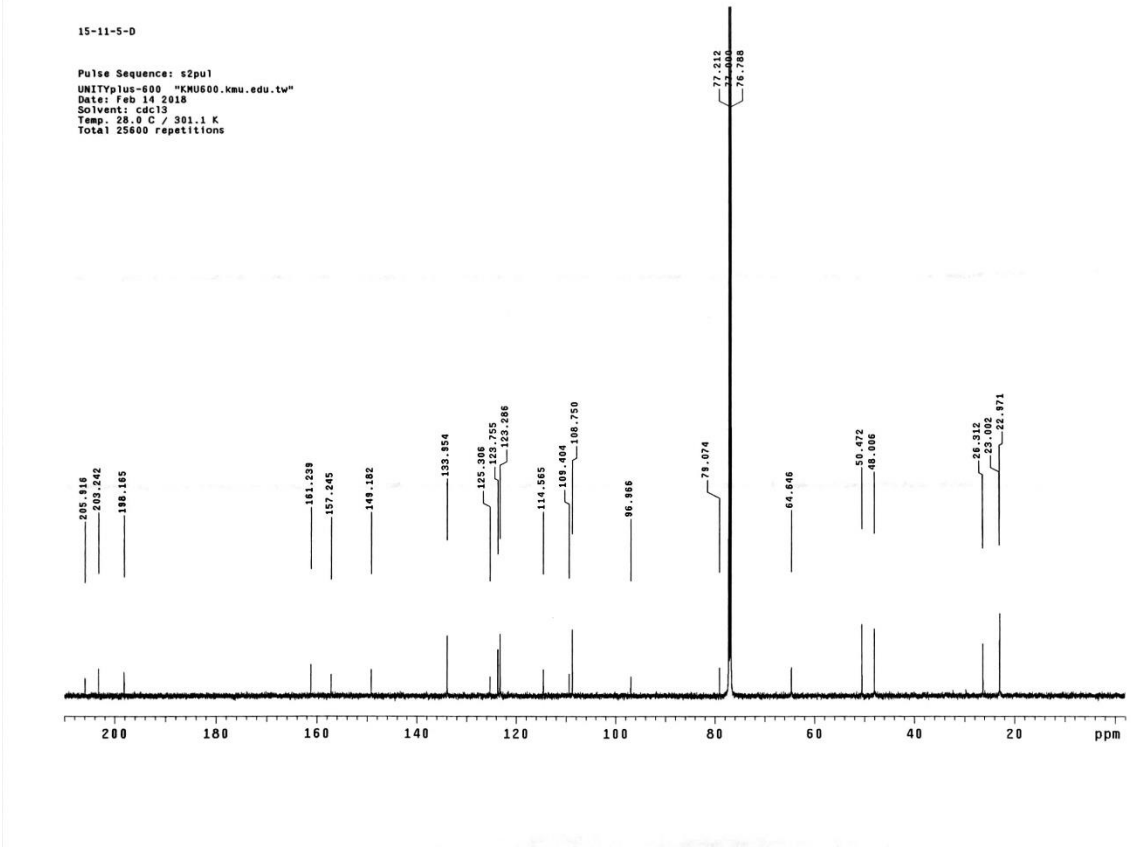


Figure S25. ^{13}C NMR spectrum of monasxanthone B (**4**) in $CDCl_3$ at 125 MHz

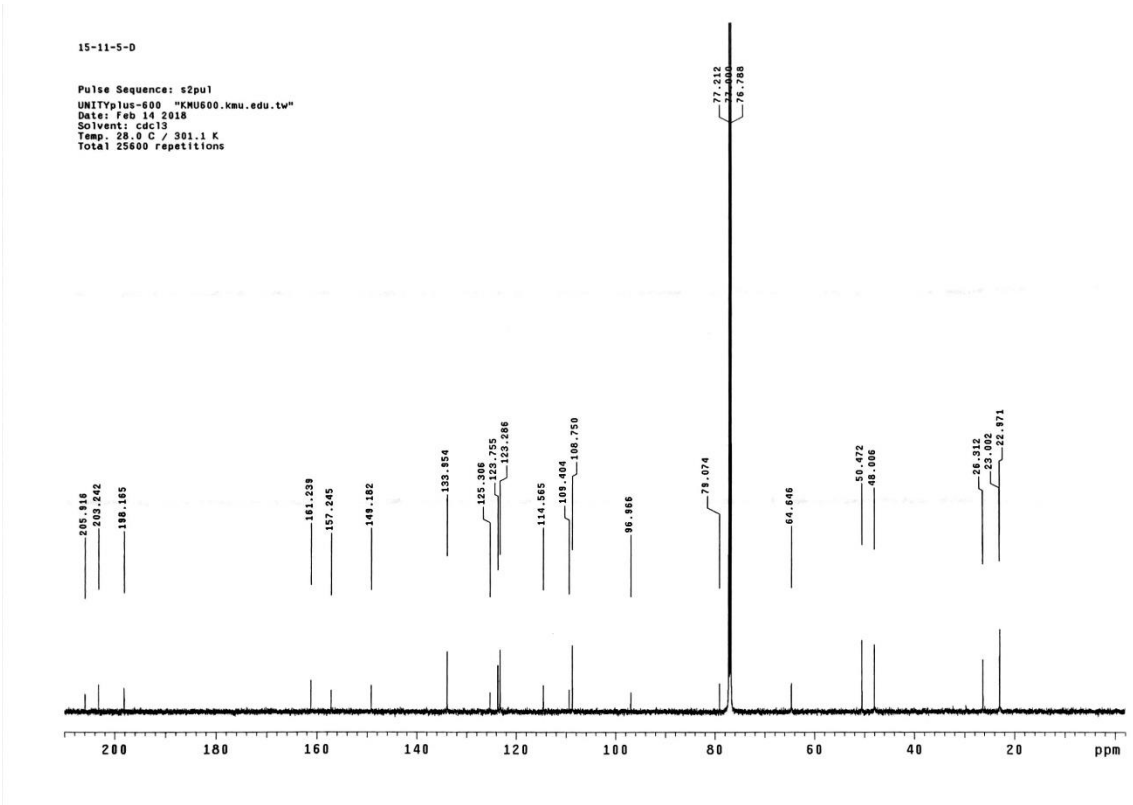


Figure S26. DEPT spectrum of monasxanthone B (**4**)

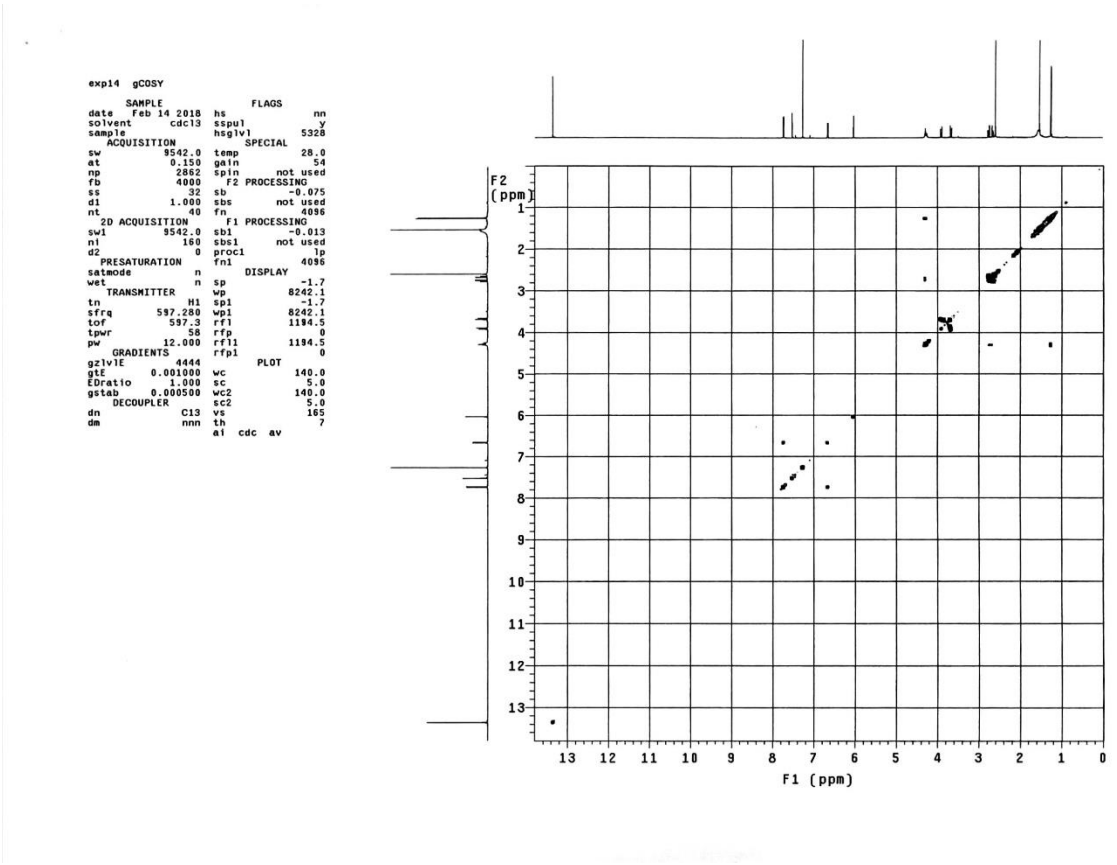


Figure S27. COSY spectrum of monasxanthone B (**4**)

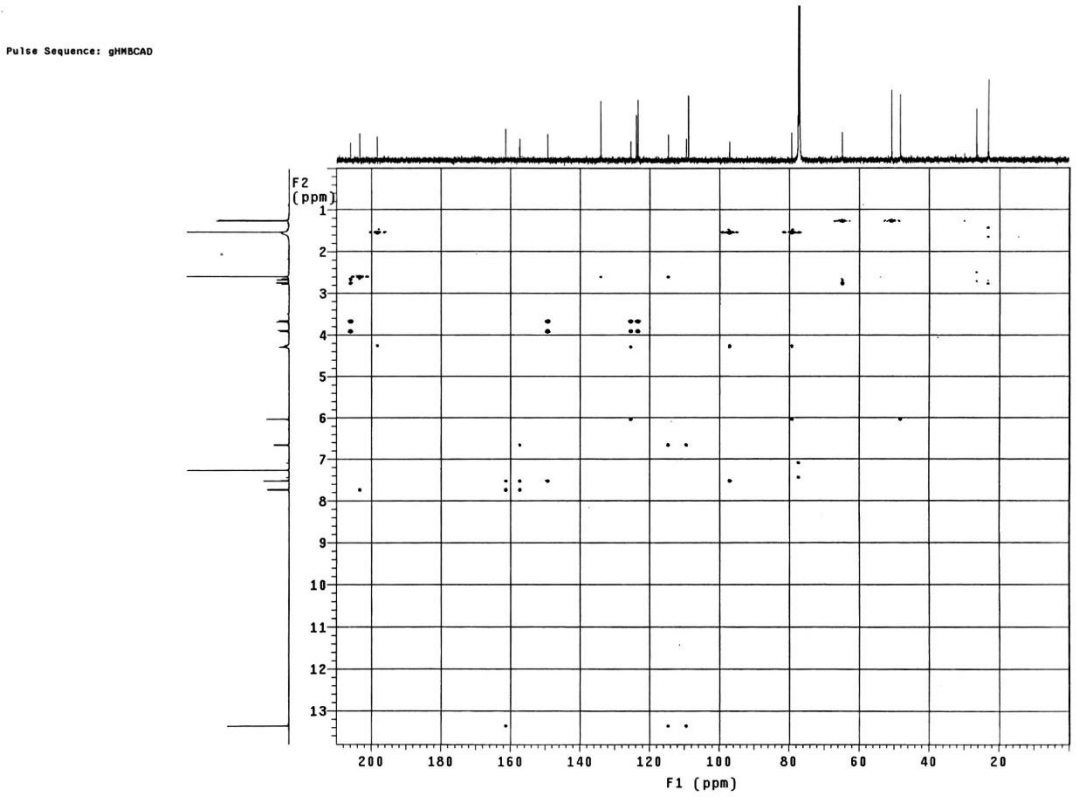


Figure S28. HMBC spectrum of monasxanthone B (**4**)

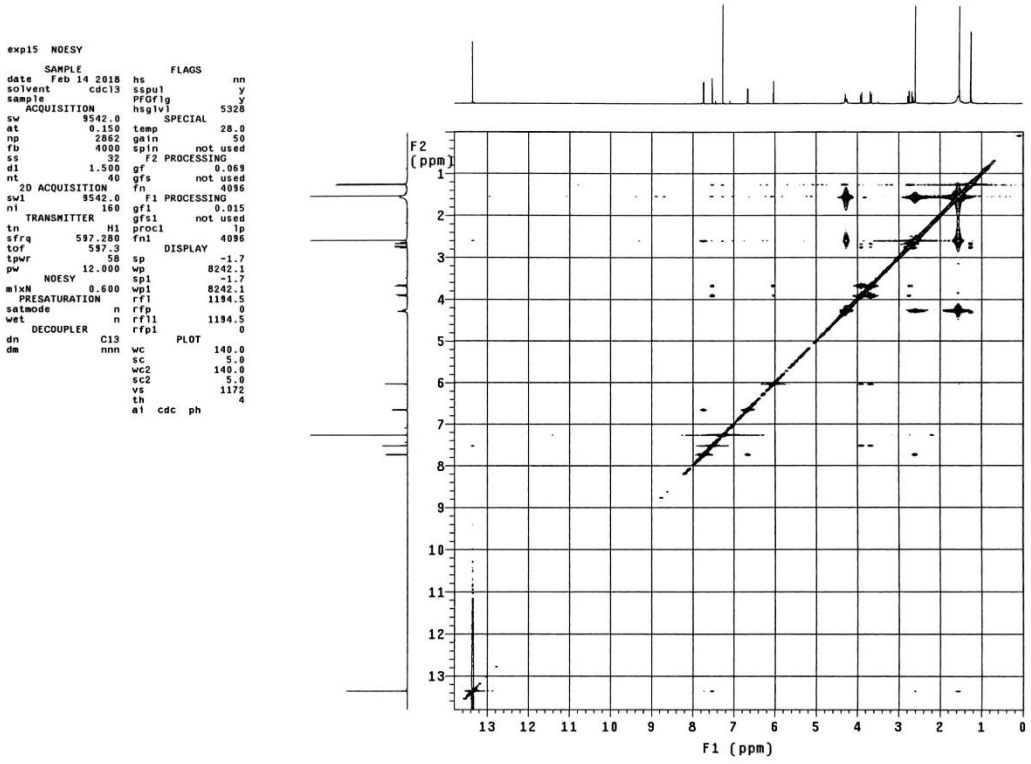


Figure S29. NOESY spectrum of monasxanthone B (**4**)

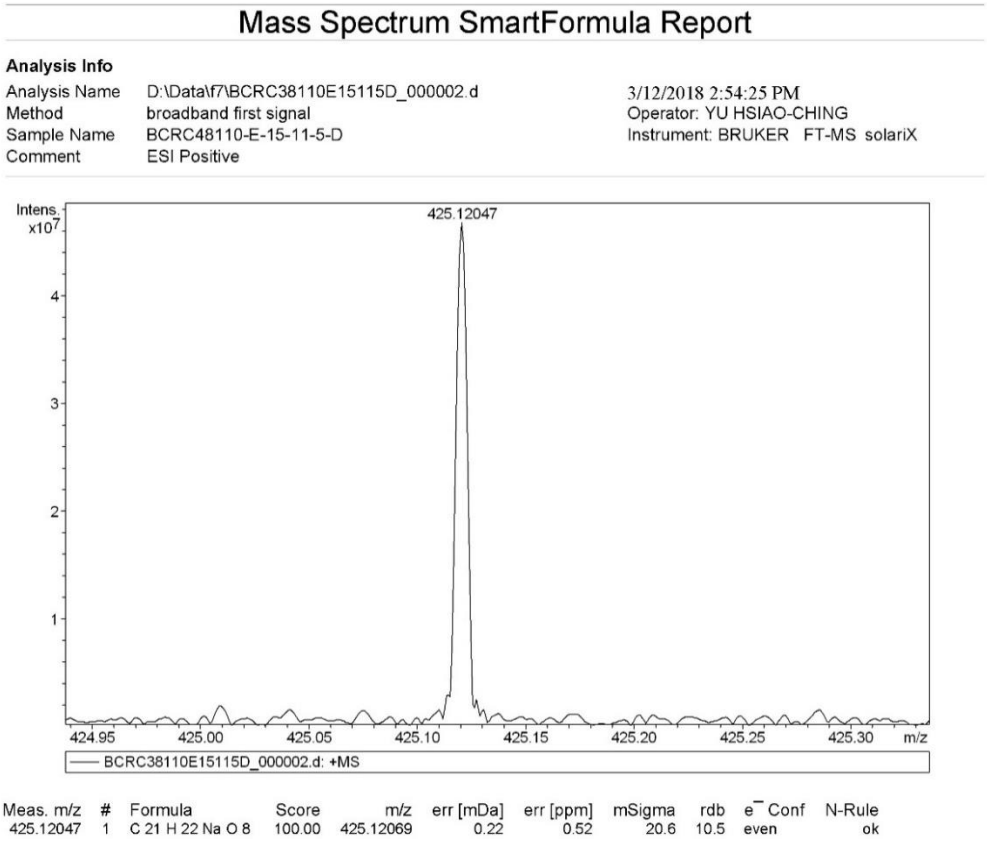


Figure S30. HRESIMS spectrum of monasxanthone B (**4**)

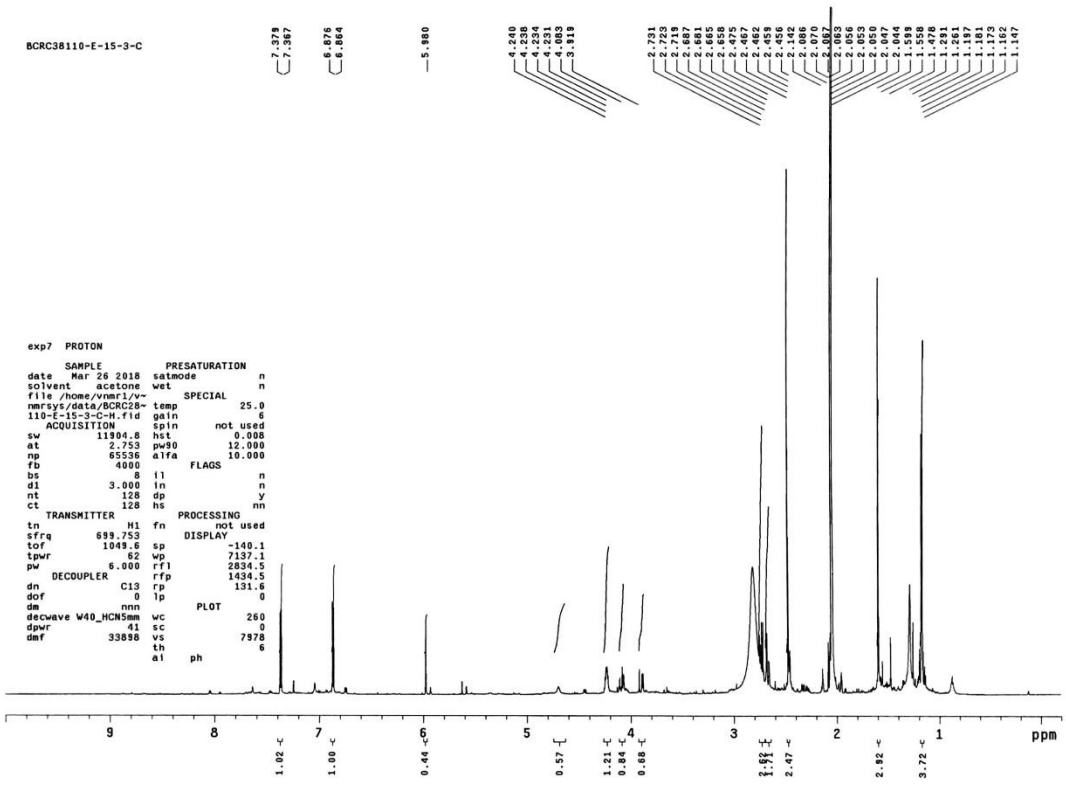


Figure S31. ^{1}H NMR spectrum of monasnaphthalenone (**5**) in acetone-d_6 at 600 MHz

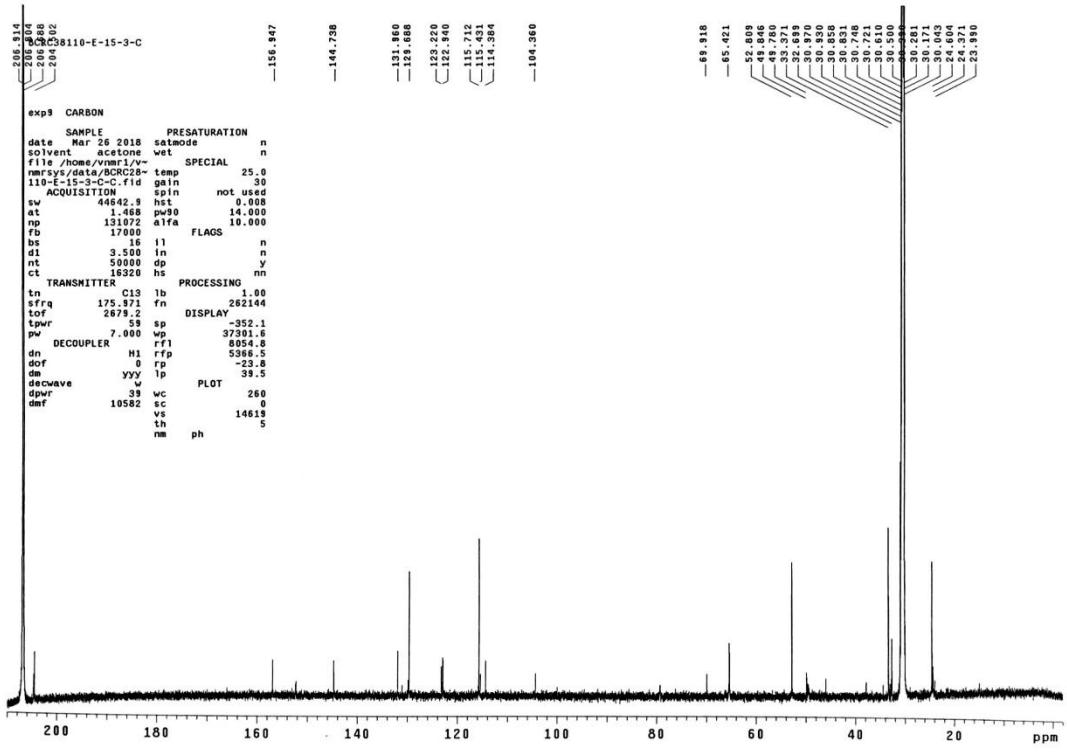


Figure S32. ^{13}C NMR spectrum of monasnaphthalenone (**5**) in acetone-d_6 at 125 MHz

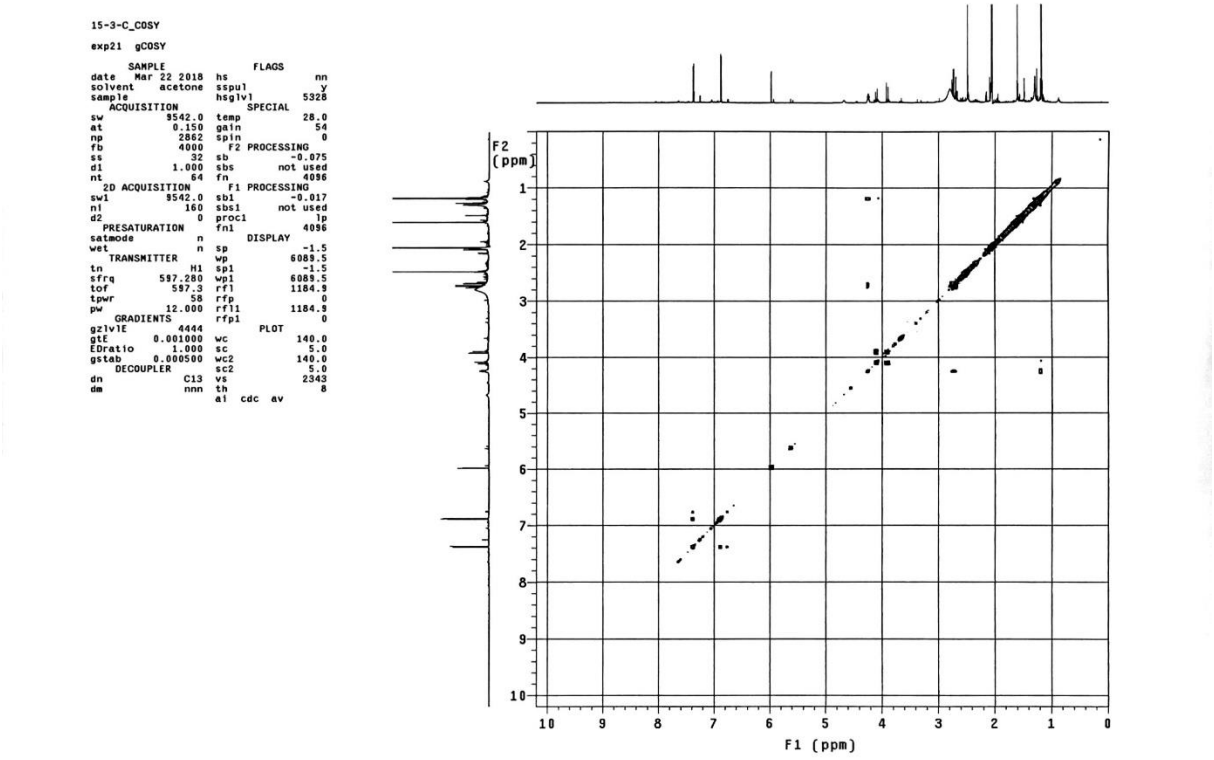


Figure S33. COSY spectrum of monasnaphthalenone (**5**)

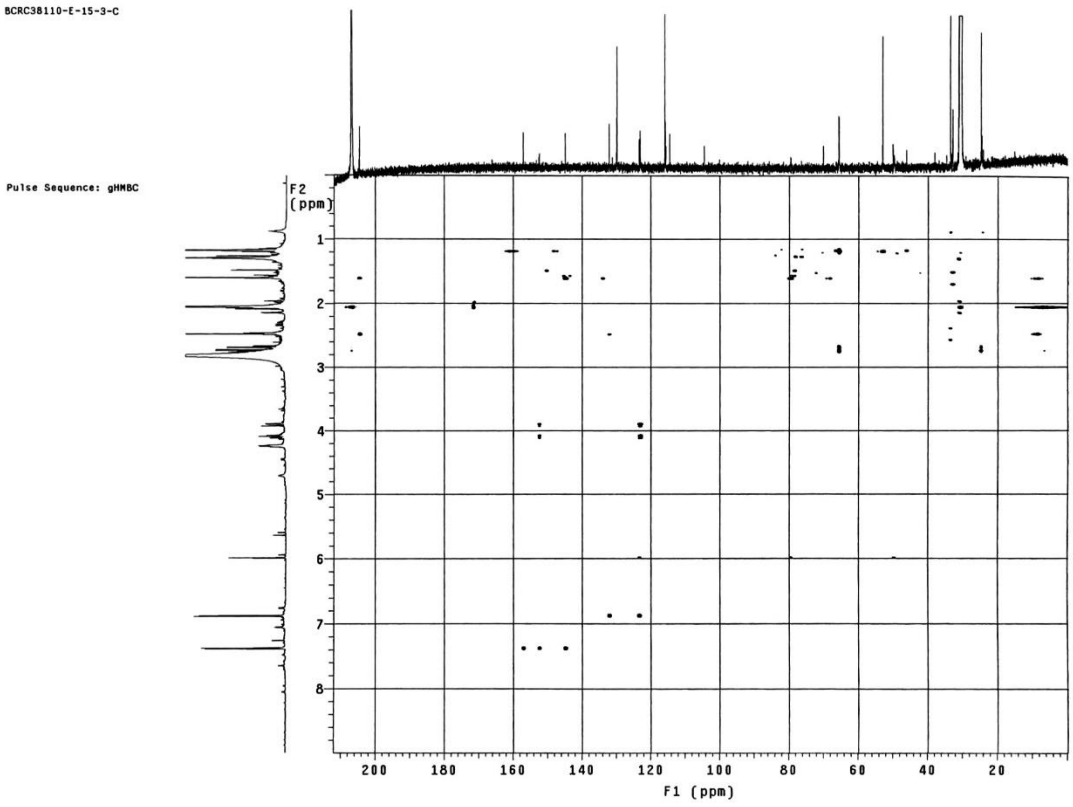


Figure S34. HMBC spectrum of monasnaphthalenone (**5**)

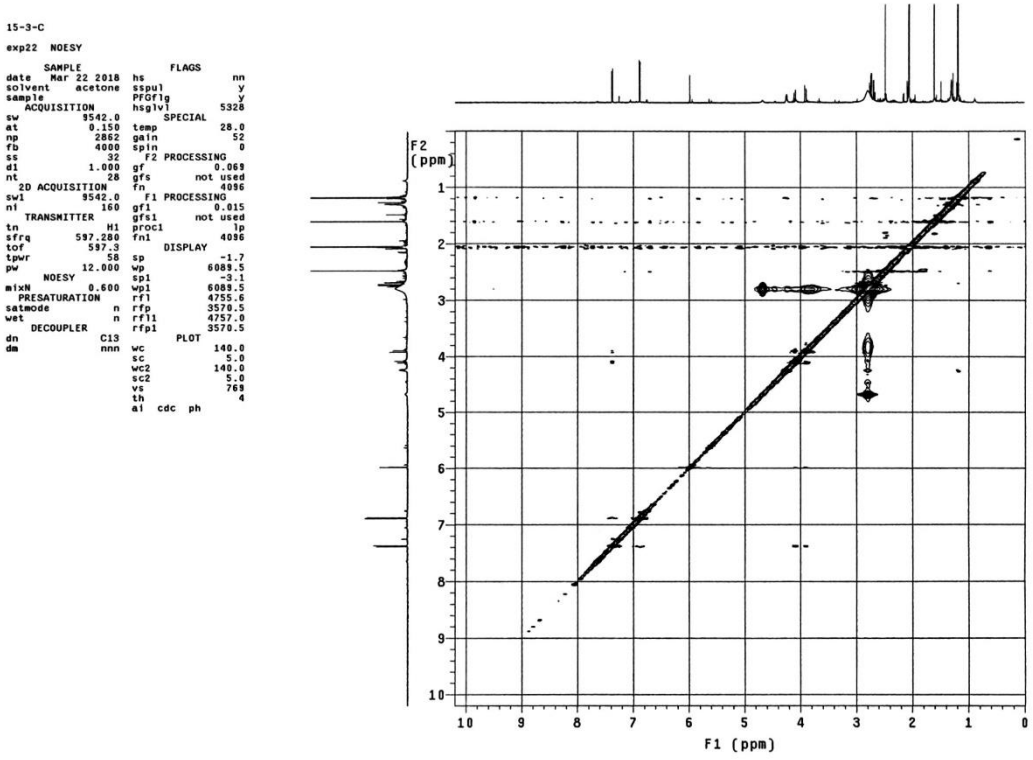
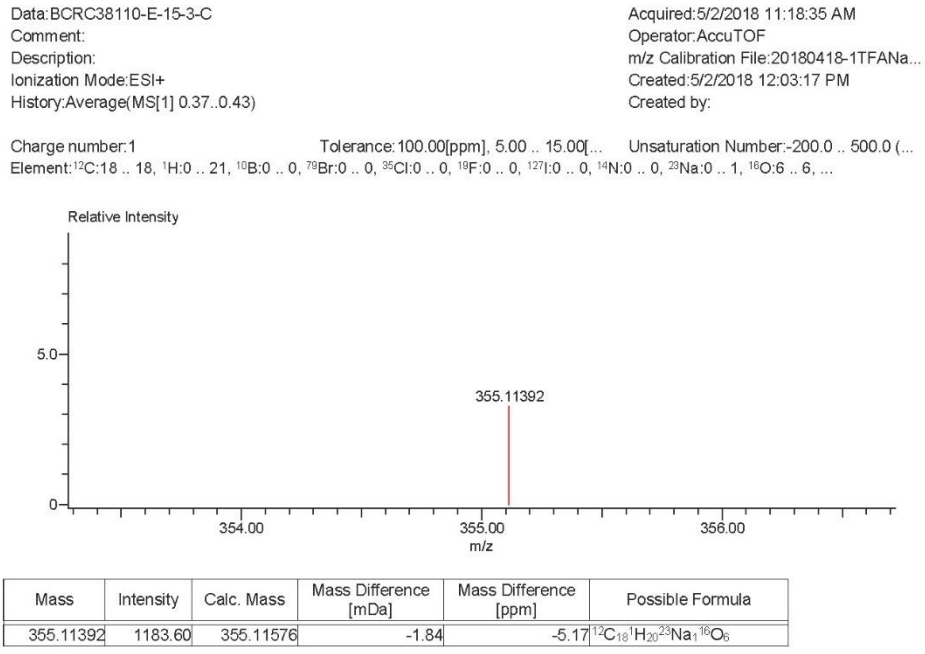


Figure S35. NOESY spectrum of monasnaphthalenone (**5**)



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**)

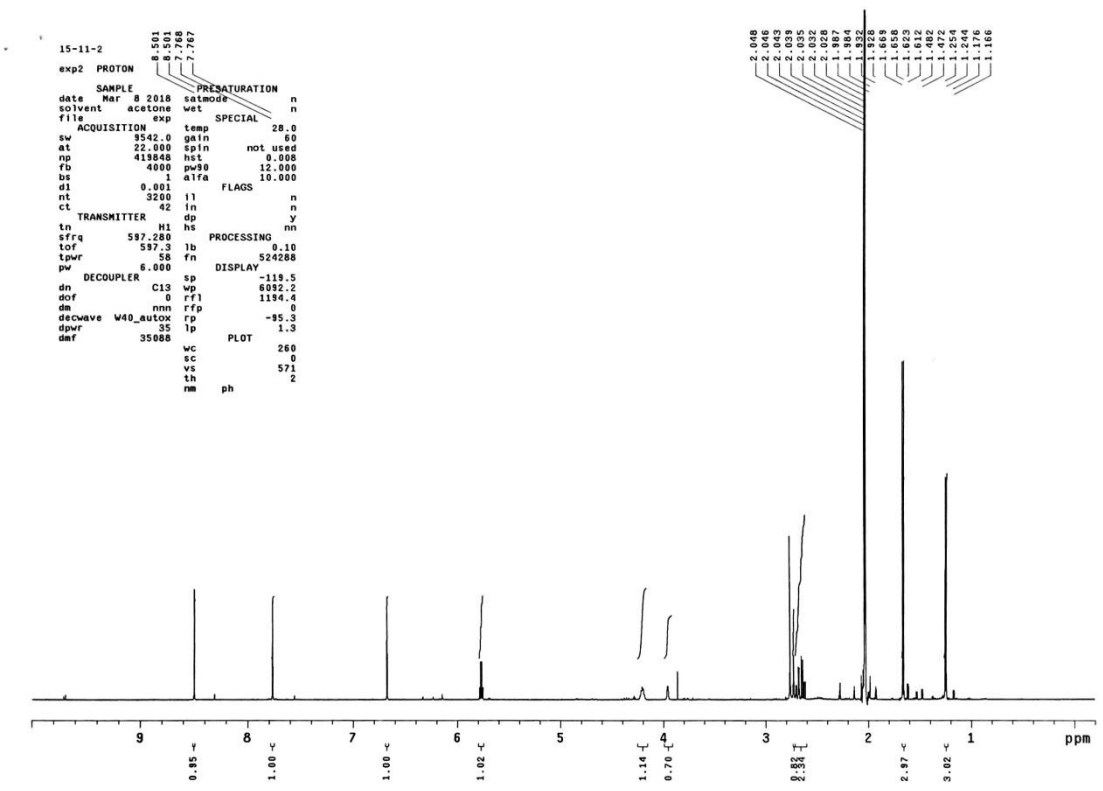


Figure S37. ^{1}H NMR spectrum of monapurpurin (**6**) in acetone-d_6 at 600 MHz

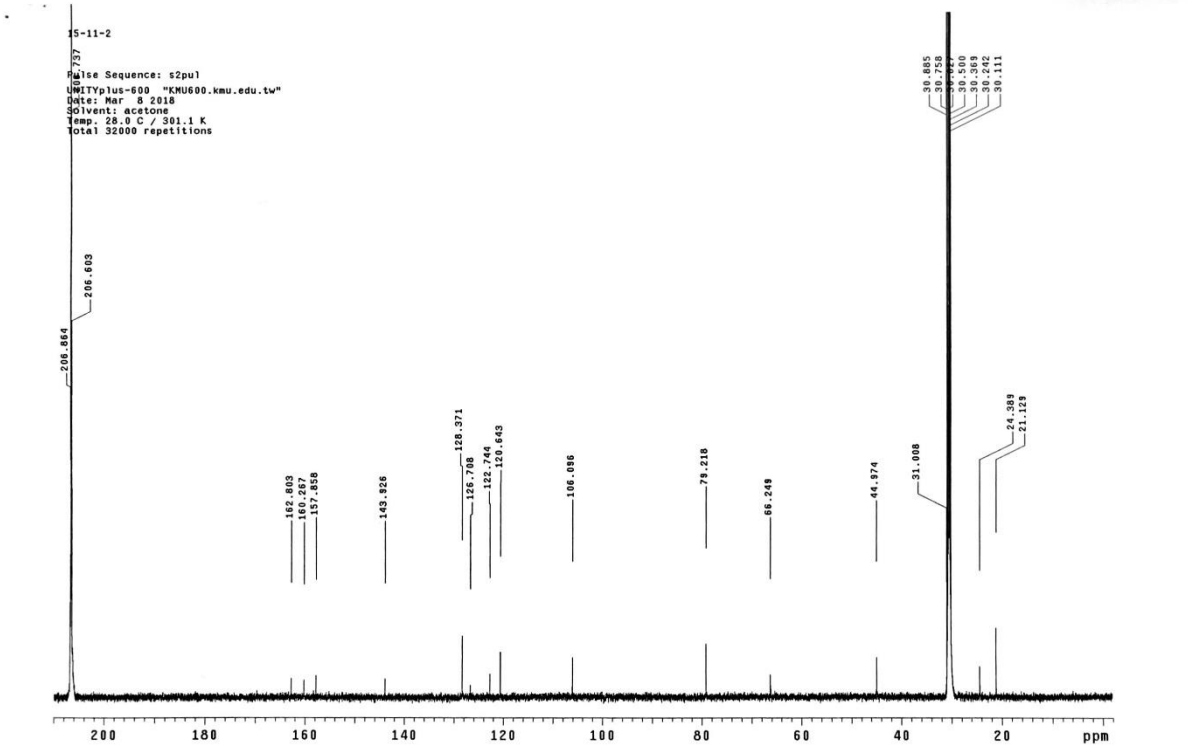


Figure S38. ^{13}C NMR spectrum of monapurpurin (**6**) in acetone-d_6 at 125 MHz

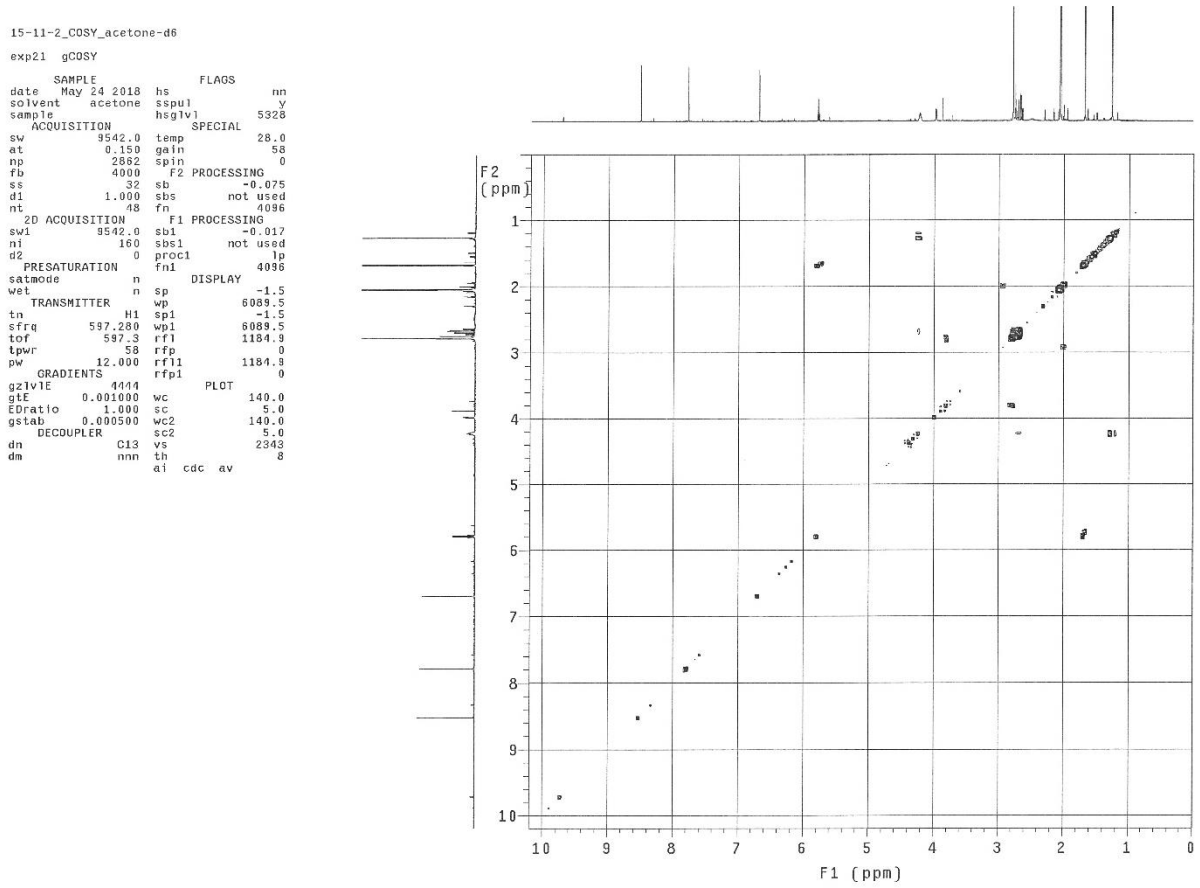


Figure S39. COSY spectrum of monapurpurin (**6**)

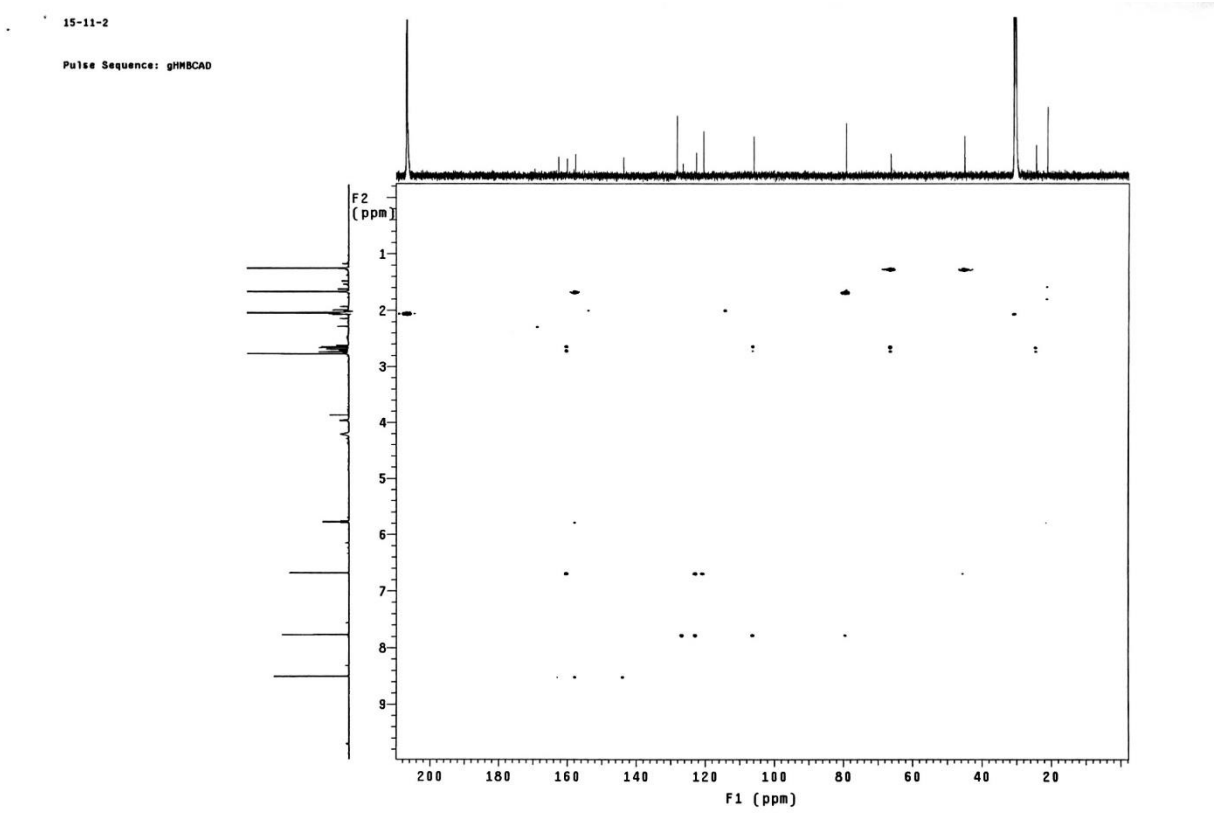


Figure S40. HMBC spectrum of monapurpurin (**6**)

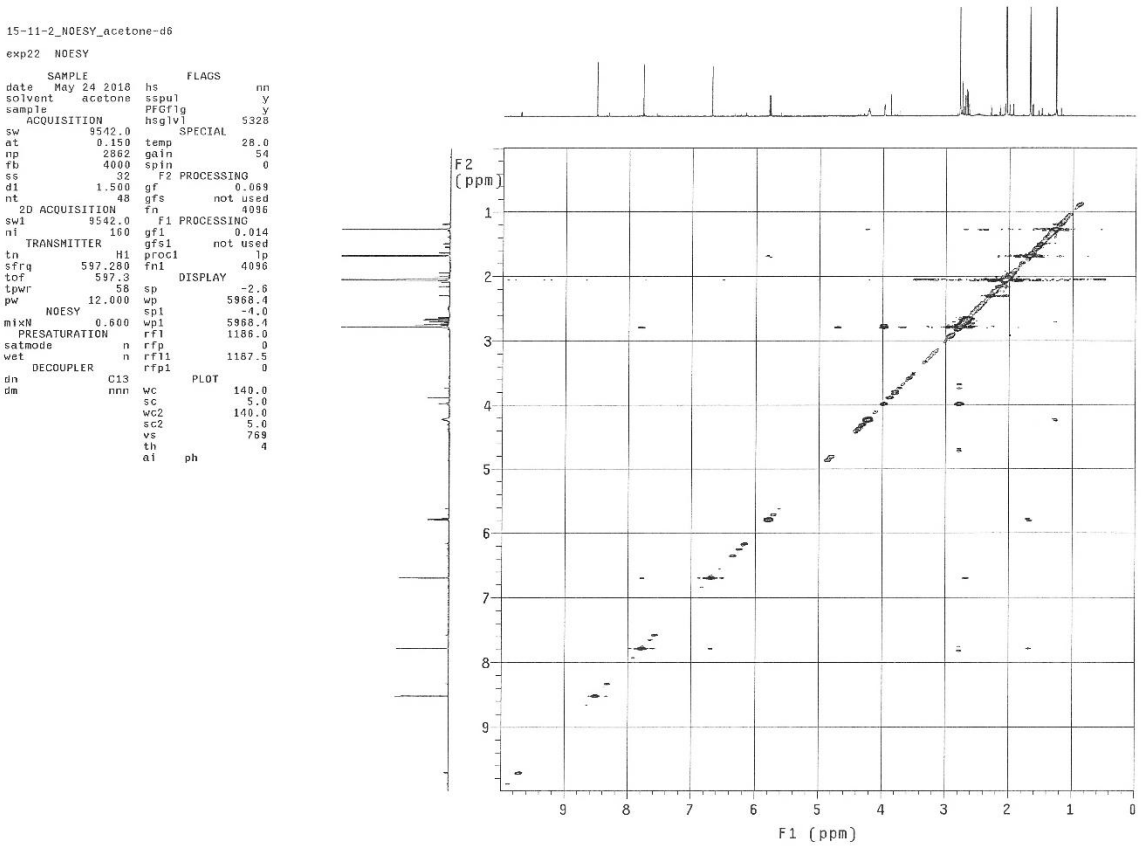


Figure S41. NOESY spectrum of monapurpurin (**6**)

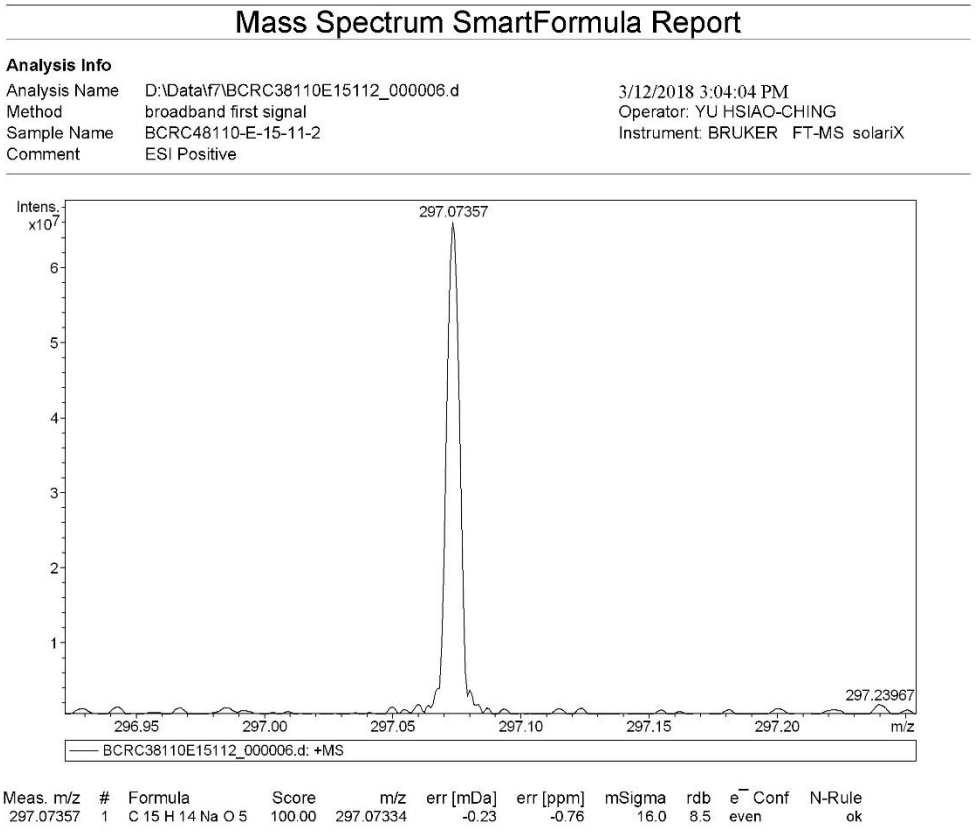


Figure S42. HRESIMS spectrum of monapurpurin (**6**)