

Supplementary Materials

Cytotoxic xanthones from *Hypericum stellatum*, an ethnomedicine in southwest China

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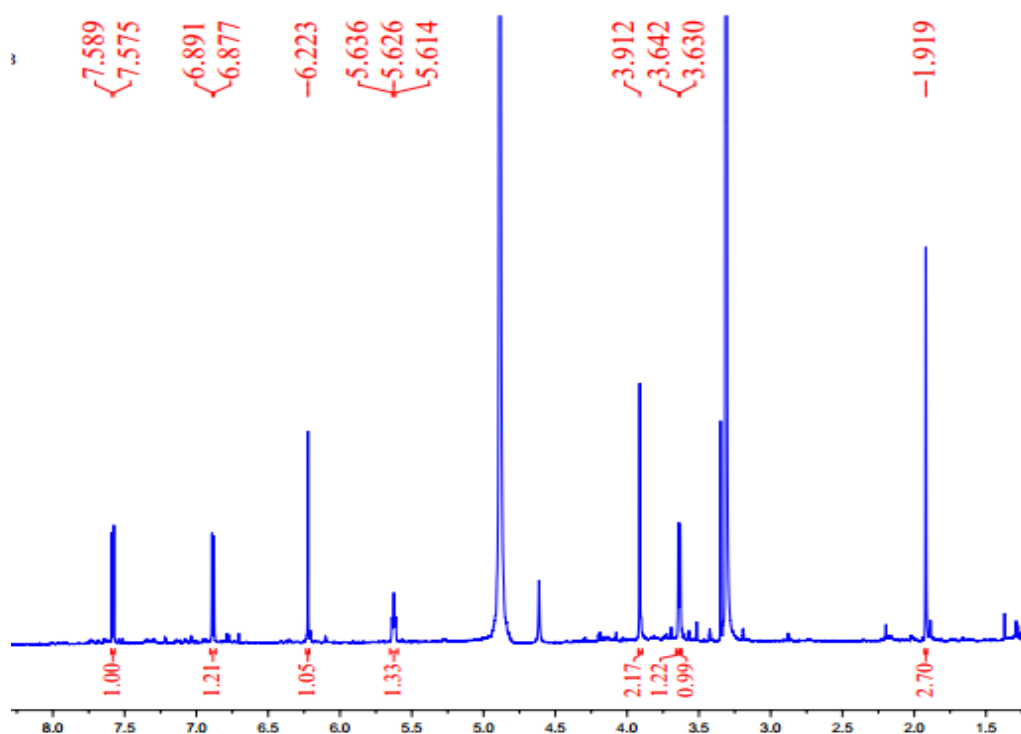


Figure S1. ¹H-NMR spectrum of hypxanthone A in methanol-*d*₄ (600 MHz).

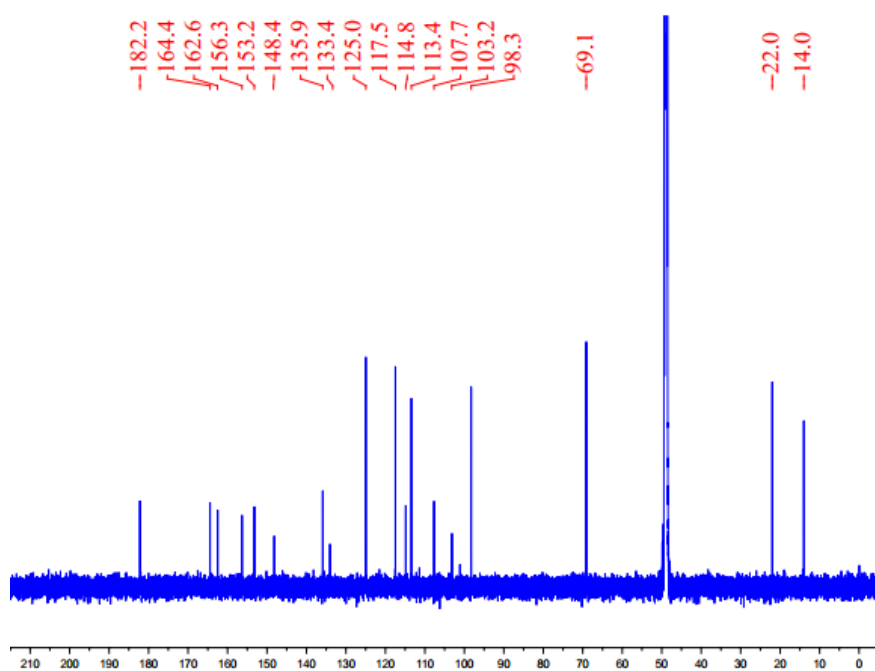


Figure S2. ^{13}C -NMR spectrum of hypxanthone A in methanol- d_4 (151 MHz).

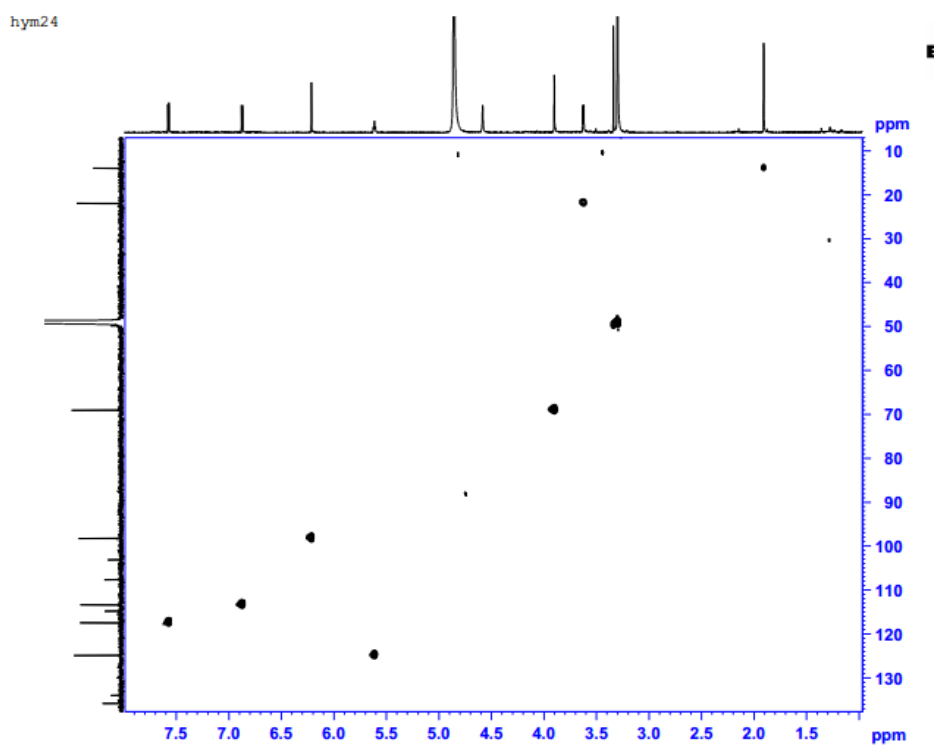


Figure S3. HSQC spectrum of hypxanthone A.

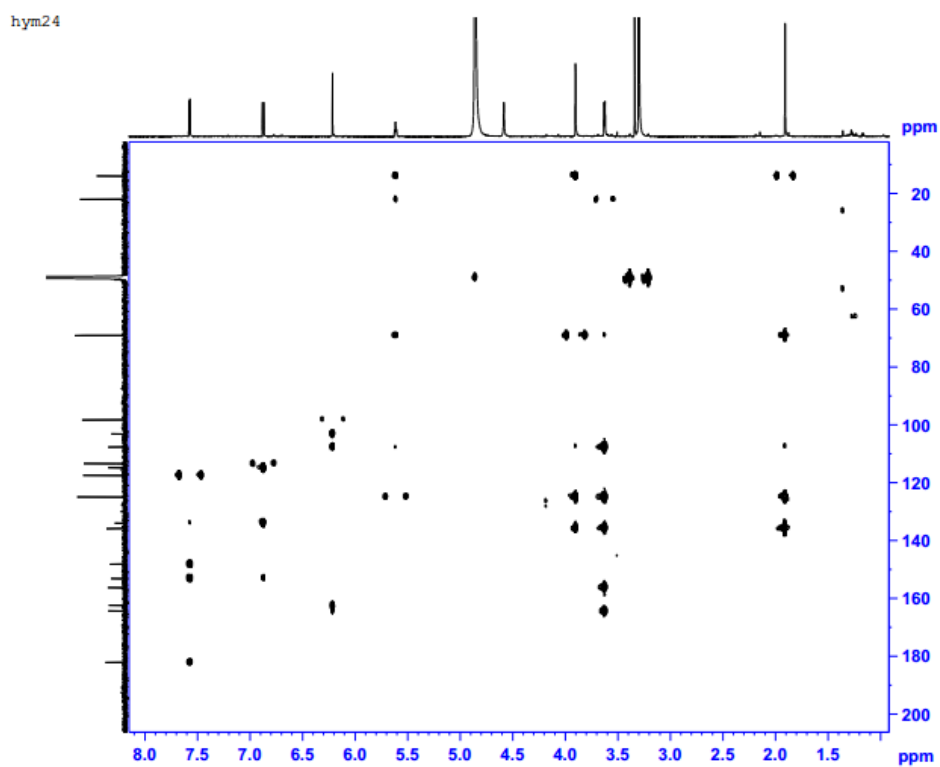


Figure S4. HMBC spectrum of hypxanthone A.

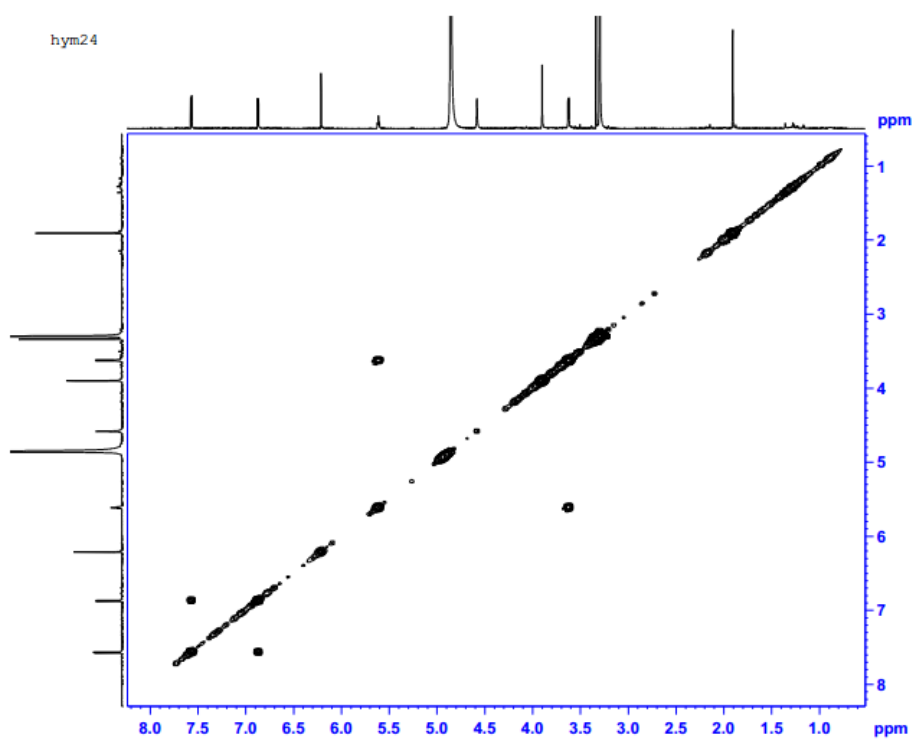


Figure S5. ^1H - ^1H COSY spectrum of hypxanthone A.

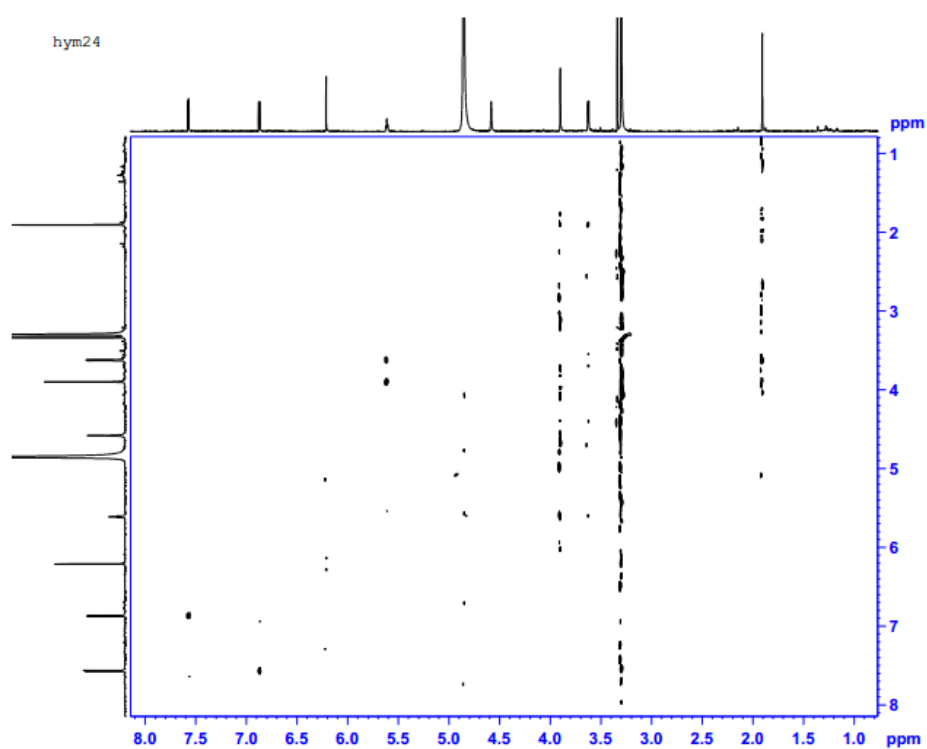


Figure S6. ROESY spectrum of hypxanthone A.

Formula Predictor Report - Hym24.lcd

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Data File: E:\DATA\2018\0305\Hym24.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	100	O	2	0	50	Si	4	0	0	Br	1	0	0	H
C	4	10	50	F	1	0	0	S	2	0	0	I	3	0	0	
N	3	0	0	Na	1	0	0	Cl	1	0	0					

Error Margin (ppm): 5

HC Ratio: unlimited

Max Isotopes: all

MSn Iso RI (%): 75.00

DBE Range: -2.0 - 100.0

Apply N Rule: yes

Isotope RI (%): 1.00

MSn Logic Mode: AND

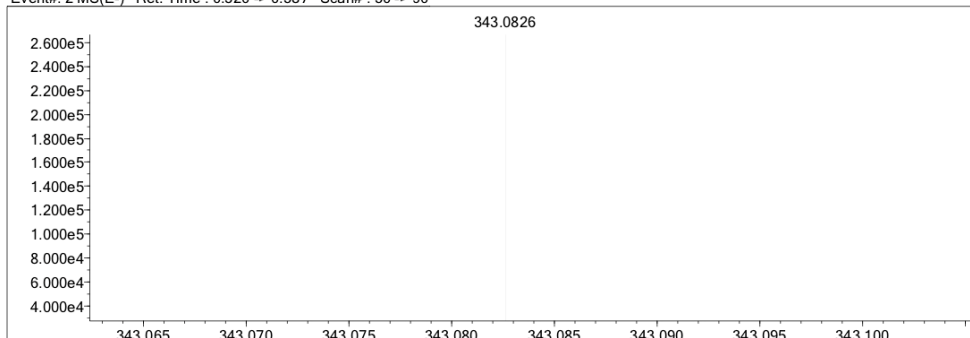
Electron Ions: both

Use MSn Info: yes

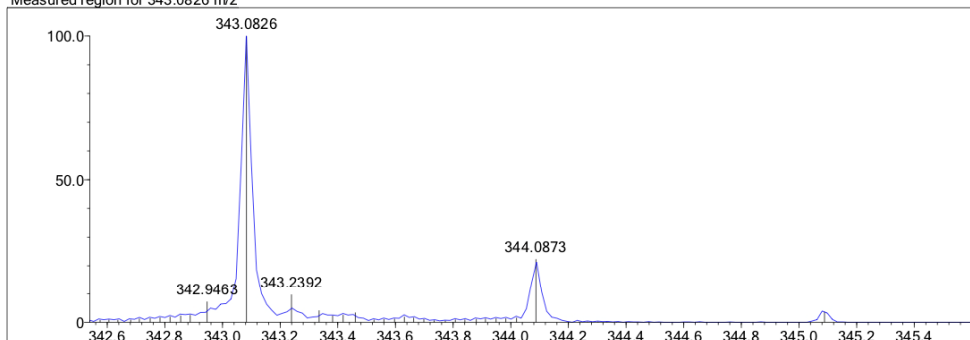
Isotope Res: 10000

Max Results: 10

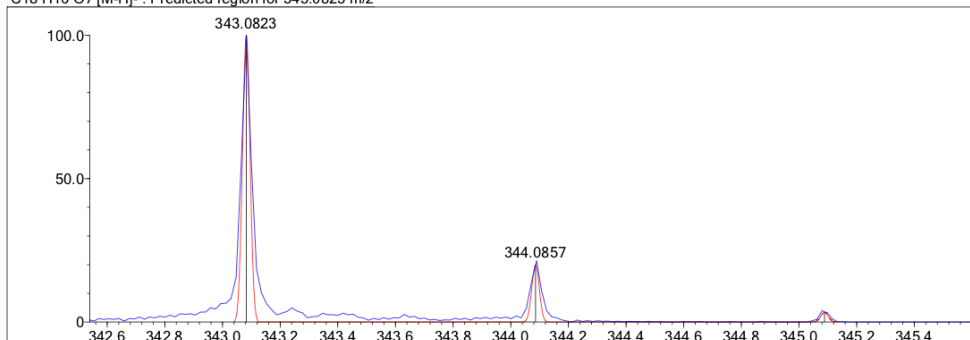
Event#: 2 MS(E-) Ret. Time : 0.320 -> 0.587 Scan#: 50 -> 90



Measured region for 343.0826 m/z



C18 H16 O7 [M-H]- : Predicted region for 343.0823 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C18 H16 O7	[M-H]-	343.0826	343.0823	0.3	0.87	11.0

Figure S7. HR-ESI-MS spectrum of hypxanthone A.

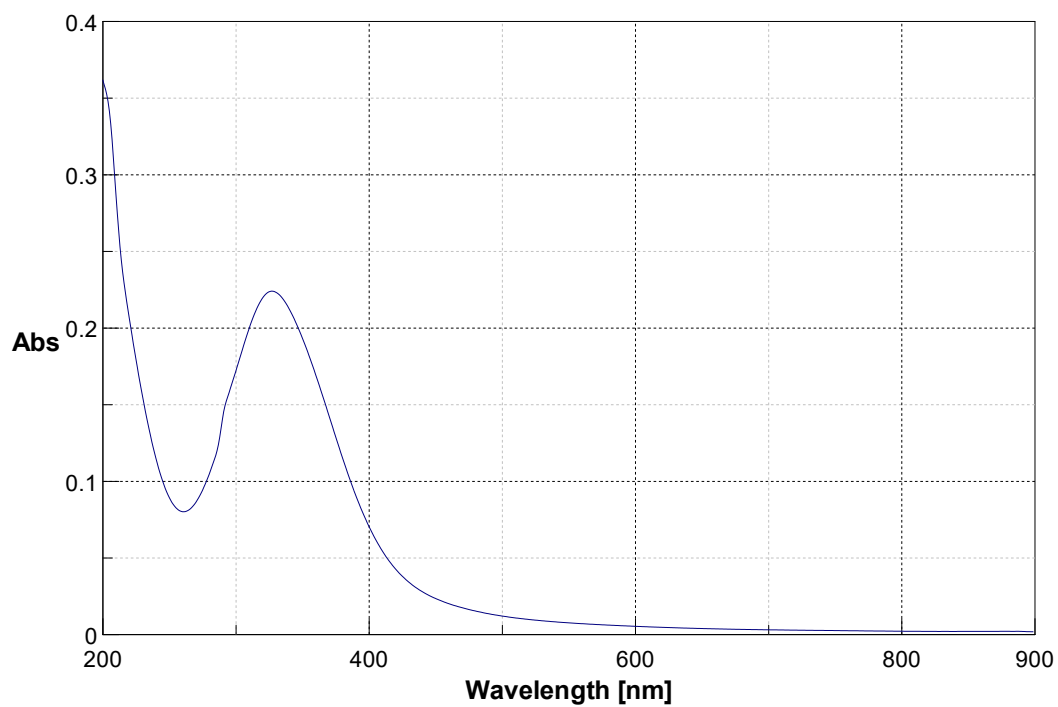


Figure S8. The UV spectrum of hypxanthone A.

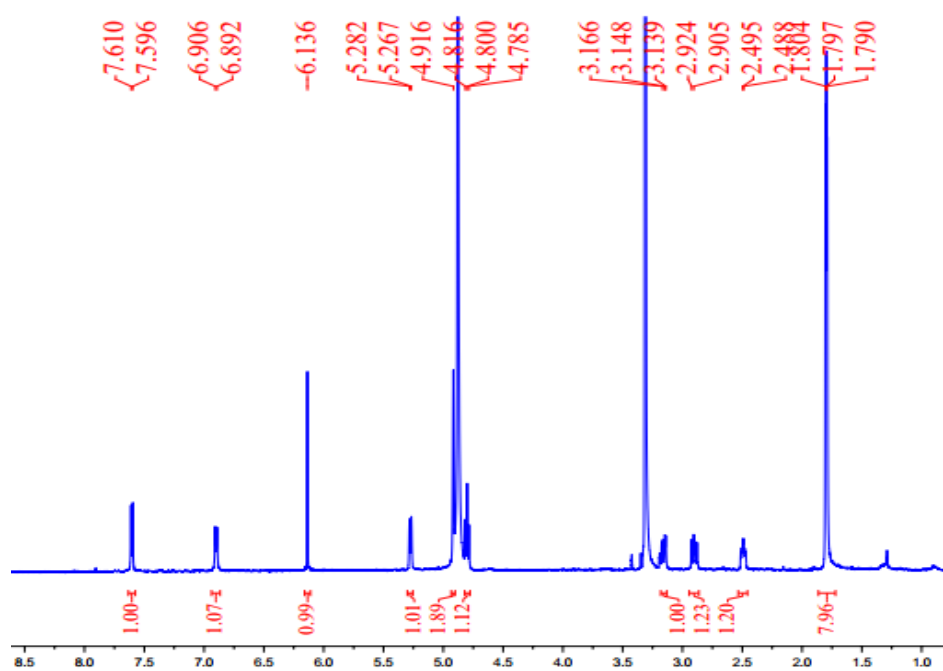


Figure S9. ¹H-NMR spectrum of hypxanthone B in methanol-*d*₄ (600 MHz).

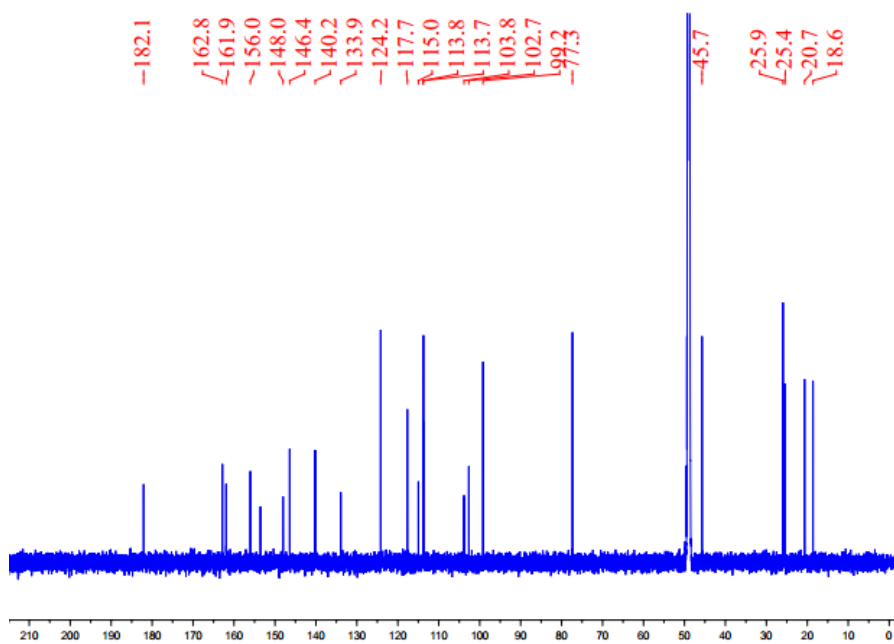


Figure S10. ¹³C-NMR spectrum of hypxanthone B in methanol-*d*₄ (151 MHz).

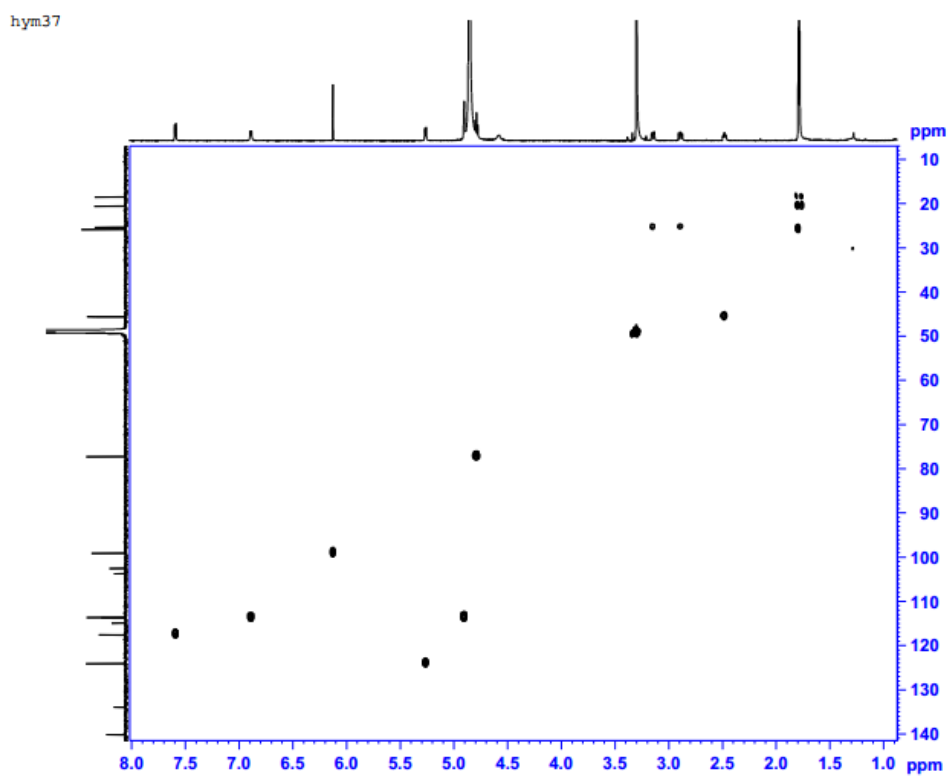


Figure S11. HSQC spectrum of hypxanthone B.

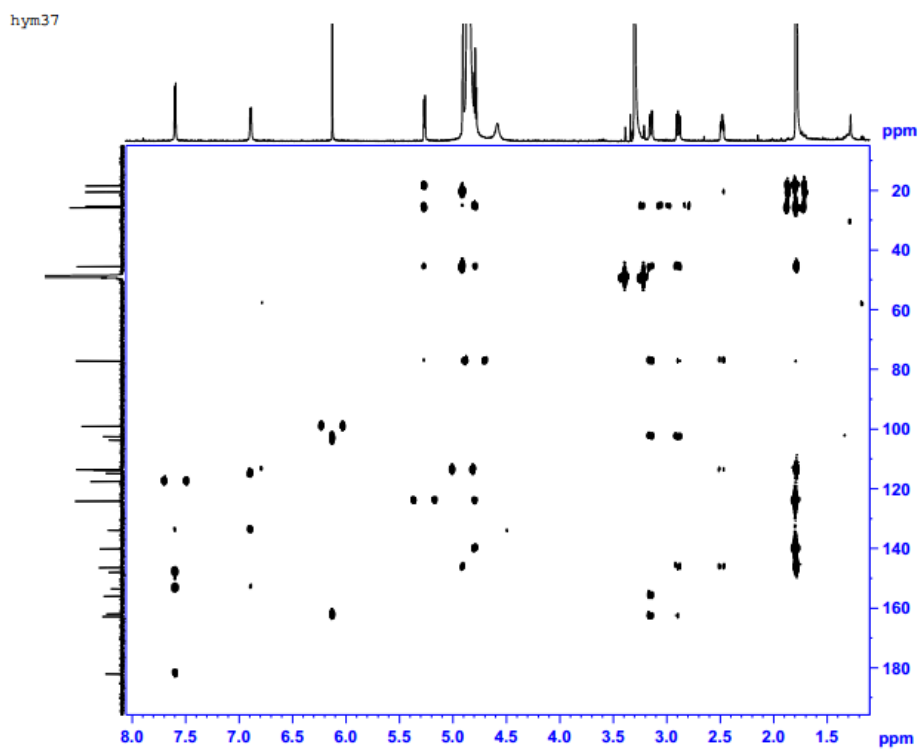
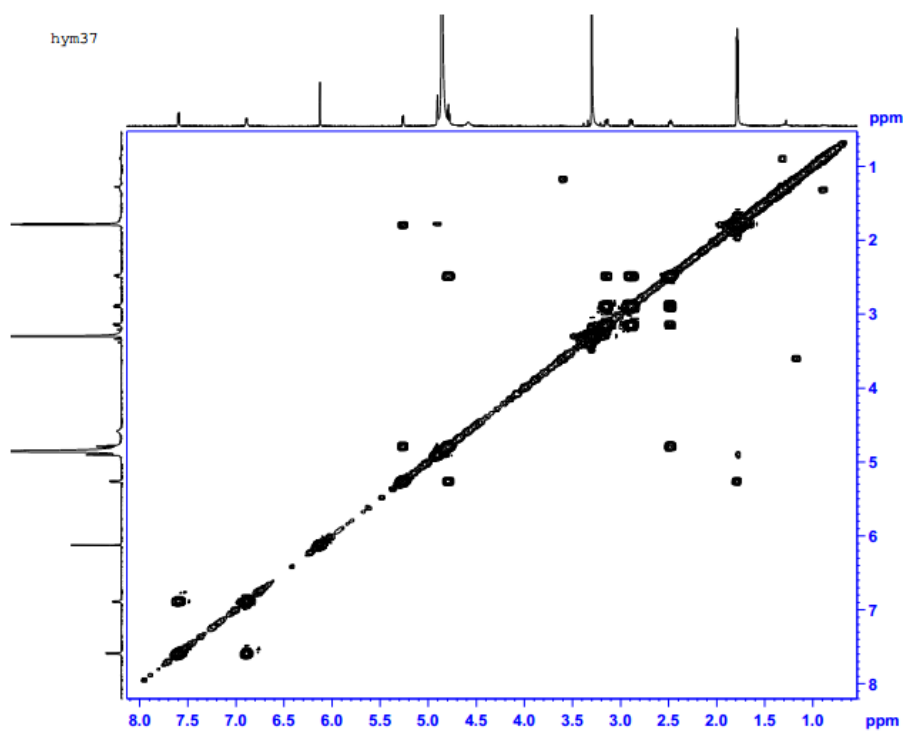


Figure S12. HMBC spectrum of hypxanthone B.

Figure S13. ^1H - ^1H COSY spectrum of hypxanthone B.

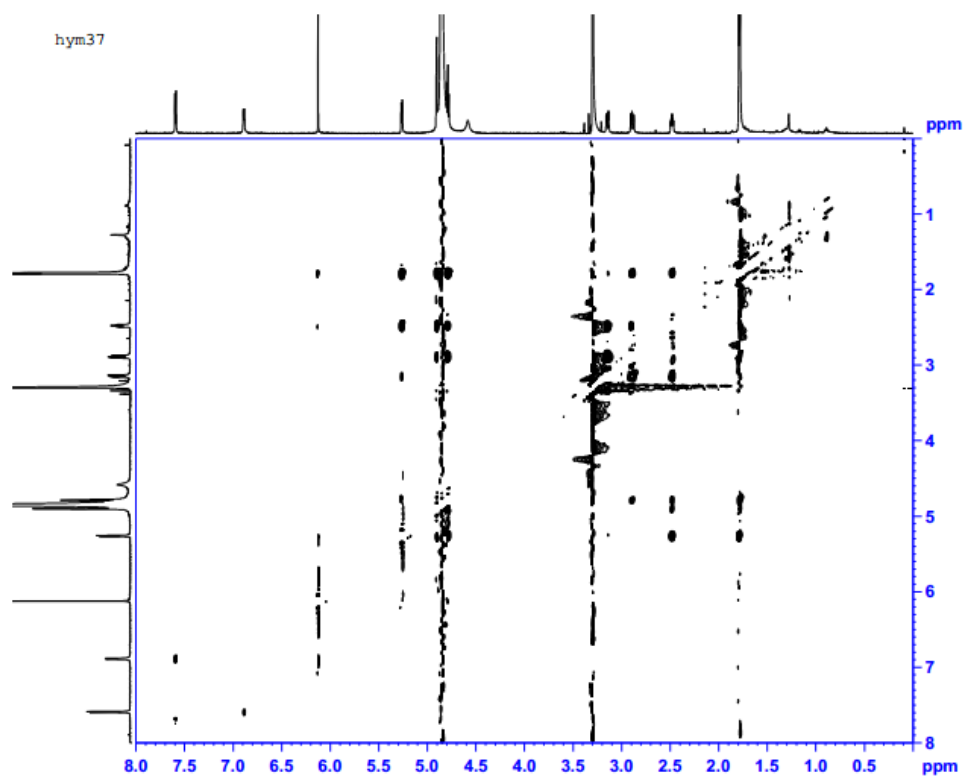


Figure S14. ROESY spectrum of hypoxanthone B.

Formula Predictor Report - Hym37.lcd

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Data File: E:\DATA\2018\0305\Hym37.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	10	100	O	2	0	50	Si	4	0	0	Br	1	0	0	H
C	4	10	50	F	1	0	0	S	2	0	0	I	3	0	0	
N	3	0	0	Na	1	0	0	Cl	1	0	0					

Error Margin (ppm): 10

HC Ratio: unlimited

Max Isotopes: all

MSn Iso RI (%): 75.00

DBE Range: -2.0 - 100.0

Apply N Rule: yes

Isotope RI (%): 1.00

MSn Logic Mode: AND

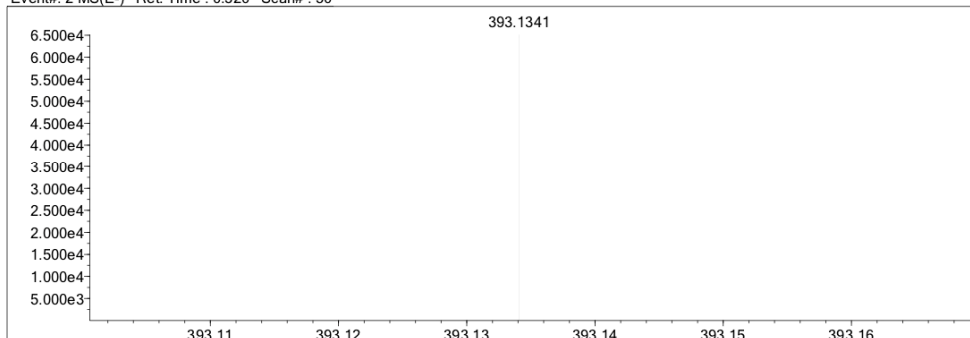
Electron Ions: both

Use MSn Info: yes

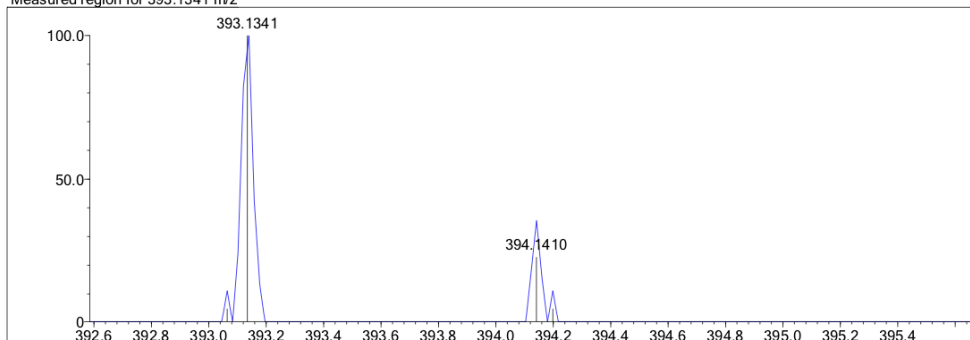
Isotope Res: 10000

Max Results: 10

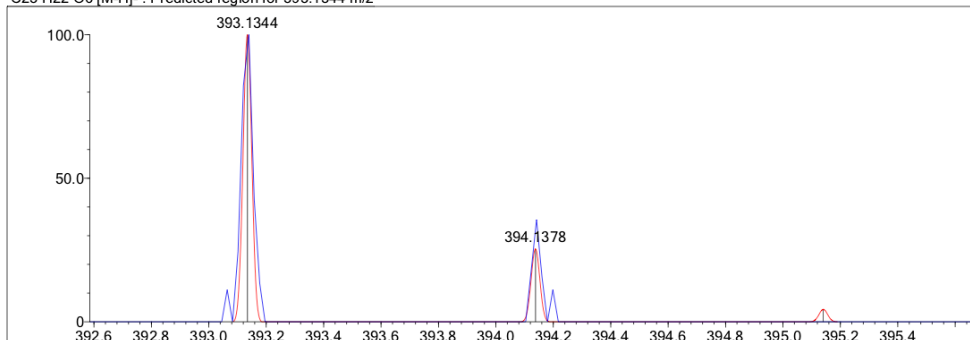
Event#: 2 MS(E-) Ret. Time : 0.320 Scan#: 50



Measured region for 393.1341 m/z



C23 H22 O6 [M-H]- : Predicted region for 393.1344 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C23 H22 O6	[M-H]-	393.1341	393.1344	-0.3	-0.76	13.0

Figure S15. HR-ESI-MS spectrum of hypxanthone B.

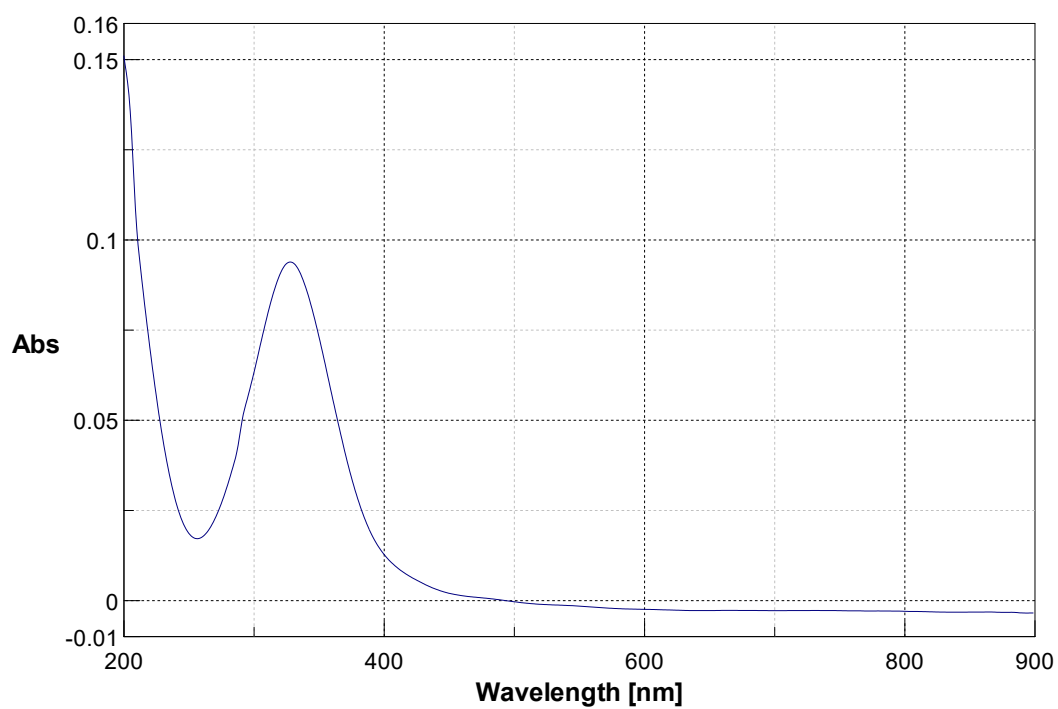


Figure S16. The UV spectrum of hypxanthone B.