

SUPPLEMENTARY MATERIAL

Cytotoxic indole alkaloids from Nauclea orientalis

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ABSTRACT

A new indole alkaloid, nauclorenine (**1**), along with seven known alkaloids (**2-8**), were isolated from the stems and leaves of *Nauclea orientalis*. Among them, nauclorenine (**1**) was a new indole alkaloid holding a rare corynanthe-type skeleton, and the known compounds (**2-8**) were isolated from *N. orientalis* for the first time. Their structures were elucidated on the basis of extensive spectroscopic data analyses. All isolated compounds were evaluated for their cytotoxicities against five human cancer cell lines: HL-60, SMMC-7721, A-549, MCF-7 and SW480 *in vitro*. Alkaloids **1-4** exhibited significant inhibitory effects against various human cancer cell lines with IC₅₀ values comparable to those of cisplatin.

Keywords: *Nauclea orientalis*; indole alkaloid; nauclorenine; cytotoxicities.

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Figure S1. Selected 2D NMR correlations for nauclorenine (**1**).

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Figure S3. ^{13}C -NMR spectrum of nauclorenine (**1**) in $\text{DMSO-}d_6$.

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Figure S7. ROESY spectrum of nauclorenine (**1**) in $\text{DMSO-}d_6$.

Figure S8. HRESIMS spectrum of nauclorenine (**1**).

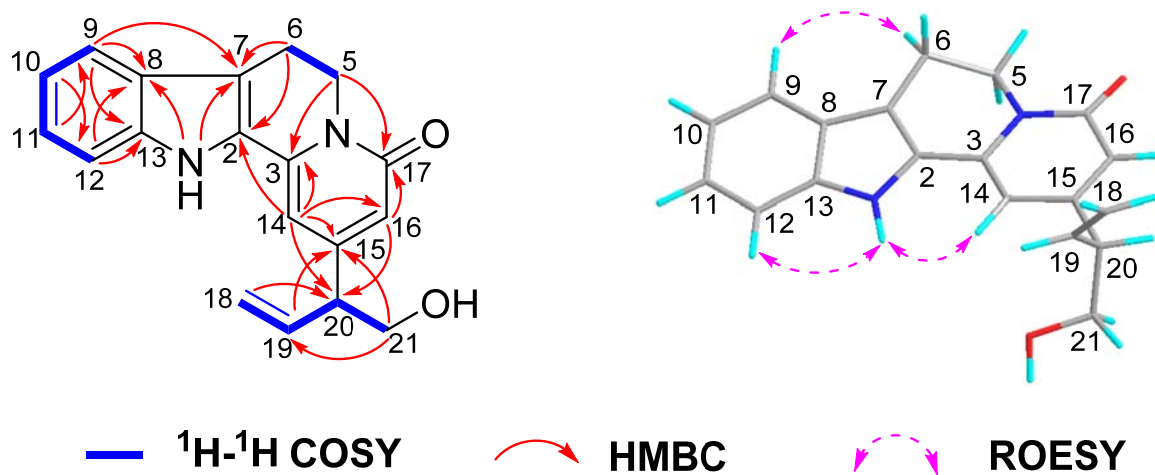


Figure S1. Selected 2D NMR correlations for nauclorenine (**1**).

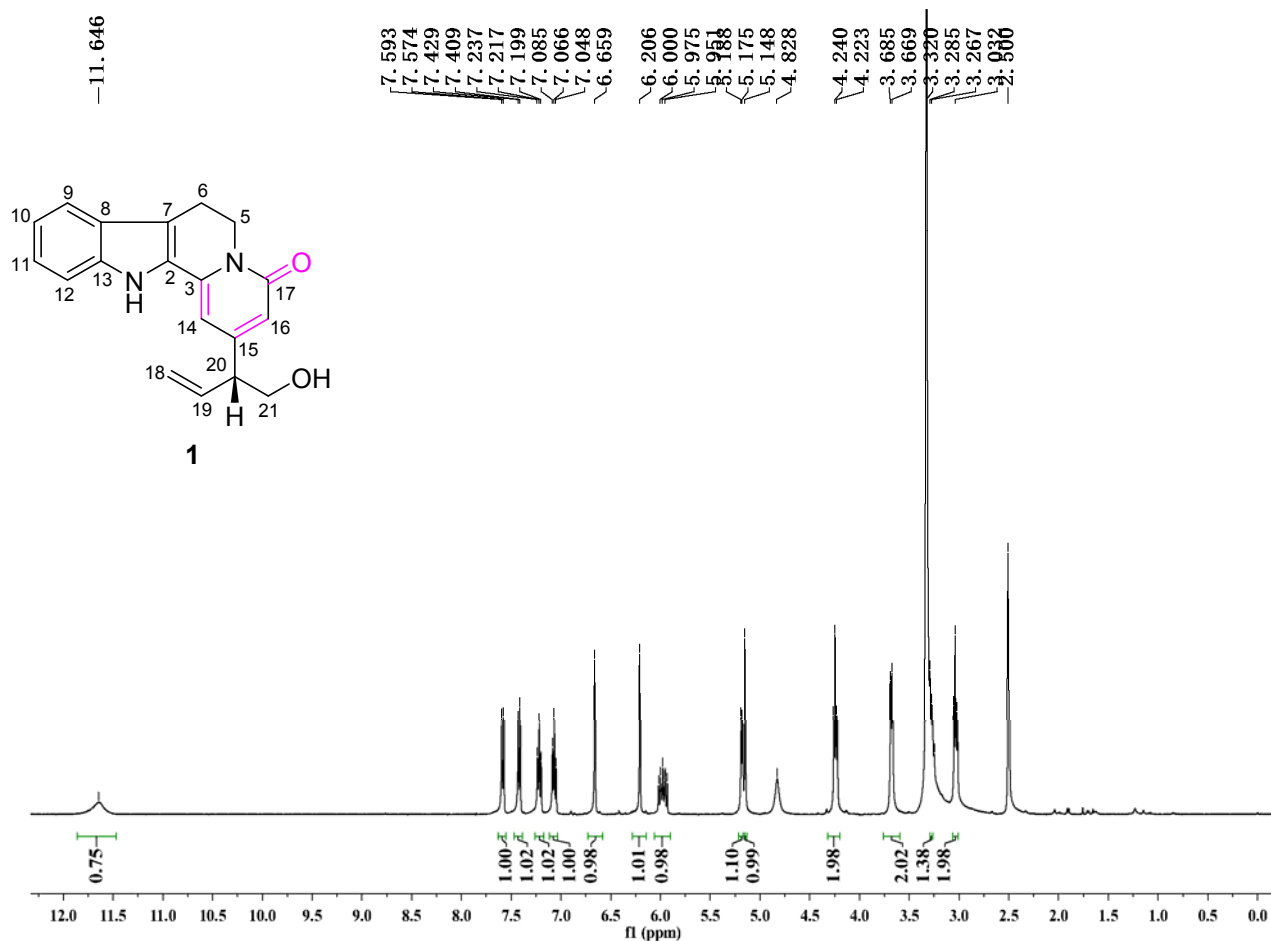


Figure S2. ^1H -NMR spectrum of nauclorenine (**1**) in DMSO- d_6 .

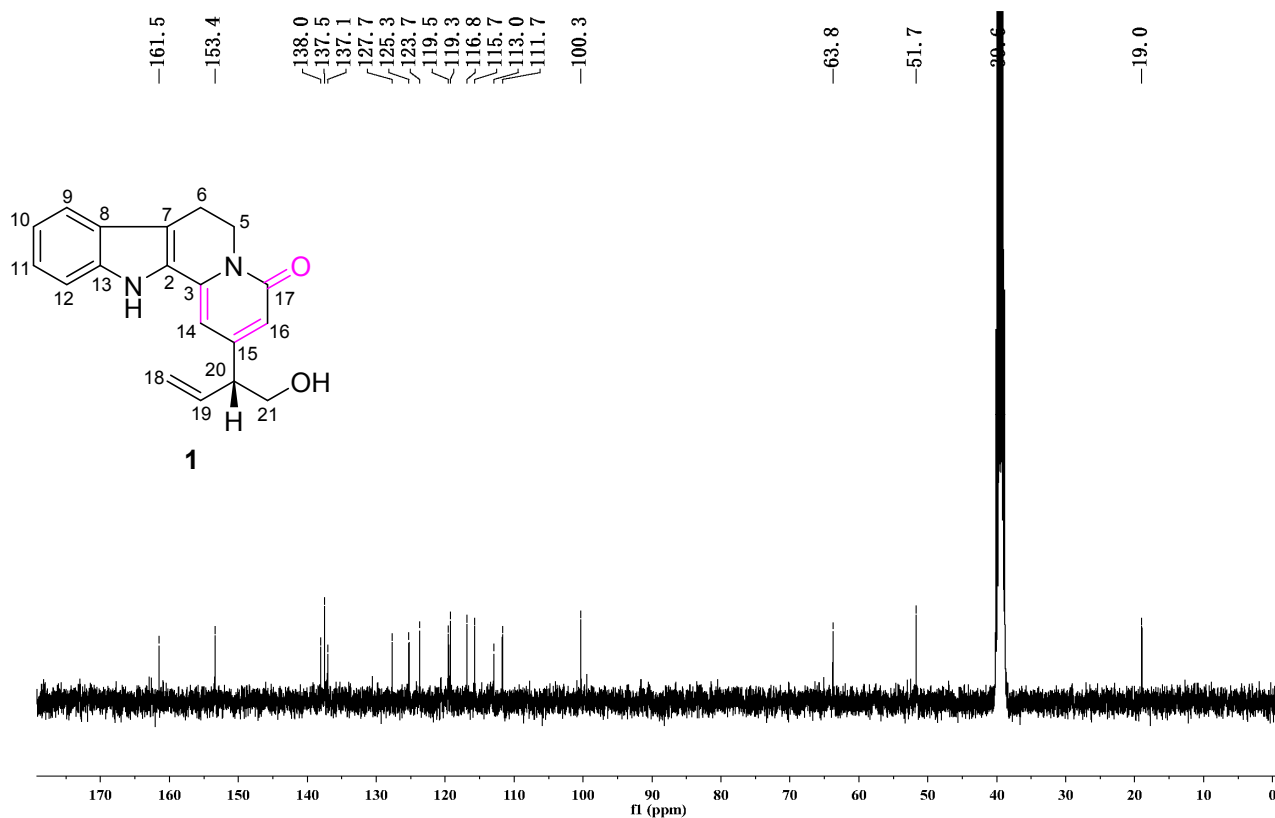


Figure S3. ^{13}C -NMR spectrum of nauclorenine (**1**) in $\text{DMSO}-d_6$.

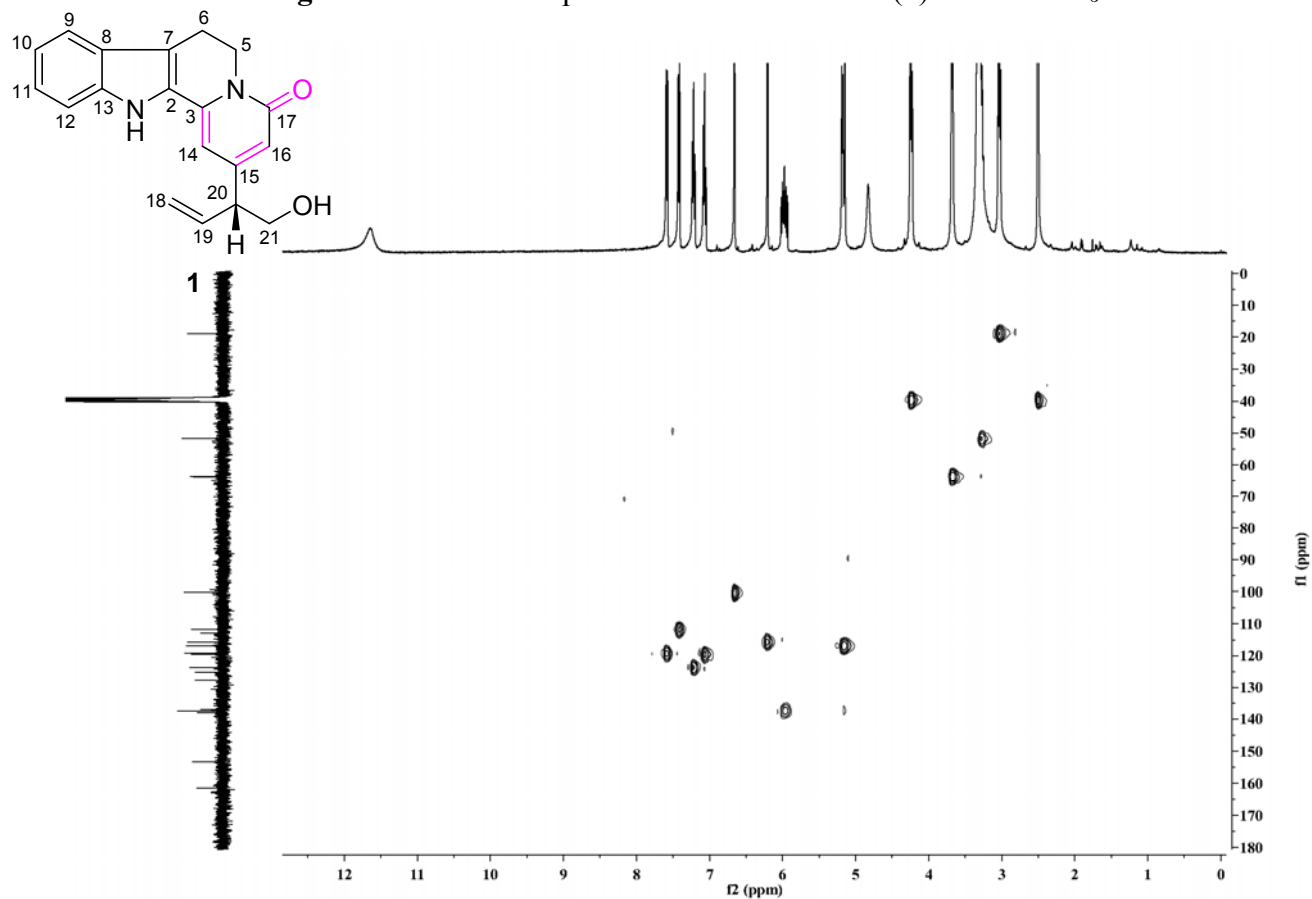


Figure S4. HSQC spectrum of nauclorenine (**1**) in $\text{DMSO}-d_6$.

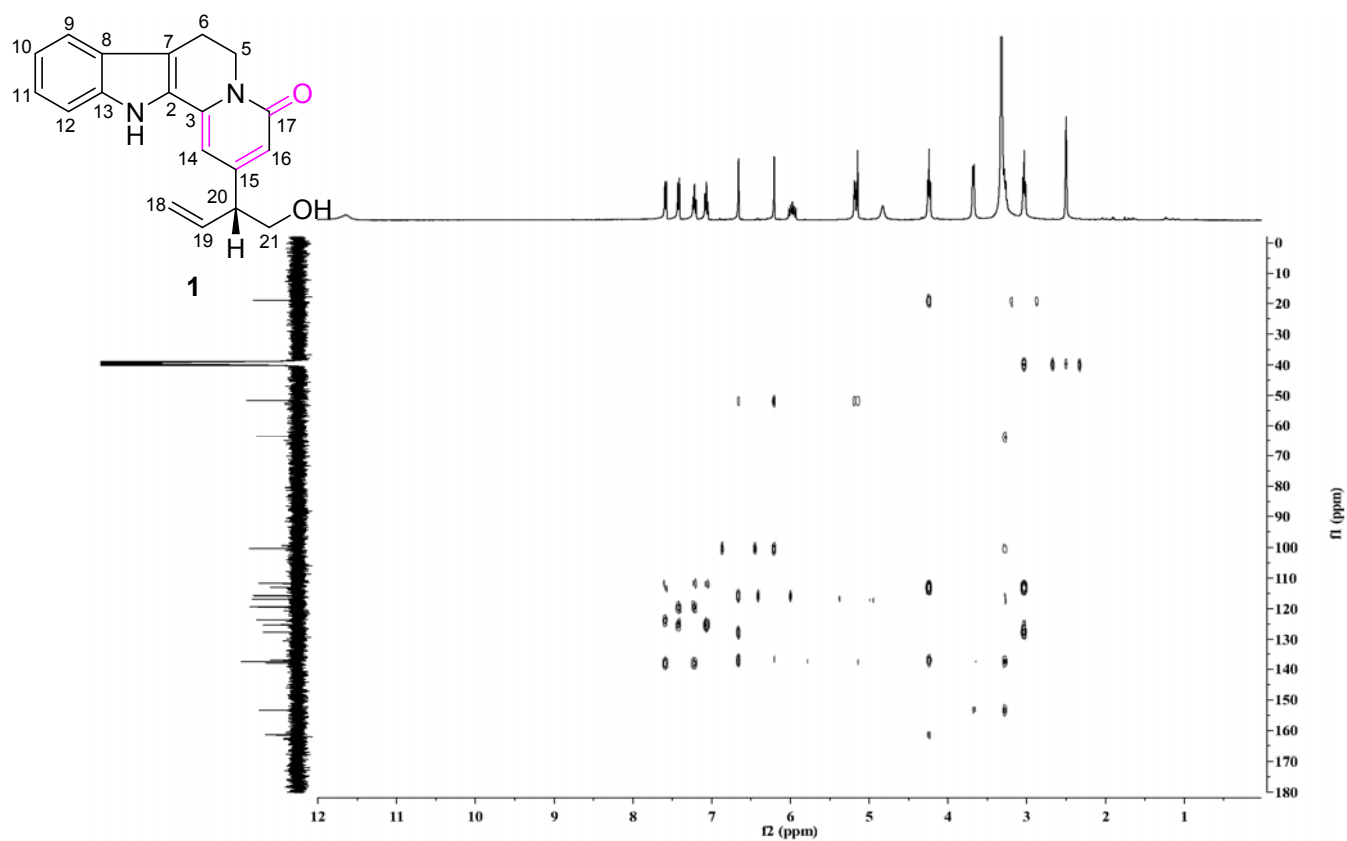


Figure S5. HMBC spectrum of nauclorenine (**1**) in DMSO- d_6 .

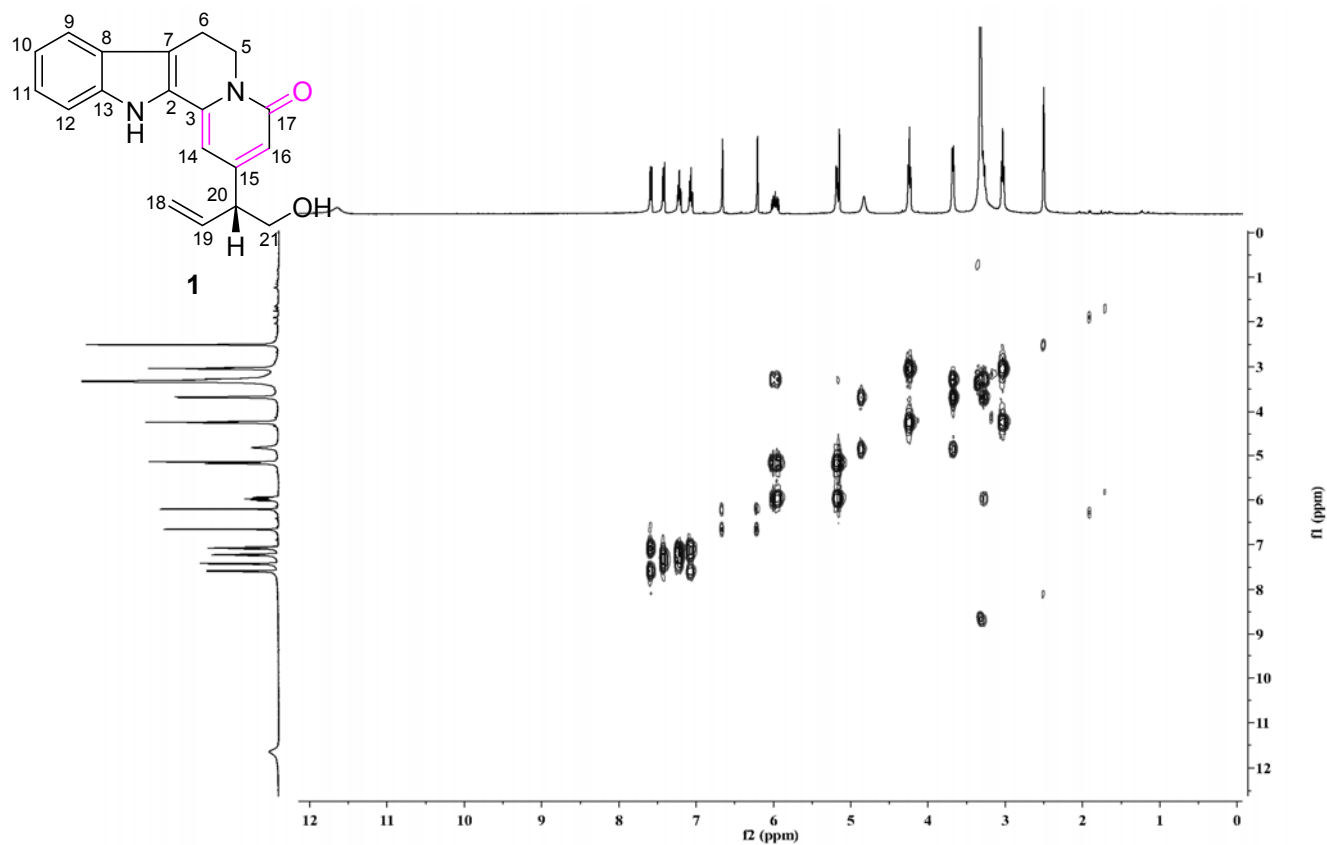


Figure S6. ^1H - ^1H COSY spectrum of nauclorenine (**1**) in DMSO- d_6 .

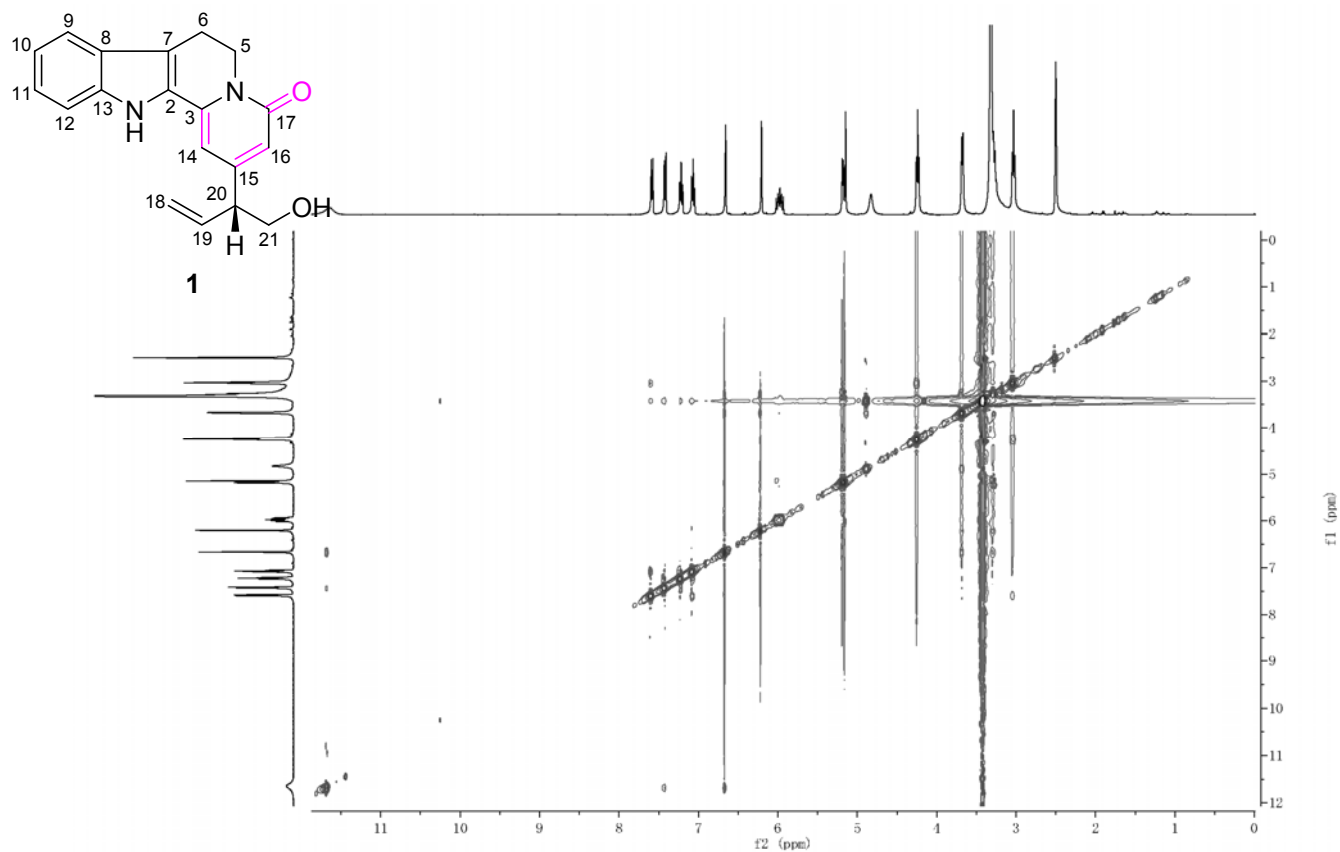


Figure S7. ROESY spectrum of nauclorenine (**1**) in DMSO- d_6 .

Data File: E:\DATA\2017\0906\HMNO6.lcd

Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Elmt	Val.	Min	Max	Use Adduct
H	1	0	150	O	2	0	50	P	3	0	0	Br	1	0	0	H
B	3	0	0	F	1	0	0	S	2	0	0	I	3	0	0	
C	4	0	50	Na	1	0	0	Cl	1	0	0	Pt	2	0	0	
N	3	0	10	Mg	2	0	0	Fe	2	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

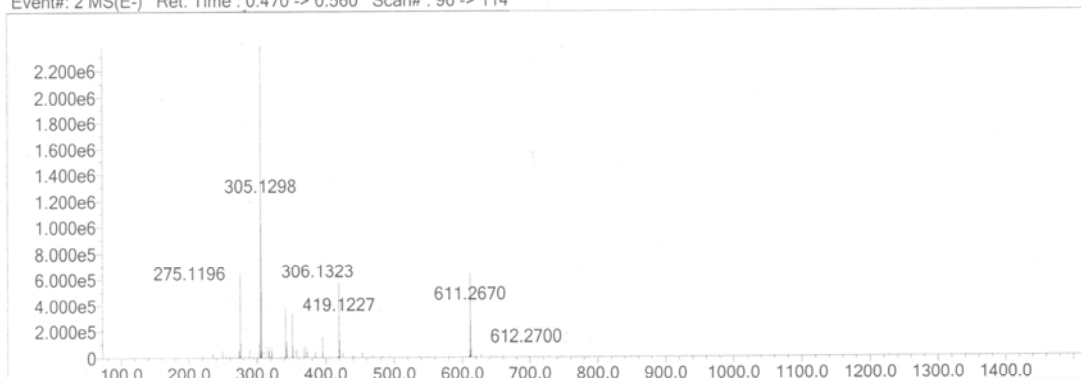
Electron Ions: both

Use MSn Info: yes

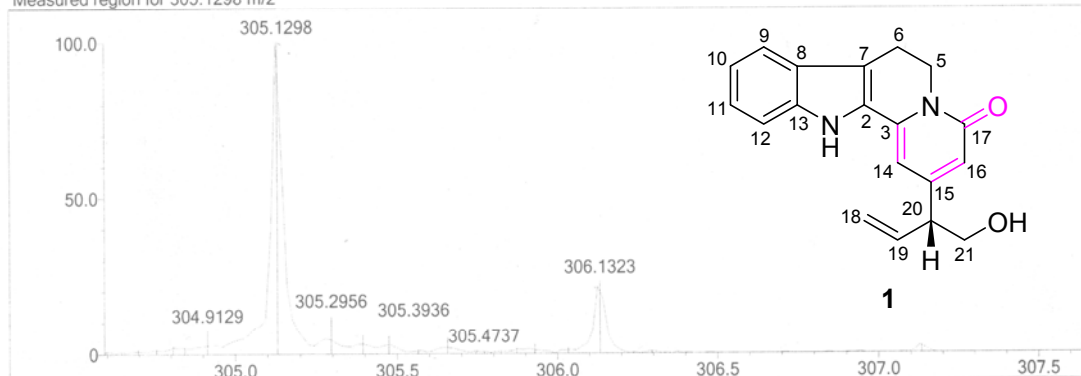
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Max Results: 10

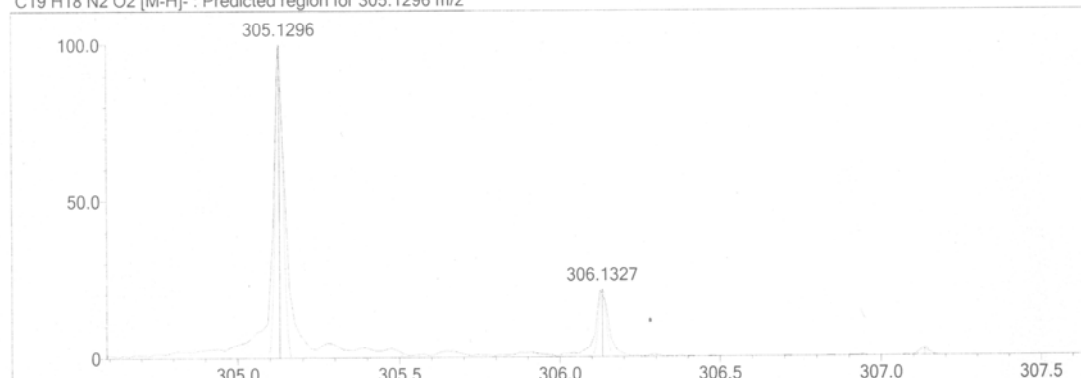
Event#: 2 MS(E-) Ret. Time : 0.470 -> 0.560 Scan#: 96 -> 114



Measured region for 305.1298 m/z



C19 H18 N2 O2 [M-H]- : Predicted region for 305.1296 m/z



Formula (M)	Ion	Meas. m/z	Pred. m/z	Df. (mDa)	Df. (ppm)	DBE
C19 H18 N2 O2	[M-H]-	305.1298	305.1296	0.2	0.66	12.0

Figure S8. HRESIMS spectrum of nauclorenine (1).