Supplementary Materials: Cytotoxic Alkaloid from the Stem of *Xylopia laevigata*

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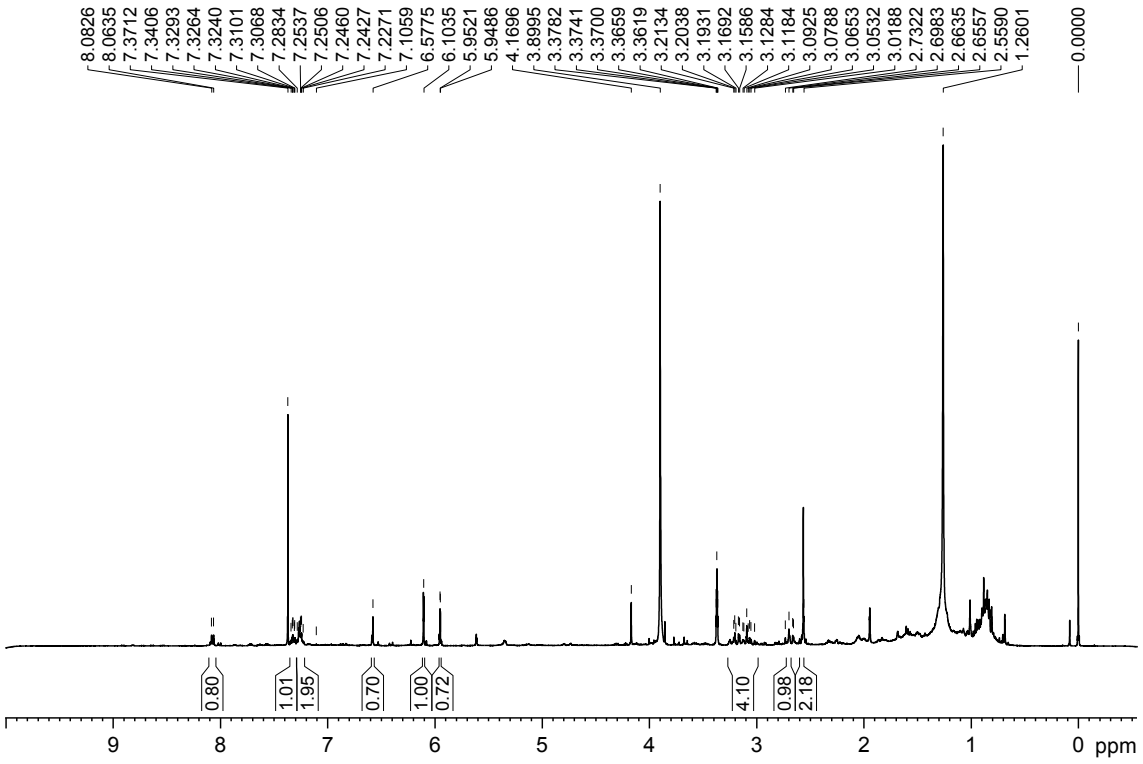

Figure S1. ^{1}H NMR spectrum of alkaloid **(-)-roemerine** ($CDCl_3$ + drops of CD_3OD at 400 MHz).

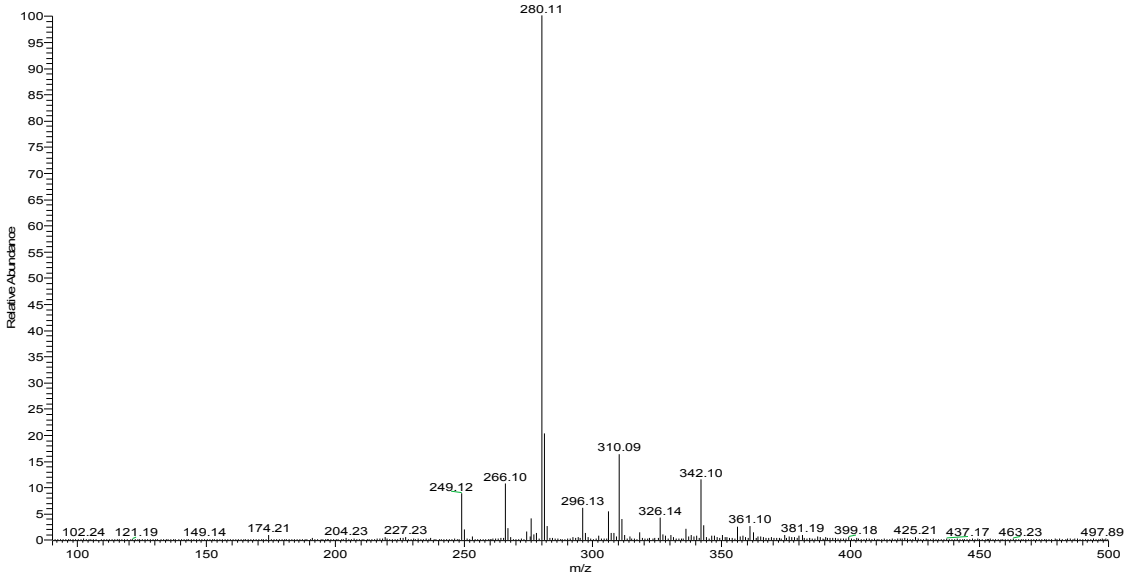

Figure S2. MS of alkaloid **(–)-roemerine** (*m*/*z* 280.11 $[M + H]^+$).

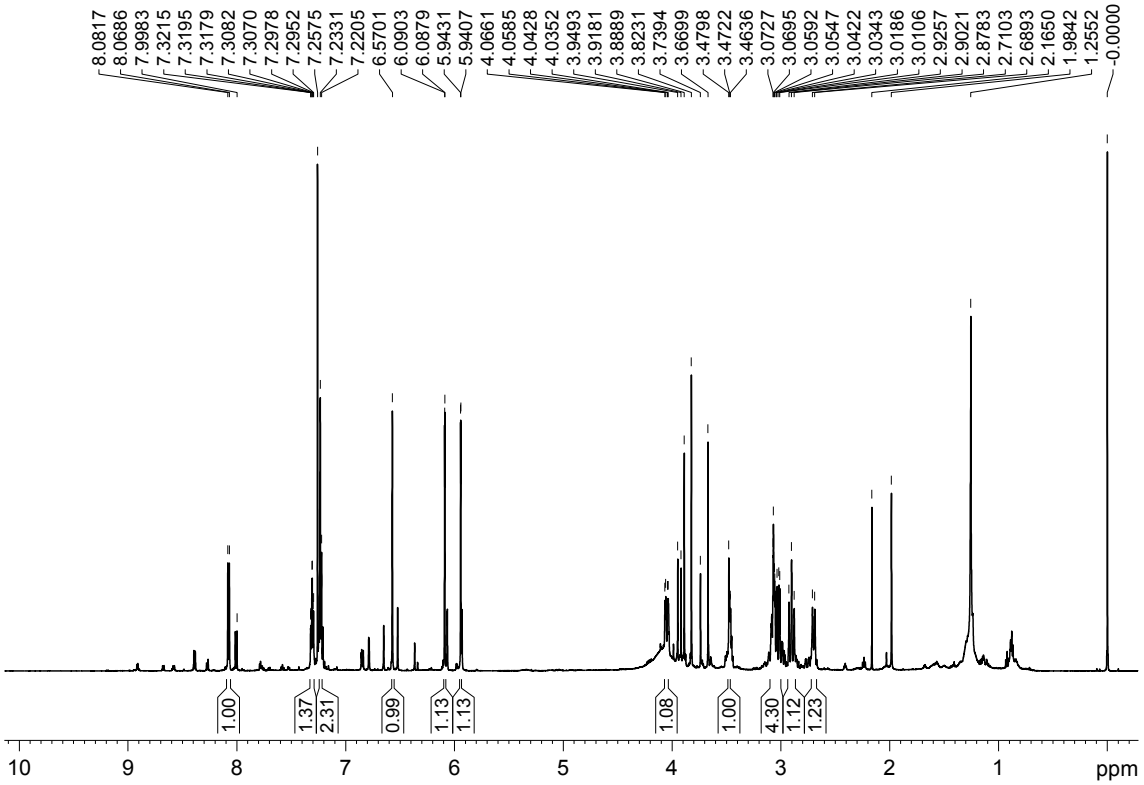

Figure S3. ^{1}H NMR spectrum of alkaloid **(+)-anonaine** ($CDCl_3$ at 400 MHz).

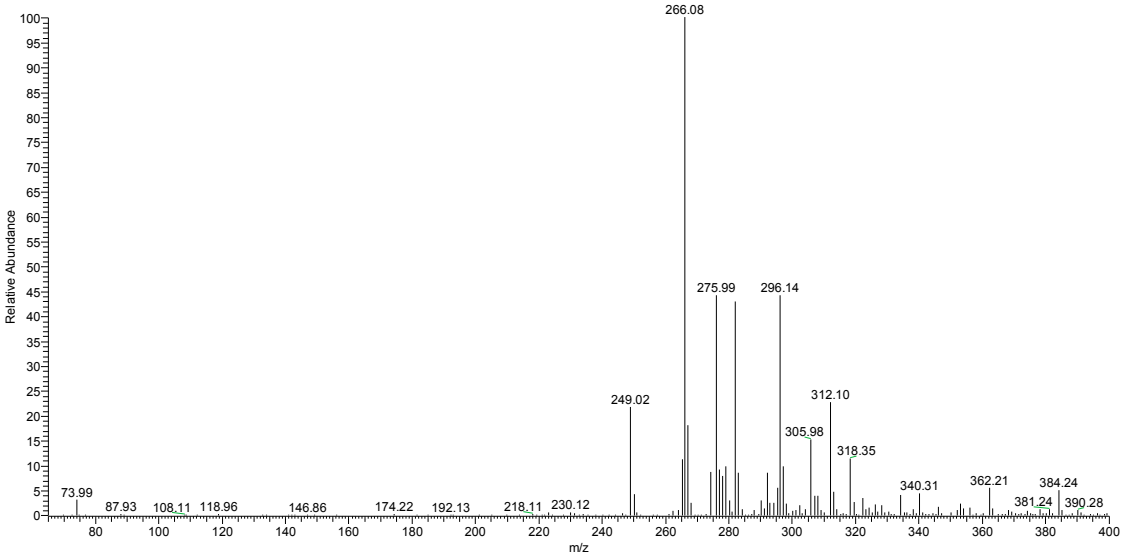

Figure S4. MS of alkaloid **(+)-anonaine** (*m*/*z* 266.08 $[M + H]^+$).

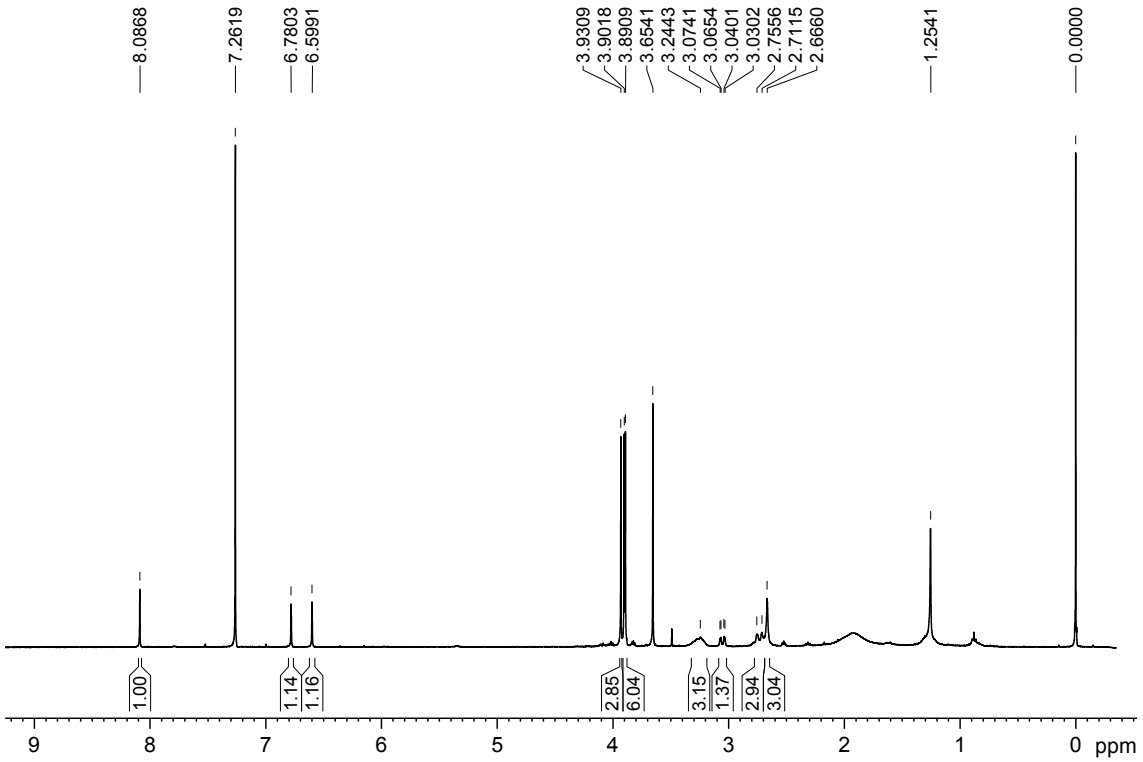

Figure S5. ^{1}H NMR spectrum of alkaloid **(+)-glaucine** ($CDCl_3$ + drops of CD_3OD at 400 MHz).

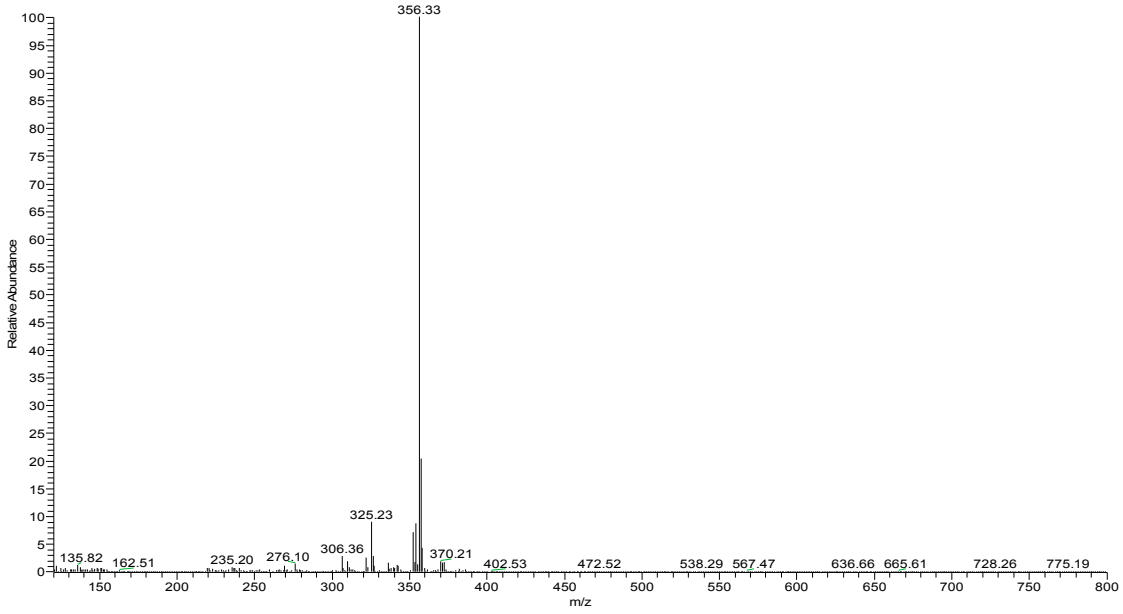

Figure S6. MS of alkaloid **(+)-glaucine** (*m*/*z* 356.33 $[M + H]^+$).

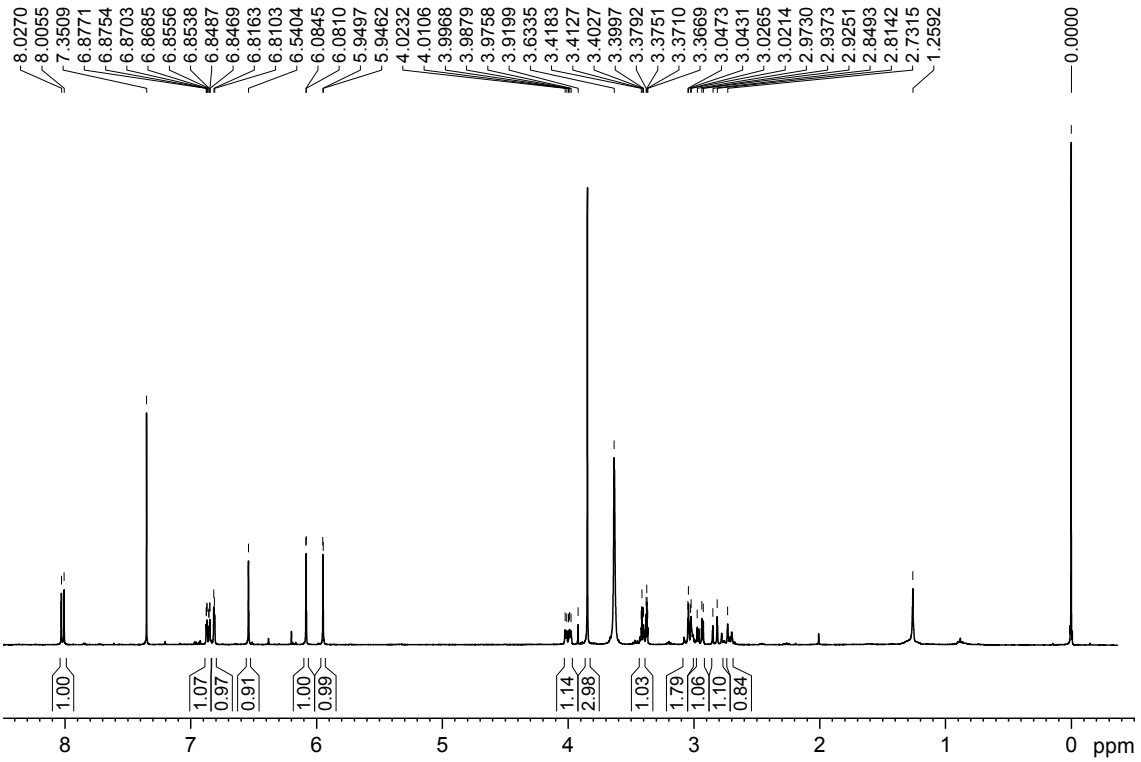

Figure S7. ^{1}H NMR spectrum of alkaloid **(+)-xylopine** ($CDCl_3$ + drops of CD_3OD at 400 MHz).

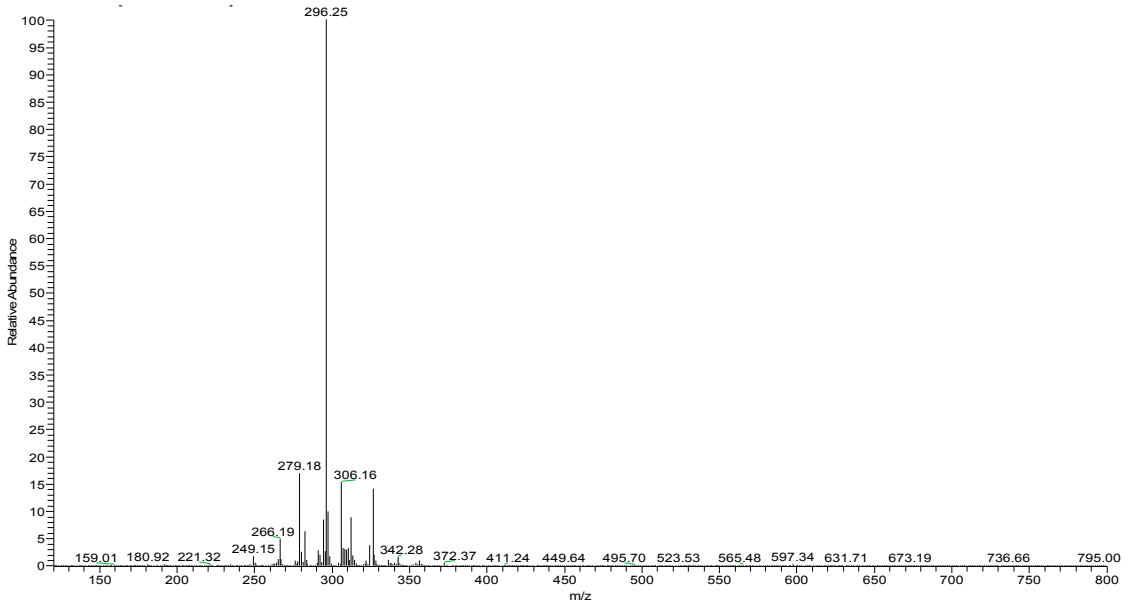

Figure S8. MS of alkaloid **(+)-xylopine** (*m*/*z* 296.25 $[M + H]^+$).

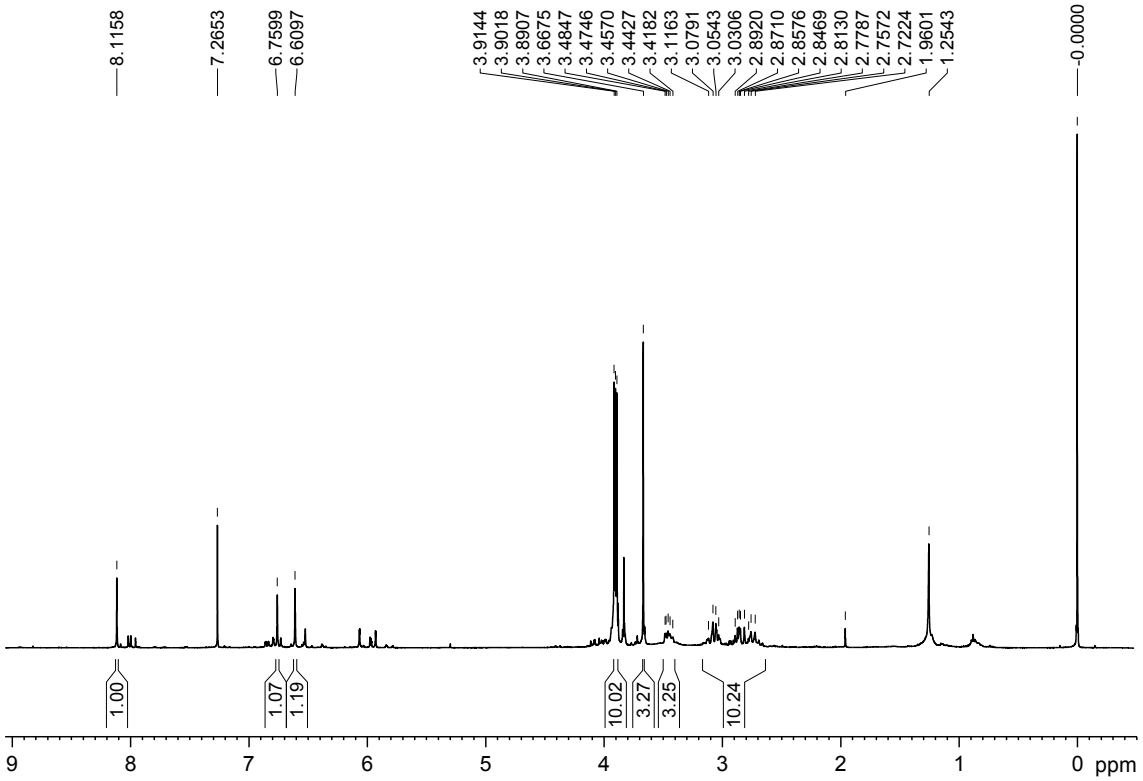

Figure S9. ^{1}H NMR spectrum of alkaloid **(+)-norglaucine** ($CDCl_3$ + drops of CD_3OD at 400 MHz).

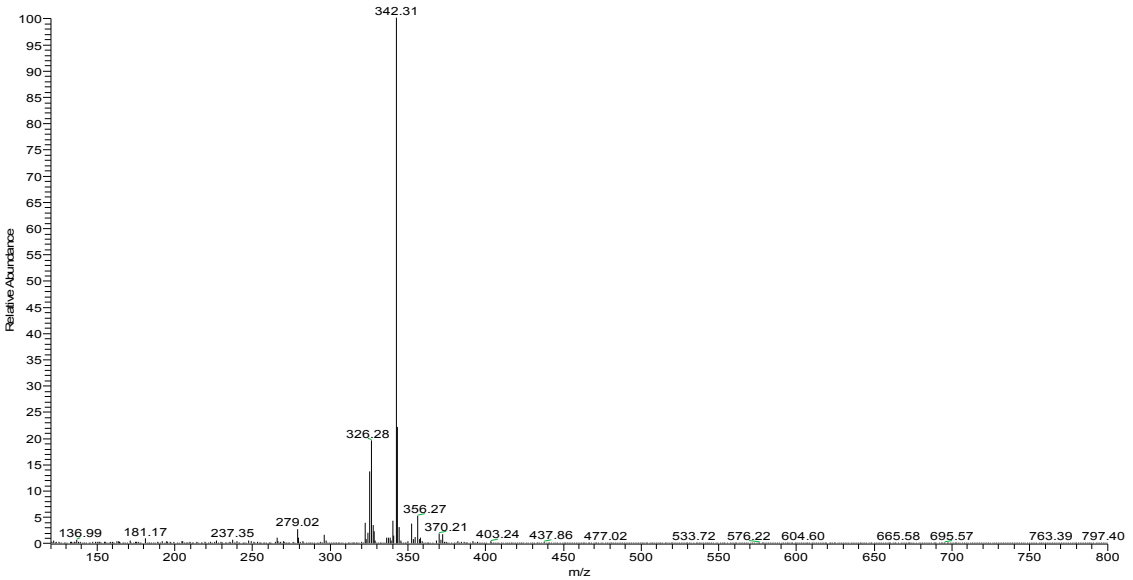

Figure S10. MS of alkaloid **(+)-norglaucine** (*m*/*z* 342.31 $[M + H]^+$).

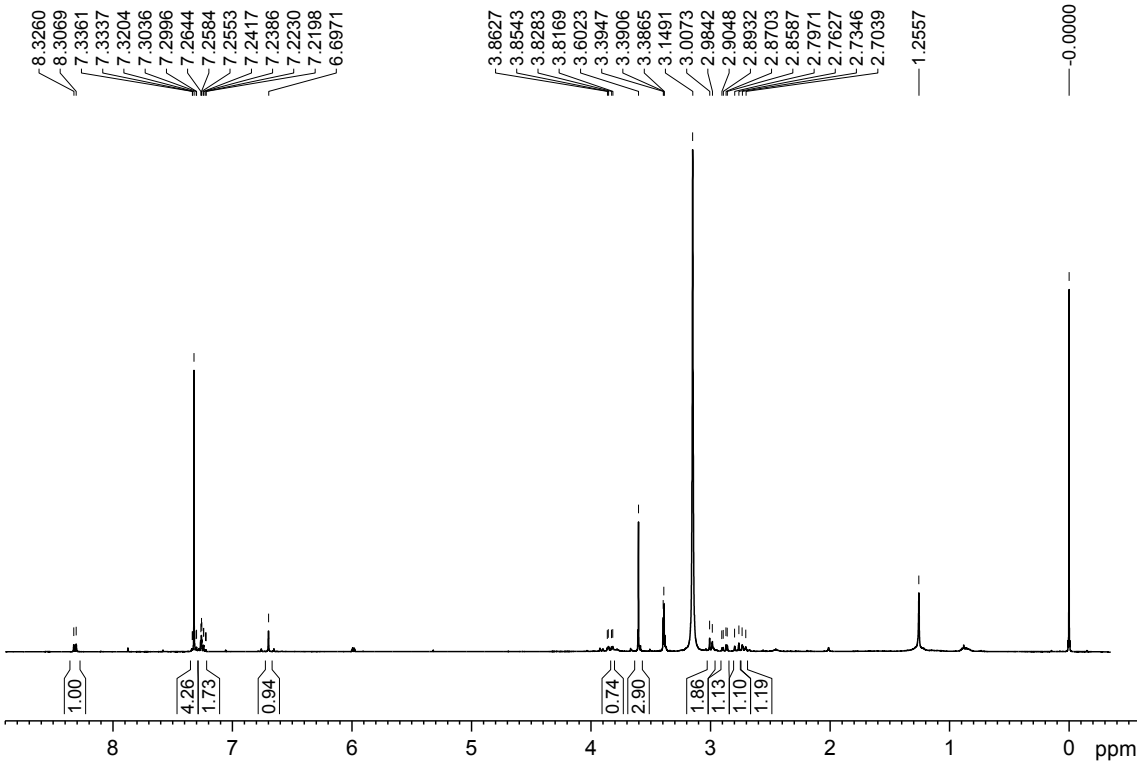

Figure S11. ^{1}H NMR spectrum of alkaloid **asimilobine** ($CDCl_3$ + drops of CD_3OD at 400 MHz).

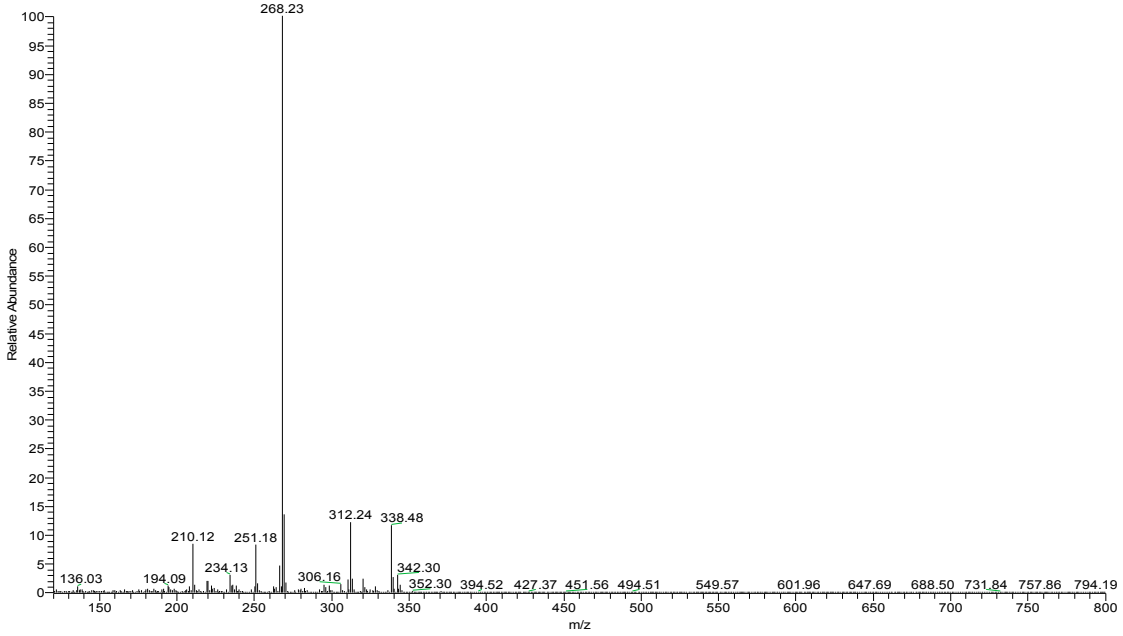

Figure S12. MS of alkaloid **asimilobine** (*m*/*z* 268.23 $[M + H]^+$).

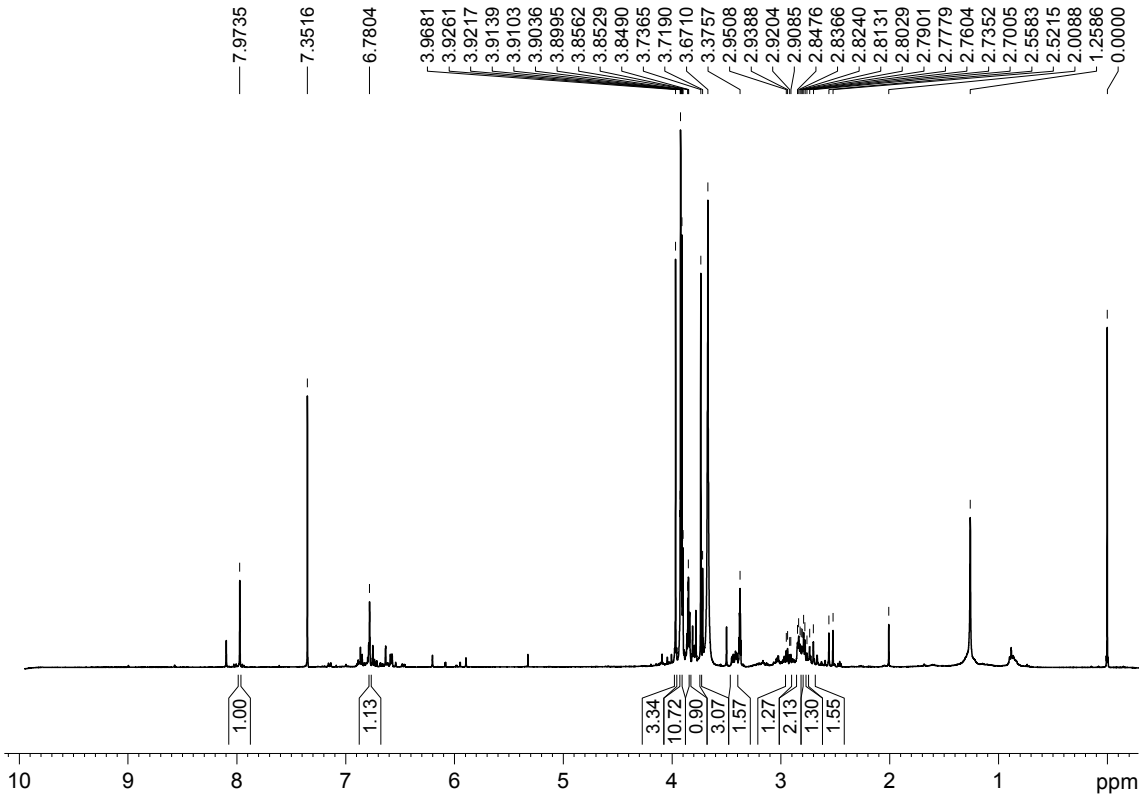

Figure S13. ^{1}H NMR spectrum of alkaloid **(+)-norpurpureine** ($CDCl_3$ + drops of CD_3OD at 400 MHz).

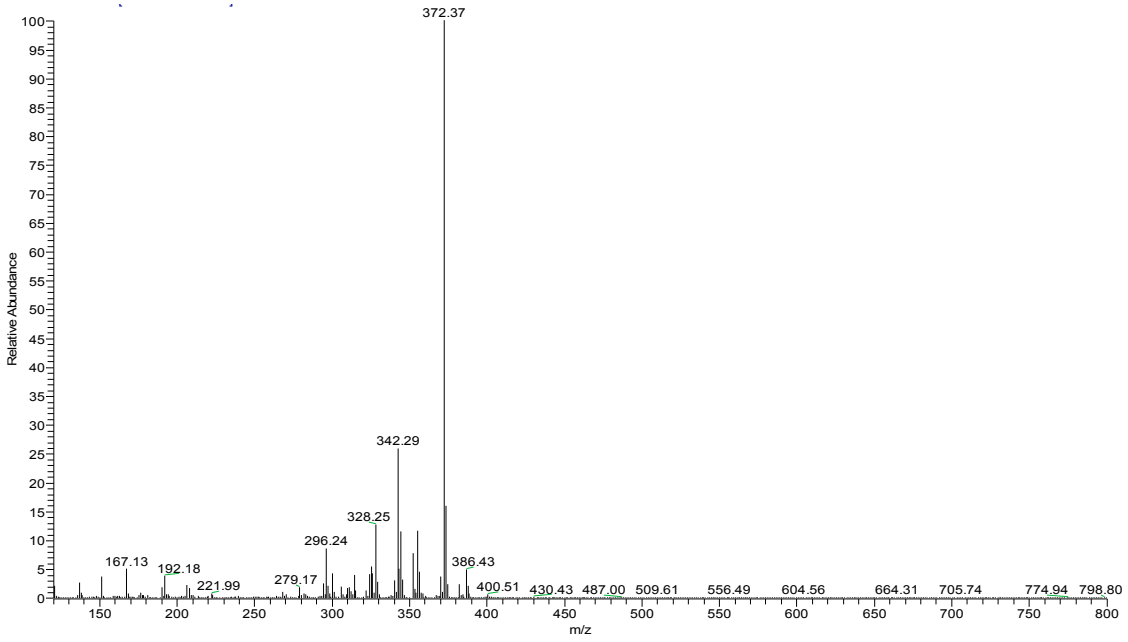

Figure S14. MS of alkaloid **(+)-norpurpureine** (*m*/*z* 372.37 [M + H]$^{+}$).

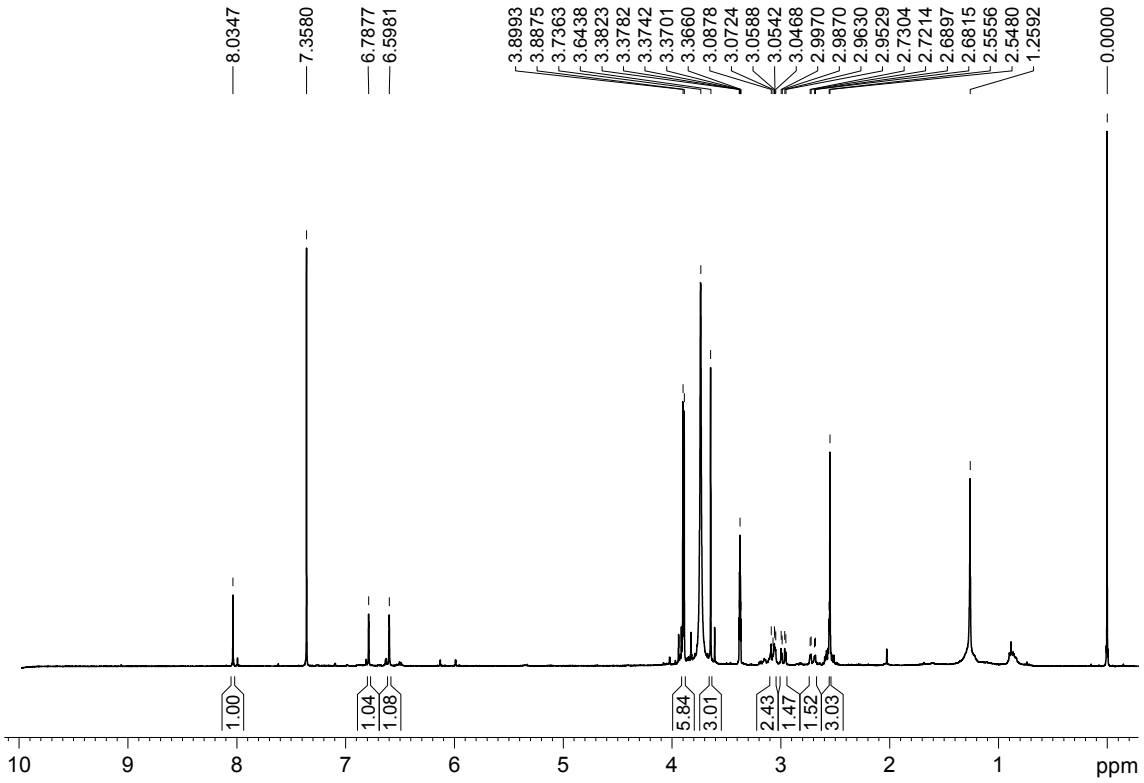

Figure S15. ^{1}H NMR spectrum of alkaloid **(+)-*N*-methyllaurotetanine** ($CDCl_3$ + drops of CD_3OD at 400 MHz).

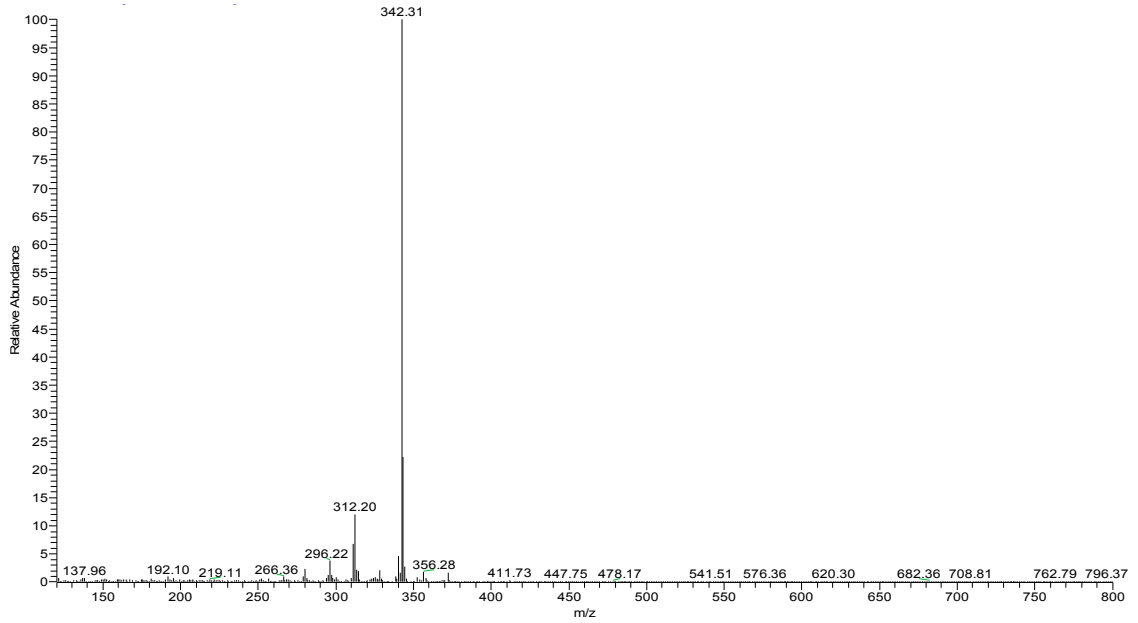

Figure S16. MS of alkaloid **(+)-*N*-methyllaurotetanine** (*m*/*z* 342.31 $[M + H]^+$).

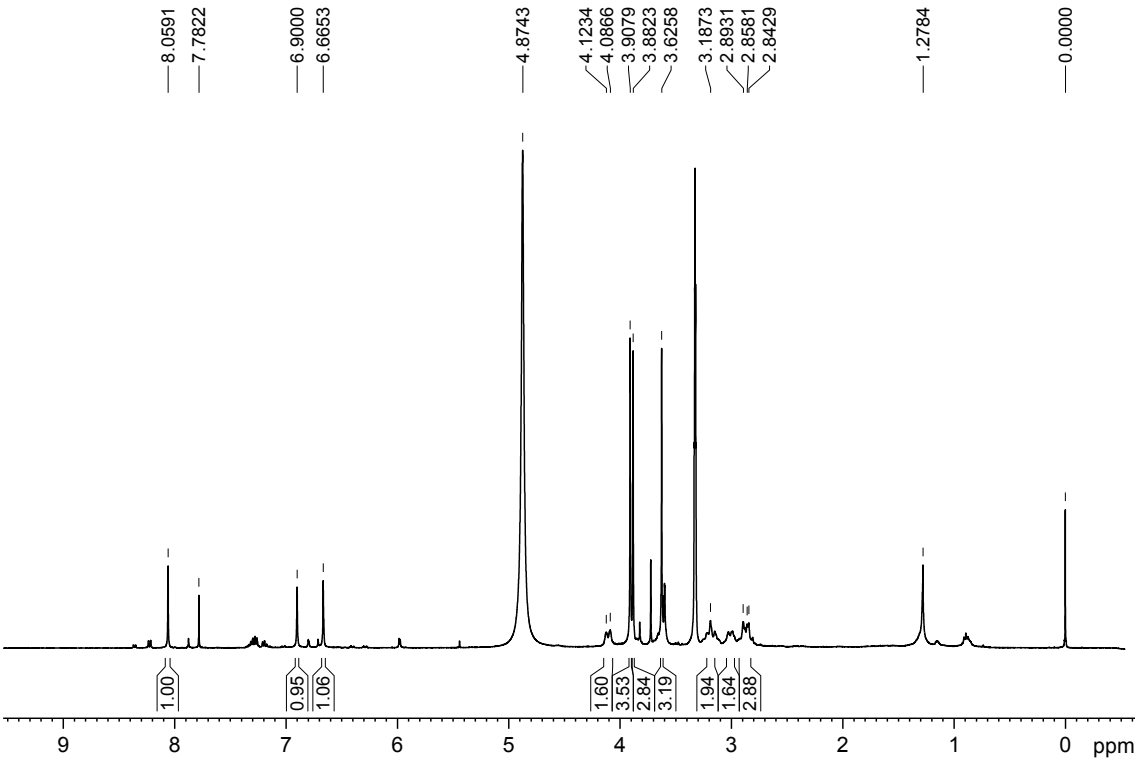

Figure S17. ^{1}H NMR spectrum of alkaloid **(+)-norpredicentrine** (CD_3OD + drops of $CDCl_3$ at 400 MHz).

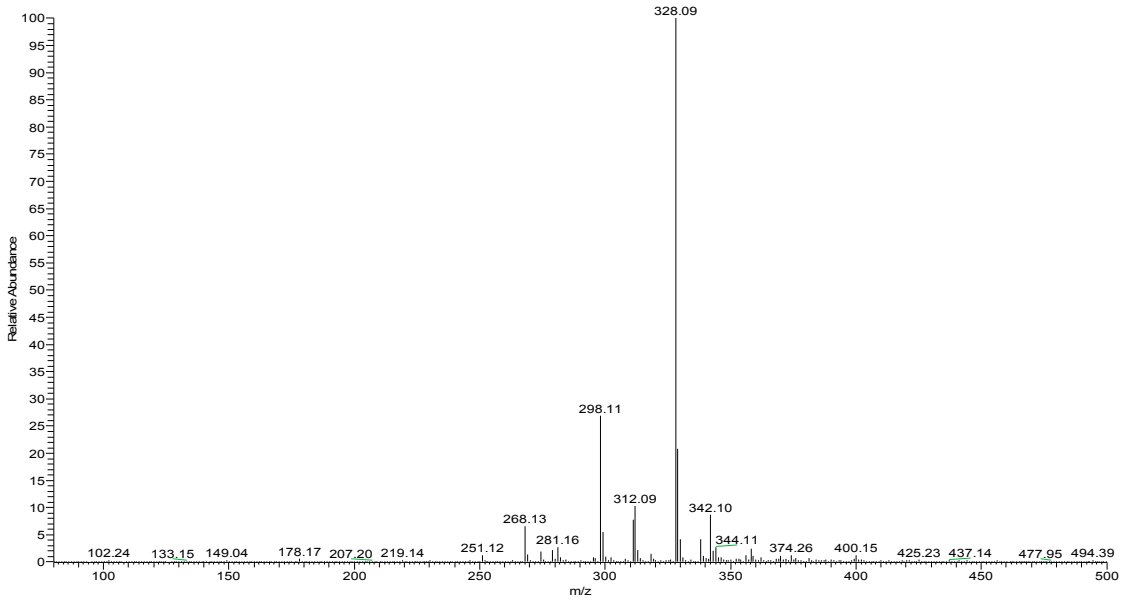

Figure S18. MS of alkaloid **(+)-norpredicentrine** (*m*/*z* 328.09 $[M + H]^+$).

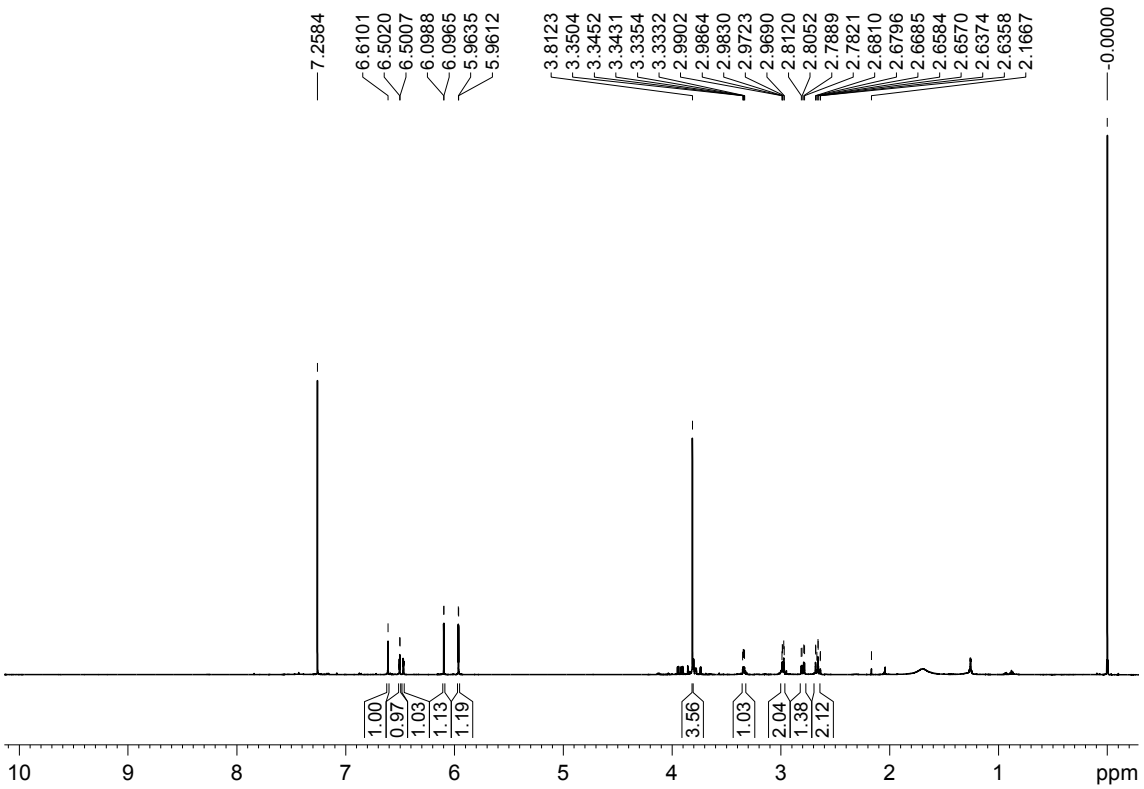

Figure S19. ^{1}H NMR spectrum of alkaloid **(+)-calycinine** ($CDCl_3$ at 400 MHz).

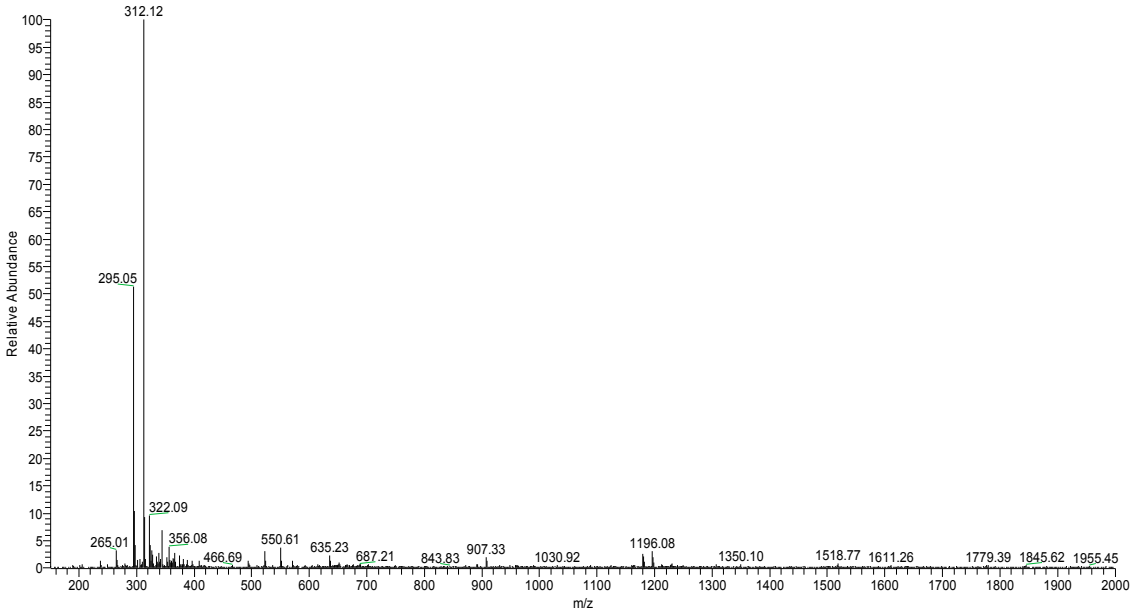

Figure S20. MS of alkaloid **(+)-calycinine** (*m*/*z* 312.12 $[M + H]^+$).

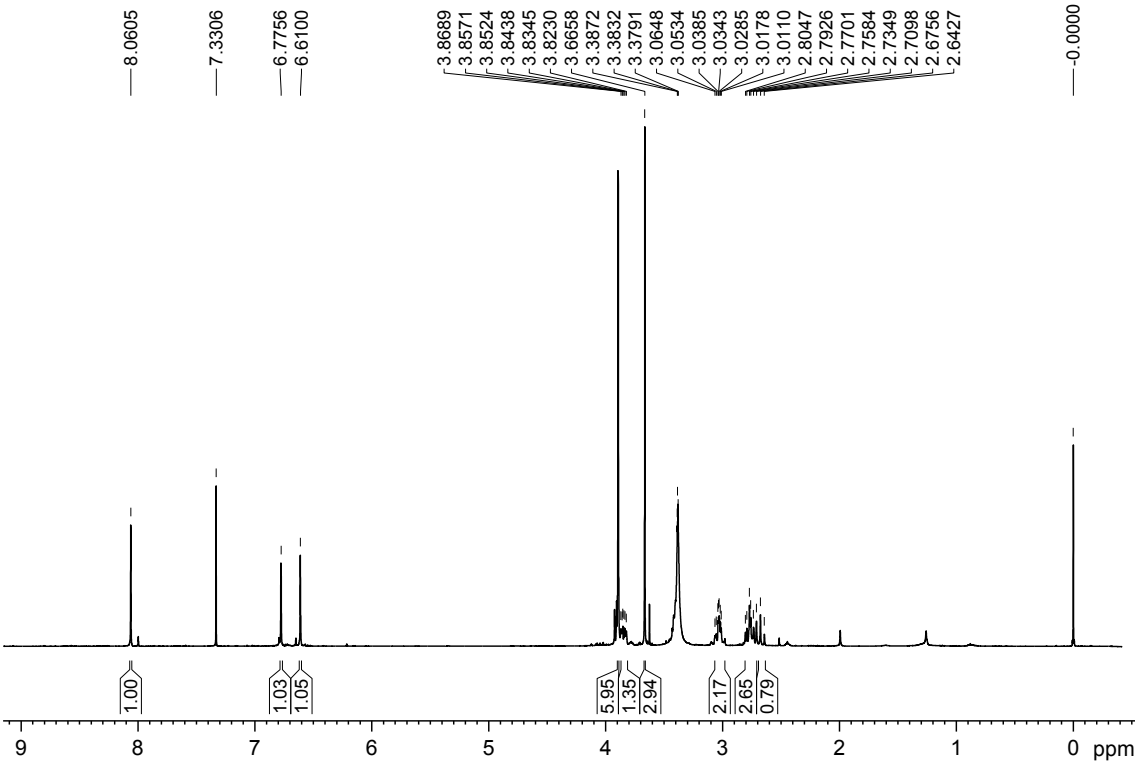

Figure S21. ^{1}H NMR spectrum of alkaloid **(+)-laurotetanine** ($CDCl_3$ + drops of CD_3OD at 400 MHz).

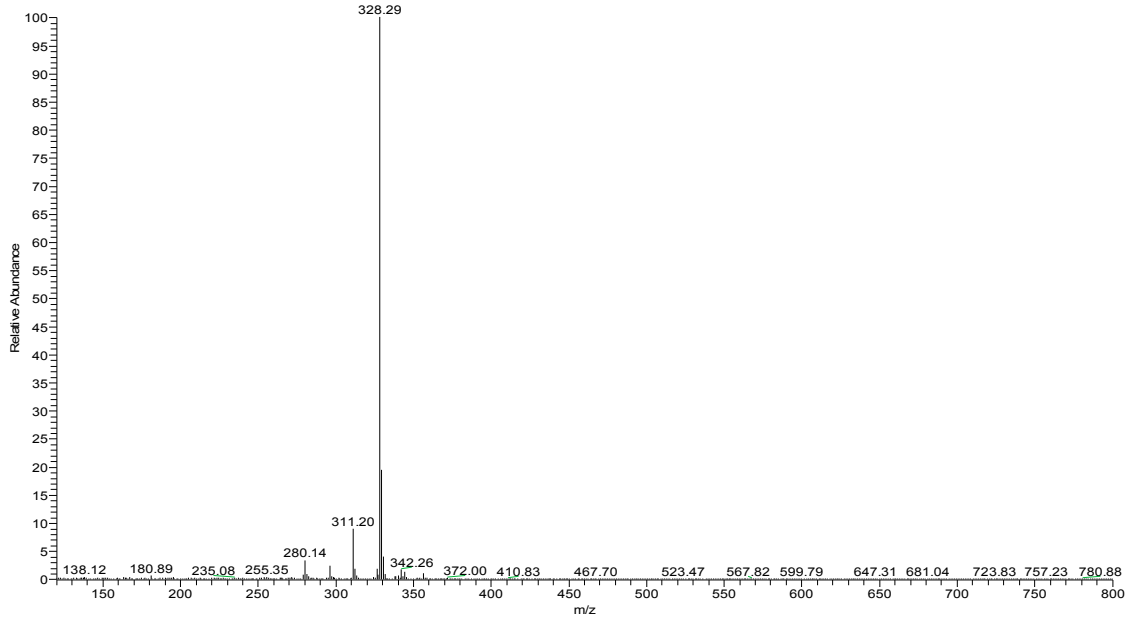

Figure S22. MS of alkaloid **(+)-laurotetanine** (*m*/*z* 328.29 $[M + H]^+$).

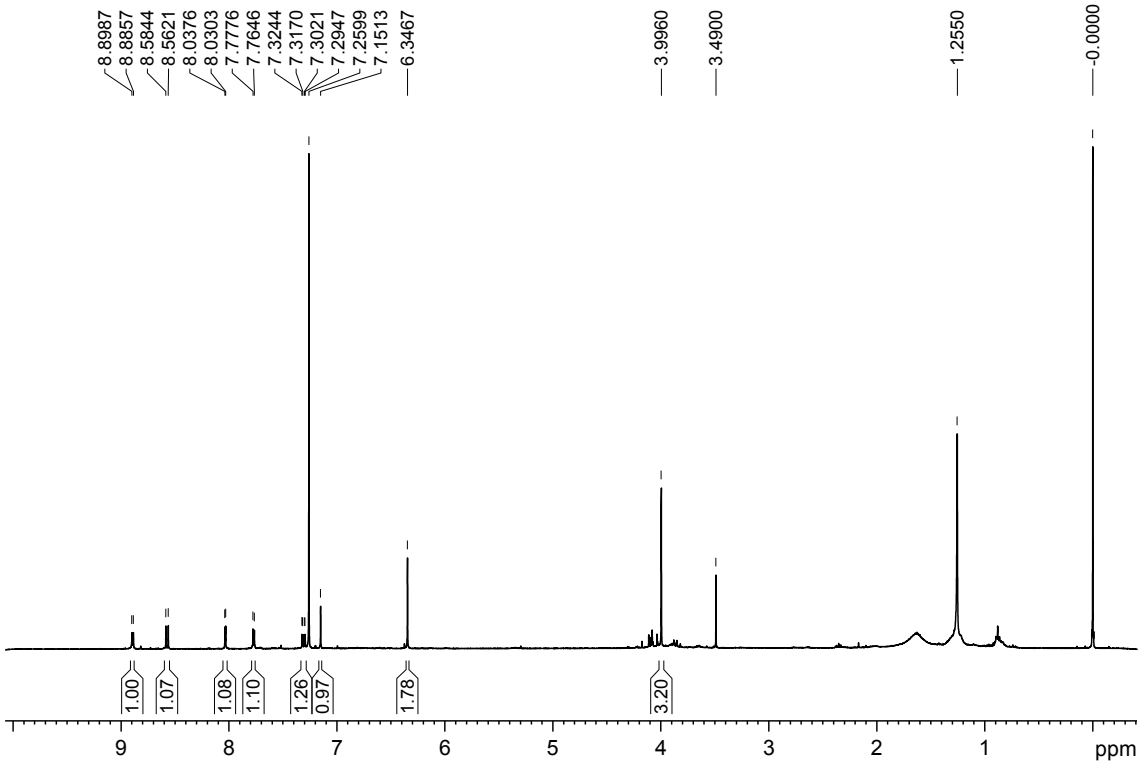

Figure S23. ^{1}H NMR spectrum of alkaloid **lanuginosine** ($CDCl_3$ + drops of CD_3OD at 400 MHz).

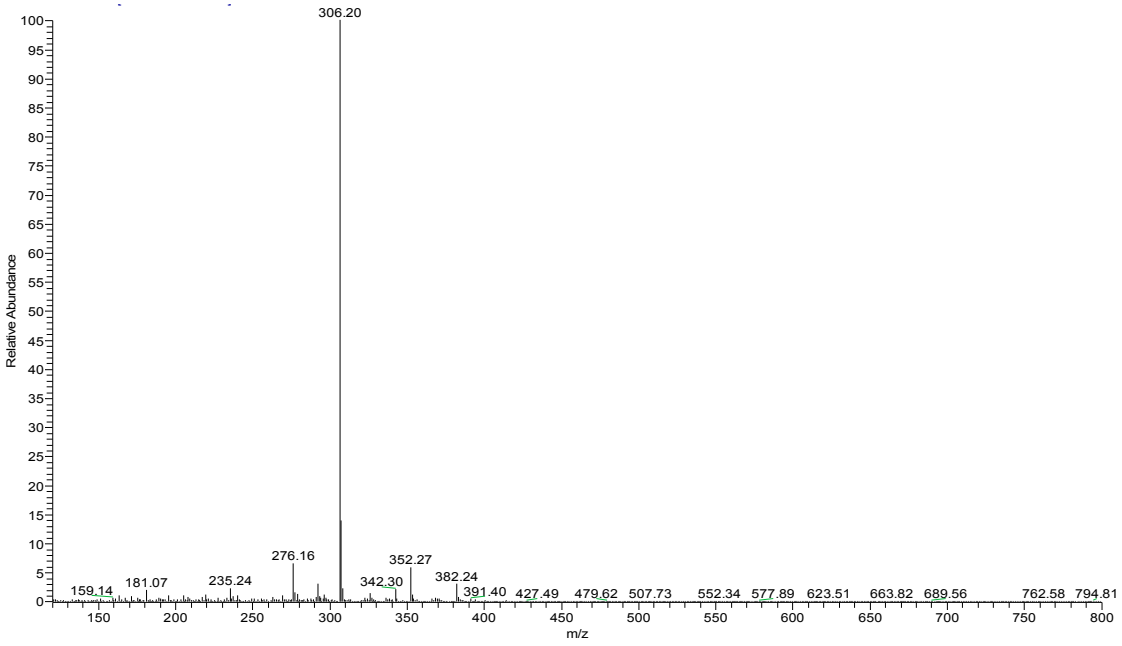

Figure S24. MS of alkaloid **lanuginosine** (*m*/*z* 306.20 $[M + H]^+$).

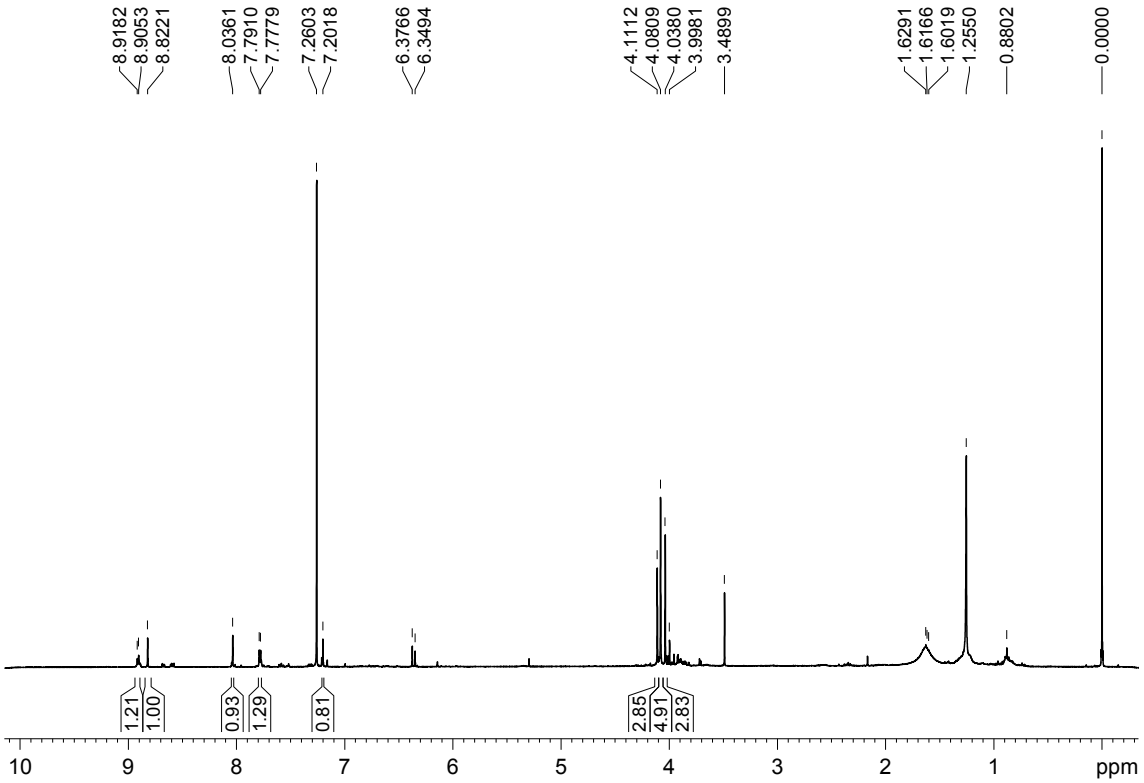

Figure S25. ^{1}H NMR spectrum of alkaloid **oxoglaucine** ($CDCl_3$ + drops of CD_3OD at 400 MHz).

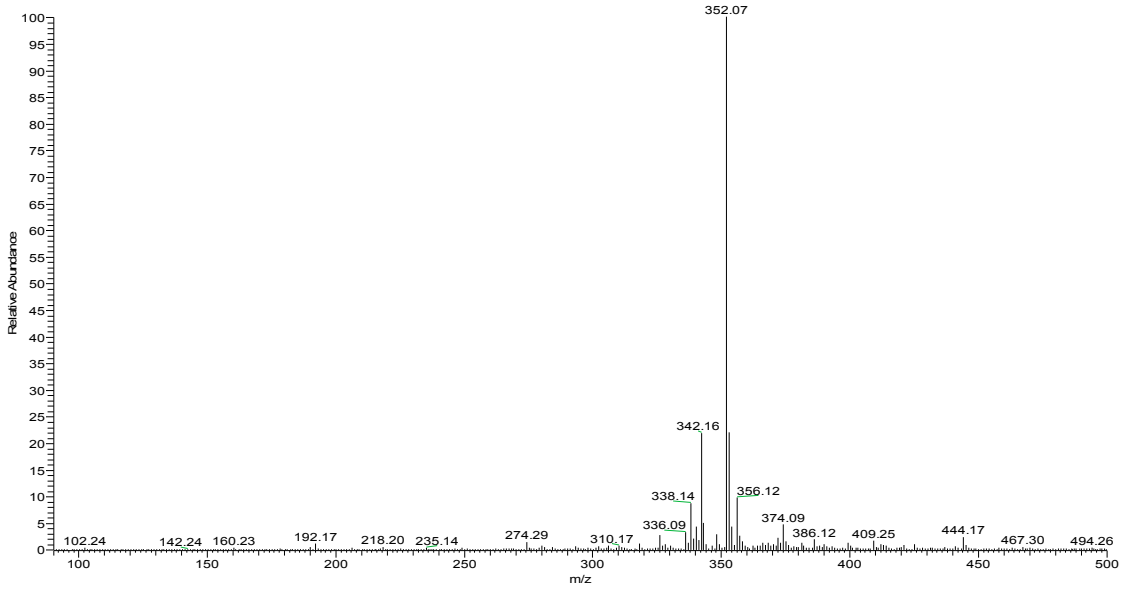

Figure S26. MS of alkaloid **oxoglaucine** (*m*/*z* 352.07 $[M + H]^+$).

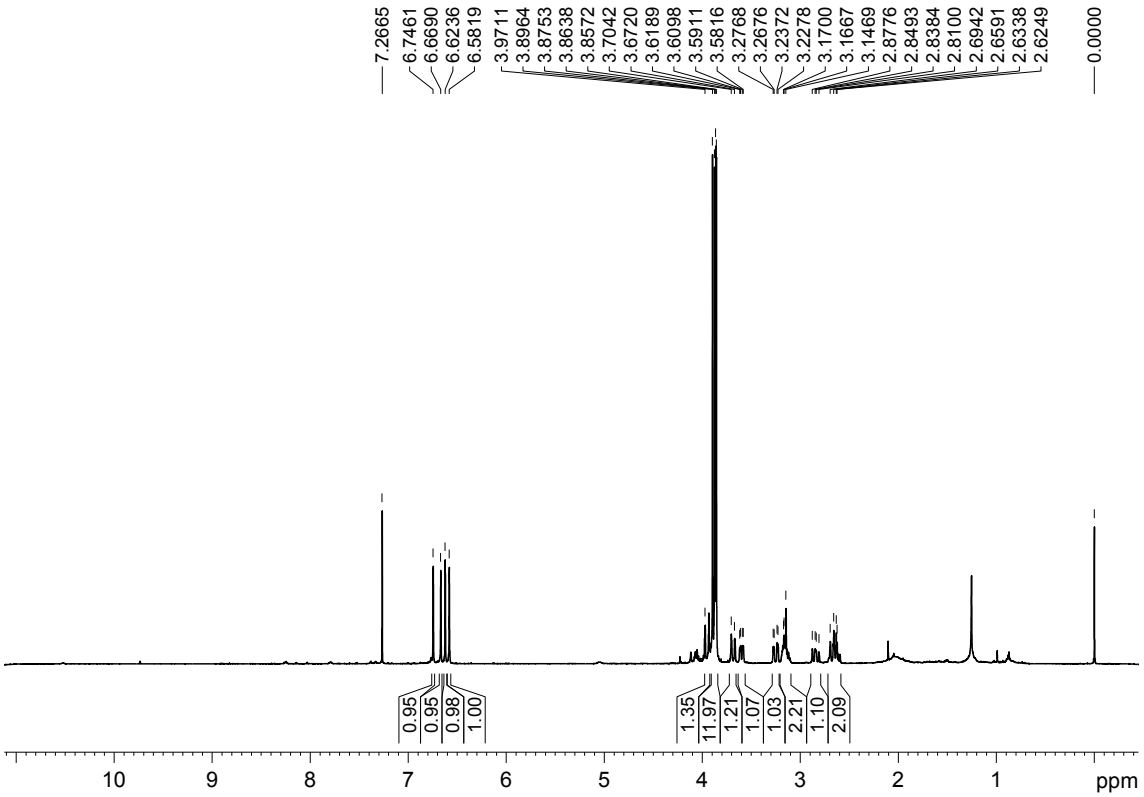

Figure S27. ^{1}H NMR spectrum of alkaloid **(–)-xylopinine** ($CDCl_3$ + drops of CD_3OD at 400 MHz).

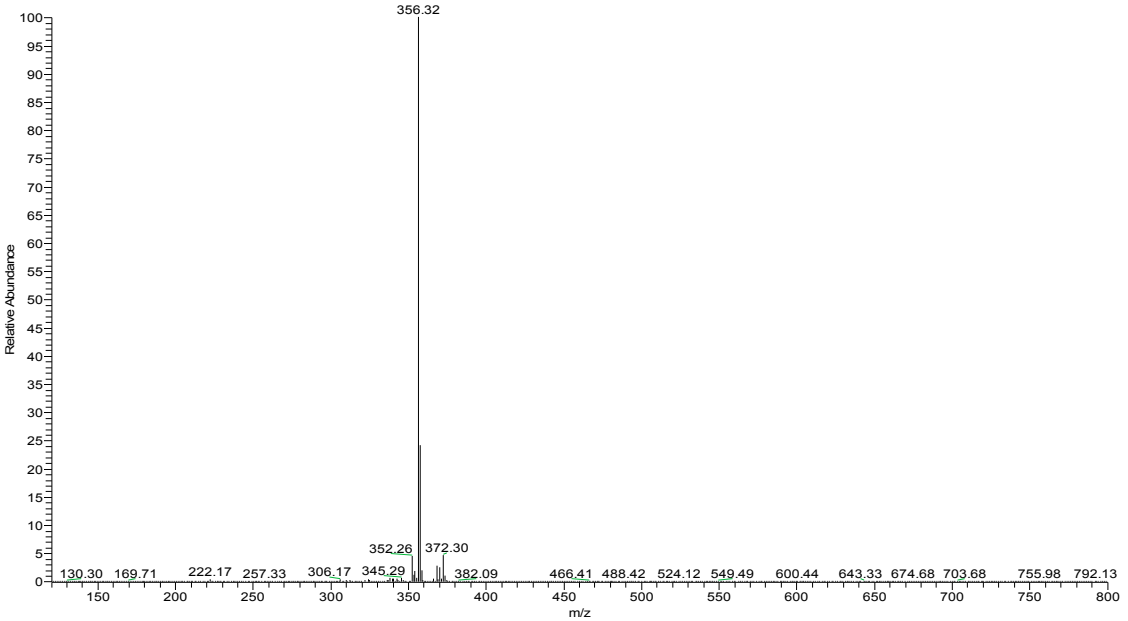

Figure S28. MS of alkaloid **(–)-xylopinine** (*m*/*z* 356.32 $[M + H]^+$).

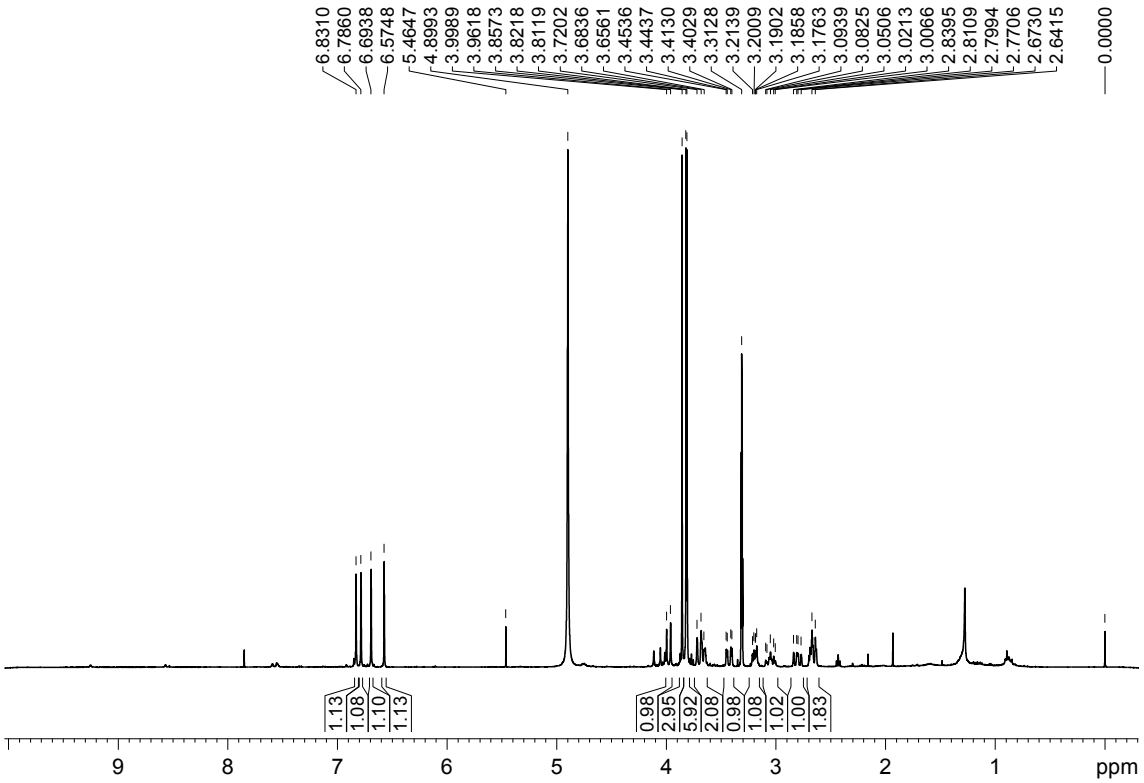

Figure S29. ^{1}H NMR spectrum of alkaloid **(+)-discretine** (CD_3OD + drops of $CDCl_3$ at 400 MHz).

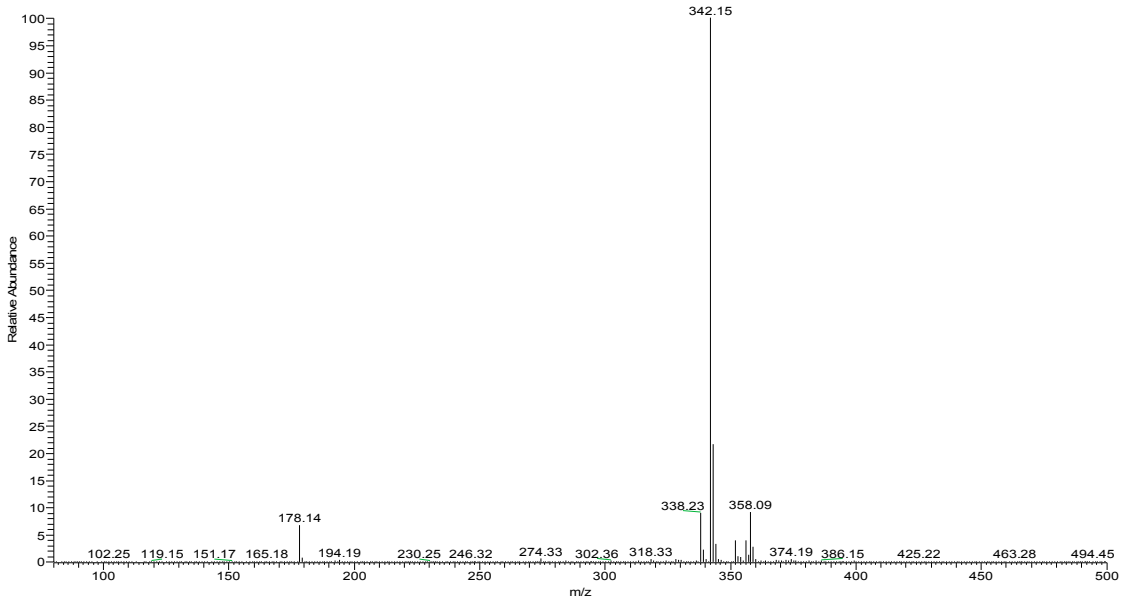

Figure S30. MS of alkaloid **(+)-discretine** (*m*/*z* 342.15 $[M + H]^+$).

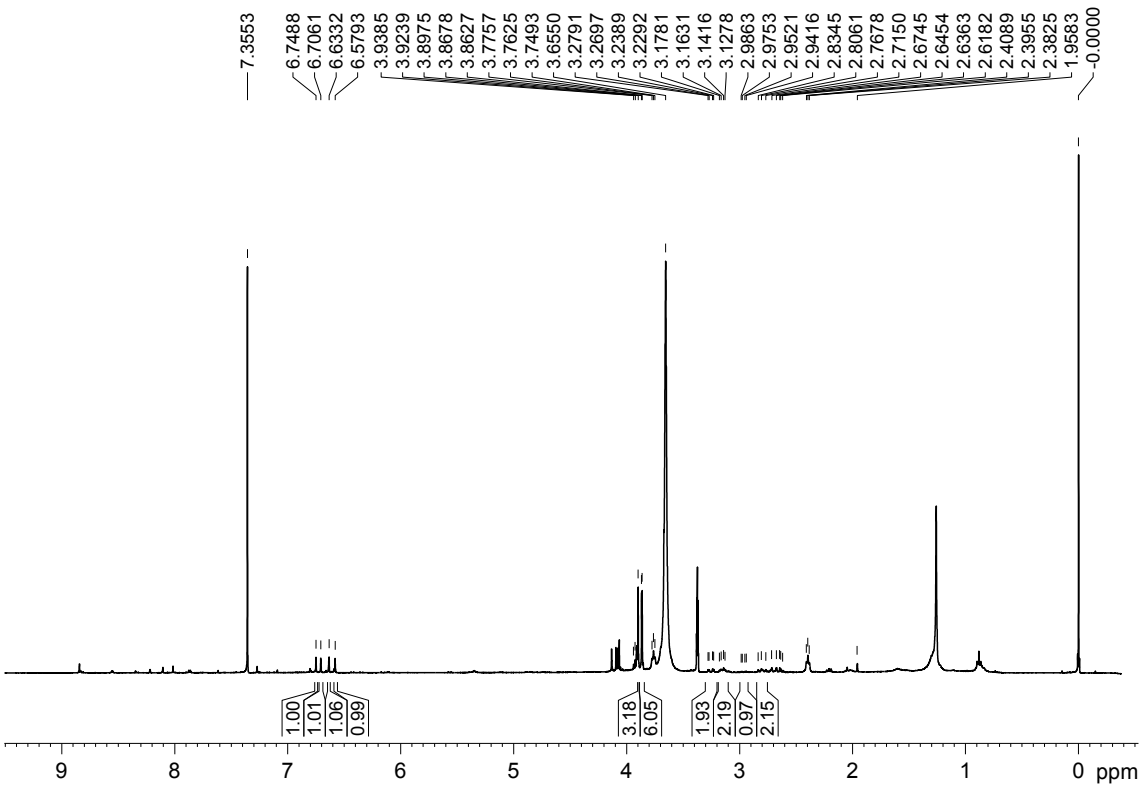

Figure S31. ^{1}H NMR spectrum of alkaloid **(–)-corytenchine** ($CDCl_3$ + drops of CD_3OD at 400 MHz).

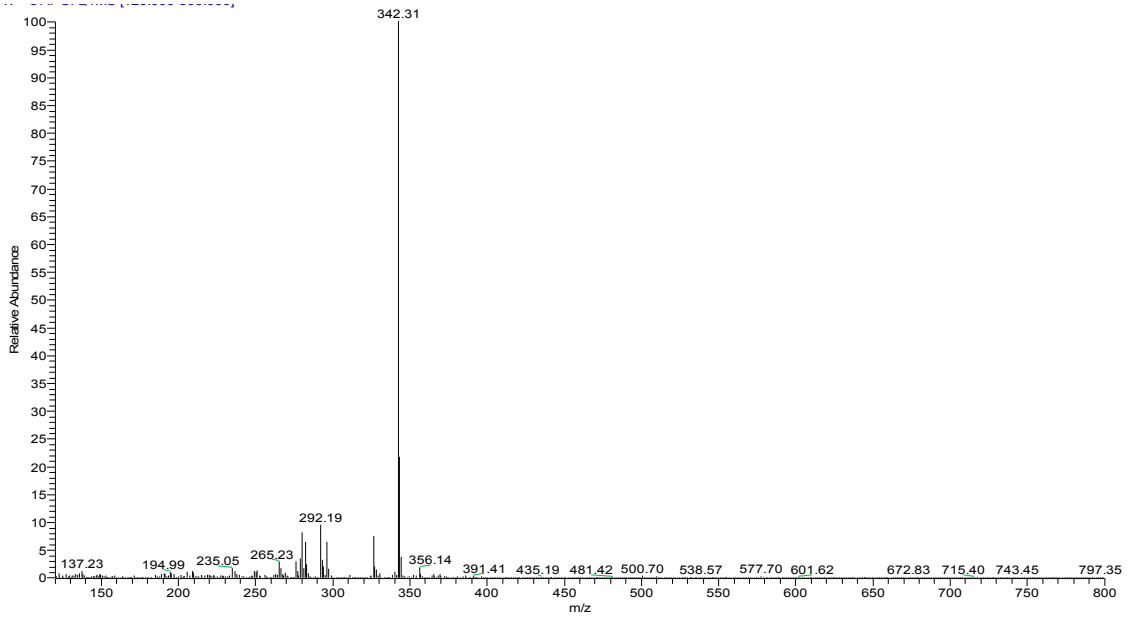

Figure S32. MS of alkaloid **(–)-corytenchine** (*m*/*z* 342.31 $[M + H]^+$).

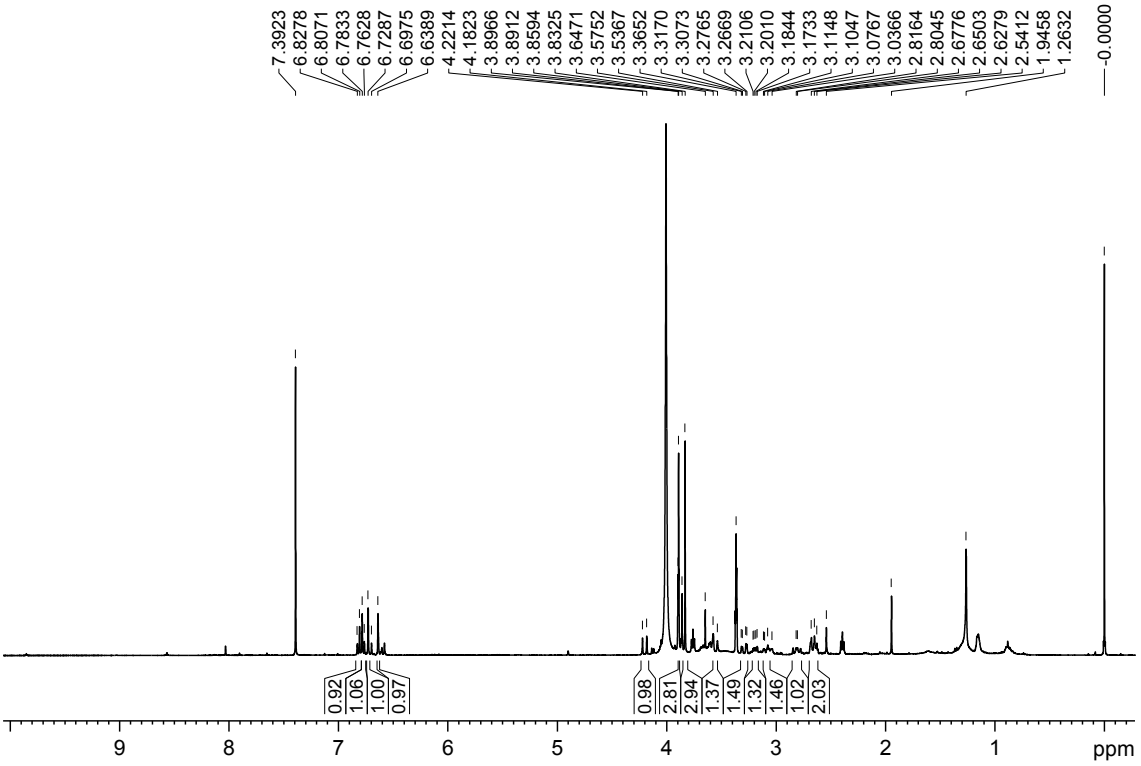

Figure S33. ^{1}H NMR spectrum of alkaloid **(+)-discretamine** ($CDCl_3$ + drops of CD_3OD at 400 MHz).

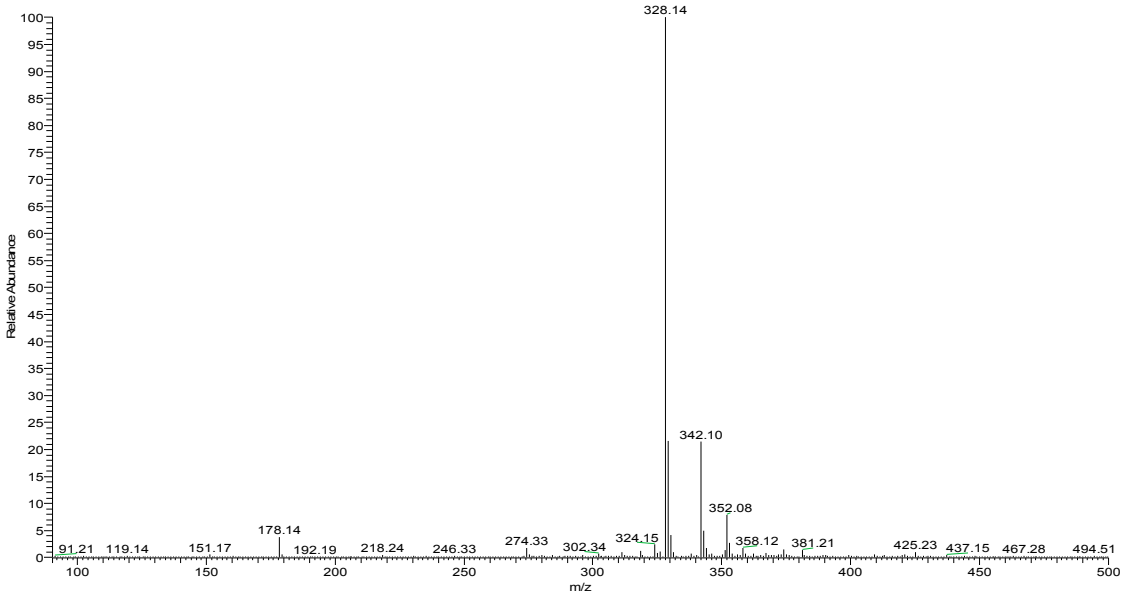

Figure S34. MS of alkaloid **(+)-discretamine** (*m*/*z* 328.14 $[M + H]^+$).

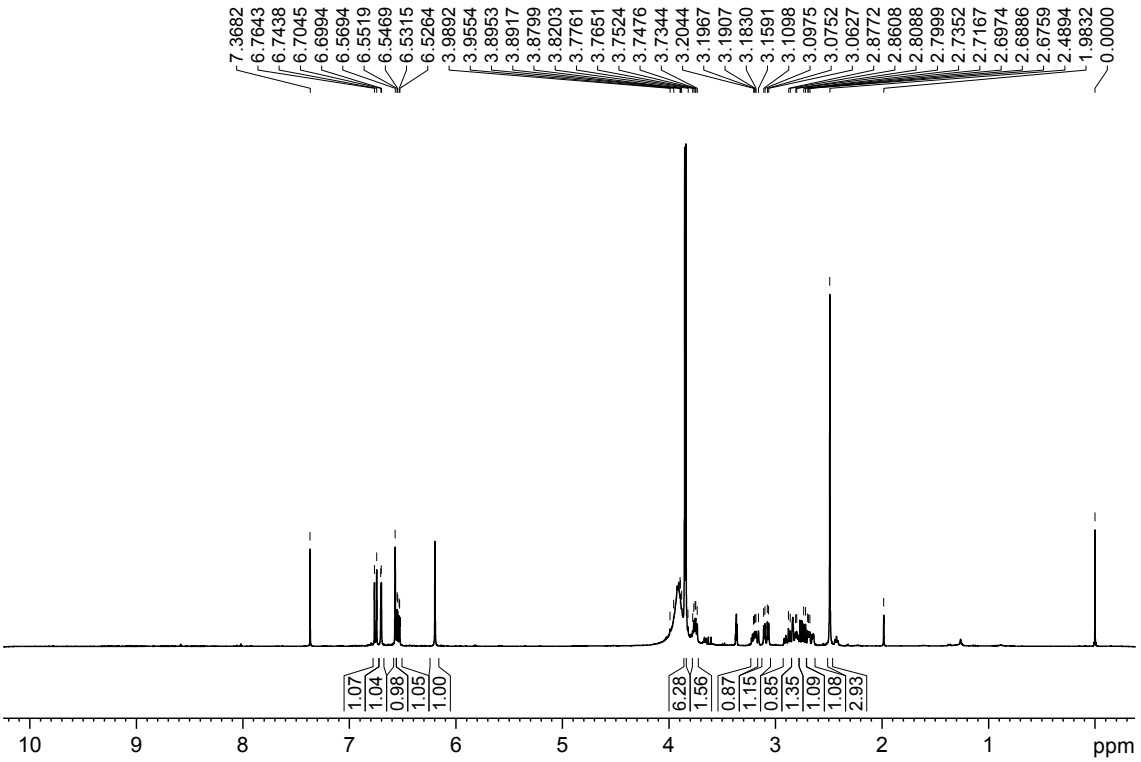

Figure S35. ^{1}H NMR spectrum of alkaloid **(+)-reticuline** ($CDCl_3$ + drops of CD_3OD at 400 MHz).

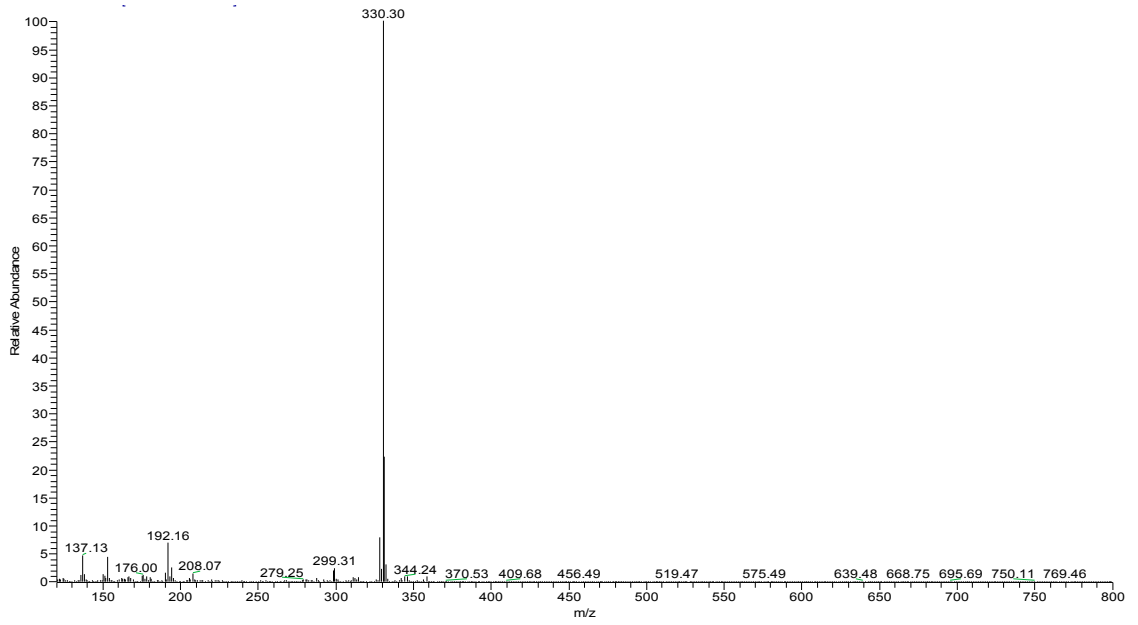

Figure S36. MS of alkaloid **(+)-reticuline** (*m*/*z* 330.30 $[M + H]^+$).

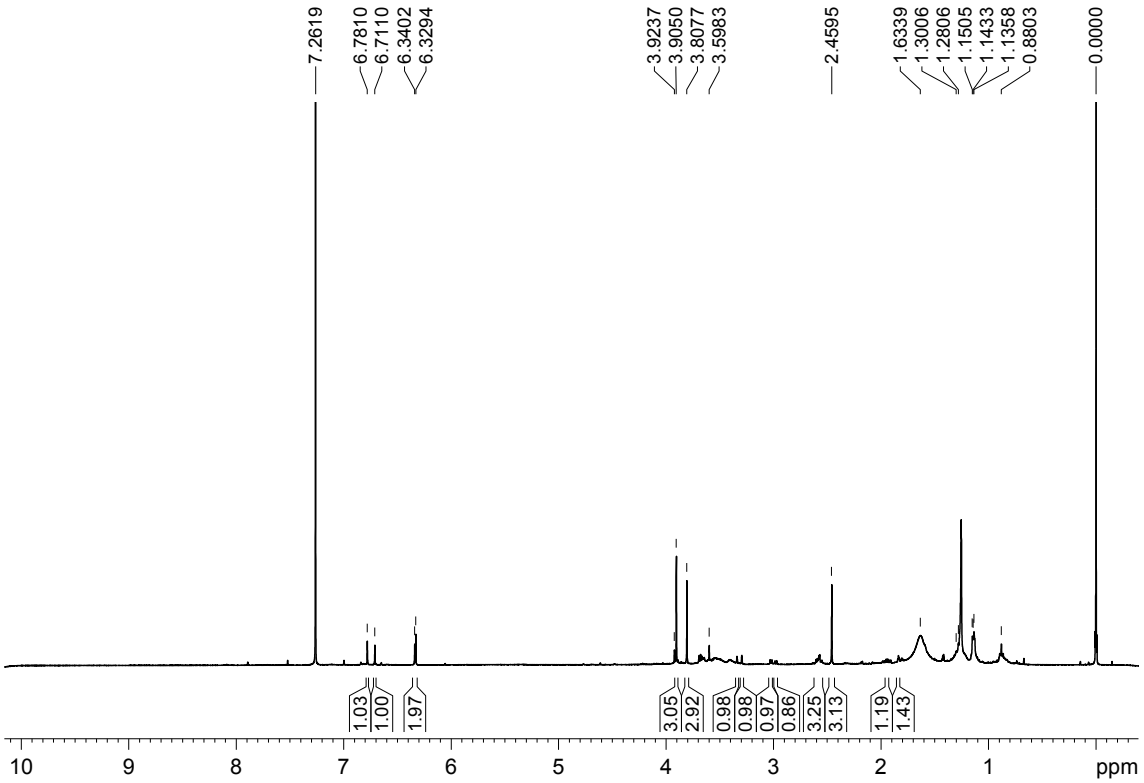

Figure S37. ^{1}H NMR spectrum of alkaloid **(+)-flavinantine** ($CDCl_3$ + drops of CD_3OD at 400 MHz).

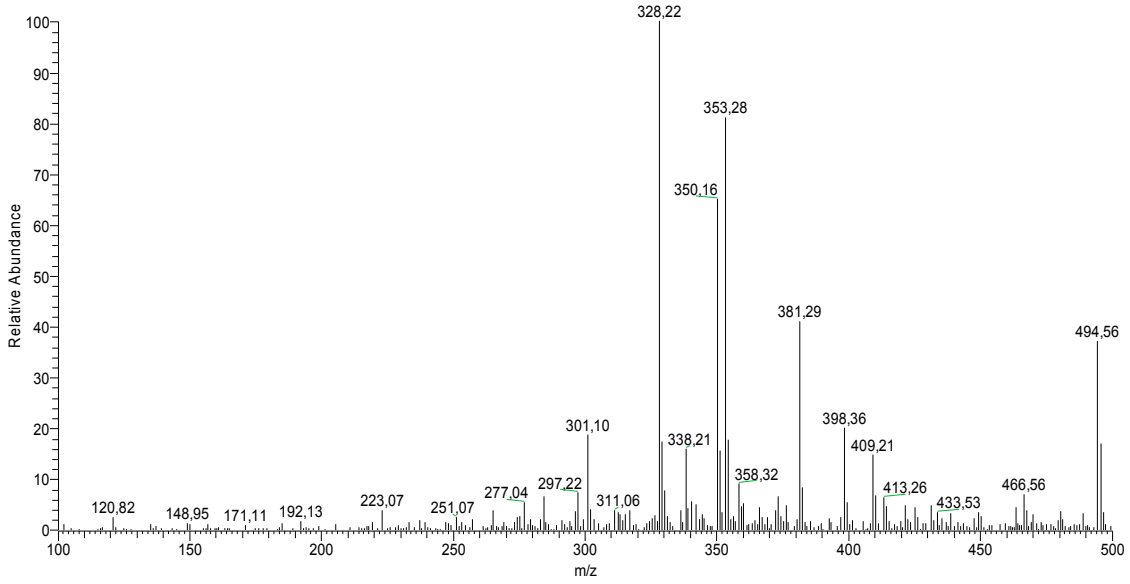

Figure S38. MS of alkaloid **(+)-flavinantine** (*m*/*z* 328.22 $[M + H]^+$).

Table S1: ^{1}H NMR data for alkaloids from the stem *X. laevigata* (δ in ppm and *J* values in (Hz))

no.	Roemerine [a]	Glaucine [a]	Xylopine [a]	Norglaucine [a]	Norpurpureine [a]	*N*-methyllaurotetanine [a]	Norpredicentrine [b]	Calycinine [c]
3	6.57 s	6.59 s	6.54 s	6.61 s		6.59 s	6.66 s	6.61 s
4	2.67 m	2.72 m	2.71 m	3.06 m	2.83 m	2.70 dd (16.3; 3.6)	3.16 m	2.70 ddd (16.0; 4.0; 1.1)
	3.14 m	3.26 m	3.03 m	2.73 m	2.83 m	3.15 m	2.86 m	3.07 ddd (16.0; 12.3; 5.8)
5	2.57 m	3.19 m	3.40 m	3.45 m	3.41 m	3.06 m	3.59 m	3.41 ddd (12.1; 5.8; 1.1)
	3.07 m	2.68 m	3.02 m	2.06 m	2.94 m	2.55 m	3.19 m	3.00 ddd (12.3; 12.1; 4.0)
6a	3.23 m	3.22 m	4.00 dd (14.1; 5.0)	3.90 m	3.83 m	3.07 d (13.6)	4.10 d (13.8)	3.85 dd (13.6; 4.1)
7	3.17 dd (13.7; 4.1)	2.73 m	2.81 t (14.1)	2.86 m	2.70 m	2.54 m	3.00 m	2.76 dddd (13.7; 13.6; 1.2; 0.9)
	2.69 t (13.7)	3.04 dd (13.7; 3.6)	2.95 dd (14.1; 5.0)	2.79 m	2.78 m	2.97 dd (13.6; 4.0)	2.85 m	2.89 dd (13.7; 4.1; 0.5)
8	7.25 m	6.78 s	6.81 dd (2.7; 0.7)	6.76 s	6.78 s	6.78 s	6.90 s	6.41 ddd (2.7; 1.2; 0.7)
9	7.25 m							
10	7.32 m		6.86 ddd (8.6; 2.7; 0.7)					6.50 dd (2.7; 0.9)
11	8.07 d (8.0)	8.08 s	8.01 d (8.6)	8.11 s	7.97 s	8.03 s	8.05 s	
OCH_3-1		3.65 s		3.66 s	3.73 s	3.64 s	3.62 s	
OCH_3-2		3.89 s		3.89 s	3.96 s	3.88 s		
OCH_3-3					3.91 s			
OCH_3-9		3.93 s	3.84 s	3.91 s	3.92 s		3.90 s	3.81 s
OCH_3-10		3.90 s		3.90 s	3.92 s	3.89 s	3.88 s	
N-CH_3	2.56 s	2.66 s				2.54 s		
(OCH_2O)1–2	6.10 d (1.4)		5.94 d. (1.4)					5.96 d. (1.4)
	5.95 d (1.4)		6.08 d. (1.4)					6.09 d. (1.4)

[a] The experiments were obtained at 303 K with TMS as internal reference (0.00 ppm) in $CDCl_3$ + drops of CD_3OD. [b] In CD_3OD + drops of $CDCl_3$. [c] In $CDCl_3$.

Table S2: ^{13}C NMR data for alkaloids from the stem *X. laevigata* (δ in ppm)

no.	Roemerine [a]	Glaucine [a]	Xylopine [a]	Norglaucine [a]	Norpurpureine [a]	*N*-methyllaurotetanine [a]	Norpredicentrine [b]	Calycinine [c]
1	142.9	144.9	142.2	144.6	149.5	144.3	144.8	138.9
1a	116.5	127.1	116.3	126.7	122.6	127.4	125.5	114.0
2	147.2	152.3	147.3	152.4	145.7	152.3	151.6	146.0
3	107.6	110.4	107.1	110.9	150.1	110.5	115.5	107.5
3a	126.5	125.5	125.7	128.5	122.8	128.7	127.9	127.6
3b	126.7	125.4	125.9	126.8	130.5	126.5	122.3	128.3
4	28.9	28.1	28.3	28.5	23.2	28.7	26.7	28.9
5	53.5	52.8	42.9	42.8	42.4	53.3	42.8	42.7
6a	62.2	62.2	53.3	53.6	53.9	62.6	54.3	53.5
7	34.5	33.7	36.5	36.3	36.1	33.8	34.9	38.2
7a	134.9	128.4	136.2	128.6	128.2	129.6	127.9	138.5
8	128.5	110.9	113.7	110.9	111.0	114.5	112.1	107.8
9	127.7	148.1	159.1	148.2	147.6	145.3	149.6	160.8
10	127.4	147.6	112.5	147.6	147.6	146.1	149.0	102.7
11	127.2	111.6	128.6	111.8	111.5	111.9	112.6	154.9
11a	131.1	124.2	133.8	124.5	124.5	123.7	125.2	110.9
OCH_3-1		60.2		60.3	60.7	60.2	60.3	
OCH_3-2		55.7		55.9	61.1	56.0		
OCH_3-3					60.5			
OCH_3-9		55.9	55.4	55.9	55.9		56.3	55.3
OCH_3-10		55.9		55.9	56.1	56.2	56.5	
N-CH_3	43.6	42.9				43.6		
(OCH_2O)1–2	101.0		100.8					100.2

[a] The experiments were obtained at 303 K with TMS as internal reference (0.00 ppm) in $CDCl_3$ + drops of CD_3OD. [b] In CD_3OD + drops of $CDCl_3$. [c] In $CDCl_3$.

Table S3. Specific rotation of alkaloids from *X. laevigata*.

Compounds	$[\alpha]_D^{20}$	***c***
Roemerine	−11.0°	0.2133
Anonaine	+12.9°	0.2700
Glaucine	+16.9°	0.0800
Xylopine	+42.9°	0.2133
Norglaucine	+181.7°	0.0666
Norpurpureine	+91.2°	0.0600
N-methyllaurotetanine	+28.3°	0.0733
Norpredicentrine	+81.4°	0.1333
Calycinine	+98.0°	0.1000
Laurotetanine	+54.6°	0.0333
Xylopinine	-207.9°	0.0266
Discretine	+45.2°	0.2066
Corytenchine	−3.7°	0.0533
Discretamine	+192.4°	0.0666
Reticuline	+74.1°	0.1733
Flavinantine	+45.5°	0.0530

Note: All the measured were realized in $CHCl_3$