

Table S1 The isotope pattern of compound **1**.

Isotopologue	Abundance (%)
M	100
M+1	34.5
M+2	5.8

Table S2 Elemental constitutes of major ions observed in Figure 1.

Solvent	Ions	Formula	Calculated	Observed	Error(ppm)
Methanol	[M-H] ⁺	C ₃₁ H ₂₃ N ₂	423.1856	423.1850	1.3
	[M] ⁺ •	C ₃₁ H ₂₄ N ₂	424.1934	424.1910	-
			424.1889^a		
	[M+H] ⁺	C ₃₁ H ₂₅ N ₂	425.2012		
			425.1966^b	425.1948	-
			425.1921^c		
Acetonitrile	[M+Na] ⁺	C ₃₁ H ₂₄ N ₂ Na	447.1832	447.1826	1.3
	[M+K] ⁺	C ₃₁ H ₂₄ N ₂ K	463.1571	463.1564	1.6
	[M-3] ⁺	C ₃₁ H ₂₁ N ₂	421.1699	421.1702	-0.7
	[M-2] ⁺ •	C ₃₁ H ₂₂ N ₂	422.1778	422.1768	-
			422.1732^d		
	[M-H] ⁺	C ₃₁ H ₂₃ N ₂	423.1856	423.1860	-0.9
Dichloromethane	[M] ⁺ •	C ₃₁ H ₂₄ N ₂ O	424.1934	424.1920	-
			424.1889		
	[M-3] ⁺	C ₃₁ H ₂₁ N ₂	421.1699	421.1699	0.1
	[M-2] ⁺ •	C ₃₁ H ₂₂ N ₂	422.1778	422.1755	-
			422.1732		
	[M-H] ⁺	C ₃₁ H ₂₃ N ₂	423.1856		
			423.1810^e	423.1850	-
			423.1764^f		
	[M] ⁺ •	C ₃₁ H ₂₄ N ₂ O	424.1934	424.1988	-
			424.1889		
	[M+13] ⁺	C ₃₁ H ₂₁ N ₂ O	437.1648	437.1627	4.8

^a (M+1) isotope of C₃₁H₂₃N₂; ^b (M+1) isotope of C₃₁H₂₄N₂; ^c (M+2) isotope of C₃₁H₂₃N₂; ^d (M+1)

isotope of C₃₁H₂₁N₂; ^e (M+1) isotope of C₃₁H₂₂N₂; ^f (M+2) isotope of C₃₁H₂₁N₂.

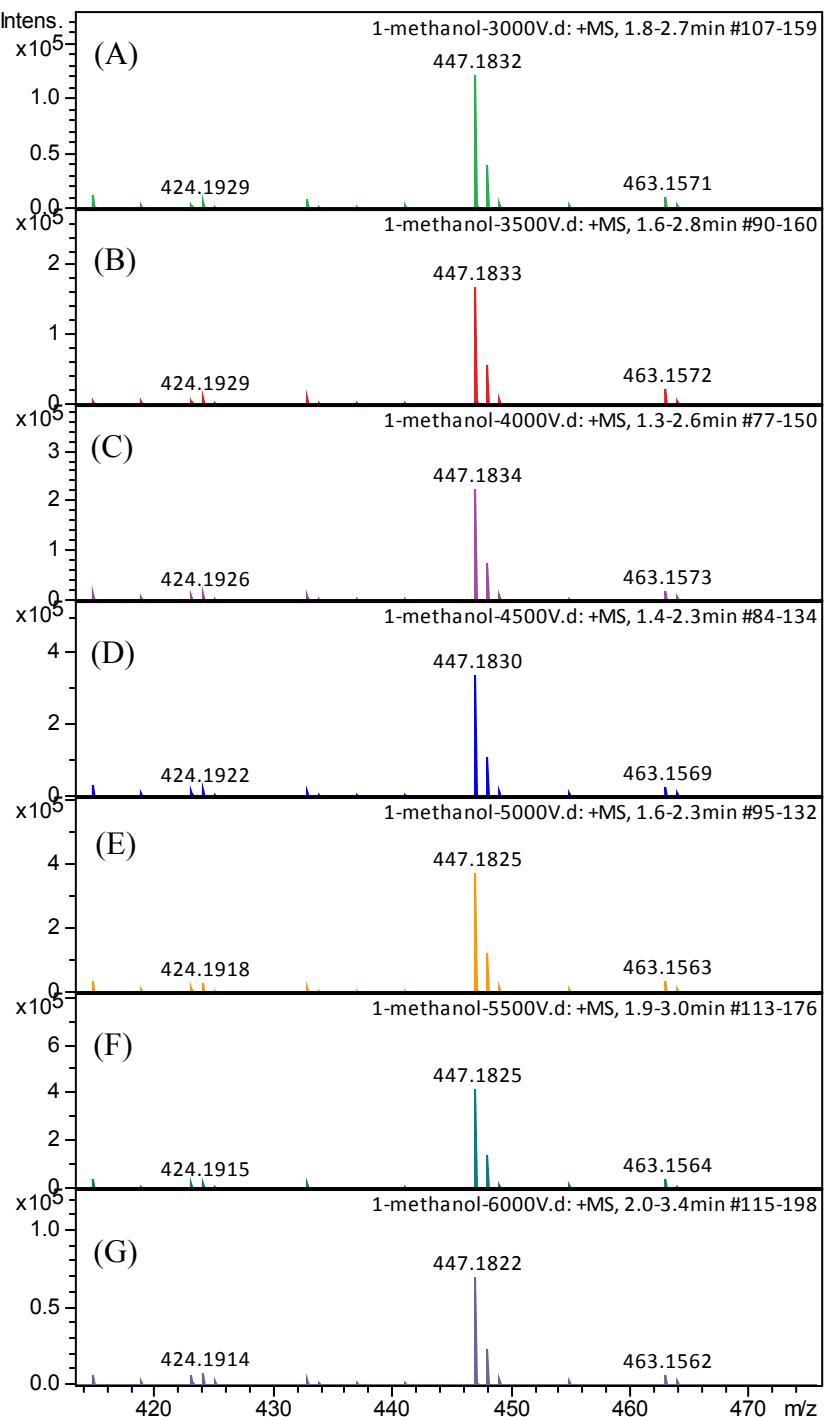


Fig. S1 The full-scan mass spectra of compound 1 with methanol as the solvent, capillary voltage was set as (A) 3.0 kV, (B) 3.5 kV, (C) 4.0 kV, (D) 4.5 kV, (E) 5.0 kV, (F) 5.5 kV and (G) 6.0 kV.

Table S3 The oxidation ratio (%) with capillary voltage over the range from 3.0-6.0 kV with the methanol as the solvent for compound 1.

capillary voltage (kV)	$I_{m/z\ 423}\%$	I_a	$I_{m/z\ 447}\%$	$I_{m/z\ 463}\%$	Oxidation ratio (%) ^b
<i>m/z</i>					
424%					
3.0	3	5.7	100	10.2	7.3
3.5	4.8	6.7	100	13.3	9.2
4.0	5.7	5	100	10.4	8.8
4.5	6.3	5.4	100	9.8	9.6
5.0	6.4	6.7	100	10	10.6
5.5	7	5	100	10.7	9.9
6.0	9.3	8.7	100	10.7	14

^a $I_{m/z\ 424}\% = I_{m/z\ 424}\% \text{ (observed)} - I_{m/z\ 423}\% \text{ (observed)} \times \text{Isotope Ratio}_{(m+1)} \text{ (theory)}$, Isotope Ratio_(m+1)=0.345.

^b Oxidation ratio = $(I_{m/z\ 423}\% + I_{m/z\ 424}\%) / (I_{m/z\ 423}\% + I_{m/z\ 424}\% + I_{m/z\ 425}\% + I_{m/z\ 447}\% + I_{m/z\ 463}\%) \times 100\%$, because the intensity of $m/z\ 425$ ($[M + H]^+$ ion) is too low, $I_{m/z\ 425}\%$ was neglected.

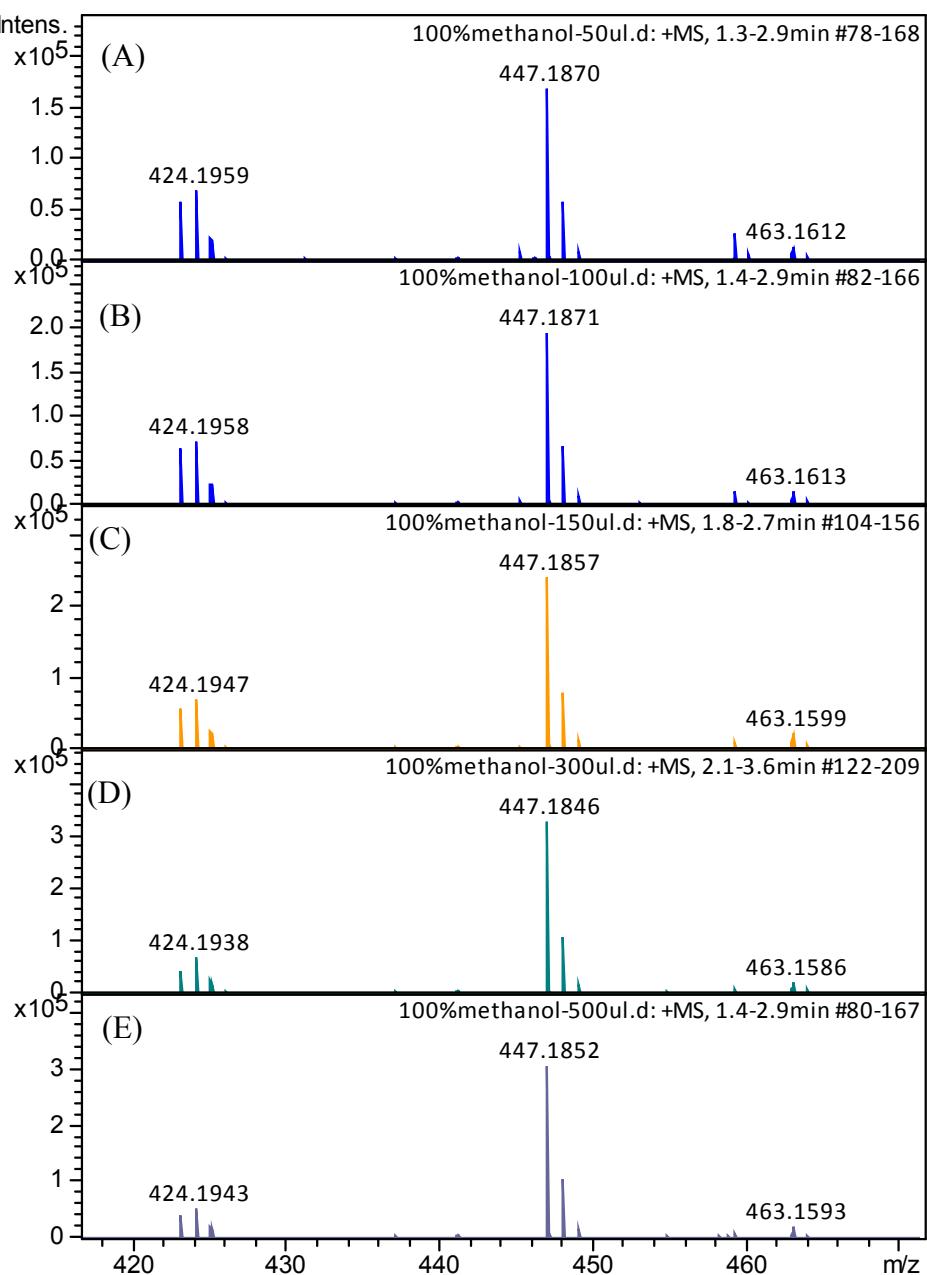


Fig. S2 The full-scan mass spectra of compound 1 with methanol as the solvent, the sample introduction rate was set as (A) 50 μ L/h, (B) 100 μ L/h, (C) 150 μ L/h, (D) 300 μ L/h and (E) 500 μ L/h.

Table S4 The oxidation ratio (%) with sample introduction rate over the range from 50-500 $\mu\text{L}/\text{h}$ with the methanol as the solvent for compound 1.

Sample introduction rate ($\mu\text{L}/\text{h}$)	$I_{m/z\ 423}\%$	I_a	$I_{m/z\ 447}\%$	$I_{m/z\ 463}\%$	Oxidation ratio (%) ^b
<i>m/z</i>					
424%					
50	34.6	29.5	100	9.2	37
150	23.8	21.3	100	9.8	29
300	16	16.7	100	8.8	23
500	14.2	12.8	100	7.5	20

^a $I_{m/z\ 424}\% = I_{m/z\ 424}\% \text{ (observed)} - I_{m/z\ 423}\% \text{ (observed)} \times \text{Isotope Ratio}_{(m+1)} \text{ (theory)}$, Isotope Ratio_(m+1)=0.345.

^b Oxidation ratio = $(I_{m/z\ 423}\% + I_{m/z\ 424}\%) / (I_{m/z\ 423}\% + I_{m/z\ 424}\% + I_{m/z\ 447}\% + I_{m/z\ 463}\%) \times 100\%$, because the intensity of *m/z* 425 ([M + H]⁺ ion) is too low, $I_{m/z\ 425}\%$ was neglected.

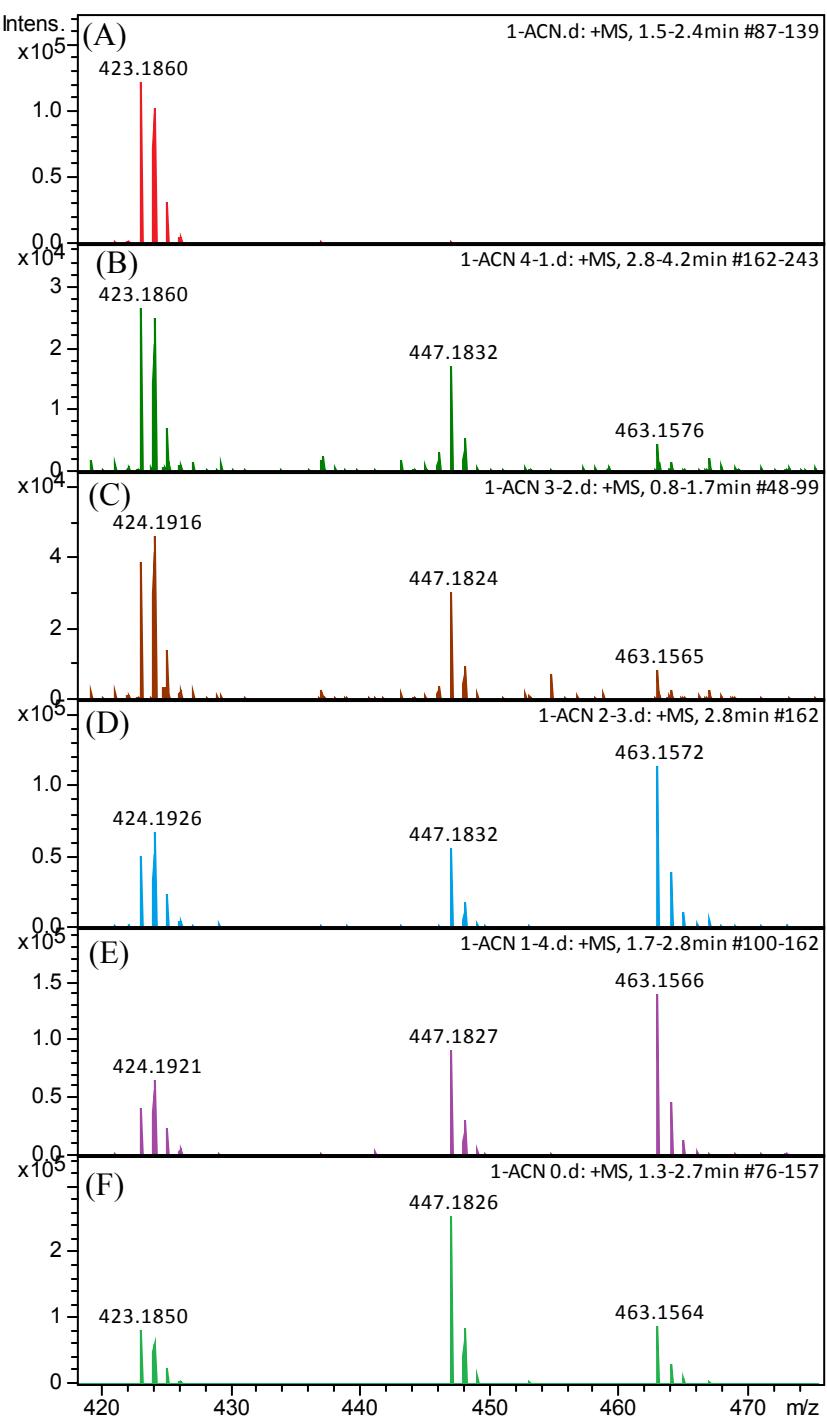


Fig. S3 The full-scan mass spectra of compound 1 with methanol/acetonitrile solvent mixtures (v/v) as the solvent, and the volume ratio of methanol to the solution is (A) 0 %, (B) 20 %, (C) 40 %, (D) 60 %, (E) 80 %, (F) 100 %.

Table S5 The oxidation ratio (%) with the volume ratio of methanol to the solution (methanol/acetonitrile solvent mixtures) for compound 1.

Volume ratio of methanol (%)	$I_{m/z\ 423}\%$	I_a	$I_{m/z\ 447}\%$	$I_{m/z\ 463}\%$	Oxidation ratio (%) ^b
424%					
0	100	49	2	1	98
20	100	61	67	18	66
40	85	71	66	19	65
60	83	71	83	98	46
80	30	37	65	100	29
100	33	13	100	35	25

^a $I_{m/z\ 424}\% = I_{m/z\ 424}\% \text{ (observed)} - I_{m/z\ 423}\% \text{ (observed)} \times \text{Isotope Ratio}_{(m+1)} \text{ (theory)}$, Isotope Ratio_(m+1)=0.345.

^b Oxidation ratio = $(I_{m/z\ 423}\% + I_{m/z\ 424}\%) / (I_{m/z\ 423}\% + I_{m/z\ 424}\% + I_{m/z\ 447}\% + I_{m/z\ 463}\%) \times 100\%$, because the intensities of $m/z\ 421$, $m/z\ 422$ and $m/z\ 425$ ($[M + H]^+$ ion) are too low, $I_{m/z\ 421}\%$, $I_{m/z\ 422}\%$ and $I_{m/z\ 425}\%$ are neglected.

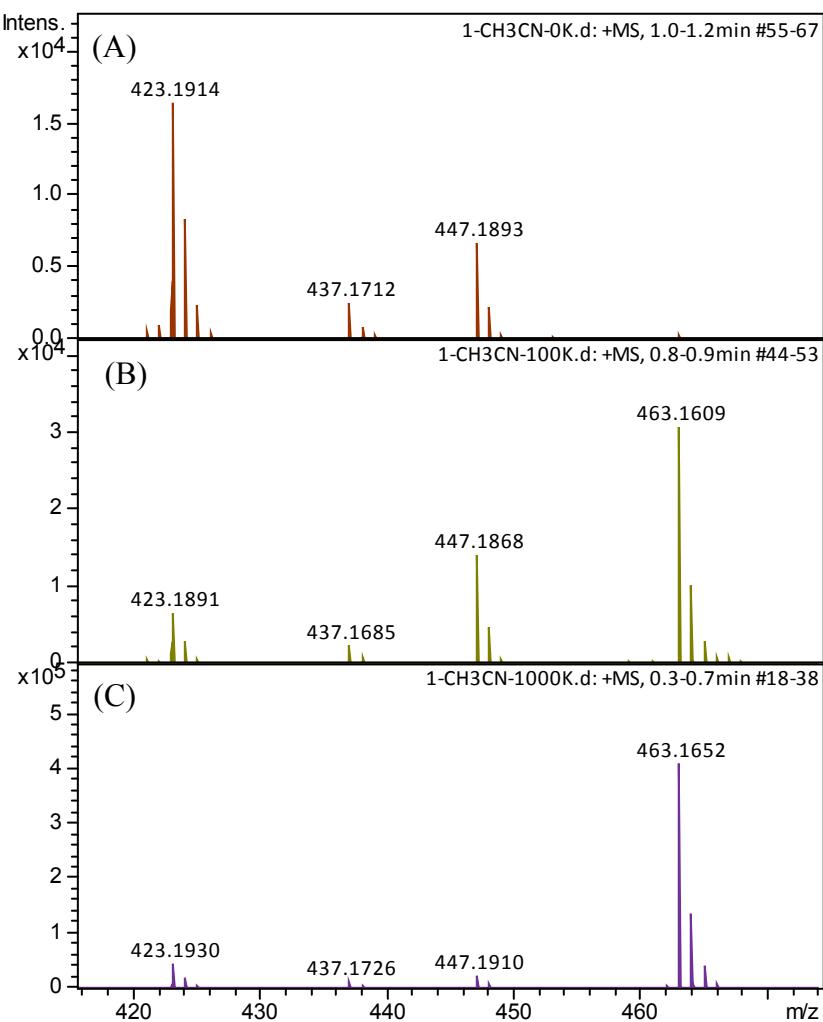


Fig. S4 Effect of K₂CO₃ addition on the abundance of [M-H]⁺ at *m/z* 423 for compound 1 with acetonitrile as the solvent (A) add 0.5 % (v/v) water; (B) add 0.5 % (v/v) 10⁻⁴ mol/L K₂CO₃ aqueous solution; (C) add 0.5 % (v/v) 10⁻³ mol/L K₂CO₃ aqueous solution.

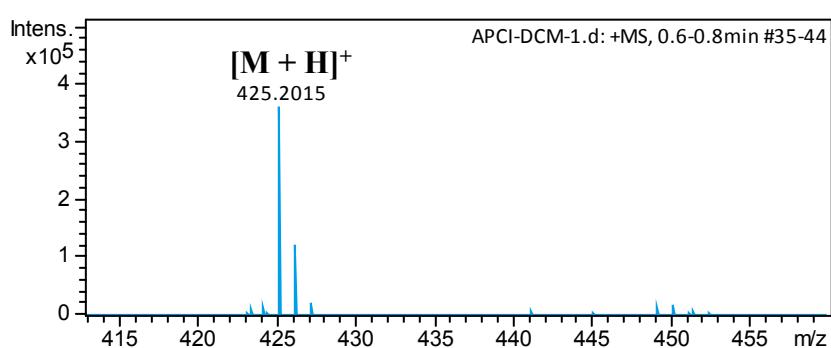


Fig. S5 The APCI spectrum of compound **1** with dichloromethane as the solvent, and the conditions of APCI source in positive-ion mode were as follows: end plate offset, 500 V; capillary, 4000 V; corona, 4000 nA; nebulizer, 2.0 bar; dry gas, 1.5 L/min; the dry gas temperature, 180 °C and vaporizer temperature, 200 °C.

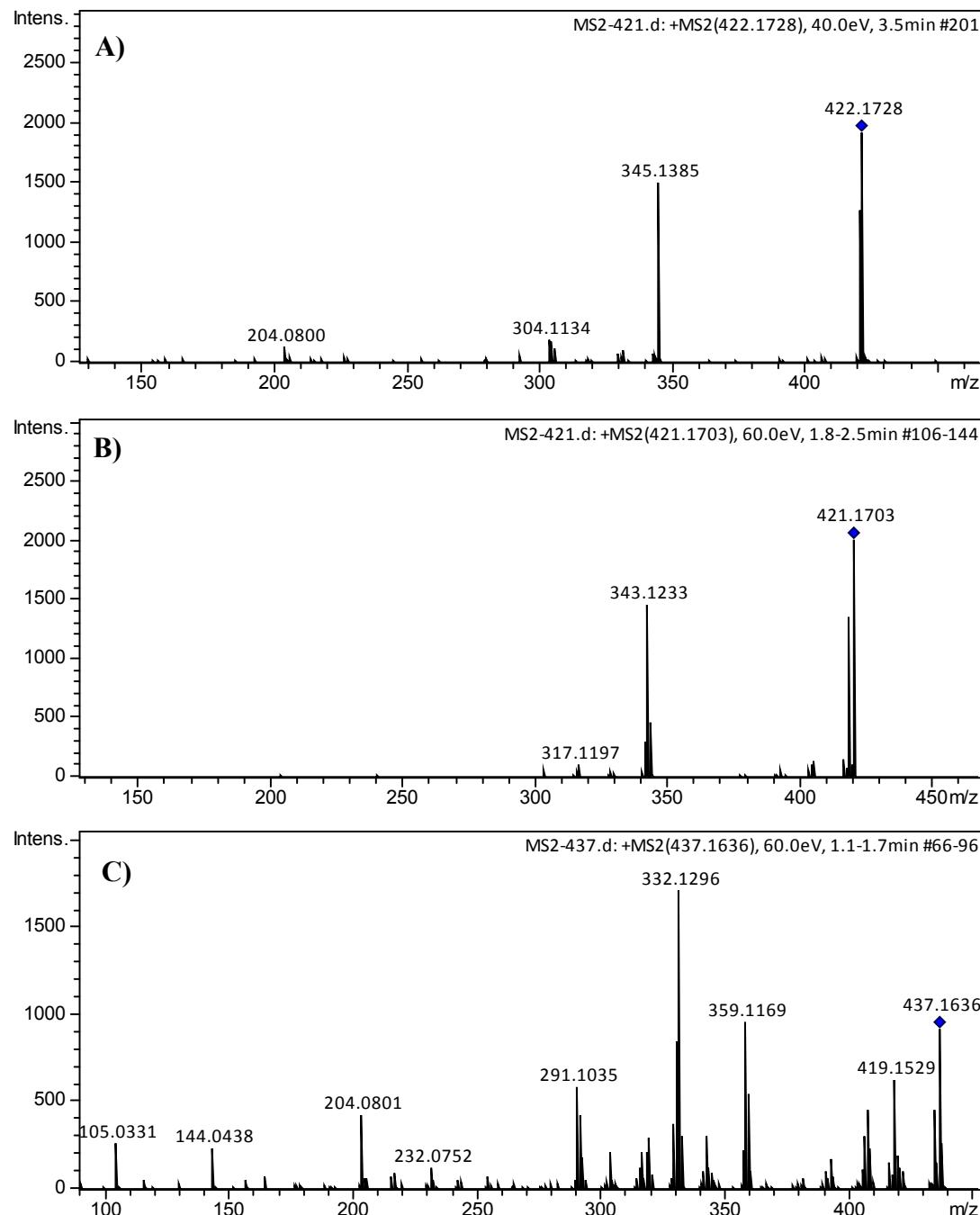
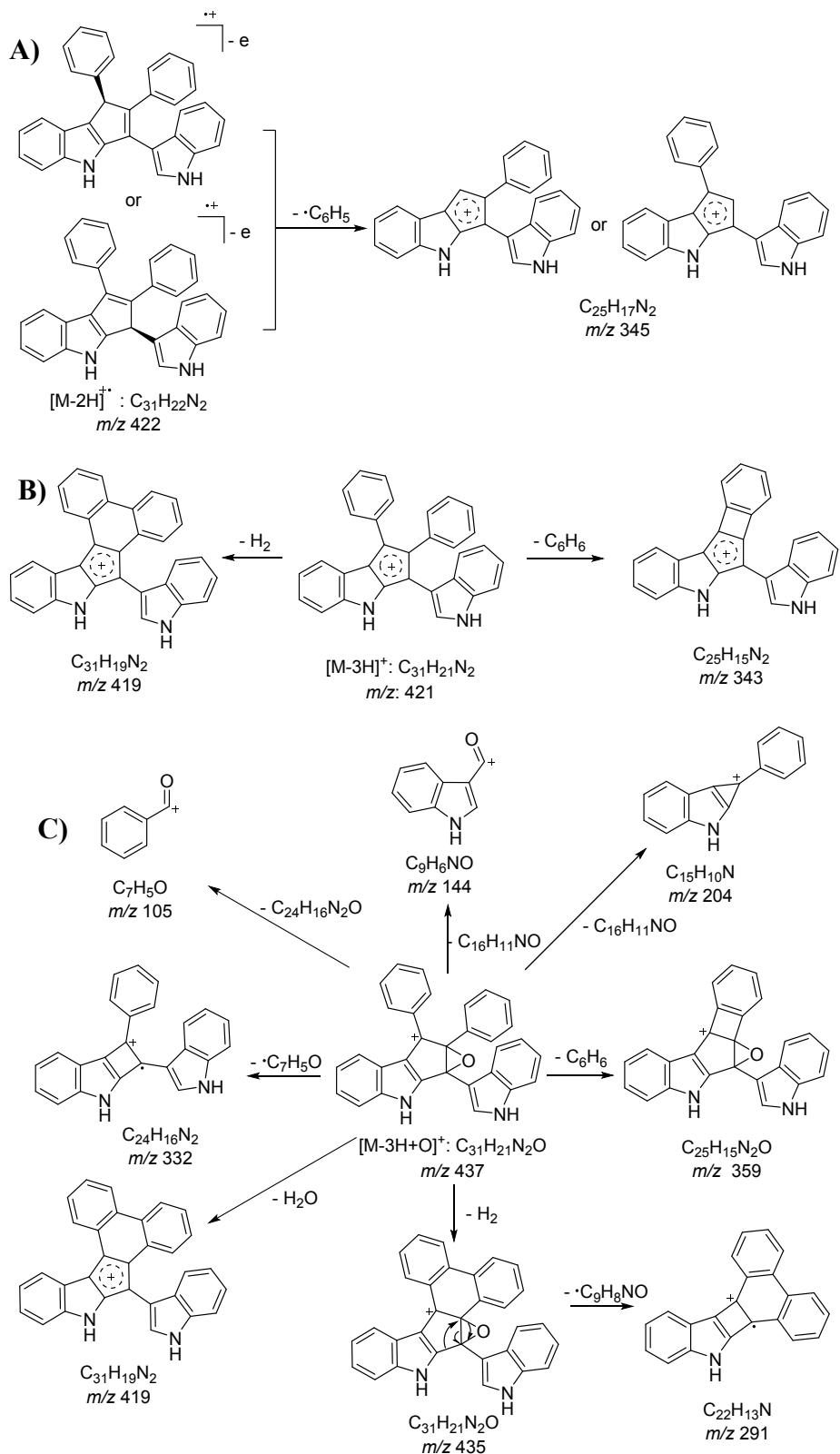


Fig. S6 The MS/MS spectra of selected precursor ions from compound **1**: (A) $[M-2H]^{+}$ at m/z 422 (collision energy: 40 eV; Isol. Width: 1 u); (B) $[M-3H]^{+}$ at m/z 421 (collision

energy: 60 eV; Isol. Width: 1 u); (C) [M-3H+O]⁺ at *m/z* 437 (collision energy: 60 eV; Isol. Width: 1 u).



Scheme S1. Major fragmentation patterns of (A) $[M-2H]^\bullet$, (B) $[M-3H]^+$ and (C) $[M-3H+O]^\bullet$ for compound **1**.

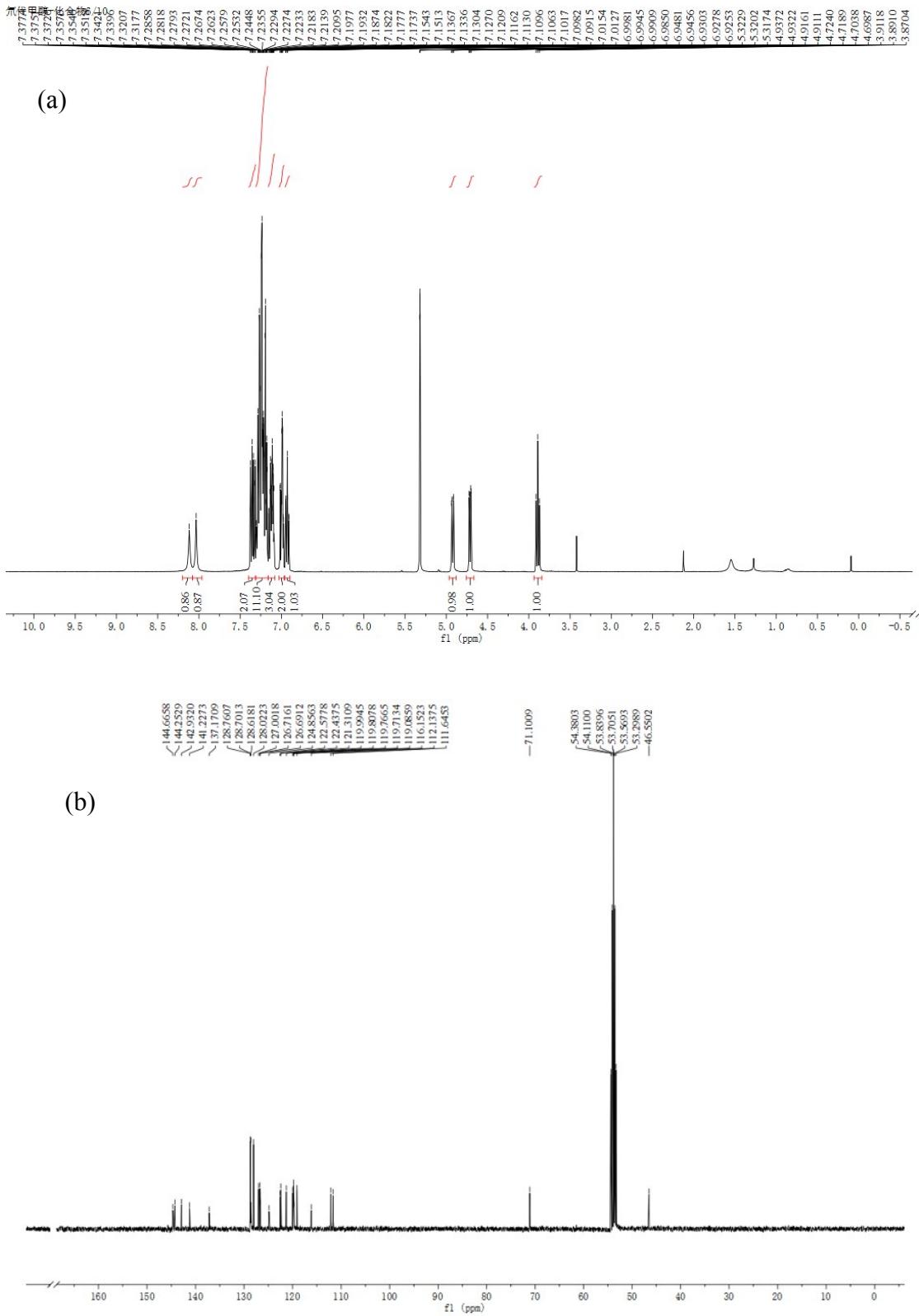


Fig. S7 (a) ^1H NMR spectrum of compound 1; (b) ^{13}C NMR spectrum of compound 1.