

## Supporting Information

*Rec. Nat. Prod.* **10:2** (2016) 221-227

### **Pyrrolizidine Alkaloids from *Onosma kaheirei* Teppner (Boraginaceae)**

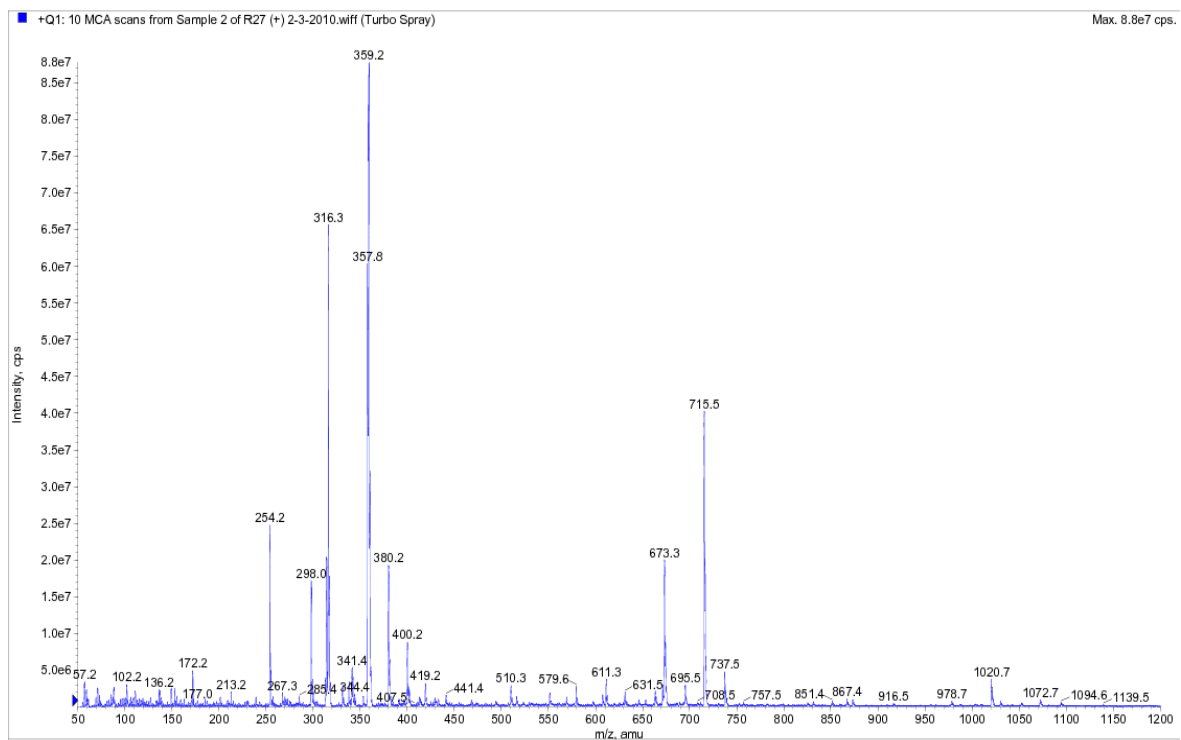
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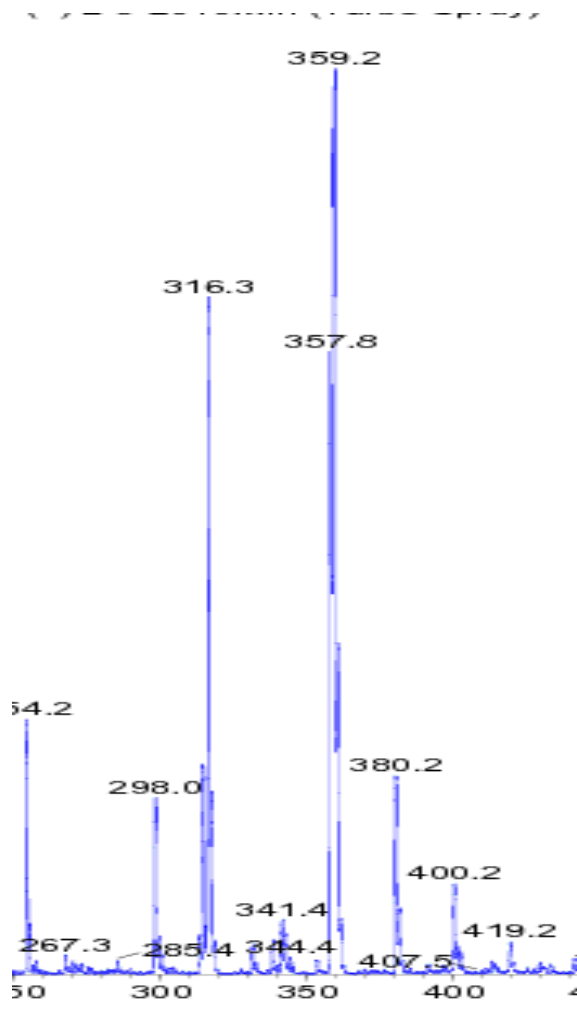
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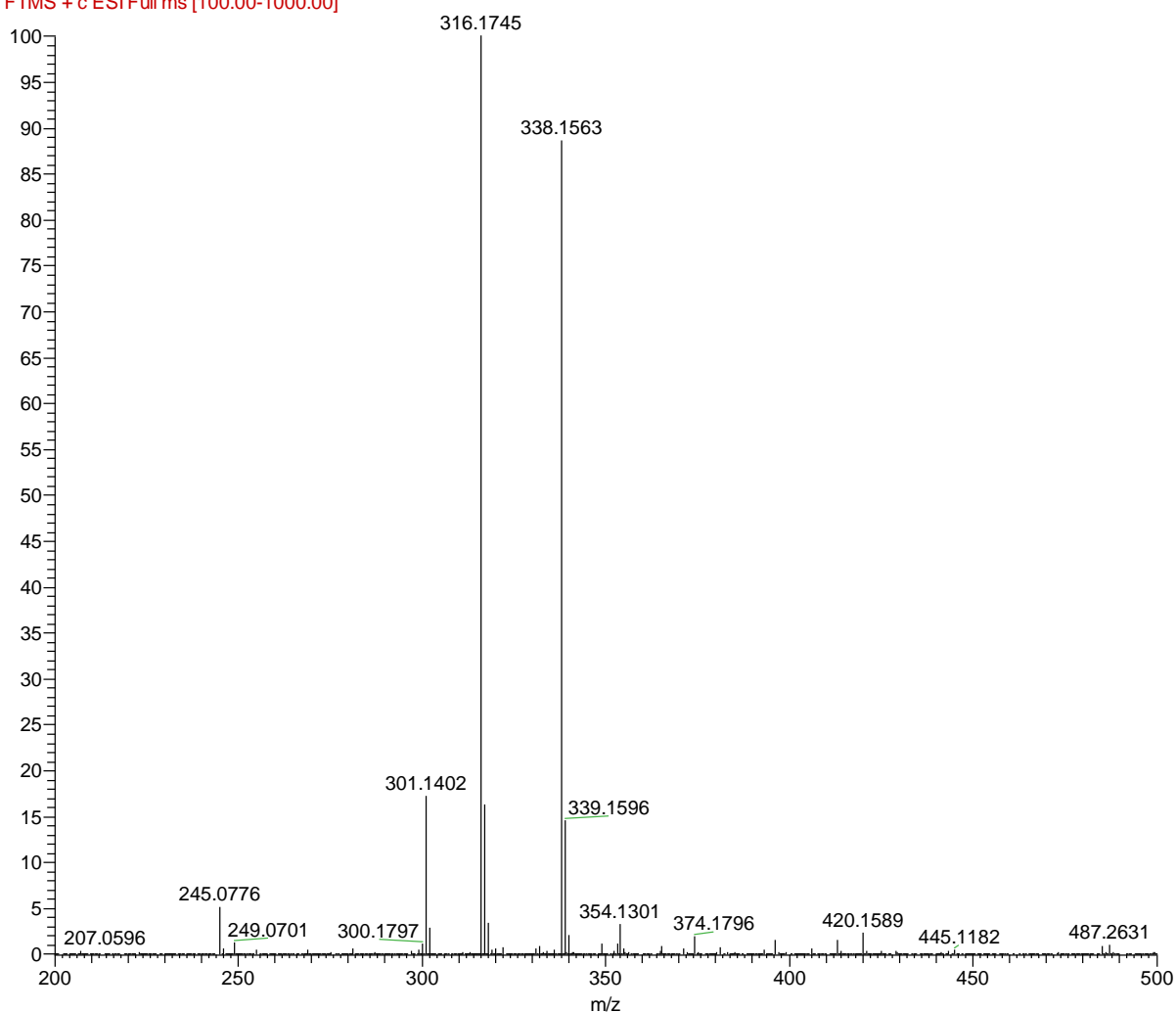


### S1: ESI-MS Spectrum of Compound 7 ((-)-3'-O-acetyechinatine N-oxide)



**S2:** Expansion of ESI-MS Spectrum of Compound **7** ((-)-3'-*O*-acetyechinatine *N*-oxide)

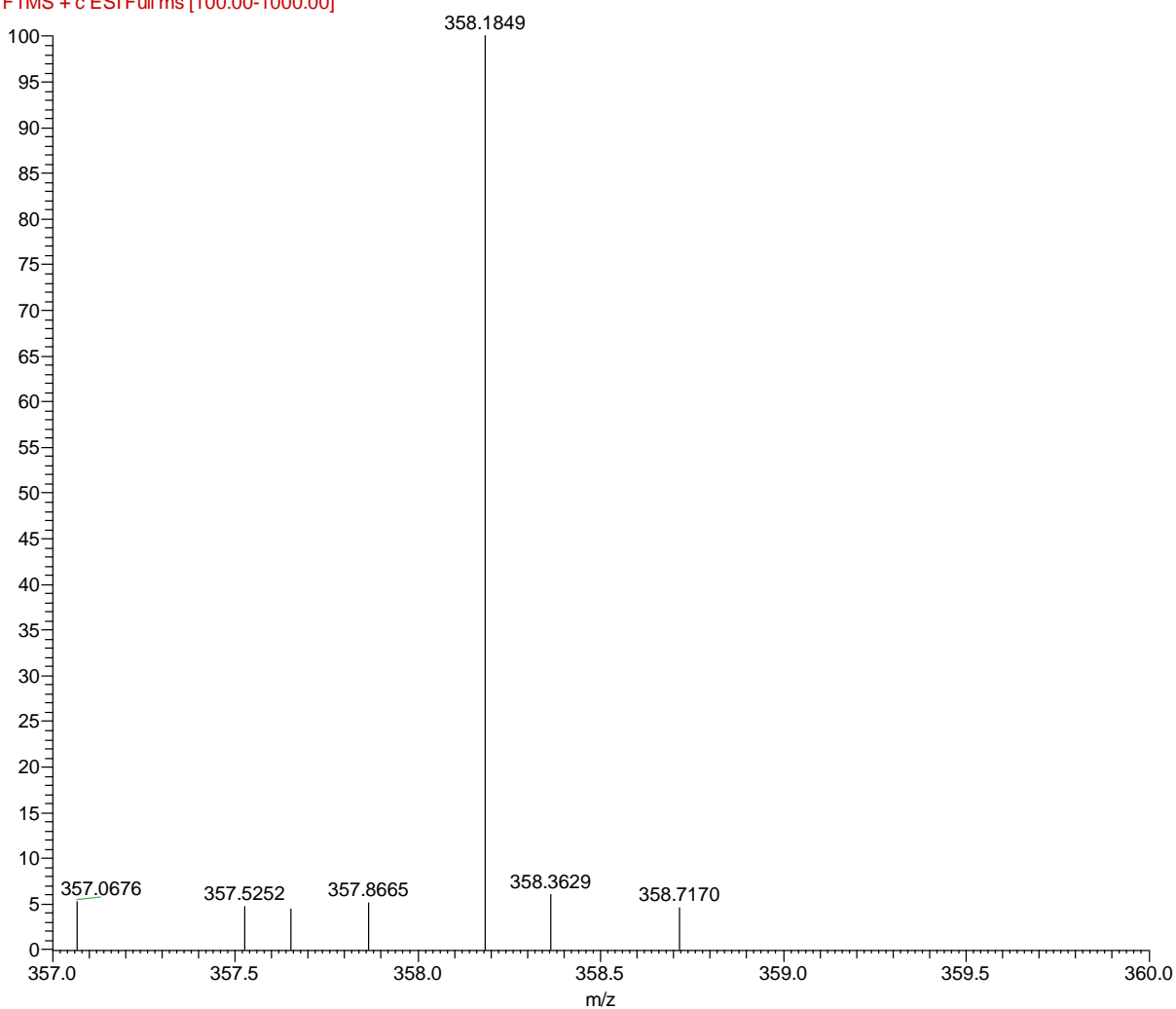
OKM\_30013B\_H2O\_MeOH\_FTMS\_2\_ESI(+) #2-29 RT: 0.01-0.23 AV: 28 NL: 4.37E7  
 F: FTMS + c ESI Full ms [100.00-1000.00]



<i>m/z</i>	Intensity	Relative Abundance	Delta (ppm)	RDB equiv.	Composition
245.0776	2242609.0	5.13	-13.23	8.5	C14 H13 O4
249.0701	526424.3	1.21	-23.72	9.0	C14 H12 O2 N Na
300.1797	493270.8	1.13	-2.75	3.5	C15 H26 O5 N
301.1402	7536284.5	17.25	-2.90	5.5	C16 H22 O4 Na
302.1435	1274941.6	2.92	-17.77	5.0	C16 H23 O4 Na
316.1745	43678848.0	100.00	-3.04	3.5	C15 H26 O6 N
317.1778	7105779.0	16.27	-17.30	3.0	C15 H27 O6 N
318.1801	525292.1	1.20	-34.53	2.5	C15 H28 O6 N
318.1899	1458730.9	3.34	-3.89	2.5	C15 H28 O6 N
338.1563	38701536.0	88.60	-3.36	3.5	C15 H25 O6 N Na
339.1596	6349374.0	14.54	-16.47	3.0	C15 H26 O6 N Na
340.1713	888915.3	2.04	-5.31	2.5	C15 H27 O6 N Na
349.1093	503649.3	1.15	-11.10	6.0	C15 H20 O7 N Na
353.2650	494714.1	1.13	68.47	0.0	C16 H35 O7 N
354.1301	1449406.6	3.32	-62.82	3.5	C15 H25 O7 N Na
354.1511	499539.8	1.14	-3.43	3.5	C15 H25 O7 N Na
374.1796	870001.9	1.99	-94.35	0.5	C16 H33 O7 N Na

**S3:** HR-ESI-MS Spectrum of Compound **7** ((-)-3'-*O*-acetylochinateine *N*-oxide)

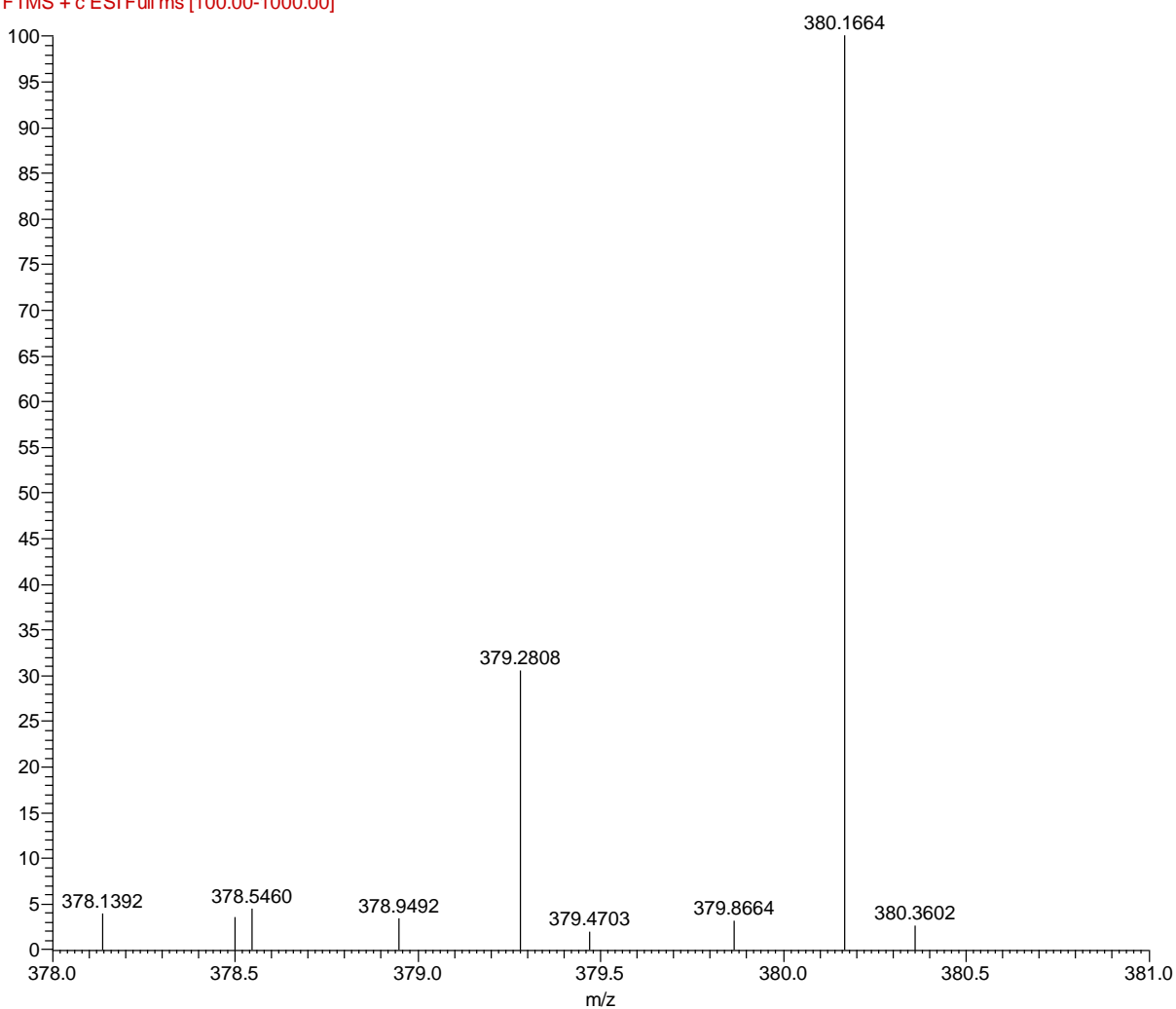
OKM\_30013B\_H2O\_MeOH\_FTMS\_2\_ESI(+) #2-29 RT: 0.01-0.23 AV: 28 NL: 4.96E4  
 F: FTMS + c ESI Full ms [100.00-1000.00]



m/z	Intensity	Relative Abundance	Delta (ppm)	RDB equiv.	Composition
357.0676	2628.0	5.30	-40.05	9.0	C16 H16 O7 N Na
357.5252	2329.3	4.69			
357.6513	2225.5	4.49			
357.8665	2516.2	5.07			
358.1849	49618.3	100.00	-3.18	4.5	C17 H28 O7 N
358.3629	2994.2	6.03			
358.7170	2288.6	4.61			

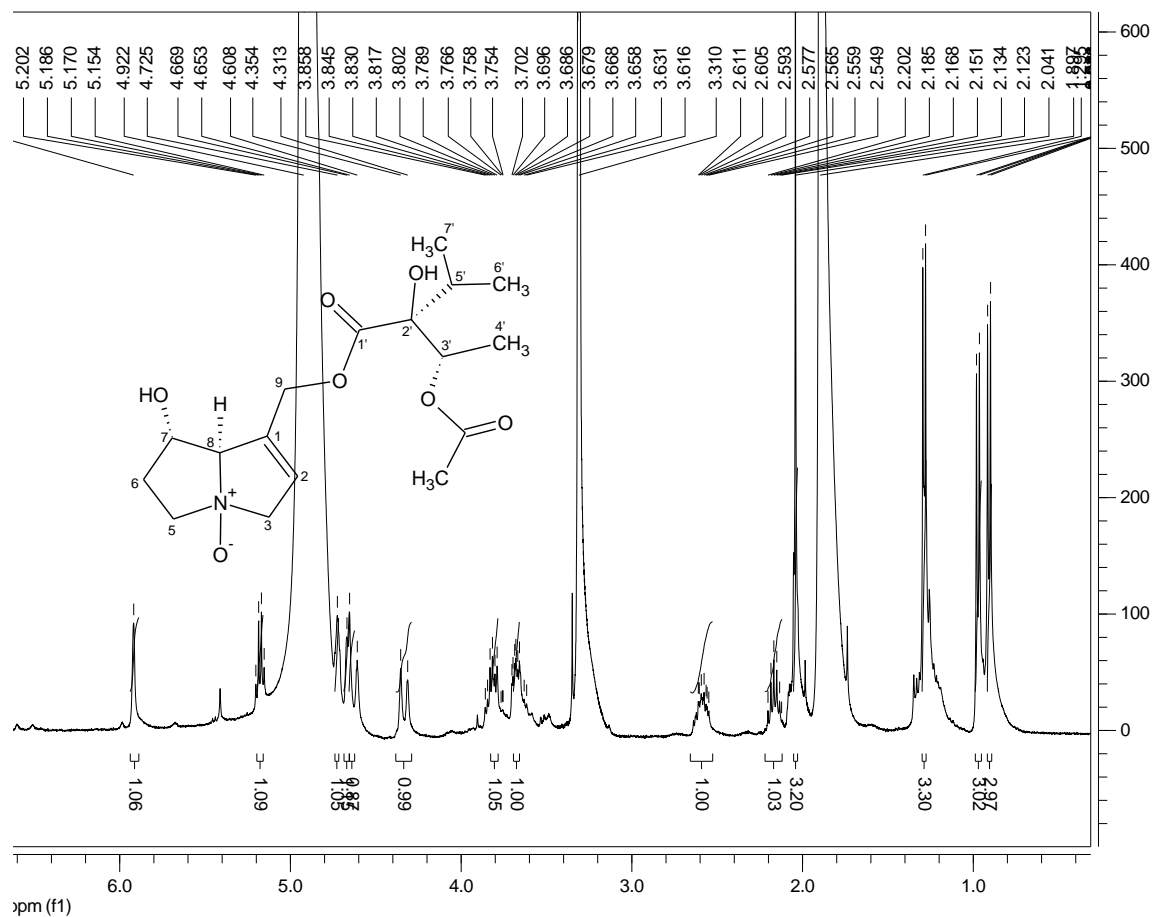
**S4:** Expansion of HR-ESI-MS Spectrum of Compound **7** ((-)-3'-O-acetylechinate *N*-oxide)

OKM\_30013B\_H2O\_MeOH\_FTMS\_2\_ESI(+) #2-29 RT: 0.01-0.23 AV: 28 NL: 9.94E4  
 F: FTMS + c ESI Full ms [100.00-1000.00]



<i>m/z</i>	Intensity	Relative Abundance	Delta (ppm)	RDB equiv.	Composition
378.1392	3954.3	3.98	-34.73	5.5	C17 H25 O7 N Na
378.5009	3510.5	3.53			
378.5460	4433.2	4.46			
378.9492	3388.2	3.41			
379.2808	30364.1	30.55	64.29	1.0	C18 H37 O7 N
379.4703	1921.4	1.93			
379.8664	3126.2	3.15			
380.1664	99397.0	100.00	-4.11	4.5	C17 H27 O7 N Na
380.3602	2519.3	2.53			

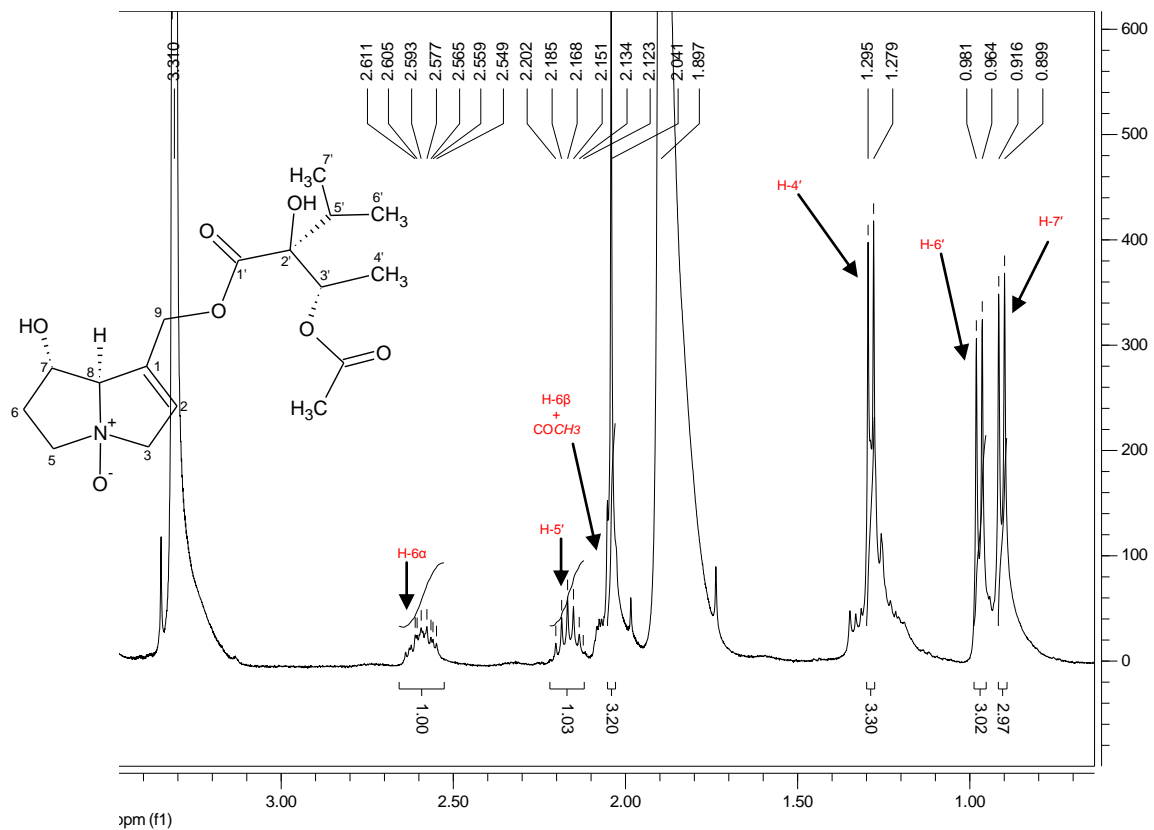
**S5:** Expansion of HR-ESI-MS Spectrum of Compound **7** ((-)-3'-*O*-acetylechinate *N*-oxide)



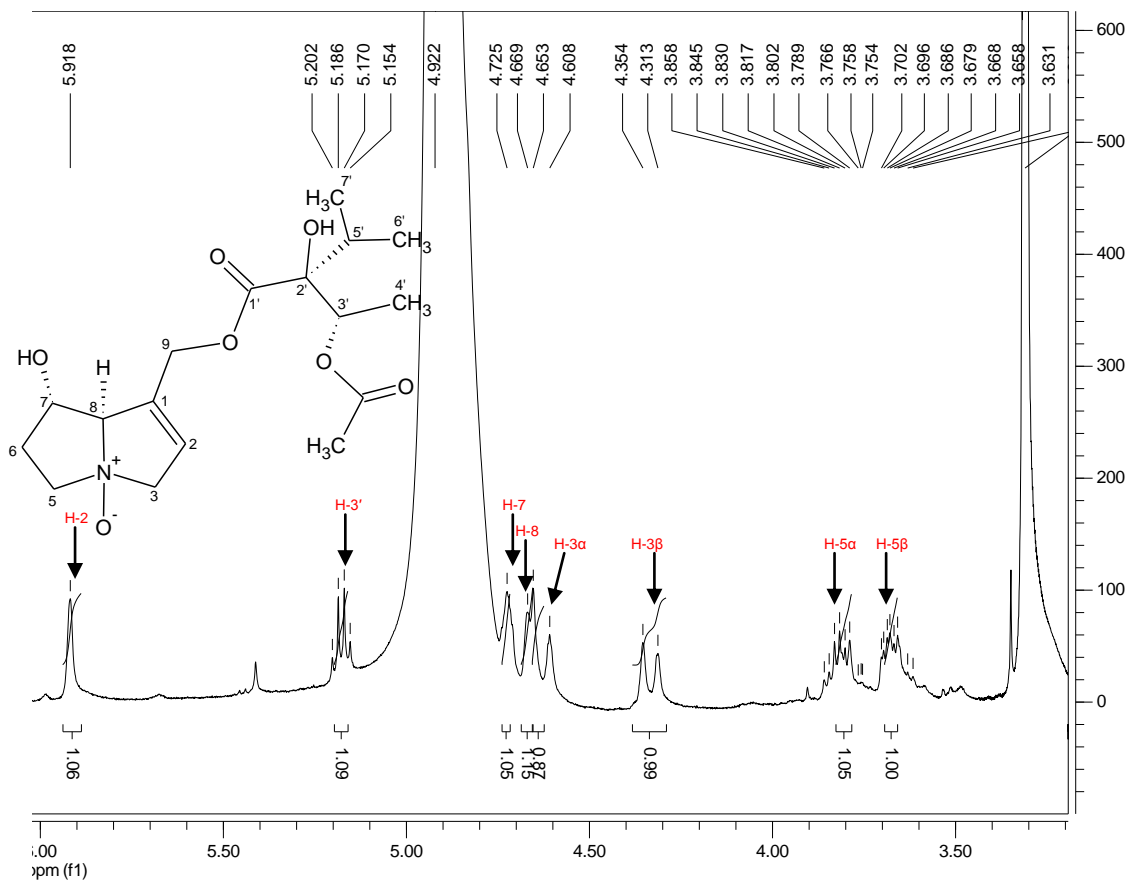
**S6:** <sup>1</sup>H-NMR Spectrum (400 MHz, MeOH-d<sub>4</sub>) of Compound 7 ((-)-3'-O-acetylechinatine N-oxide)

(-)-3'-O-acetylechinatine N-oxide (7): Pale yellow gum. <sup>1</sup>H-NMR (MeOH-d<sub>4</sub>, 400 MHz), δ: 0.91 (3H, d, H-7'), 0.97 (3H, d, H-6'), 1.29 (3H, d, H-4'), 2.04 (3H, s, COCH<sub>3</sub>), 2.08 (1H, m, H-6β), 2.17 (1H, sept, H-5'), 2.60 (1H, m, H-6α), 3.68 (1H, m, H-5β), 3.83 (1H, m, H-5α), 4.33 (1H, d, H-3β), 4.63 (1H, d, H-3α), 4.67 (1H, brs, H-8), 4.73 (1H, m, H-7), 4.85 (2H, brs, H-9), 5.18 (1H, q, H-3'), 5.92 (1H, brs, H-2). <sup>13</sup>C-NMR (MeOH-d<sub>4</sub>, 50 MHz), δ: 16.6 (C-4'), 17.5 (C-6'), 18.3 (C-7'), 18.5 (COCH<sub>3</sub>), 33.9 (C-5'), 35.7 (C-6), 62.4 (C-9), 70.2 (C-5), 70.8 (C-7), 71.9 (C-3'), 79.1 (C-3), 82.0 (C-2'), 97.2 (C-8), 123.5 (C-2), 133.7 (C-1), 170.6 (C-1'), 172.0 (COCH<sub>3</sub>). ESI-MS: *m/z* = 380.4 [M+Na]<sup>+</sup> for formula C<sub>17</sub>H<sub>27</sub>NO<sub>7</sub>Na.

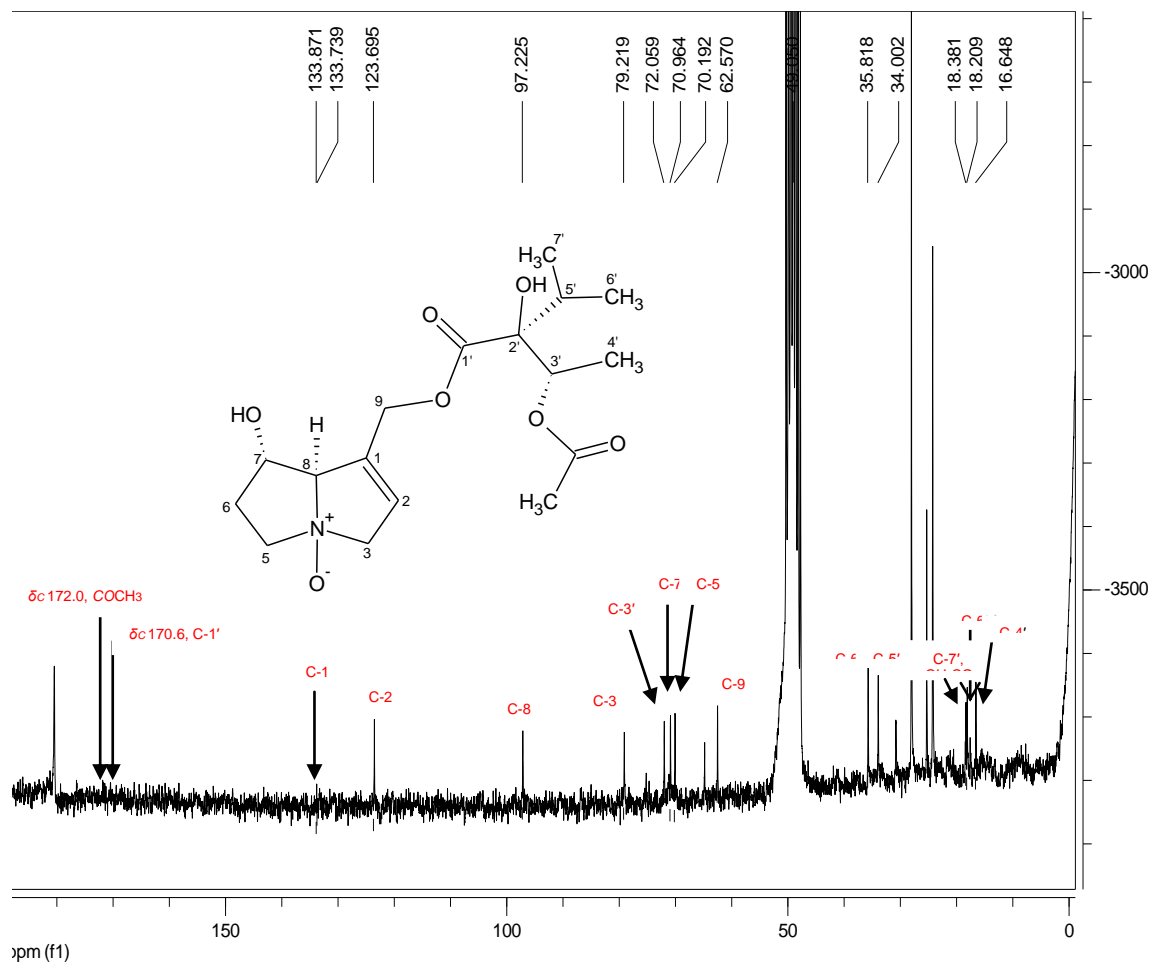




**S7:** Expansion of <sup>1</sup>H-NMR Spectrum of Compound **7** ((-)-3'-O-acetylchinatine N-oxide) (from 0.00 to 3.40 ppm)

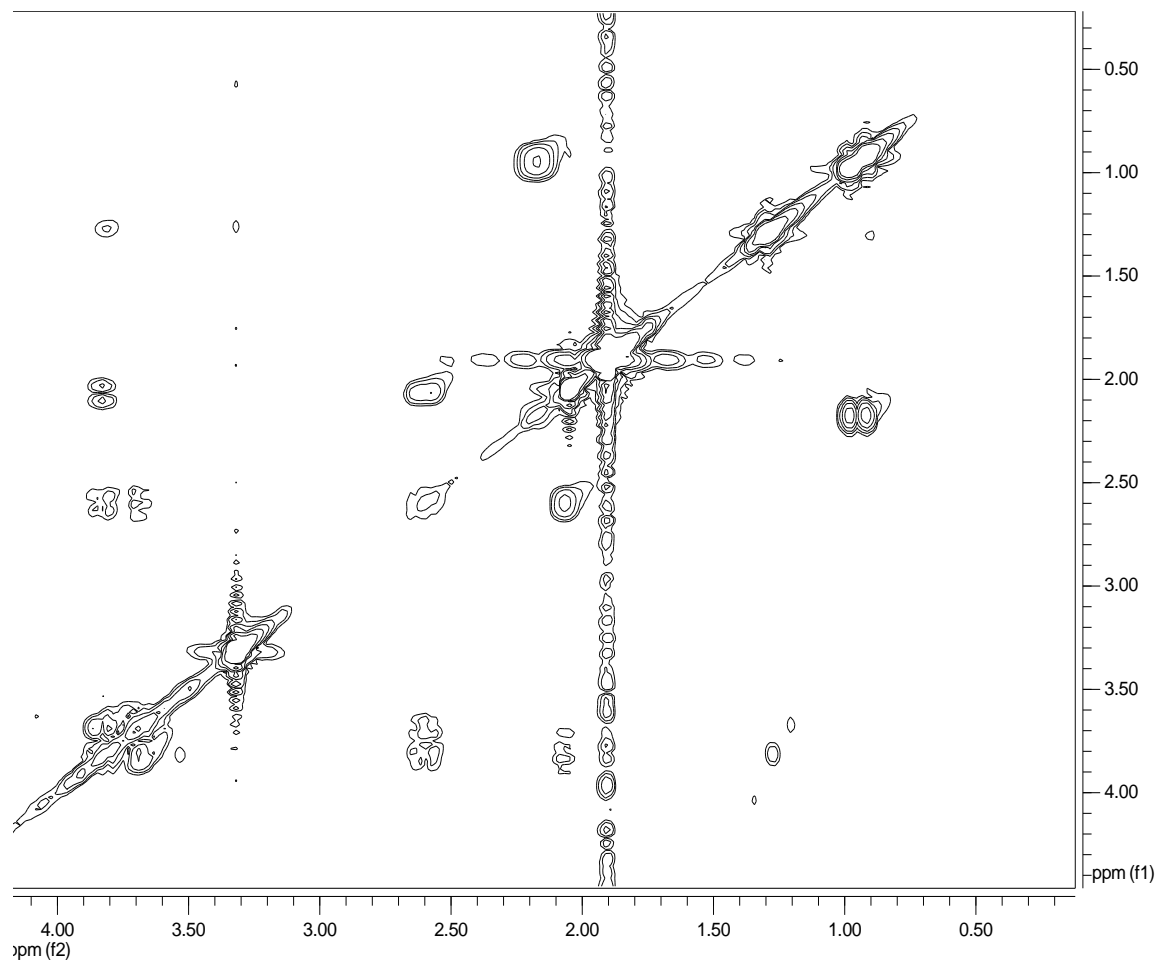


**S8:** Expansion of <sup>1</sup>H-NMR Spectrum of Compound 7 ((-)-3'-O-acetylchinatine N-oxide) (from 3.40 to 6.00 ppm)

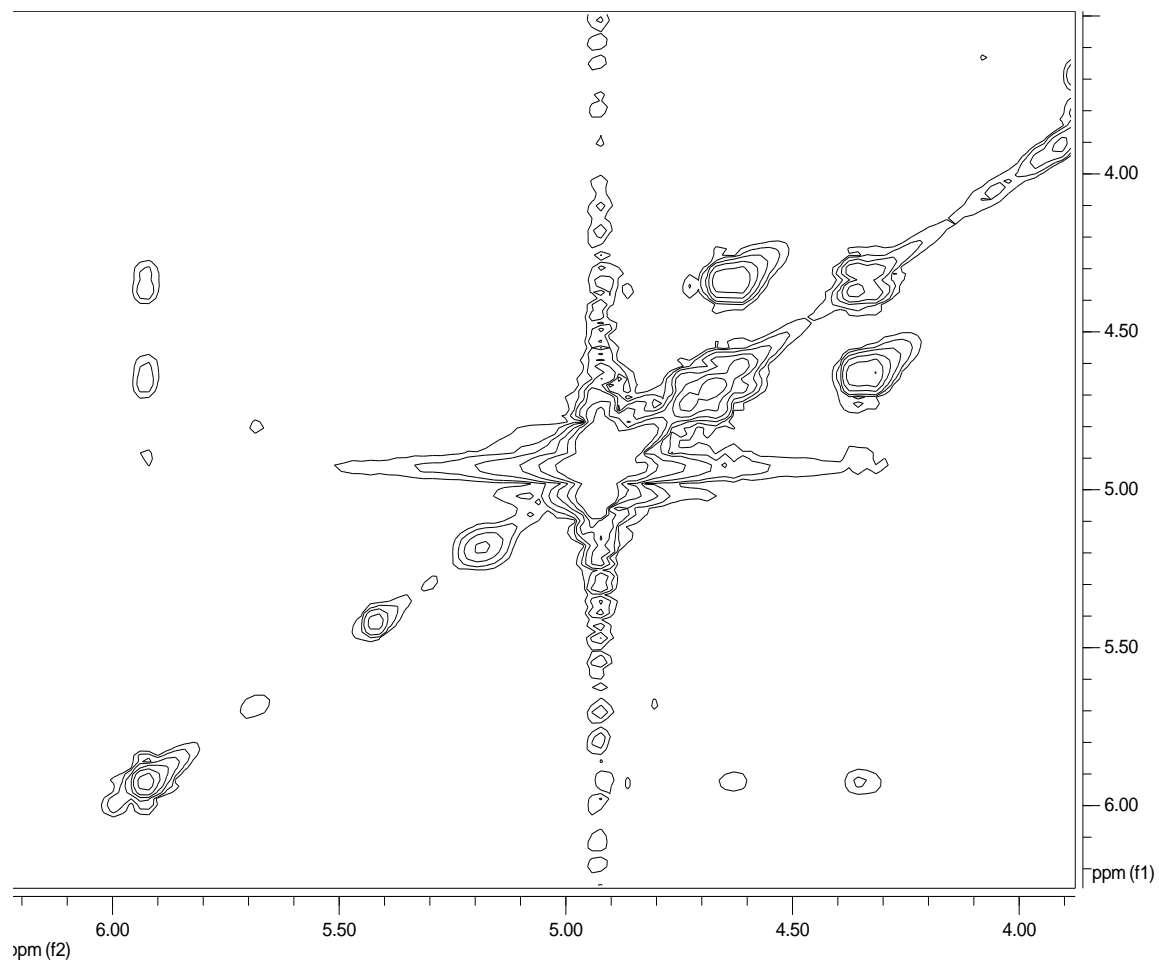


**S9:**  $^{13}\text{C}$ -NMR Spectrum (50 MHz, MeOH- $d_4$ ) of Compound 7 ((-)-3'-O-acetylchinate N-oxide)

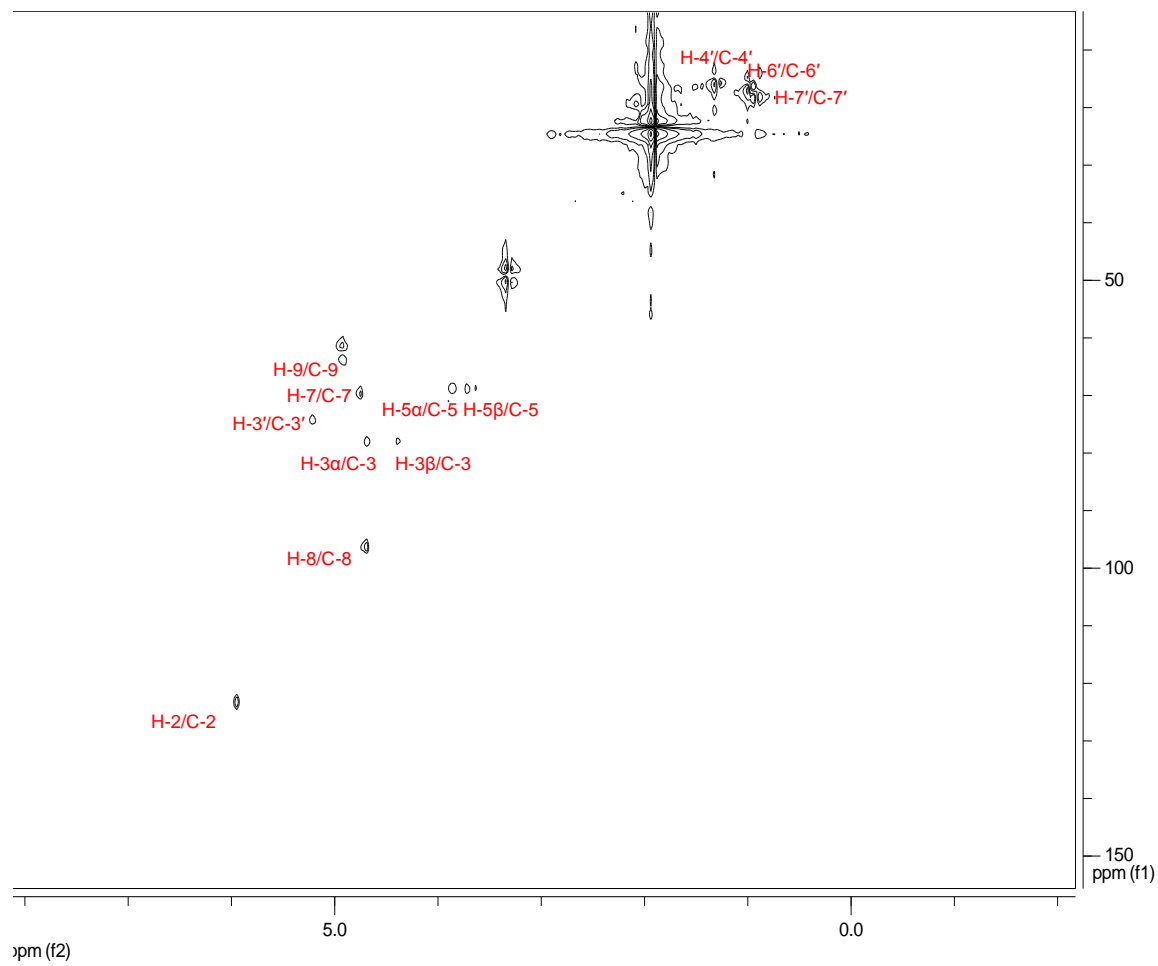




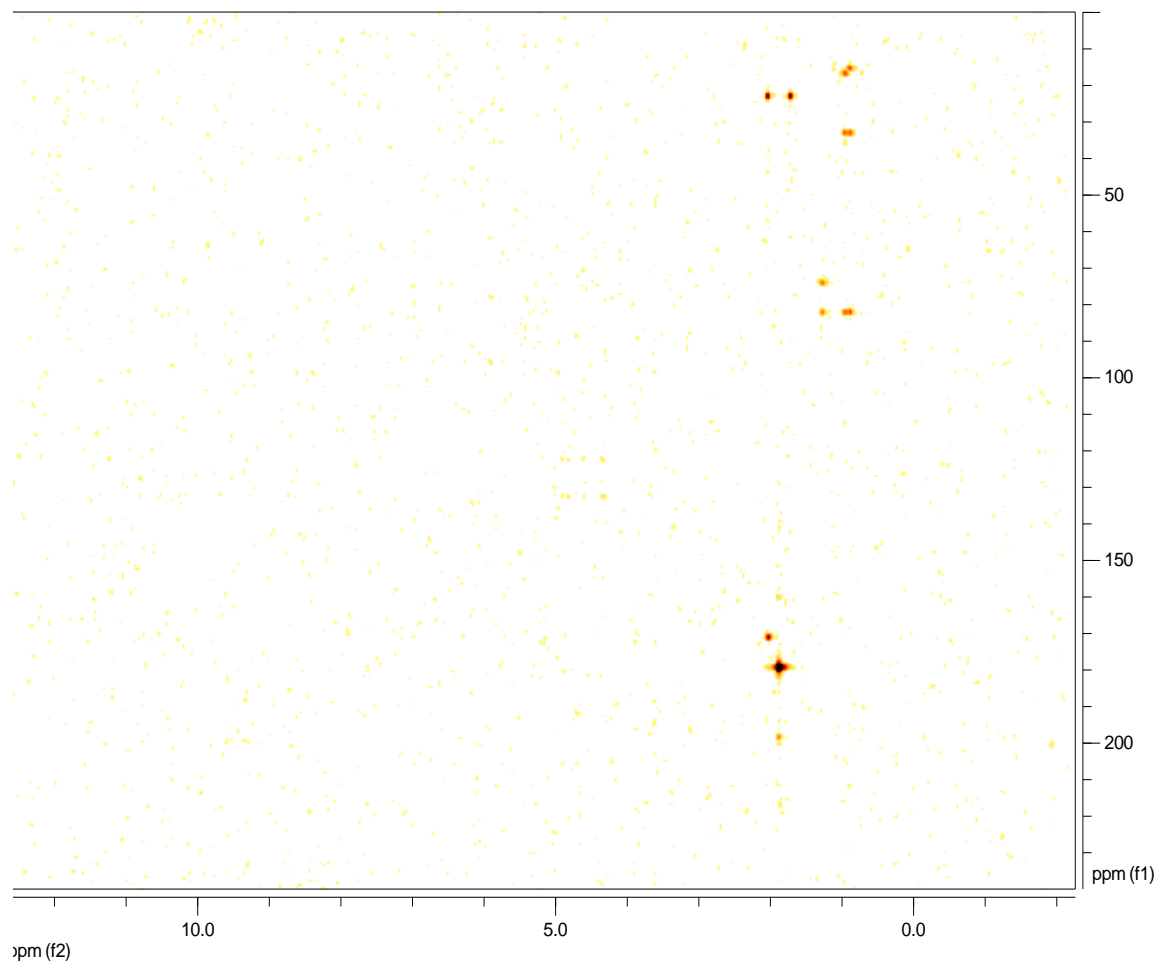
**S11:** Expansion of COSY Spectrum (400 MHz) of Compound **7** ((-)-3'-*O*-acetyechinatine *N*-oxide) (from 0.00 to 4.00 ppm)



**S12:** Expansion of COSY Spectrum (400 MHz) of Compound **7** ((-)-3'-*O*-acetylechinate *N*-oxide) (from 4.00 to 6.00 ppm)

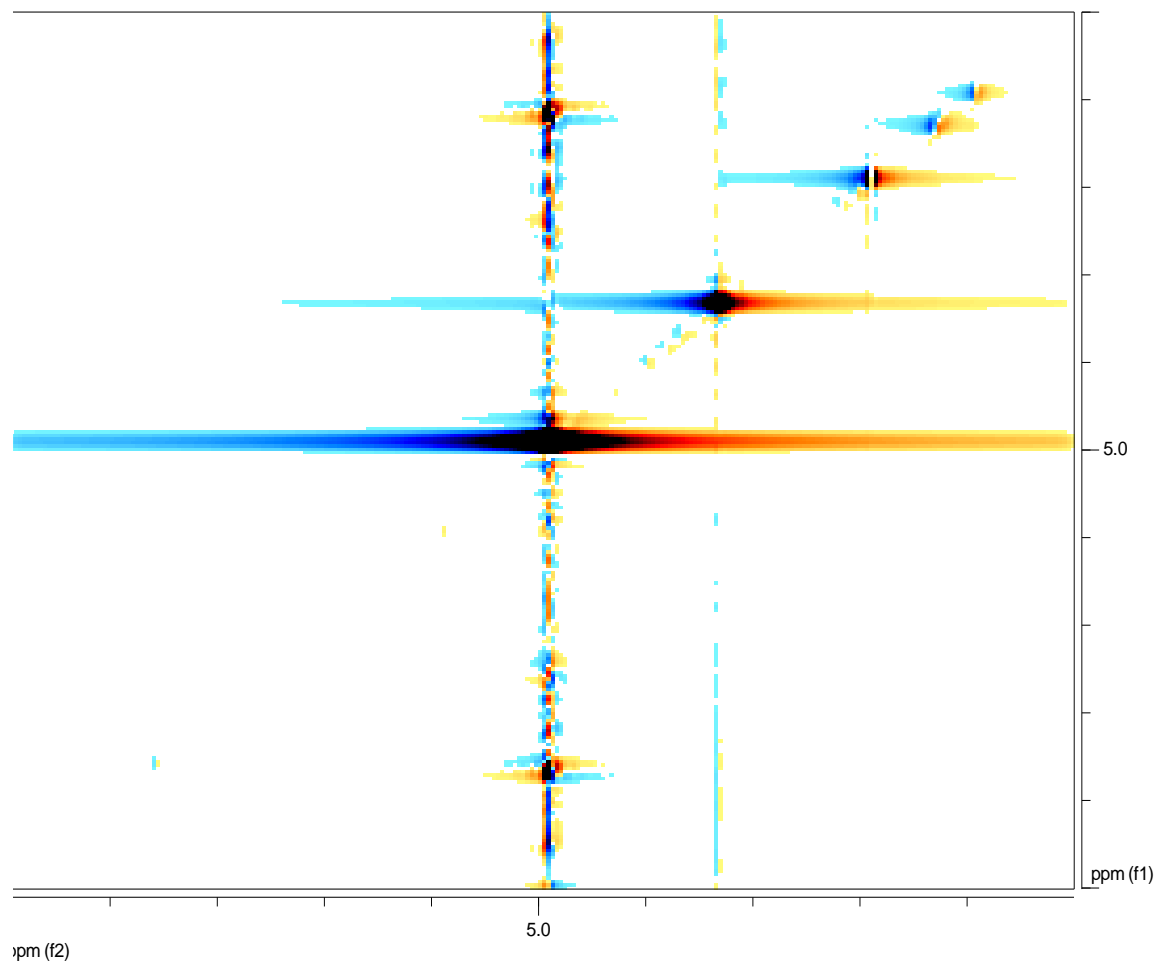


**S13:** HSQC-DEPT Spectrum (400 MHz) of Compound **7** ((-)-3'-*O*-acetylechinate *N*-oxide)



**S14:** HMBC Spectrum (400 MHz) of Compound **7** ((-)-3'-*O*-acetylechinate *N*-oxide)





**S15:** NOESY Spectrum (400 MHz) of Compound **7** ((-)-3'-*O*-acetylechinate *N*-oxide)