Supporting Information

Melohemsines A-I, melodinus-type alkaloids from *Melodinus hemsleyanus*

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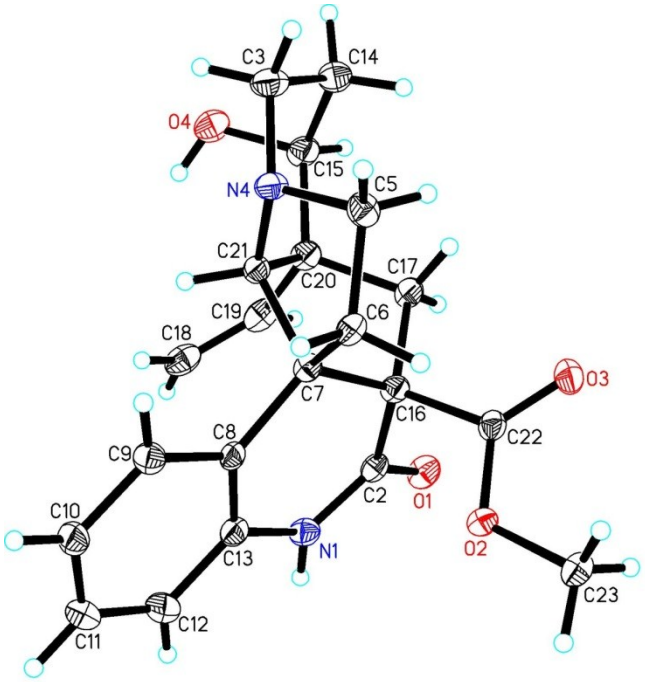
List of Supporting Information

X-ray Crystallographic Analysis of 4. A colourless blocks crystal suitable for X-ray analysis was from MeOH. The X-ray data of compound 4 were collected at 173(2) K with Cu Kα radiation (λ = 1.54184 Å) on Agilent Gemini S Ultra CCD diffractometer. Crystal data: formula: $C_{21}H_{24}N_2O_4$, tetragonal, space group $P4_3$; a = 12.31578 (8) Å, b = 12.31578 (8) Å, c = 13.37214 (14) Å, $\alpha = \beta = \gamma = 90.00°$; V = 2028.27 (3) Å, T = 173(2) K, Z = 4, Dc = 1.207 mg/mm^3, $F(000)$ = 784. A total of 16235 reflections were collected in the range $6.06 \leq \theta \leq 62.78$, of which 3149 unique reflections with $I > 2\sigma(I)$ were collected for the analysis. The structure was refined by full-matrix least squares on F^2 using SHELXL-97 package software. The final reliability factors are: R = 0.0464, R_W = 0.1314, S = 1.105, and Flack paremeter = 0.0 (3). Crystallographic data for the structure reported in this paper had been deposited at the Cambridge Crystallographic Data Centre under the reference number CCDC 1454869.

Single crystal X-ray data and structure of 4

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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
;
# SQUEEZE RESULTS (APPEND TO CIF)
# Note: Data are Listed for all Voids in the P1 Unit Cell
# i.e. Centre of Gravity, Solvent Accessible Volume,
# Recovered number of Electrons in the Void and
# Details about the Squeezed Material
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O3 O 0.19196(17) 0.57773(18) 0.12518(16) 0.0378(5) Uani 1 1 d . . .
O4 O -0.21495(17) 0.56849(19) 0.43905(18) 0.0411(5) Uani 1 1 d . . .
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N1 N 0.19031(19) 0.31932(18) 0.35630(19) 0.0288(5) Uani 1 1 d . . .
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C3 C -0.0755(2) 0.7514(3) 0.4140(3) 0.0374(7) Uani 1 1 d . . .
H3A H -0.0687 0.8289 0.4028 0.045 Uiso 1 1 calc R . .
H3B H -0.1113 0.7412 0.4779 0.045 Uiso 1 1 calc R . .
N4 N 0.03466(18) 0.70336(19) 0.41944(18) 0.0283(5) Uani 1 1 d . . .
C5 C 0.1128(2) 0.7437(2) 0.3456(2) 0.0312(6) Uani 1 1 d . . .
H5A H 0.1344 0.8178 0.3601 0.037 Uiso 1 1 calc R . .
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C6 C 0.2065(2) 0.6656(2) 0.3592(2) 0.0255(6) Uani 1 1 d . . .
H6A H 0.2512 0.6872 0.4154 0.031 Uiso 1 1 calc R . .
H6B H 0.2513 0.6636 0.2996 0.031 Uiso 1 1 calc R . .
C7 C 0.1536(2) 0.5522(2) 0.3788(2) 0.0233(6) Uani 1 1 d . . .
C8 C 0.2176(2) 0.4843(2) 0.4528(2) 0.0241(6) Uani 1 1 d . . .
C9 C 0.2587(2) 0.5306(2) 0.5412(2) 0.0286(6) Uani 1 1 d . . .
H9A H 0.2497 0.6046 0.5522 0.034 Uiso 1 1 calc R . .
C10 C 0.3123(2) 0.4689(3) 0.6121(2) 0.0332(7) Uani 1 1 d . . .
H10A H 0.3393 0.5014 0.6697 0.040 Uiso 1 1 calc R . .
C11 C 0.3256(3) 0.3578(3) 0.5968(3) 0.0411(8) Uani 1 1 d . . .
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C12 C 0.2853(3) 0.3120(3) 0.5118(3) 0.0389(7) Uani 1 1 d . . .
H12A H 0.2935 0.2378 0.5013 0.047 Uiso 1 1 calc R . .
C13 C 0.2320(2) 0.3746(2) 0.4406(2) 0.0277(6) Uani 1 1 d . . .
C14 C -0.1461(2) 0.7033(3) 0.3324(3) 0.0387(7) Uani 1 1 d . . .
H14A H -0.2173 0.7368 0.3337 0.046 Uiso 1 1 calc R . .
H14B H -0.1137 0.7173 0.2675 0.046 Uiso 1 1 calc R . .
C15 C -0.1565(2) 0.5832(3) 0.3486(2) 0.0348(7) Uani 1 1 d . . .
H15A H -0.1991 0.5524 0.2935 0.042 Uiso 1 1 calc R . .
C16 C 0.1289(2) 0.4903(2) 0.2775(2) 0.0253(6) Uani 1 1 d . . .
C17 C 0.0130(2) 0.5240(2) 0.2501(2) 0.0284(6) Uani 1 1 d . . .
H17A H -0.0202 0.4719 0.2051 0.034 Uiso 1 1 calc R . .
H17B H 0.0117 0.5952 0.2193 0.034 Uiso 1 1 calc R . .
C18 C -0.0380(3) 0.3598(2) 0.4671(3) 0.0391(7) Uani 1 1 d . . .
H18A H -0.0021 0.3980 0.5171 0.047 Uiso 1 1 calc R . .
H18B H -0.0551 0.2869 0.4765 0.047 Uiso 1 1 calc R . .
C19 C -0.0644(2) 0.4083(3) 0.3838(2) 0.0353(7) Uani 1 1 d . . .
H19A H -0.1002 0.3652 0.3372 0.042 Uiso 1 1 calc R . .
C20 C -0.0451(2) 0.5252(2) 0.3523(2) 0.0291(6) Uani 1 1 d . . .
C21 C 0.0375(2) 0.5836(2) 0.4203(2) 0.0240(6) Uani 1 1 d . . .
H21A H 0.0298 0.5573 0.4891 0.029 Uiso 1 1 calc R . .
C22 C 0.2108(2) 0.5213(2) 0.1960(2) 0.0265(6) Uani 1 1 d . . .
C23 C 0.3921(2) 0.5018(3) 0.1419(2) 0.0326(6) Uani 1 1 d . . .
H23A H 0.4586 0.4673 0.1617 0.049 Uiso 1 1 calc R . .
H23B H 0.4028 0.5789 0.1382 0.049 Uiso 1 1 calc R . .

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C3 0.0308(15) 0.0327(15) 0.0486(18) 0.0023(14) 0.0057(13) 0.0073(13)
N4 0.0253(12) 0.0253(11) 0.0342(14) 0.0009(10) 0.0032(10) 0.0039(9)
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C7 0.0215(13) 0.0252(13) 0.0234(15) -0.0040(11) -0.0003(10) -0.0014(10)
C8 0.0196(12) 0.0327(14) 0.0199(13) 0.0008(11) 0.0041(11) 0.0011(10)
C9 0.0257(13) 0.0307(14) 0.0295(15) -0.0003(12) -0.0016(12) -0.0008(11)
C10 0.0249(14) 0.0477(17) 0.0269(16) -0.0006(13) -0.0042(12) 0.0020(12)
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C15 0.0222(13) 0.0470(18) 0.0351(17) -0.0045(14) -0.0022(12) 0.0037(12)
C16 0.0191(13) 0.0317(14) 0.0250(14) -0.0036(11) -0.0018(10) 0.0002(10)
C17 0.0224(13) 0.0387(16) 0.0240(15) -0.0068(12) -0.0043(11) 0.0004(11)
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C19 0.0240(14) 0.0396(17) 0.0424(19) -0.0119(14) 0.0054(13) -0.0092(12)
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N1 C2 1.342(4) . ?
N1 C13 1.414(4) . ?
N1 H1A 0.8600 . ?
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C3 N4 1.481(4) . ?
C3 C14 1.516(5) . ?
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N4 C21 1.475(3) . ?
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C6 H6B 0.9700 . ?
C7 C8 1.516(4) . ?
C7 C21 1.583(4) . ?
C7 C16 1.583(4) . ?
C8 C13 1.372(4) . ?
C8 C9 1.407(4) . ?
C9 C10 1.382(4) . ?
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C10 C11 1.393(5) . ?
C10 H10A 0.9300 . ?
C11 C12 1.362(5) . ?
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C15 H15A 0.9800 . ?
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N4 C3 C14 113.9(2) . . ?
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N4 C3 H3B 108.8 . . ?
C14 C3 H3B 108.8 . . ?
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C21 N4 C3 114.9(2) . . ?
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H6A C6 H6B 108.7 . . ?
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C17 C16 C2 109.0(2) . . ?
C22 C16 C2 103.5(2) . . ?
C17 C16 C7 104.7(2) . . ?
C22 C16 C7 111.2(2) . . ?
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C16 C17 C20 102.9(2) . . ?
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C19 C18 H18B 120.0 . . ?
H18A C18 H18B 120.0 . . ?
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O2 C23 H23B 109.5 . . ?
H23A C23 H23B 109.5 . . ?

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C2 N1 C13 C12 179.1(3) . . . . ?
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C18 C19 C20 C15 -111.1(3) . . . . ?
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C16 C17 C20 C15 166.2(2) . . . . ?
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O4 C15 C20 C17 171.0(2) . . . . ?
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O4 C15 C20 C21 -73.0(3) . . . . ?
C14 C15 C20 C21 47.1(3) . . . . ?
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C3 N4 C21 C20 38.7(3) . . . . ?
C5 N4 C21 C7 23.8(3) . . . . ?
C3 N4 C21 C7 155.7(2) . . . . ?
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C6 C7 C21 C20 124.6(2) . . . . ?
C16 C7 C21 C20 8.3(3) . . . . ?
C23 O2 C22 O3 -1.1(4) . . . . ?
C23 O2 C22 C16 179.8(2) . . . . ?
C17 C16 C22 O3 9.6(4) . . . . ?
C2 C16 C22 O3 126.9(3) . . . . ?
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HPLC analysis graphics of 1 ~ 8.

Detecting conditions:

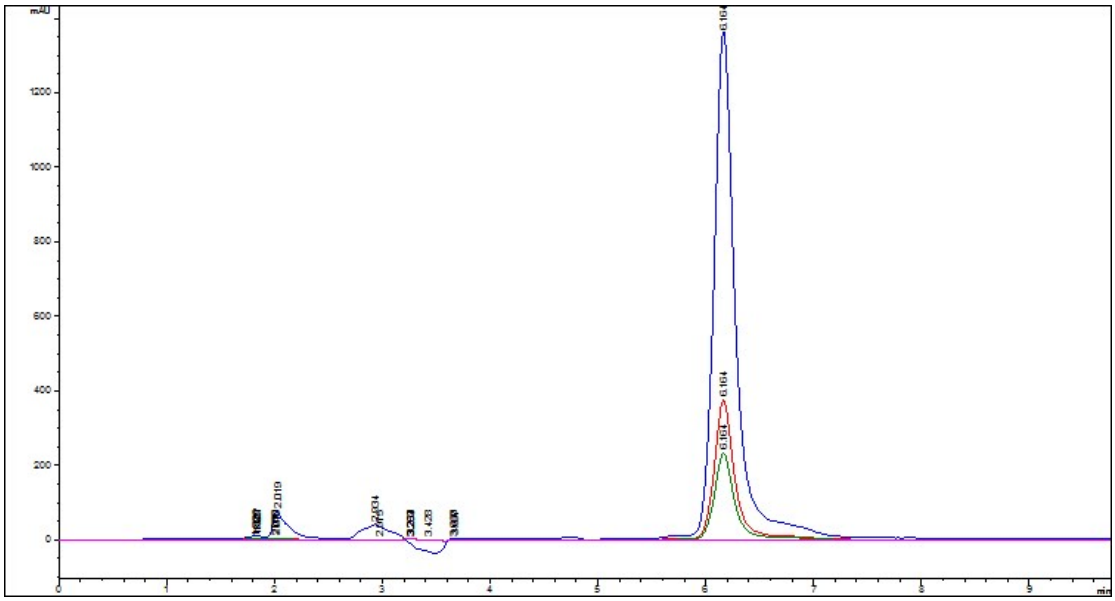
Column: Waters Xbridge^{TM} C18 reversed-phase column (4.6 × 250 mm, 5μm, USA).

UV wavelength: 210, 254, 280, 365 nm

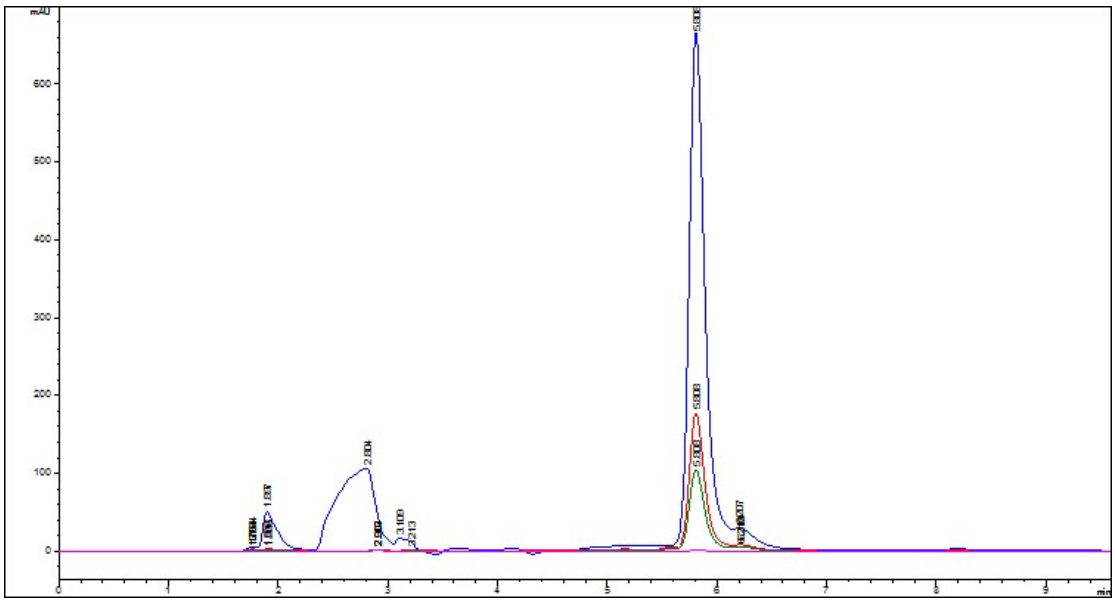
Mobile phase: acetonitrile-water

Temperature: 30 ℃

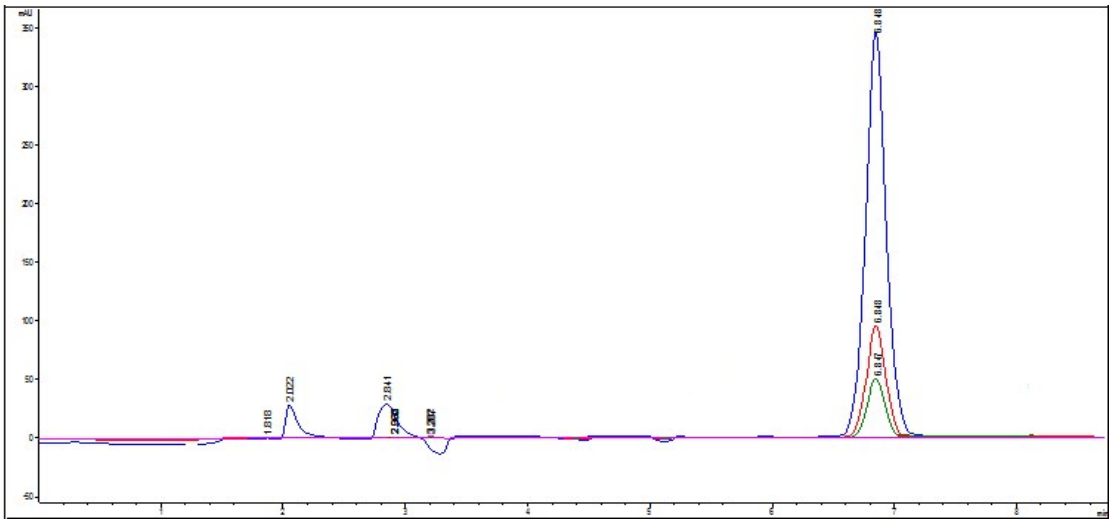
The retention time between 2~3.5 minutes of peaks are the solvent peaks.



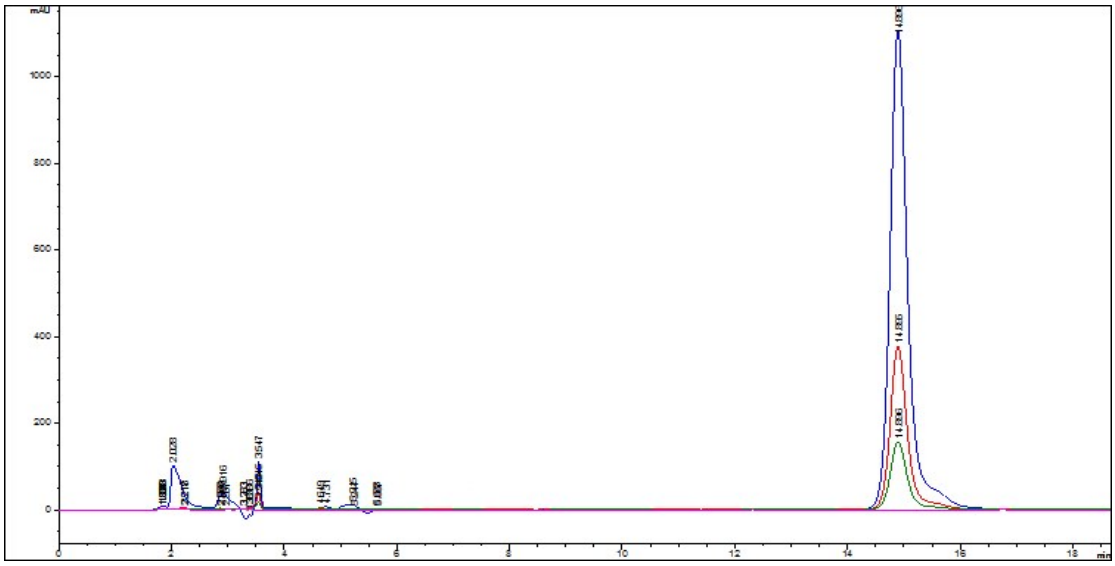
HPLC analysis graphics of **1**



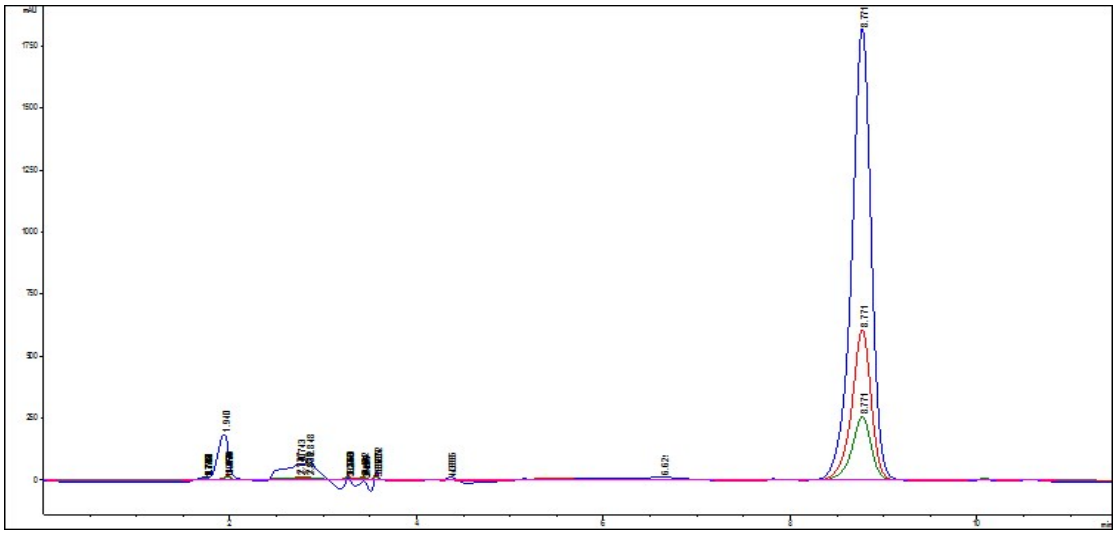
HPLC analysis graphics of **2**



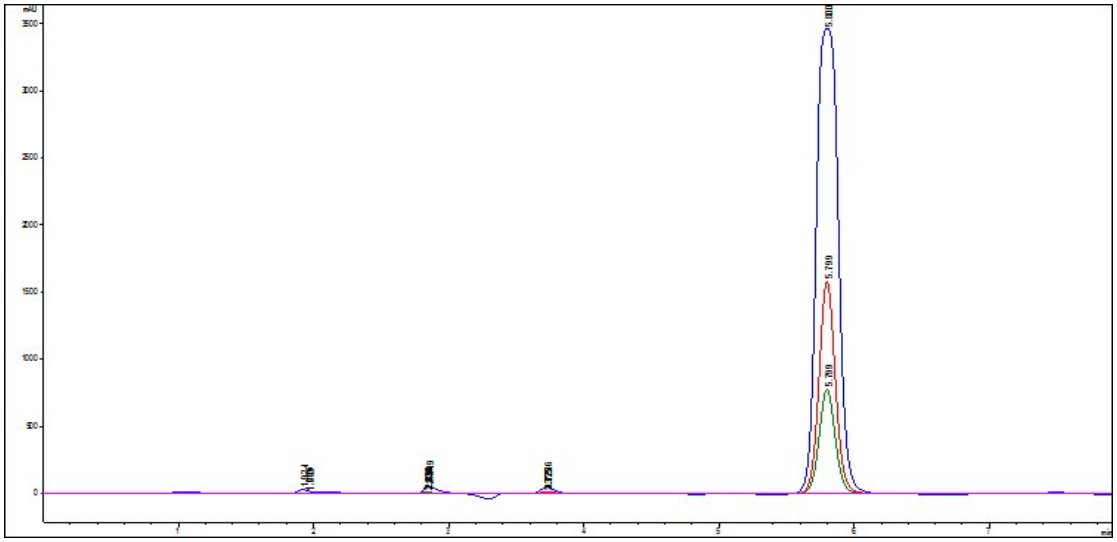
HPLC analysis graphics of **3**



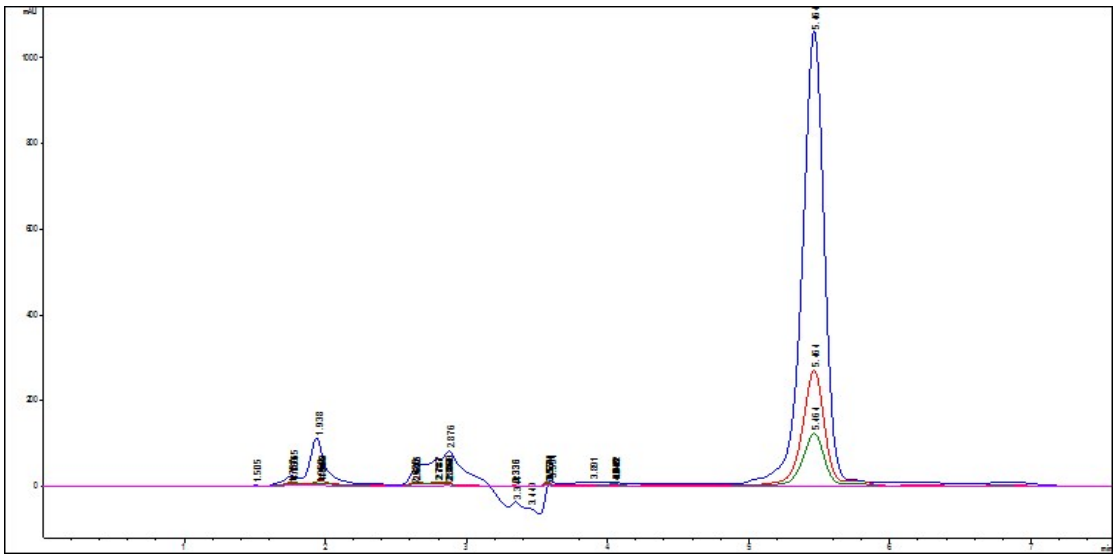
HPLC analysis graphics of **4**



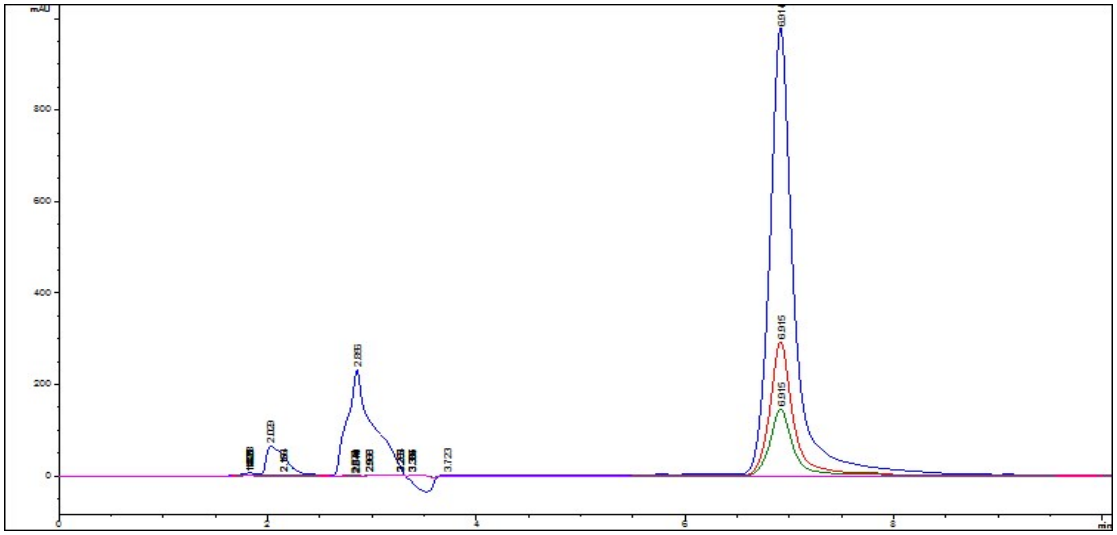
HPLC analysis graphics of **5**



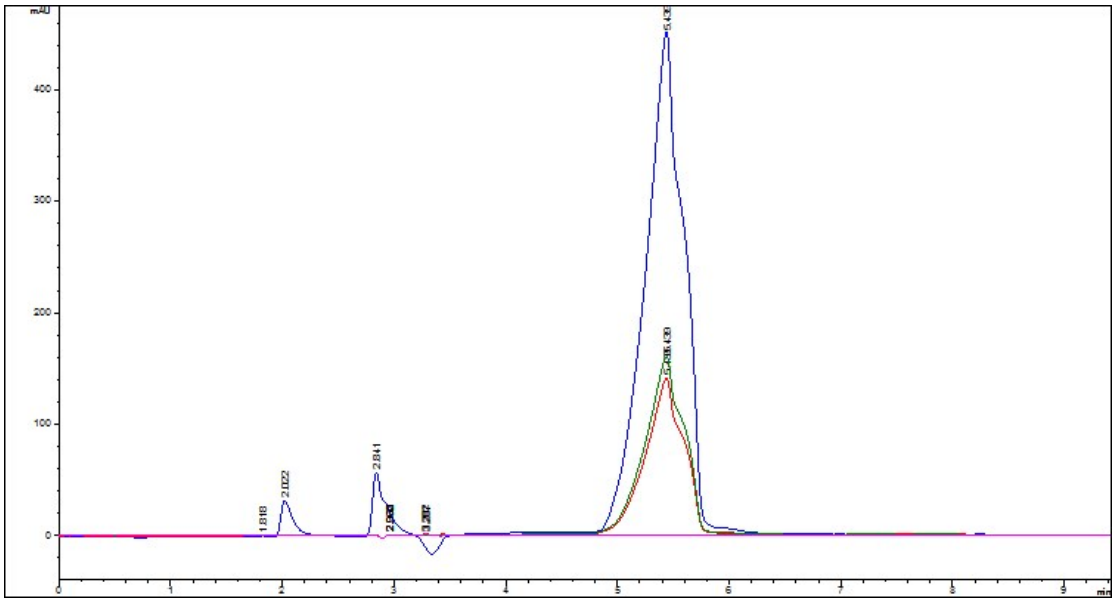
HPLC analysis graphics of **6**



HPLC analysis graphics of **7**



HPLC analysis graphics of **8**



HPLC analysis graphics of **8**

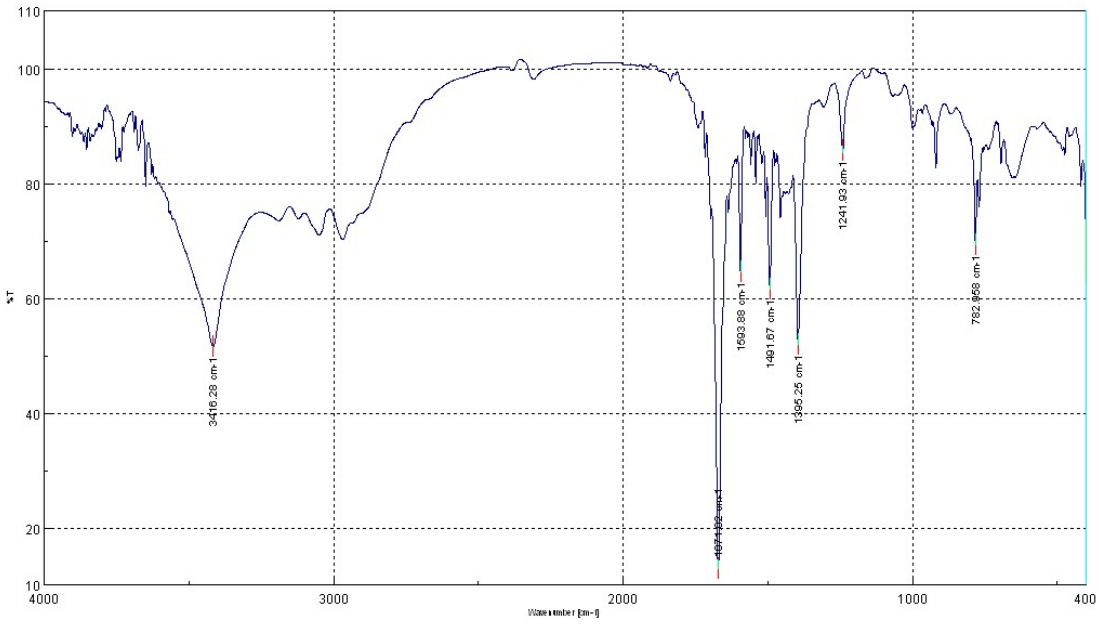
(Because of the compound properties caused the peak pattern bad, but the compound of **8** is very pure)

IR data and graphics of 15 ~ 17

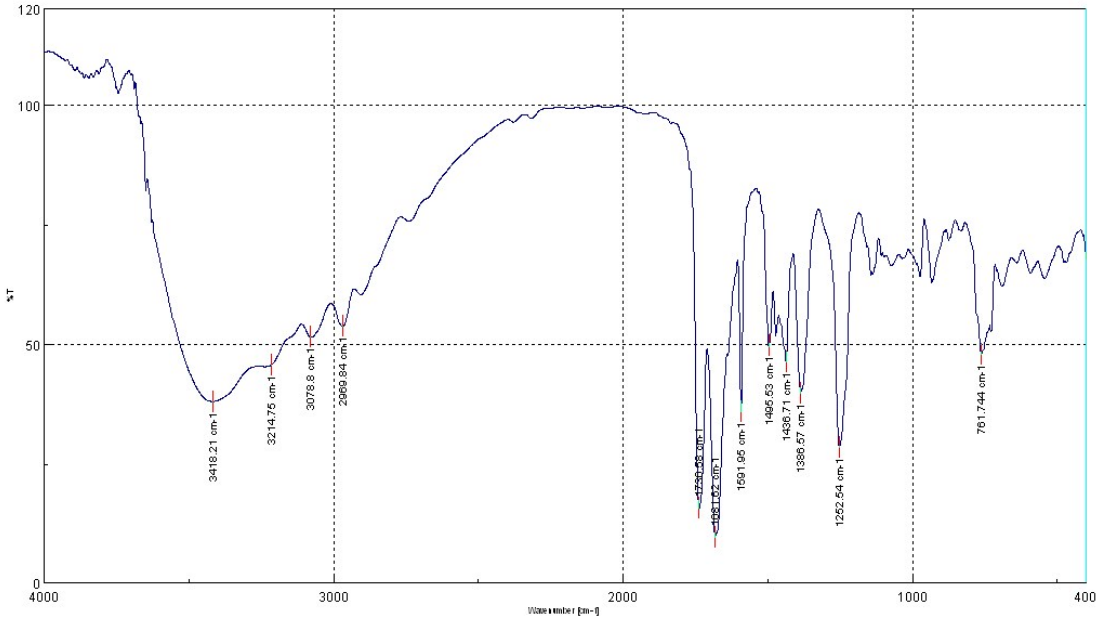
meloscine N_4-oxide (**15**): IR (KBr): 3416, 2969, 1671, 1593, 1491, 1395, 1241, 782 cm^{-1}.

scandine N_4-oxide (**16**) : IR (KBr): 3418, 2969, 1730, 1681, 1591, 1495, 1386, 1252, 761 cm^{-1}.

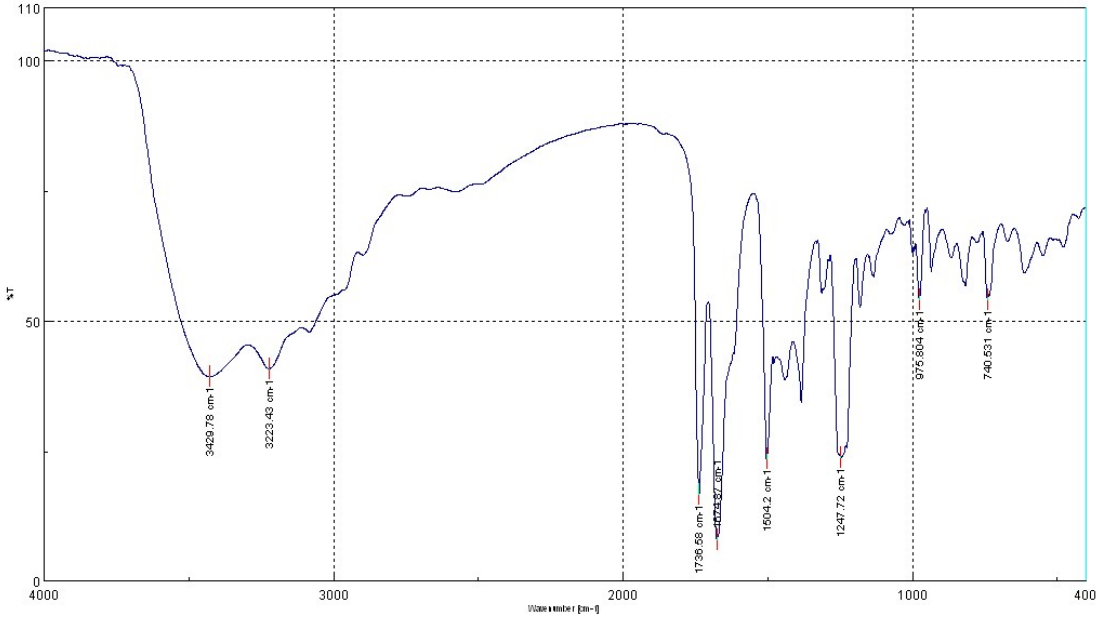
melodinine U (**17**) : IR (KBr): 3429, 3223, 1736, 1674, 1504, 1247, 975, 740 cm^{-1}.



IR graphic of **15**



IR graphic of **16**



IR graphic of **17**

Computational data of 1 and 2. The systematic random conformational analysis of two pairs of enantiomers (7*S*,14*R*,15*R*,16*R*,19*S*,20*S*,21*S*-**1**, 7*R*,14*S*,15*S*,16*S*,19*R*,20*R*,21*R*-**1**, 7*S*,16*R*,20*R*,21*S*-**2**, 7*R*,16*S*,20*S*,21*R*-**2**)were performed in the SYBYL 8.1 program by using MMFF94s molecular force field, which afforded 9 and 13 conformers for **1** and **2** respectively, with an energy cutoff of 10 kcal mol^{-1} to the global minima. All of the obtained conformers were further optimized using DFT at the B3LYP/6-31+G(d) level in gas phase by using Gaussian09 software.[1] All of the optimized stable conformers were used for TDDFT computation of the excited stats at the same levels, with the consideration of the first 50 excitations. The overall ECD curves of **2** were weighted by Boltzmann distribution of each conformer (with a half-bandwidth of 0.3 eV). The calculated ECD spectra of **1** and **2** were subsequently compared with the experimental ones. The ECD spectra were produced by SpecDis 1.6 software.[2]

Coordinates of computations (method: B3LYP/6-31G (d))

Cartesian coordinate of 7*S*,14*R*,15*R*,16*R*,19*S*,20*S*,21*S*-1 optimized:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.552489	3.334798	-0.810513
2	6	0	3.298117	3.233987	0.364769
3	6	0	3.094683	2.151414	1.218921
4	6	0	2.148484	1.171549	0.896471
5	6	0	1.402888	1.238134	-0.295252
6	6	0	1.617972	2.344407	-1.126131
7	7	0	1.922039	0.119996	1.799679
8	6	0	1.248329	-1.042923	1.549436
9	6	0	0.618108	-1.196040	0.148880
10	6	0	0.326398	0.191206	-0.550276
11	6	0	-0.785438	-1.825285	0.296458
12	6	0	-1.699358	-0.646570	0.622816
13	6	0	-1.036272	0.636336	0.089270
14	6	0	-3.212056	-0.742930	0.508132
15	6	0	-4.015669	0.362112	-0.183922
16	6	0	-3.149525	1.567092	-0.656825
17	7	0	-1.764269	1.268919	-1.010383

18	8	0	1.168784	-1.926678	2.395273
19	1	0	-0.884941	1.376272	0.882930
20	6	0	-0.050471	0.016474	-2.064317
21	6	0	-1.529983	0.434267	-2.190189
22	6	0	-2.556689	-0.608653	1.871311
23	8	0	-4.779219	-0.188100	-1.273798
24	6	0	-2.713530	0.602495	2.770589
25	6	0	1.556454	-2.091366	-0.673184
26	8	0	1.197497	-2.992255	-1.402600
27	8	0	2.845668	-1.735123	-0.514488
28	6	0	3.816446	-2.508496	-1.248684
29	1	0	2.688496	4.180727	-1.478415
30	1	0	4.032376	3.992963	0.621018
31	1	0	3.665985	2.062607	2.140775
32	1	0	1.026130	2.458780	-2.027575
33	1	0	2.396954	0.144699	2.696151
34	1	0	-1.062034	-2.296399	-0.652722
35	1	0	-0.782926	-2.601867	1.065737
36	1	0	-3.621852	-1.730820	0.296019
37	1	0	-4.790974	0.744708	0.490093
38	1	0	-3.651452	2.023407	-1.517385
39	1	0	-3.122167	2.325699	0.136629
40	1	0	0.589844	0.633386	-2.696301
41	1	0	0.085975	-1.014582	-2.397475
42	1	0	-2.158044	-0.476297	-2.212984
43	1	0	-1.746569	1.002012	-3.102670
44	1	0	-2.542900	-1.543714	2.432202
45	1	0	-4.181824	-0.679819	-1.859180
46	1	0	-3.635662	0.521373	3.359831
47	1	0	-1.875447	0.673837	3.475455
48	1	0	-2.763059	1.547200	2.220533
49	1	0	3.764757	-3.558265	-0.949169
50	1	0	3.631953	-2.425616	-2.322777
51	1	0	4.782885	-2.077495	-0.987446

Cartesian coordinate of 7*R*,14*S*,15*S*,16*S*,19*R*,20*R*,21*R*-1 optimized:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.552489	3.334798	-0.810513
2	6	0	-3.298117	3.233987	0.364769
3	6	0	-3.094683	2.151414	1.218921
4	6	0	-2.148484	1.171549	0.896471
5	6	0	-1.402888	1.238134	-0.295252
6	6	0	-1.617972	2.344407	-1.126131
7	7	0	-1.922039	0.119996	1.799679
8	6	0	-1.248329	-1.042923	1.549436
9	6	0	-0.618108	-1.196040	0.148880
10	6	0	-0.326398	0.191206	-0.550276
11	6	0	0.785438	-1.825285	0.296458
12	6	0	0.699358	-0.646570	0.622816
13	6	0	1.036272	0.636336	0.089270
14	6	0	3.212056	-0.742930	0.508132
15	6	0	4.015669	0.362112	-0.183922
16	6	0	3.149525	1.567092	-0.656825
17	7	0	1.764269	1.268919	-1.010383

18	8	0	-1.168784	-1.926678	2.395273
19	1	0	0.884941	1.376272	0.882930
20	6	0	0.050471	0.016474	-2.064317
21	6	0	1.529983	0.434267	-2.190189
22	6	0	2.556689	-0.608653	1.871311
23	8	0	4.779219	-0.188100	-1.273798
24	6	0	2.713530	0.602495	2.770589
25	6	0	-1.556454	-2.091366	-0.673184
26	8	0	-1.197497	-2.992255	-1.402600
27	8	0	-2.845668	-1.735123	-0.514488
28	6	0	-3.816446	-2.508496	-1.248684
29	1	0	-2.688496	4.180727	-1.478415
30	1	0	-4.032376	3.992963	0.621018
31	1	0	-3.665985	2.062607	2.140775
32	1	0	-1.026130	2.458780	-2.027575
33	1	0	-2.396954	0.144699	2.696151
34	1	0	1.062034	-2.296399	-0.652722
35	1	0	0.782926	-2.601867	1.065737
36	1	0	3.621852	-1.730820	0.296019
37	1	0	4.790974	0.744708	0.490093
38	1	0	3.651452	2.023407	-1.517385
39	1	0	3.122167	2.325699	0.136629
40	1	0	-0.589844	0.633386	-2.696301
41	1	0	-0.085975	-1.014582	-2.397475
42	1	0	2.158044	-0.476297	-2.212984
43	1	0	1.746569	1.002012	-3.102670
44	1	0	2.542900	-1.543714	2.432202
45	1	0	4.181824	-0.679819	-1.859180
46	1	0	3.635662	0.521373	3.359831
47	1	0	1.875447	0.673837	3.475455
48	1	0	2.763059	1.547200	2.220533
49	1	0	-3.764757	-3.558265	-0.949169
50	1	0	-3.631953	-2.425616	-2.322777
51	1	0	-4.782885	-2.077495	-0.987446

Cartesian coordinate of 7*S*,16*R*,20*R*,21*S*-2 optimized:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.855369	2.794120	1.037028
2	6	0	-3.736755	2.467254	0.005498
3	6	0	-3.403477	1.451416	-0.888444
4	6	0	-2.193729	0.762476	-0.747970
5	6	0	-1.303716	1.052831	0.301258
6	6	0	-1.656047	2.089705	1.173573
7	7	0	-1.855504	-0.213679	-1.701824
8	6	0	-0.835028	-1.115134	-1.628691
9	6	0	0.021087	-1.085047	-0.340436
10	6	0	0.031396	0.323668	0.369006
11	6	0	1.500227	-1.307109	-0.718443
12	6	0	1.939411	0.074227	-1.250974
13	6	0	1.152886	1.121917	-0.400956
14	6	0	3.425109	0.322387	-1.274700
15	6	0	4.001287	1.352674	-0.643765

16	6	0	3.201502	2.326671	0.197132
17	7	0	1.922020	1.786700	0.654705
18	8	0	-0.634190	-1.932409	-2.520922
19	1	0	0.728733	1.893450	-1.053746
20	6	0	0.617311	0.201575	1.821127
21	6	0	2.005062	0.861831	1.787656
22	1	0	1.577480	0.148889	-2.288196
23	6	0	-0.615443	-2.168895	0.540432
24	8	0	-1.774427	-2.143601	0.903001
25	8	0	0.239754	-3.158098	0.861848
26	6	0	-0.311881	-4.232454	1.650955
27	1	0	-3.093978	3.593505	1.732982
28	1	0	-4.677545	2.999062	-0.108033
29	1	0	-4.079499	1.188428	-1.699474
30	1	0	-0.972640	2.375984	1.966101
31	1	0	-2.461129	-0.328146	-2.508006
32	1	0	1.607204	-2.106992	-1.454422
33	1	0	2.074533	-1.584507	0.169883
34	1	0	4.030290	-0.366268	-1.864680
35	1	0	5.075244	1.516908	-0.726071
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37	1	0	3.012576	3.249810	-0.373835
38	1	0	-0.034539	0.696865	2.541512
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40	1	0	2.797343	0.102864	1.661269
41	1	0	2.227738	1.418962	2.705999
42	1	0	-1.135007	-4.709072	1.112825
43	1	0	0.511816	-4.931220	1.797924
44	1	0	-0.676191	-3.852284	2.608893

Cartesian coordinate of 7*R*,16*S*,20*S*,21*R*-2 optimized:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.855369	2.794120	1.037028
2	6	0	3.736755	2.467254	0.005498
3	6	0	3.403477	1.451416	-0.888444
4	6	0	2.193729	0.762476	-0.747970
5	6	0	1.303716	1.052831	0.301258
6	6	0	1.656047	2.089705	1.173573
7	7	0	1.855504	-0.213679	-1.701824
8	6	0	0.835028	-1.115134	-1.628691
9	6	0	-0.021087	-1.085047	-0.340436
10	6	0	-0.031396	0.323668	0.369006
11	6	0	-1.500227	-1.307109	-0.718443
12	6	0	-1.939411	0.074227	-1.250974
13	6	0	-1.152886	1.121917	-0.400956
14	6	0	-3.425109	0.322387	-1.274700

15	6	0	-4.001287	1.352674	-0.643765
16	6	0	-3.201502	2.326671	0.197132
17	7	0	-1.922020	1.786700	0.654705
18	8	0	0.634190	-1.932409	-2.520922
19	1	0	-0.728733	1.893450	-1.053746
20	6	0	-0.617311	0.201575	1.821127
21	6	0	-2.005062	0.861831	1.787656
22	1	0	-1.577480	0.148889	-2.288196
23	6	0	0.615443	-2.168895	0.540432
24	8	0	1.774427	-2.143601	0.903001
25	8	0	-0.239754	-3.158098	0.861848
26	6	0	0.311881	-4.232454	1.650955
27	1	0	3.093978	3.593505	1.732982
28	1	0	4.677545	2.999062	-0.108033
29	1	0	4.079499	1.188428	-1.699474
30	1	0	0.972640	2.375984	1.966101
31	1	0	2.461129	-0.328146	-2.508006
32	1	0	-1.607204	-2.106992	-1.454422
33	1	0	-2.074533	-1.584507	0.169883
34	1	0	-4.030290	-0.366268	-1.864680
35	1	0	-5.075244	1.516908	-0.726071
36	1	0	-3.777199	2.631872	1.080043
37	1	0	-3.012576	3.249810	-0.373835
38	1	0	0.034539	0.696865	2.541512
39	1	0	-0.692669	-0.841068	2.141715
40	1	0	-2.797343	0.102864	1.661269
41	1	0	-2.227738	1.418962	2.705999
42	1	0	1.135007	-4.709072	1.112825
43	1	0	-0.511816	-4.931220	1.797924
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[1] Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K.

N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

[2] T. Bruhn, A. Schaumlöffel, Y. Hemberger, G. Bringmann, SpecDis version 1.60, University of Wuerzburg, Germany, 2012.

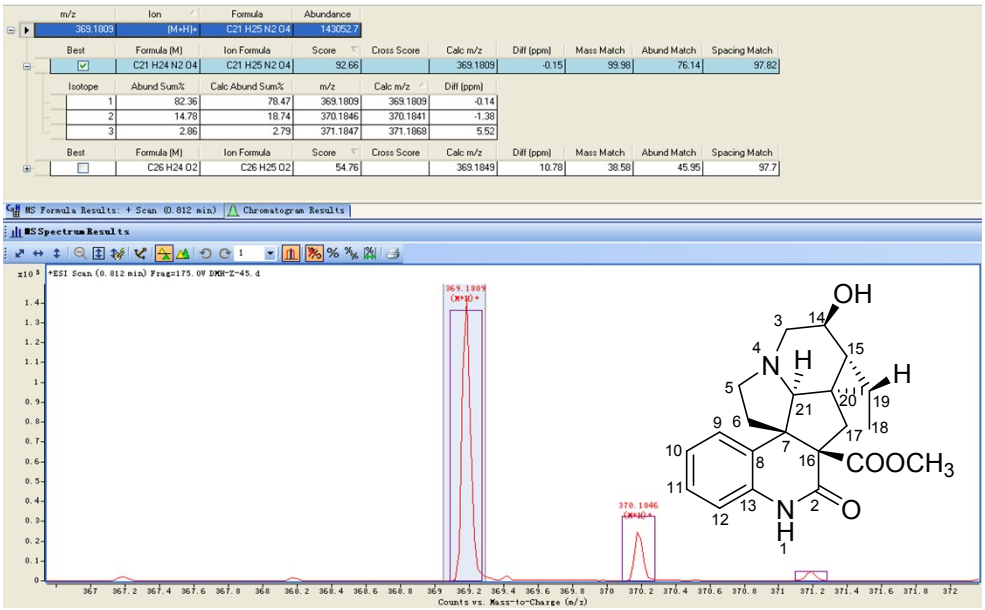
Evaluation of cytotoxicity activities of 1-17

The cytotoxic effects of compounds **1-17** on the viability of three human cancer cell lines were determined by the MTT assay. However, the results showed that all these melodinus-type alkaloids exhibit weak cytotoxicity with IC_{50} values over 50 μM.

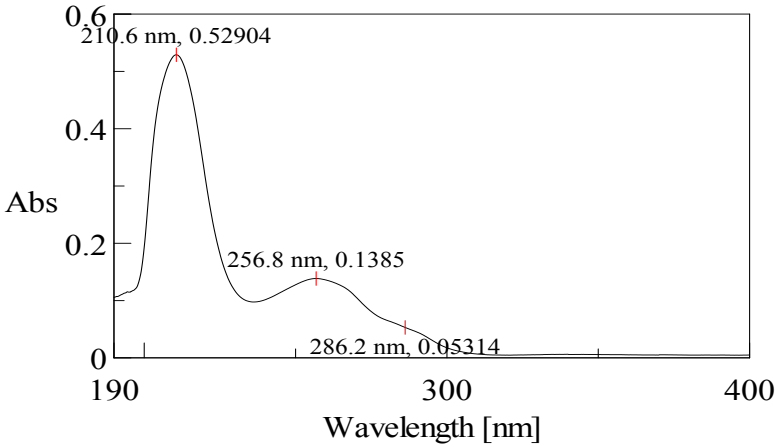
Cytotoxicity assay

Human breast cancer MCF-7, hepatocellular carcinoma HepG2, and lung cancer A-549 cell lines were obtained from the American Type Culture Collection (ATCC). The three cells were cultured in the RPMI 1640 medium containing 100 units/ml penicillin and 100 ug/ml streptomycin with 10% FBS in a humidified atmosphere of 95% air and 5% CO_2 (v/v) at 37℃. The three human cancer cell lines were grown in 96-well culture plates for 48 h. After that, the cells were treated with compounds **1-17** at various concentrations for 72 h. A 30 μL aliquot of MTT solution (5 mg/mL) was added into each well and incubated for another 4 h. Subsequently, the medium was

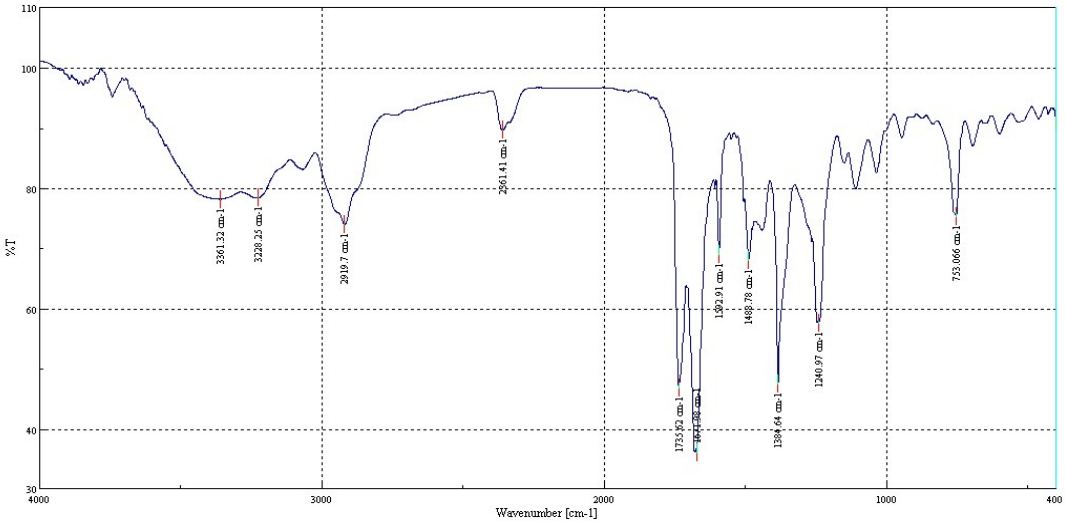
removed and adding 100 μL of DMSO to dissolve the purple formazan, the absorbance was recorded at 570 nm using a microplate Reader (Thermo scientific multiskan MK3, USA). Each well was performed in triplicate in 3 independent experiments. The concentration giving 50% inhibiton (IC_{50}) was determined from the dose-response curves using Prism software and expressed as the mean ± SD.



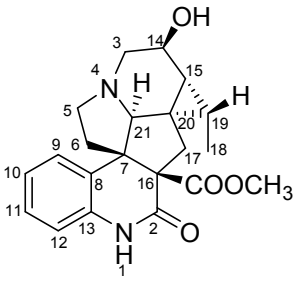
HRESIMS spectrum of **1**

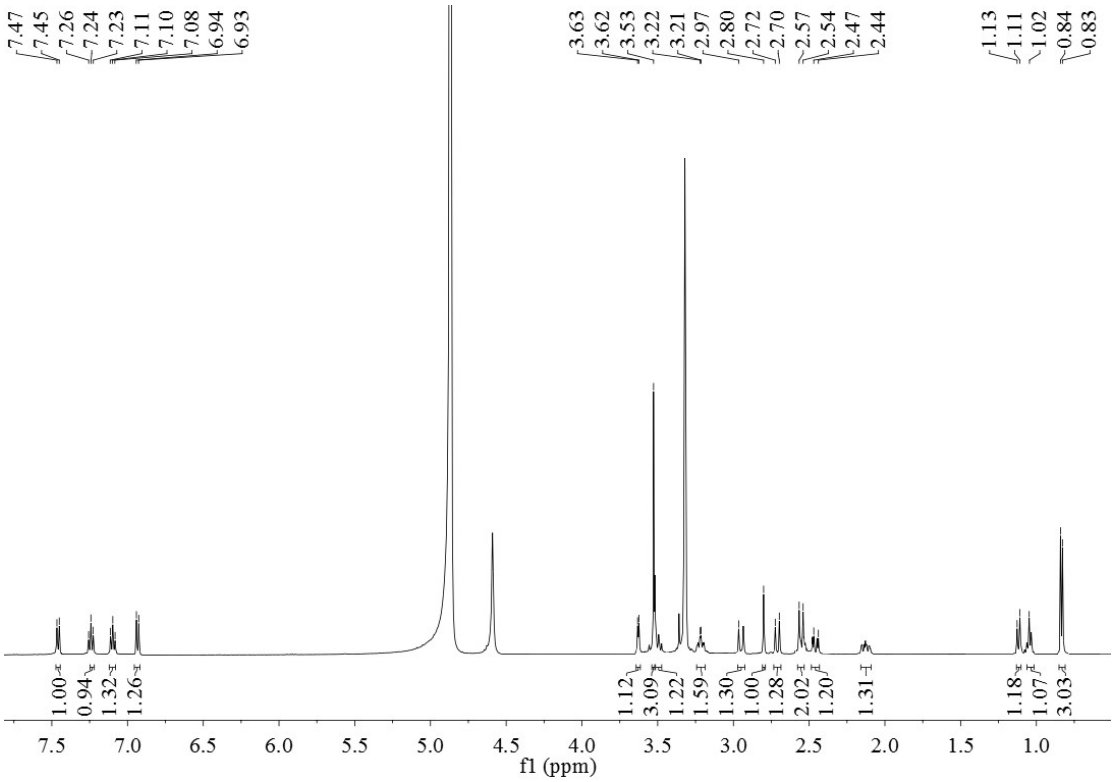


UV spectrum of **1** (MeOH)

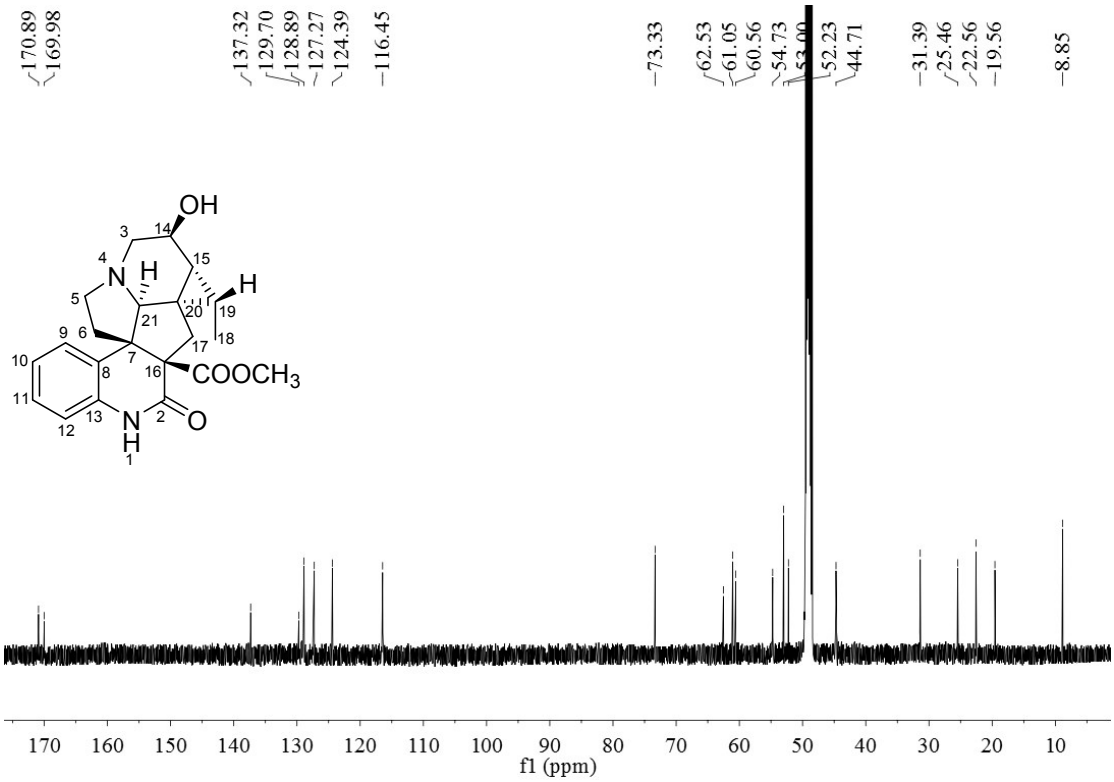


IR spectrum of **1** (KBr disc)

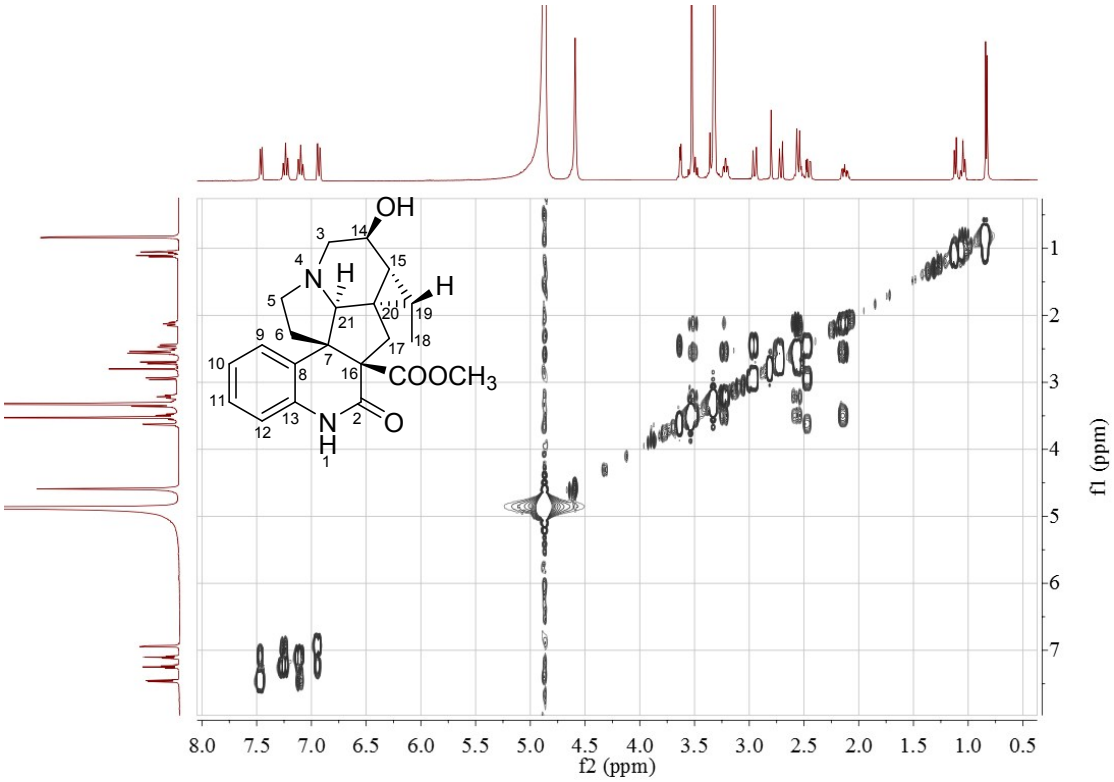




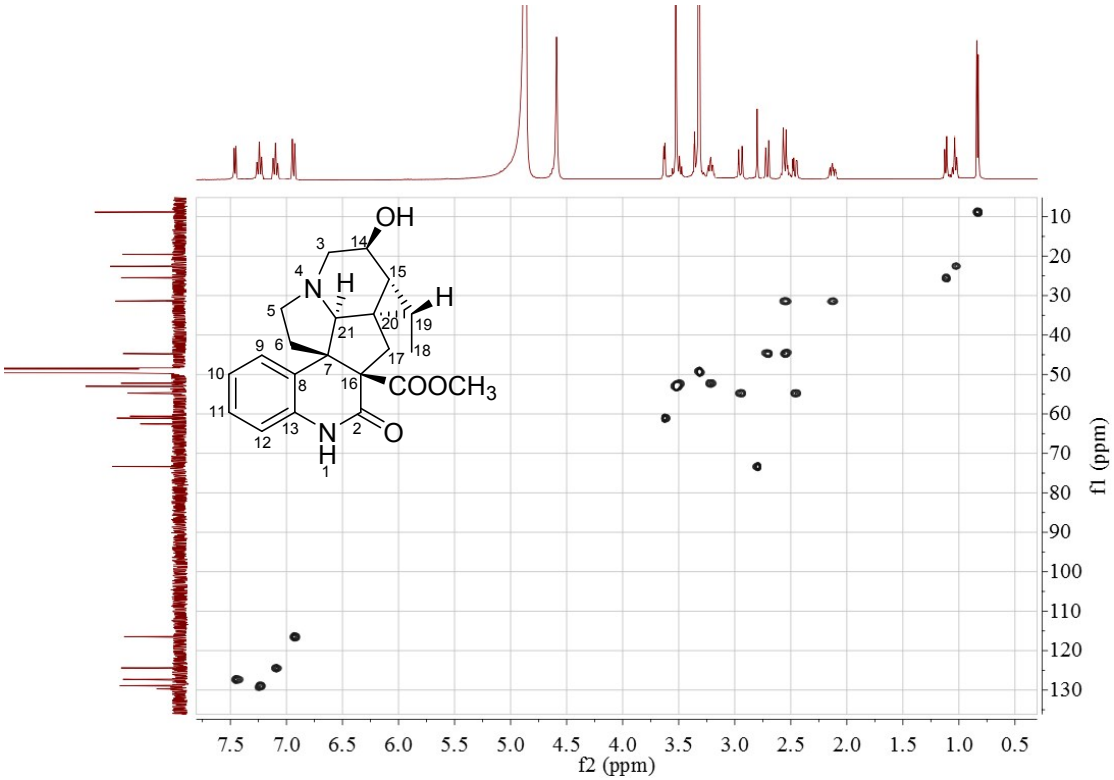
^{1}H NMR spectrum of **1** (500 Hz, CD_3OD)



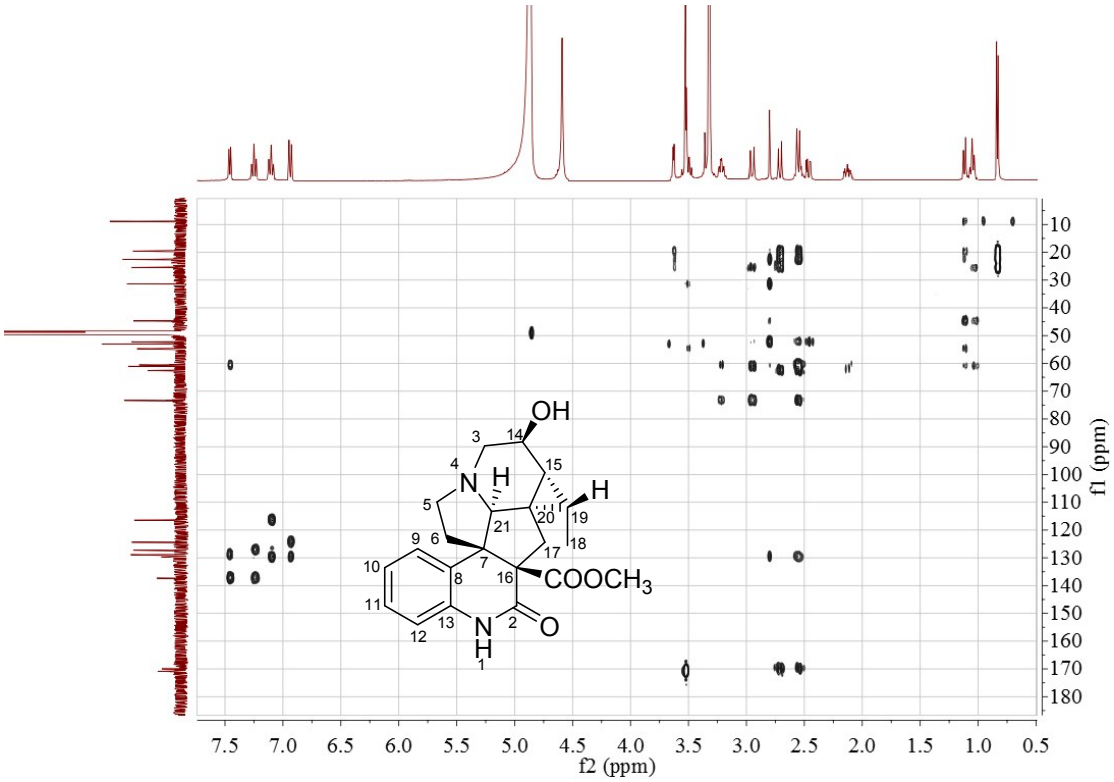
^{13}C NMR spectrum of **1** (125 Hz, CD_3OD)



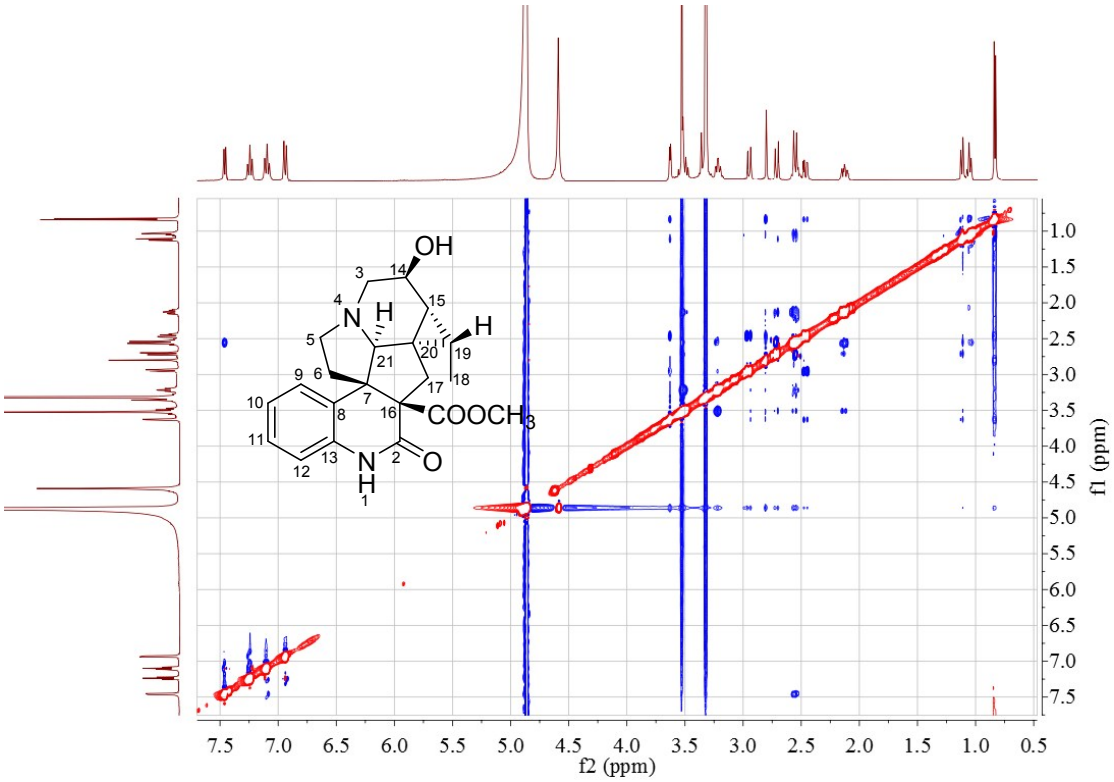
^{1}H-^{1}H COSY spectrum of **1** (CD_3OD)



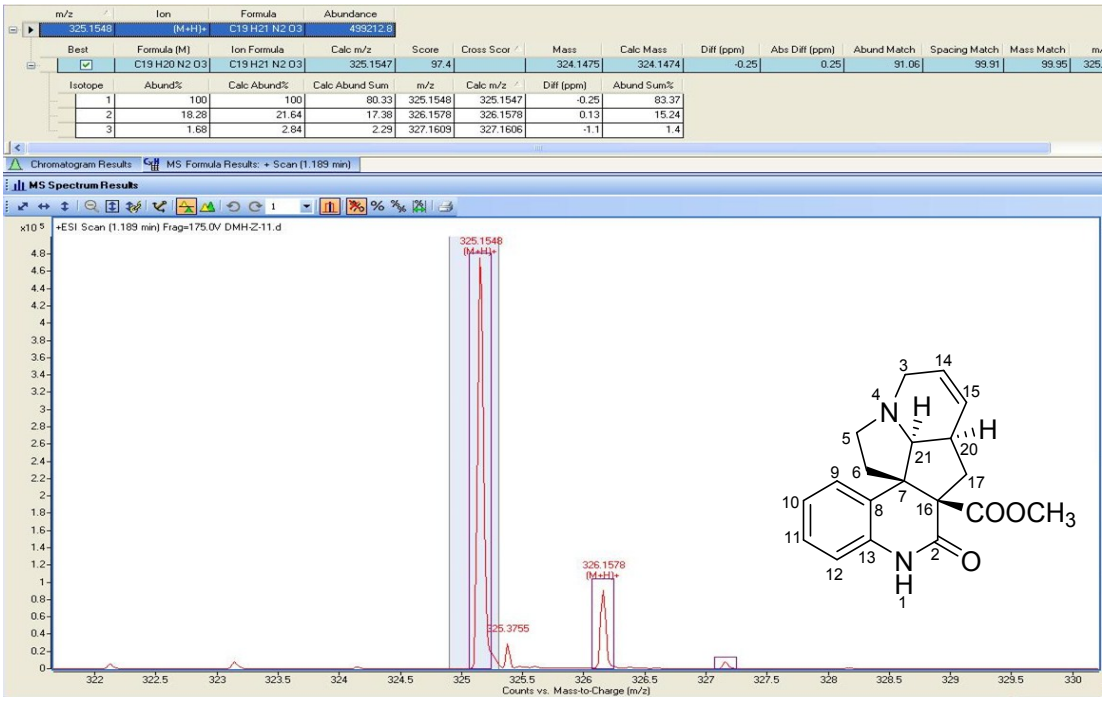
HSQC spectrum of **1** (CD_3OD)



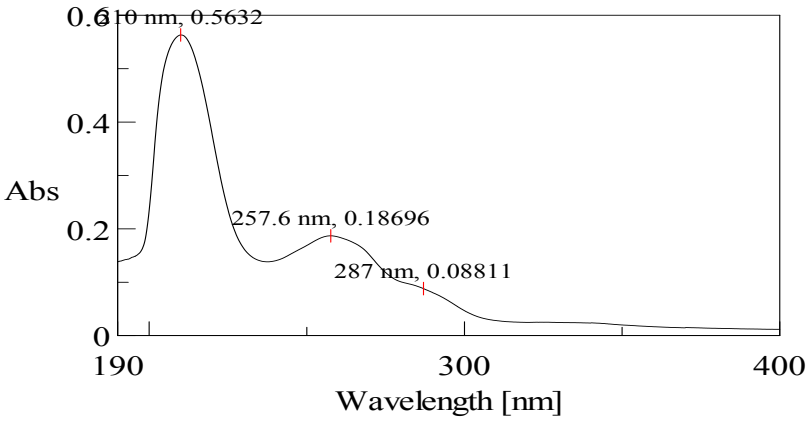
HMBC spectrum of **1** (CD_3OD)



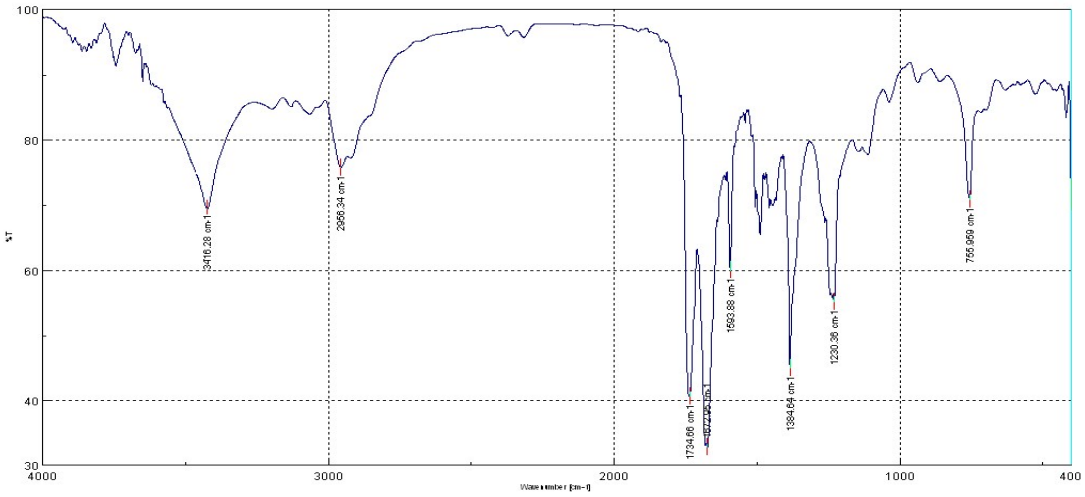
NOESY spectrum of **1** (CD_3OD)



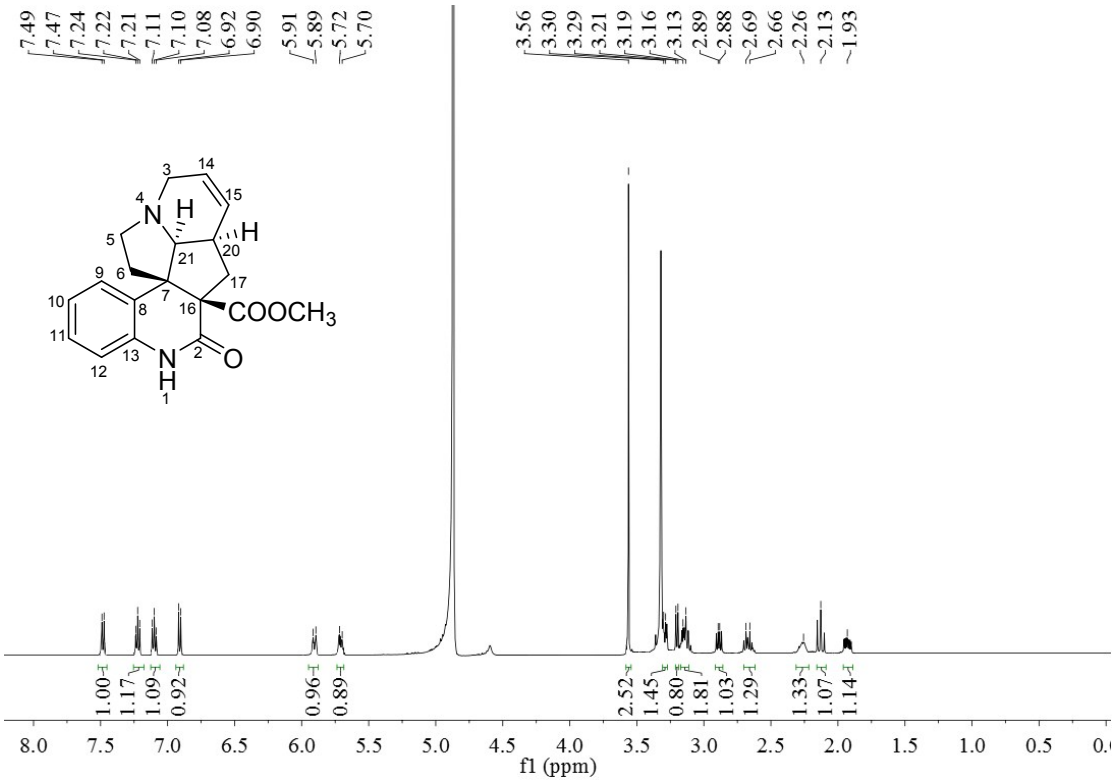
HRESIMS spectrum of **2**



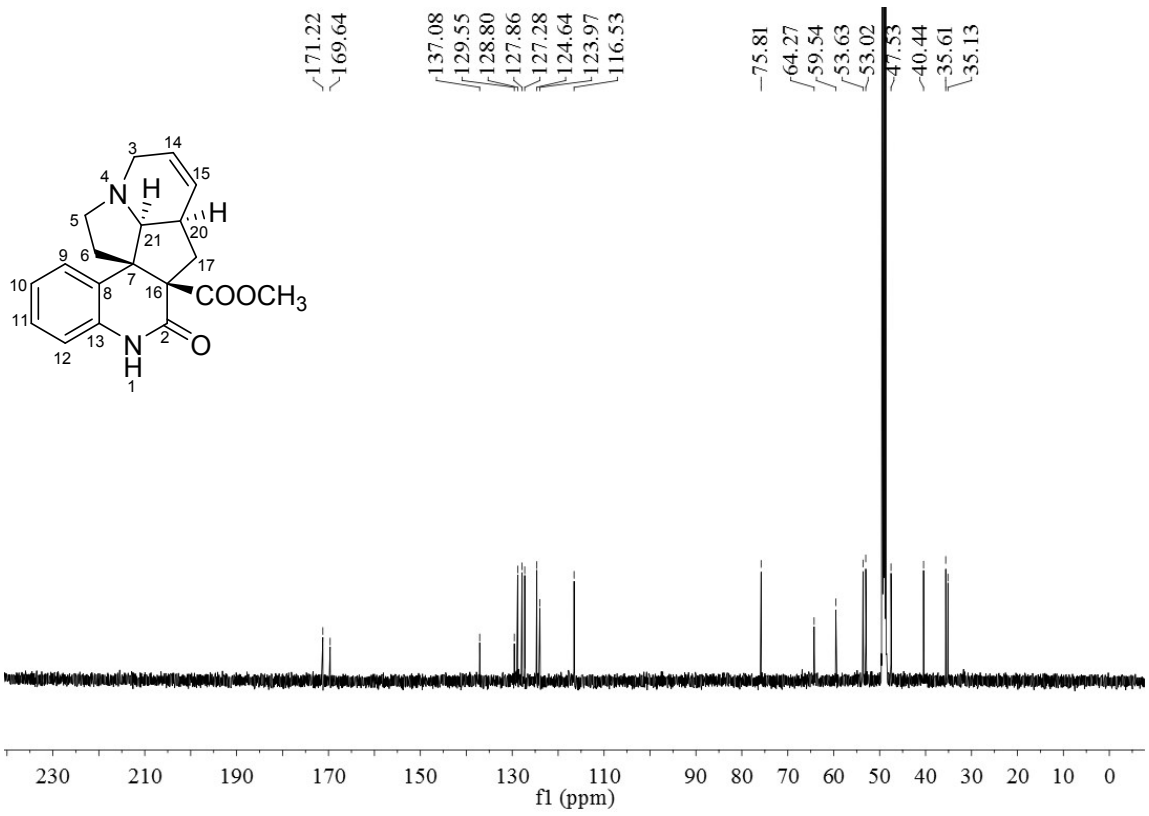
UV spectrum of **2** (MeOH)



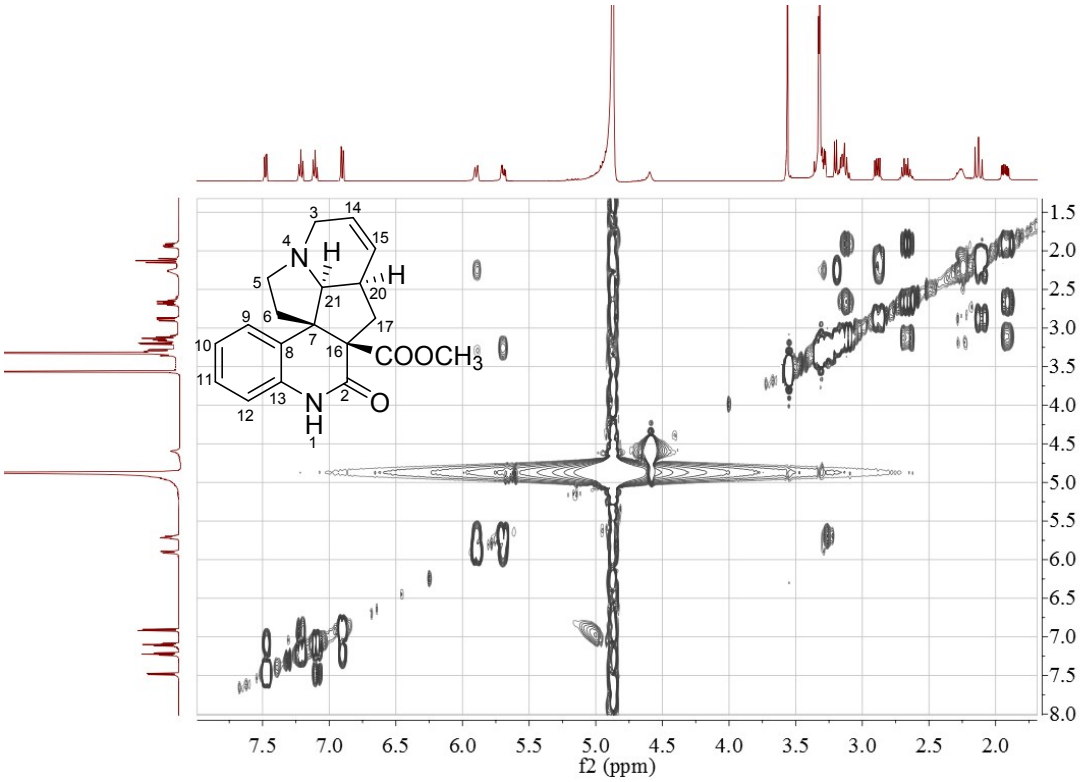
IR spectrum of **2** (KBr disc)



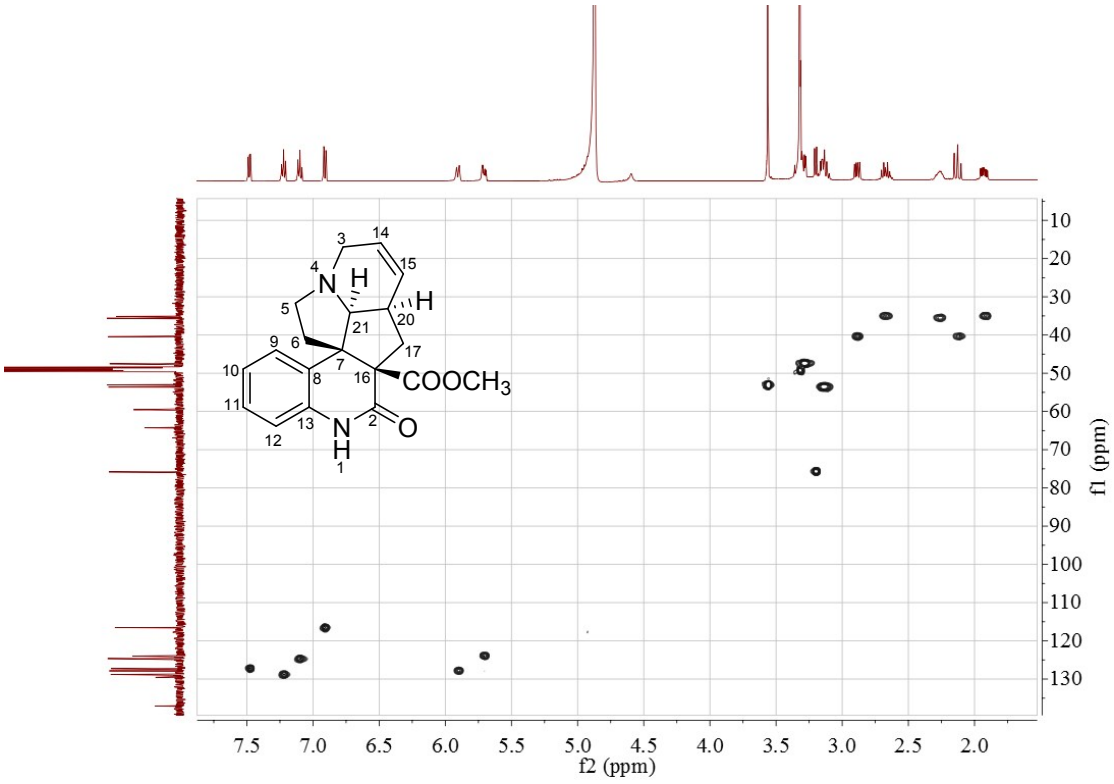
^{1}H NMR spectrum of **2** (500 Hz, CD_3OD)



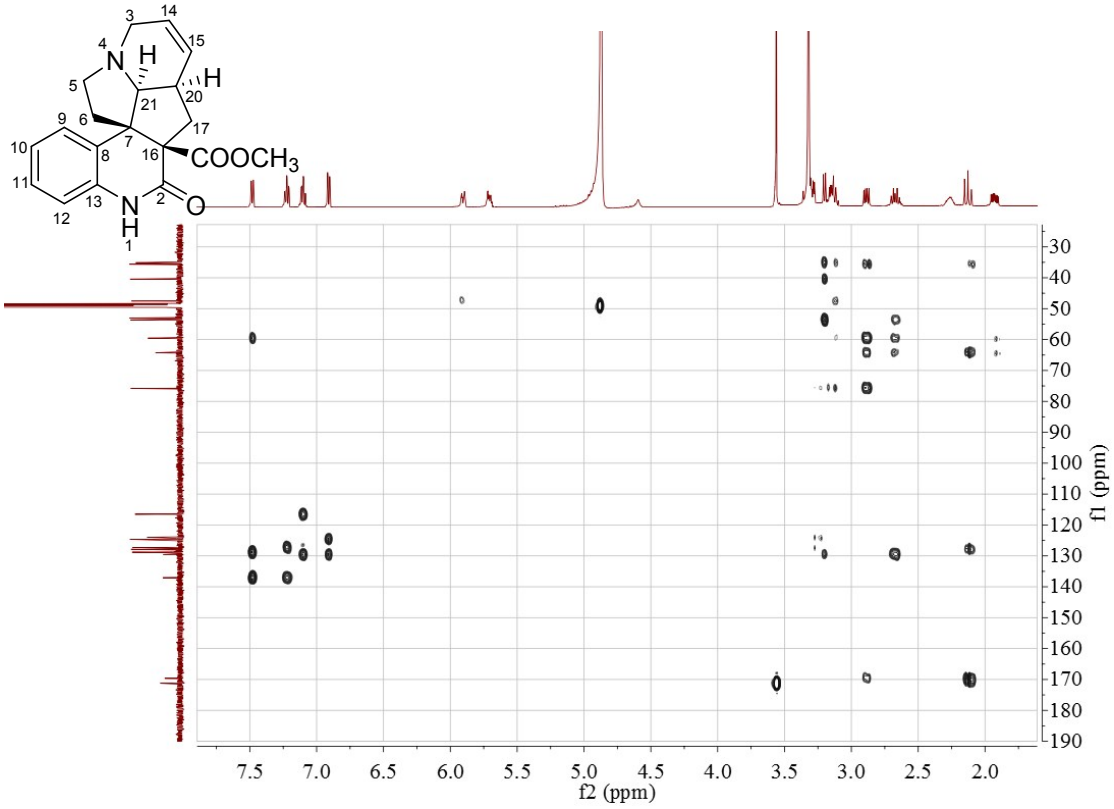
^{13}C NMR spectrum of **2** (125 Hz, CD_3OD)



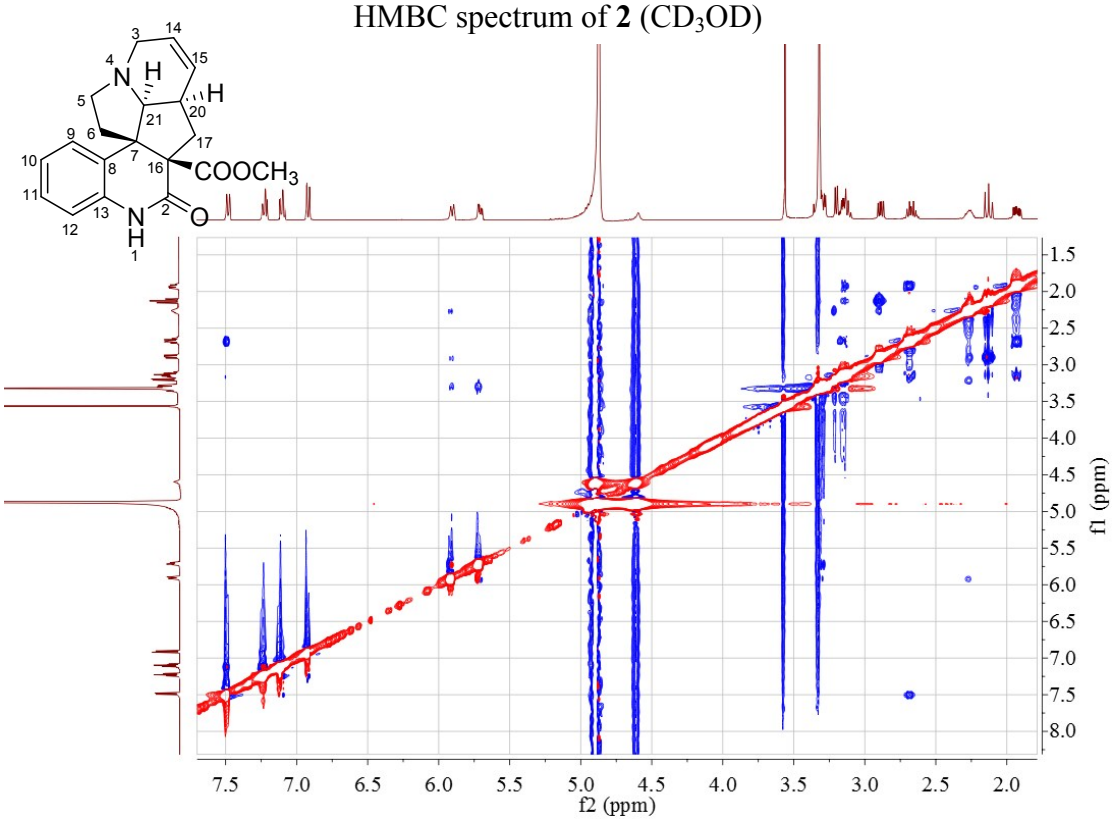
^{1}H-^{1}H COSY spectrum of **2** (CD_3OD)



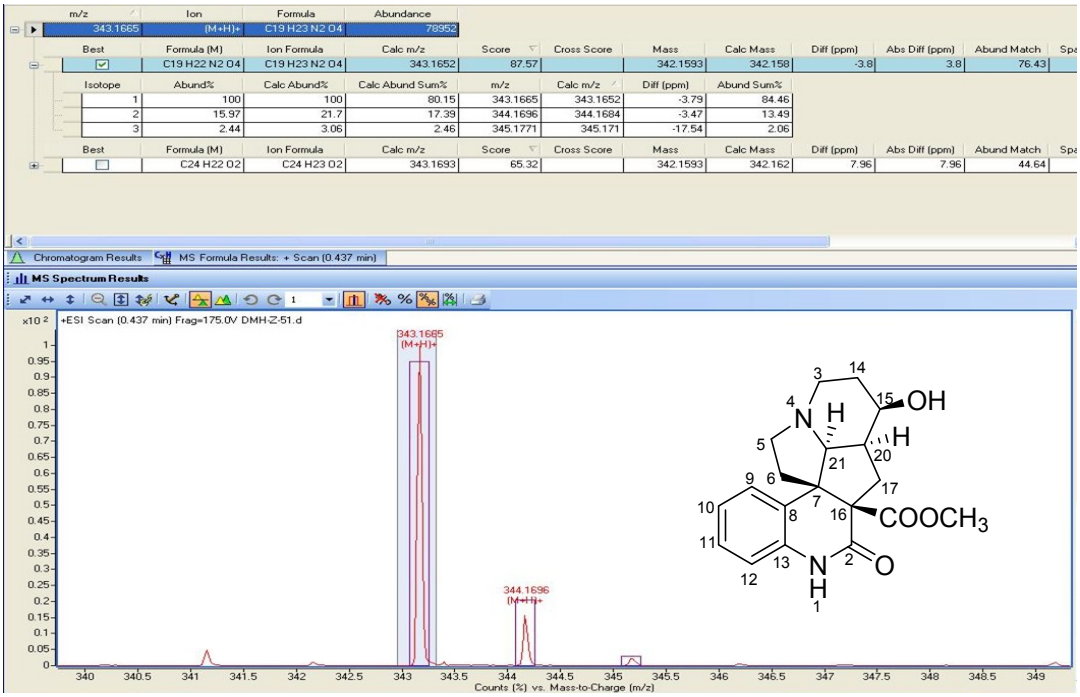
HSQC spectrum of **2** (CD_3OD)



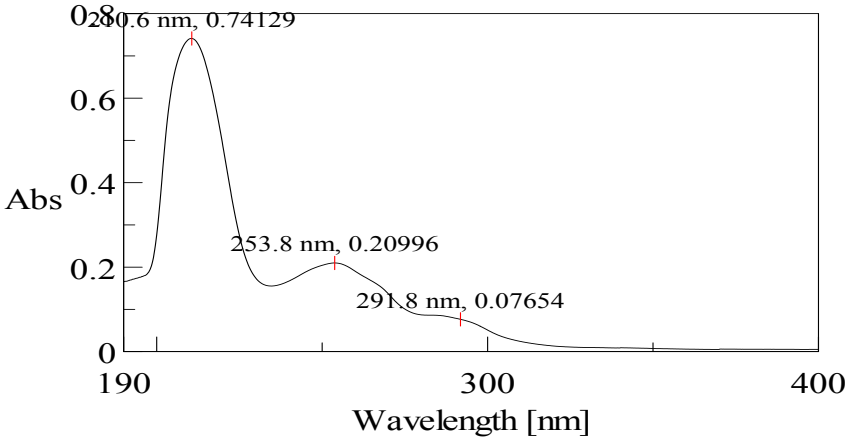
HMBC spectrum of **2** (CD_3OD)



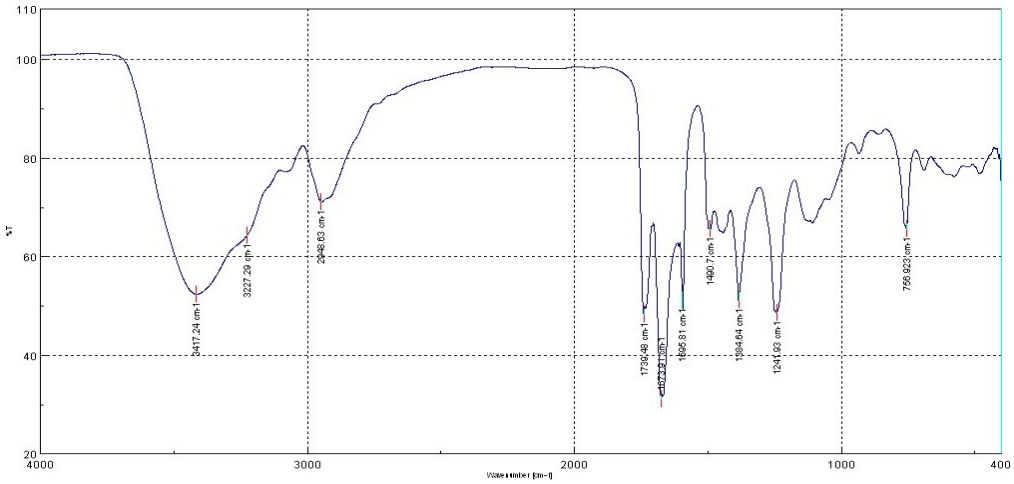
NOESY spectrum of **2** (CD_3OD)



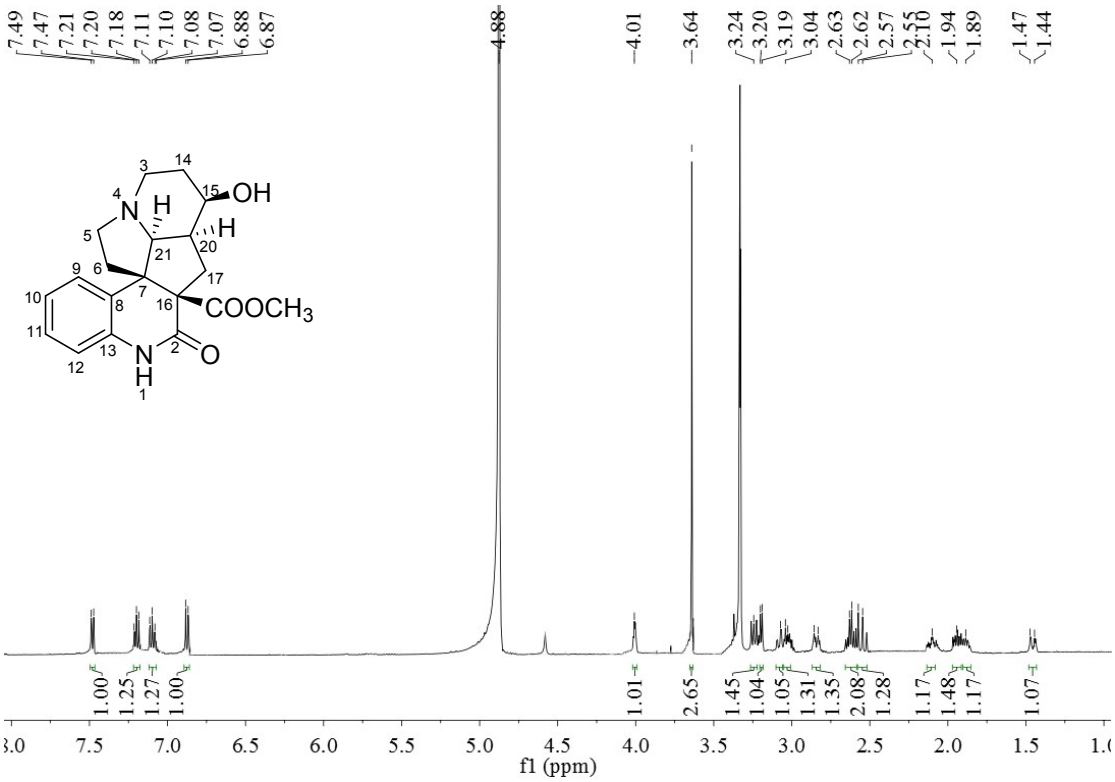
HRESIMS spectrum of **3**



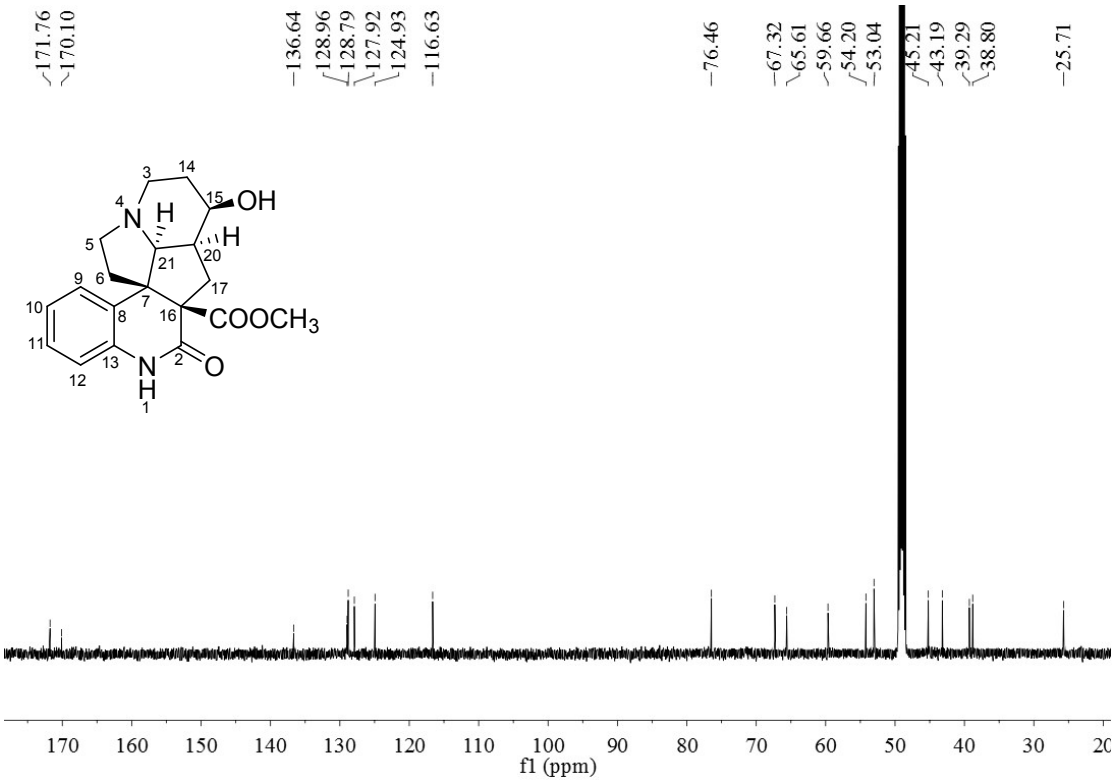
UV spectrum of **3** (MeOH)



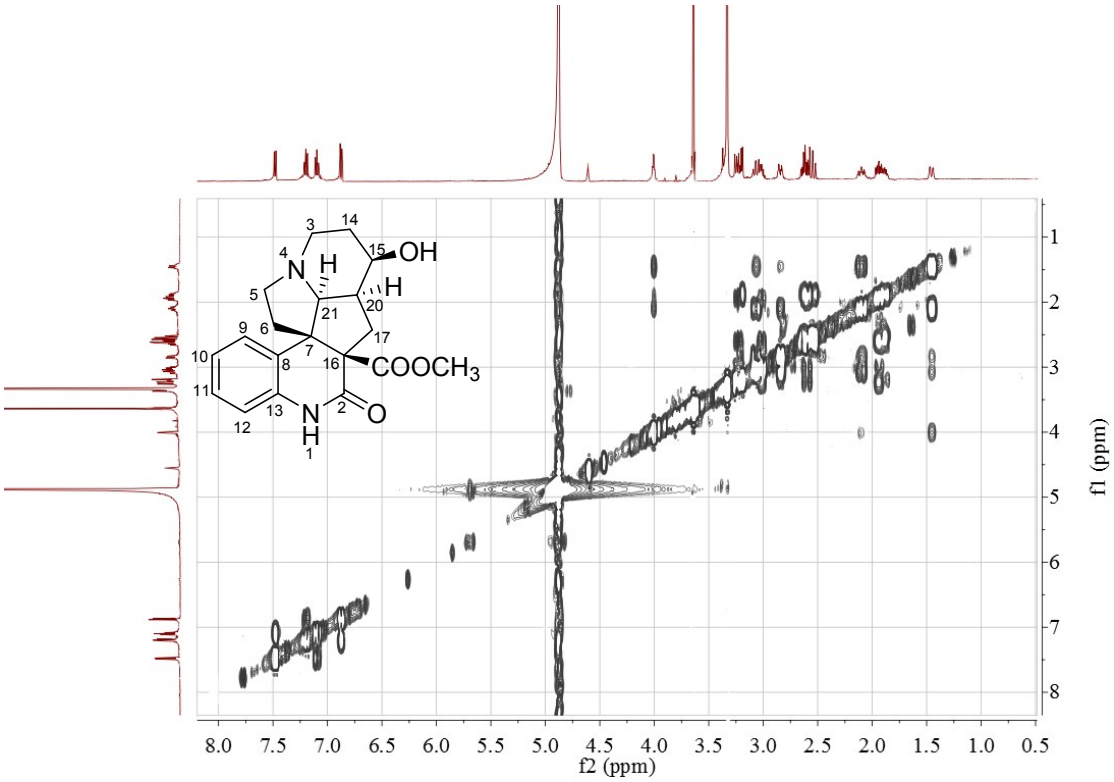
IR spectrum of **3** (KBr disc)



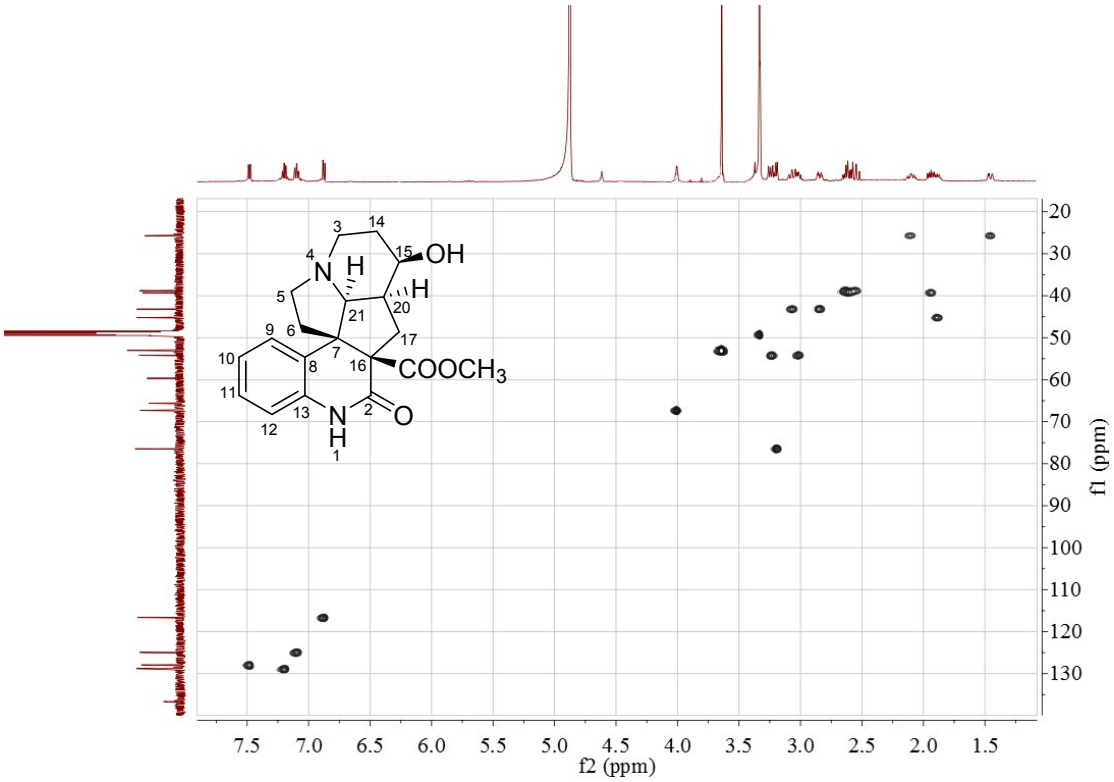
^{1}H NMR spectrum of **3** (500 Hz, CD_3OD)



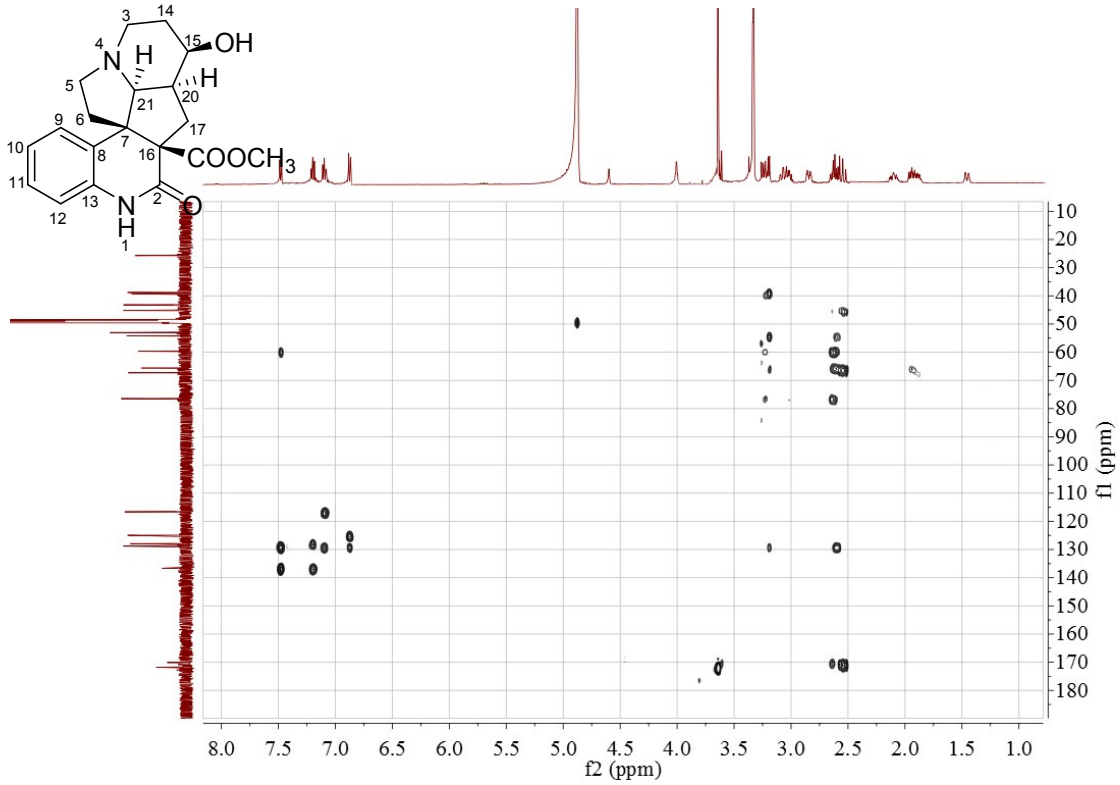
^{13}C NMR spectrum of **3** (125 Hz, CD_3OD)



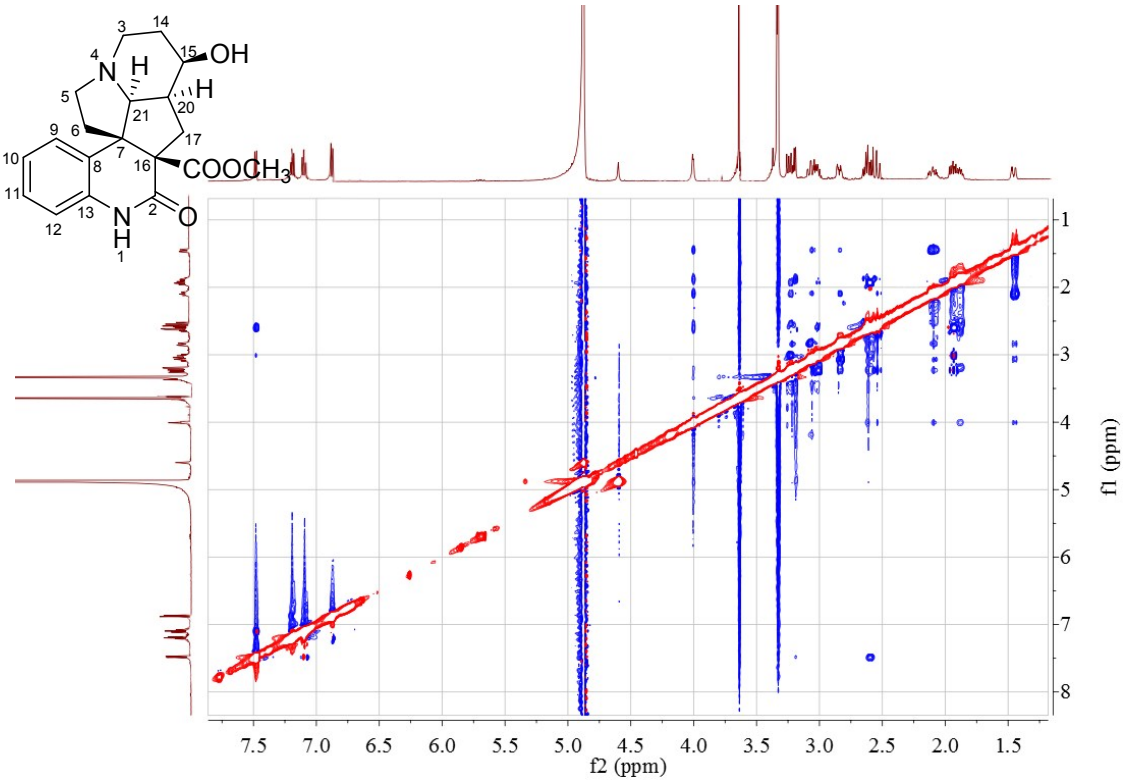
^{1}H-^{1}H COSY spectrum of **3** (CD_3OD)



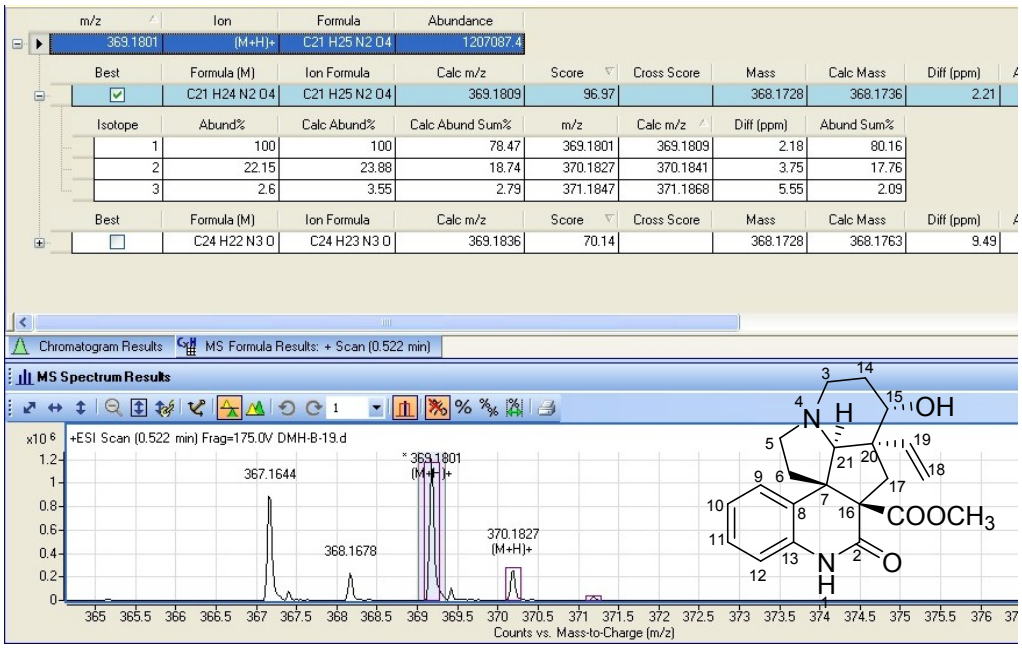
HSQC spectrum of **3** (CD_3OD)



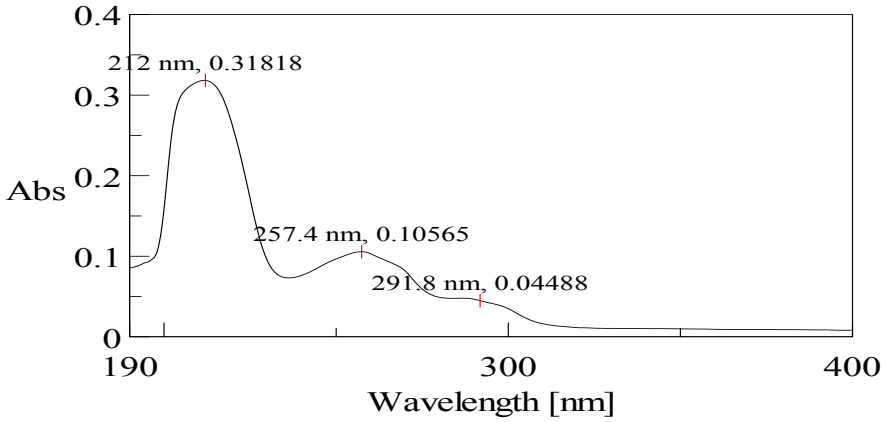
HMBC spectrum of **3** (CD_3OD)



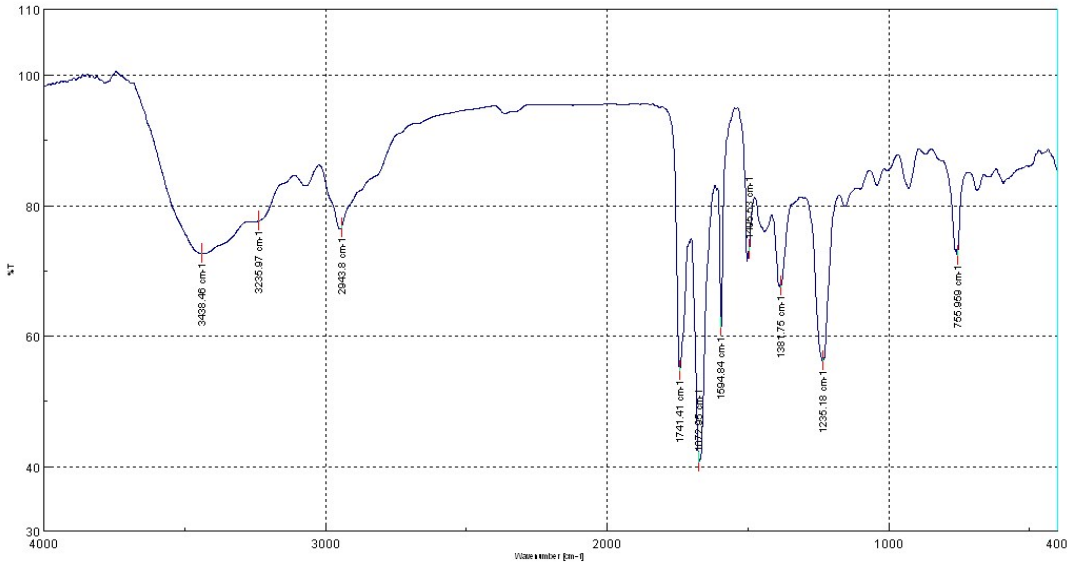
NOESY spectrum of **3** (CD_3OD)



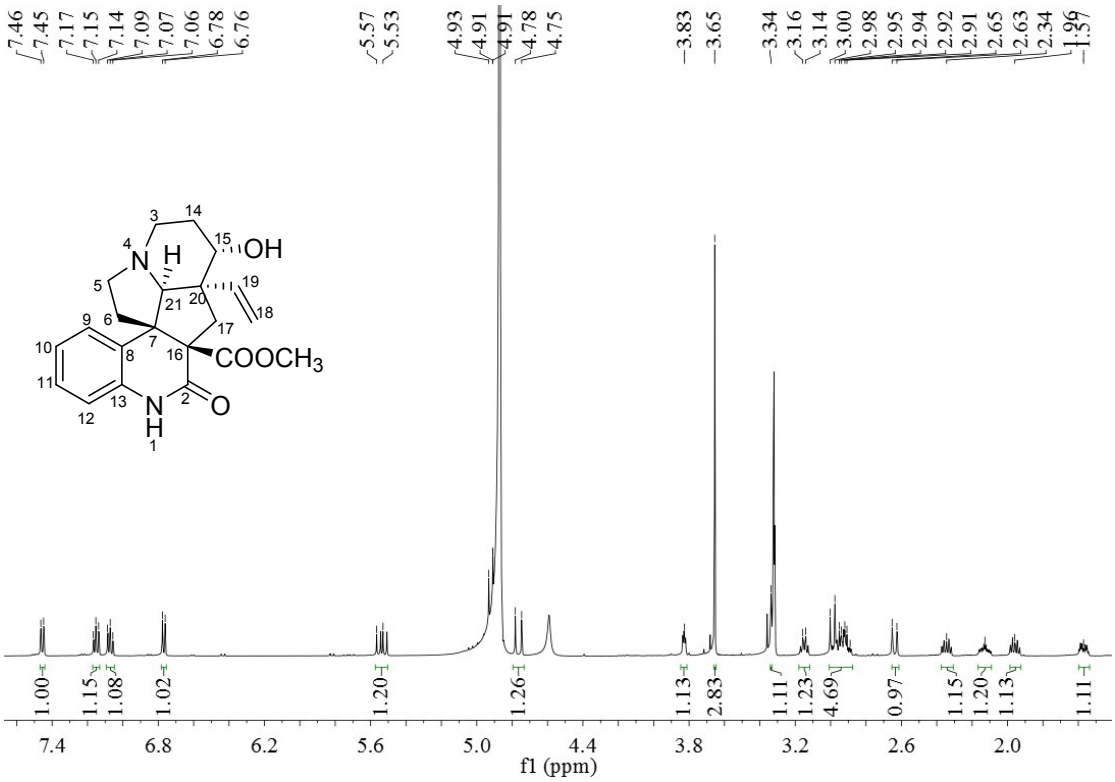
HRESIMS spectrum of **4**



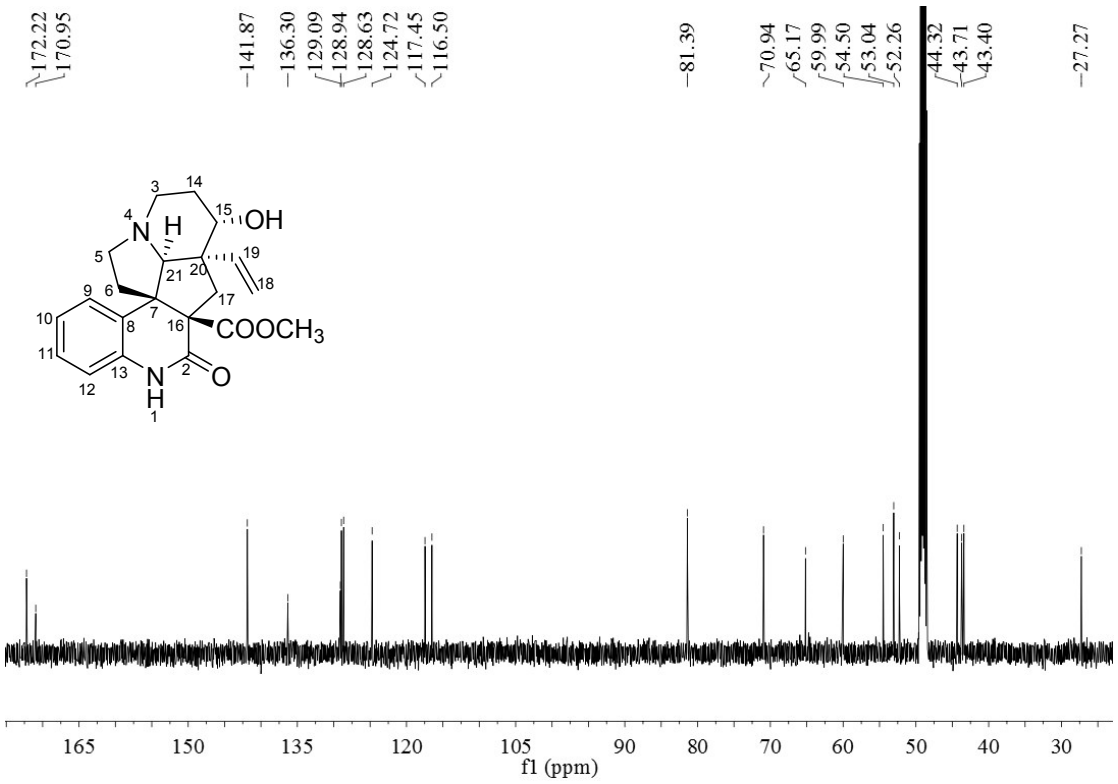
UV spectrum of **4** (MeOH)



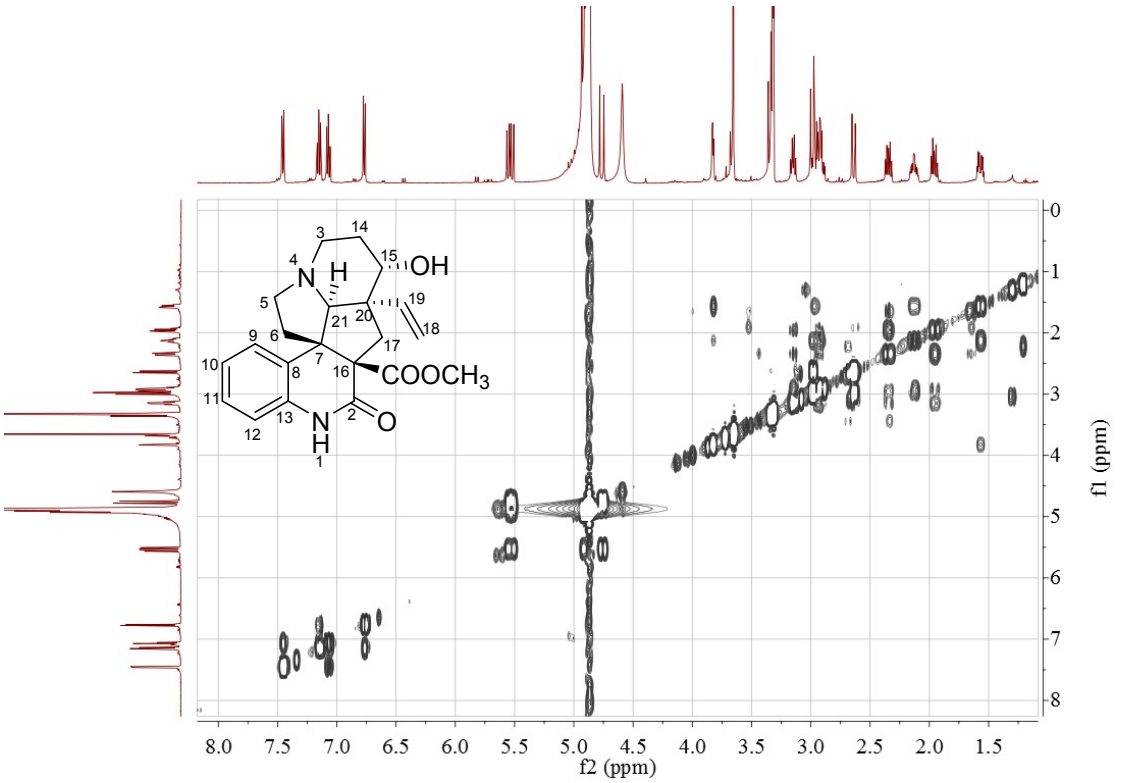
IR spectrum of **4** (KBr disc)



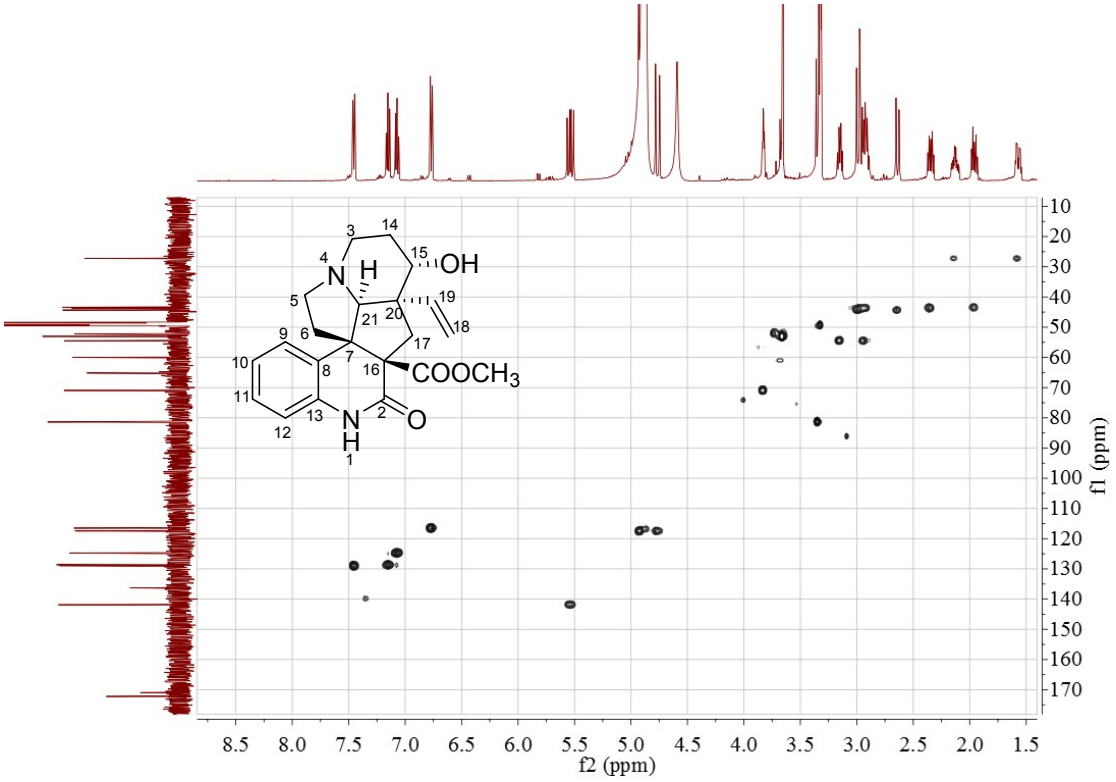
^{1}H NMR spectrum of **4** (500 Hz, CD_3OD)



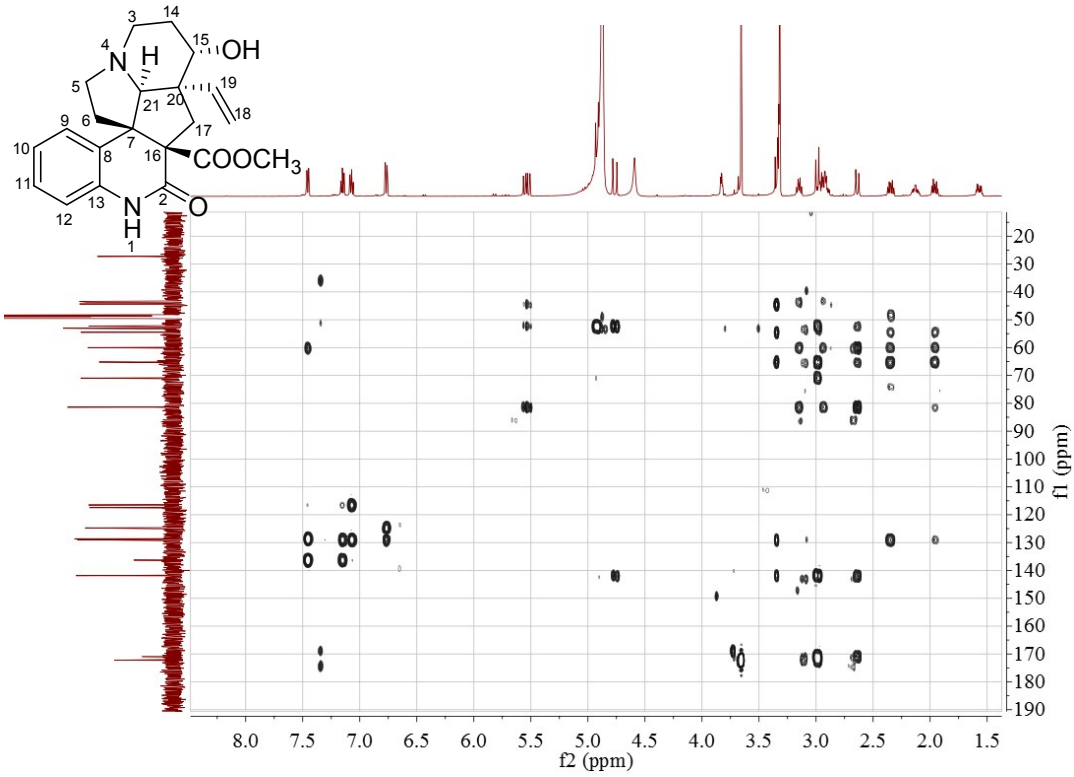
^{13}C NMR spectrum of **4** (125 Hz, CD_3OD)



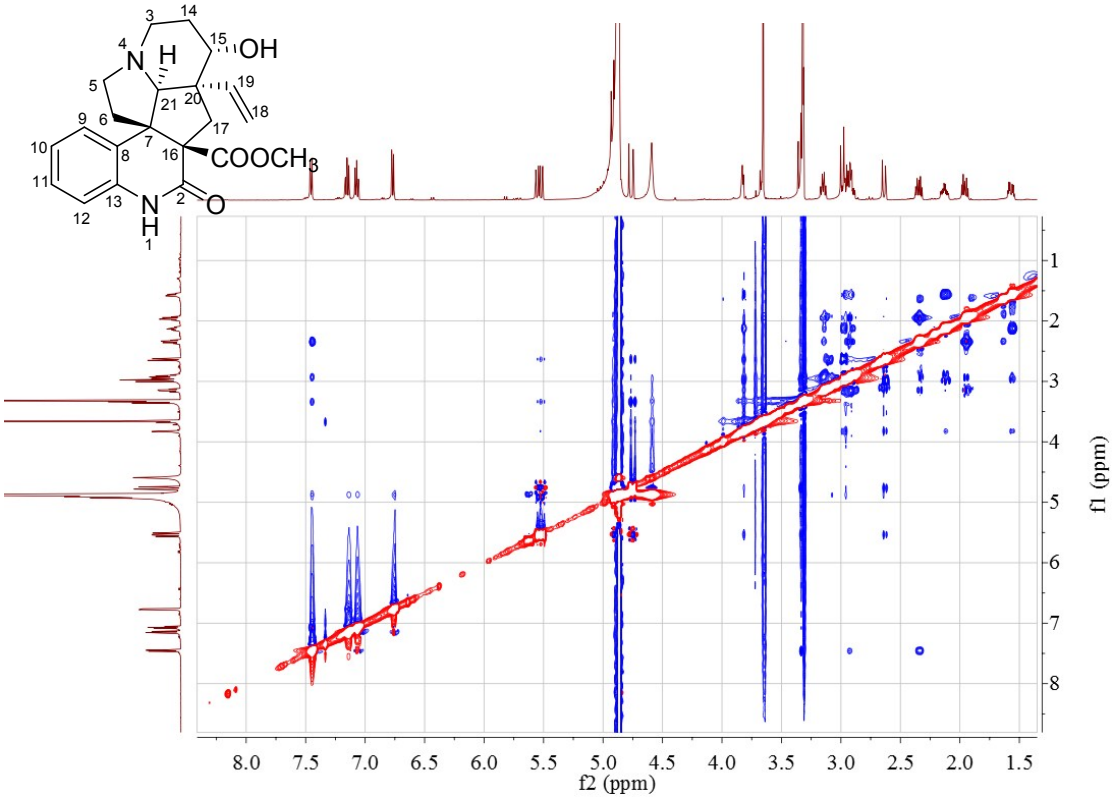
^{1}H-^{1}H COSY spectrum of **4** (CD_3OD)



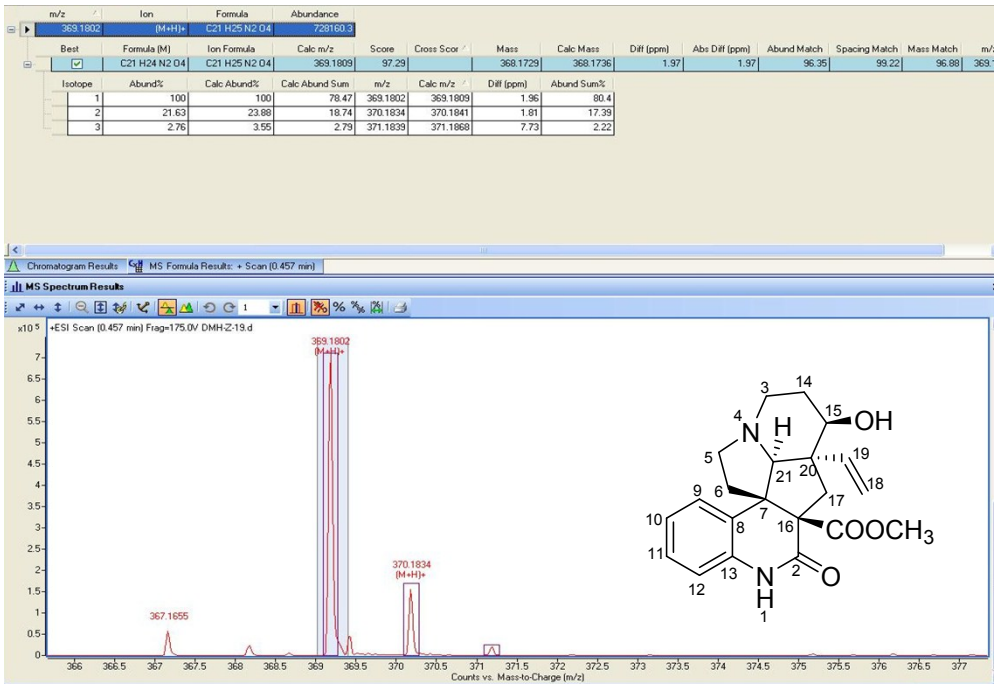
HSQC spectrum of **4** (CD_3OD)



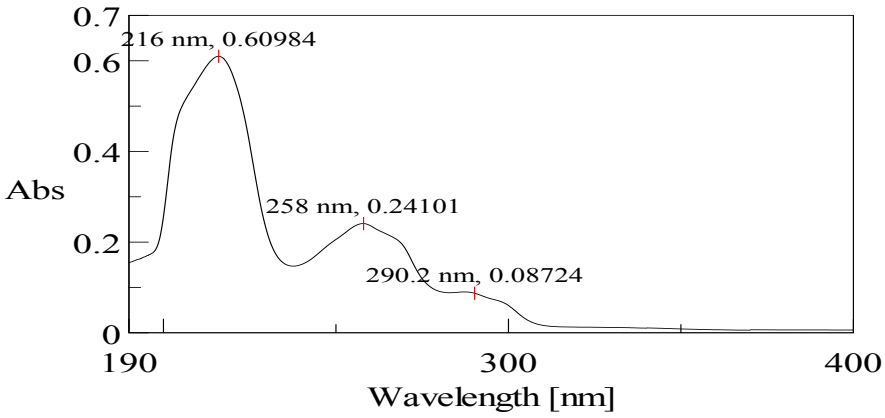
HMBC spectrum of **4** (CD_3OD)



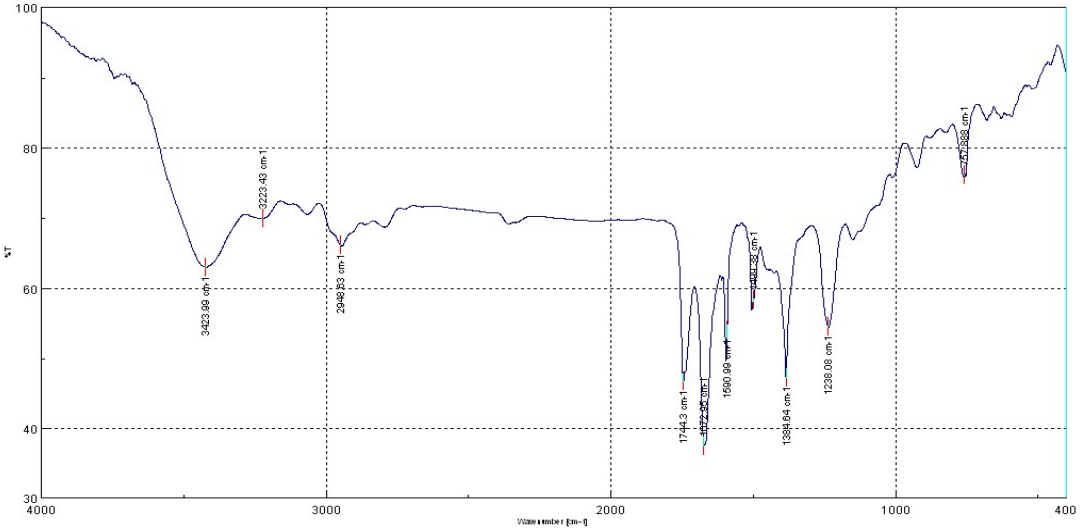
NOESY spectrum of **4** (CD_3OD)



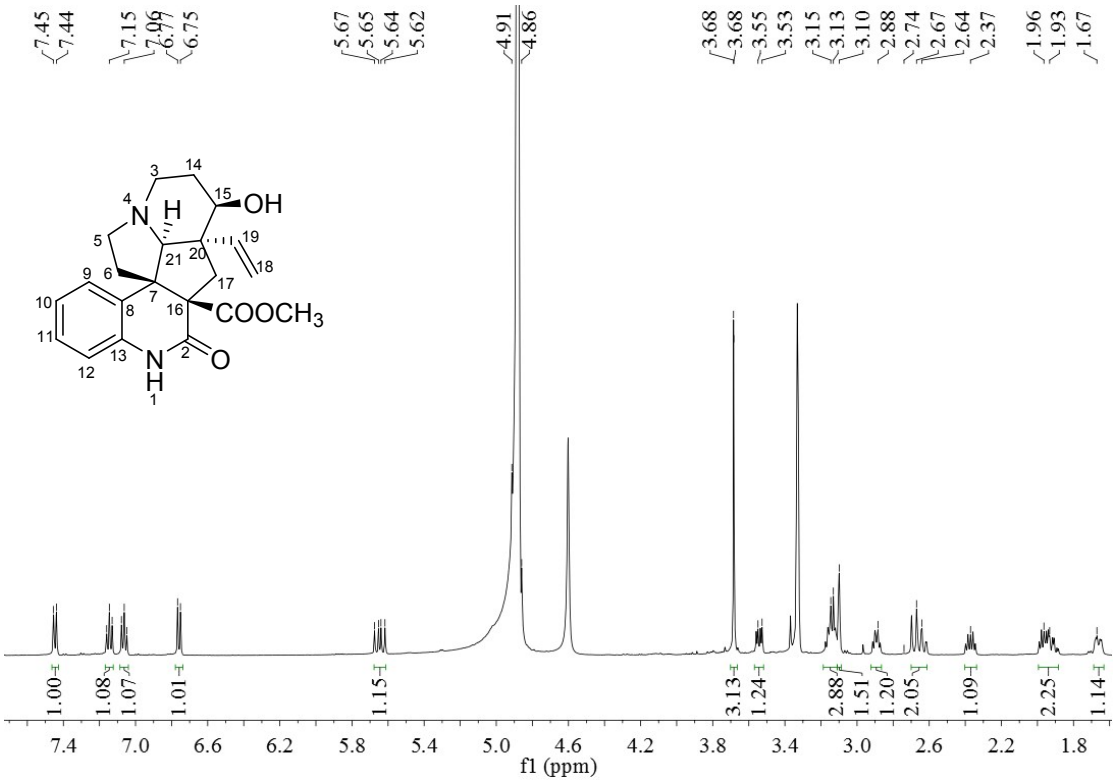
HRESIMS spectrum of **5**



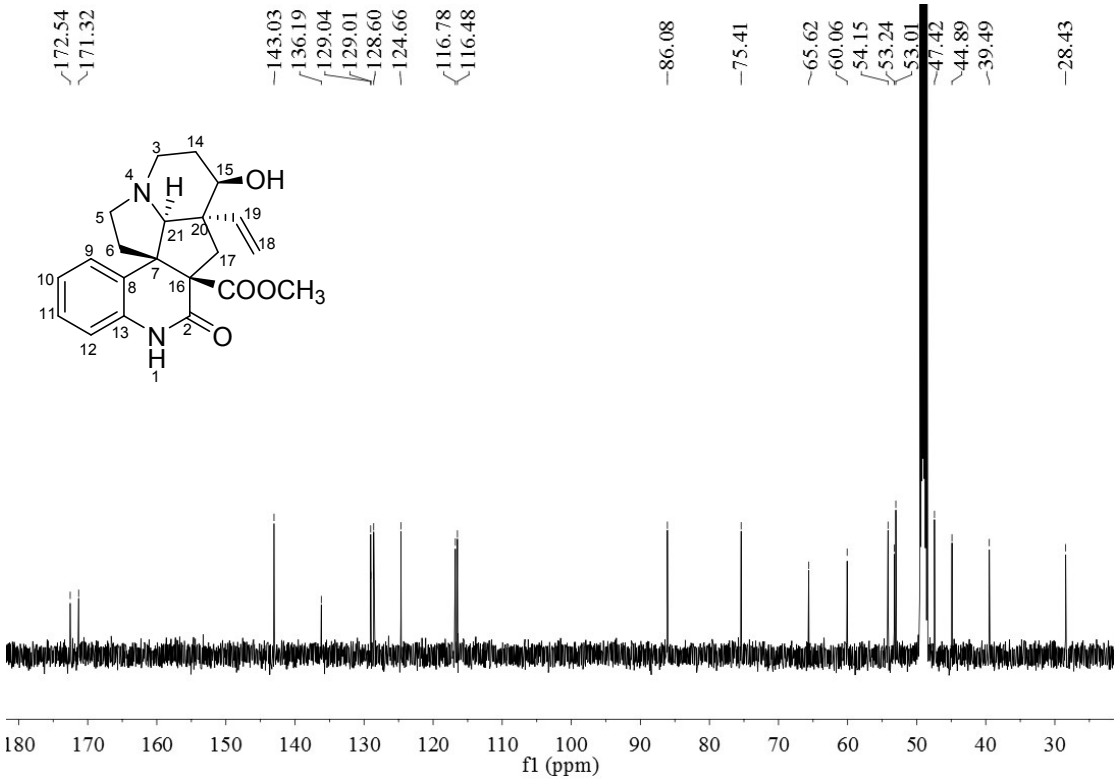
UV spectrum of **5** (MeOH)



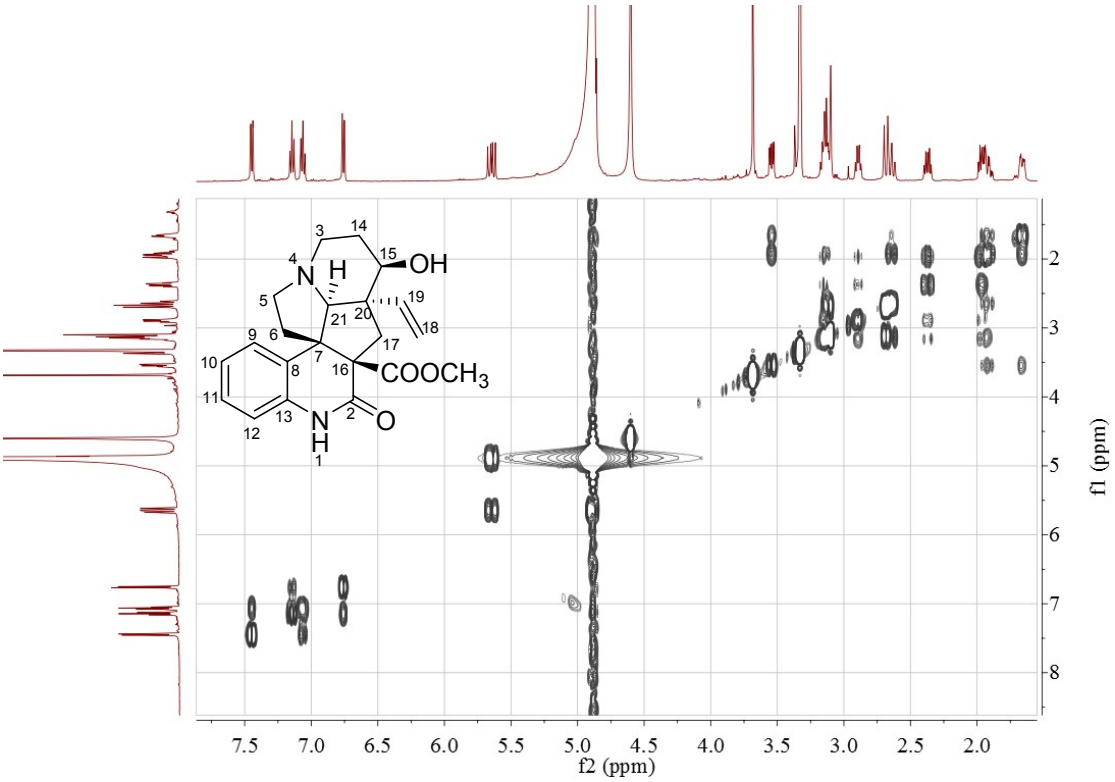
IR spectrum of **4** (KBr disc)



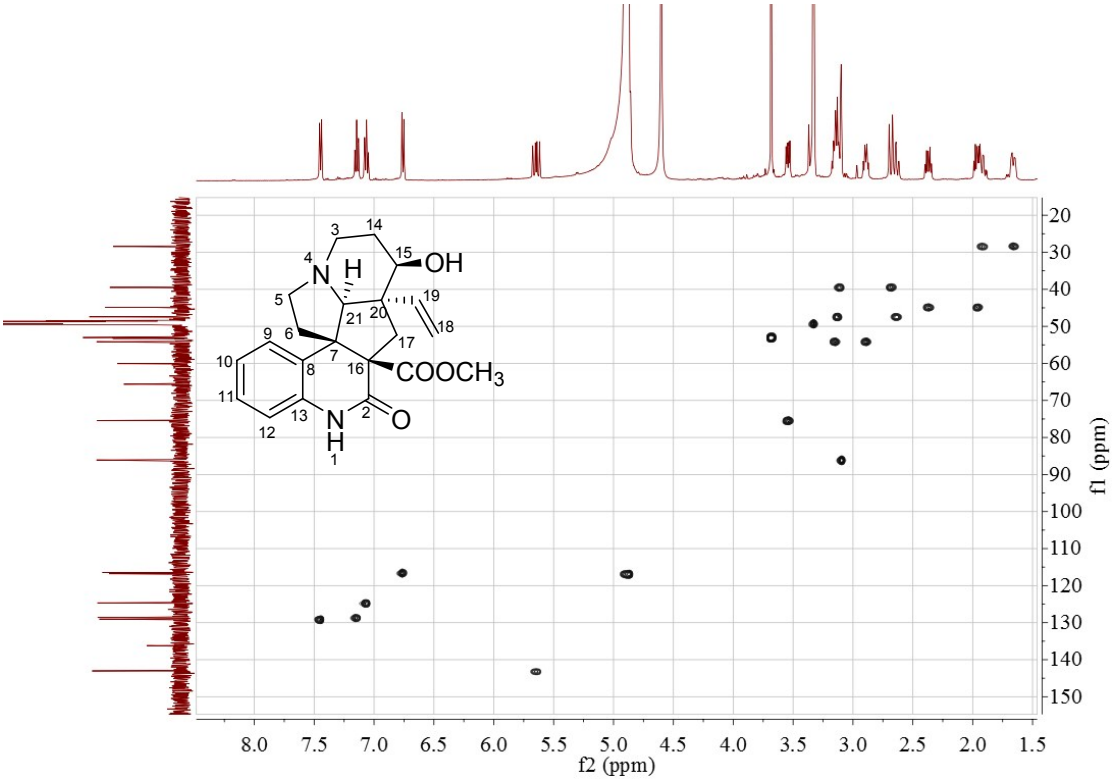
^{1}H NMR spectrum of **5** (500 Hz, CD_3OD)



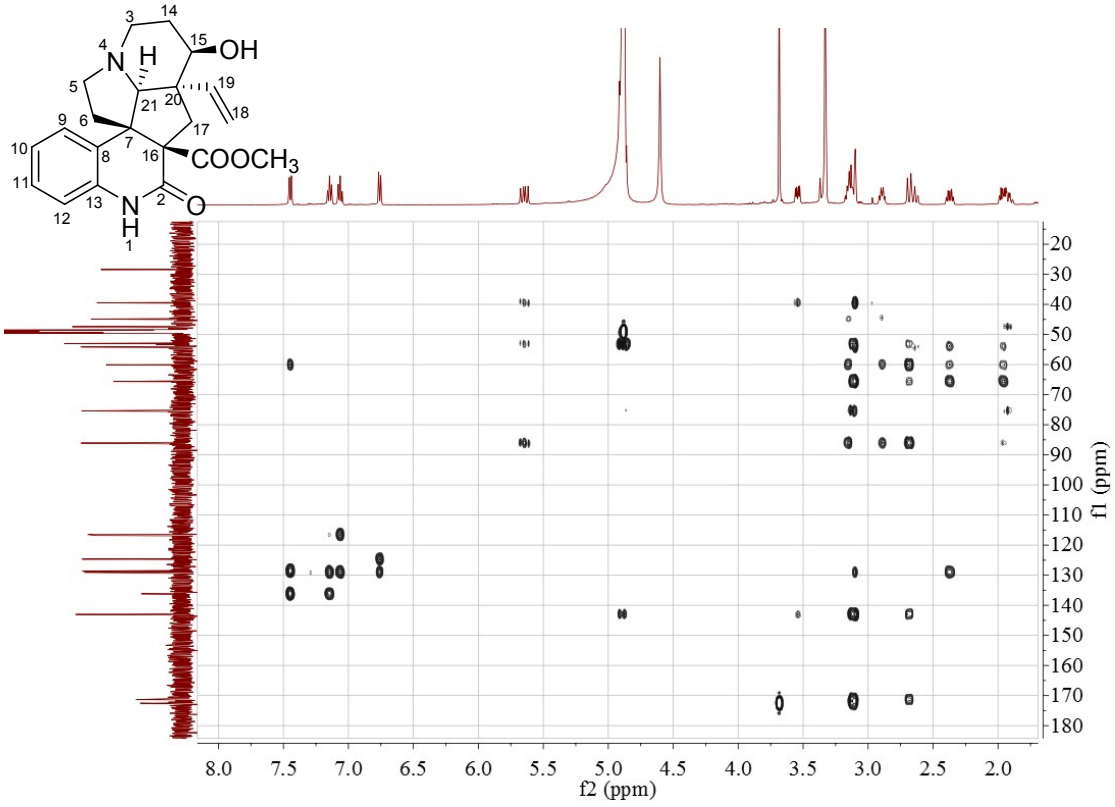
^{13}C NMR spectrum of **5** (125 Hz, CD_3OD)



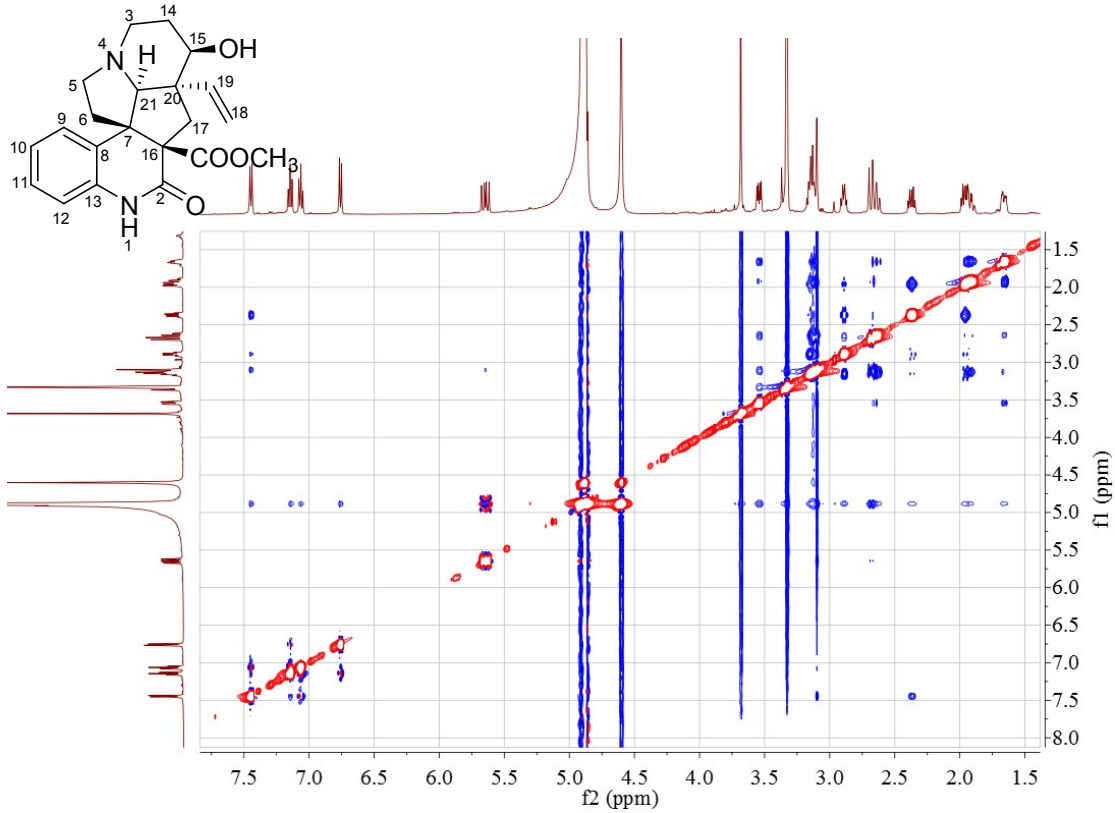
^{1}H-^{1}H COSY spectrum of **5** (CD_3OD)



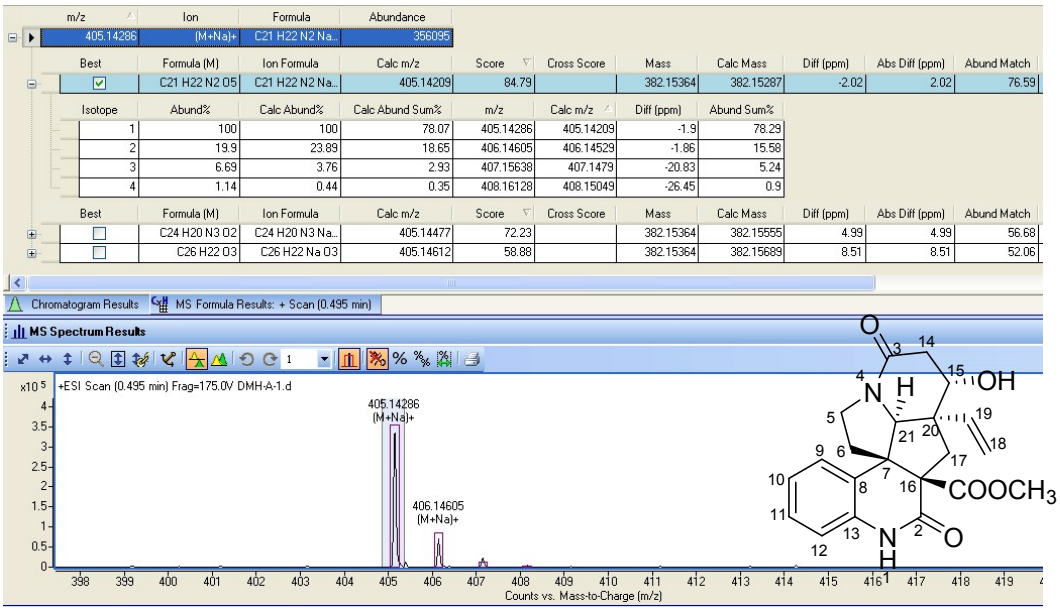
HSQC spectrum of **5** (CD_3OD)



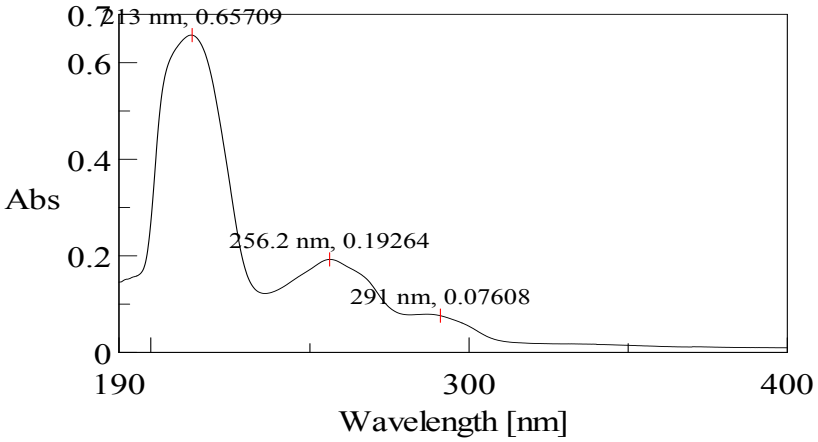
HMBC spectrum of **5** (CD_3OD)



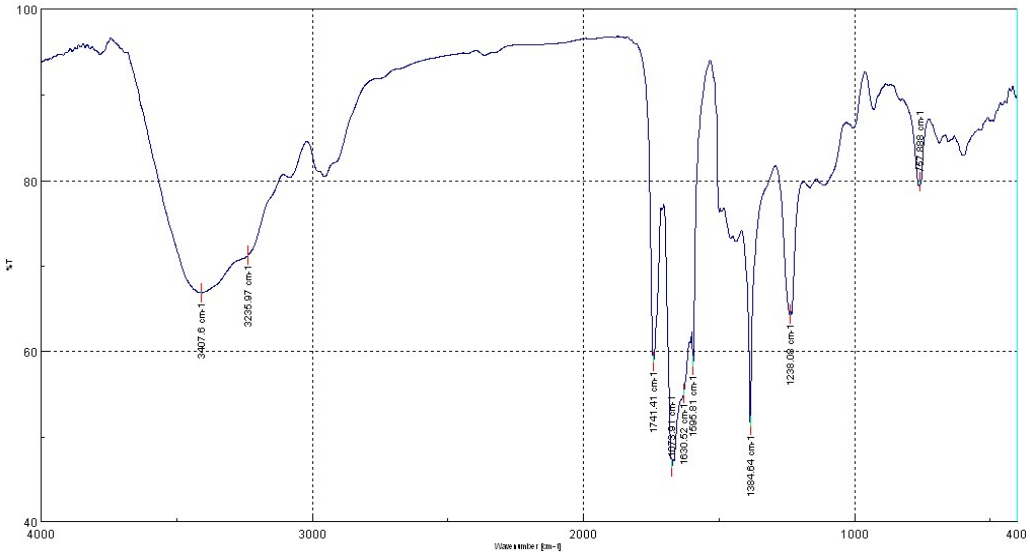
NOESY spectrum of **5** (CD_3OD)



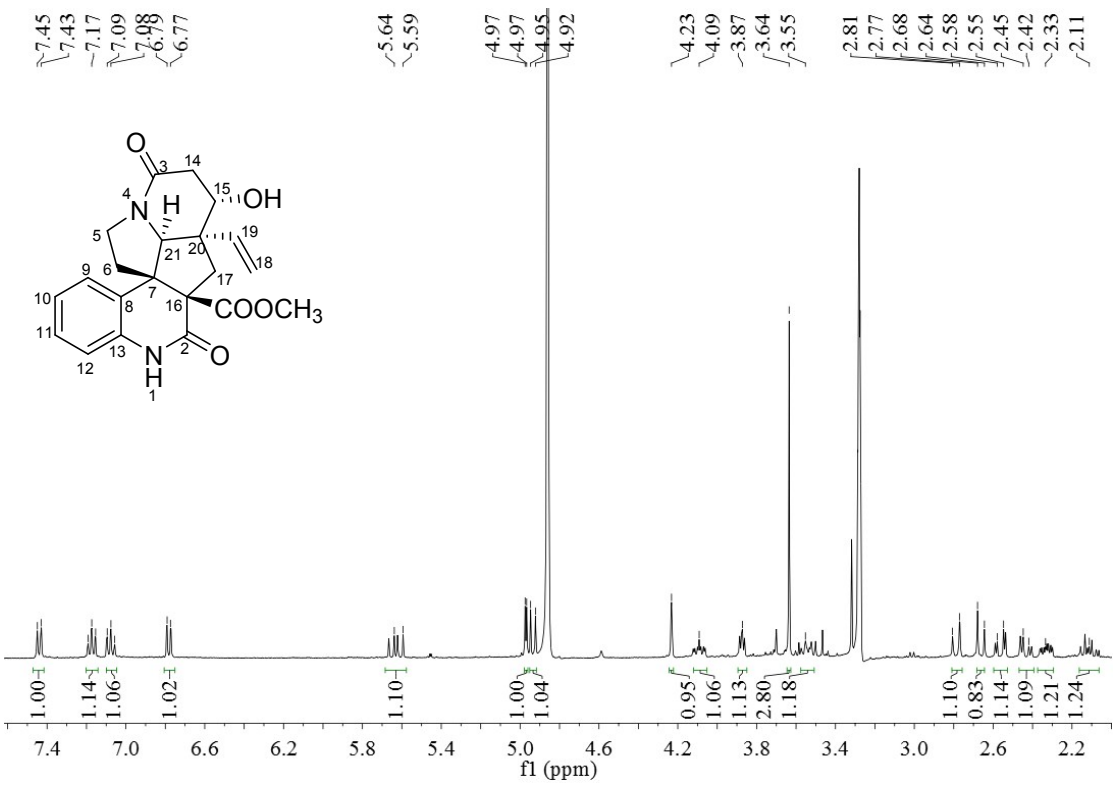
HRESIMS spectrum of **6**



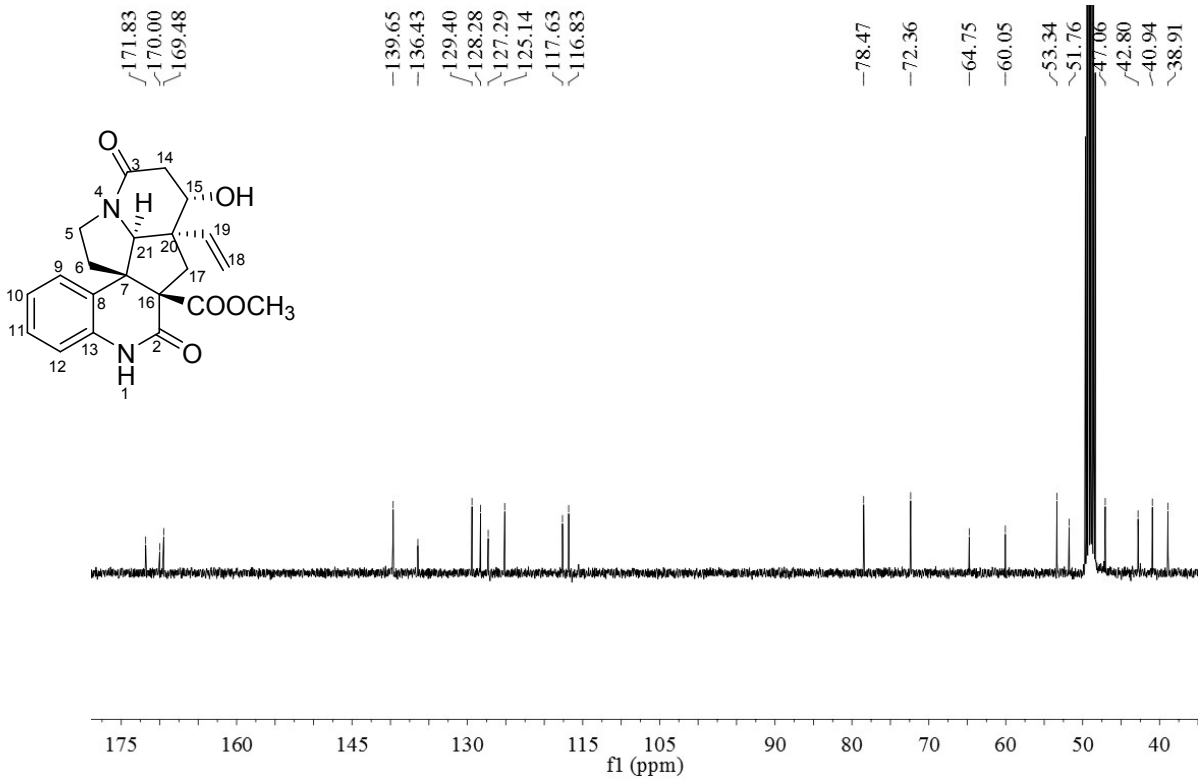
UV spectrum of **6** (MeOH)



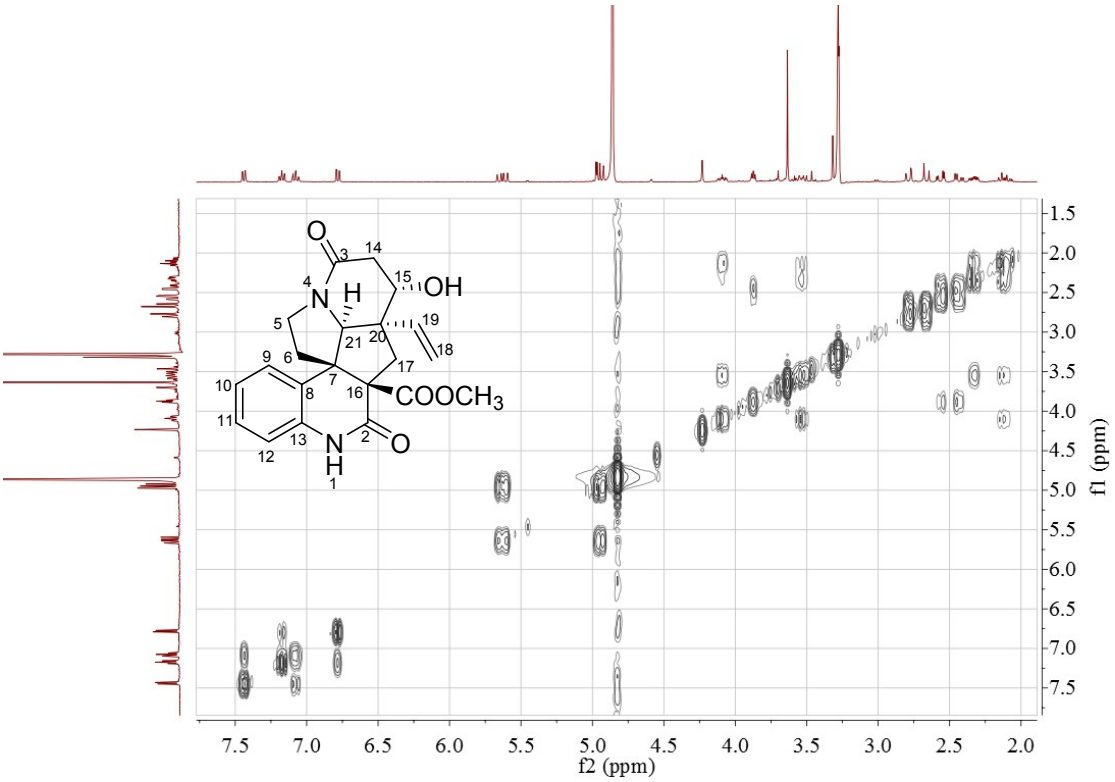
IR spectrum of **6** (KBr disc)



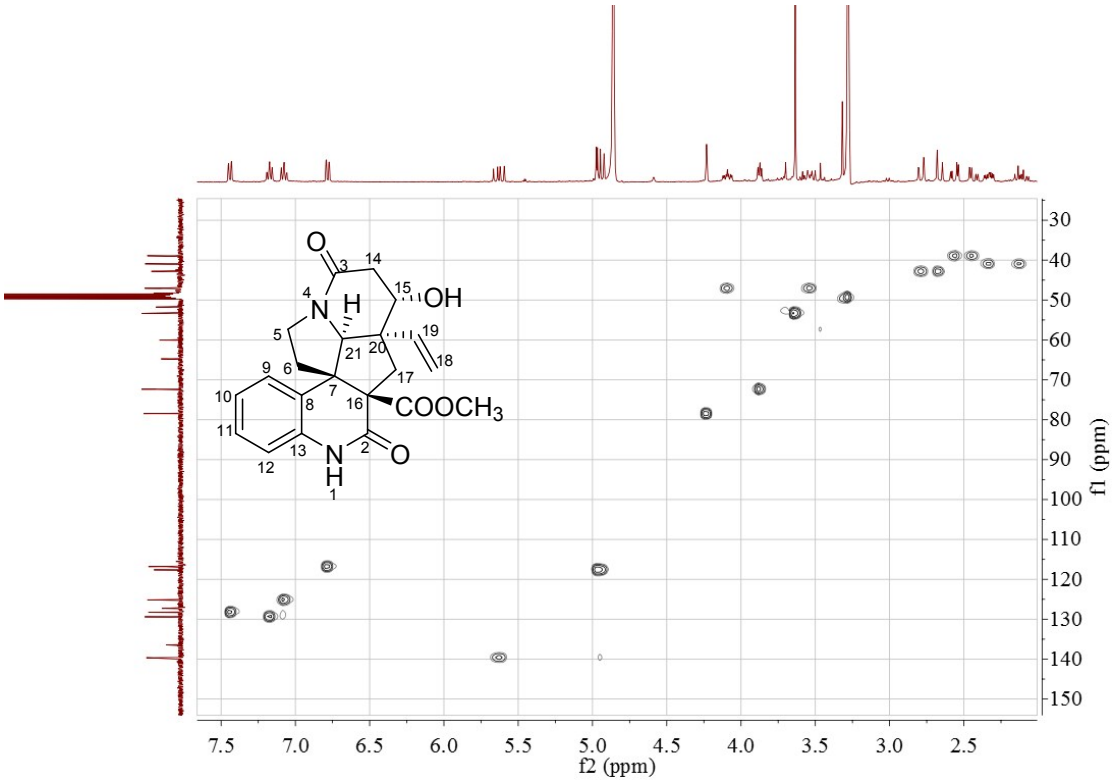
^{1}H NMR spectrum of **6** (400 Hz, CD_3OD)



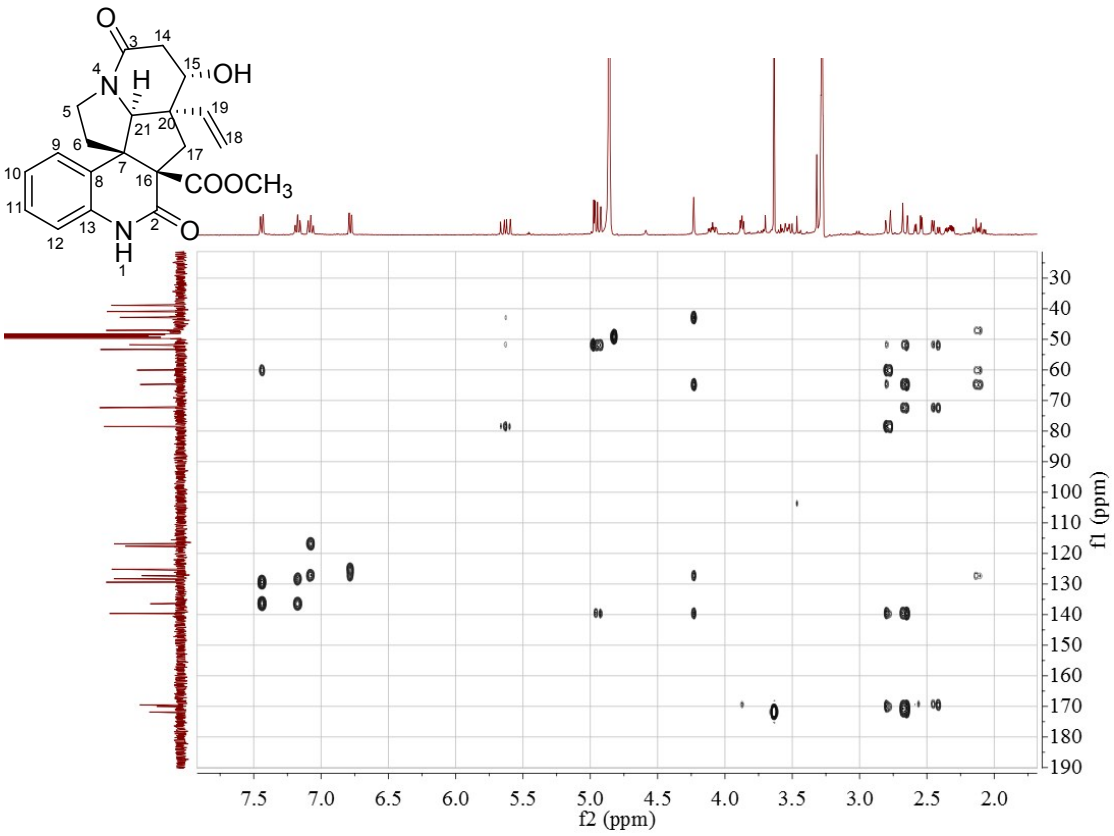
^{13}C NMR spectrum of **6** (100 Hz, CD_3OD)



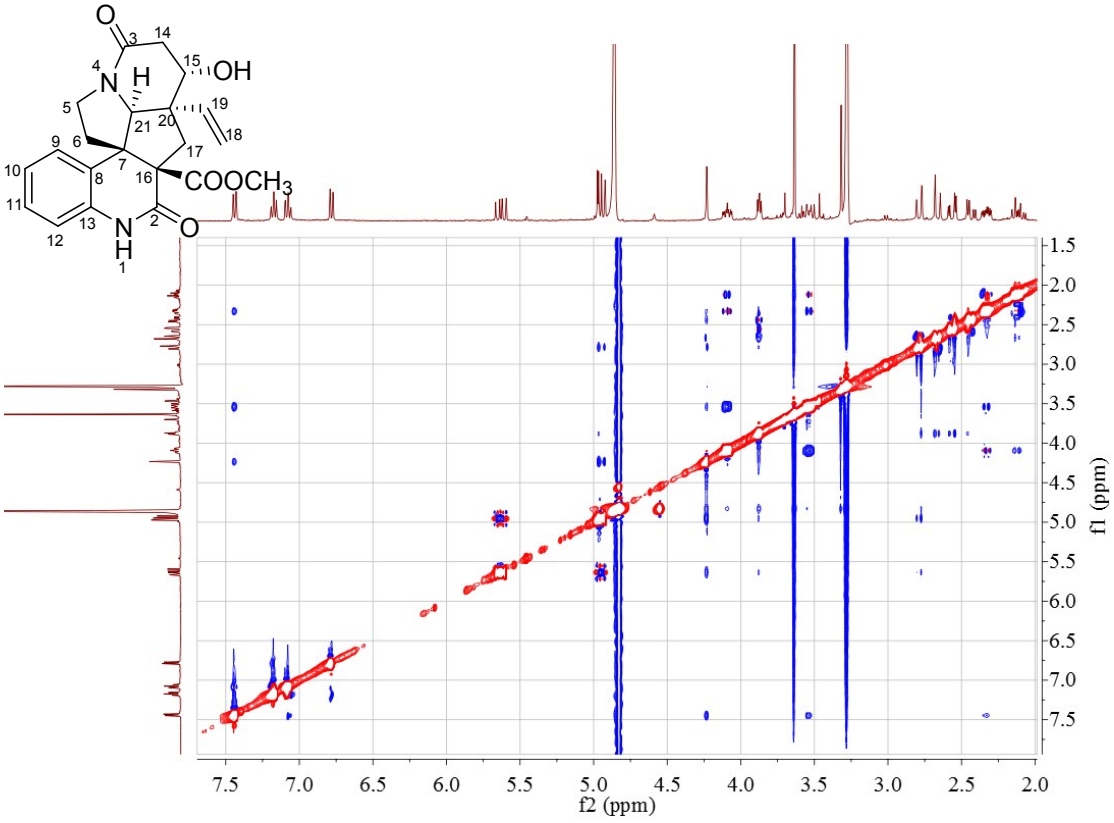
^{1}H-^{1}H COSY spectrum of **6** (CD_3OD)



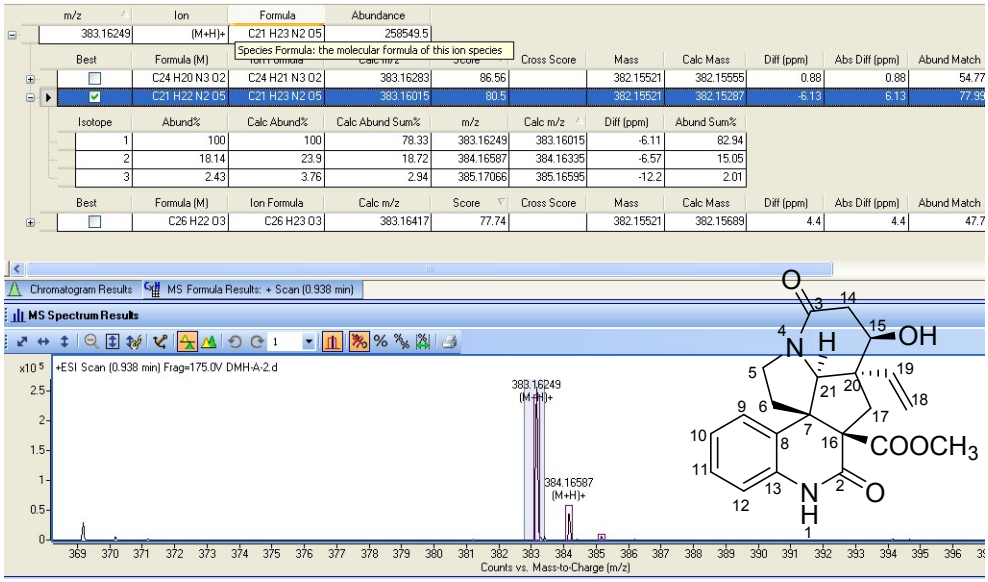
HSQC spectrum of **6** (CD_3OD)



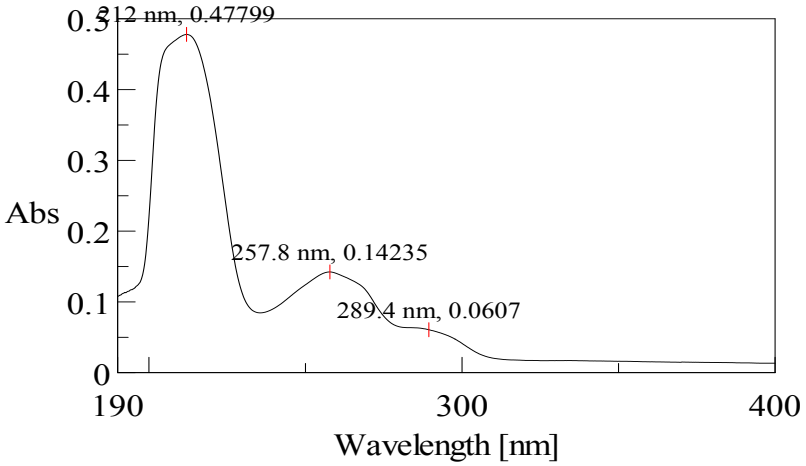
HMBC spectrum of **6** (CD_3OD)



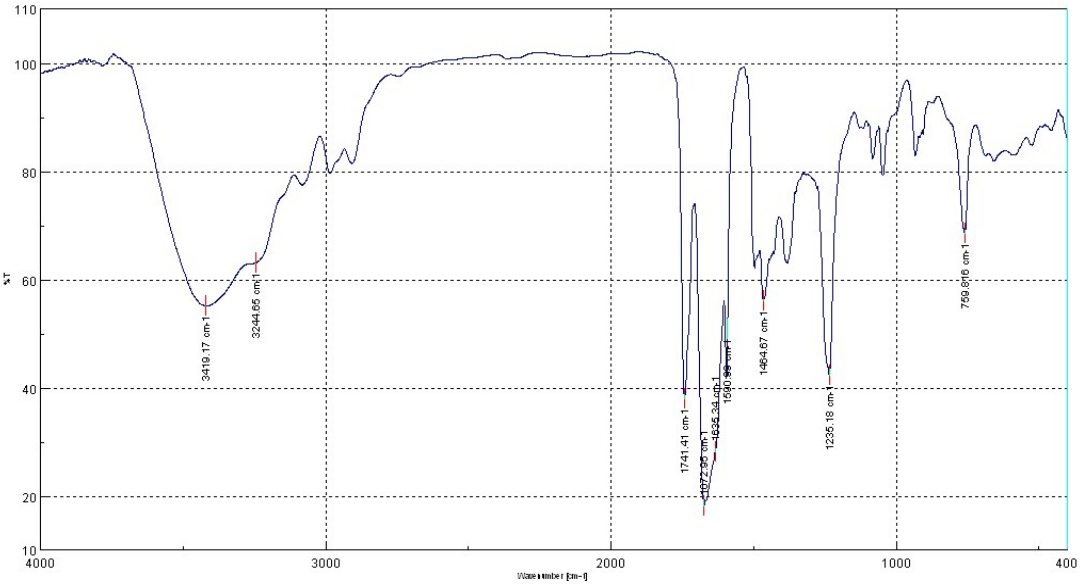
NOESY spectrum of **6** (CD_3OD)



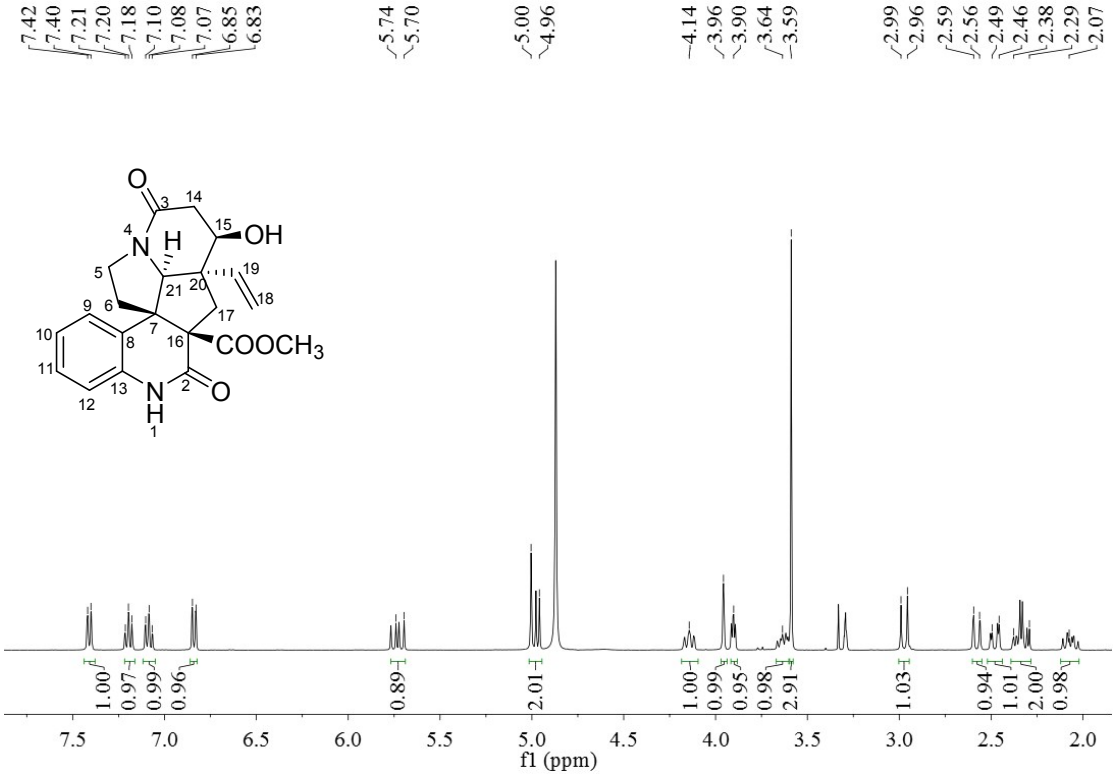
HRESIMS spectrum of **7**



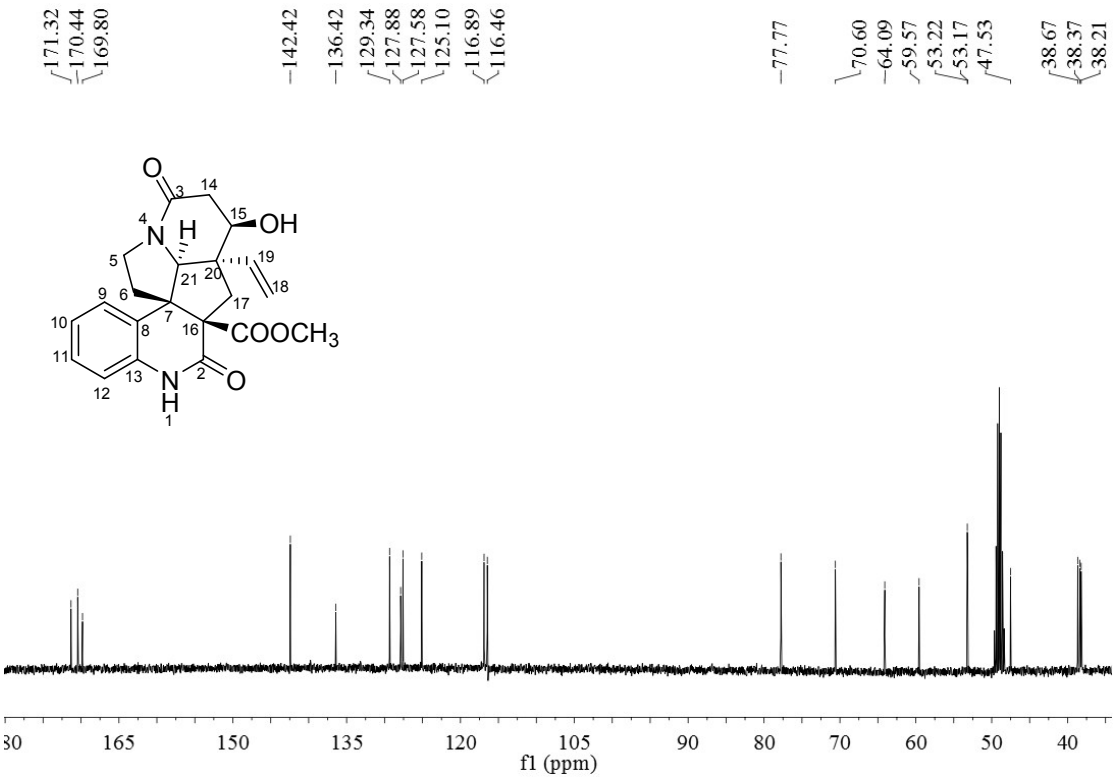
UV spectrum of **7** (MeOH)



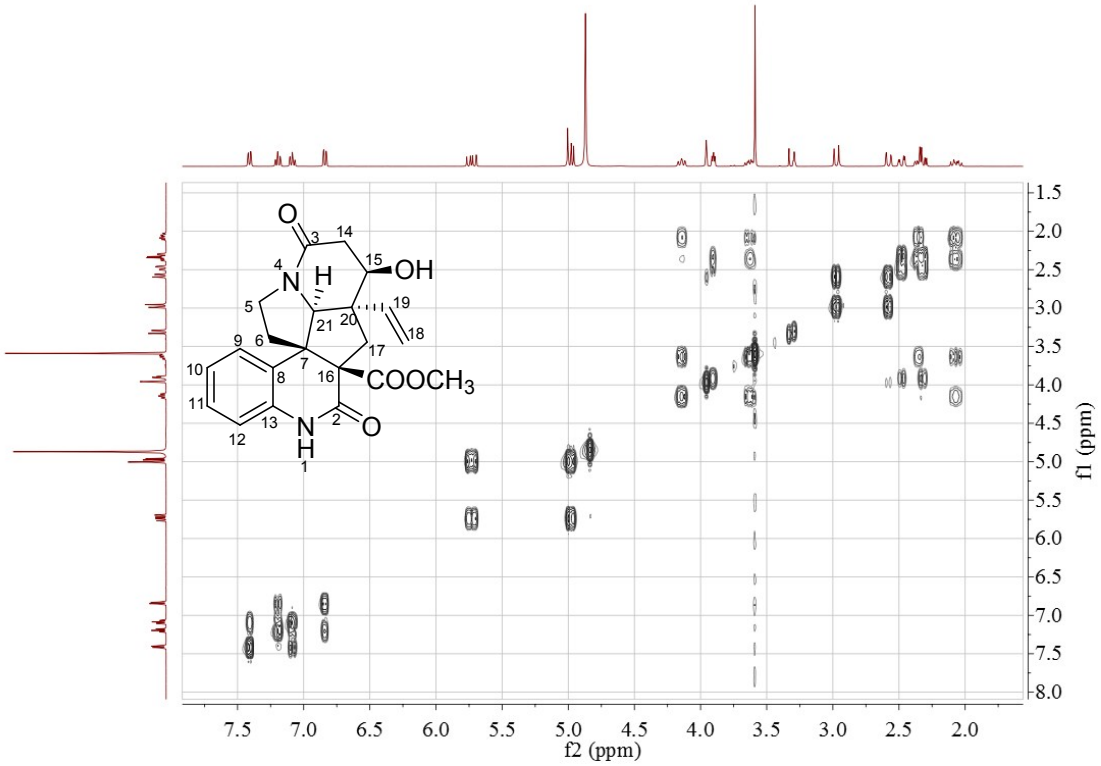
IR spectrum of **7** (KBr disc)



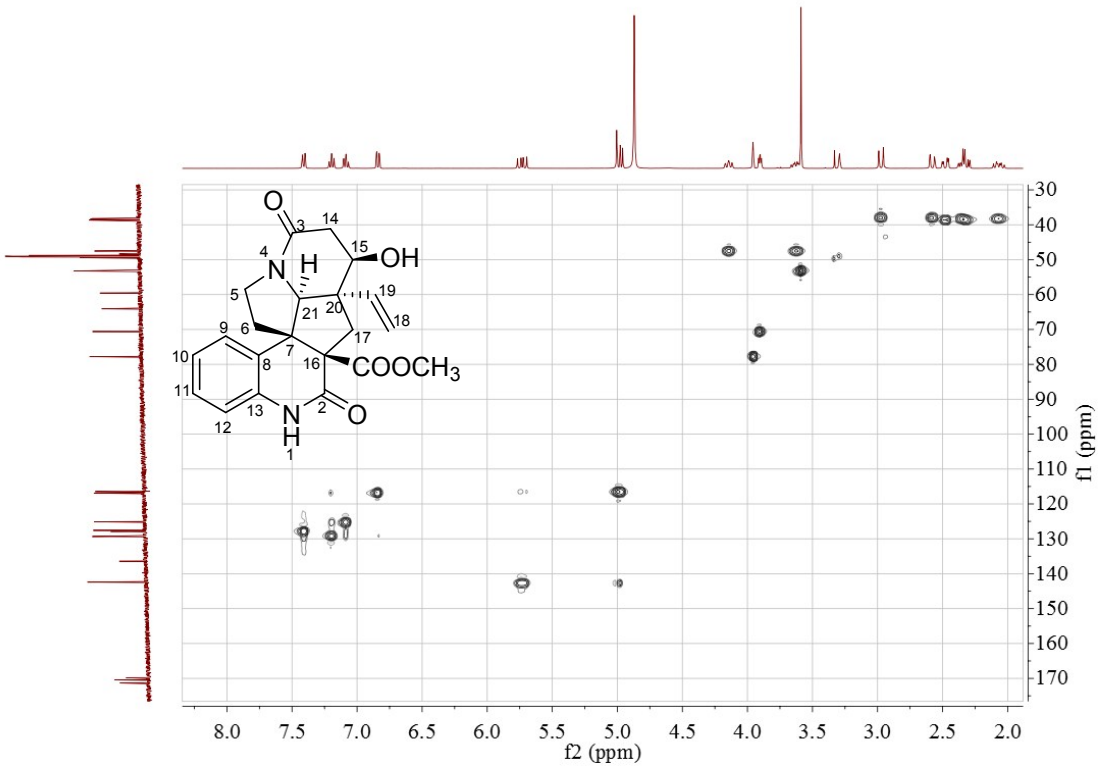
^{1}H NMR spectrum of **7** (400 Hz, CD_3OD)



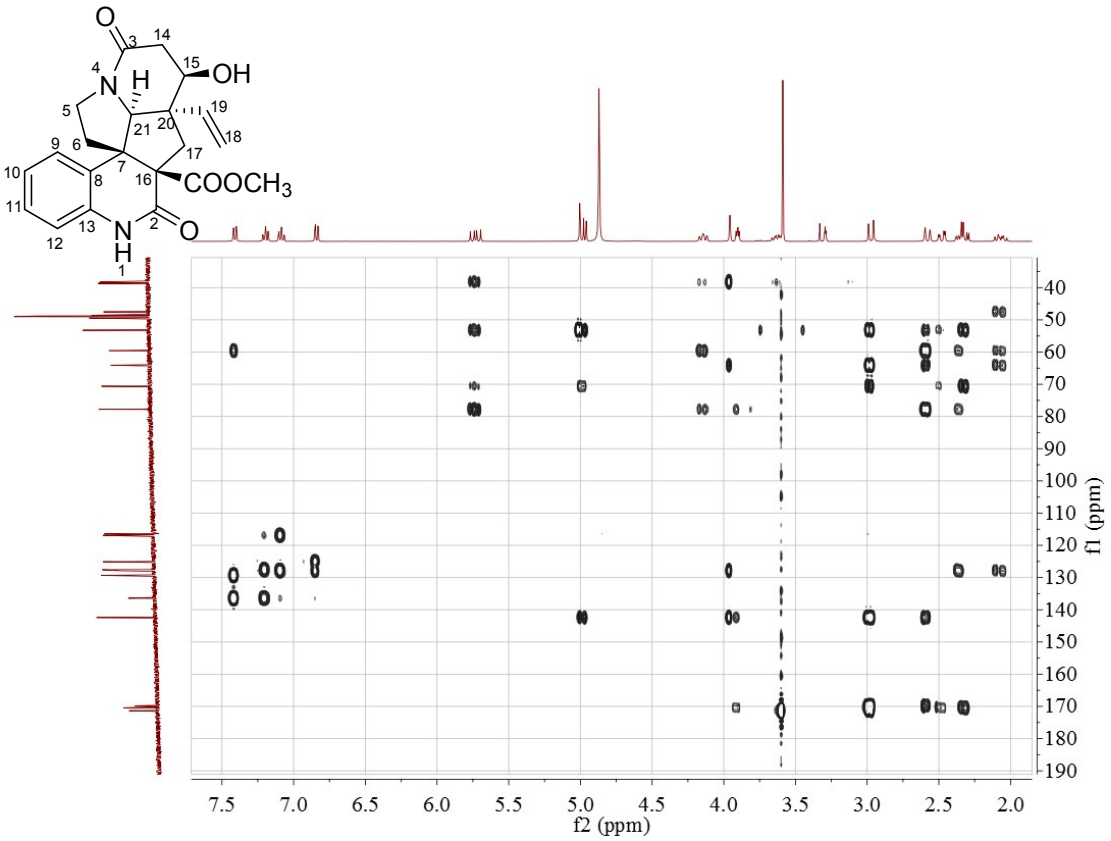
^{13}C NMR spectrum of **7** (100 Hz, CD_3OD)



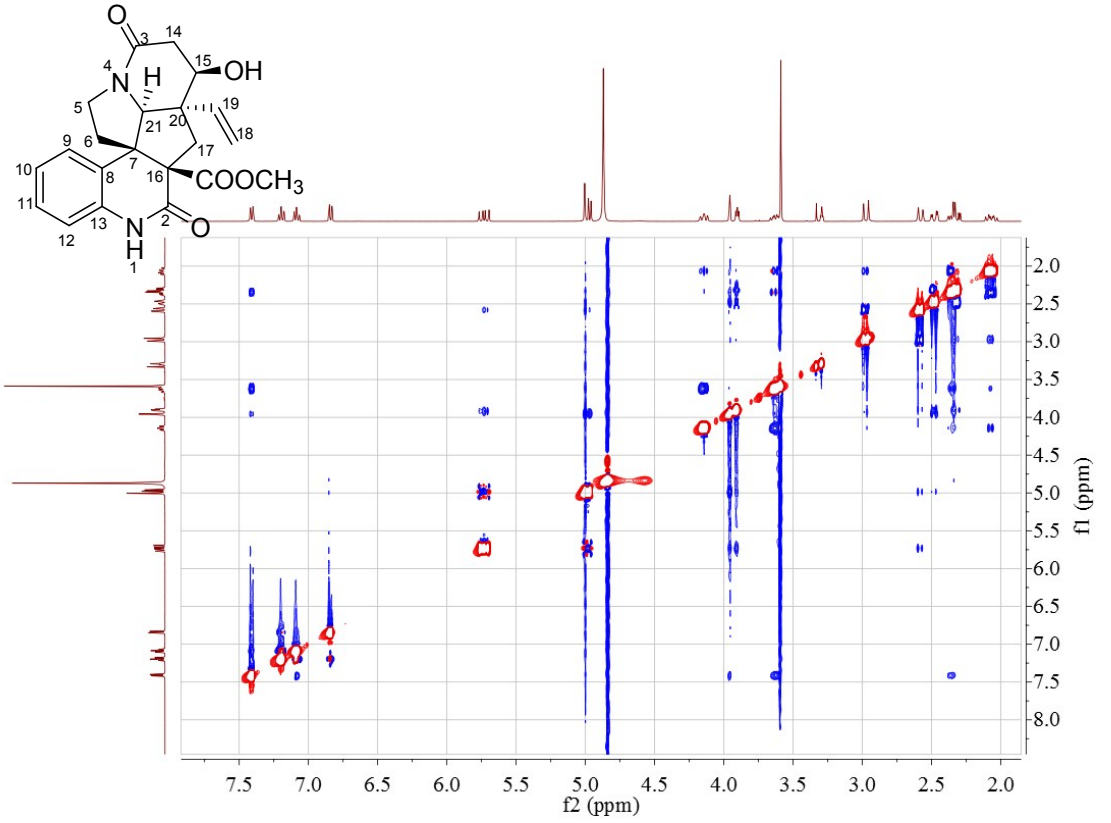
^{1}H-^{1}H COSY spectrum of **7** (CD_3OD)



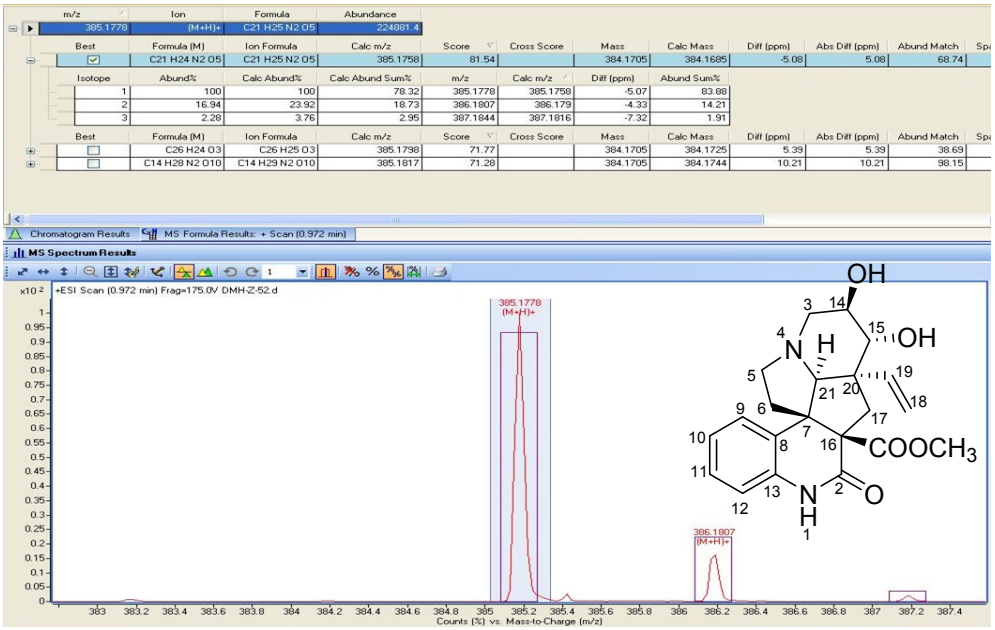
HSQC spectrum of **7** (CD_3OD)



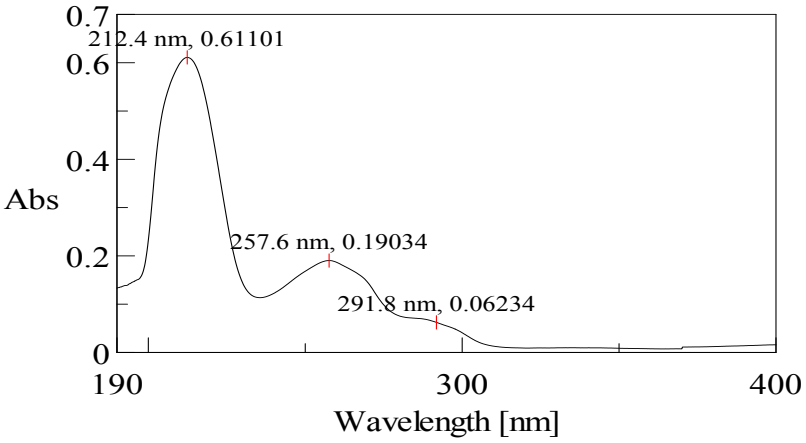
HMBC spectrum of **7** (CD_3OD)



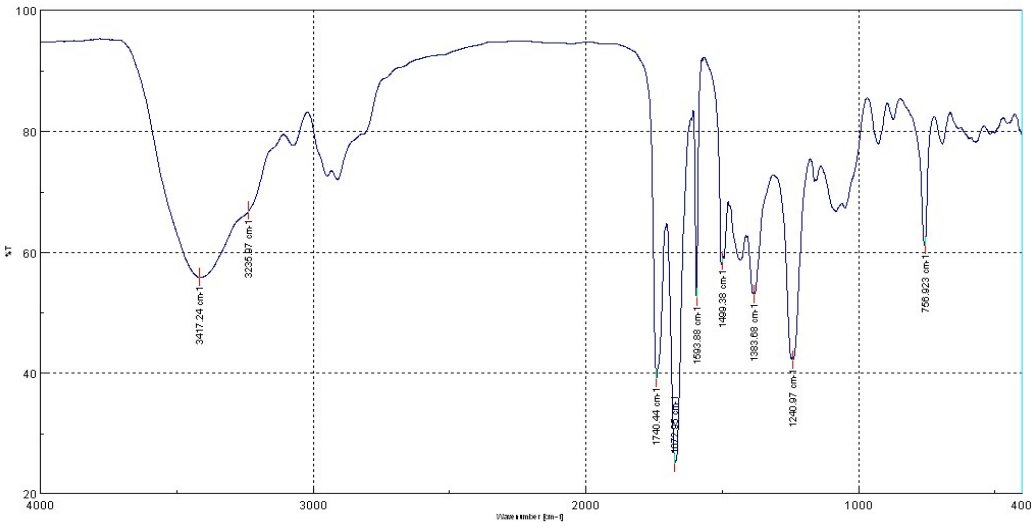
NOESY spectrum of **7** (CD_3OD)



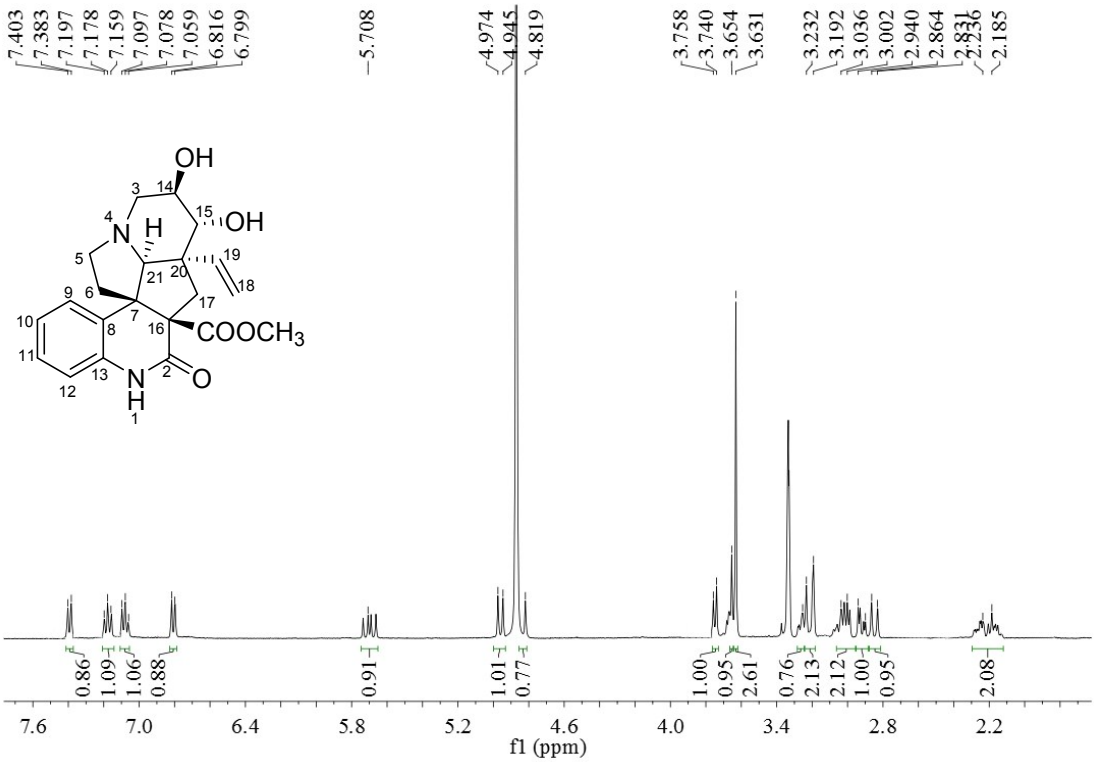
HRESIMS spectrum of **8**



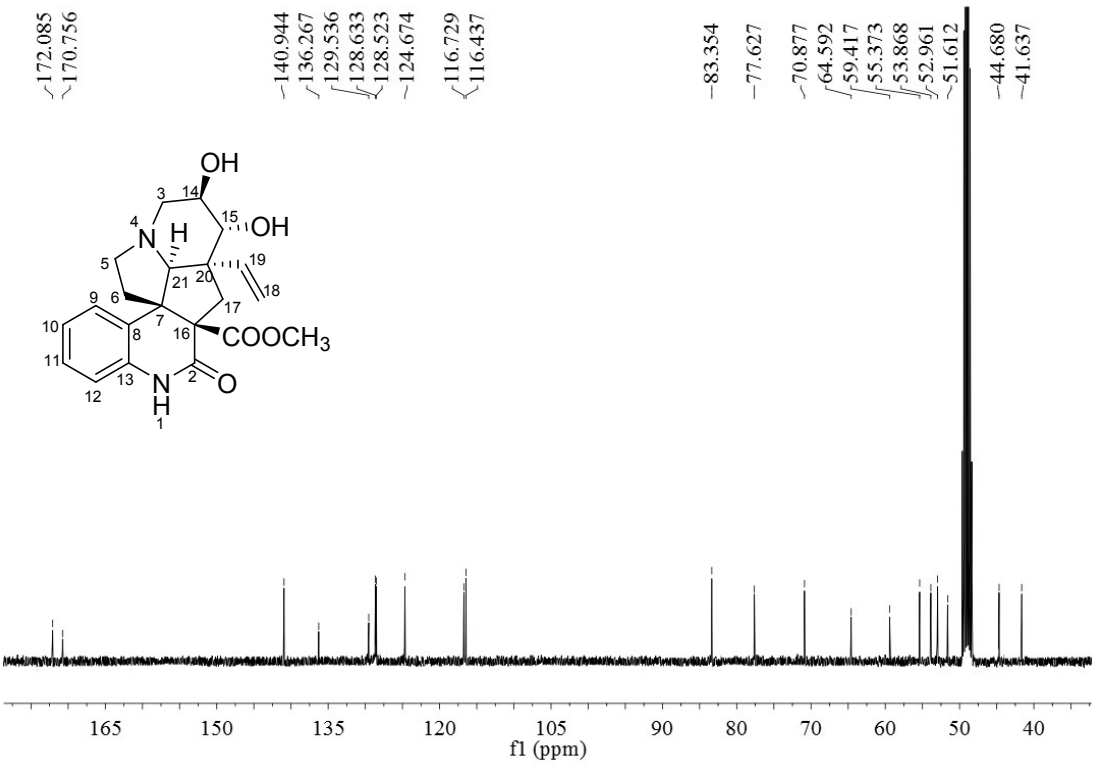
UV spectrum of **8** (MeOH)



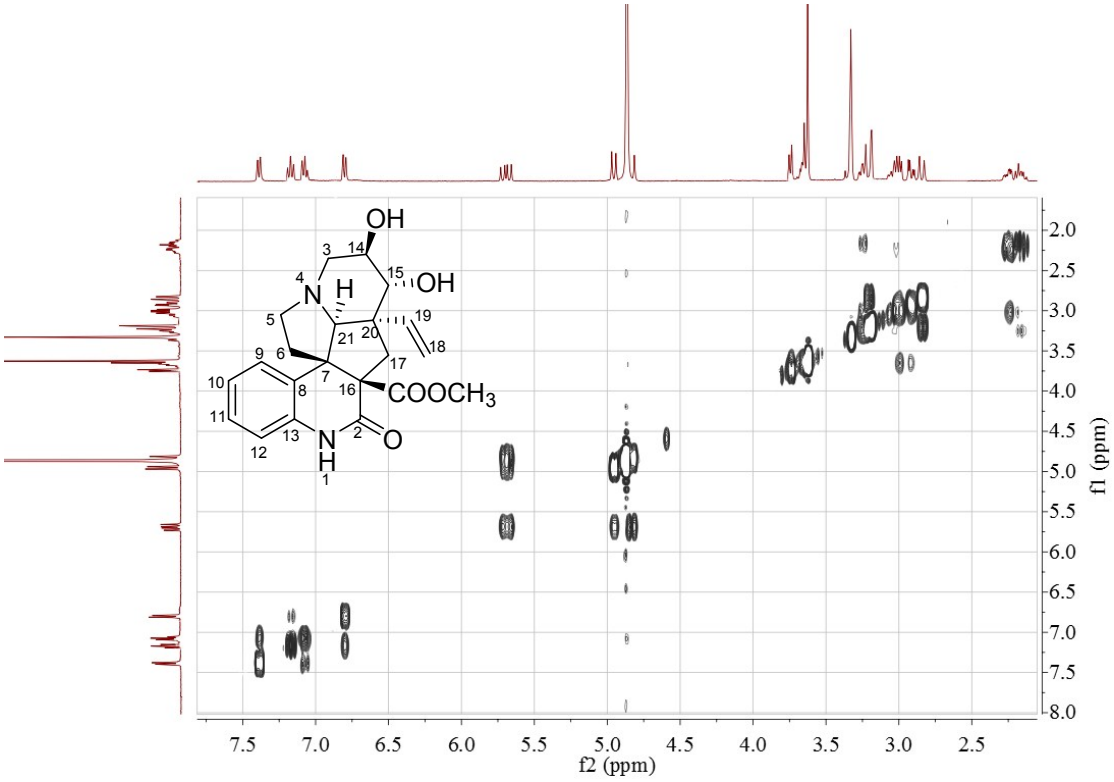
IR spectrum of **8** (KBr disc)



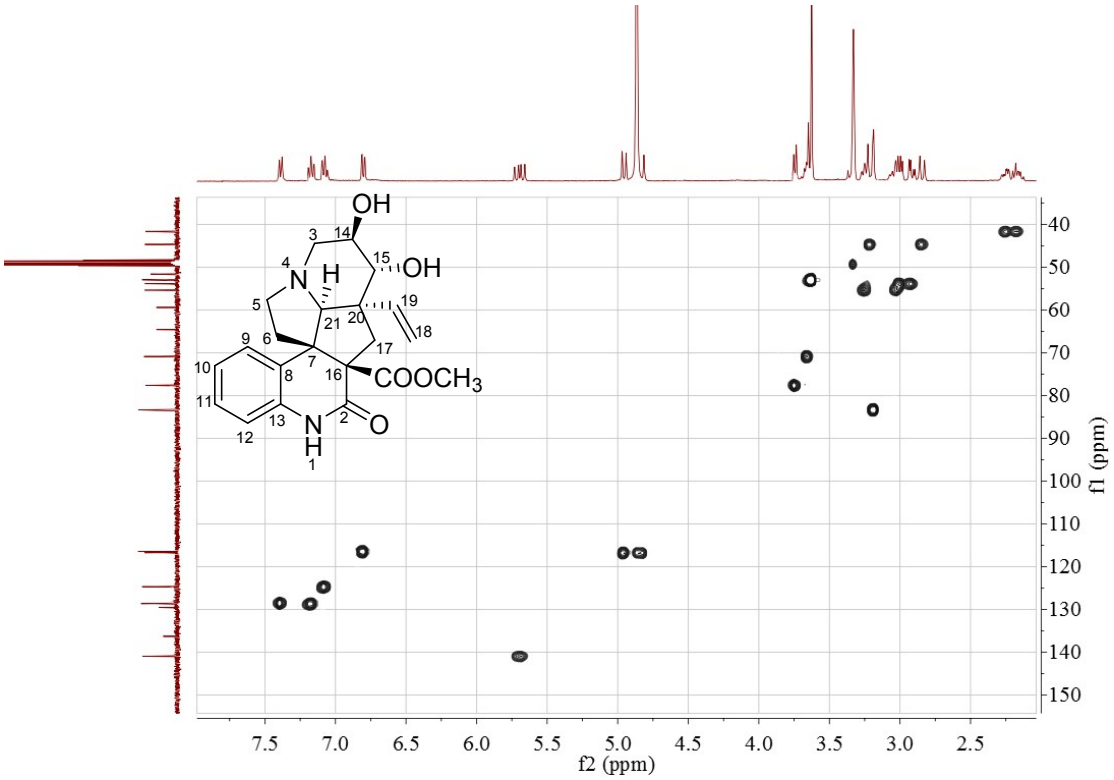
^{1}H NMR spectrum of **8** (400 Hz, CD_3OD)



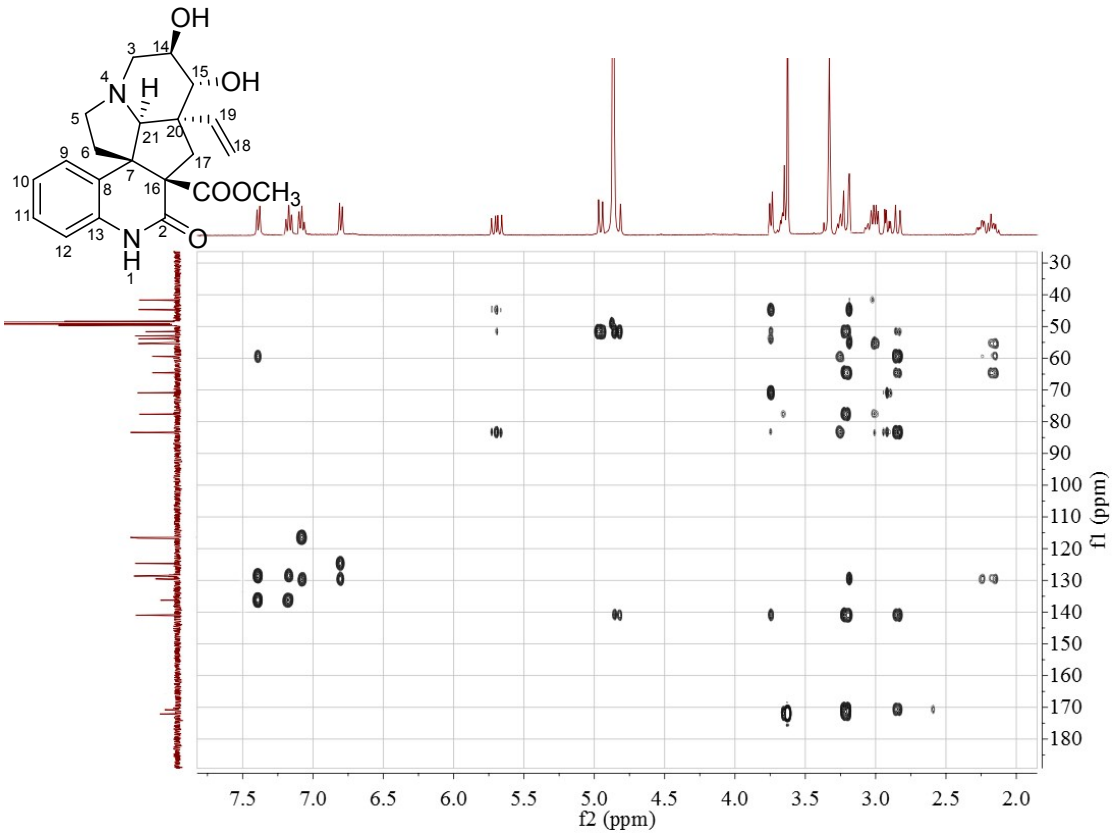
^{13}C NMR spectrum of **8** (100 Hz, CD_3OD)



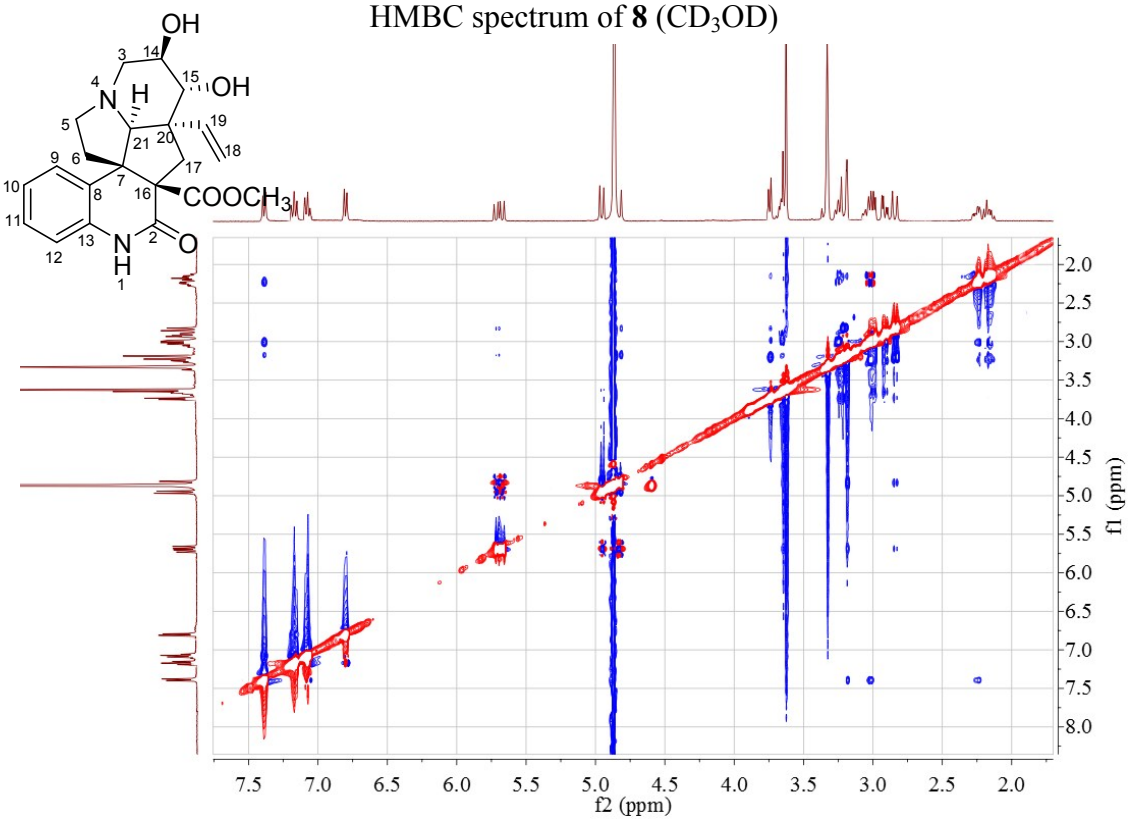
^{1}H-^{1}H COSY spectrum of **8** (CD_3OD)



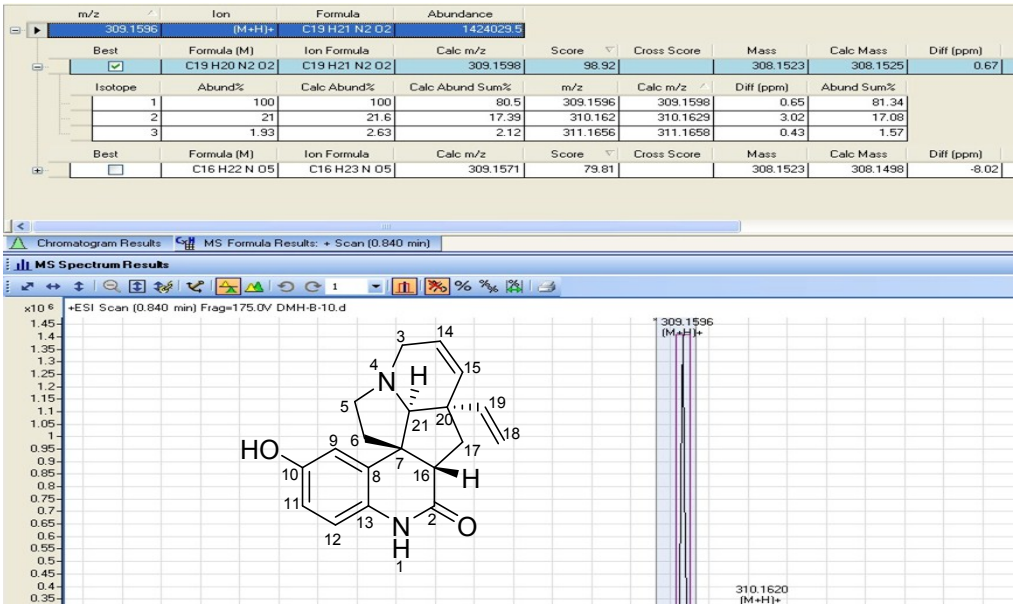
HSQC spectrum of **8** (CD_3OD)



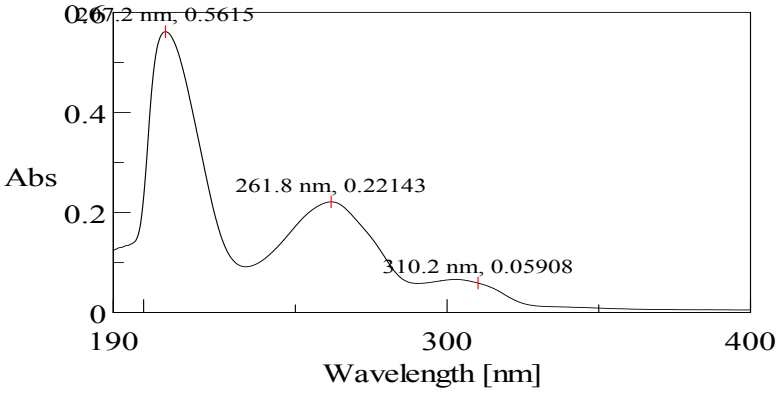
HMBC spectrum of **8** (CD_3OD)



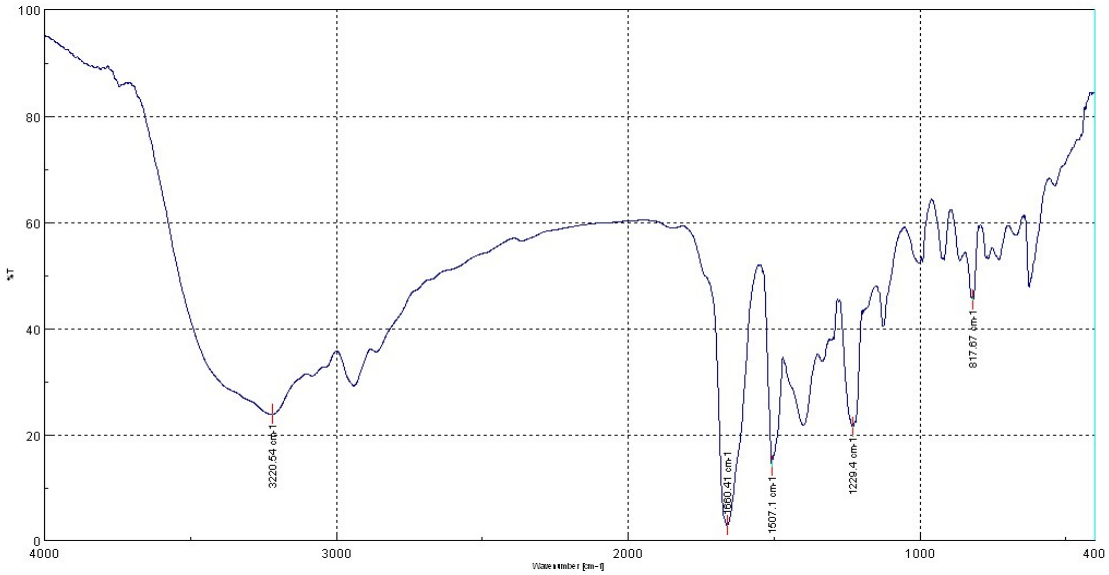
NOESY spectrum of **8** (CD_3OD)



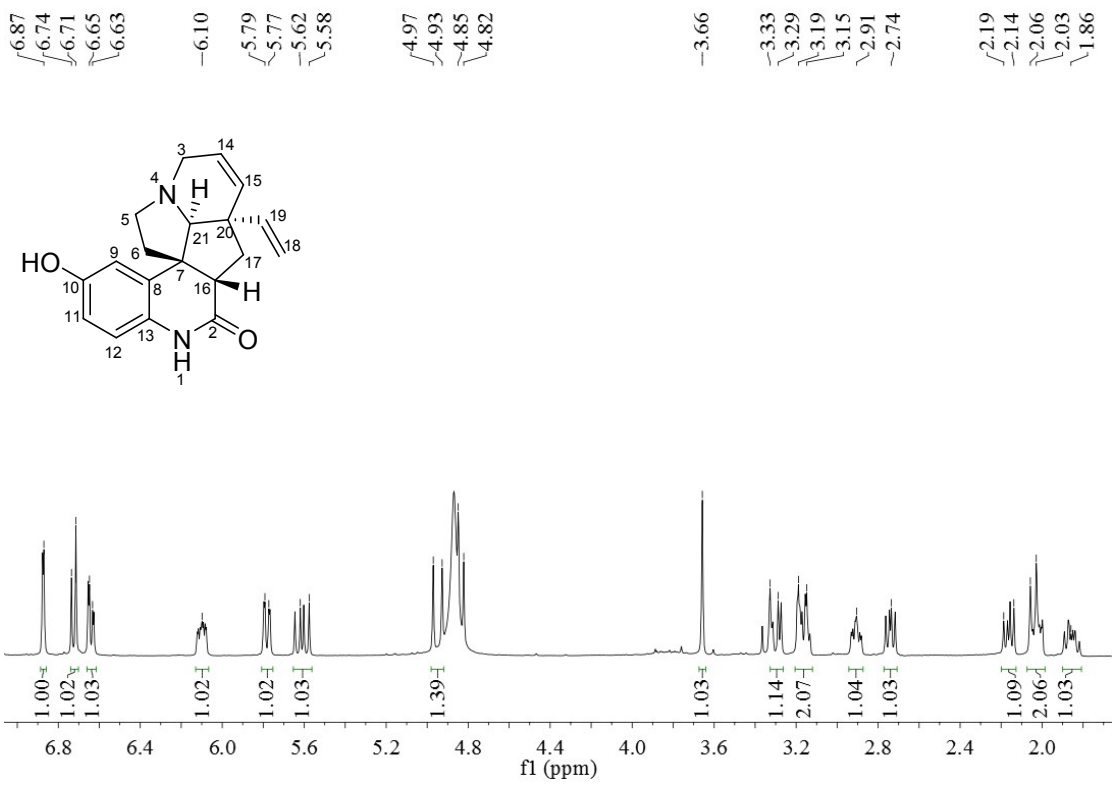
HRESIMS spectrum of **9**



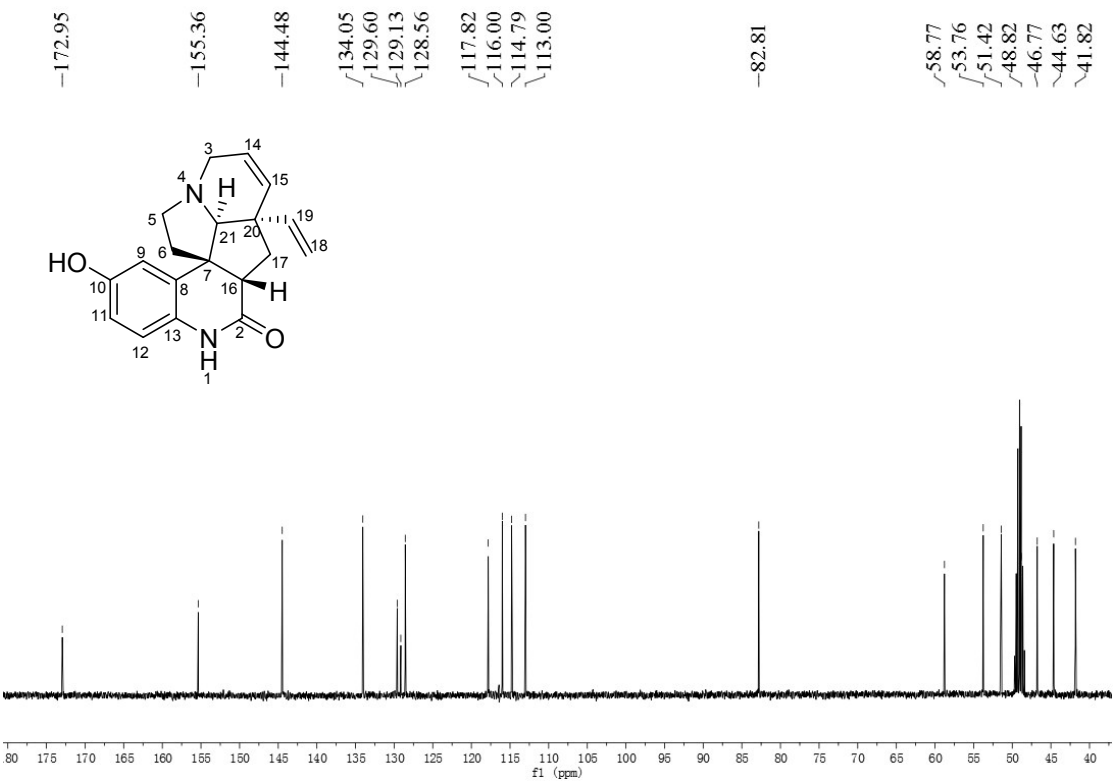
UV spectrum of **9** (MeOH)



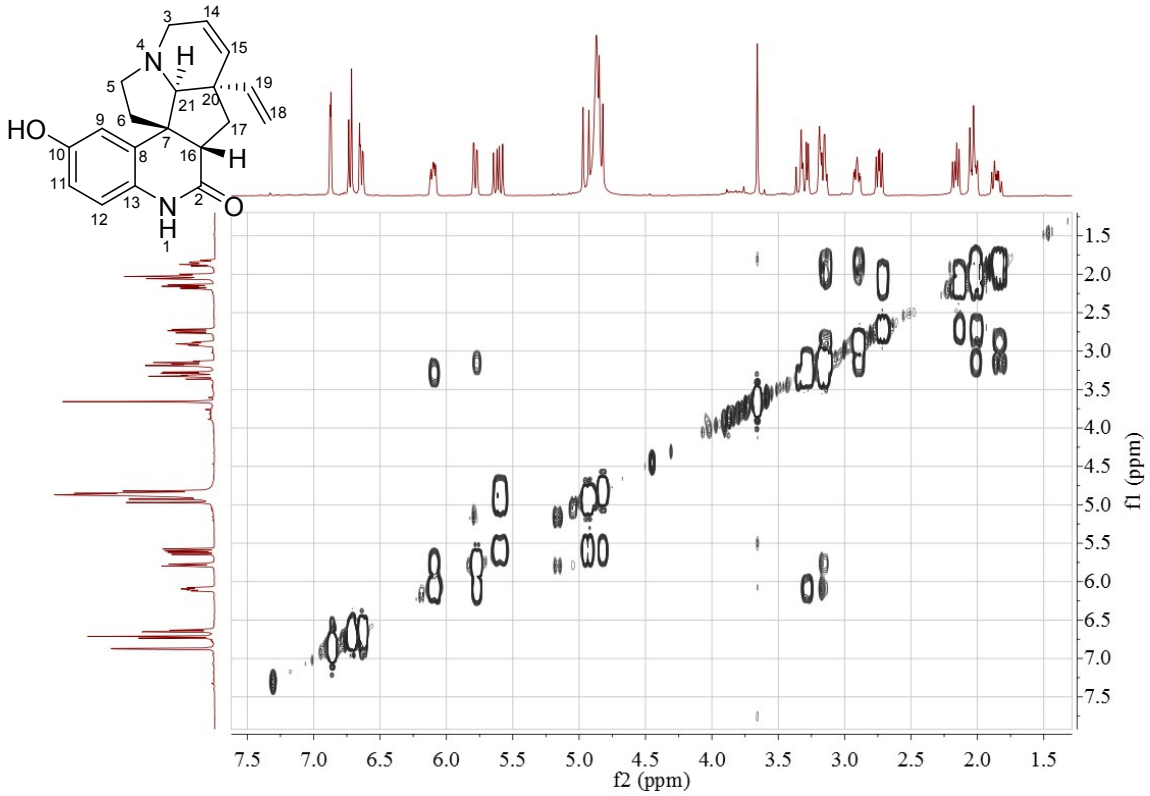
IR spectrum of **9** (KBr disc)



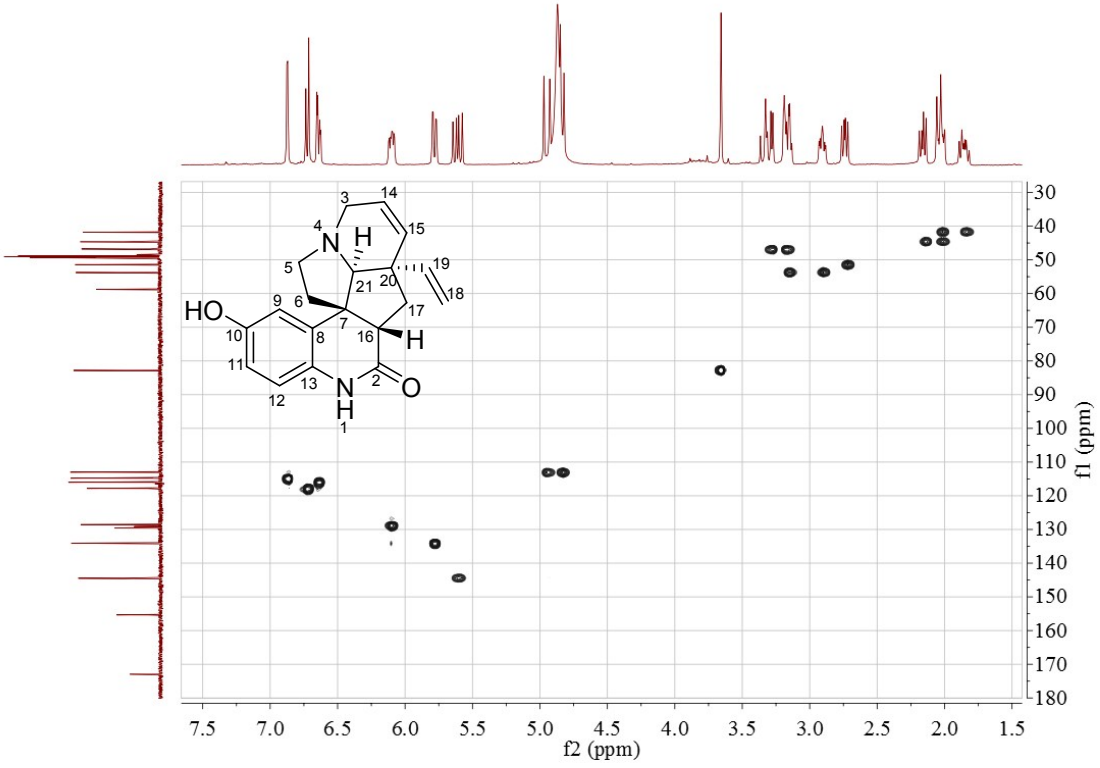
^{1}H NMR spectrum of **9** (400 Hz, CD_3OD)



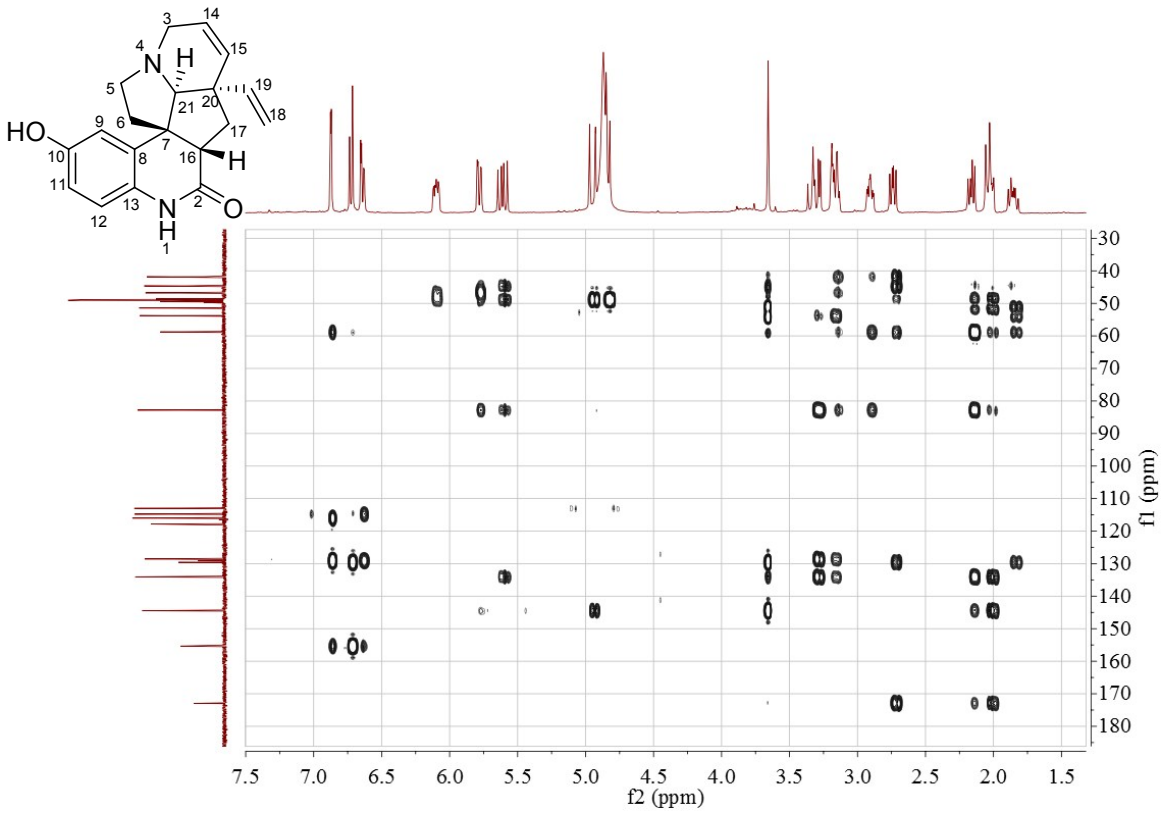
^{13}C NMR spectrum of **9** (100 Hz, CD_3OD)



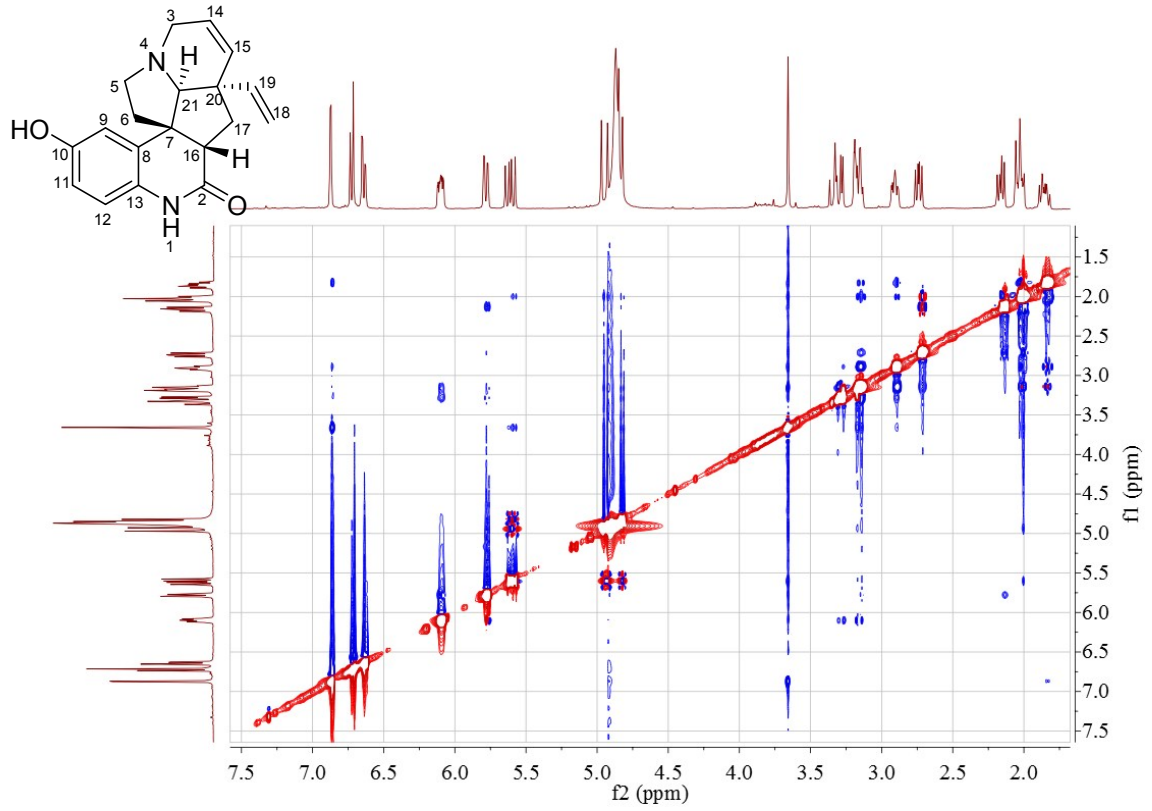
^{1}H-^{1}H COSY spectrum of **9** (CD_3OD)



HSQC spectrum of **9** (CD_3OD)



HMBC spectrum of **9** (CD_3OD)



NOESY spectrum of **9** (CD_3OD)