Supporting Information

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Chemical Constituents from the Roots of *Clausena excavata* and Their Cytotoxicity

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Isolations of compounds **1**-**18**

The air-dried roots of *C. excavata* were extracted with acetone over a period of 3 days at room temperature. Removal of the solvent under reduced pressure provided acetone extract (288.02 g) which was further chromatographed by quick column chromatography (QCC) over silica gel eluting with a gradient of *n*-hexane-acetone (100% *n*-hexane to 100% acetone) to afford 19 fractions (A-S). Fraction G (10.68 g) was performed by QCC with 2% EtOAc-*n*-hexane to 100% EtOAc yielded 6 subfractions (G1-G6). Subfraction G2 (23.9 mg) was fractionated by repeated column chromatography (CC) with 24% CH_2Cl_2-*n*-hexane to give compound **11** (2.6 mg) whereas compounds **3** (17.3 mg), **5** (30.0 mg) and **18** (39.8 mg) were obtained from subfraction G4 (1.82 g) by repeated CC using 6% EtOAc-*n*-hexane. Subfraction G6 (400.5 mg) was washed with *n*-hexane to give compound **2** (308. 0 mg).

Fraction J (5.74 g) was subjected to QCC with a gradient of EtOAc and *n*-hexane (100% *n*-hexane to 100% EtOAc) afforded 8 subfractions (J1-J8). Subfraction J5 (292.7 mg) was further purified by QCC with 12% EtOAc-*n*-hexane to give compound **13** (46.0 mg) and 10 subfractions (J5.1-J5.10). Subfraction J5.5 (10.0 mg) was washed with *n*-hexane to yield compound **17** (4.4 mg). Compounds **7** (4.6 mg) and **11** (29.1 mg) were obtained from subfractions J5.9 (22.8 mg) and J5.7 (35.5 mg), respectively by CC with 12% acetone-*n*-hexane. Subfraction J5.7 (2.50 g) was recrystallized with CH_2Cl_2 to yield compound **4** (2.24 g). Subfraction J5.9 (192.7 mg) was subjected to CC with 4% acetone-CH_2Cl_2 to effort 6 subfractions (J5.9.1-J5.9.6). Compounds **1** (4.4 mg) and **12** (13.5 mg) were obtained from subfractions J5.9.3 (22.0 mg) and J5.9.4 (38.0 mg), respectively by recrystallized with CH_2Cl_2 while compound **8** (2.9 mg) was isolated from subfraction J5.9.6 (17.0 mg) by CC with 22% acetone-*n*-hexane. Subfraction J5.10 (59.1 mg) was further purified by CC with 3% acetone-*n*-hexane to give compound **9** (8.5 mg).

Fraction N (8.11 g) was chromatographed by QCC with 20% EtOAc-*n*-hexane to 100% EtOAc afforded 5 subfractions (N1-N5). Subfraction N5 (200.0 mg) was purified by CC with 90% CH_2Cl_2-*n*-hexane to yield 5 subfractions (N5.1-N5.5). Compounds **6** (8.1 mg) and **14** (12.0 mg) were obtained from subfractions N5.3 (10.0 mg) and N5.1 (20.0 mg), respectively, by recrystallization with CH_2Cl_2. Compound **16** (17.6 mg) was isolated from subfraction 5.5 (32.0 mg) by CC with 30% acetone-*n*-hexane whereas compound **15** (39.0 mg) was isolated from fraction S (1.05 g) by CC with 30% acetone-*n*-hexane.

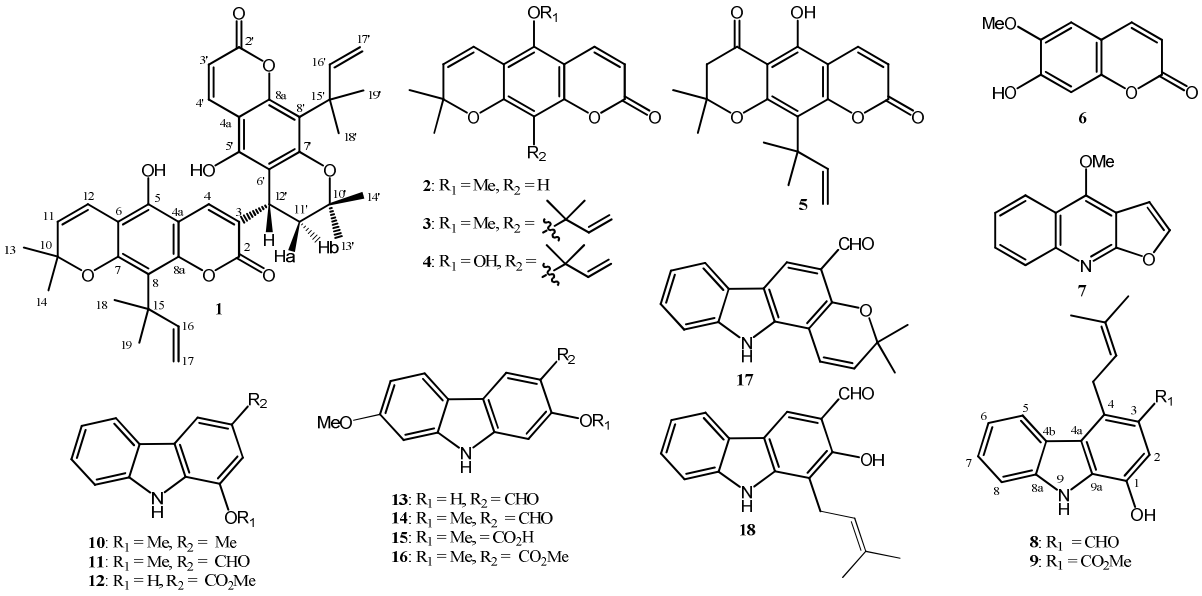


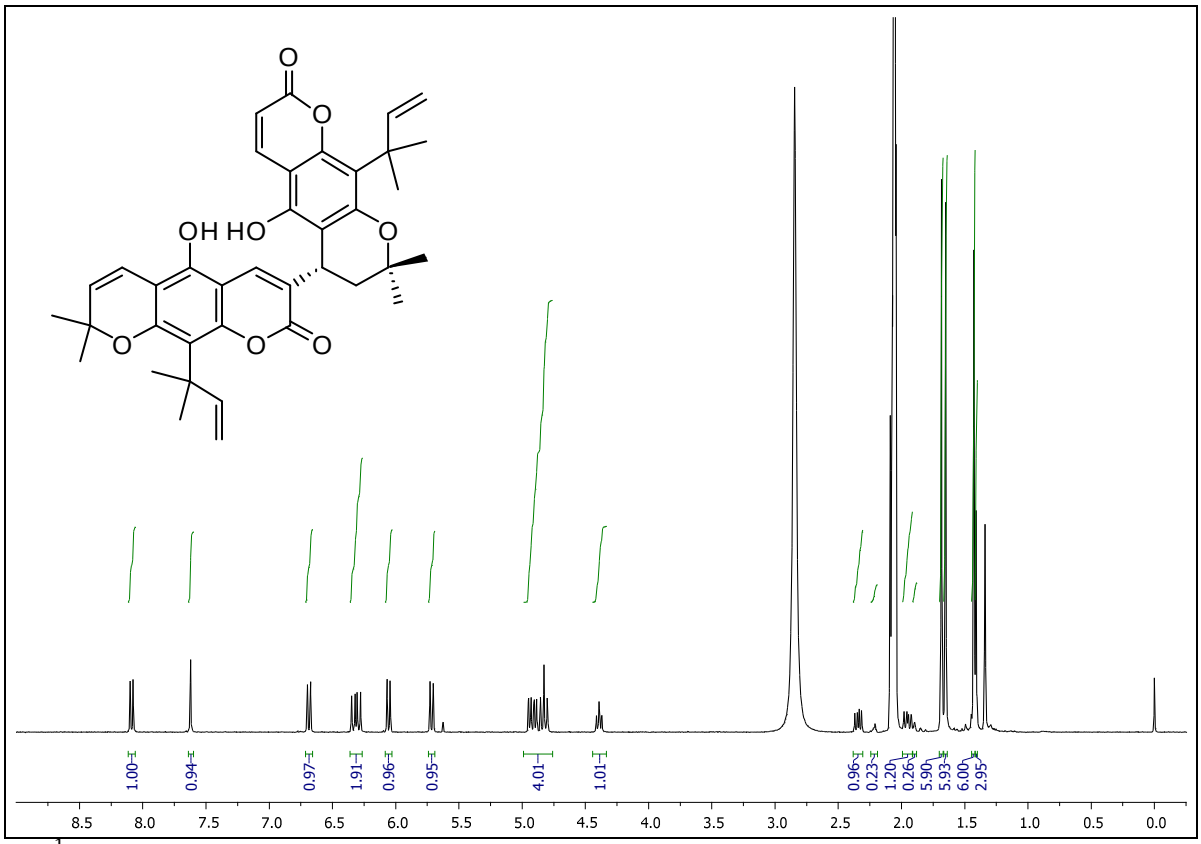
Figure 1. The structures of compounds **1**-**18**.

Table 2. ^{1}H, ^{13}C NMR and HMBC spectral data of **1** in acetone-d_6

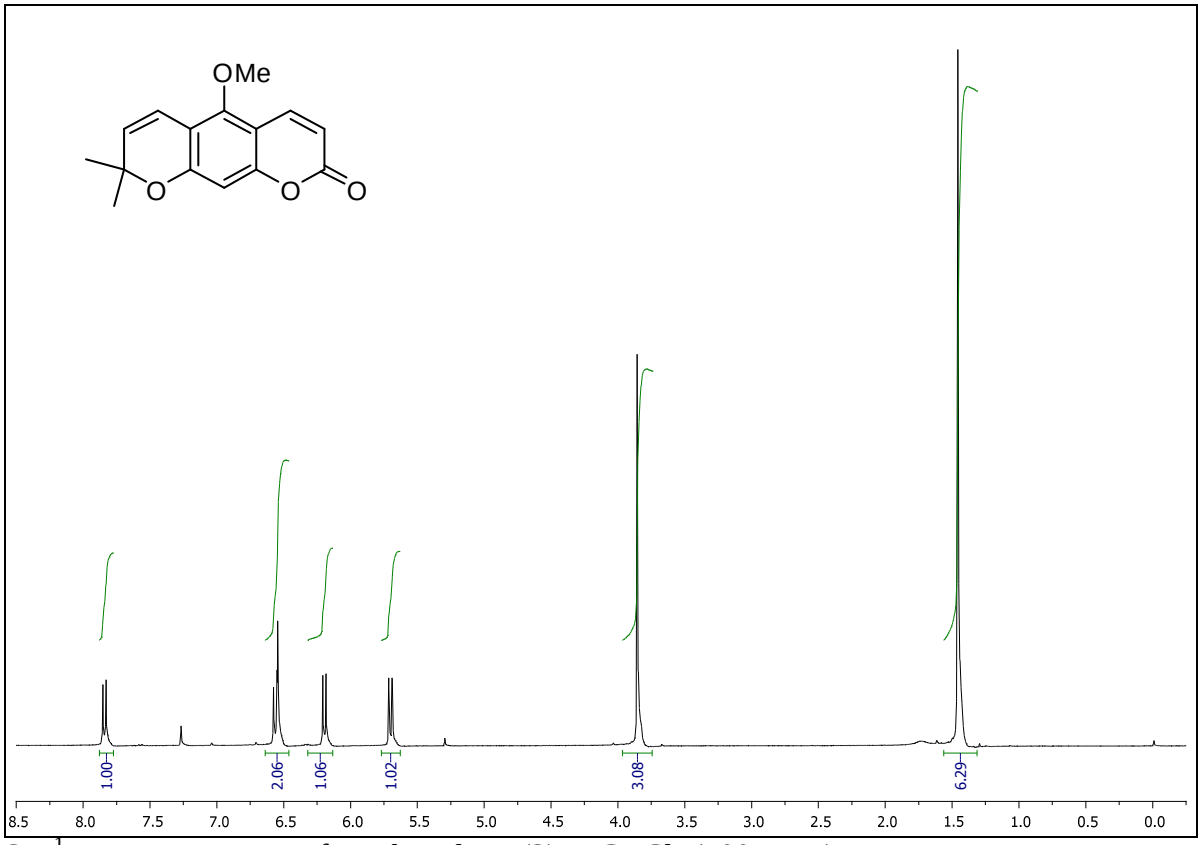
Position	δ_H (mult., *J* in Hz)[a]	δ_C[b]	HMBC
2	-	161.2[1]	-
3	-	126.2	-
4	7.61 (1H, s)	133.9	C-2, C-3,C-4a, C-5, C-8a, C-12'
4a	-	107.6[2]	-
5	-	151.1[3]	-
6	-	108.1[4]	-
7	-	159.9[5]	-
8	-	115.7	-
8a	-	156.3[6]	-
10	-	76.6[7]	-
11	5.71 (1H, d, 10.0)	129.7	C-6, C-10, C-13, C-14
12	6.68 (1H, d, 10.0)	117.0	C-5, C-6, C-7, C-10
13 and 14	1.42 (6H,s)	27.4	C-10, C-11, C-13, C-14
15	-	41.8[8]	-
16	6.29 (1H, dd, 16.8, 10.0)	153.1[9]	C-15, C-18, C-19
17	4.91 (1H, dd, 16.8, 1.2) 4.82 (1H, dd, 10.0, 1.2)	110.1[10]	C-15, C-16
18 and 19	1.64 (6H, s)	30.3	C-8, C-15, C-16, C-18, C-19
2'	-	160.7[1]	-
3'	6.05 (1H, d, 9.6)	110.4	C-2', C-4'a
4'	8.08 (1H, d, 9.6)	140.1	C-2', C-5', C-4'a, C-8'a
4'a	-	107.5[2]	-
5'	-	151.2[3]	-
6'	-	107.8[4]	-
7'	-	159.0[5]	-
8'	-	115.7	-
8'a	-	155.1[6]	-
10'	-	77.1[7]	-

11'a	2.33 (1H, dd, 13.6, 7.6)	40.3	C-3, C-6', C-12', C-10' C-13', C-14'
11'b	1.94 (1H, dd, 13.6, 8.8)		
12'	4.38 (1H, dd, 7.6, 8.8)	31.7	C-2, C-3, C-4, C-6', C-7', C-11'
13'	1.40 (3H, s)	30.1	C-10', C-11', C-14'
14'	1.33 (3H, s)	24.9	C-10', C-11', C-13'
15'	-	41.5[8]	-
16'	6.29 (1H, dd, 16.8, 10.0)	151.6[9]	C-15', C-18', C-19'
17'	4.91 (1H, ddd, 16.8, 1.2)	108.3[10]	C-15', C-16'
	4.82 (1H, dd, 10.0, 1.2)		
18' and 19'	1.67 (6H, s)	27.6	C-8', C-15', C-16', C-18', C-19'
5-OH	8.49 (1H, brs)[11]	-	-
5'-OH	8.76 (1H, brs)[11]	-	-

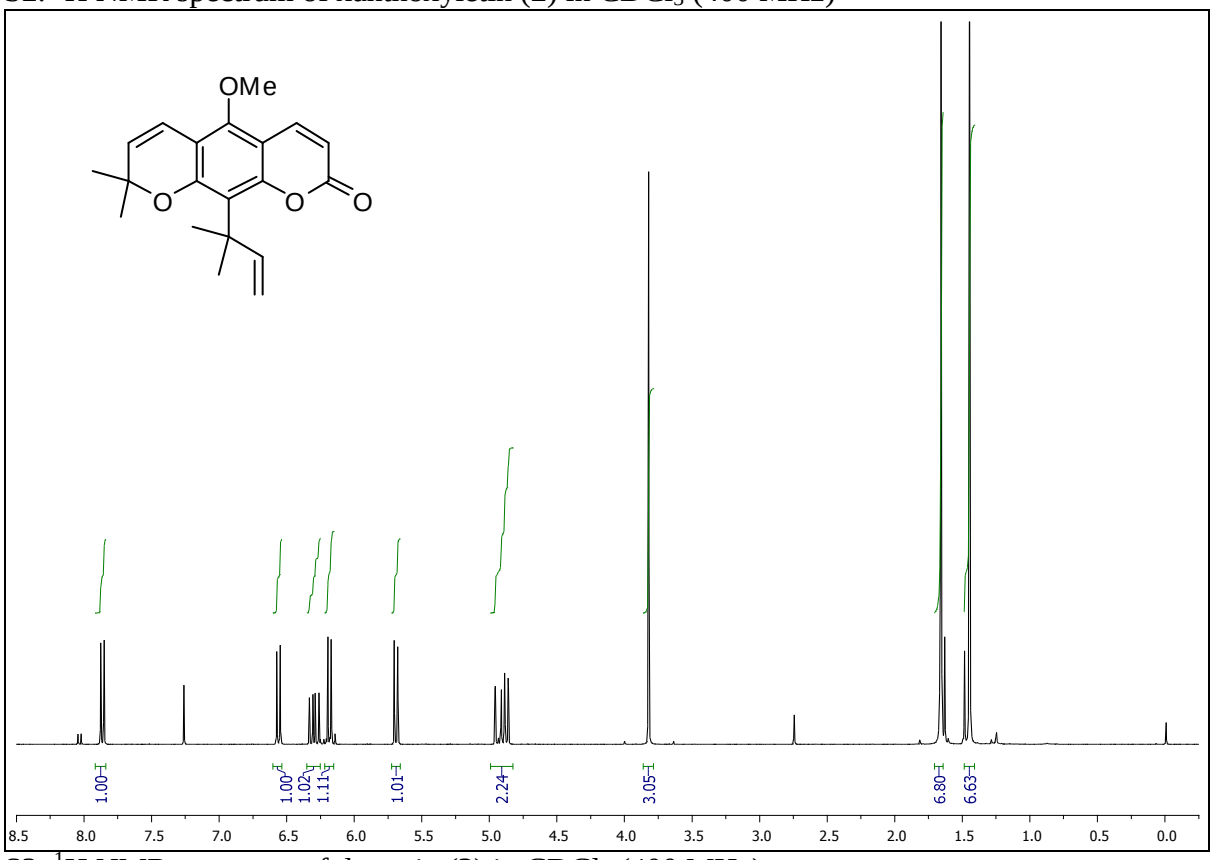
[a]Recorded on 400 MHz Bruker FTNMR Ultra Shield spectrometer. [b]Recorded on 500 MHz Varian UNITY INOVA spectrometer. [1-11] Signal assignment may be interchangeable.



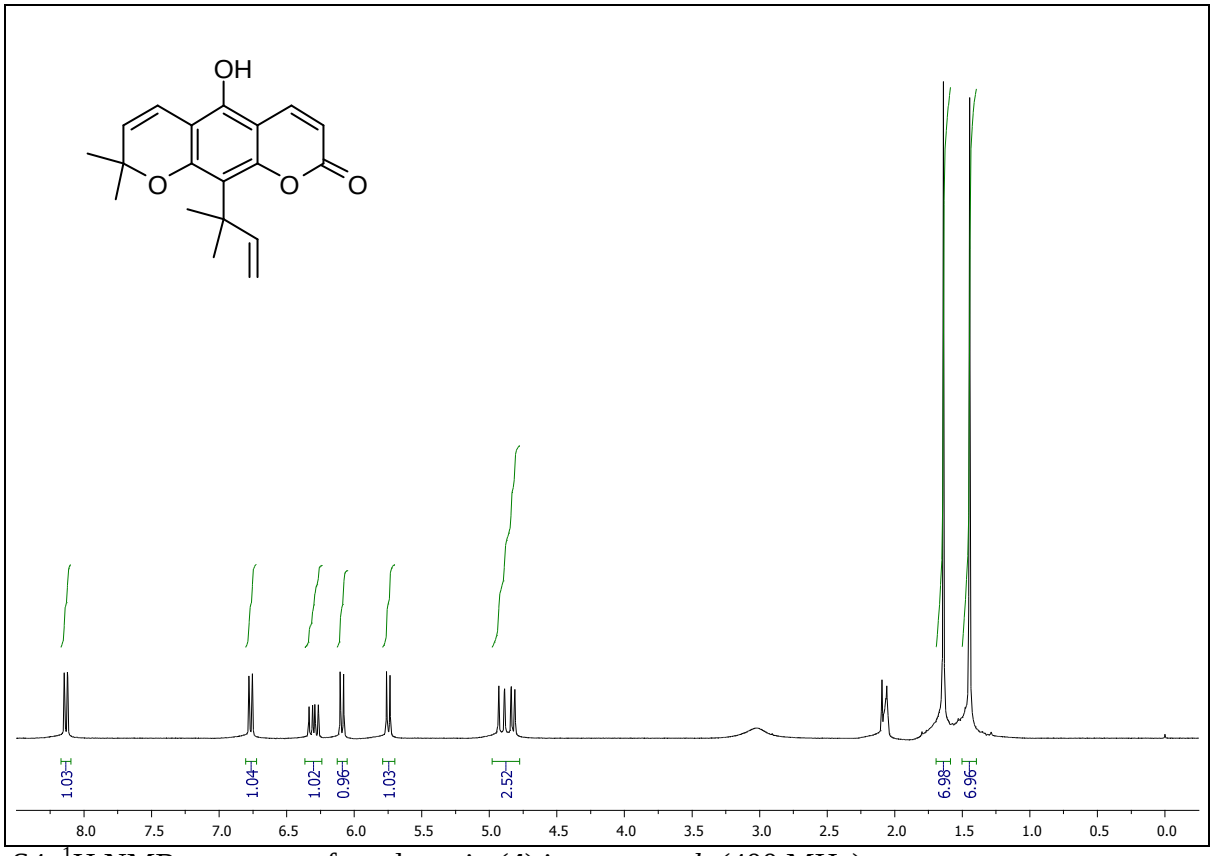
S1. ^{1}H NMR spectrum of binorponcitrin (**1**) in $CDCl_3$ (400 MHz)



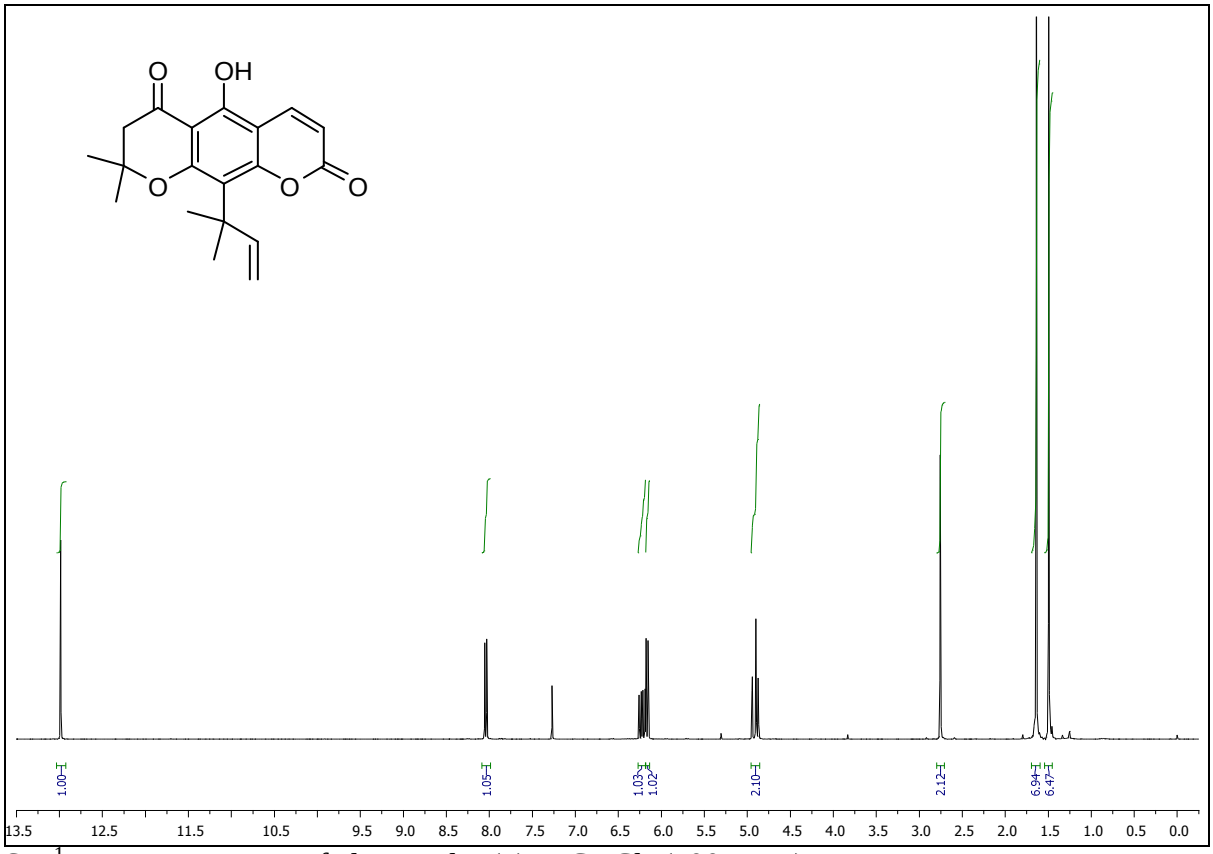
S2. ^{1}H NMR spectrum of xanthoxyletin (**2**) in $CDCl_3$ (400 MHz)



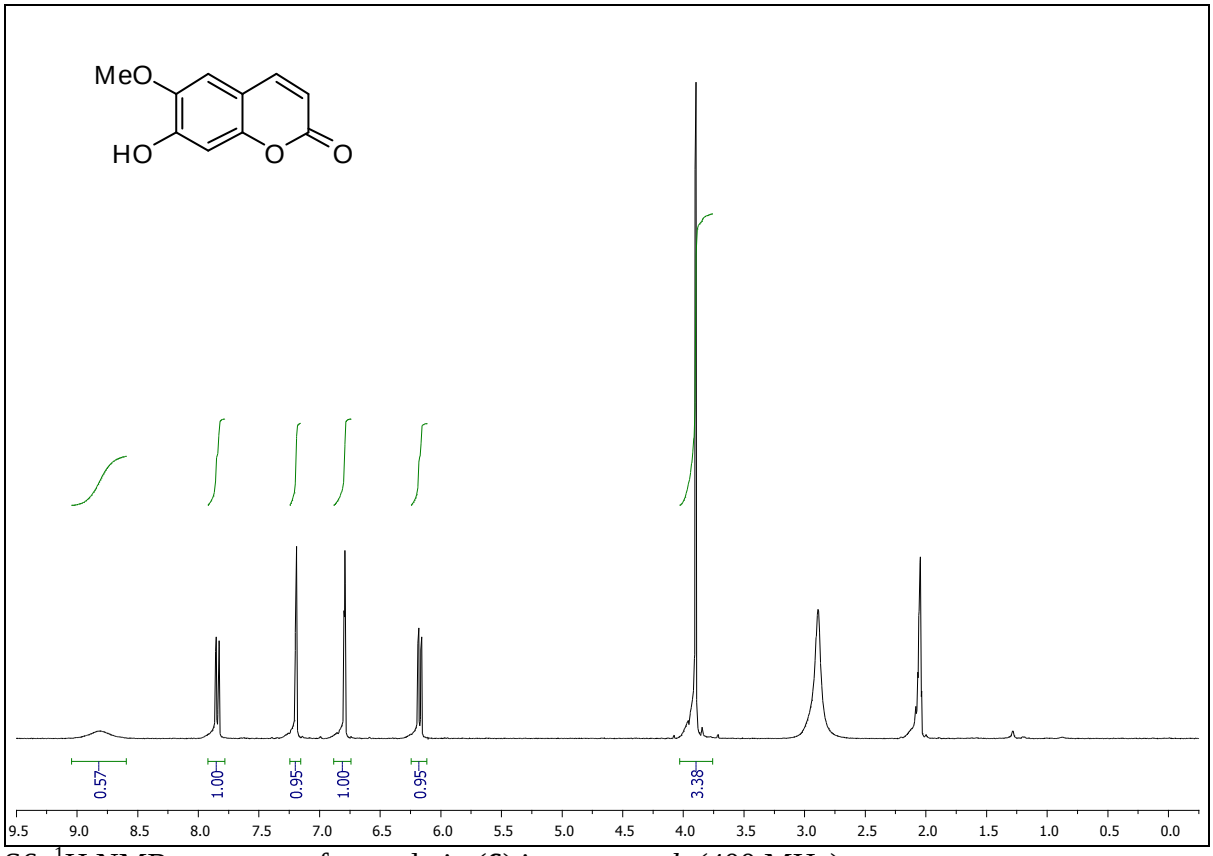
S3. ^{1}H NMR spectrum of dentatin (**3**) in $CDCl_3$ (400 MHz)



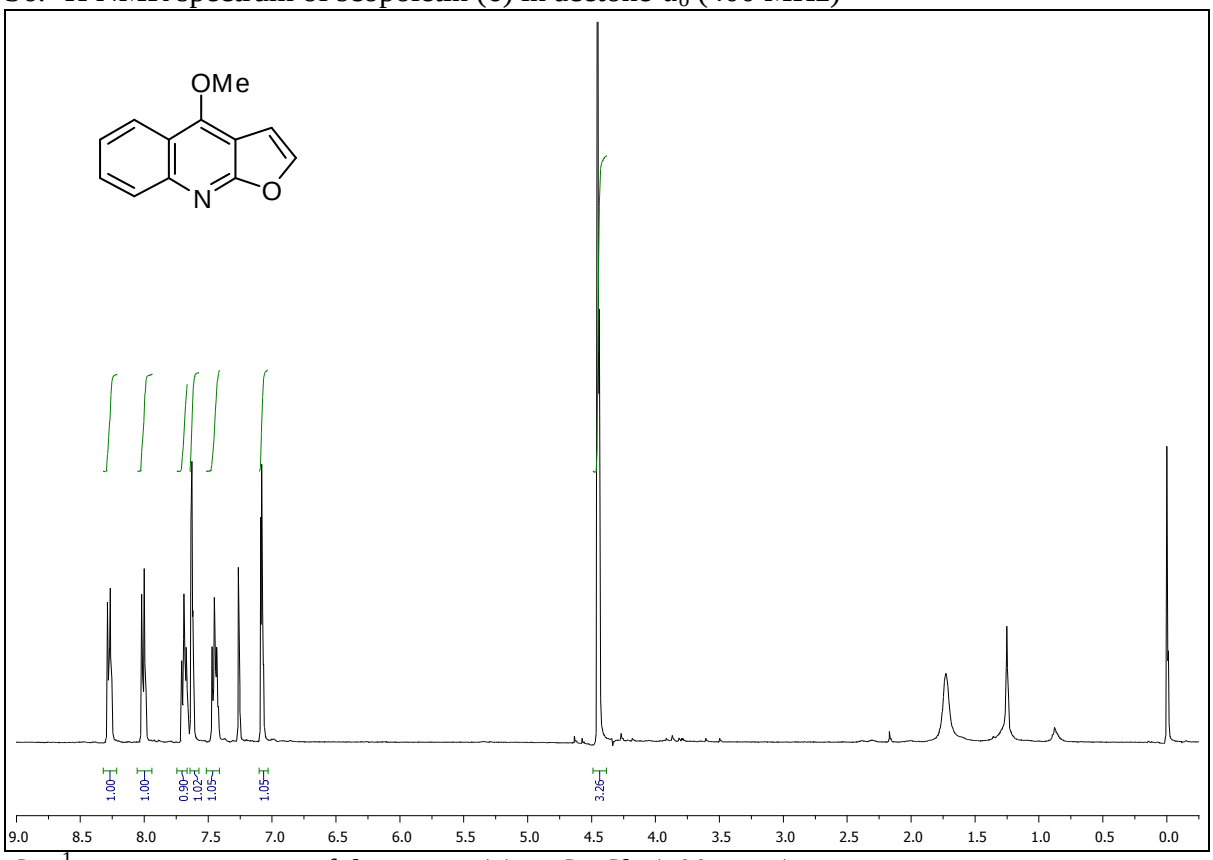
S4. ^{1}H NMR spectrum of nordentatin (**4**) in acetone-d_6 (400 MHz)



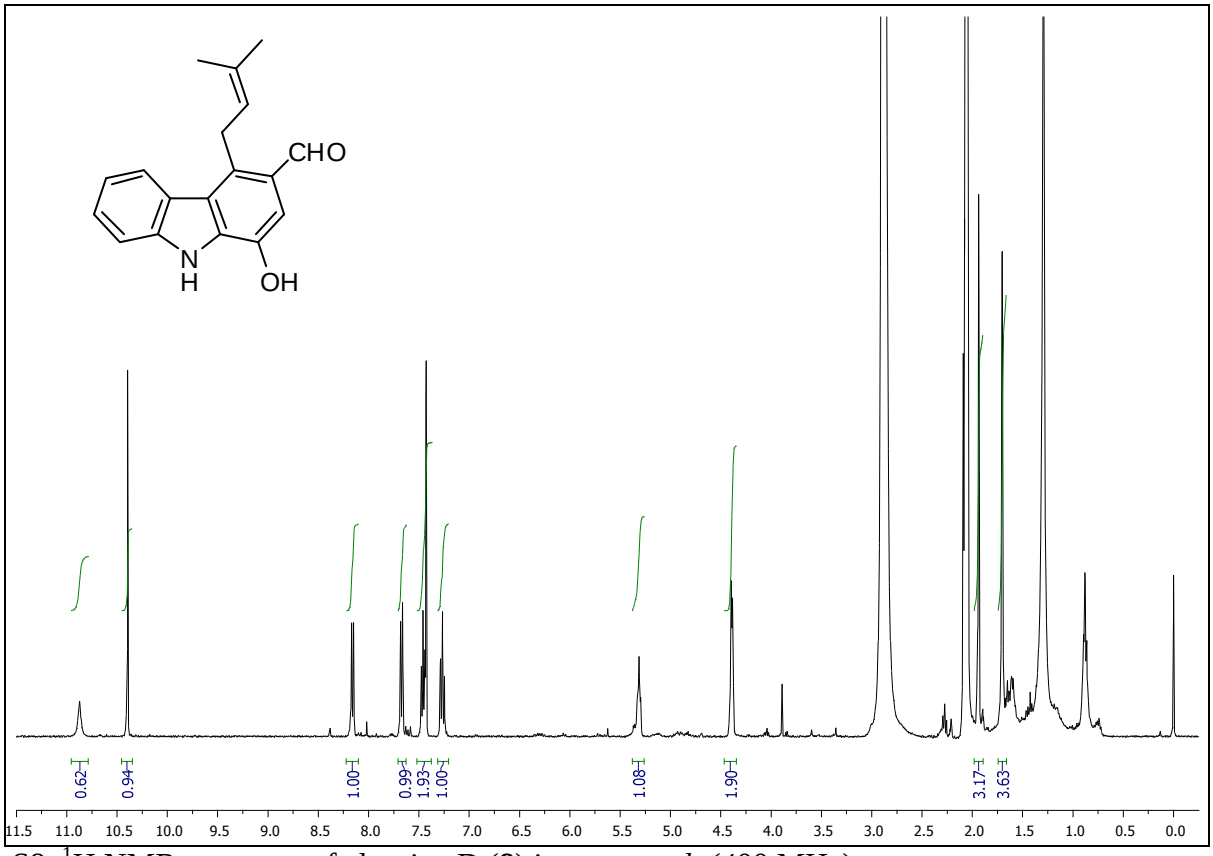
S5. ^{1}H NMR spectrum of clausenidin (**5**) in $CDCl_3$ (400 MHz)



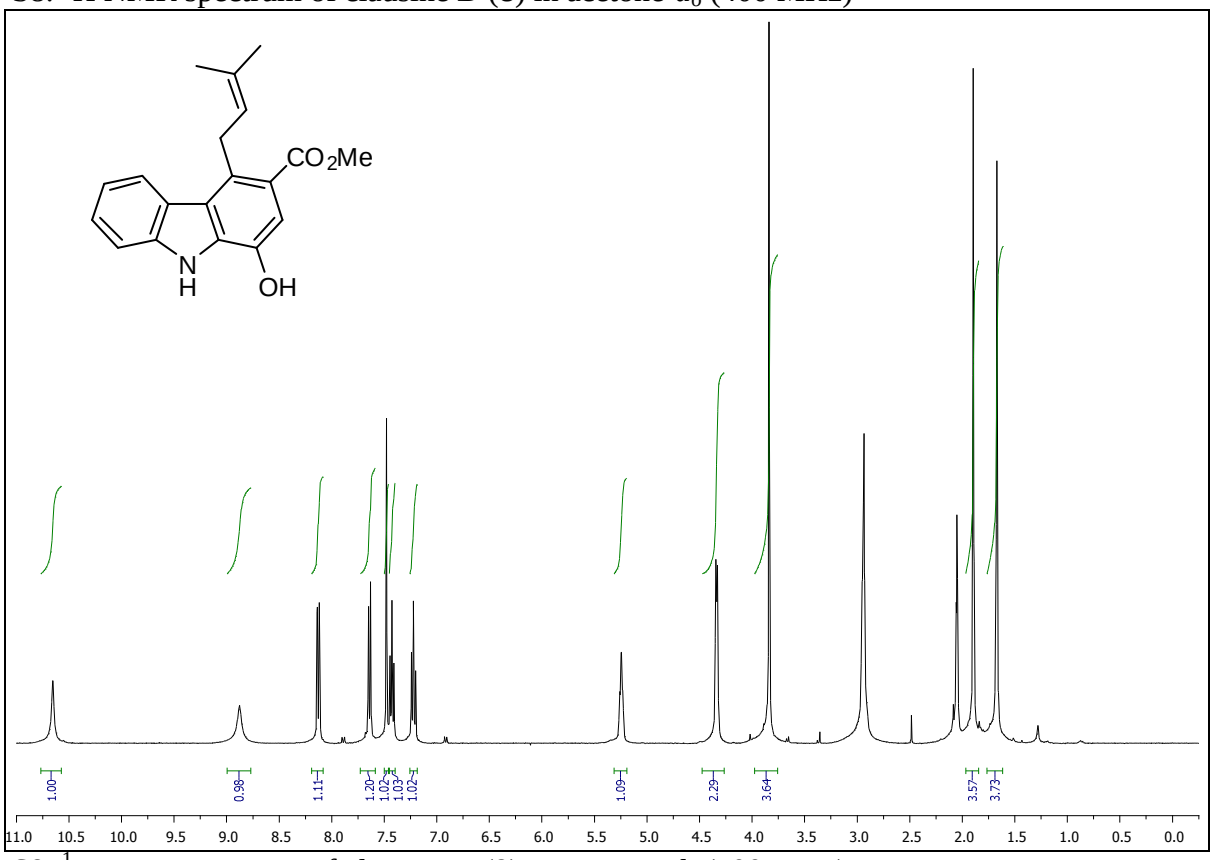
S6. ^{1}H NMR spectrum of scopoletin (**6**) in acetone-d_6 (400 MHz)



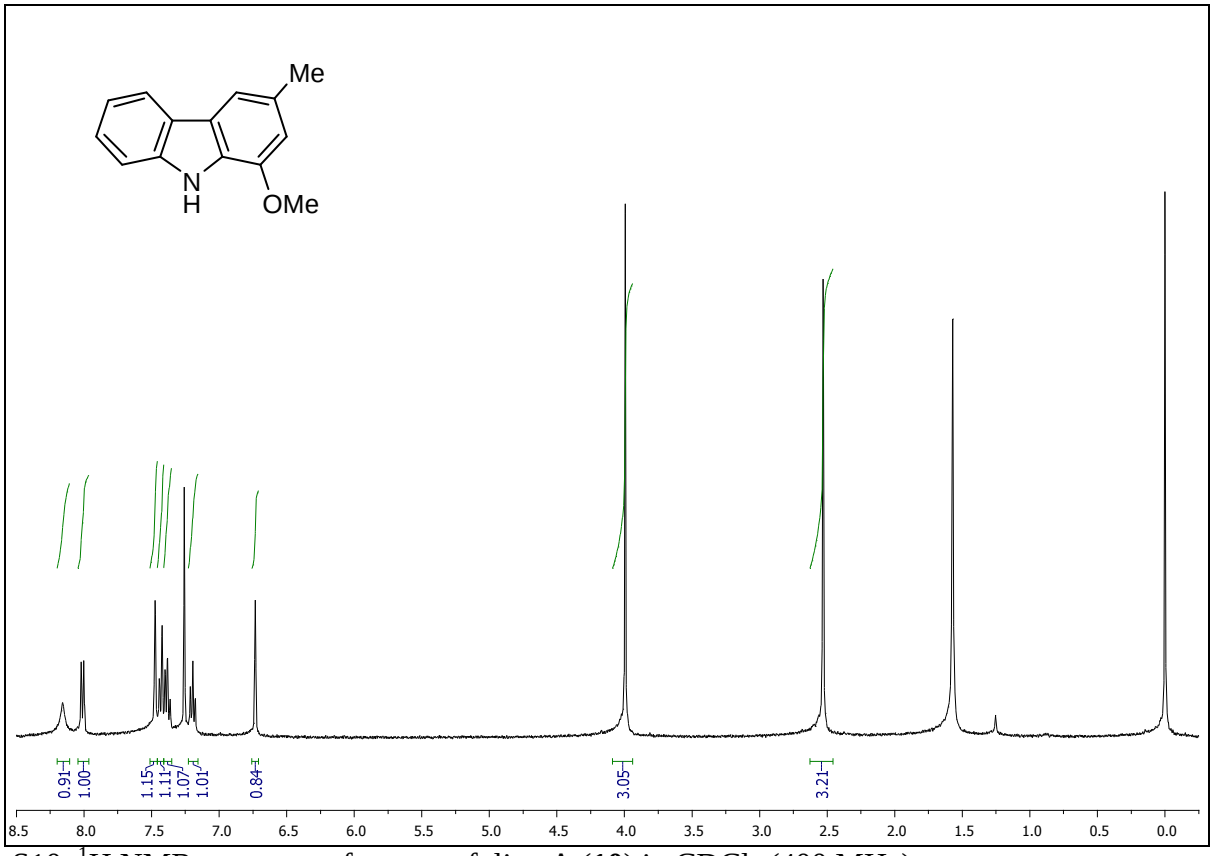
S7. ^{1}H NMR spectrum of dictamine (**7**) in $CDCl_3$ (400 MHz)



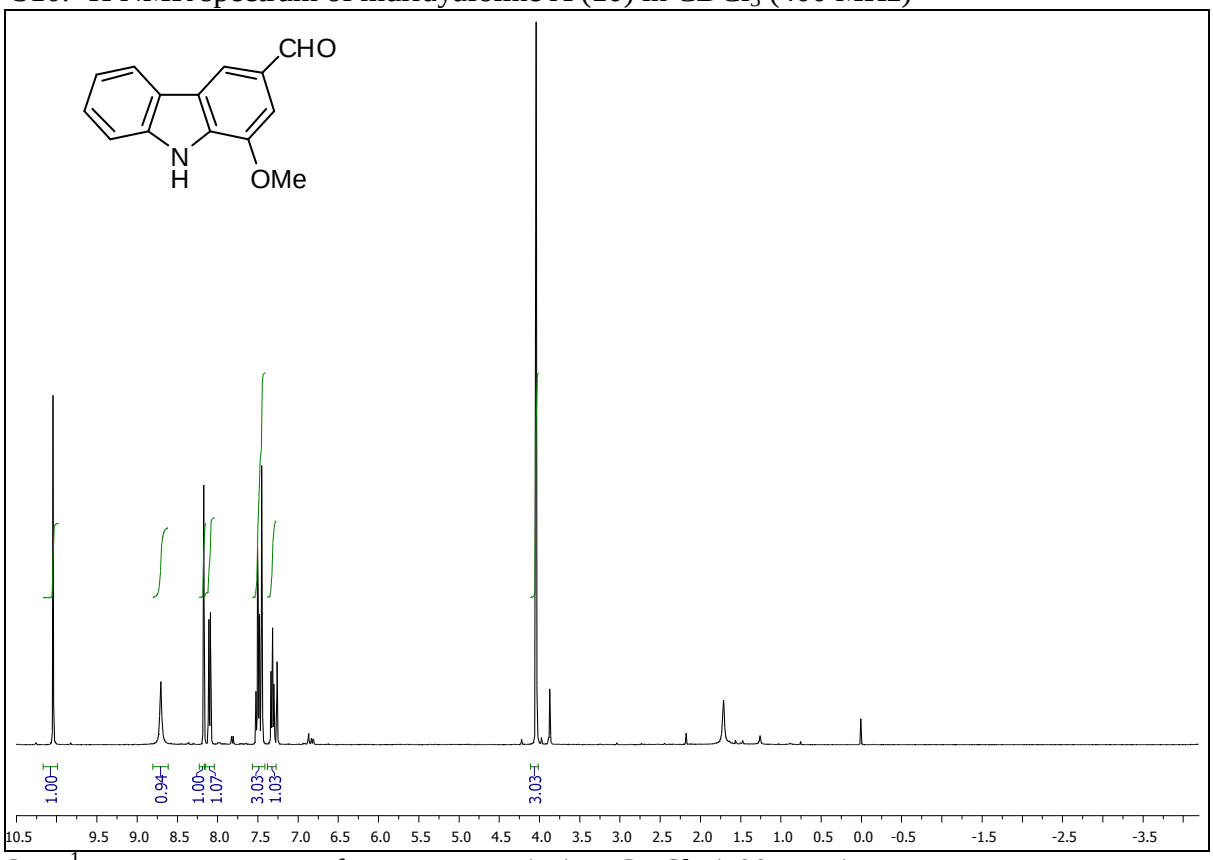
S8. ^{1}H NMR spectrum of clausine D (**8**) in acetone-d_6 (400 MHz)



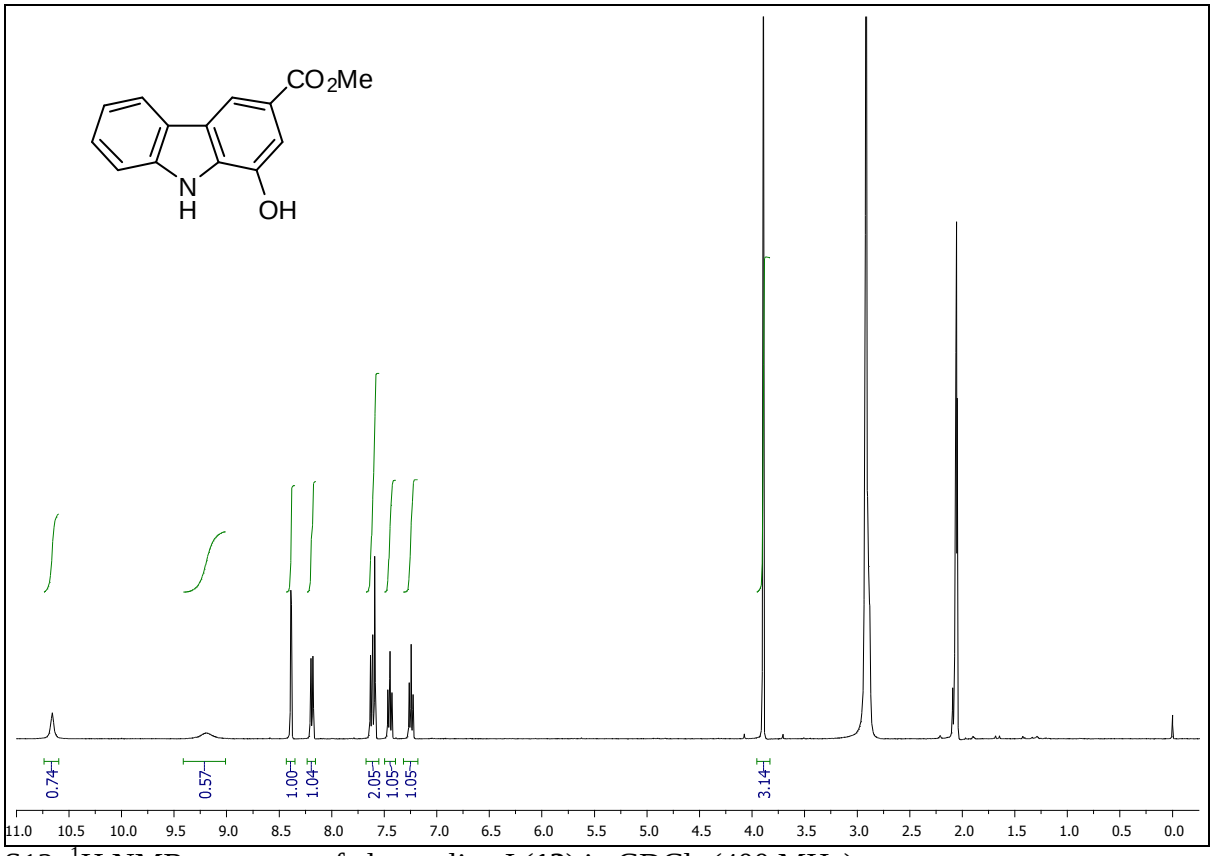
S9. ^{1}H NMR spectrum of clausine F (**9**) in acetone-d_6 (400 MHz)



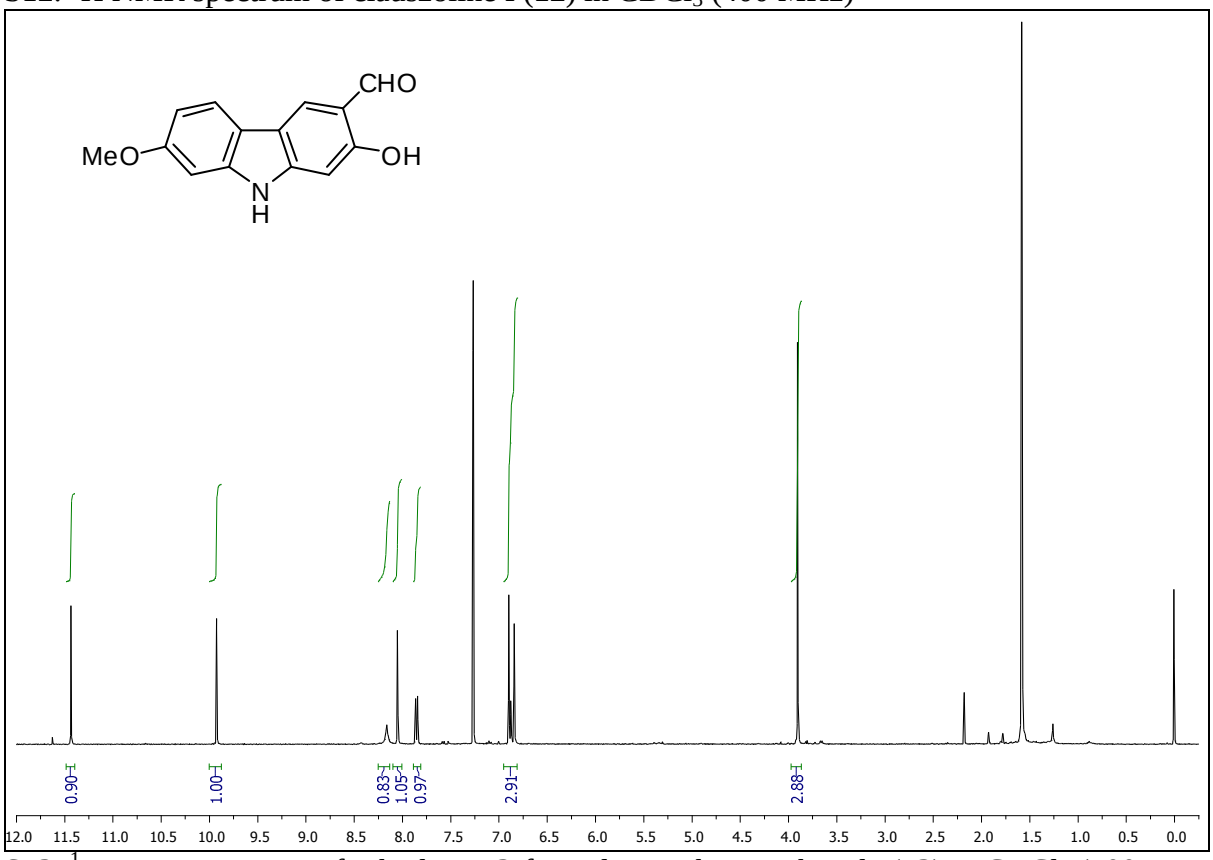
S10. ^{1}H NMR spectrum of murrayafoline A (**10**) in $CDCl_3$ (400 MHz)



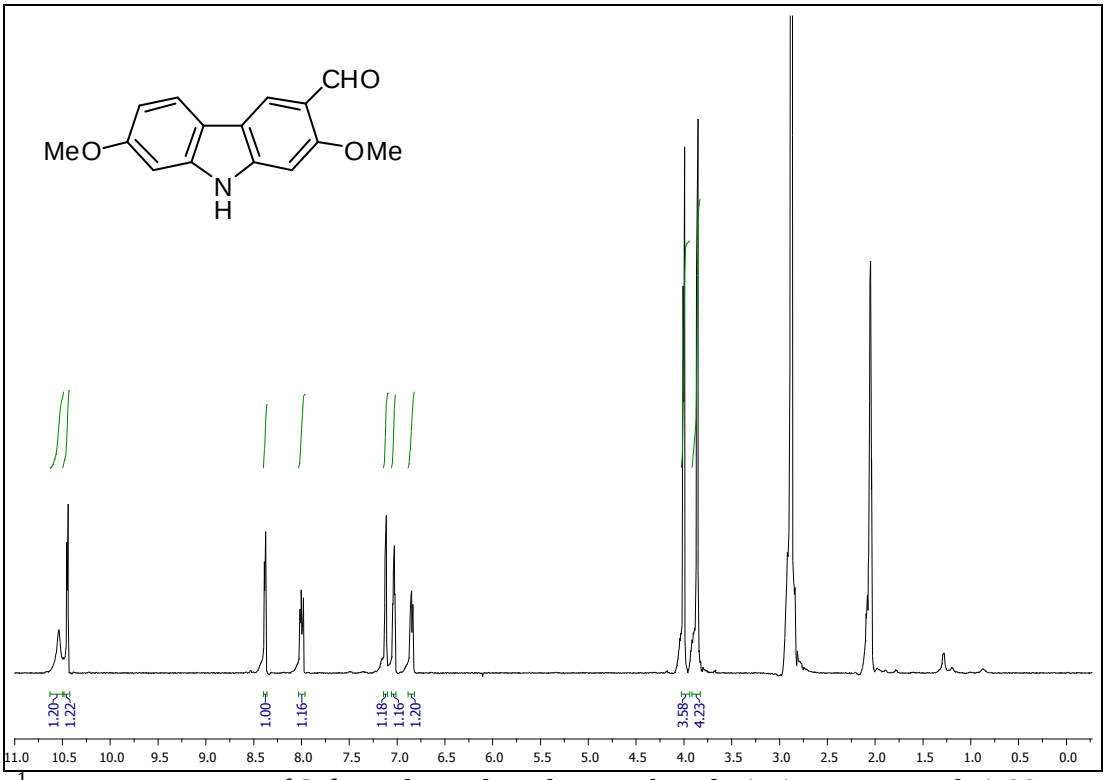
S11. ^{1}H NMR spectrum of murrayanine (**11**) in $CDCl_3$ (400 MHz)



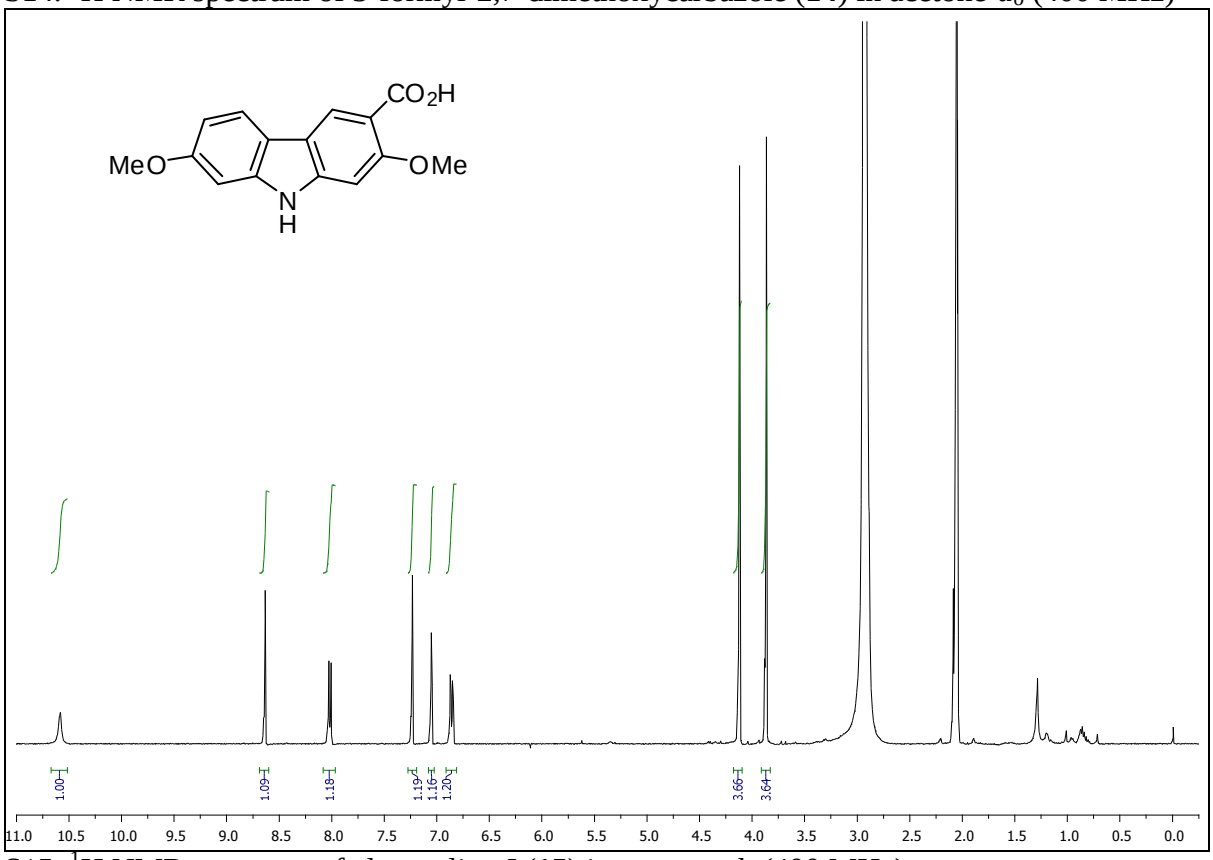
S12. ^{1}H NMR spectrum of clauszoline I (**12**) in $CDCl_3$ (400 MHz)



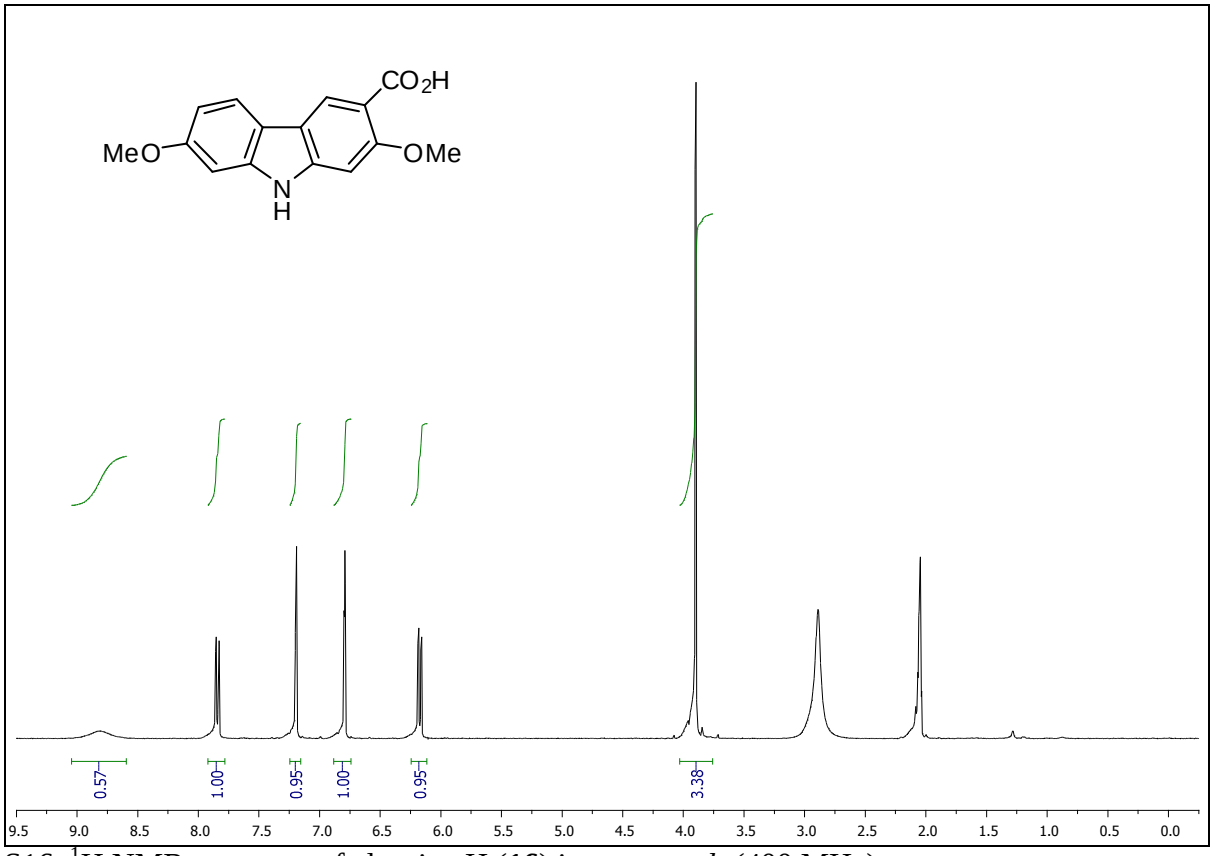
S13. ^{1}H NMR spectrum of 2-hydroxy-3-formyl-7-methoxycarbazole (**13**) in $CDCl_3$ (400 MHz)



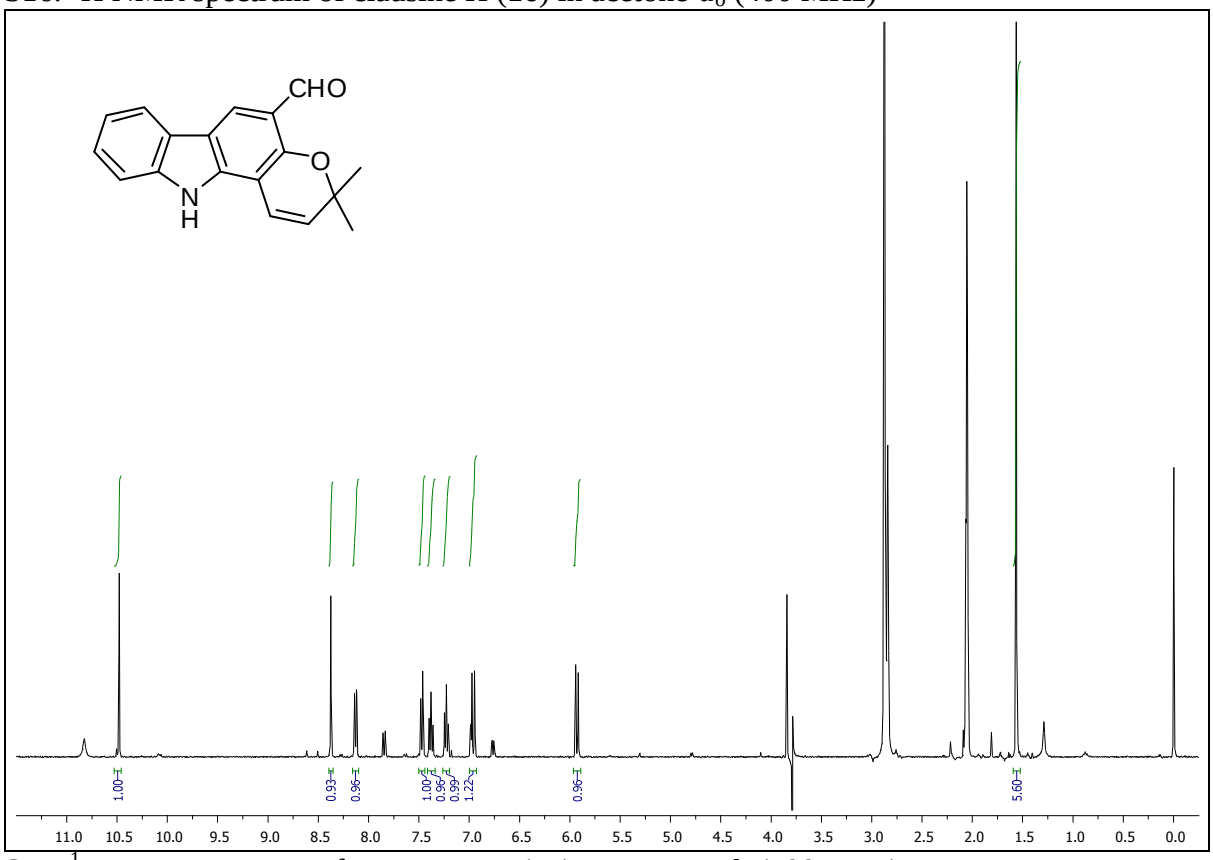
S14. ^{1}H NMR spectrum of 3-formyl-2,7-dimethoxycarbazole (**14**) in acetone-d_6 (400 MHz)



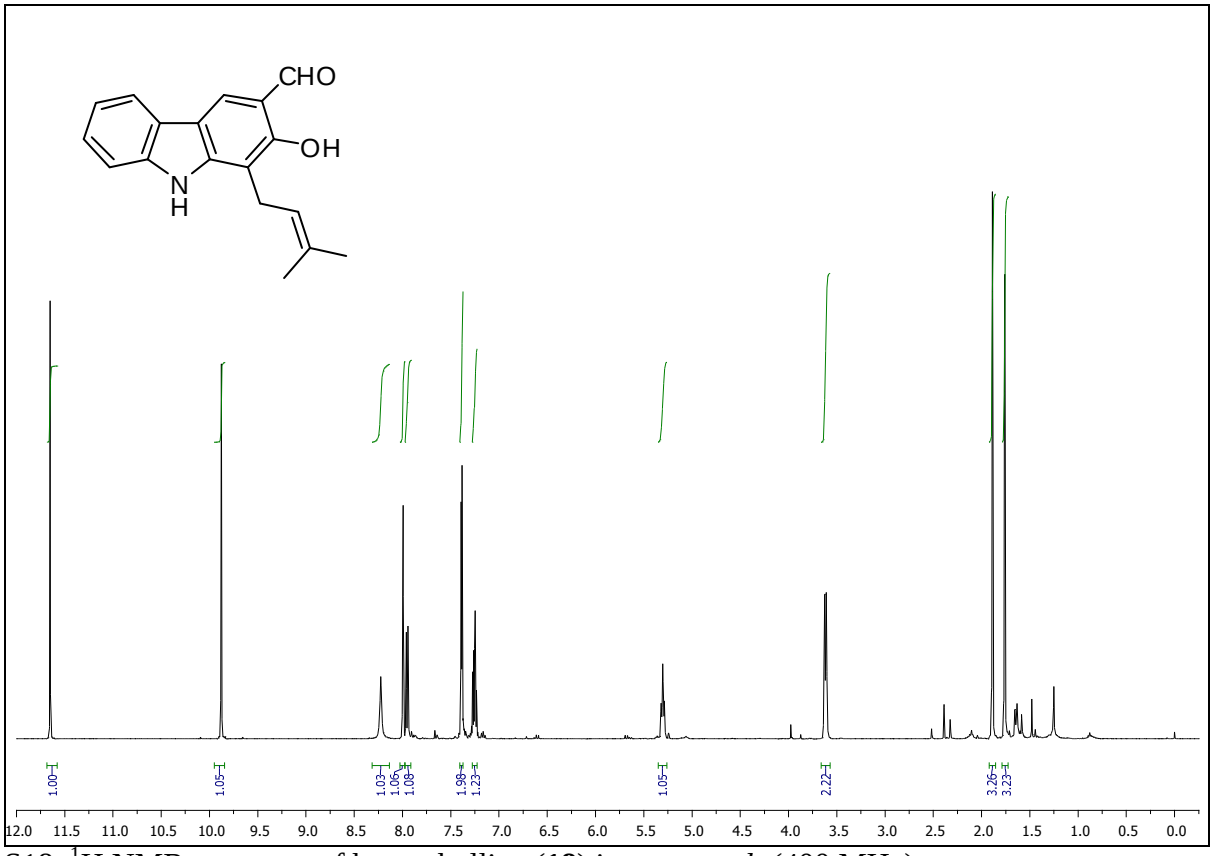
S15. ^{1}H NMR spectrum of clauszoline J (**15**) in acetone-d_6 (400 MHz)



S16. ^{1}H NMR spectrum of clausine H (**16**) in acetone-d_6 (400 MHz)



S17. ^{1}H NMR spectrum of murrayacine (**17**) in acetone-d_6 (400 MHz)



S18. ^{1}H NMR spectrum of heptaphylline (**18**) in acetone-d_6 (400 MHz)