SUPPLEMENTARY MATERIAL

Article

Bioactive metabolites of the stem bark of *Strychnosaff. darienensis* and evaluation of their antioxidant and UV protection activity in human skin cell cultures

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Figure S1: The extraction procedure using different pH treatments

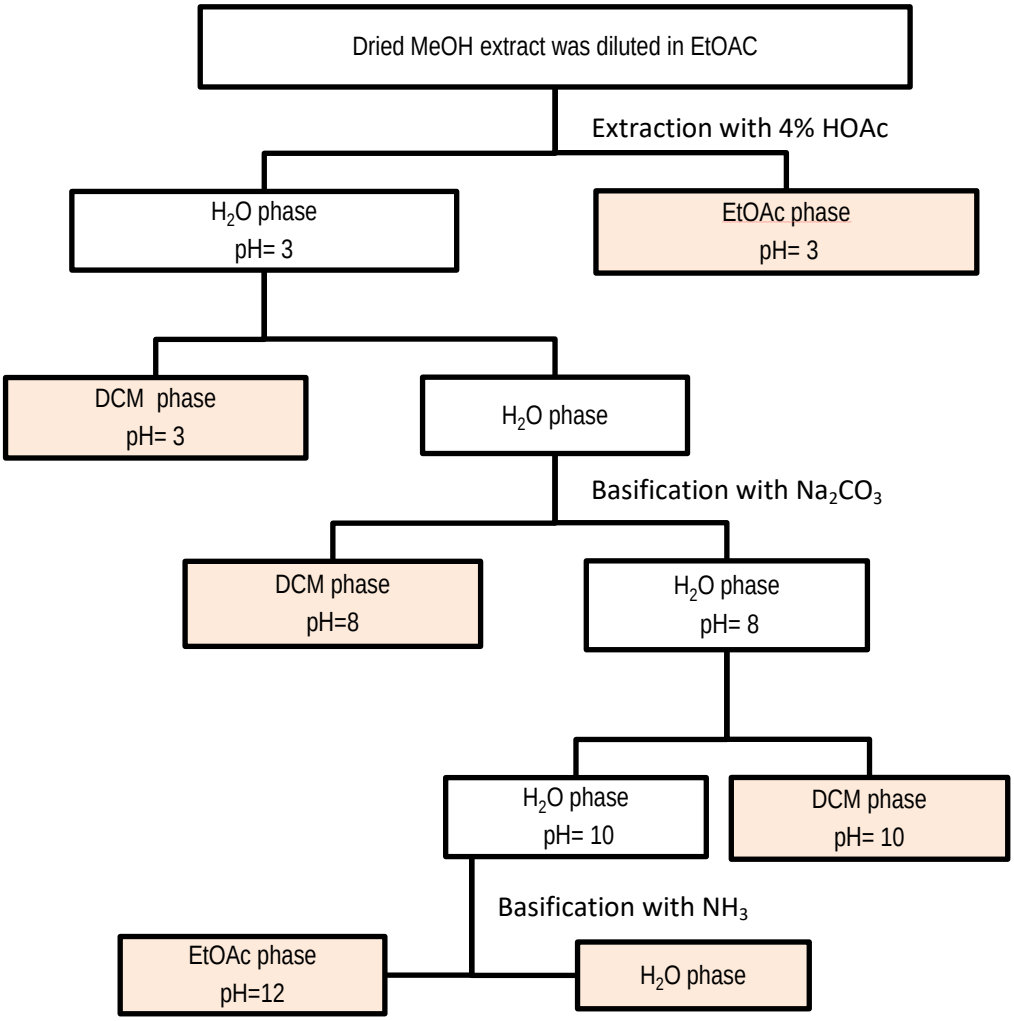
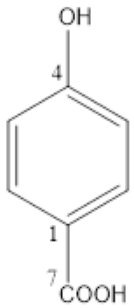


Table S1: FCPC gradient system used for separation of fraction M1.

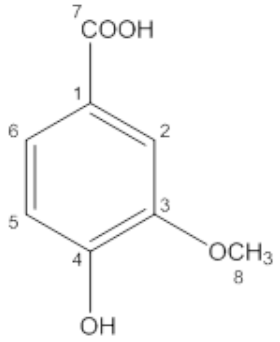
Gradient System	Solvents			
	C-Hex	EtOAc	EtOH	H_2O
S1	14	1	5	10
S2	12	3	5	10
S3	10	5	5	10
S4	7	8	5	10
S5	5	10	5	10
S6	3	12	5	10
S7	1	14	5	10

Table S2: NMR spectral data of p-hydroxybenzoic acid (**1**), (δ(ppm) and *J* (Hz), CD_3OD), recorded in a 600 MHz instrument (600MHz for ^1H and 150 MHz for ^{13}C).



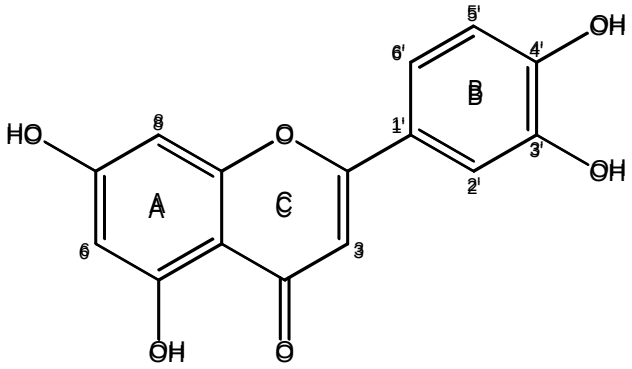
	^1H NMR **δ (ppm) / *J* (Hz)**	^{13}C NMR **δ (ppm)**
1	–	125.4
2 / 6	7.86 (2H, d, *J*= 8.6)	115.2
3 / 5	6.78 (2H, d, *J*= 8.6)	132.5
4	–	161.6
7	–	172.8

Table S3: NMR spectral data of vanillic acid (**2**), (δ (ppm) and J (Hz), CD_3OD), recorded in a 600 MHz instrument (600MHz for ^1H and 150 MHz for ^{13}C).



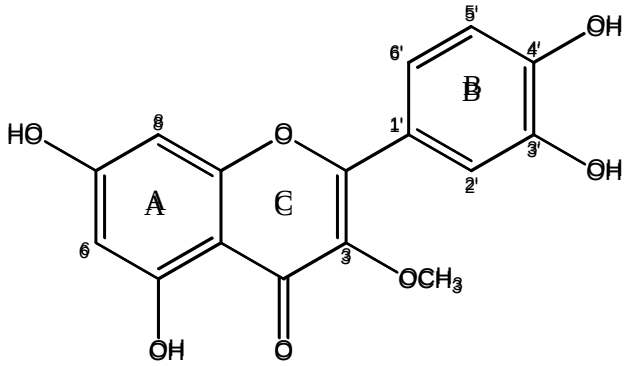
	^1H NMR **δ (ppm) / J (Hz)**	^{13}C NMR **δ (ppm)**
1	–	125.4
2	7.58 (1H, d, J=1.9)	113.4
3	–	148.3
4	–	151.3
5	7.55 (1H, dd, J= 8.2 / 1.9)	124.5
6	6.85 (1H, d, J= 8.2)	115.3
7	–	171.6
OCH_3	3.91 (3H, s)	56.1

Table S4: NMR spectral data of luteolin (**3**) (δ (ppm) and J (Hz), CD_3OD), recorded in a 600 MHz instrument (600MHz for ^1H and 150 MHz for ^{13}C).



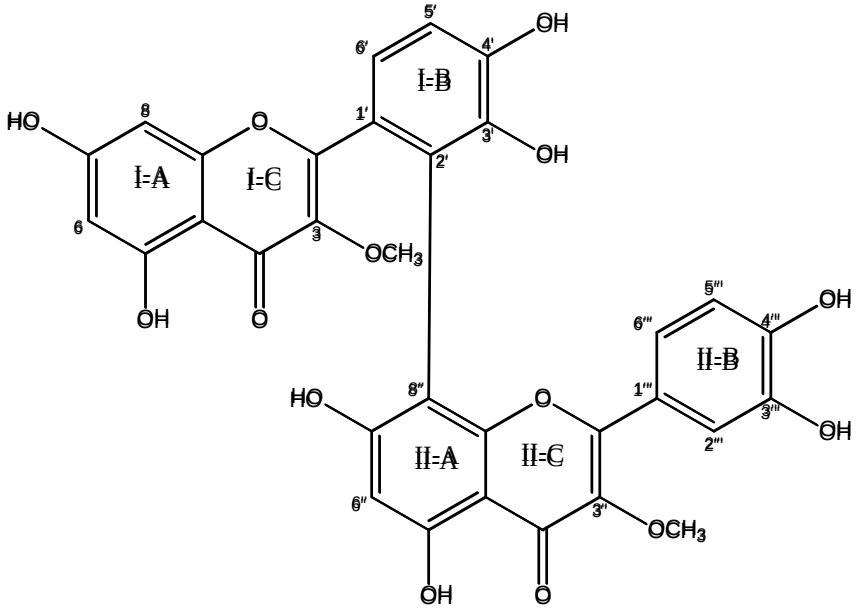
	^1H NMR **δ (ppm) / J (Hz)**	^{13}C NMR **δ (ppm)**
2	–	166.1
3	6.57 (1H, s)	103.9
4	–	183.9
5	–	163.2
6	6.23 (1H, d, J= 2.1)	100.1
7	–	166.4
8	6.47 (1H, d, J= 2.1)	95.0
9	–	158.4
10	–	105.3
1'	–	123.7
2'	7.40 (1H, d, J= 2.0)	114.2
3'	–	147.0
4'	–	151.0
5'	6.93 (1H, d, J=8.2)	116.1
6'	7.41 (1H, dd, J= 8.2/ 2.0)	120.3

Table S5: NMR spectral data of 3-*O*-methyl quercetin (**4**), (δ (ppm) and *J* (Hz), CD_3OD), recorded in a 600 MHz instrument (600MHz for ^1H and 150 MHz for ^{13}C).



	^1H NMR **δ (ppm) / *J* (Hz)**	^{13}C NMR **δ (ppm)**
2	–	157.4
3	–	139.1
4	–	179.9
5	–	163.1
6	6.18 (1H, d, *J*= 2.0)	100.3
7	–	165.9
8	6.40 (1H, d, *J*= 2.0)	95.0
9	–	158.3
10	–	105.1
1'	–	122.7
2'	7.61 (1H, d, *J*= 2.2)	116.1
3'	–	146.1
4'	–	149.9
5'	6.91 (1H, d, *J*= 8.4)	116.2
6'	7.55 (1H, dd, *J*= 8.4/ 2.2)	122.1
3–OCH_3	3.80 (3H, s)	60.2

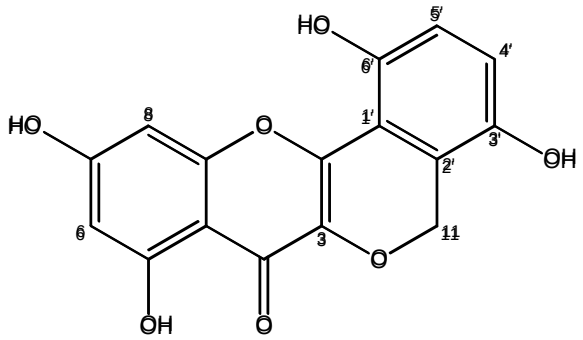
Table S6: NMR spectral data of strychnobiflavone (**5**), (δ (ppm) and J (Hz), CD_3OD), recorded in a 600 MHz instrument (600MHz for ^1H and 150 MHz for ^{13}C).



	^1H NMR **δ (ppm) / *J* (Hz)**	^{13}C NMR **δ (ppm)**
2	–	160.7
3	–	138.9
4	–	179.0
5	–	162.8
6	6.05 (1H, d, *J*= 1.8)	99.5
7	–	166.1
8	5.69 (1H, d, *J*= 1.8)	94.3
9	–	158.1
10	–	105.1
1'	–	123.6
2'	–	121.3
3'	–	145.4
4'	–	149.4
5'	7.01 (1H, d, *J*=8.3)	114.8
6'	7.15 (1H, d, *J*=8.3)	122.7
2"	–	157.4
3"	–	139.6
4"	–	179.1
5"	–	161.8
6"	6.16 (1H, s)	99.8
7"	–	164.2

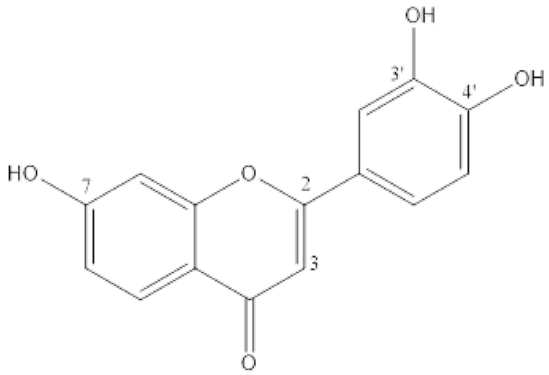
8''	–	103.6
9''	–	155.5
10''	–	104.6
1'''	–	122.7
2'''	7.55 (1H, d, *J*=2.2)	116.7
3'''	–	145.9
4'''	–	149.6
5'''	6.72 (1H, d, *J*= 8.5)	115.9
6'''	7.16 (1H, dd, *J*= 2.2 / 8.5)	122.2
3–OCH_3	3.72 (3H, s)	60.1
3''–OCH_3	3.37 (3H, s)	60.6

Table S7: NMR spectral data of minaxin (**6**) (δ (ppm) and *J* (Hz), DMSO), recorded in a 600 MHz instrument (600MHz for ^{1}H and 150 MHz for ^{13}C).



	^{1}H NMR **δ (ppm) / *J* (Hz)**	$^{13}CNMR$ **δ (ppm)**
2	–	149.9
3	–	132.8
4	–	174.2
5	–	161.6
6	6.16 (1H, d, *J*= 1.9)	98.7
7	–	163.9
8	6.42 (1H, d, *J*= 1.9)	93.9
9	–	156.0
10	–	104.4
11	5.17 (2H, s)	63.1
1'	–	119.9
2'	–	115.5
3'	–	140.9
4'	6.89 (1H, d, *J*=8.3)	114.9
5'	7.19 (1H, d, *J*=8.3)	114.3
6'	–	149.1

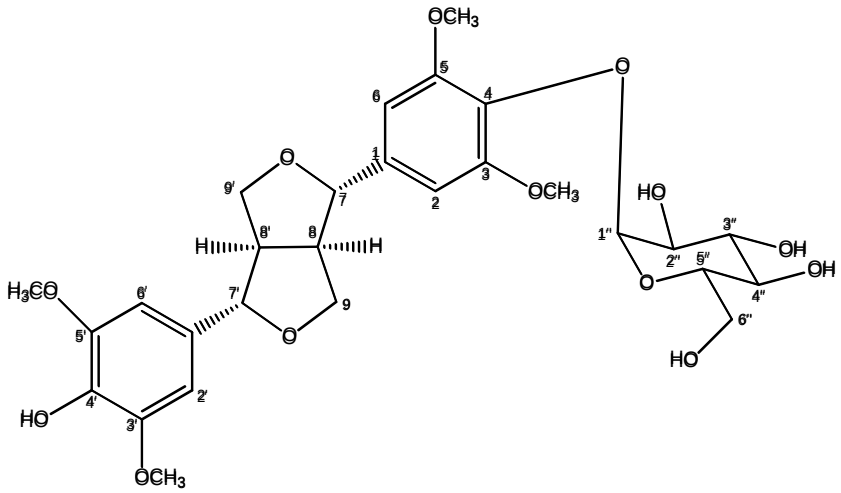
Table S8: NMR spectral data of 3′,4′,7-trihydroxyflavone (**7**)(δ (ppm) and *J* (Hz), CD_3OD), recorded in a 600 MHz instrument (600MHz for ^1H and 150 MHz for ^{13}C).



	^1H NMR **δ (ppm) / *J* (Hz)**	^{13}C NMR **δ (ppm)**
2	–	166.2
3	6.62 (1H, s)	105.4
4	–	180.2
5	7.97 (1H, d, *J*= 8.0)	127.8
6	6.95 -6.91 (1H, *)	116.5
7	–	165.0
8	6.95 -6.91 (1H, *)	103.6
9	–	159.3
10	–	117.4
1'	–	123.9
2'	7.39 (1H, *)	114.7
3'	–	147.1
4'	–	150.8
5'	6.95 -6.91 (1H, *)	116.7
6'	7.40 (1H, *)	120.4

*These ^1H NMR signals are overlapped

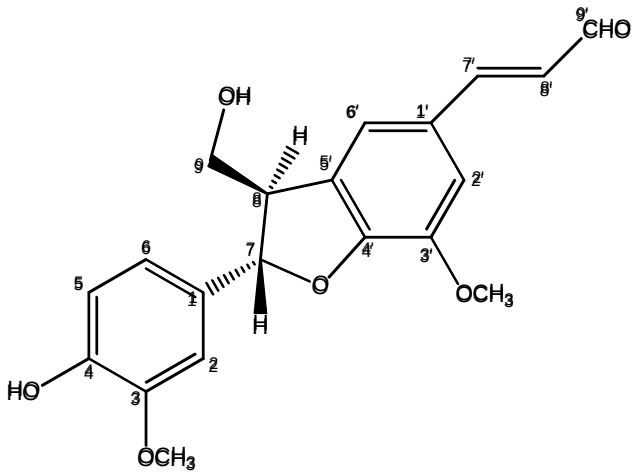
Table S9: NMR spectral data of syringaresinol-*β*-D-glucoside (**8**), (δ (ppm) and *J* (Hz), CD_3OD), recorded in a 600 MHz instrument (600MHz for ^1H and 150 MHz for ^{13}C).



	^1H NMR **δ (ppm) / *J* (Hz)**	^{13}C NMR **δ (ppm)**
1	-	138.5
2 / 6	6.61 (1H, s)	103.1
3 / 5	-	152.8
4	-	134.5
7	4.76 (1H,d, *J*= 4.4)	86.0
8	3.09 (1H, m)	54.6
9	H-9a 4.30 (1H, m) H-9b 3.93 (1H, m)	72.2
1'	-	131.7
2' / 6'	6.58 (1H, s)	102.9
3' / 5'	-	146.9
4'	-	134.0
7'	4.74 (1H, d, *J*= 4.5)	86.5
8'	3.09 (1H, m)	54.6
9'	4.30 (1H, m) 3.93 (1H, m)	72.2
3-OMe / 5-OMe	3.90 (6H, s)	56.7
3'-OMe / 5'-OMe	3.89 (6H, s)	56.7
1"	4.54 (1H, d, *J*=7.7)	106.6
2"	3.67 (1H, *)	74.0
3"	3.59 (1H, *)	77.0
4"	3.63 (1H, *)	70.7
5"	3.40 (1H, m)	76.5
6"	3.93 (1H, *) 3.81 (1H, dd, 11.9 / 5.2 Hz)	62.8

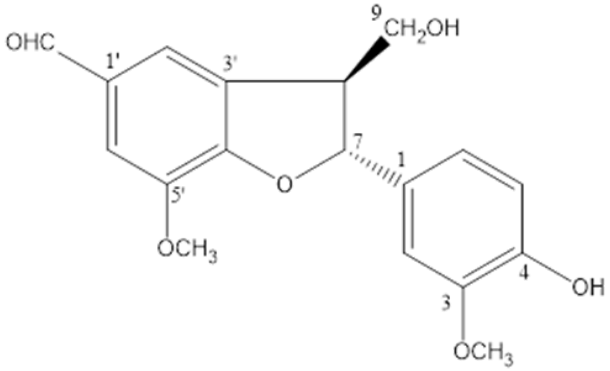
*These ^1H NMR signals are overlapped

Table S10: NMR spectral data of balanophonin (**9**), (δ (ppm) and J (Hz), CD_3OD), recorded in a 600 MHz instrument (600MHz for ^1H and 150 MHz for ^{13}C).



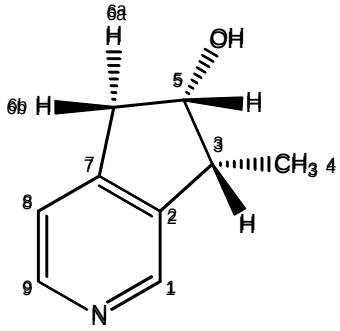
	^1H NMR **δ (ppm) / J (Hz)**	^{13}C NMR **δ (ppm)**
1	–	133.5
2	6.97 (1H,d, J=1.6)	110.3
3	–	148.4
4	–	147.7
5	6.81 (1H, d, J=8.0)	116.0
6	6.84 (1H, dd, J= 8.0/ 1.6)	119.6
7	5.62 (1H, d, J=6.8)	89.7
8	3.59 (1H, m)	54.6
9	3.87 (2H, m)	64.3
1'	–	129.2
2'	7.25 (1H, s)	114.1
3'	–	145.8
4'	–	152.7
5'	–	130.8
6'	7.31 (1H, brs)	120.2
7'	7.64 (1H, d, J=15.7)	156.0
8'	6.71 (1H, dd, J=15.7 / 7.8)	126.8
9'	9.61 (1H, d, J=7.8)	195.6
3'–OCH_3	3.93 (3H, s)	56.7
3–OCH_3	3.84 (3H, s)	56.3

Table S11: NMR spectral data of ficusal (**10**), (δ (ppm) and J (Hz), $(CD_3)_2CO$), recorded in a 600 MHz instrument (600MHz for ^1H and 150 MHz for ^{13}C).



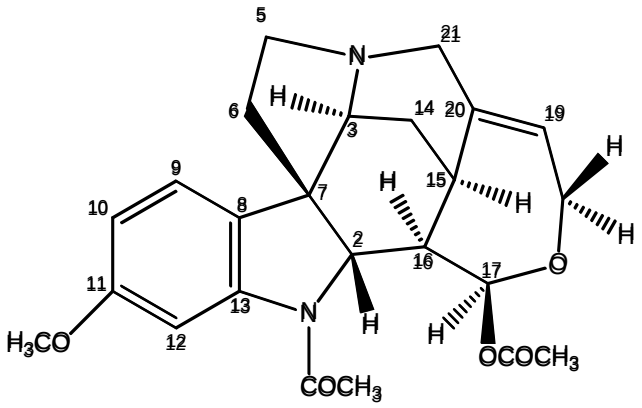
	^1H NMR **δ (ppm) / J (Hz)**	^{13}C NMR **δ (ppm)**
1	–	133.5
2	7.03 (1H,d, *J*=1.6)	110.3
3	–	147.9
4	–	148.4
5	6.82 (1H, d, *J*=8.0)	116.1
6	6.87 (1H, dd, *J*= 8.0/ 1.6)	119.8
7	5.67 (1H, d, *J*=6.8)	89.7
8	3.66 (1H, m)	54.1
9	3.91 (2H, m)	64.1
1'	–	132.4
2'	7.53 (1H, brs)	121.2
3'	–	130.8
4'	–	154.9
5'	–	145.8
6'	7.42 (1H, s)	113.5
7	7.64 (1H, d, *J*=15.7)	156.0
8	6.71 (1H, dd, *J*=15.7 / 7.8)	126.8
9	9.81 (1H, d, *J*=7.8)	191.2
5'–OCH_3	3.91 (3H, s)	56.7
3–OCH_3	3.82 (3H, s)	56.3

Table S12: NMR spectral data of venoterpine (**11**), (δ (ppm) and *J* (Hz), CDCl3,), recorded in a 600 MHz instrument (600MHz for ^{1}H and 150 MHz for ^{13}C).



	^{1}H NMR **δ (ppm) / *J* (Hz)**	^{13}C NMR **δ (ppm)**
1	8.40 (1H, s)	146.0
2	–	141.9
3	3.26 (1H, qd, *J*= 7.2/ 2.6)	43.7
4	1.37 (3H, d, *J*=7.2)	12.4
5	4.59 (1H, ddd, *J*= 5.4/ 2.6/ 2.2)	75.9
6	3.13 (1H, dd, *J*= 16.9/ 5.4)	42.0
	2.94 (1H, dd, *J*= 16.9/ 2.2)	
7	–	151.3
8	7.21 (1H, d, *J*=4.9)	121.3
9	8.38 (1H, d, *J*=4.9)	147.1

Table S13: NMR spectral data of 11-methoxyhenningsamine (**12**), (δ (ppm) and *J* (Hz), $CDCl_3$), recorded in a 600 MHz instrument (600MHz for ^1H and 150 MHz for ^{13}C).

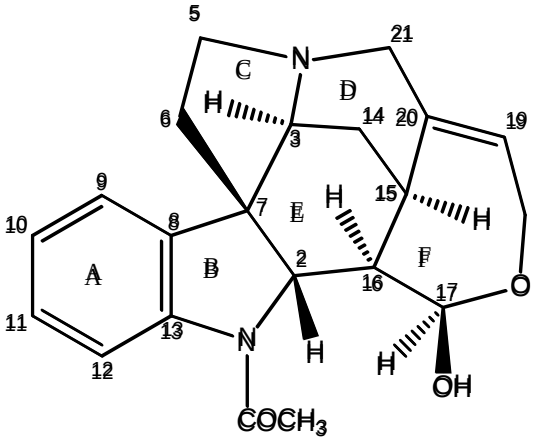


	^1H NMR **δ (ppm) / *J* (Hz)**	^{13}C NMR **δ (ppm)**
2	4.36 (1H, d, *J*=10.4)	63.5
3	4.19 (1H, brs)	59.5
4	–	–
5	3.60 (1H, m)	51.4
	2.96 (1H, *)	
6	2.04 (1H, m)	37.4
	1.77 (1H, dd, *J*= 12.7/4.6)	
7	–	53.2
8	–	123.7
9	7.03 (1H, d, *J*=8.3)	122.0
10	6.63 (1H, dd, *J*=8.3/2.1)	110.3
11	–	160.3
12	7.68 (1H, d, *J*=2.1)	105.6
13	–	143.2
14	1.68 (1H, d, *J*=14.9)	25.5
	2.34 (1H, ddd, *J*=14.9/ 3.5/ 2.8)	
15	2.87 (1H, brs)	32.8
16	1.87 (1H, d, *J*=10.4)	44.5
17	5.86(1H, s)	101.7
18	4.39 (1H, m)	64.2
	4.12 (1H, dd, *J*=14.3/4.5)	
19	6.09 (1H, brs)	129.3
20	–	138.0
21	3.95 (1H, d, *J*=15.6)	53.2
	2.97 (1H, *)	
11-OCH_3	3.81 (3H, s)	55.6
O$\underline{CO}CH_3$	–	168.5
OCO$\underline{CH_3}$	2.09 (3H, s)	20.8

$N\underline{C}O\underline{C}H_3$	-	170.1
$NCO\underline{C}\underline{H}_3$	2.37 (3H, s)	24.1

* Overlapping of ^1H NMR signals was observed

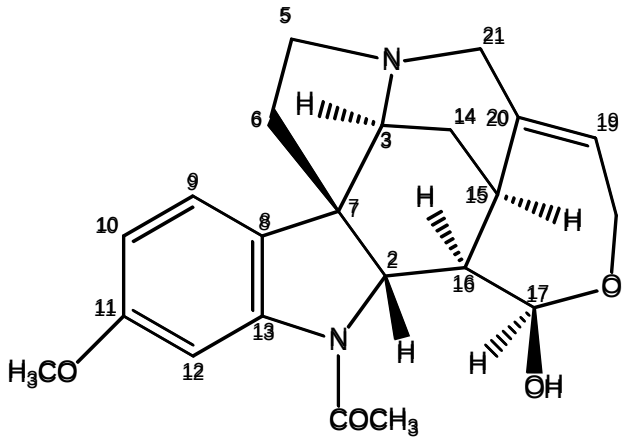
Table S14: NMR spectral data of diaboline (**13**), (δ (ppm) and *J* (Hz), CDCl3), recorded in a 600 MHz instrument (600MHz for ^{1}H and 150 MHz for ^{13}C).



	^{1}H NMR **δ (ppm) / *J* (Hz)**	^{13}C NMR **δ (ppm)**
2	4.94 (1H, d, *J*=11.9)	63.5
3	4.54 (1H, brs)	60.6
4	–	–
5	4.03 (1H, m)	51.5
	3.21 (1H, *)	
6	2.09 (1H, m)	37.2
	1.98 (1H, m)	
7	–	53.2
8	–	132.8
9	7.30 (1H, d, *J*=7.5)	122.93
10	7.20 (1H, *)	125.7
11	7.35 (1H, t, *J*=7.5)	129.5
12	7.21 (1H, *)	117.9
13	–	140.9
14	1.60 (1H, m)	24.0
	2.37 (1H, m)	
15	3.62 (1H, brs)	27.9
16	1.71 (1H, m)	49.3
17	5.34 (1H, s)	96.5
18	4.77 (1H, d, *J*=15.4)	51.4
	4.12 (1H, *)	
19	6.12 (1H, brs)	134.4
20	–	138.0
21	4.14 (1H, *)	52.7
	3.24 (1H, *)	
$NCOCH_3$	–	169.6
$NCOCH_3$	2.40 (3H, s)	23.2

* Overlapping of ^{1}H NMR signals was observed

Table S15: NMR spectral data of 11-methoxy diaboline (**14**), (δ (ppm) and J (Hz), CDCl3), recorded in a 600 MHz instrument (600MHz for ^{1}H and 150 MHz for ^{13}C).



	^{1}H NMR **δ (ppm) / *J* (Hz)**	^{13}C NMR **δ (ppm)**
2	4.91 (1H, d, *J*=11.0)	63.9
3	4.48 (1H, brs)	60.5
4	–	–
5	3.99 (1H, m)	51.5
	3.18 (1H, m)	
6	2.07 (1H, m)	37.1
	1.95 (1H, m)	
7	–	52.9
8	–	124.1
9	7.19 (1H, d, *J*=8.2)	123.3
10	6.69 (1H, d, *J*=8.2)	109.1
11	–	160.5
12	6.74 (1H, s)	105.9
13	–	143.2
14	1.62 (1H, m)	23.3
	2.35 (1H, m)	
15	3.60 (1H, brs)	27.6
16	1.69 (1H, d, *J*=11.0)	46.0
17	5.32 (1H, s)	96.4
18	4.77 (1H, m)	51.5
	4.05 (1H, dd, *J*=14.3/4.5)	
19	6.11 (1H, brs)	134.3
20	–	143.1
21	4.13 (1H, d, *J*=14.0)	52.6
	3.24 (1H, m)	
OCH_3	3.83 (3H, s)	55.6
$N\underline{CO}CH_3$	–	169.4
$NCO\underline{CH_3}$	2.39 (3H, s)	23.3