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Supplementary Material

CHEMICAL AND BIOLOGICAL INVESTIGATION OF *Cattleya nobilior* Rchb. F. (Orchidaceae): TARGETING ON PHENANTHRENE AND STILBENOID DERIVATIVES

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Table 1S. Plant material parts collected of *Cattleya nobilior* and the description of their weights

Part	Material *in natura* / g	Dried material / g
Leaves	431.80	41.61
Roots	179.32	121.75
Rhizomes	129.80	34.90
Pseudobulb	530.37	69.18

Table 2S. Extraction solvents and extract yields obtained from *Cattylea nobilor*

Material	Code	Extraction solvent	Yield / %
Roots	CnRo-DM5	DCM:MeOH 95:5	38.2
	CnRo-DM50	DCM:MeOH 1:1	17.64
	CnRo-M	MeOH 100%	15.9
Leaves	CnLf-DM5	DCM:MeOH 95:5	21.3
	CnLf-DM50	DCM:MeOH 1:1	6.9
	CnLf-M	MeOH 100%	14.9
Rhizome	CnRh-DM5	DCM:MeOH 95:5	36.8
	CnRz-DM50	DCM:MeOH 1:1	21.4
	CnRz-M	MeOH 100%	17.3
Pseudobulb	CnBb-DM5	DCM:MeOH 95:5	6.2
	CnBb-DM50	DCM:MeOH 1:1	14.1
	CnBb-M	MeOH 100%	34.1

Table 3S. ^{1}H NMR chemical shift values (δ), multiplicities (mult.), coupling constants (J), ^{13}C NMR, and HMBC (heteronuclear multiple bond correlation) data for batatasin III (**32**)

H/C	^{1}H (δ) mult. (J)	^{13}C (δ)	HMBC
1	–	143.5	H: 2, 6
2	6.24[a]	106.8	H: 6, 4, 2a
3	–	156.5	H: 2, 4, 6
4	6.30 s	99.0	H: 6, 2
5	–	161.0	H: 6, 4, OCH_3
6	6.24[a]	106.8	H: 2, 4, 2a
7 (OCH_3)	3.73 s	55.7	–
2a (CH_2)	2.80 m	37.7	H: 2a', 2, 6
2a' (CH_2)	2.80 m	37.7	H: 2a, 2',6'
1'	–	143.5	H: 2', 5',6'
2'	6.65[a]	115.0	H: 4', 5', 6', 2a'
3'	–	155.5	H: 2', 4', 5', 6'
4'	6.65[a]	112.0	H: 2', 5', 6'
5'	7.13 dd (7.9, 7.5)	129.4	H: 6', 4'
6'	6.75[a]	120.0	H: 2', 4', 5', 2a'

[a]Overlapped signals. $CDCl_3$, 500 MHz.

Table 4S. ^{1}H NMR shift values (δ), multiplicities (mult), coupling constants (J), ^{13}C NMR, and HMBC (heteronuclear multiple bond correlation) data of gigantol (**33**)

H/C	^{1}H (δ) mult. (J)	^{13}C (δ)	HMBC
1	–	144.2	H: 2, 6
2	6.23[a]	107.6	H: 6, 4, 2a
3	–	156.0	H: 2, 4, 6
4	6.23[a]	99.8	H: 6, 2
5	–	160.3	H: 6, 4, OCH_3
6	6.30[a]	106.4	H: 2, 4, 2a
7 (OCH_3)	3.73 s	55.8	–
7' (OCH_3)	3.82 s	56.3	–
2a (CH_2)	2.78 m	37.9	H: 2a', 2, 6
2a' (CH_2)	2.80 m	37.0	H: 2a, 2', 6'
1'	–	133.3	H: 2', 5' ,6'
2'	6.60 s	110.7	H: 4', 5', 6', 2a'
3'	–	145.8	H: 2', 4', 5', 6'
4'	–	143.1	H: 2', 5',6'
5'	6.80 d (8.1)	113.6	H: 6', 4'
6'	6.66 d (8.1)	120.5	H: 2', 4', 5', 2a'

[a]Overlapped signals. $CDCl_3$, 500 MHz.

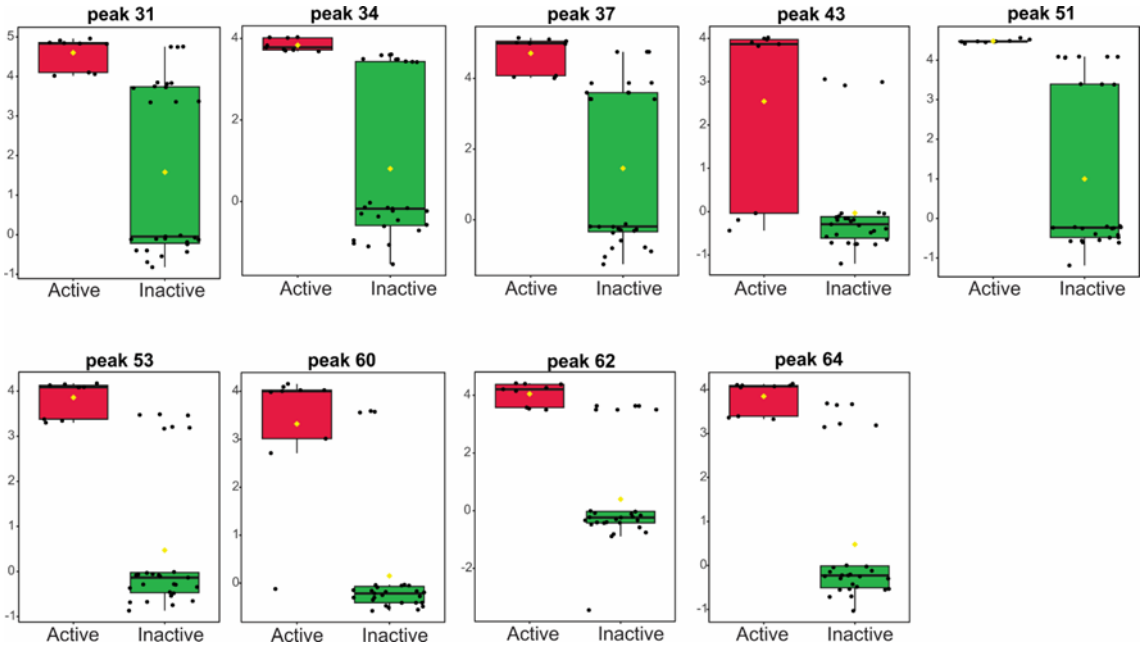

Figure 1S. *Box plots of the annotated features that exhibited $p \leq 0.05$ in the active extracts from the volcano plot*

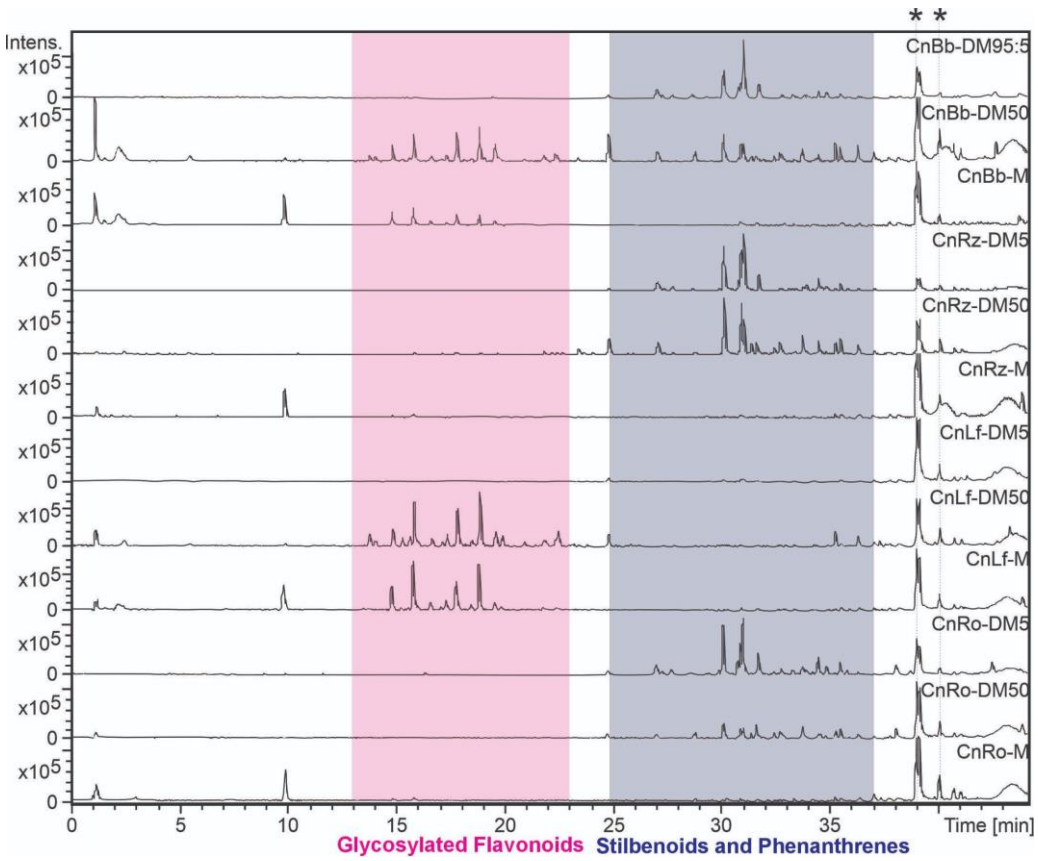

Figure 2S. *Chromatograms (270 nm) of the different extracts obtained from the C. nobilior. CnLf: C. nobilior leaf extract; CnBb: C. nobilior pseudobulb extract; CnRo: C. nobilior root extract; CnRz: C. nobilior rhizome extract; DM5: dichloromethane and methanol 95:5; DM50: dichloromethane and methanol 1:1; M: methanol 100%.*

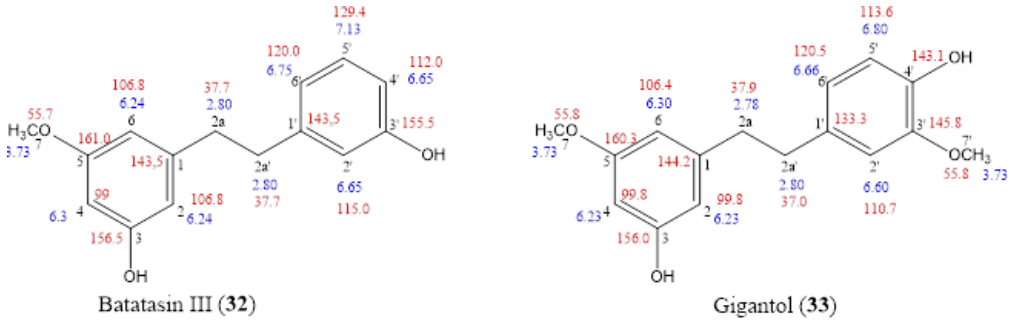

Figure 3S. *Chemical structures of batatasin III (**32**) and gigantol (**33**) and their ^{1}H and ^{13}C chemical shifts*