

Supplementary Information

Construction of a potato fraction library for the investigation of functional secondary metabolites

Toshihiko Nogawa¹, Yushi Futamura¹, Akiko Okano¹, Mari Suto², Junya Nakamura²,
Katsuyuki Ishihara², Hiroyuki Osada^{†1}

¹*RIKEN Center for Sustainable Resource Science, Chemical biology Research Group,
2-1 Hirosawa, Wako, Saitama 351-0198, Japan*

²*R&D Center, Calbee Inc., 23-6 Kiyohara-kogyodanchi,
Utsunomiya, Tochigi 321-3231, Japan*

[†] Corresponding author

Mailing address:

RIKEN CSRS, Chemical Biology Research Group, 2-1 Hirosawa, Wako, Saitama 351-0198, Japan

Phone: (+81) 48-467-9541/Fax: (+81) 48-462-4669/E-mail: hisyo@riken.jp

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Table S1. Samples used for the preparation of a potato fraction library.

cultivar	part	prefecture	collected weight		MeOH for extraction (L) (3 times)	extract (g)	extraction rate (%)	extract used for partitioning (g)
			wet (kg)	dry (g)				
KH: Kitahime	flower	Hokkaido		18.6	0.1	9.3	49.9	2.9
KH: Kitahime	leaf	Hokkaido	1.06			46.1	4.3	3.0
KH: Kitahime	stem	Hokkaido		245.0	1.2	38.5	15.7	3.1
KH: Kitahime	roots	Hokkaido		77.6	0.4	13.7	17.6	3.0
KH: Kitahime	tuber-peel	Hokkaido		893.5	4.5	28.9	3.2	3.2
KH: Kitahime	tuber	Hokkaido		3072.0	15.4	26.1	0.8	3.1
PI: Pilka	flower	Hokkaido		3.4	0.02	1.7	50.3	1.6
SF: Sakurafubuki	flower	Hokkaido		6.1	0.03	2.9	47.9	2.8
AT: Atrantic	leaf	Hokkaido		31.8	0.2	10.2	32.1	2.8
AT: Atrantic	stem	Hokkaido		40.0	0.2	10.4	26.0	3.0
AT: Atrantic	roots	Hokkaido		9.1	0.05	1.2	13.7	–
TS-H: Toyoshiro	leaf	Hokkaido	1.46			59.1	4.1	3.0
TS-H: Toyoshiro	stem	Hokkaido		293.3	1.5	57.3	19.5	3.1
TS-H: Toyoshiro	roots	Hokkaido		94.4	0.5	18.1	19.2	3.1
TS-H: Toyoshiro	tuber-peel	Hokkaido		2118.0	10.6	69.1	3.3	3.0
TS-H: Toyoshiro	tuber	Hokkaido		3101.0	15.5	26.9	0.9	3.0
TS-I: Toyoshiro	leaf	Ibaraki	2.18			86.9	4.0	3.0
TS-I: Toyoshiro	stem	Ibaraki		384.8	1.9	76.5	19.9	3.2
TS-I: Toyoshiro	roots	Ibaraki		46.8	0.2	7.3	15.6	3.0
TS-I: Toyoshiro	tuber-peel	Ibaraki		1206.0	6.0	36.3	3.0	3.1
TS-I: Toyoshiro	tuber	Ibaraki		3090.0	15.5	33.8	1.1	3.2
SD: Snowden	leaf	Hokkaido	1.98			92.7	4.7	3.3
SD: Snowden	stem	Hokkaido		549.6	2.7	111.3	20.3	2.9
SD: Snowden	roots	Hokkaido		117.7	0.6	21.9	18.6	3.1
SD: Snowden	tuber	Hokkaido		3001.0	15.0	28.2	0.9	2.8
KM: Kitamurasaki	tuber	Hokkaido		3064.0	15.3	38.2	1.2	2.9
NR: Northern Ruby	tuber	Hokkaido		2331.0	11.7	35.9	1.5	2.9

Table S2. Biological activities of extracts and partitioned extracts at 0.3, 3, and 30 $\mu\text{g/mL}$.

sample	extract	HeLa		HL60		mammal		srcfs-NRK		C3H10T1/2		gram +		gram -		A.fumigatus		fungi		Calbicans		malaria					
		0.3	3	30	0.3	3	30	0.3	3	30	0.3	3	30	0.3	3	30	0.3	3	30	0.3	3	30	0.3	3	30		
KH	flower	extract	0	0	3	0	0	3	0	3	0	3	0	1	0	0	0	0	0	0	0	0	0	0	0	0	
		hexane	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0		
		EIOAc	0	0	3	0	0	3	0	0	3	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	
	leaf	BuOH	0	1	3	0	1	3	0	0	3	0	2	3	0	0	0	0	0	0	0	0	0	0	0	0	
		H ₂ O	0	0	1	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		extract	0	0	0	0	2	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
	stem	hexane	0	0	2	0	0	3	0	0	2	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		EIOAc	0	0	2	0	0	3	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		BuOH	0	0	3	0	0	3	0	0	3	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
	roots	H ₂ O	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		extract	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		hexane	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
PI	flower	EIOAc	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		BuOH	0	0	3	0	0	3	0	0	3	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	
		H ₂ O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
	tuber-peel	extract	0	0	1	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		hexane	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		EIOAc	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
	tuber	BuOH	0	0	3	0	0	3	0	0	2	0	0	2	0	0	1	0	0	0	0	0	0	0	0	0	
		H ₂ O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		extract	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
	SF	flower	hexane	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
			EIOAc	0	0	3	0	0	3	0	0	3	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0
			BuOH	0	0	3	0	1	3	0	0	3	0	2	3	0	0	0	0	0	0	0	0	0	0	0	0
leaf		H ₂ O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		extract	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		hexane	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
stem		EIOAc	0	0	3	0	0	3	0	0	3	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	
		BuOH	0	0	3	0	0	3	0	0	3	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	
		H ₂ O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
AT		flower	extract	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
			hexane	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
			EIOAc	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	leaf	BuOH	0	0	3	0	0	3	0	0	3	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	
		H ₂ O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		extract	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
	stem	hexane	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		EIOAc	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		BuOH	0	0	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
	TS-H	flower	H ₂ O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
			extract	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
			hexane	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
leaf		EIOAc	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		BuOH	0	0	2	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		H ₂ O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
stem		extract	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		hexane	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		EIOAc	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
TS-I		flower	BuOH	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
			H ₂ O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
			extract	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
	leaf	hexane	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		EIOAc	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		BuOH	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
	stem	H ₂ O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		extract	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		hexane	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
	NR	flower	EIOAc	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
			BuOH	0	0	3	0	0	3	0	0	3	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0
			H ₂ O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
leaf		extract	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		hexane	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		EIOAc	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
stem		BuOH	0	0	3	0	0	3	0	0	3	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	
		H ₂ O	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		extract	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
tuber		hexane	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		EIOAc	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
		BuOH	0	0	3	0	0	3	0	0	3	0	0	3	0	0	0	0	0	0	0	0	0	0	0	0	

Activity was expressed by the index of 0, 1, 2, and 3 for 0 - 20%, 20 - 50%, 50 - 80%, and >80% of growth inhibition

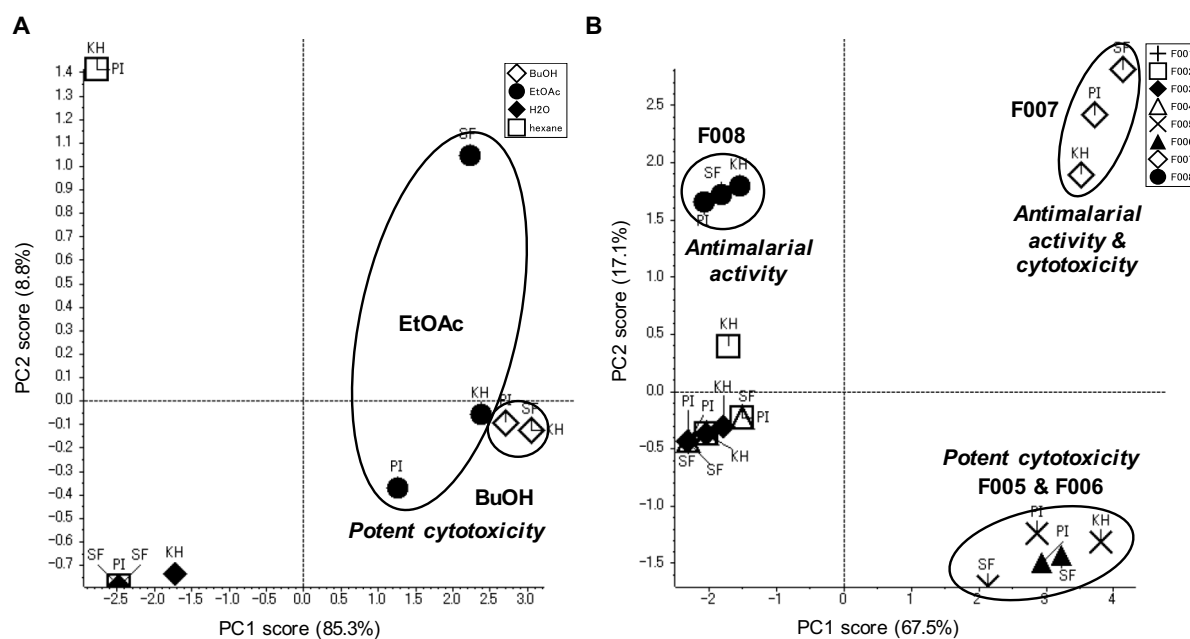
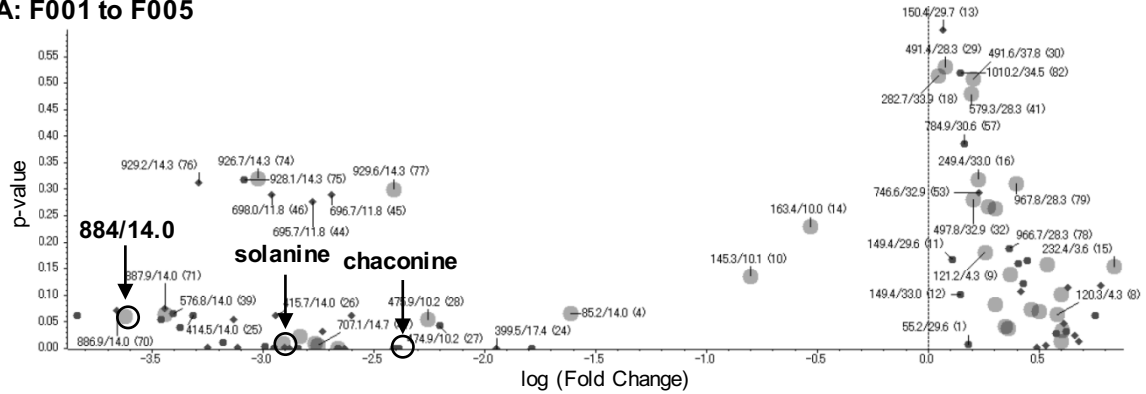


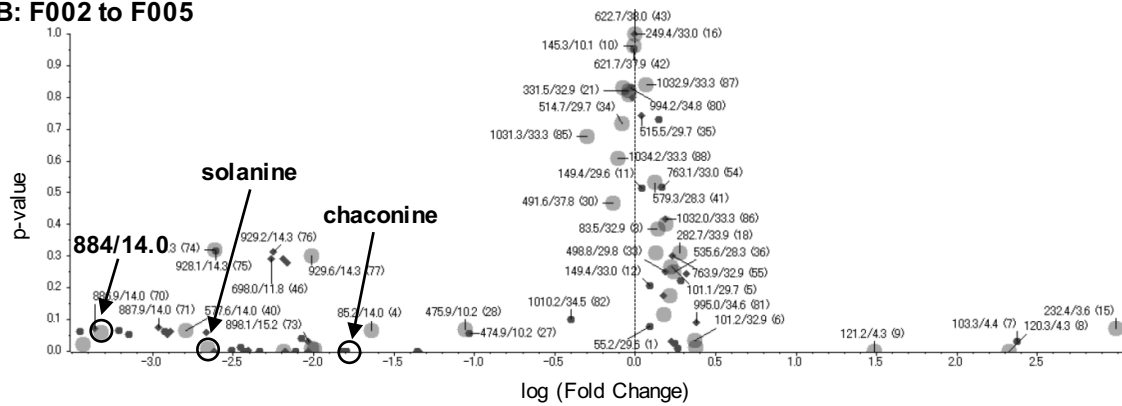
Figure S1. PCA results of partitioned extracts and BuOH fractions of flower extracts based on biological activities.

A: PCA score plot for partitioned extracts. **B:** PCA score plot for BuOH fractions.

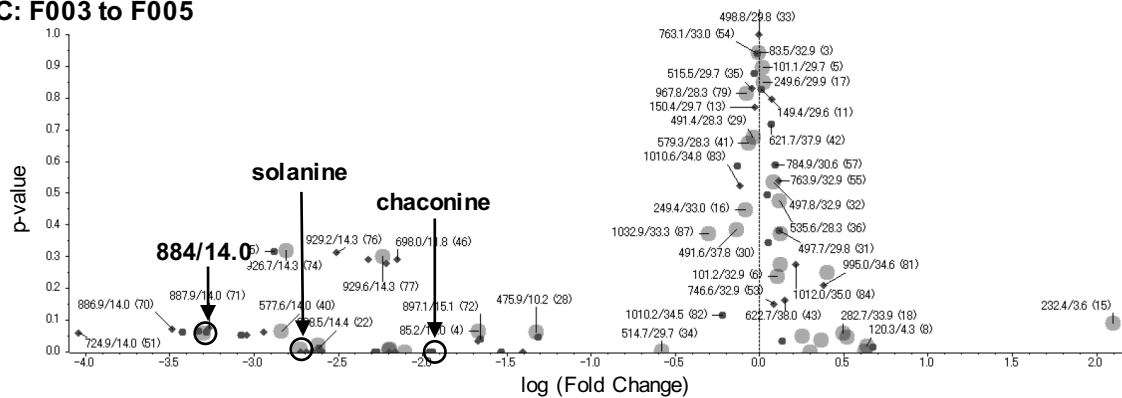
A: F001 to F005



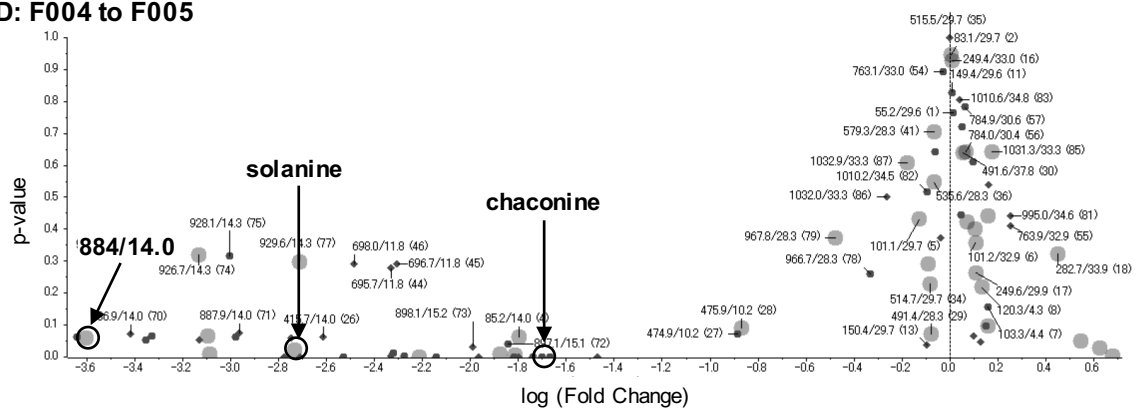
B: F002 to F005



C: F003 to F005



D: F004 to F005



[illegible]

F005 to F007

solanine → 854.0/14.4 (59)

← **chaconine** 884/14.0

log (Fold Change)

F005 to F008

log (Fold Change)

solanine

chaconine

884/14.0

1203.7/4.3 (8)

121.2/4.3 (9)

103.3/4.4 (7)

232.4/3.6 (15)

926.7/14.3 (74)

928.1/14.3 (75)

929.2/14.3 (76)

163.4/10.0 (14)

399.5/17.4 (24)

145.3/1.0 (10)

884/14.0 (71)

897.1/15.1 (72)

698.0/11.8 (46)

696.7/11.8 (45)

475.9/10.2 (28)

474.9/10.2 (27)

149.4/33.0 (12)

150.4/29.7 (13)

995.0/34.6 (81)

994.2/34.8 (80)

579.3/28.3 (41)

621.7/37.9 (42)

622.7/38.0 (43)

1010.2/34.5 (82)

835.3/32.9 (83)

A: Inactive fraction F001 to active fraction F005. **B:** Inactive fraction F002 to active fraction F005. **C:** Inactive fraction F003 to active fraction F005. **D:** Inactive fraction F004 to active fraction F005. **E:** Active fraction F005 to active fraction F006. **F:** Active fraction F005 to active fraction F007. **G:** Active fraction F005 to weak active fraction F008.

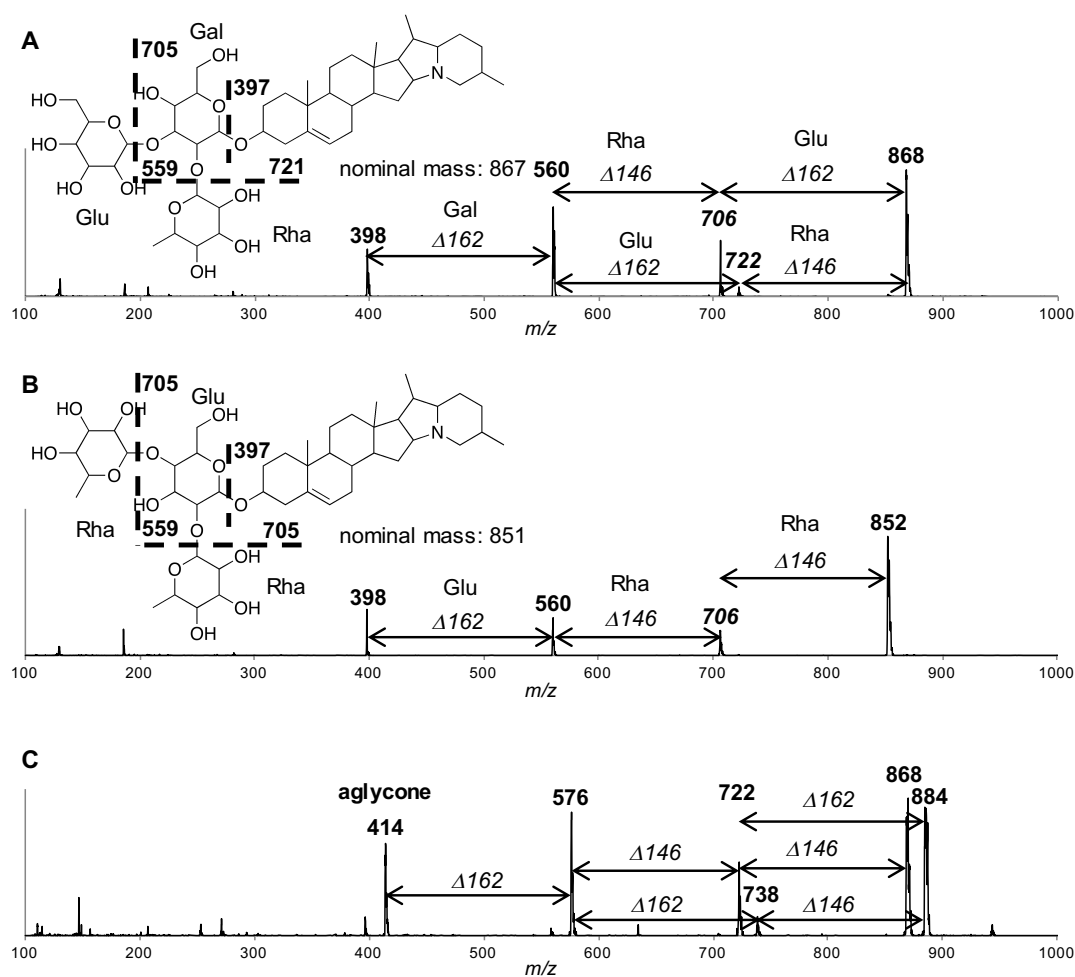


Figure S3. Mass spectra of solanine and chaconine standards and the characteristic peak found by PCA-DA recorded by positive mode.

A: mass spectrum of solanine standard and the structure with supposed fragmentation pattern, which suggested the possible two types of fragmentation pattern including 868/722/560/398 and 868/706/560/398. **B:** mass spectrum of chaconine standard with supposed fragmentation pattern. **C:** mass spectrum extracted from the characteristic peak found by PCA-DA.

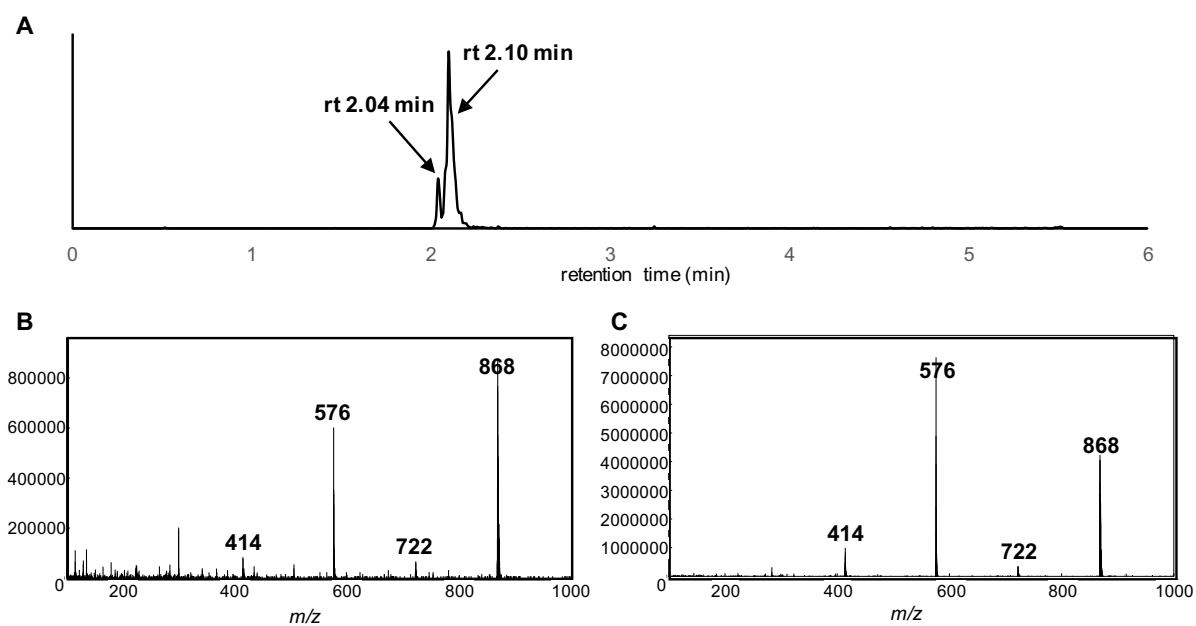


Figure S4. UPLC/MS result of co-injection of **1** and standard solamargine.

A: Mass chromatogram recorded by m/z : 868. **B:** Mass spectrum of **1** at t_R 2.04 min. **C:** Mass spectrum of solamargine at t_R 2.10 min.

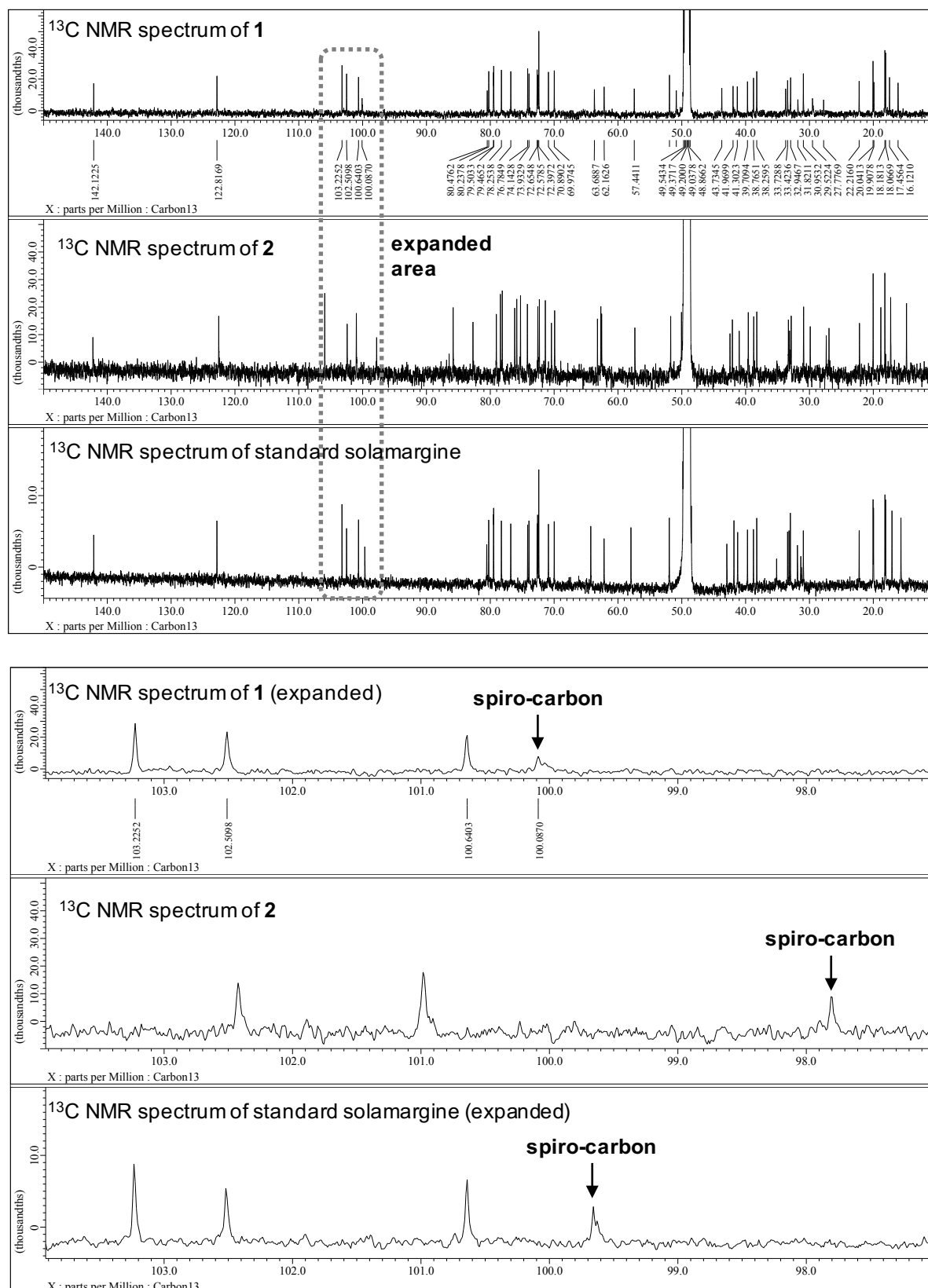


Figure S5. Comparison of ^{13}C NMR spectra of **1**, **2**, and standard solamargine in methanol- d_4 at 125 MHz.

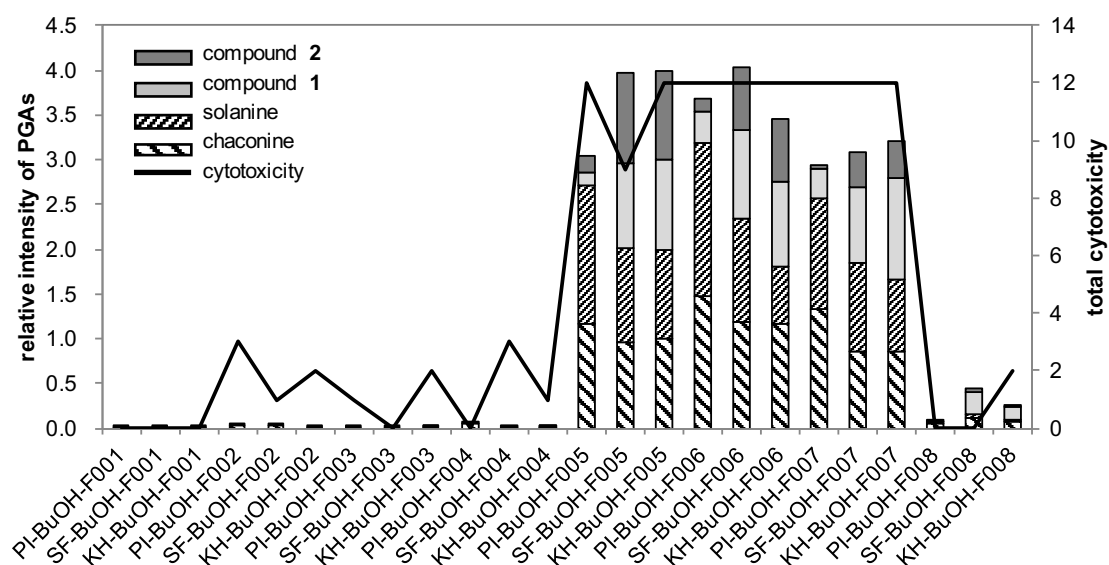


Figure S6. The relative quantities for 4 PGAs and total cytotoxicity for flower BuOH fractions.

The quantities of 4 PGAs were calculated based on the area of ion strength observed in the mass chromatogram recorded by the related m/z value. The relative quantities were calculated against KH BuOH-F005 and total cytotoxicity was sum of the activity index against 5 mammalian cells at 30 $\mu\text{g/mL}$.