Supplementary Information

Chemical Constituents of *Psychotria nemorosa* Gardner and Antinociceptive Activity

Nivea O. Calixto,[a] Millena S. Cordeiro,[b] Thais B. S. Giorno,[b] Gibson G. Oliveira,[c] Norberto P. Lopes,[c] Patricia D. Fernandes,[b] Angelo C. Pinto[†,a] and Claudia M. Rezende*[,a]

[a]Instituto de Química and [b]Instituto de Ciências Biomédicas, Universidade Federal do Rio de Janeiro, 21949-900 Rio de Janeiro-RJ, Brazil

[c]NPPS - Faculdade de Ciências Farmacêuticas de Ribeirão Preto, Universidade de São Paulo, 14040-903 Ribeirão Preto-SP, Brazil

Table S1. Fractions from silica gel 60 (70-230 mesh) column chromatography from EE *P. nemorosa* leaves

Number	Fraction	Elution	Mass / g
1	1 (1-3)	hexane	0.112
2	5 (4-5)	hexane/EtOAc 5%	0.150
3	8 (6-8)	hexane/EtOAc 10%	0.132
4	9 (9-10)	hexane/EtOAc 10%	0.050
5	11 (11-13)	hexane/EtOAc 10%	0.010
6	15 (14-15)	hexane/EtOAc 20%	0.003
7	16	hexane/EtOAc 20%	0.035
8	18 (17-18)	hexane/EtOAc 1:1	0.082
9	19 (19-21)	hexane/EtOAc 1:1	0.067
10	22 (22-25)	hexane/EtOAc 1:1	0.005
11	26 (26-29)	EtOAc	1.691
12	32 (30-35)	MeOH	2.826
–	–	Total	5.081

*e-mail: claudia.rezendeufrj@gmail.com

[†]*In memoriam*

Table S2. Phytochemical profile of *P. nemorosa* obtained by GC-MS (column: DB-1 30 m × 0.25 mm × 0.25 mm)

Peak No.	Fraction	Compound	R_t / min	$[M]^{+\cdot}$
1	1	cinnamic acid	14.95	148
2	1	1-hexadecene	16.96	224
3	1	dihydroactinidiolide	17.90	180
4	1	hexadecane, 1-chloro	18.14	260
5	1	4-hydroxy-β-ionone	18.87	208
6	1	phytol	20.15	296
7	1	*n*-tetracosane	23.27	338
8	1	*n*- octacosane	24.47	394
9	1	*n*-nonacosane	24.70	408
10	1	2-methyloctacosane	24.98	408
11	1	*n*- triacontane	26.27	562
12	5	isophytol	19.60	296
13	5	13-methyl-tetradecanoate, ethyl ester	20.09	270
14	5	8,11-octadecadienoic acid, methyl ester	20.74	294
15	5	stearic acid, methyl ester	20.98	298
16	5	stearic acid, ethyl ester	21.39	312
17	5	18-methylnonadecanoate, methyl ester	22.21	326
18 a	5	β-amyrone[a]	31.35	424
18 b	5	α -amyrone[a]	32.11	424
19	5	lupeol[b]	32.58	426
20 a	5	β-amyrin acetate[a]	33.40	468
20 b	5	α-amyrin acetate[a]	34.79	468
21 a	5	3,11-dioxo-β-amyrene[a]	35.99	438
21 b	5	3,11-dioxo-α-amyrene[a]	36.87	438
22	8	1-heptacosanol	19.59	396
23	8	oxalic acid, heptadecyl hexyl ester	20.71	412
24	8	oxalic acid, hexadecyl isohexyl ester	20.82	398
25	8	10-methylundec-2-en-4-olide	21.08	196
26	8	n.i.	22.25	–
27	8	4,8,12,16-tetramethylheptadecan-4-olide	22.33	324
28	8	campesterol	29.80	400
29	8	stigmasterol	30.26	412
30	8	γ-sitosterol	31.23	414
31 a	8	β-amyrin[b]	31.87	426
31 b	8	α-amyrin[b]	32.68	426
32	8	stigmast-4-en-3-one	33.65	412
33	9	*n*-hexadecanoic acid	19.83	256
34	9	2,6,10,14-tetramethyl-7-(3-methylpent-4-enylidene) pentadecane	22.25	348
35	9	triethylene glycol di(2-ethylhexoate)	22.95	402

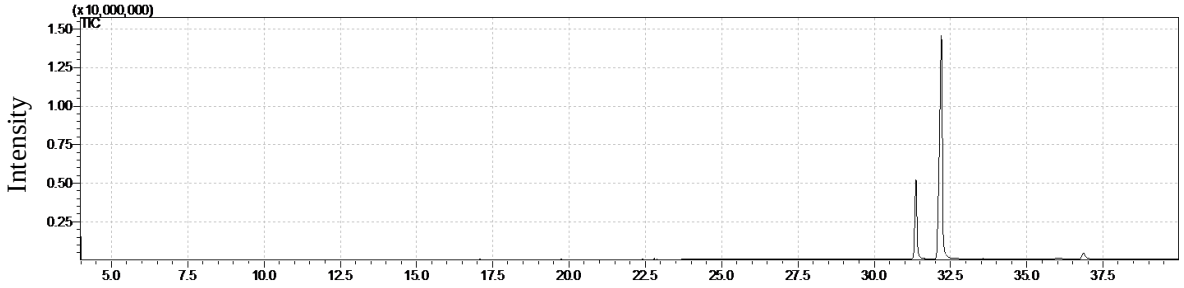
[a,b]Identities confirmed by injection of standards obtained by chemical transformations of [a]natural products or [b]isolated substances from natural sources. n.i.: not identified.

Table S3. GC-MS data from the compounds identified in *Psychotria nemorosa* leaves

Compound[a]	MS *m/z* / %
Cinnamic acid	148 (82), 147 (100), 131 (21), 103 (56), 102 (21), 91 (20), 77 (34), 51 (28), 50 (13)
Dihydroactinidiolide	180 (23), 165 (7), 152 (11), 137 (38), 124 (10), 111 (100), 110 (23), 109 (42), 69 (20), 67 (30)
4-Hydroxy-β-ionone	208 (5), 207 (22), 193 (27), 175 (8), 165 (16), 152 (83), 147 (33), 137 (77), 123 (97), 109 (100), 91 (61)
Phytol	278 (4), 263 (3), 179 (4), 123 (50), 109 (30), 95 (88), 82 (70), 68 (100), 57 (88)
Isophytol	296 (1), 281 (0), 71 (100), 57 (19)
4,8,12,16-Tetramethylheptadecan-4-olide	324 (1), 126 (16), 114 (16), 99 (100), 83 (14), 69 (24), 57 (26)
Campesterol	400 (100), 382 (56), 367 (46), 340 (12), 315 (76), 289 (60), 273 (36), 255 (44), 231 (36), 213 (56), 199 (20), 159 (40), 145 (60), 133 (40), 107 (68), 95 (64), 81 (56)
Stigmasterol	412 (81), 394 (9), 379 (13), 351 (27), 314 (9), 300 (36), 273 (32), 255 (68), 213 (32), 199 (18), 159 (54), 145 (50), 133 (57), 123 (38), 107 (32), 83 (95), 81 (72), 55 (100)
γ-Sitosterol	414 (100), 396 (76), 381 (40), 330 (16), 329 (60), 303 (46), 273 (36), 255 (44), 231 (32), 213 (72), 199 (20), 178 (20), 173 (24), 161 (38), 145 (32), 119 (36), 107 (60), 95 (56), 81 (28), 57 (76), 55 (72)
Stigmast-4-en-3-one	412 (34), 398 (6), 370 (12), 289 (24), 271 (8), 229 (48), 149 (18), 147 (22), 124 (100), 107 (18), 95 (20), 81 (16)

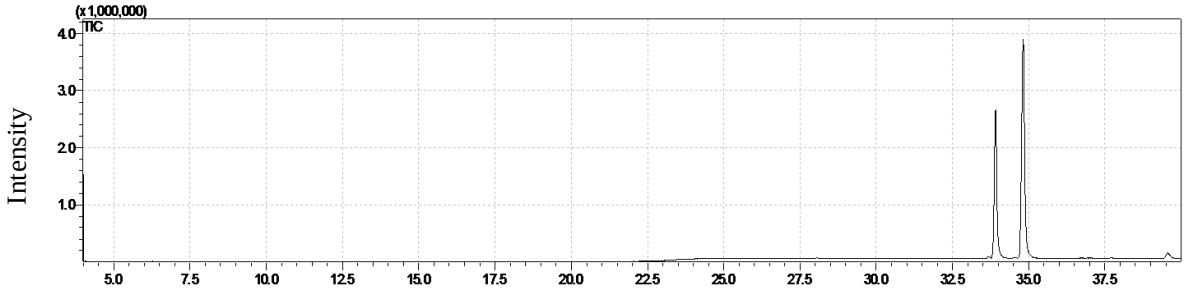
[a]Identities confirmed by comparing mass spectra and retention times with those of NIST database.

A



Time (min)

B



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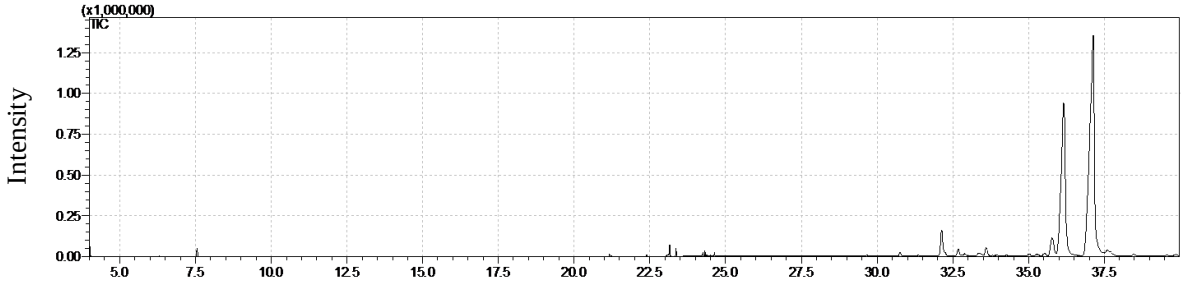

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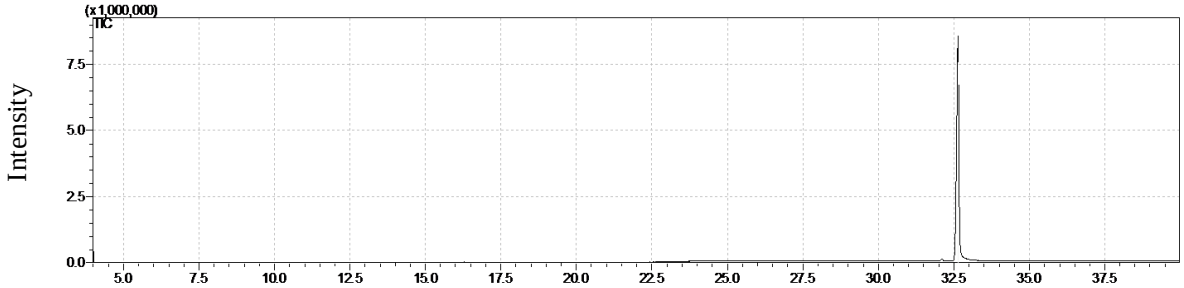

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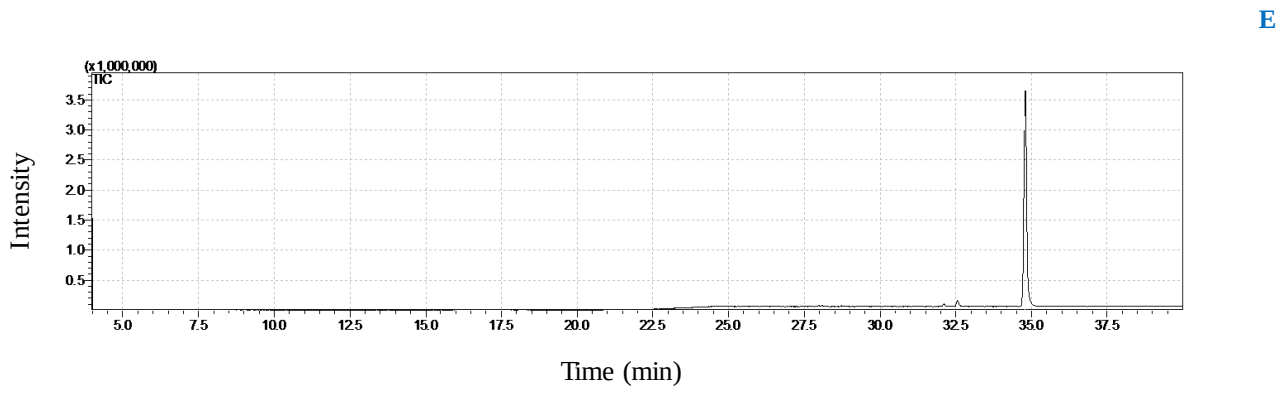


Figure S1. TIC of (A) α/β-amyrone (R_t: 31.330 min, β-isomer; R_t: 32.185min, α-isomer); (B) α/β-amyrin acetate (R_t: 33.498 min, β-isomer; R_t: 34.820 min, α-isomer); (C) 3,11-dioxo-α/β-amyrene (R_t: 36.105 min, β-isomer; R_t: 37.035 min, α-isomer); (D) lupeol (R_t: 32.630 min) and (E) lupeol acetate (R_t: 34.800 min) by GC.

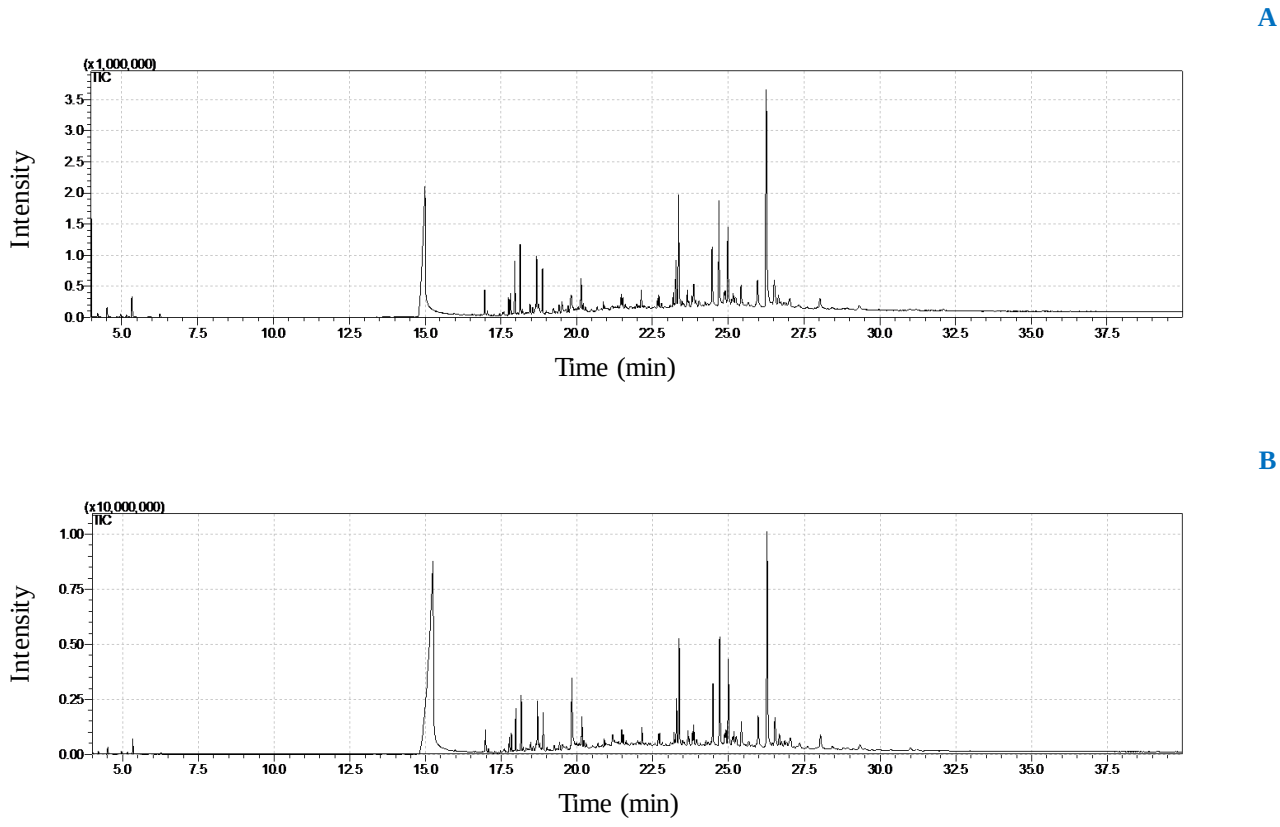
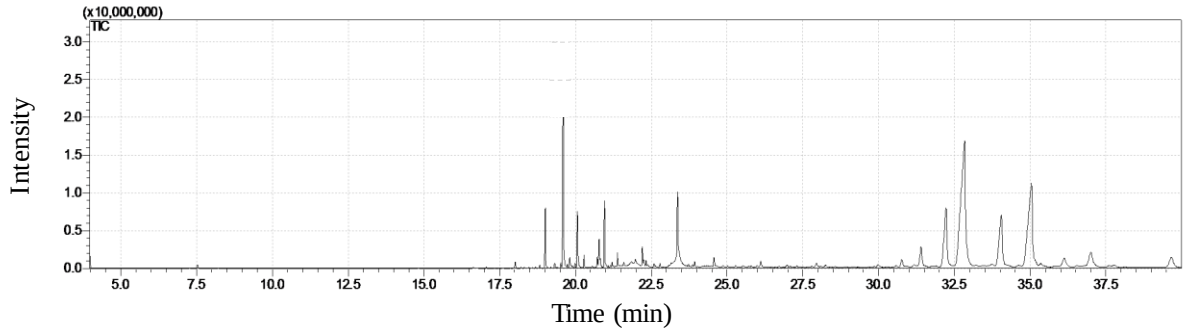


Figure S2. TIC of (A) *P. nemorosa* hexane and (B) *P. nemorosa* hexane fraction + cinnamic acid obtained by GC.

A



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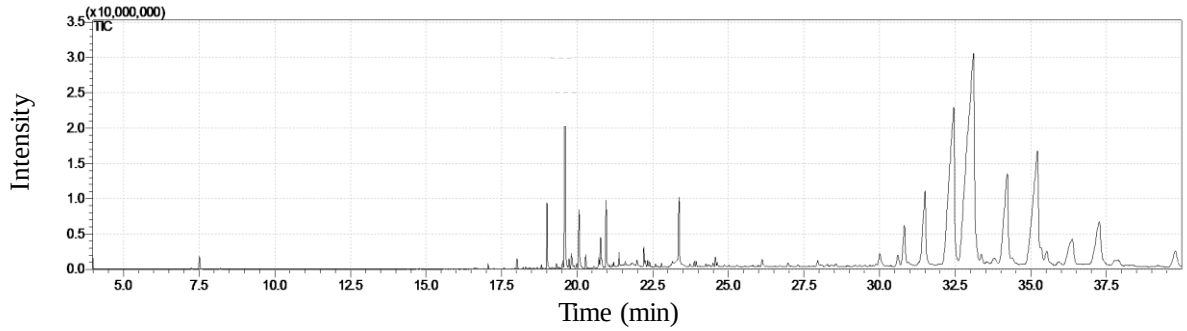
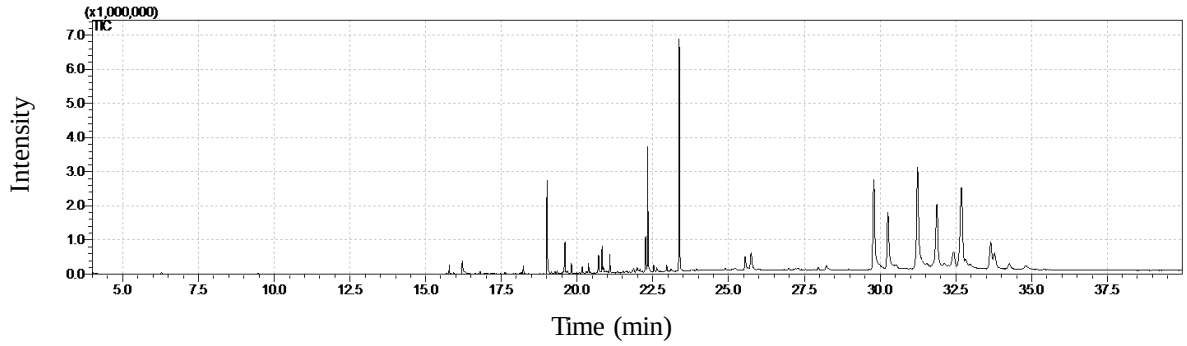


Figure S3. TIC of (A) *P. nemorosa* hexane/EtOAc 5% and (B) *P. nemorosa* hexane/EtOAc 5% + α/β amyrone, lupeol, α/β-amyrin acetate and 3,11-dioxo-α/β-amyrene obtained by GC.

A



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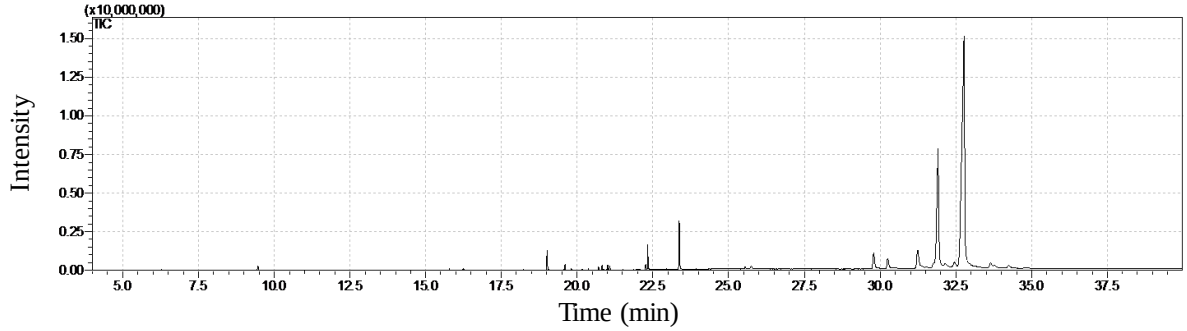

Figure S4. TIC of (A) *P. nemorosa* hexane/EtOAc 10% fraction and (B) *P. nemorosa* hexane fraction + α/β-amyrin obtained by GC.

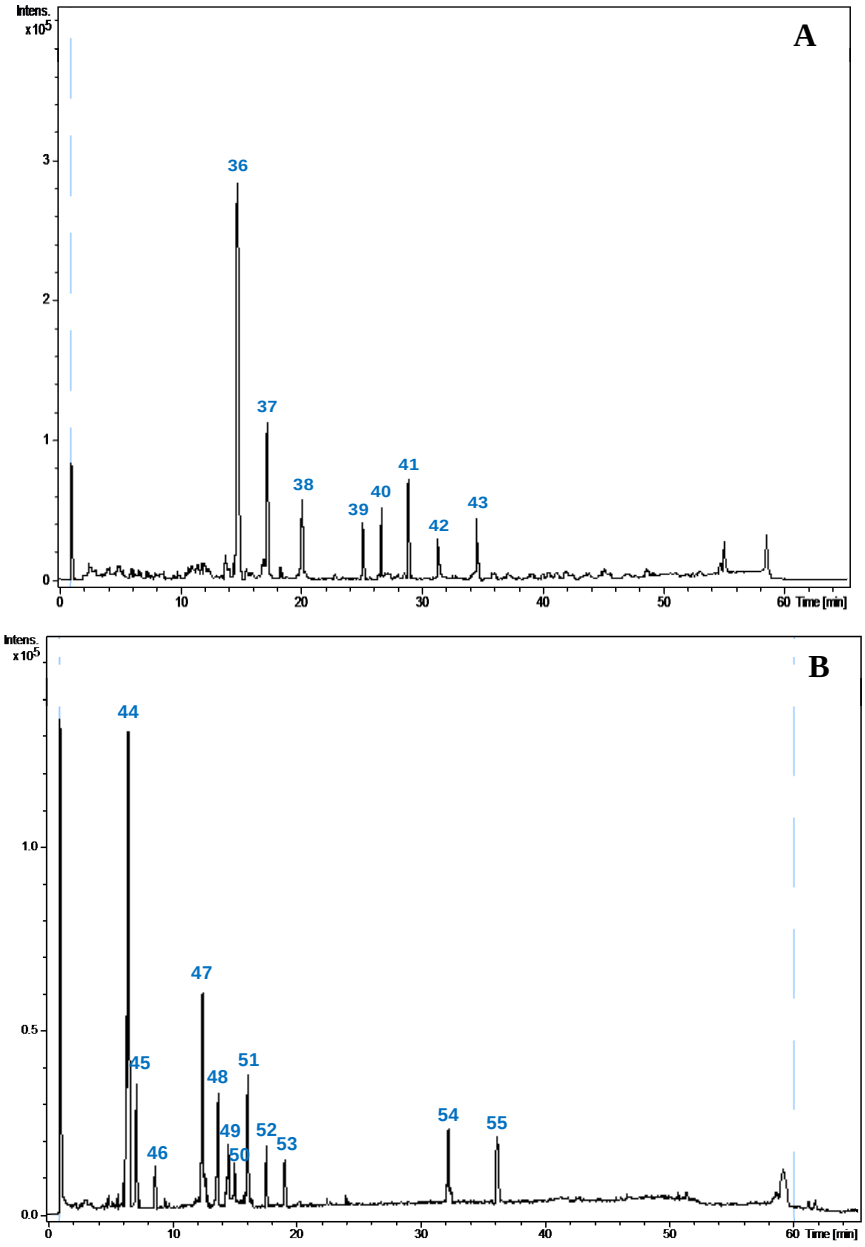

Figure S5. TIC of *P. nemorosa* EtOAc fraction in (A) positive and (B) negative modes.

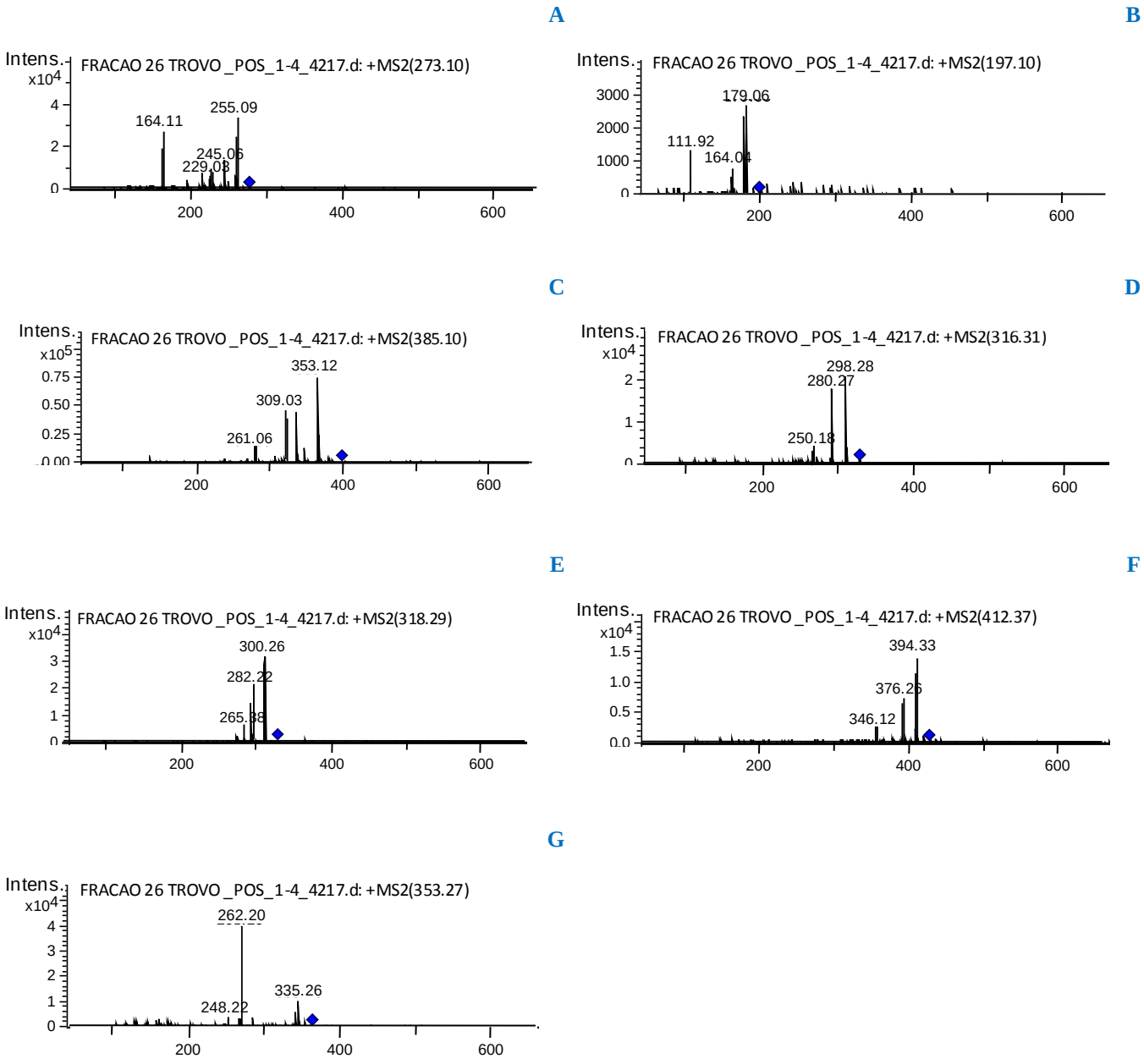

Figure S6. Product ion spectra of bioactive compounds detected in positive mode of *P. nemorosa* EtOAc fraction. (A) Butin; (B) loliolide; (C) gibberellin related compound; (D) dehydrophytosphingosine; (E) phytosphingosine; (F) 2-amino-1,3,4-docosanetriol and (G) palmitoylglycerol.

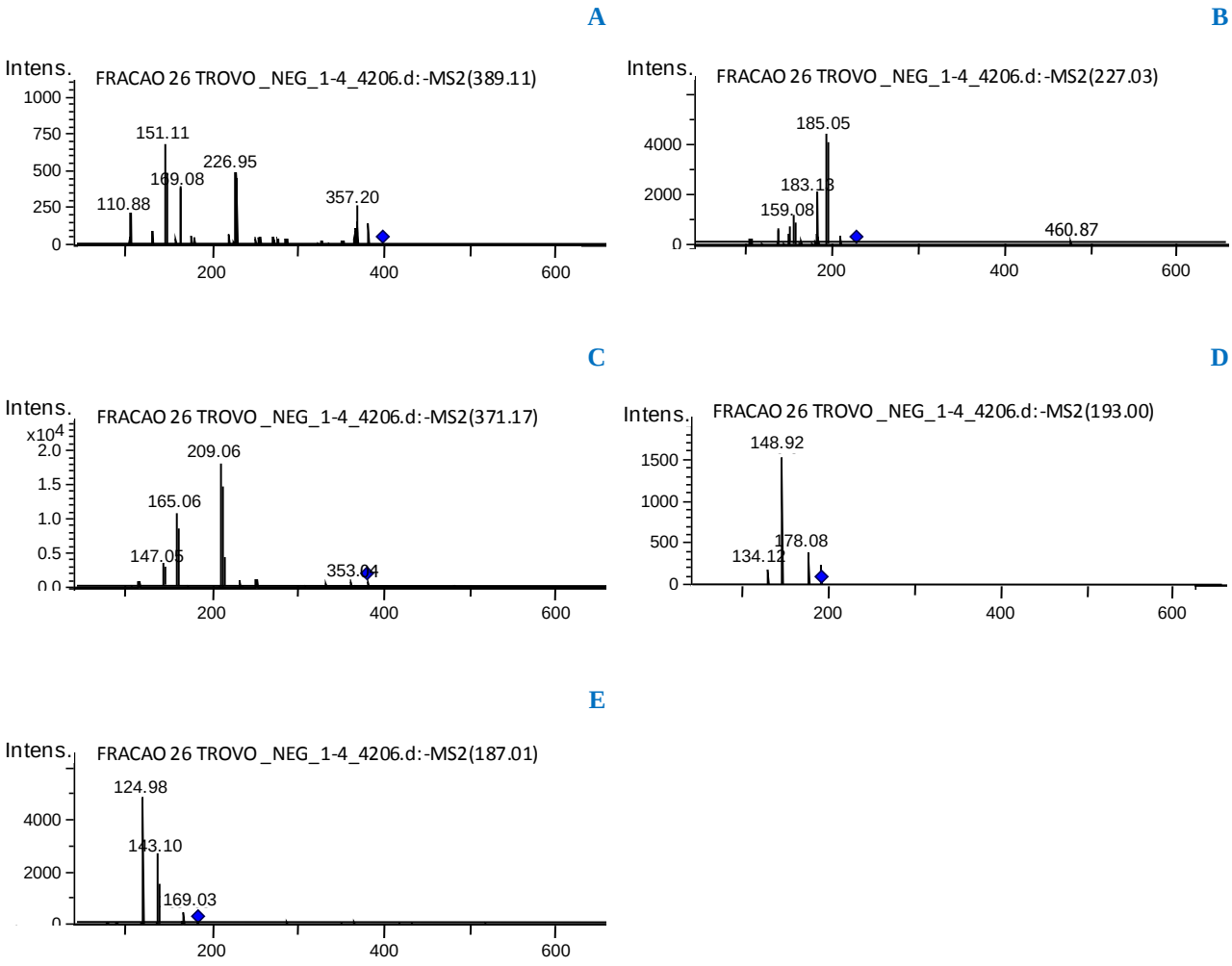

Figure S7. Product ion spectra of bioactive compounds detected in negative mode of *P. nemorosa* EtOAc fraction. (A) Epiloganin; (B) resveratrol; (C) deacetylasperuloside; (D) ferulic and (E) azelaic acids.

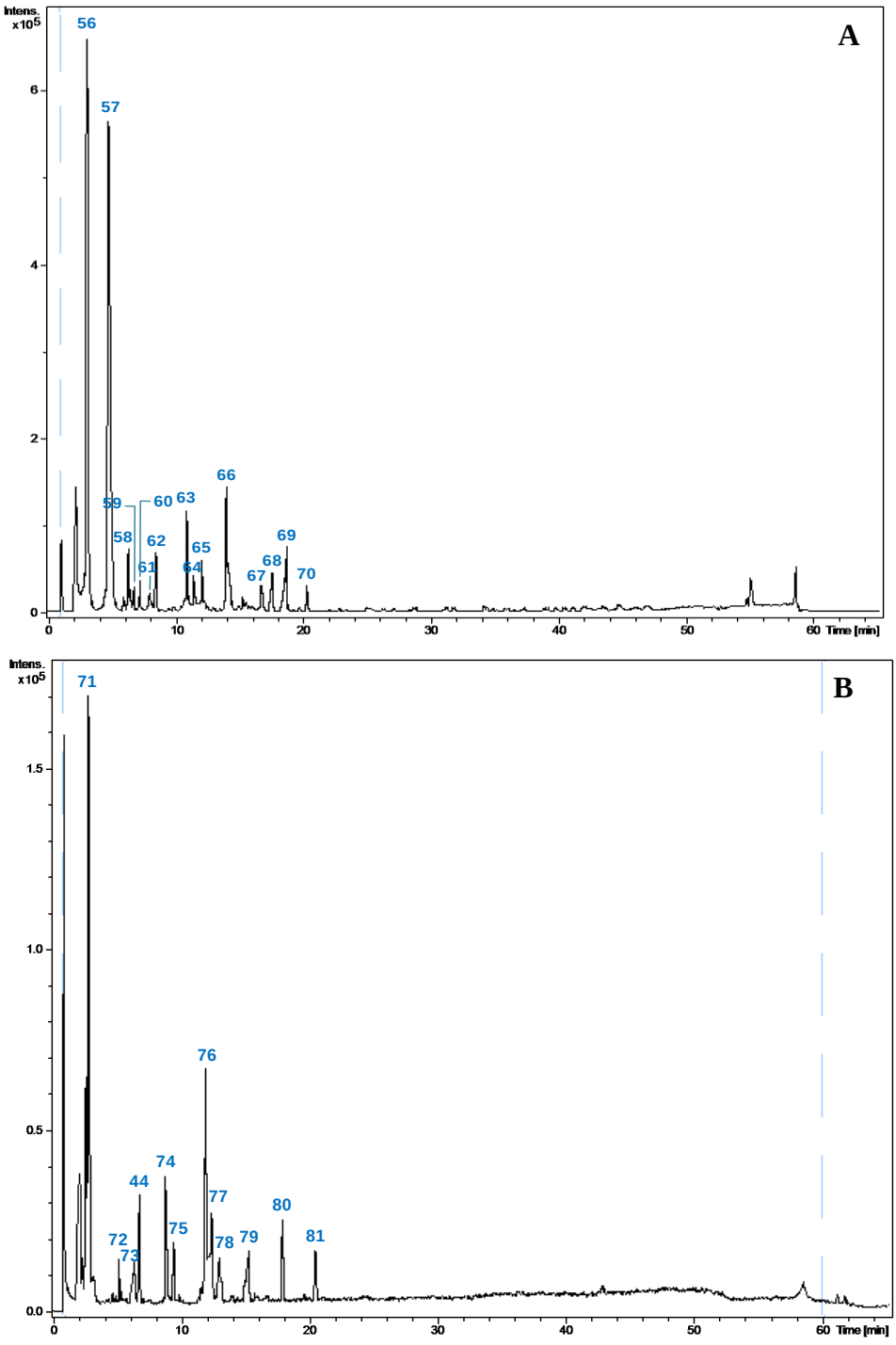

Figure S8. TIC of *P. nemorosa* MeOH fraction in (A) positive and (B) negative modes.

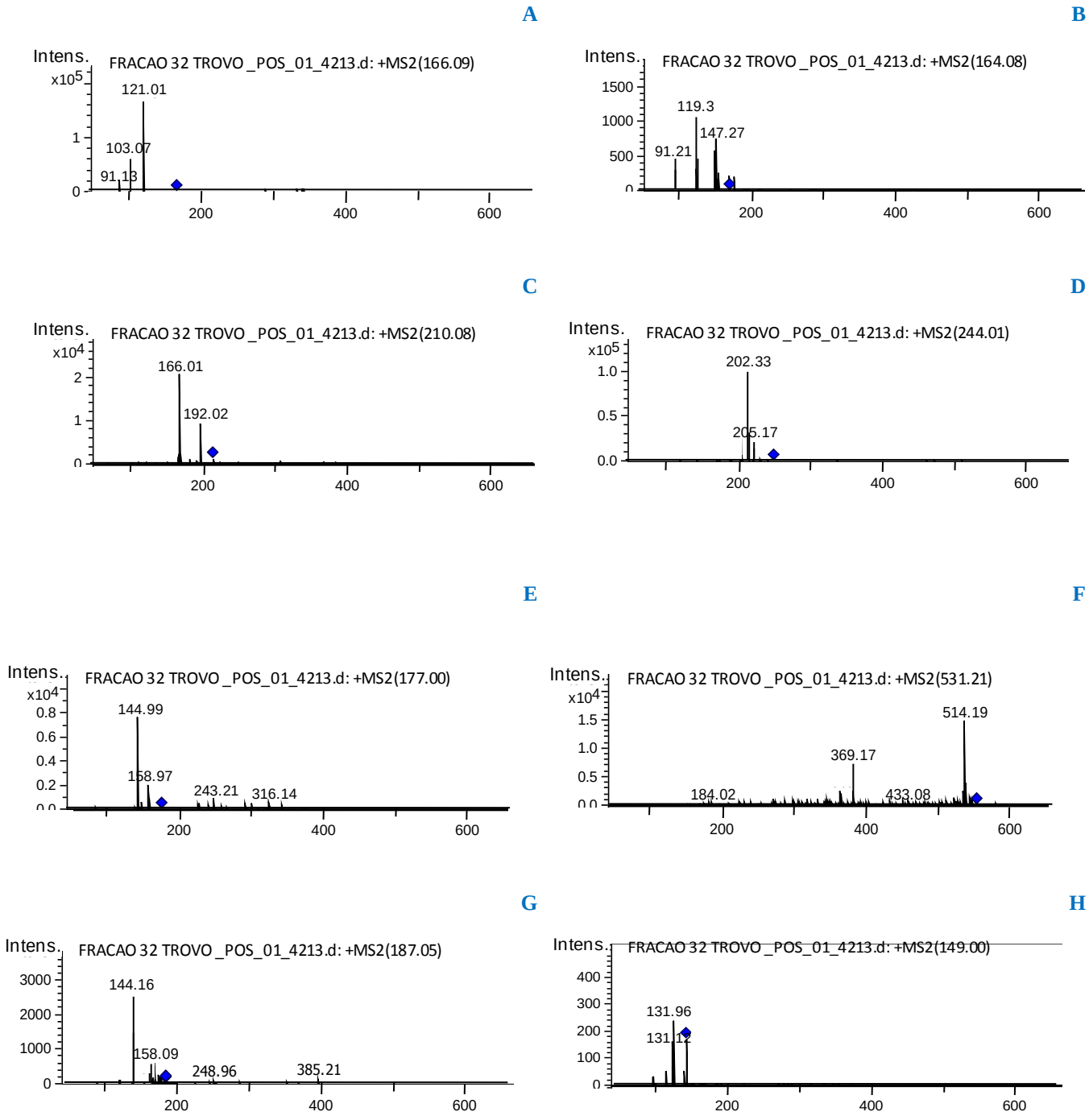

Figure S9. Product ion spectra of bioactive compounds detected in positive mode of *P. nemorosa* MeOH fraction. (A) Hordenine; (B) eusterol; (C) 8-amino-7-oxononanoic acid; (D) an amino suggar; (E) syringol/vanillic alchool/hydroxytyrosol; (F) strictosidine; (G) *N*-methyl-1,2,3,4-tetrahydro-β-carboline and (H) pyrogallol.

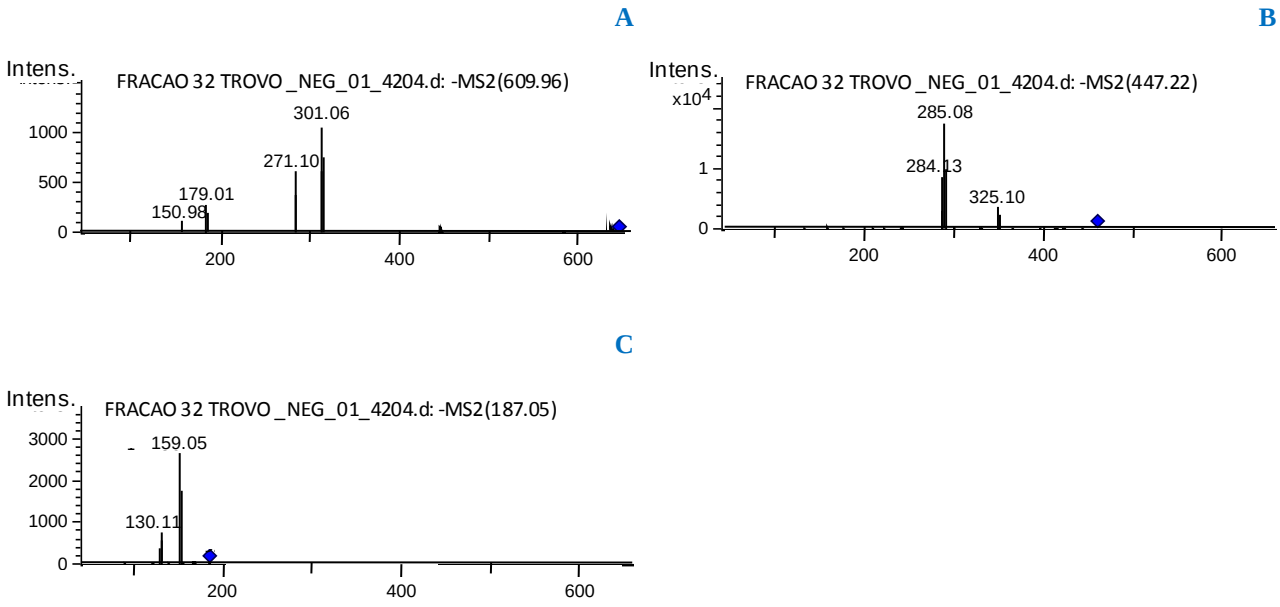

Figure S10. Product ion spectra of bioactive compounds detected in negative mode of *P. nemorosa* MeOH fraction. (A) Rutin; (B) kaempferol 7-O-β-D-glucopyranoside and (C) *N*-formyl tryptamine.