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UPLC-ESI-MS/MS Profile of The Ethyl Acetate Fraction of Aerial Parts of Bougainvillea 'Scarlett O'Hara' Cultivated in Egypt

May A. El-Sayed*, Fawkeya A. Abbas, Sara Refaat, Azza M. El-Shafae, Eman Fikry

Department of Pharmacognosy, Faculty of Pharmacy, Zagazig University, 44519 Zagazig, Egypt

Abstract

The ethyl acetate fraction of *Bougainvillea* 'Scarlett O'Hara' cultivated in Egypt did not receive enough attention in phytochemical and biological studies. This inspired the authors to investigate the phytochemicals of this fraction for the first time using UPLC-ESI-MS/MS in negative and positive ionization modes to understand the distribution of the major secondary metabolites. The analysis revealed the tentative identification of fifty-seven compounds. The detected metabolites belonged to numerous chemical classes including seven organic acids, fourteen phenolic compounds, one betacyanin, seven anthocyanins, ten flavonoids, three saponins, six tannins, four cyclic tetrapyrolic derivatives and five miscellaneous. The LC-ESI-MS methodology in negative ionization mode was the most appropriate to detect the group of saponins (22.17%), flavonoids (14.27%), free organic (12.35%) and phenolic acid derivatives (14%). It can be seen that the highest ionization rate produced for cyclic tetrapyrolic derivatives (56.41%), anthocyanins (18.8%) and tannins (3.2%) in the positive mode chromatogram.

Keywords: Bougainvillea; Nyctaginaceae*;* phytochemicals; UPLC-ESI-MS/MS.

1. Introduction

Family Nyctaginaceae (Known as the Four-O'Clock family) is a relatively small family of dicotyledonous flowering-plants comprising of about 33 genera with approximately bout 400 species distributed mainly in tropical and subtropical regions of the New World with a few species in India, Africa, and the Mascarene and Pacific Islands [1-4]. In Asia, Brazil and Mexico, plants of the family Nyctaginaceae have been used to treat diarrhea, dysentery, gastrointestinal colic, muscle discomfort and as abscess, boil and scab poultices. Roots of some indigenous species are eaten as vegetables in southern Africa, the family is best known to South Africans by the genus of *Bougainvillea* that is commonly cultivated in gardens [3]**.**

Bougainvillea is a genus of a very widespread flowering plants native to South America from Peru to West Brazil and South to Southern Argentina [5]. In 1768, at Rio-de-Janeiro, Brazil, *Bougainvillea* was discovered by French military commander *Louis Antoine de Bougainville*, who introduced the plant to Europe [6]. Plants of this genus are reported to have a broad range of medicinal properties such as insecticide, antidiarrheal, anti-ulcer, antiviral, antibacterial, antioxidant, anti-inflammatory, antidiabetic, antifertility and also considered to be larvicidal, a hepatoprotective plant and also used for the treatment of hypotension [7, 8].

Bougainvillea has about eighteen species. Just four species (B. buttiana, B. glabra, B. spectabilis and B. peruviana) have been well studied and economically used. However, there are also more than 100 cultivars and three hybrids which have not yet been recognized [9]. *Bougainvillea* plants have been regularly hybridized due to their commercialization, driving to the development of more than 400 new varieties with complex genetic background [10].

The growth habit of *Bougainvillea* and its beautiful showy bracts make it a common plant for landscaping for agriculture, beautification, pharmaceutical, and

*Corresponding author e-mail: Mayalsayed@zu.edu.eg.; (May A. El-Sayed)
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environmental industries [11]. In addition to its ornamental value in landscaping, it has recently been found that *Bougainvillea* is a plant that is pollution-tolerant and can assist in reducing air pollution (greenhouse gases) [12].

Plants of this genus are spread in quick growing ornamental shrubs or small trees, sometimes climbers. Due to the presence of beautiful colorful foliage bracts and large compliance with various soil and climatic conditions, they are commonly used in tropical or subtropical gardens. They bloom throughout the year [13, 14].

One of the best and most hardy *Bougainvillea* cultivars is 'Scarlett O'Hara' which is the plant of concern for this genus. It is a tropical and subtropical woody, shrubby, thorny ornamental vine with a heavy growth habit. The effectively scrambling shrubs flower most vigorously in the hot, full sun showing colourful bracts up and down the branches. It has a spreading, usually multi-trunked or with clumping, stems with a height and spread of up to 12 meters. It climbs by sending out slim arching canes armed with stiff curved thorns covered with a dark waxy material. In contrast to the deep red bracts, broad deep green leaves contrast well. The colour shifts to hot magenta when the bracts are open completely.

As there is no report in the available literature about the pharmacognostical, phytochemical studies and the biological screening of this plant, it is deemed of interest to carry out our study on this plant.

Therefore, the main objective of the current study was to use UPLC-ESI-MS/MS to phytochemically characterize the fraction of ethyl acetate obtained from the aerial components of *Bougainvillea* 'Scarlett O'Hara'.

2. Experimental

2.1. Plant Material:

The fresh aerial parts (leaves, stems and flowers) of *Bougainvillea* 'Scarlett O'Hara' were collected from Zagazig- Benha road, Sharkia province, Egypt during June 2016. Taxonomical authentication of plant sample was performed by Eng. Therese Labib, Consultant of plant taxonomy at Ministry of Agriculture and the former director of El-Orman Botanical Garden, Giza, Egypt. Voucher specimen for plant (#BSO-2016) was kept in the herbarium of Pharmacognosy Department, Faculty of Pharmacy, Zagazig University, Egypt.

2.2. Preparation of Extracts:

The air-dried powdered aerial parts of *Bougainvillea* 'Scarlett O'Hara' (10 kg) was extracted by cold maceration with 90% ethanol (3 x 20 L) at room temperature till complete exhaustion. The combined alcoholic extract was evaporated under vacuum to yield 160 g of total ethanolic residue. This residue was suspended in methanol-water mixture (1: 9, 1 L) and successively partitioned against light petroleum, chloroform and ethyl acetate (5 x 500 ml) to afford 66 g, 3 g and 6 g of light petroleum, dichloromethane and ethyl acetate fractions, respectively**.**

2.3. Chemicals and Reagents:

The solvent used in this work viz.: petroleum ether, dichloromethane, ethyl acetate and ethanol (90%) were of analytical grade. Sigma Aldrich (Hamburg, Germany) provided HPLC grade methanol (≥ 99.9%), acetonitrile, water and formic acid for ESI-MS analysis.

2.4. *UPLC- ESI- MS/MS instrument and separation technique*:

Ultra-performance liquid chromatography with electrospray ionization quadrupole- linear ion trap-tandem mass spectrometry analysis, performed on ESI-MS positive and negative ion acquisition modes, was carried out on a XEVO TQD triple quadruple instrument. Method in a multiple-reaction monitoring (MRM) mode was employed for the quantitative determination of phytochemicals. The ethyl acetate fraction of *Bougainvillea* was analyzed by UPLC, to obtain chromatographic profile of the more polar portions of the extracts, which contain phenolic and flavonoid compounds. The sample was dissolved in HPLC grade methanol, filtered through 0.2 µm membrane disc filter, and the resulting solution concentration was 100 *µg*/ mL, then subjected to LC-ESI-MS analysis. The UPLC system was a mass spectrometer, Waters Corporation, Milford, USA. The reverse-phase separations were performed (ACQUITY UPLC BEH C_{18} Column, 1.7µm- 2.1 × 50 mm; 50 mm × 1.2 mm inner diameter; 1.7 µm particle size) at 0.2 m/mL flow rate. A previously reported gradient program was applied for the analysis [15, 16]. The mobile phase consisted of acidified water containing 0.1% formic acid (A) and acidified methanol containing 0.1% formic acid (B). The employed elution conditions were as follows: 0–2 min, isocratic elution at 10% B; 2–5 min, linear gradient from 10 to 30% B; 5–15 min, linear gradient from 30% to 70% B; 15–22 min, linear gradient from 70% to 90% B; and 22–25 min, isocratic elution at 90% B;

finally, washing and reconditioning of column were done. To obtain more data, electrospray ionization (ESI) was performed in both negative and positive ion modes. The parameters for analysis were set using negative ion mode as follows: cone voltage 30 eV, capillary voltage 3 kV, cone gas flow 50 L/h, source temperature 150°C, desolvation temperature 440°C and desolvation gas flow 900 L/hr. Mass spectra were detected in the ESI between *m/z* 100 and 1000 atomic mass units. Chemical constituents were identified by their ESI–QqQLIT–MS/MS spectra and fragmentation patterns. The peaks and spectra were processed using the MassLynx 4.1 software and tentatively identified by comparing their retention time (R_t) and mass spectrum with reported data.

3. *Results and discussion:*

In this study, structural identification of polyphenols and other constituents of ethyl acetate fraction of *Bougainvillea* 'Scarlett O'Hara' was analyzed by UPLC-ESI-MS/MS, operating in both positive and negative ionization modes. The identification of abundant compounds of this fraction was based on mass fragmentation patterns and the standard data reported in the published available literature and database. The compounds were arranged according to R_t. Fifty-seven compounds were tentatively identified including seven organic acids, fourteen phenolic compounds, one betacyanin, seven anthocyanins, ten flavonoids, three saponins, six tannins, four cyclic tetrapyrolic derivatives and five miscellaneous. The respective total ion chromatograms (TICs) are shown in Fig. **1.** It is possible to check the distribution of the determined secondary metabolites in the analyzed sample in Table **1** and **2.** The 39 detected compounds with UPLC-ESI-MS/MS in negative mode are listed in Table **1** while the 18 compounds detected in the positive mode are described in table **2**. Both tables include names of the compounds, retention times (R_t) of the assigned peaks, molecular ion value either $[M-H]^-$ or $[M+H]^+$, respectively as well as MS/MS fragments and the used published references that confirm the proposed identification in addition to the area percentage of identified compounds in the tested fraction. The sum of peak areas achieved for the compounds that have been identified in *Bougainvillea* 'Scarlett O'Hara' ethyl acetate fraction with the two evaluated methods (LC-ESI-MS $^{(-/+)}$) is shown in Fig. **2.** Pie charts presented in Fig. **3** display the percentage (in terms of area) corresponding to each chemical category over the total area of the chromatograms obtained by means of the two methodologies used in this study. Structures of the identified compounds detected in the fraction under investigation are shown in Fig. **4.** While Fig. **5** showed fragmentation patterns for some detected metabolites**.**

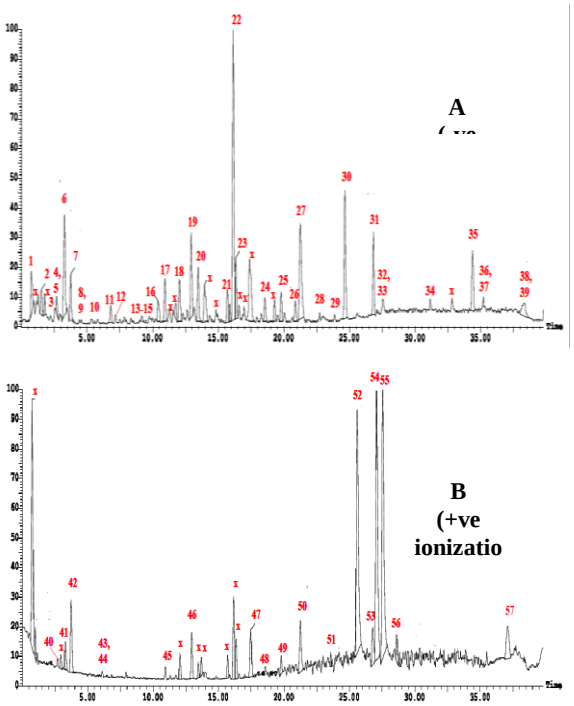

Fig. 1: Total ion chromatograms of the ethyl acetate fraction of *Bougainvillea* 'Scarlett O'Hara'. (A): negative mode; (B): positive mode. x=unidentified compounds

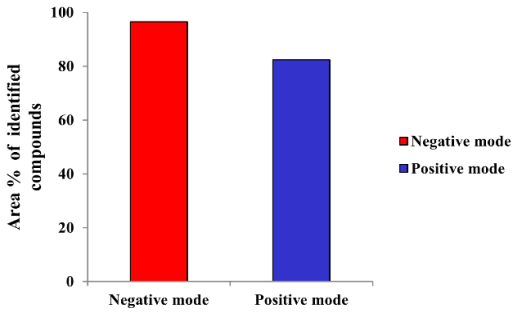

Fig. 2: Bars graph representing the sum of areas (in a normalized axis) of the identified compounds found in *Bougainvillea* 'Scarlett O'Hara' ethyl acetate fraction.

Table 1: Metabolites identified in *Bougainvillea* 'Scarlett O'Hara' aerial parts ethyl acetate fraction using UPLC-ESI-MS/MS analysis in negative ionization mode.

Comp. no.	Compound name	Rt (min.)	$[M-H]^-$ (*m/z*)	MS^2 fragments (*m/z*)	Area %	Ref.
1	Sucrose	0.76	341	179, 161, 131	2.60	[17]
2	Coumaric acid	1.53	163	119	1.56	[18]
3	*p*-Hydroxy benzoic acid hexoside	2.54	299	137 $(M-H-Glc)^-$, 93 $(M-H-Glc-CO_2)^-$	0.90	[19]
4	Caffeic acid derivative	2.70	377	341, 332, 179, 215	0.92	[20]
5	Tetramethoxy flavone	2.81	341	326, 311, 285	1.56	[21]
6	Syringic acid	3.17	197	197, 182 $(M-H-CH_3)^-$, 167 $(M-H-2CH_3)^-$, 153 $(M-H-CO_2)^-$	6.74	[19, 22, 23]
7	Trihydroxyursolic acid derivative	3.74	711	503 (100%), 441$[M-H-H_2O-COOH]^-$, 485 $(M-H-H_2O)^-$,456, 455 (ursolic acid), 393, 357	2.67	[24]
8	Methoxycinnamic acid hexoside	4.09	339	177 (100%) $(M-H-Hex.)^-$	0.32	[19]
9	Caffeic acid hexoside	4.60	341	179 $(M-H-Hex.)^-$, 135	0.26	[25]
10	Delphinidin hexosyl pentosyl malonate	5.18	681	595, 301	0.27	[26]
11	Syringic acid isomer	6.17	197	197, 182 $(M-H-CH_3)^-$, 167 $(M-H-2CH_3)^-$, 153 $(M-H-CO_2)^-$	0.95	[19, 22, 23]
12	Acacetin-7-*O*-glucoside	7.52	445	283 $(M-H-Glc.)^-$	0.45	[27]
13	Liquirtigenin-7-*O*-glucoside	8.14	711	549 $(M-H-Glc.)^-$	0.27	[28]
14	Luteolin-3'-*O*-(*O*-acetyl) *β*-*D*-glucuronide	9.04	503	399, 285	0.32	[29]
15	3-*O*-glucuronide-29-hydroxyoleanolic acid	9.14	647	629$(M-H-H_2O)^-$, 471 $(M-H-176)^-$, 439 $(M-H-176-CH_3OH)^-$	0.27	[30]
16	Quercetin-3-*O*-glucuronide (miquelianin)	9.54	477	301, 151, 135	1.62	[31]
17	Chrysoeriol methyl ether	9.60	313	283	2.65	[32]
18	Fraxiresinol hexoside	11.44	565	403 $(M-H-Glc.)^-$, 373$(M-H-Glc.-CH_2O)^-$, 343 $(M-H-Glc.-2CH_2O)^-$, 299 $(M-H-Glc.-2CH_2O-CO_2)^-$, 181, 166	2.91	[23]
19	Hexahydroxydiphenoyl (HHDP) galloylglucose	12.56	633	481, 421, 339, 301, 249	5.13	[33]
20	Quercetin-3-*O*-methacrylate	13.42	385	301	3.22	[34]
21	Salvianolic acid B	15.08	717	519 (100%), 339, 313, 179	2.02	[35]
22	Chikusetsusaponins (CSs) Iva	17.11	793	631 $(M-H-Glc.)^-$, 569 $(M-H-Glc.-H_2O-CO_2)^-$, 455	18.30	[30, 36, 37]
23	Chikusetsusaponins (CSs) Iva isomer	17.30	793	631 $(M-H-Glc.)^-$, 569 $(M-H-Glc.-H_2O-CO_2)^-$	3.60	[30, 36, 37]
24	*p*-Hydroxybenzoic acid	18.84	137	93	1.45	[19]
25	Sinapic acid-3-*O*-glucoside	19.81	385	223$(M-H-Glc.)^-$, 179	1.76	[38]
26	Methyl trigalloyl glucose	20.28	649	497 $(M-H-152)^-$, 479	1.33	[33]
27	Delphinidin hexosyl pentosyl malonate isomer	21.33	681	595, 301	8.71	[26]
28	Ethyl gallate	23.49	197	169, 124	0.58	[39]
29	Methoxy benzoic acid hexoside	24.25	313	151 $(M-H-Hex.)^-$	0.43	[19]
30	*N*-Feruloyl tyramine	24.66	312	312	7.74	[40]
31	Lanopalmitic acid	26.84	271	225	4.24	[18]
32	Chebulic acid	27.06	355	337, 249	1.19	[41, 42]
33	*N*-Feruloyl tyramine isomer	27.26	312	312	0.45	[40]

34	Ethyl gallate isomer	31.43	197	169, 124	1.23	[39]
35	Quercetin	34.35	301	217, 191, 151	4.18	[17]
36	Sinapic acid-3-*O*-glucoside isomer	35.14	385	223 (M-H-Glc.)$^-$, 179	1.21	[38]
37	Acetyl-*O*-galloyl glucose	35.38	373	313, 169, 151	0.35	[38]
38	Ferulic acid derivative	38.13	367	295, 235, 193, 149	0.52	[20]
39	Protocatechualdehyde	38.90	137	137	1.64	[23]
Total area % of identified compounds					96.52	

Glc. = Glucose; Hex. = Hexose

Table 2: Metabolites identified in *Bougainvillea* 'Scarlett O'Hara' aerial parts ethyl acetate fraction using UPLC-ESI-MS/MS analysis in positive ionization mode.

Comp. no.	Compound name	Rt (min.)	$[M+H]^+$ (*m/z*)	MS^2 fragments (*m/z*)	Area %	Ref.
40	Ferulic acid	2.65	195	177 $(M+H-H_2O)^+$	0.54	[43]
41	Ferulic acid isomer	3.16	195	177	1.33	[43]
42	Cyanidin-3-*O*- acetyl-glucoside	3.74	491	287, 137	4.56	[39]
43	*O*-Galloyl arbutin	5.06	425	273	0.22	[17]
44	5"-*O*- salicyl-2'-*O*-glucosyl-betanin Or 5"-O- salicyl-2'-O-glucosyl-isobetanin	5.69	833	713 $(M+H-120)^+$ (M+H-salicylated)$^+$, 671 (M+H-Glc.)$^+$, 551 (M+H-120-Glc.)$^+$, 389	0.31	[44]
45	Apigenin glucuronide	10.61	447	271	0.55	[17]
46	Guaiacyl pyrano malvidin 3-*O*-glucoside	13.15	639	477, 462	3.15	[39]
47	Cyanidin-3-*O*- acetyl-glucoside isomer	18.17	491	287, 137	3.48	[39]
48	Tri-galloyl-hexoside	18.95	637	483, 465, 169	0.56	[17]
49	Myricitin derivative	20.19	657	319	0.86	[17]
50	Cyanidin-3-*O*- acetyl-glucoside isomer	21.21	491	287, 137	4.30	[39]
51	Caffeoylquinic acid	23.97	355	337 $(M+H-OH)^+$	0.34	[43]
52	13^2–Hydroxypheophorbide-*β*-methyl ester (Petasiphyll-A)	25.49	637	559	18.60	[45]
53	Trigalloyllevoglucosan	27.01	619	303, 153, 109	2.42	[17]
54	13^2–Hydroxypheophorbide-*α*-methyl ester	27.29	623	605, 573, 545, 503, 485, 459	16.78	[45, 46]
55	13^2–Hydroxypheophorbide-*α*-methyl ester isomer	28.39	623	605, 573, 545, 503, 485, 459	19.77	[45, 46]
56	13^2–Hydroxypheophorbide-*β*-methyl ester isomer	29.19	637	619, 587, 559, 531, 499	1.26	[45]
57	Malvidin-3-*O*-caffeoyl-glucoside	36.22	655	331, 315	3.31	[39]
Total area % of identified compounds					82.34	

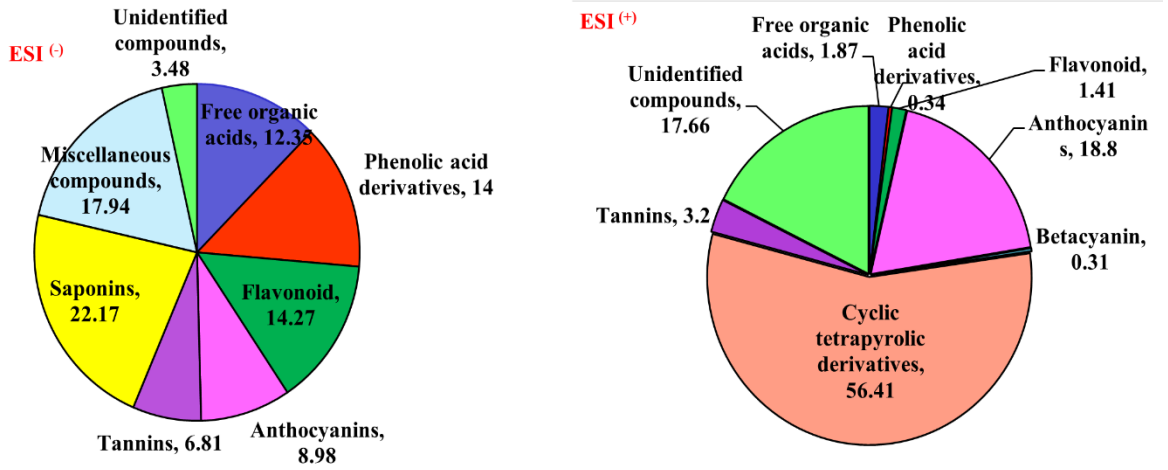

Fig. 3: Pie charts showing the share of every chemical class (in terms of area (% of the total area)) in the chromatograms obtained either in negative ESI (-) or positive ESI (+) modes.

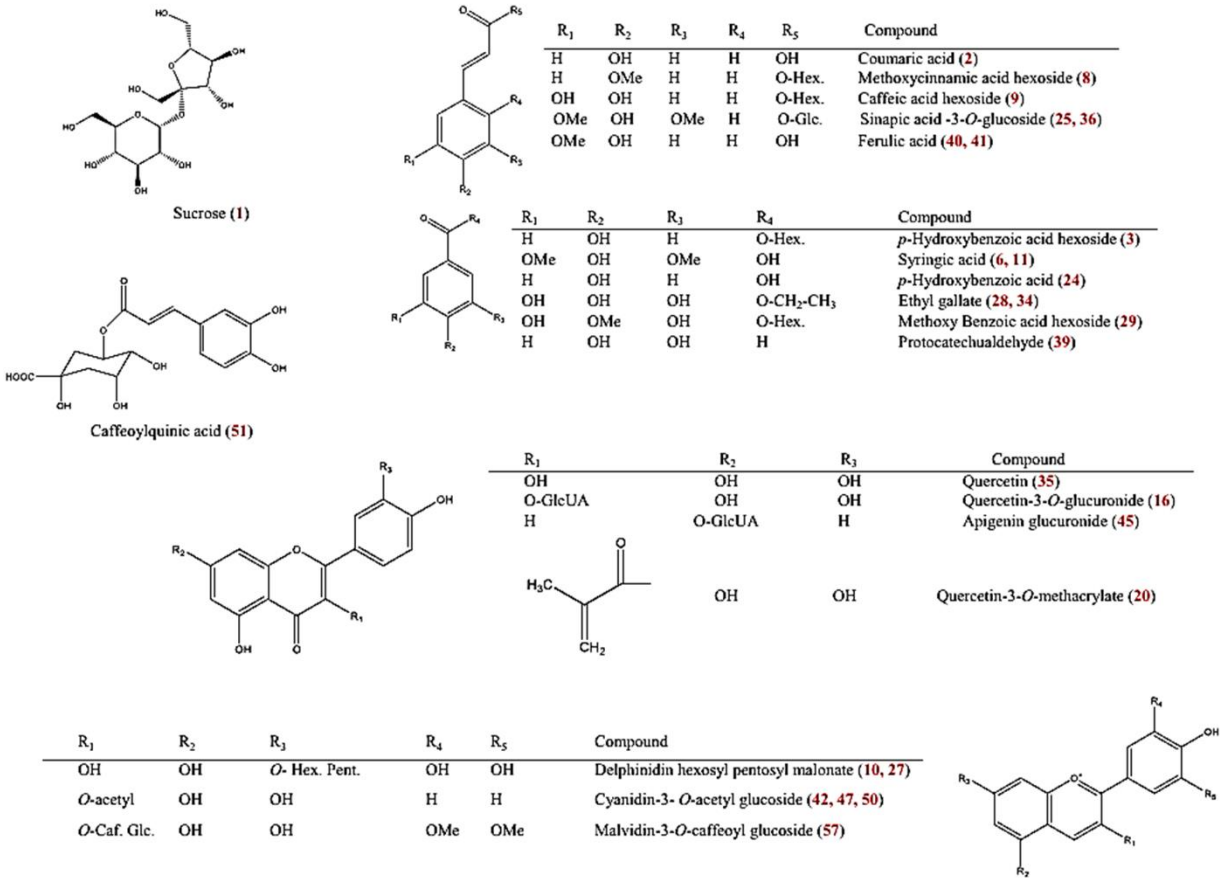

Fig. 4: Continued

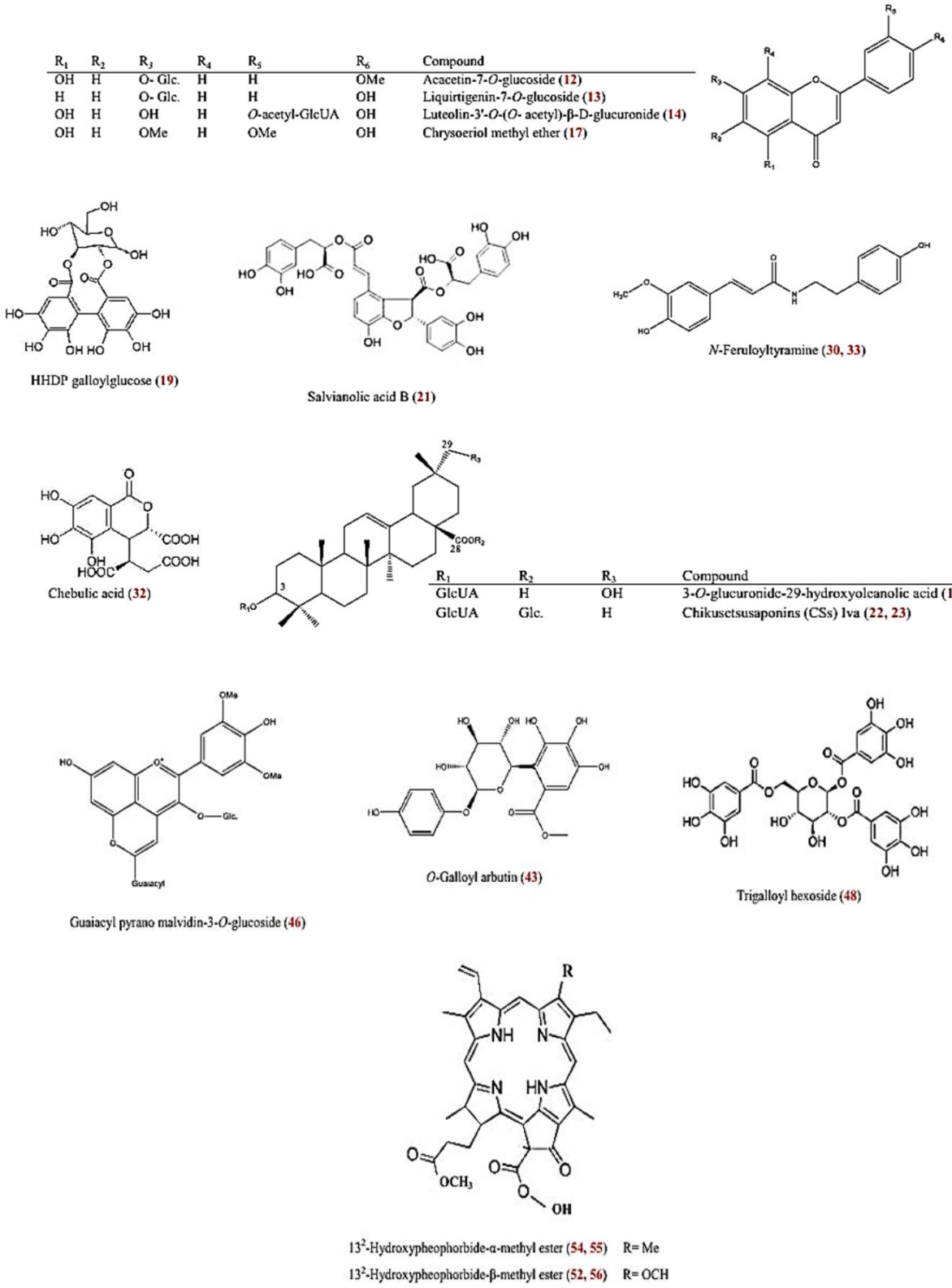

Fig. 4: Metabolites identified in *Bougainvillea* 'Scarlett O'Hara' ethyl acetate fraction using UPLC-ESI-MS in negative and positive ionization modes.
Caf. = Caffeoyl; Glc. = Glucose; GlcUA= Glucuronyl; Hex. = Hexose; Me= Methyl; Pen. = Pentosyl.

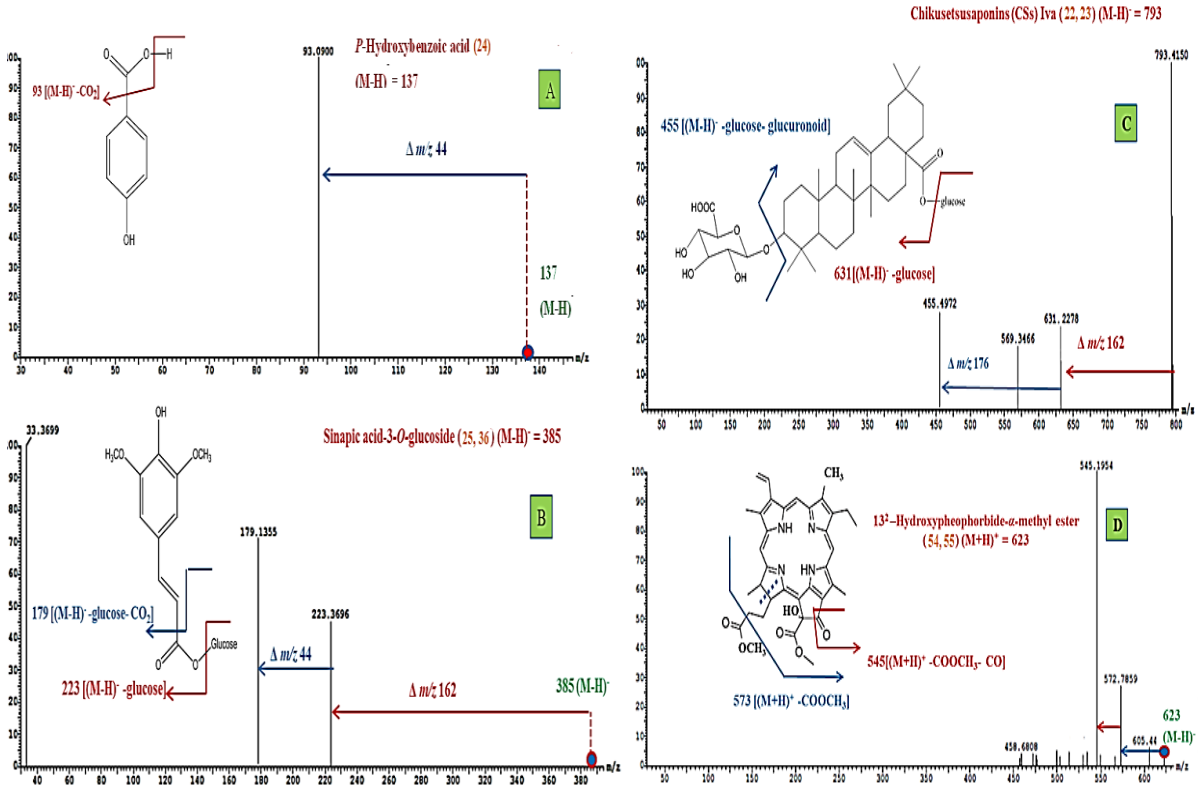

Fig. 4: Product ions (MS^2) spectra of different compounds in negative and positive ion modes ESI-MS from Table 1 and 2.
A= *p*-Hydroxybenzoic acid $(M-H)^-$ = 137; B= sinapic acid-3-*O*-glucoside $(M-H)^-$ = 385; C= chikusetsu saponins (CSs) Iva $(M-H)^-$ = 793; D= 13^2 –hydroxypheophorbide-*α*-methyl ester $(M+H)^+$ = 623.

3.1.Free organic acids

Free organic acids as syringic (**6**) and its isomer (**11**) [19, 22, 23], salvianolic acid B (**21**) [35], *p*-hydroxybenzoic (**24**) [19], ferulic (**40**) and its isomer (**41**) [43] and chebulic acid (**32**) [41, 42] were identified as previously published.

3.2. Phenolic acid derivatives

Most of the phenolic acid derivatives are glycosides, their first stage of fragmentation is the cleavage of the glycosidic bond to produce the *m/z* of the phenolic acid and the respective neutral mass loss of sugar molecules, and then neutral mass losses of methyl, hydroxyl or carboxylic groups helped to identify the specific phenolic acid. Coumaric acid (**2**) [18], *p*-hydroxybenzoic hexoside (**3**) [19], caffeic acid derivative (**4**) and ferulic acid derivative (**38**) [20], trihydroxyursolic acid derivative (**7**) [24], methoxycinnamic acid hexoside (**8**) and methoxy benzoic acid hexoside (**29**) [19], caffeic acid hexoside (**9**) [25], sinapic acid-3-*O*-glucoside (**25**) and its isomer (**36**) [38], ethyl gallate (**28**) and its isomer (**34**) [39], protocatechualdehyde (**39**) [23] and caffeoylquinic acid (**51**) [43] were identified.

3.3. Flavonoid-O-glycosides

Compound (**12**) showed a deprotonated molecular ion at *m/z* 445 with characteristic MS^2 fragment ion at *m/z* 283 $[M-H-glc.]^-$ which related to deprotonated acacetin and consequently it was tentatively identified as acacetin-7-*O*-glucoside [27]. Compound (**13**) was tentatively identified as liquirtigenin-7-*O*-glucoside as

it exhibited a $[M-H]^-$ ion at *m/z* 711 and MS^2 base peak ion at *m/z* 549 $[M-H-162]^-$ after the neutral loss of glucosyl moiety (162 Da) [28]. Quercetin-*O*-methacrylate was proposed for compound (**20**) at R_t 13.42 min (*m/z* 385, $[M-H]^-$). In the MS^2 spectrum, a fragment ion at *m/z* 301, which corresponds to quercetin in structure after methacrylate unit loss [34].

3.4. Flavonoid glucuronides

Three flavonoid-*O*-glucuronides were detected in the analyzed sample: luteolin-3'-*O*-(*O*-acetyl) *β-D*-glucuronide (**14**), quercetin-3-*O*-glucuronide (miquelianin) (**16**) and apigenin glucuronide (**45**)**.** They characterized by neutral loss of 176 u (glucuronide moiety).
Compound (**14**) showed mass spectrum with a precursor ion at *m/z* 503 $[M - H]^-$. This precursor ion showed MS/MS spectrum with a product ion at *m/z* 285 [M-H-218 (176+ 42)]$^-$ (luteolin) after the neutral loss of glucuronyl- acetyl moiety (218 Da) and was tentatively identified as luteolin-3'-*O*-(*O*-acetyl) *β-D*-glucuronide [29].

Compound (**16**) was identified as quercetin derivative as it exhibited a $[M-H]^-$ ion at *m/z* 477 and MS^2 base peak ion at *m/z* 301 $[M-H-176]^-$ (quercetin) after the neutral loss of glucuronyl moiety (176 Da) and was tentatively identified as quercetin-3-*O*-glucuronide (miquelianin) [31].

The precursor ion of compound (**45**) was detected at *m/z* 447 $[M+H]^+$ and its characteristic MS^2 fragment ion at *m/z* 271 $[M+H-176]^+$ suggesting the neutral loss of glucuronide moiety and was tentatively identified as apigenin glucuronide [17].

3.5. Flavonoid aglycones

Quercetin (**35**) was recognized by comparing its MS/MS fragmentation pattern with the previously reported data [17]. Tetramethoxy flavone (**5**) [21], chrysoeriol methyl ether (**17**) [32] and myricitin derivative (**49**) [17] were tentatively identified as well.

3.6. Anthocyanins

A total of five anthocyanin derivatives have been detected in *Bougainvilleae* 'Scarlett O'Hara'. Thus, mass data of compounds (**42**) and its isomers (**47**, **50**) showed a molecular ion peak at *m/z* 491 and MS^2 ion at *m/z* 287 $[M+H-162-42]^+$. These were indicative for a cyanidine with glucose (162 Da) and acetyl (42 Da) moieties. This compound (**42**) and its isomers (**47**, **50**) were proposed to be cyanidin-3-*O*- acetyl- glucoside by comparing its MS^2 data with the published study [39].

Compound **10** and its isomer (**27**) were tentatively assigned as delphinidin hexosyl pentosyl malonate ($C_{29}H_{29}O_{19}$). The ESI-MS/MS spectrum showed a precursor ion at *m/z* 681 $[M-H]^-$ with main MS^2 fragment ions at *m/z* 595 $[M-H-86]^-$ and 301 $[(M-H-86-294]^-$ corresponding to loss of a malonic acid moiety (86 Da) and hexose + pentose moieties (294 Da), respectively. Depending on the consequent loss of malonic acid followed by the two sugars together, the acyl and sugar residues are bound to the same position [26]. Compound related to peak (**46**) was identified as guaiacyl pyrano malvidin-3-*O*-glucoside. It exhibited a protonated molecular ion at m/z 639 and intense fragment ions at *m/z* 477 (loss of 162, loss of glucose moiety) [39].
Positive-ion ESI-MS for compound (**57**) showed a molecular ion of *m/z* 655 $[M+H]^+$. MS^2 of the molecular ion gave a daughter ion at *m/z* 331 $[M+H-324]^+$; corresponding to the loss of caffeoyl-glucose moieties (2x 162 Da) [39].

3.7. Betacyanins

UPLC-ESI-MS/MS analysis revealed the presence of 5"-*O*- salicyl -2'-*O*-glucosyl betanin /isobetanin (compound **44**) as a salicylated betacyanin in ESI^+ mode with ions at *m/z* 833. The appearance of fragment ions at *m/z* 713, $[M+H-120]^+$ suggested the presence of a salicylated moeity, *m/z* 671, $[M+H-162]^+$, attributed to a hexose moiety loss, *m/z* 551, $[M+H-120-162]^+$ and *m/z* 389, $[M+H-120-162-162]^+$ suggested the presence of a salicylated and dihexose moieties. A loss of one glucose (*m/z* 671) and a further cleavage of the salicyl moiety (*m/z* 551 [M+H-glc.-salicyl]$^+$) indicated the location of the salicyl residue on the first glucose unit [44].

3.8. Saponins

Compound (**15**) was identified as 3-*O*-glucuronide-29- hydroxyoleanolic acid (MS^1 at *m/z* 647 $[M-H]^-$, MS^2 at *m/z* 629 $[M-H-H2O]^-$, *m/z* 471$[M-H-176]^-$ revealing the loss of glucuronide molecule (176 Da)) [30, 36, 37].
Compound (**22**) and its isomer (**23**) were oleanolic acid-type ginsenoside as a pseudomolecular ion was observed at *m/z* 793 which fragmented to produce MS^2 base peak at *m/z* 631$[M-H-glc]^-$ revealing the loss of glucose molecule (162 Da), *m/z* 569 $[M-H-glc-H_2O-CO_2]^-$ and *m/z* 455 $[M-H-162-176]^-$ corresponding to additional loss of glucuronyl moiety (176 Da), therefore, it was identified as chikusetsu saponins (CSs) Iva that called 3- *O- β- D*-glucuronopyranosyl-28- *O- β- D* glucopyranosyl oleanolic acid or can be known as 3- *O*- glucuronide oleanolic acid- 28- *O*-hexose and its isomer, respectively [30, 36, 37].

3.9. Hydrolysable tannins derivatives

Hexahydroxydiphenoyl (HHDP) galloylglucose is proposed for compound (19) ([M-H]- at m/z 633). MS2 spectral data showed a fragment ion at m/z 481 [M-H -152]-, indicating the neutral loss of galloyl moiety. The fragment at m/z 301 [M-H- 332]- corresponding to HHDP indicated the loss of galloylglucose unit [33].

Compound (**26**) with a molecular ion at *m/z* 649 in ESI^- mode was tentatively identified as methyl trigalloyl glucose. In MS^2 spectrum for this compound, we observed the product ions at *m/z* 497 due to a neutral loss of galloyl moiety $[M-H-152]^-$ and at *m/z* 479 $[M-H-152-18]^-$ which is attributed to loss of galloyl group in addition to a water molecule [33]. While compound (**37**) was identified as acetyl-*O*-galloyl-glucose. It demonstrated the molecular ion peak $[M-H]^-$ at *m/z* 373 and the daughter ions at *m/z* 313, 169 and 151 as previously reported [38].

Compound (**43**) exhibited molecular ion at *m/z* 425 in MS spectrum. However, the product ion in MS/MS spectrum was at *m/z* 273 corresponding to arbutin in structure and to the neutral loss of galloyl moiety $[M+H-152]^+$. Therefore, the compound was assigned to *O*-galloyl arbutin [17].

Compound (**48**) with a precursor ion $[M+H]^+$ at *m/z* 637 was tentatively suggested as trigalloyl hexoside. The characterization was based on the acceptable MS and MS/MS data, in addition to literature [17]. While compound (**53**) (R_t 27.01 min, respectively) with the precursor ion at *m/z* 619 has been assigned to be trigalloyl levoglucosan relying on the MS^1 and MS/MS spectra [17].

3.10. Cyclic tetrapyrrolic derivatives

Cyclic tetrapyrrolic derivatives such as 13^2-hydroxypheophorbide-α- methyl ester (**54** and **55**) and 13^2- hydroxypheophorbide-β- methyl ester (**52** and **56**) were identified according to [45].

A couple of isomers (**54** and **55**) with a precursor ion $[M+H]^+$ at *m/z* 623 were tentatively suggested as 13^2-hydroxypheophorbide-*α*- methyl ester ($C_{36}H_{38}N_4O_6$). The characterization was based on the acceptable MS and MS/MS data (*m/z* 605, 573, 545, 503, 485 and 459), in addition to literature [45, 46]. This compound was previously detected in *Bougainvilleae* leaves, while 13^2- hydroxypheophorbide-*β*- methyl ester (**52** and **56**), known as petasiphyll-A according to Lin, Li and Wu [47], is less common [45]. To our knowledge, it is the first time to detect 13^2- hydroxypheophorbide-*β*- methyl ester in *Bougainvillea.*

3.11. Miscellaneous compounds

Other compounds were also characterized in *Bougainvillea* 'Scarlett O'Hara', like sucrose (**1**), fraxiresinol hexoside (**18**), lanopalmitic acid (**31**), *N*-feruloyl tyramine (**30**) and its isomer (**33**). Moreover, compound (**1**) was suggested to be sucrose (MS^1 at *m/z* 341 $[M-H]^-$, MS^2 at *m/z* 179 $[M-H-glc.]^-$, 161, 131) according to [48].
Compound (**18**) showed a deprotonated molecular ion at *m/z* 565 and intense fragment at *m/z* 403, attributed to the loss of hexoside moiety. Further, MS analysis of the *m/z* 403 ion produced identical product ions as syringyl (8-O-4') guaiacyl dilignol as it yields fragments suggested syringyl and guaiacyl units connected by a structure of resinol bonding. Compound (**18**) was tentatively identified as *β*-aryl ether dilignol hexoside known as fraxiresinol hexoside [23].
One fatty acid, lanopalmitic acid (**31**) was identified as previously reported [18]. *N*-Feruloyl tyramine (**30**) and its isomer (**33**) were recognized by comparing its MS/MS fragmentation pattern with the reported data [40].
This is the first preliminary UPLC–ESI-MS/MS tentative identification of secondary metabolite of ethyl acetate fraction of this plant based on the survey of the literatures.
As revealed from **Fig. 2** and by previous studies, most flavonoids and phenolic compounds showed much cleaner mass spectral background and higher sensitivity in the negative mode than those obtained in the positive mode [49-52]. Unlike flavonoids or polyphenols, anthocyanins and cyclic tetrapyrolic derivatives exist in cationic forms; hence the positive ion mode was more sensitive for their analysis. Due to the positive charge and phenolic groups of anthocyanins, these compounds can easily donate protons to free radicals and show much cleaner mass spectral background in the positive mode [45, 53]. Such reported studies are compatible with the results shown in our study.

As revealed from **Fig. 3**, although some compounds remained as "unidentified compounds" saponins represented the largest area fraction of the ethyl acetate chromatogram acquired with the ESI source in LC-MS negative mode, followed by the rest of flavonoids and phenolic acid derivatives in different proportions. The area corresponding to unknown peaks was also appreciable, accounting for 3.48% and 17.66% of the total area in negative and positive polarity, respectively. As revealed in **Fig. 3**, LC-MS $^{(-)}$ of ethyl acetate fraction, one quarter of the whole chromatogram area corresponded to saponins, and 14.27% was taken up by flavonoids, 14% to phenolic acid derivatives and around 12.35% to free organic acids. The LC-ESI-MS methodology in negative

ionization mode was the most appropriate one to detect the group of saponins and flavonoids although it also showed relatively good efficiency when detecting free organic and phenolic acid derivatives. It can be seen that the chromatogram of ethyl acetate fraction obtained by means of the LC-MS $^{(+)}$ produced the highest ionization rate for cyclic tetrapyrolic derivatives and anthocyanins. Cyclic tetrapyrolic derivatives recorded for 56.41%, anthocyanins for 18.8% and tannins for 3.2% of the chromatogram area.

4. Conclusion

The first report on the phytochemical components of *Bougainvillea* 'Scarlett O'Hara' cultivated in Egypt is presented in the current research. Organic acids, phenolic compounds, betacyanin, anthocyanins, flavonoids, saponins, tannins and cyclic tetrapyrolic derivatives were characterized in this plant using UPLC-ESI-MS/MS technique. Further studies are needed to isolate and classify the bioactive secondary metabolites from this fraction, for future *in vitro* and *in vivo* biological investigation, using different spectroscopic and spectrometric techniques.

Authors' Contributions

All authors made considerable contributions to the manuscript. FA, AE, ME, EF and SR designed the study. FA, ME, EF and SR performed the experiments. FA, AE, ME, EF and SR interpreted the results. ME, FA, EF and SA wrote the manuscript. All authors revised the manuscript and approved it for publication.

Conflicts of interest

There are no conflicts to declare.

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كروماتوجرافيا السائل فائق الآداء المقترن بمطياف الكتلة لخلاصة خلات الاثيل للأجزاء الهوائية من الجهنمية "سكارليت أوهارا" المنزرعة في مصر

مي أحمد محمد أحمد السيد[1] (مي السيد)
فوقية عبدالله عباس[1] (فوقية عباس)
سارة رفعت مصطفى شريف[1] (سارة رفعت)
عزة محمد ابراهيم الشافعي[1] (عزة الشافعي)
ايمان فكري أحمد حسن[1] (ايمان فكري)
قسم العقاقير ، كلية الصيدلة ، جامعة الزقازيق ، 44519 الزقازيق ، مصر

تحليل تجزئة خلاصة خلات الايثيل لنبات الجهنمية "سكارليت أوهارا" المنزرع في مصر لم يحظ بالاهتمام الكافي في الدراسات الكيميائية والبيولوجية فقام الباحثون بالتحقق من المركبات الكيميائية لهذا الجزء لأول مرة باستخدام كروماتوجرافيا السائل فائق الأداء المتصلة بمطياف الكتلة في أوضاع التأين السالبة و الموجبة لفهم توزيع المركبات الكيميائية الرئيسية المكتشفة في الجهنمية "سكارليت أوهارا". حيث تم التعرف على 57 مركبًا من نواتج الأيض الثانوية والتي تنتمي إلى العديد من الفئات الكيميائية مثل الأحماض العضوية (7) ، المركبات الفينولية (14) ، وبيتاسيانين (1) ، أنثوسيانين (7) ، مركبات الفلافونويدات (10) ، السابونين (3) ، التانينات (6) ، و مشتقات دورية رباعي البيروليك (4) وخمس مركبات متنوعة. كان وضع التأين السالب هو الأنسب للكشف عن مجموعة السابونين (22.17٪ من مخطط الكروماتوجرام) والفلافونويدات (14.27٪) و مشتقات الأحماض العضوية (12.35٪) والفينولية الحرة (14٪). يمكن ملاحظة أن المخطط الكروماتوجرافي لجزء خلات الإيثيل الذي تم الحصول عليه في وضع التأين الايجابي أنتج أعلى معدل تأين لمشتقات رباعي البيروليك (56.41٪ من الكروماتوجرام) والأنثوسيانين (18.8٪) والتانين بنسبة 3.2٪ .