LC/MS characterization of flavonoids glycosides from leaves ethanolic extract of Bougainvillea spectabilis cultivated in Iraq.

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Abstract

Objective: The goal of this study was to detect the major compounds found in the leaves ethanolic extract of Iraqi cultivated *Bougainvillea spectabilis*. Methods: Plant materials were collected from Baghdad, Iraq, deffated with n-hexane, and extracted with ethanol. Then, the leaves ethanolic extract was analyzed by Liquid Gas Chromatography/Mass Spectroscopy (LC/Mass). Results: Flavonoid glycosides (Kaempferol-3-O-glucoside, Kaempferol-3-O-rutinoside, 3-Rha-7-Rha Quercetin, 3-O-Neohesperidoside Quercetin) were the major compounds obtained from the LC/Mass analyses. The structure was characterized using standard retention times, [M-H] data, and MS/MS fragmentation peaks. Conclusion: This study found that Iraqi cultivated *Bougainvillea spectabilis* differs from those grown in other soils in that it lacks free flavonoids and instead contains sugar conjugated flavonoids linked via glycosidic linkage.

Keywords: LC/MS characterization, flavonoids glycosides, ethanolic, Bougainvillea spectabilis

Introduction

Plants are essential for the survival of the planet and all living creatures. They are necessary components of human well-being. Plants produce a variety of chemical compounds known as secondary metabolites, which have been demonstrated to have a variety of biological effects, providing a basis for the use of herbs in the treatment of a variety of diseases[(1)]. *Bougainvillea spectabilis* (figure 1) is a member of the Nyctaginaceae family. Nyctaginaceae, or the four o'clock plant family, is a Caryophyllales order flowering plant family with approximately 30 genera and 400 species. It is found primarily in tropical and subtropical regions of the world, with the majority of its distribution in tropial America [(2)]. *Bougainvillea spectabilis* was named after French explorer Louis Antionede Bougainville (1729-1811), who discovered the plant in Brazil in 1786 and popularized it around the world [(3)]. The bracts of *B. spectabilis* are papery and thin, earning it the nickname "Paper Flower"[(4)]. Great Bougainvillea (English) is the preferred common name, and *Bougainvillea spectabilis* Willd is the scientific name. *B.spectabilis* is an aggressive climbing shrub or vine that can reach a height of more than 10 meters. The flowers are white or creamy in color and, form three axillary clusters with a pink, purple, red, or orange bract beneath each blossom. Leaves are green, simple, leathery, and long-lasting. The stems are woody perennial vines with narrow,

long thorns in the leaf axils [5]. *Bougainvillea spectabilis* has been shown to possess a large number of phytochemical constituents. Alkaloids, flavonoids, phenols, glycosides, saponins, steroids, and terpenoids have all been discovered in this plant [6].

Figure1: *Bougainvillea spectabilis*

Materials and methods

B.spectabilis leaves were collected from the Almansour neighborhood of Baghdad, Iraq, washed with tap water, dried in the shade at room temperature, and pulverized into a powder. A Soxhlet apparatus was used to extract shade-dried pulverized plant leaves (50 g) with hexane (500 ml), the defatted plant material was then extracted with 90 percent ethanol (500 ml). The extract was filtered, and the solvent was evaporated under reduced pressure using a rotary evaporator, and the results were examined using Liquid Gas Chromatography/Mass Spectroscopy (LC/Mass) [7,8].

Liquid Chromatography/ Mass Spectrometry (LC/MS):

Liquid mass detection was performed at the College of Pharmacy/Zarqa University in Jordan, utilizing a Bruker Daltonik Impact II ESI-Q-TOF System in conjunction with a Bruker Daltonik Elute UPLC system (Bremen, Germany) for screening numerous compounds of interest.The device was powered by an Ion Source Apollo II ion funnel electrospray source. The capillary voltage was 2500 V, the nebulizer gas pressure was 2.0 bar, the dry gas flow rate was 8 L/min, and the dry temperature was 200°C. The TOF repetition rate was up to 20 kHz, and the mass resolution was 50000 FSR (Full Sensitivity Resolution). The mass precision was less than one part in a million. Standards for Bruker TOF MS and stock solutions for high-resolution m/z identification were made by dissolving the required amount of material in dimethyl sulfoxide-DMSO (analytical grade), diluting with acetonitrile, and using for MS and retention time identification.

Results and discussion

LC-MS spectra can be a valuable technique for evaluating component molecular weights. A compound's pattern of fragmentation of different groups can give information about its structure. LC-MS was used to analyse chromatograms of the *Bougainvillea spectabilis* leaves ethanolic extract, resulting in spectra with discrete peaks. Each component's molecular mass was assessed, and each chromatogram's molecular mass was determined. The structure was characterized using standard retention times, [M-H] data, MS/MS fragmentation peaks, and published data.

The LC chromatogram with peaks indicated in the order of their retention time was shown in figure 2. In addition, LC chromatogram of each individual peak of the major compounds is shown in figure 3. The major compounds obtained were flavonoid glycosides (Kaempferol-3-O-glucoside, Kaempferol-3-O-rutinoside, 3-Rha-7-Rha Quercetin, 3-O-Neohesperidoside Quercetin), table 1 (1-4). Figure 4 also shows the fragmentation patterns of these glycosides.

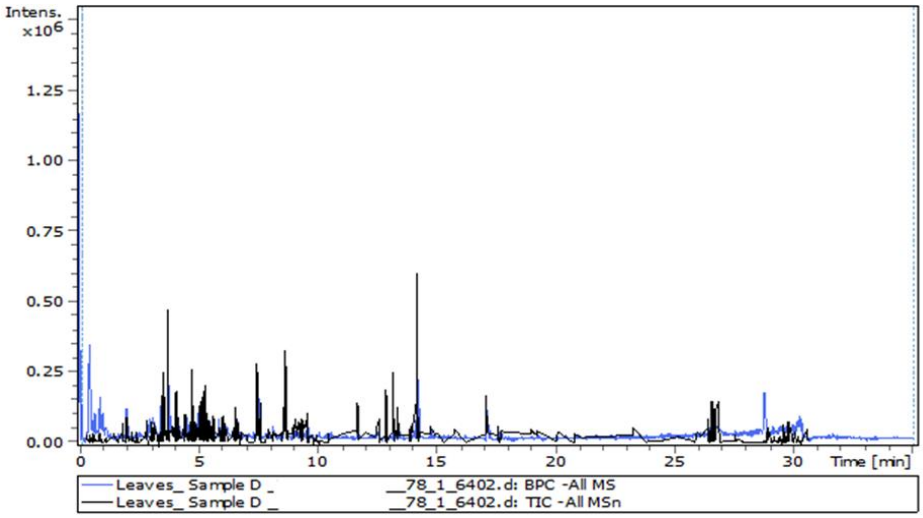


Figure 2: LC-chromatogram obtained from leaves ethanolic extract of *Bougainvillea spectabilis*

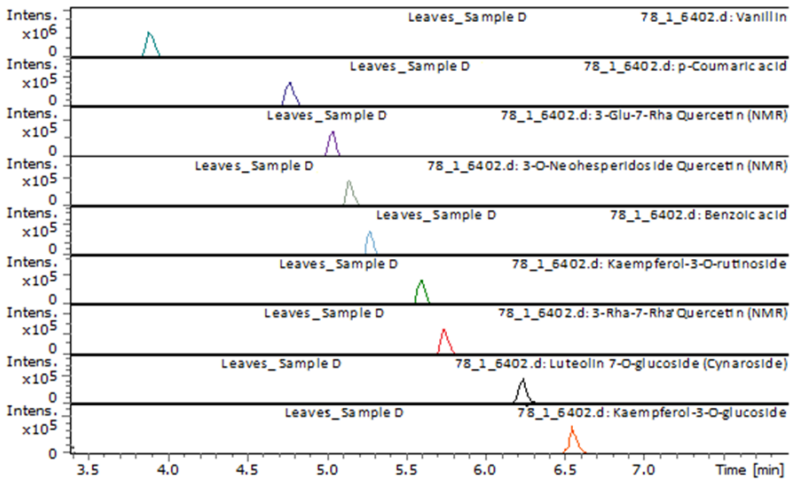
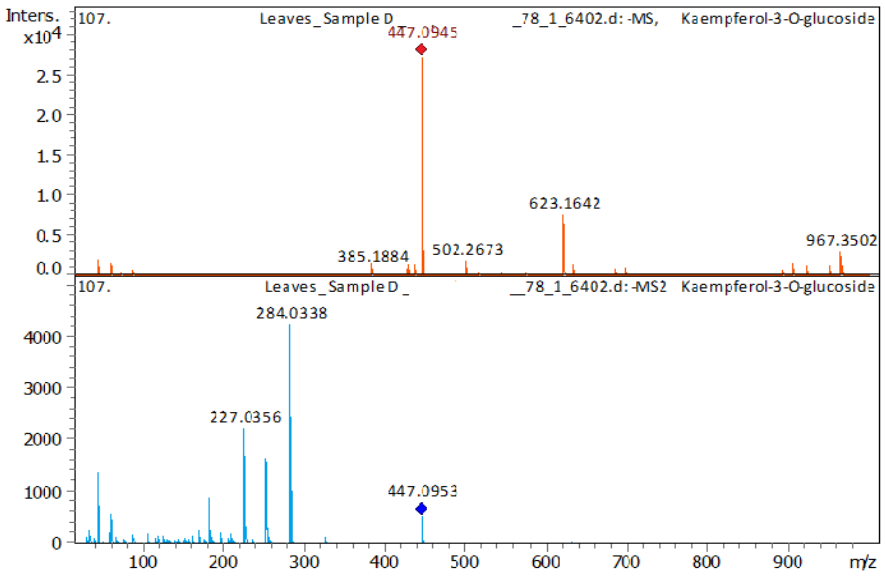


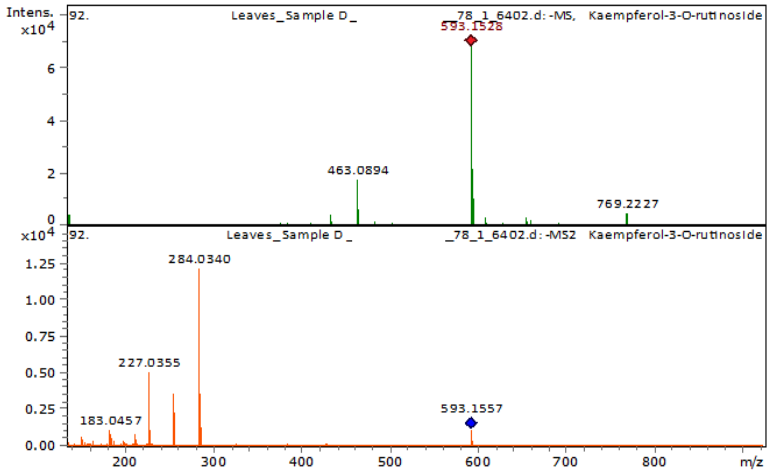
Figure 3: LC-chromatogram of each individual peak of the main compounds obtained from leaves ethanolic extract of *Bougainvillea spectabilis*

Table (1): the retention time, m/z measures, M measures, [M − H]− peaks, molecular formula for each compound (1-4).

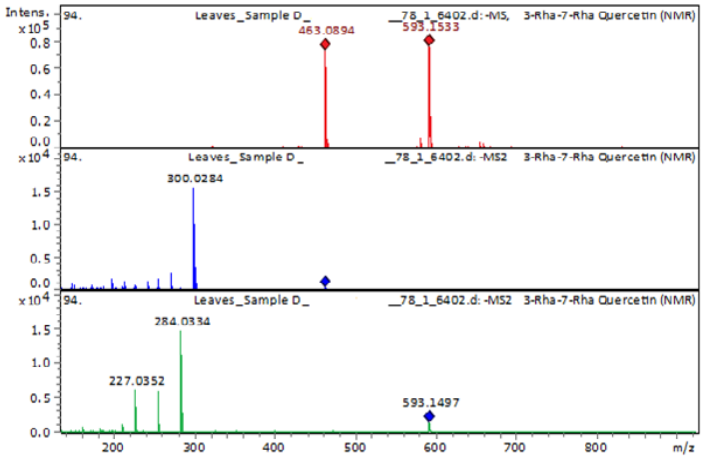
	Compound	Molecular formula	Ions	M meas.	M/Z meas.	RT (min)
1-	Kaempferol-3-O-glucoside	C21H20O11	[M-H]-	448.1009	447.0936	6.53
2-	Kaempferol-3-O-rutinoside	C27H30O15	[M-H]-	594.158	593.1508	5.61
3-	3-Rha-7-Rha Quercetin	C27H30O15	[M-H]-	594.1583	593.151	5.75
4-	3-O-Neohesperidoside Quercetin	C27H30O16	[M-H]-	610.1535	609.1463	5.05



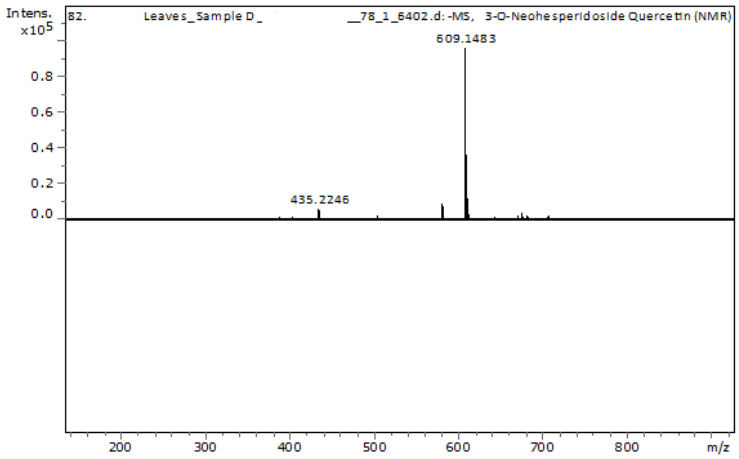
(1)



(2)



(3)



(4)

Figure 4: fragmentation pattern of flavonoid glygosides obtained from LC/Mass analysis of *Bougainillea spectabilis* leaves ethanolic extract. (1) Kaempferol-3-O-glucoside, (2) Kaempferol-3-O-rutinoside, (3) 3-Rha-7-Rha Quercetin, (4) 3-O-Neohesperidoside Quercetin.

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