Structural Investigation on the Leaf Parts of Rumex Abyssinicus Jacq.

Birhanu Ayalew Tebeje*

Department of Chemistry College of Natural and Computational Science,
Post Box 196, University of Gondar, Ethiopia.

Abstract: *Rumex abyssinicus Jacq. is a rich source of important secondary metabolites. Besides, it is a medicinal plant and still used in traditional medicine.In this study, a phytochemical study of Rumex abyssinicus Jacq.has been under taken.Chemicalinvestigation on the solvent extract of the plant has been conducted.The ethanolic extract of the leaf parts of Rumex abyssinicus Jacq.led to isolation of one compound.The compound were identified to be (**BUOG1**). Structural determination was accomplished by means of spectroscopic methods(UV,H^{1}NMR,^{13} C NMR and Dept NMR).*

I. Introduction

Natural products, as the term implies, are those chemical compounds derived from living organisms, plants, animals, insects, and the study of natural products is the investigation of their structure, formation, use, and purpose in the organism.[1]Natural products became a necessity to mankind. They have been immensely utilized for various purposes, such as, foodstuff, as weapons, treatment of diseases, in their crude form[2]. The contribution of Natural products to the development of medicine could be demonstrated by the amount of plant derived drugs being used. In general 40% of modern drugs are said to be of natural origin.[3]

Until the 1950's, the structures of natural products were determined by degradative techniques, and a structure was not proven until the compound had been synthesized in an unambiguous manner. Stereochemistry was not often determined. Now, structures are elucidated primarily by spectroscopic techniques, and the stereochemistry is an important feature of the structure.[4]

Phytochemical studies of plants especially of medicinal plants are of great importance in developing drugs. They are useful in the study of chemotaxonomy and plant biodiversity as well as in documenting knowledge. Enhancing the knowledge of biological and pharmacological effects of plant constituents and determination of the structures of the active principles may help in sustaining the use of these products.[1]Natural products are secondary metabolites of an organism. In most instances they appear to be non-essential to the plant, insect or microorganism producing them in marked contrast to the other organic compounds in nature (sugars, amino acids, nucleotides and the polymers derived from them) which are both essential and ubiquitous.[5, 6]

Plants and animals produce an amazingly diverse range of chemicals. These chemical products of plants and animals can be classified into primary and secondary metabolites. Primary metabolites are those which are common to all species and can be subdivided into proteins, carbohydrates, lipids and nucleic acids. These four groups of materials are defined according to the chemical structures of their members. The secondary metabolites are often referred to as "natural products". These can be subdivided into terpenoids, alkaloids, shikimates and polyketides. The classification is based on the means by which the materials were made.
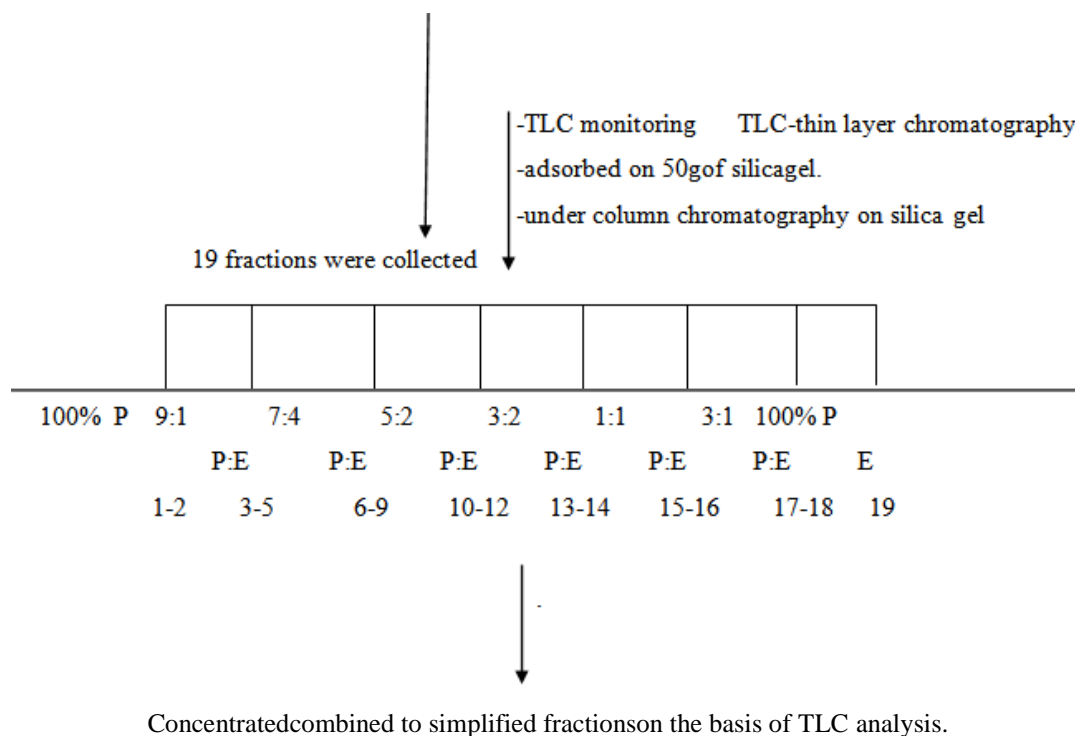
The main objectives of this studywas to isolate and characterized the constituents of the ethanolic extract of the leaf parts of Rumex abyssinicus Jacq. The plant was selected for the study because it has variety of uses especially for the treatment of avariety of diseases.

II. Experimental

Sample collection, Extraction and Isolation

Rumex abyssinicus Jacq. was collected from Gondar town in June 2019. The leaf part of the plant was dried with air and powdered; 1kg of powderedRumex abyssinicus Jacq. was soaked with 2.5L of ethanol (78^{0}c) for 7 days. The extract, on removal of the solvent by using rotaryevaporator afforded 25g of greyjelly material and labeled as **BUOG1**.This extracted sample was subjected to column chromatography using different solvent ratios and 19 fractions were found. Finally one single spot were found from frequent checkup of each fractions by tin layer chromatography.

25.g of crude sample

-TLC monitoring   TLC-thin layer chromatography

-adsorbed on 50gof silicagel.

-under column chromatography on silica gel

19 fractions were collected

100% P	9:1	7:4	5:2	3:2	1:1	3:1	100% P
	P:E	P:E	P:E	P:E	P:E	P:E	E
1-2	3-5	6-9	10-12	13-14	15-16	17-18	19

Concentratedcombined to simplified fractionson the basis of TLC analysis.

Instrumental

UV spectrum was measured with GENEY'S spectrometer (200-400) in $CHCl_3$ at room temperature.

^{1}H NMR, ^{13}C, and Dept NMR spectra were recorded on a Bruker Advance 400 MHZ spectrometer with TMS as internal standard. The purity of compounds was monitored on silica gel GF254. Analytical thin layer chromatograph were run on silica gel (Merck) coated on aluminum foil, 0.2mm thickness. The spots were detected by their UV fluorescence and by spraying with iodine. Silica gel with fluorescent indicator 254 nm on aluminum cards with layer thickness0.2mm used for TLC.

Silica gel 60(Merck), particle size 0.063-0.200(70-230 mesh size) used for column Chromatography.

III.   Result and discussion

3.1.General

The large number of protons at a particular position continuously joined CH_2 protons and the corresponding cis and trans coupling as a result the peak shown will also be diffused. Greater number of CH_2 groups present continuously and at different position of similar chemical environment shows diffused peaks.The existence of many CH_2 and CH_3 groups in a very closes almost similar chemical environment as well as the solvent used affects the number of hydrogen.

The carbon near to electron donating groups shows the peak high fields where as the carbon attached to most electro negative atom resonate at low field.

Carbon spectra can be used to determine the number of none equivalent carbons and to identify the types of carbon atoms (methyl, methylene, aromatic, carbonyl)that may be present in a compound.

Thus, carbon NMR provides direct information about the carbon skeleton of a molecule.some of the principles of proton NMR apply to the study of carbon NMR; however, structural determination is generally easier with carbon -13 NMR spectra than with proton NMR. Typically, both techniques are used together to determine the structureof an unknown compound.

3.2. Characterization

The isolated compoundwas characterized from the ethanolic extract of Rumex abyssinicus Jacq. Structural elucidation of the compounds was done based on the spectroscopic data obtained for the compound. The UV spectrum λmax (inCHCl_3) revealed absorption band at 274nm indicating that the molecule has conjugated double bonds in the aromatic ring and unsaturated carbonyl chromophore.

The ^{1}H NMR showed doublet of doublet at δ 7.75 integrated for one proton indicated the presence of aromatic proton.A doublet of doublet peak at δ 7.55 integrated for one protons indicated again aromatic proton. A singlet peaks at δ 7.25 integrated for one protons indicated that conjugated double bonds attached to aromatic carbon.

A multiplet peak at δ 0.96 integrated for 15 protons indicated that methyl group attached to amethylene carbon. A multiplet peak at δ 1.42 integrated for 30 protons indicated methylene group attached to methyl carbon. Again a doublet peaks at δ1.51integrated for one proton indicated that methine protons attached to atertiary carbon. A single peak at δ1.7 integrated for two protons indicated that methylene groups attached to between olefinic double bonds and atertiary carbon.

A multiplet peak at δ 2.1 integrated for eight proton indicated that methyl group attached to olefinic double bonds and one proton indicated that attached to the hydroxyl groups. A multiplet peaks at δ 2.38 integrated for four protons indicated proton attached O-substituted methylene group. A multiplet peaks at δ 2.71 integrated for four protons indicated that methylene protons attached to aromatic carbons. A doublet of doublet peaks at δ 4.1integrated for two proton indicated that mthylene group attached to the hydroxyl group.

Again adoublet of doublet peaks at δ 4.3integrated for two proton indicated that mthylene group attached to O-substituted groups. Atriplet peaks at δ 4.2 integrated for one proton indicated methine group attached to tertiary carbon. Single peaks at δ 5.48 integrated for five protons indicated that olefinic proton.

**Table 3:^{1}H, Proton Decoupled ^{13}C & DEPT spectra data of BOUG1**

^{1}H δ (PPm)	^{13}C NMR of KTS-1 δ (ppm)	DEPT
0.7(m)	10.97	-CH$_3$
0.9(m)	14.08	-CH$_3$
	14.15	-CH$_3$
	14.31	-CH$_3$
1.42(m)	20.60	-CH$_2$
	22.60	-CH$_2$
	22.71	-CH$_2$
	23.0	-CH$_2$
	23.73	-CH$_2$
	24.84	-CH$_2$
	25.53	-CH$_2$
	25.62	-CH$_2$
	27.21	-CH$_2$
	29.36	-CH$_2$
1.5(s)	38.70	-CH
1.7(s)	34.19	-CH$_2$
2.1(m)	34.02	-CH$_2$
	31.94	-CH$_2$
	30.35	-CH$_2$
2.38(m)	29.72	-CH$_2$
2.71(s)	32	-CH$_2$
4.3(t)	68.86	- CH
5.48(s)	130.01	- CH
	130.23	- CH
	130.90	- CH
	131.92	- CH
	128.81	- CH
7.25(s)	127.10	- CH
-	127.74	-
-	127.90	-
7.55(q)	128.06	- CH
-	128.23	-
7.75(q)	128.29	- CH
-	128.81	-
-	173.29	-

The proton decoupled 13C NMR spectrum showed well resolved resonance of the 42 carbon atoms. The multiplicity of each carbon atom was determined using DEPT-135 experiment, which revealed the presence of four methyl groups, 16 methylene groups, 10 methine groups (three attached to aromatic carbon atom two attached to two saturated carbons and the other is vinylic),

Six quaternary carbon (one carbonyl carbons, aromatic carbons indicating 32 hydrogen atoms attached to carbon atoms.

Based on ^{1}H NMR and proton decoupled ^{13}C NMR spectrum data of the given samplethe proposed structure of the compound is
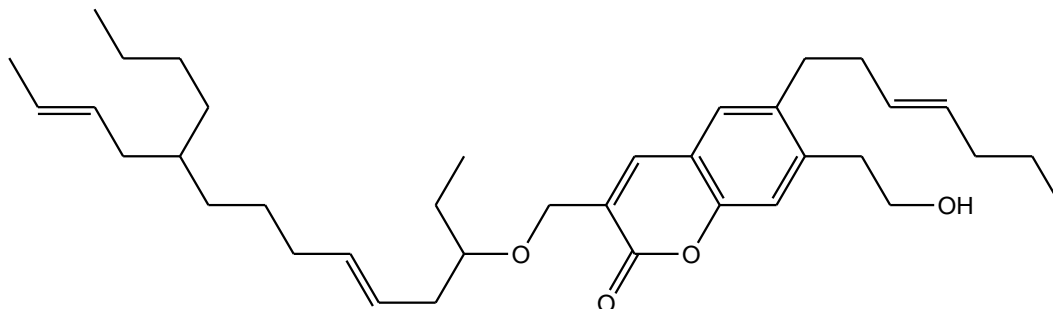
3-(((5*E*,12*E*)-10-butyltetradeca-5,12-dien-3-yloxy)methyl)-6-(((*E*)-hept-3-enyl)-7-(2-hydroxyethyl)-2*H*-chromen-2-one

Conflict of interest
The author has no conflict of interest

Acknowledgement

References
[1].   Mann. J, *Secondary metabolism* 2nd.ed. Clarendon Press,Oxford,**1987**. **1986.**
[2].   Koskinen A., *Asymmetric synthesis of natural products*, **1993**, John Wiley & Sons Ltd, University of Oulu, Oulu, Finland.
[3].   http://www.people.vcu.edu
[4].   P. w. Atkins, J. S. E., Holker, A. K, Holliday *Secondary metabolism*: 2nd edition
[5].   Paul, M. Dewick, Medicinal *Natural Product* 2nd ed.Stockholm, **2004.**
[6].   R. Zeichen de Sa, A. Rey, E. Arganaraz and E. Bindstein (2000). J Ethnopharmacol., 69(2), 93–98.
[7].   P.H.D. Edinburgh (1967). Flora of Turkey, Vol. 2, p. 495. Edinburgh University Press, North America.
[8].   SM Ahmed; MB Uddin; M R Tito. Int J For Usuf Mngt. 2007, 8(2), 50-63.
[9].   S Hosseinzadeh; A Jafarikukhdan; A Hosseini; R Armand. Int J Clin Med. 2015, 6, 635-642.
[10].   T Sandhya; KM Lathika; BN Pandey; KP Mishra. Cancer letters. 2006, 231(02), 206-214.
[11].   MA Hannah; S Krishnakumari. J Med Plants Studies. 2015, 3(5), 107-111.
[12].   B Abera. J Ethnobiol Ethnomed. 2014, 10(40), 1-15