

Extraction of chemical composition of volatile oil of *Ferula Gummosa* using carbon nanotube profile

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ABSTRACT: Multi-wall carbon nanotubes were used to extract the essential oil of the *Ferula gummosa* stem bark through non-covalent interactions between the surface of MWCNTs and oil segments. Analyzing the absorbed volatile oil using GC and GC-MS showed that it is containing twenty-nine different compounds major compound such as β -moaliene (19.431%), β -Guriunene (10.23%), Allo-aromadendrene (7.518%), Aromandrene (6.528%) total compound identified is 84.903%. A comparison of the chemical composition of the oil was made with that of others methods on aerial parts of *Ferula gummosa* using nano tube and hydrodistillaion methods. MWCNTs were washed by water and organic solvents and they were used repeatedly. This method is a new, fast and easy method.

KEY WORDS: *Ferula gummosa*; Volatiles; Composition; MWCNT.

INTRODUCTION

Carbon nanotubes (CNTs) have attracted much attention because of their unique atomic structure, high surface area-to-volume ratio and excellent electronic, mechanical and thermal properties [1]. They have a wide range of potential applications including nanoelectronic, sensors, fillers in composites materials and others [2-4]. Due to the high surface area-to-volume ratio, high hydrophobicity and electronic structure of CNTs, they can be used to absorb and deliver variety of molecules and macromolecules through "noncovalent" interactions. This approach is based on poor vander Waals or π - π interactions between CNTs and guest molecules such as polymers and small organic molecules and without disrupting the primary structure, thus maintaining electronic and mechanical properties of nanotubes [7]. In some cases the modification of surface of CNTs is essential for improving their interactions with polymers and the interfacial adhesion to the matrix and finally a good dispersion in the polymer matrix. To have a good interaction with the surface of a CNT, an essential structural factor in a polymer is the presence of hydrophobic segments or π -bonds which can interact with the hydrophobic surface and π -bonds of CNTs. An advantage of this procedure is the use of macromolecules containing two or more types of functional groups in which one type interacts with sidewall of CNT and others can be used to react with other molecules [8]. With increasing production and application of carbon nanotubes (CNTs), it becomes necessary to understand the interaction between CNTs and aromatic compounds, an important group of organic contaminants and structural components of large organic molecules in biological systems. However, so far few experimental studies have been conducted to systematically investigate the sorption mechanism of polar aromatics to CNTs. Therefore, cyclohexanol, phenol, catechol, pyrogallol, 2-phenylphenol, 1-naphthol, and naphthalene were selected to investigate the role of aromatic structure and -OH substitution in the polar aromatics-CNTs system. Sorption affinity of these compounds by CNTs increased with increasing number of aromatic rings, with an order of cyclohexanol < phenol < 2-phenylphenol < 1-naphthol, and was greatly enhanced by -OH substitution, with an order of phenol (1 -OH) < catechol (2 -OH) < pyrogallol (3-OH). Four possible solute-sorbent interactions, i.e., hydrophobic effect, electrostatic interaction, hydrogen bonding, and π - π bonds, were discussed to address the underlying mechanism of the enhanced sorption affinity by -OH substitution. It was evident that electron-donating substitution on the aromatic rings strengthened the π - π interaction between the aromatics and CNTs and thus the adsorption affinity. These results will advance the understanding of the sorption behavior of CNTs in the environmental systems adsorption of Phenolic compounds by Carbon Nanotubes. CNTs have been used to study the surface-protein and protein-protein binding which may lead to develop the highly specific electronic bimolecular detectors⁹. Initiators containing aromatic segments have been supported by CNTs. The resulting CNT/initiator hybrid has been used for the polymerization of monomers leading to a nano composite containing a CNT core and polymeric shell¹⁰. Based on above explanations it can be understood that CNTs are able to form complexes with hydrophobic molecules or those containing conjugated π -bonds through non-covalent interactions, hence the volatile oil of many plants which are containing molecules and macromolecules with these characteristics can be extracted using CNTs as supporter probably. *Ferula gummosa* Boiss. (Apiaceae) is a perennial plant native to central Asia, growing in the northern and western parts of Iran and blooms once in its several years' life span¹¹. Nomads of southwest Iran call this plant 'Barijeh' and traditionally use its resin for the treatment of diarrhea. They eat a small piece of the resin and believe it to be a very effective anti-diarrheal herbal medicine⁹. In Iranian ancient medicine, the gum obtained from the aerial parts of this plant has been used for stomach pain, chorea,

epilepsy and as a wound-healing remedy¹⁰. In recent years there are some reports regarding the main effects of this plant. An anti-nociceptive activity has been shown for the hydro alcoholic extract of aerial parts¹² and acetone extract of *F. gummosa* seed and root has been reported previously¹³. Furthermore, a methanol-chloroform (1:1) extract of *F. gummosa* and its fractions have alleviated the morphine withdrawal syndrome induced by naloxone¹⁴. The anticonvulsant potential of an essential oil¹⁰ and the antibacterial activity of the seed¹⁵ and anti-inflammatory activity of the seed and root of *F. gummosa*¹³ have been reported previously. The composition of the essential oil of the fruit of the plant has been determined and it has been shown that terpenoid compounds such as alpha-pinene, betapinene, 3-carene, alpha-thujene and sabinene are abundant in this plant³.

EXPERIMENTAL SECTION

Plant material

About 1Kg of fresh aerial part of *F. gummosa* at maturity were collected from agriculture college garden of the university. The dried aerial parts were stored in a cool and dark place.

Isolation of volatile components

Fresh powdered (10g) of plant were subjected to nanotube (MWNTs 20-40 nm length 5-15 micro meter S.S area 40-300 m²/g) in a petri dish -type apparatus heated for 4h. at 40C then washed by n-hexane. The yield (V/W) of volatile oil was 0.2%. The volatile oil was dried over anhydrous sodium sulfate and stored at 4 C for analysis

GC-MS analysis

GC/MS analysis of the oil was carried out on an Agilent HP-6890 gas Chromatograph (Agilent Technologies, Palo Alto, CA, USA) equipped with an Agilent HP-5973 mass selective detector in the electron impact mode (ionization energy: 70eV), operating under the same conditions as described above, using a HP-5MS 5% phenylmethylsiloxane capillary column (30 m x 0.25 mm, 0.25 μm film thickness; Restek, Bellafonte, PA). Retention indices were calculated for all components using a homologous series of n-alkanes injected in conditions equal to the sample⁶. Identification of components of essential oil was based on retention indices (RI) relative to n-alkanes and computer matching with the Wiley⁷ and NIST libraries, as well as comparisons of the fragmentation pattern of the mass spectra with data published in the literature¹⁶. Some commercially available components of the essential oil were also co-injected for further confirmation of their identification.

RESULTS AND DISCUSSION

For the first time, the volatile oil of barks of *Ferula gummosa* was extracted by nanotube and was analyzed by GC and GC-MS. Retention indices for all compounds were determined according to the Kovats method using n-alkanes as standards¹⁶. Wherever possible, by co injection with an authentic sample and by matching their fragmentation patterns in mass spectra with those stored in NIST library and published mass spectra¹⁶ and Wiley⁷ and NIST libraries of GC/MS. The chemical composition of the *Ferula gummosa* is presented in Table I. A total of twenty-four compounds were identified, which constitute 98% of the volatile oil. The volatile oil of *Ferula gummosa* contains β-moaliene(19.431%), β-Guriunene(10.23%), Allo-aromadendrene (7.518%) and Aromandrene(6.528%) total compound identified is 84.903%.

Table1.composition of essential oil from *Ferula gummosa* by nano tube

Row	Compound	KI	RI	Percentage
1	Camphene	954	5.13	0.021
2	Beta- pinene	979	5.27	0.837
3	Myrcene	991	5.54	0.105
4	D- limonene	1029	6.11	0.219
5	Delta- 3- careen	1031	6.32	0.060
6	Allo-Ocimene	1050	7.1	0.132
7	Gamma- terpinene	1060	7.2	0.186
8	Trans- pinocarveol	1139	9.3	1.114
9	Trans propenyl sec butyl disulfide	1167	9.91	0.891
10	Myrtenal	1196	10.52	1.485
11	Myrtenol	1196	10.60	0.375
12	p-ment- 2en- 9 ol E	1199	11.08	0.699

13	Rubean	1210	11.61	0.462
14	Endobornyl acetate	1285	12.20	0.726
15	3- Caren- 4ol	1315	12.55	0.642
16	Alpha- Cabebene	1351	13.40	0.564
17	α -copaene	1377	14.03	0.141
18	β -Cubebene	1388	14.19	2.298
19	Beta- elemene	1391	14.30	0.627
20	α -Gurjunene	1410	14.90	0.420
21	Trans- caryophylene	1419	15.03	0.420
22	α -Guaiene	1440	15.13	0.393
23	Allo-aromadendrene	1460	16.35	7.518
24	α -Amorphene	1485	17.2	2.226
25	β -selinene	1490	17.89	0.558
26	α -Farnesene	1506	18.96	5.067
27	D- cadinene	1523	19.39	3.921
28	Calarene	1609	19.68	4.986
29	α -Eudesmol	1654	20.24	5.172
30	β -moaliene	1671	20.67	19.431
31	Agarospinol	1689	20.69	5.982
32	Aromandrene	1693	21.08	6.528
33	β -Guriunene	1723	21.36	10.23
34	Aristolene	1763	21.39	0.471
	Total			84.903%

CONCLUSION

Due to the high surface area-to-volume ratio and electronic structure of CNTs, they can be used to absorb and deliver a variety of molecules and macromolecules through "noncovalent" interactions. This approach is based on poor van der Waals or π - π interactions between CNTs and guest molecules. For the first time, the volatile oil of barks of *Ferula gummosa* was extracted by nanotube.

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