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Original Research Article

Chemical profile of the essential oil from *Chaerophyllum Khorossanicum* czerniak. ex schischk of Iran

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ABSTRACT

The aim of this study is to determine the chemical composition of essential oils of *Chaerophyllum khorassanicum* belonging to the Apiaceae family for the first time. Identification of essential oils is necessary, for food, cosmetics-health industry, and medicinal uses. The plant was collected at the flowering stage of Khorassan Razavi Province in Iran, Farizi Village. The shoot parts of the specimen were dried in the laboratory and crushed to particles. The essential oils were obtained by hydro-distillation using Clevenger and analyzed by GC-MS. Fifty-one components were identified in *Chaerophyllum khorassanicum* essential oils which accounted for 97.2% of the essence. The major chemical category of the volatile compounds were the monoterpene hydrocarbons (65.5%), followed by oxygenated monoterpenes (24.5%). In particular, the main components were limonene 32.1%, methyl eugenol 16.2%, and β-Ocimene 15.6%. In conclusion, monoterpene hydrocarbons are characteristic and represent excellent chemotaxonomical markers for *Chaerophyllum khorassanicum*.

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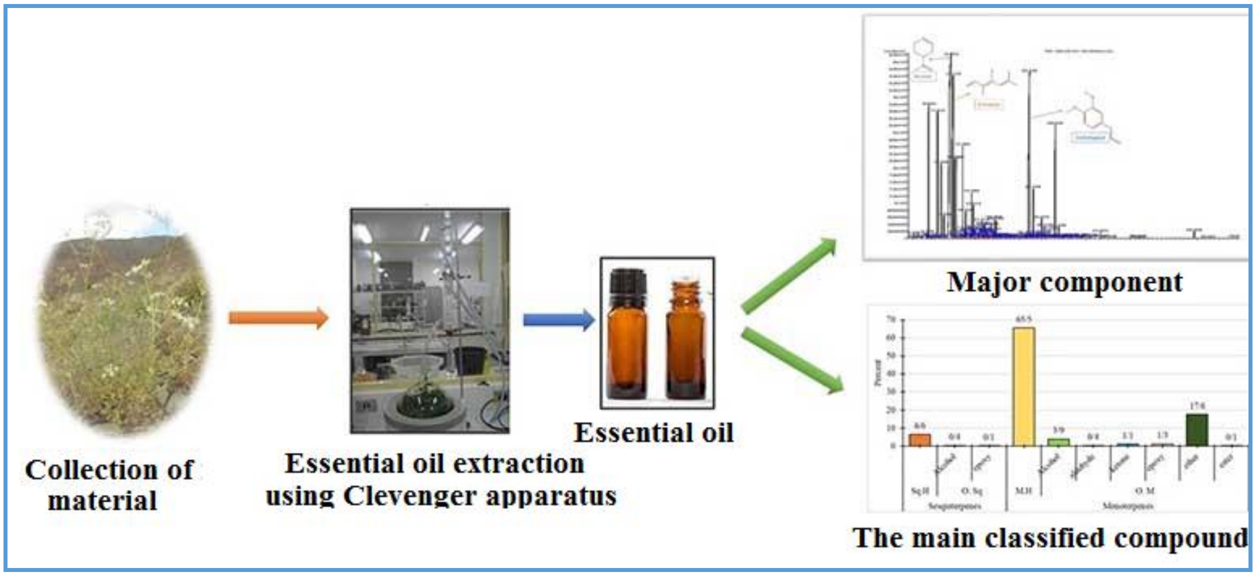
Graphical Abstract



Introduction

The genus Chaeropyllum belonged to the Apiaceae family. The Apiaceae genus, with many species in the world, is considered as one of the large plant genera with a wide distribution [1]. Iran, along with China, and Turkey, is one of the wealthiest and the most diverse regions in this genus and is probably the origin of many genera and subdivisions [2]. This genus has eight species in Iran, except for one, which is perennials. They are spread in mountainous pastures and heights almost all over Iran except in hot and humid southern regions.

Essential oils have many applications in the medical and pharmaceutical sciences. Identifying the essential oil compounds of different plant species can lead to identify specific compounds for treatments with lower drug costs, so the isolation and identification of essential oil compounds in newly discovered plants can be significant [3].

Therefore, the present study was evaluated by focusing on the identification of the essential oil of *Chaerophyllum Khorassanicum* from the Apiaceae family, which is reported for the first time.

However, the other species of the genus Chaerophyllum have been studied. Mamedova *et al.* were analyzed the essential oils of *Chaerophyllum macrospermum* in which the essential oils of flowers, leaves, and stems in Azerbaijan. Rustaiyan *et al.* analyzed the essential oils of the aerial parts of the *Chaerophyllum Macrospermum* growing in Iran by using GC and GC/MS. Sefidkon *et al.* identified the essential oils of the *Chaerophyllum macrospermum* organs collected from the Haraz Region located in Tehran Province. Kurkcuogly *et al.* investigated the chemical composition and antifungal activity of C*haerophyllum byzantinum* Boiss in Turkey.

Shafaqat *et al.* studied the constituents of essential oils of aerial parts and roots of *Chaerophyllum macropodum* Boiss.

Experimental

Plant material and isolation of the essential oils (EOs)

The aerial parts of *Chaerophyllum Khorassanicum* were collected from Kandalan Valley of Farizi Village in August 2021 from Kandalan valley of Farizi Village (Figures 1 and 2). The details of the collection place and the voucher specimen kept in the herbarium (Medicinal Plants Research Center of the Ferdowsi University of Mashhad) are represented in Table 1. The essential oil was extracted by water distillation using a Clevenger apparatus for four hours. Finally, the essential oils were collected in small and dark vials previously washed with acetone. The essential oils obtained with anhydrous sodium sulfate (Na_2SO_4) were also dehumidified. Due to the sensitivity of the essential oils to light, oxygen, and heat, the lids of these dark-colored vials were solidified and kept in the refrigerator at 4 °C for further analysis and experiments.

Essential oil analysis

The GC-MS analyses were performed on an Agilent 5975 system coupled to an MS, operating in EI mode (70 eV), by using a fused silica HP-5MS capillary column (30 m × 0.25 mm I.D., film thickness: 0.25 μM). The column heat program started at 50 °C. After stopping at the same temperature for 5 minutes, the temperature gradually increased to 3 °C until it reached 250 °C. The detector temperature was 280 °C, and helium carrier gas was used at a flow rate of 1 mL/min.The ionization current was set equal to 150 microamperes. Criminal data was collected in the range of 35 to 465. To detect the structure of the components in the essential oil, the Retention Indices (RI) of compounds were determined by comparing the retention times of a series of n-alkanes with a linear interpolation. Identification of the essential oil components was made by comparison of their mass spectra on both columns with those stored in NIST05, Pherobase, and Wiley 275 libraries, or with mass spectra from literature. the identification of each component was confirmed by comparison of its retention index either with those of authentic compounds or with data in the literature [4].

Results and Discussion

Identification of the essential oils

Essential oils were analyzed by GC/MS, and the fifty-one compounds, which in total constituted 97.2% of the total oil, were identified (see Table 2). The three major constituents of *Chaerophyllum khorassanicum* essential oil were found to be limonene (32.1%), methyl eugenol (16.2%), and β-Ocimene (15.6%) (Figure 3). Rustaiyan *et al.* identified 16 compounds from *Chaerophyllum Macrospermum.* The main components were (E)-β-Ocimene (40.0%), tricyclene (19.4%), δ-3-carene (18.3%), and myrcene.1%) [6].

Monoterpenes and Sesquiterpenes are the main components of *Chaerophyllum khorassanicum* essential oil. Monoterpenes (90.1%) had the highest share in the constituents of essential oils among them, hydrocarbon monoterpenes (65.5%) are the main components of monoterpenes, and among the oxygenated monoterpenes, Etheric monoterpenes (17.6%) have the highest amount, and the esoteric monoterpenes (0.1%) have the lowest amount (Figure 4, Table 3). Likewise, sesquiterpenes identified in these essential oils, hydrocarbon sesquiterpenes (6.6%) are the main components. Among the oxygenated sesquiterpenes, alcoholic sesquiterpenes (0.4%) have the highest amount (Table 3, Figure 4).

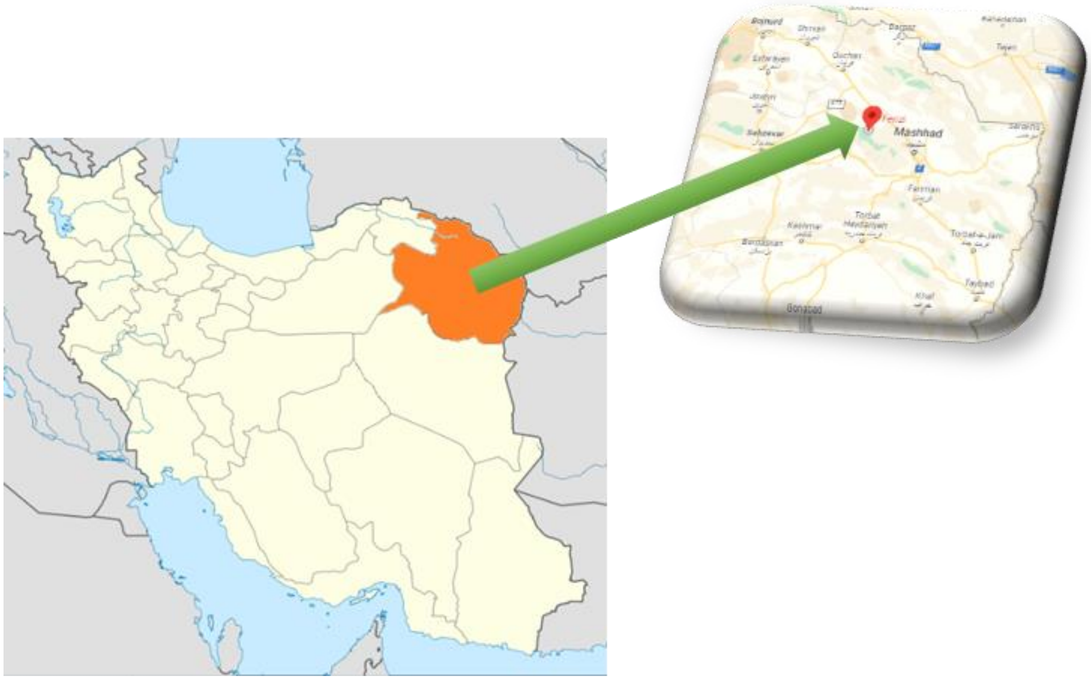


Figure 1. Map of Iran Khorassan Razavi Province in Orange, Farizi Village in Red

Figure 2. Picture of *Chaerophyllum khorassanicum*

Table 1. The collected Plant characteristics

Plant	Voucher specimenis	Used parts	Collection place
Chaerophyllum khorossanicum Czerniak. ex Schischk	13654	Aerial parts	Kandalan Valley of Farizi Village[a]

[a] Farizi is a village in Golamkan District, Chenaran City, Razavi Khorasan Province, Iran

Table 2. Chemical composition of *Chaerophyllum khorassanicum*

No.	Compound name	Molecular Formula	RI	%
1	α -thujene	$C_{10}H_{16}$ (**M.H**)	930	0.1
2	α-pinene	$C_{10}H_{16}$ (**M.H**)	939	4.4
3	camphene	$C_{10}H_{16}$ (**M.H**)	952	0.1
4	β-pinene	$C_{10}H_{16}$ (**M.H**)	979	4.9
5	myrcene	$C_{10}H_{16}$ (**M.H**)	992	2.5
6	α-terpinene	$C_{10}H_{16}$ (**M.H**)	1017	0.1
7	Limonene	$C_{10}H_{16}$ (**M.H**)	1031	32.1
8	β-Ocimene	$C_{10}H_{16}$ (**M.H**)	1041	15.6
9	γ-terpinene	$C_{10}H_{16}$ (**M.H**)	1062	1.8
10	terpinolene	$C_{10}H_{16}$ (**M.H**)	1091	2.8
11	linalool	$C_{10}H_{18}O$ (**O.M**)	1099	0.7
12	1,3,8-*p*-menthatriene	$C_{10}H_{14}$ (**M.H**)	1112	0.1
13	Trans-*p*-mentha-2,8-dienol	$C_{10}H_{16}O$ (**O.M**)	1122	0.3
14	α-campholenal	$C_{10}H_{16}O$ (**O.M**)	1128	0.1
15	allo-ocimene	$C_{10}H_{16}$ (**M.H**)	1134	1.1
16	z-epoxy-ocimene	$C_{10}H_{16}O$ (**O.M**)	1135	0.3
17	cis-*p*-mentha-2,8-dien-1-ol	$C_{10}H_{16}O$ (**O.M**)	1138	0.1
18	Trans-limonene oxide	$C_{10}H_{16}O$ (**O.M**)	1142	0.9
19	E-myroxide	$C_{10}H_{16}O$ (**O.M**)	1145	0.1
20	Cis-pinocarveol	$C_{10}H_{16}O$ (**O.M**)	1164	0.1
21	pinocarvone	$C_{10}H_{14}O$ (**O.M**)	1165	0.2
22	lavandulol	$C_{10}H_{18}O$ (**O.M**)	1170	0.3
23	Terpinene-4-ol	$C_{10}H_{18}O$ (**O.M**)	1178	0.5
24	cryptone	$C_{9}H_{14}O$ (**O.M**)	1186	0.1
25	ρ-cymen-8-ol	$C_{10}H_{14}O$ (**O.M**)	1185	0.4
26	α-terpineol	$C_{10}H_{18}O$ (**O.M**)	1189	0.3
27	myrtenal	$C_{10}H_{14}O$ (**O.M**)	1196	0.3
28	myrtenol	$C_{10}H_{16}O$ (**O.M**)	1197	0.1
29	methyl chavicol	$C_{10}H_{12}O$ (**O.M**)	1198	0.2
30	2,6-dimethyl-3,5,7-octatriene-2-ol	$C_{10}H_{16}O$ (**O.M**)	1207	0.4
31	carveol	$C_{10}H_{16}O$ (**O.M**)	1220	0.7
32	carvone	$C_{10}H_{14}O$ (**O.M**)	1230	0.5
33	thymol methyl ether	$C_{11}H_{16}O$ (**O.M**)	1237	0.3
34	Carvacrol methyl ether	$C_{11}H_{16}O$ (**O.M**)	1241	0.5
35	ρ-menth-1-en-7-al	$C_{10}H_{16}O$ (**O.M**)	1276	0.1
36	lavandulyl acetate	$C_{12}H_{20}O_2$ (**O.M**)	1288	0.1
37	α-copaene	$C_{15}H_{24}$ (**Sq.H**)	1376	0.1
38	elemene	$C_{15}H_{24}$ (**Sq.H**)	1391	1.4
39	(E)-jasmone	$C_{11}H_{16}O$ (**O.M**)	1403	0.1
40	metyl eugenol	$C_{11}H_{14}O_2$ (**O.M**)	1405	16.2
41	geranyl acetone	$C_{13}H_{22}O$ (**O.M**)	1453	0.1
42	trans-β-farnesene	$C_{15}H_{24}$ (**Sq.H**)	1458	0.1
43	Germacrene D	$C_{15}H_{24}$ (**Sq.H**)	1483	0.5
44	α-curcumene	$C_{15}H_{24}$ (**Sq.H**)	1484	0.1
45	trans-β-ionone	$C_{13}H_{20}O$ (**O.M**)	1488	0.1
46	bicyclogermacrene	$C_{15}H_{24}$ (**Sq.H**)	1498	0.3
47	trans-methyl isoeugenol	$C_{11}H_{14}O_2$ (**O.M**)	1500	0.1
48	myristicin	$C_{11}H_{12}O_3$ (**O.M**)	1520	0.3

49	Germacrene B	$C_{15}H_{24}$ (**Sq.H**)	1561	4.1
50	spathulenol	$C_{15}H_{24}O$ (**O.Sq**)	1580	0.4
51	caryophyllene oxide	$C_{15}H_{24}O$ (**O.Sq**)	1587	0.1

RI: retention indices calculated from retention times in relation to those of n-alkanes (C_5 – C_{18}) series in HP-5MS capillary column.
M.H: monoterpene hydrocarbones, O.M: oxygenated monoterpenes, Sq.H: sesquiterpene hydrocarbons, O.Sq: oxygenated sesquiterpenes.

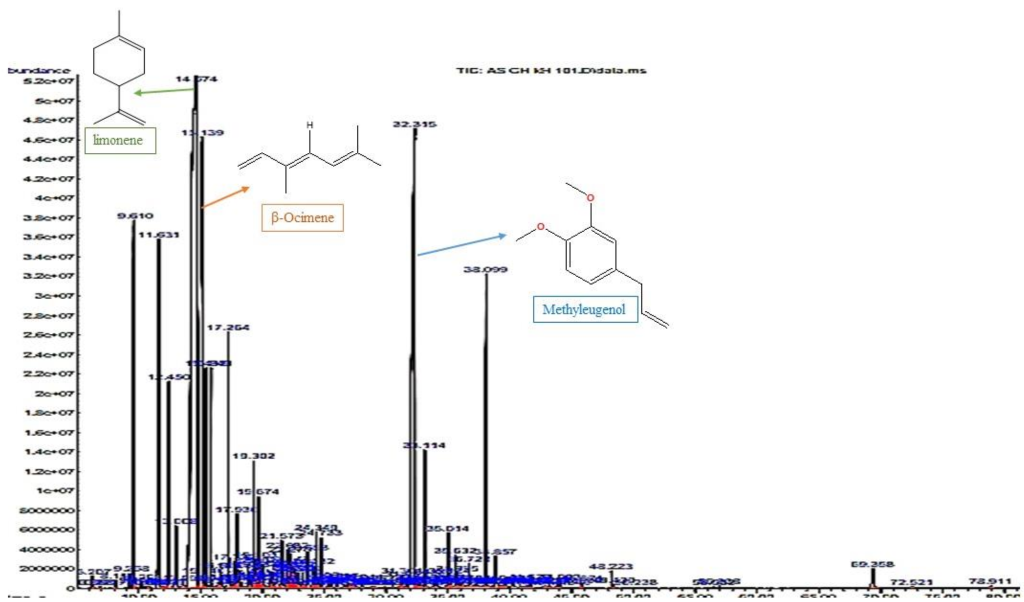


Figure 3. Chromatographic profile (GC/MS) of *Chaerophyllum khorassanicum* essential oils. The three major components are indicated, where (RT) from 14.5–15 (limonen), 15–15.5 (β-Ocimene), and 32–32.5 (methyleugenol)

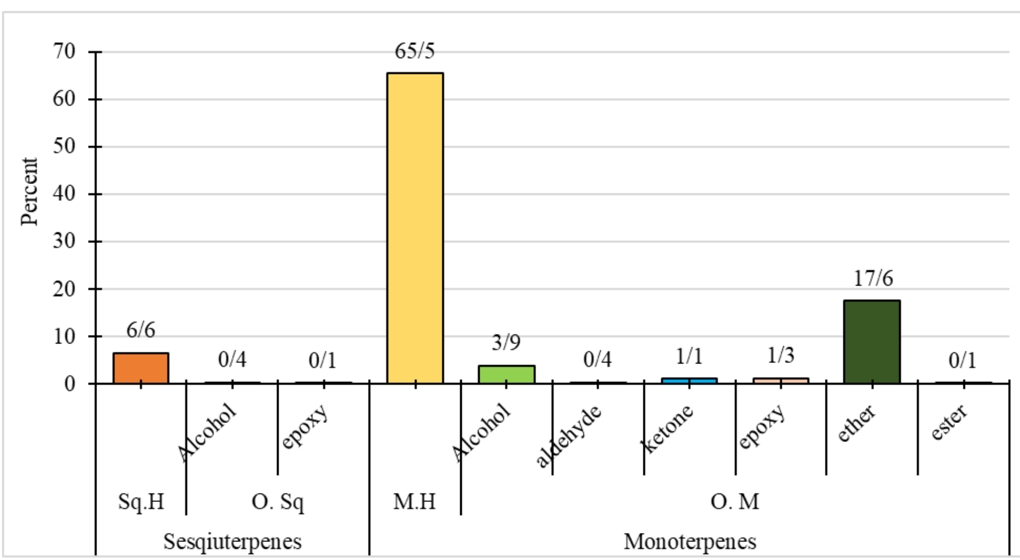


Figure 4. The mainclassified compounds

Table 3. Classification of chemical compounds of *Chaerophyllum khorassanicum* essential oils

Compounds									
Sesqiuterpenes(Sq): 7.1			Monoterpenes(M): 90.1						
Sesqiuterpene Hydrocarbons (Sq.H)	Oxygenated Sesqiuterpenes (O.Sq) 0.5		Monoterpens Hydocarbones (M.H) 65.5	Oxygenated Monoterpenes(O.M) 24.5					
6.6	Alcohol 0.4	Epoxy 0.1		Alcohol 3.9	Aldehyde 0.4	Ketone 1.1	Epoxy 1.3	Ether 17.6	Ester 0.1

The result of the study on the essential oil compounds of *Chaerophyllum macrospermum* in Azerbaijan indicated the identification of 33 compounds of the total constituents of the essential oils of flowers and 28 compounds of the total constituents of the essential oils of leaves and stems. Major compounds in flower essential oil, 1,8- cineole, linalool, Δ^3-carene, α-terpineol, and eugenol were reported. While the same compounds were present in leaf-stem essential oil with different percentages and oxygenated monoterpenes in both essential oils were the predominant compounds [5].

Aerial organs of the *chaerophyllum macrospermum* were extracted by water distillation, and then analyzed by using GC/MS. Among twenty-seven compounds identified, the major components were (E)-β-Ocimene (55.9%), terpinolene (9.8%), α-pinene (7.5%), β-phellandrene (4.3%), and β-pinene (4.2%) [7].

The study was done on the essential oils of *chaerophyllum byzantinum*, sixty-five components were identified which represents 94.6% of the essential oil compounds. Sabinene (30.0%), *p*-cymene-8-ol (16.0%), and terpinolene (11.5%) were identified as the main constituents. Essential oils were tested on five Candida species and two Candida albicans strains and showed good activity [8].

Identification of essential oil compounds of chaerophyllum macropodum Boiss that was done by shafaqat *et al.* revealed that the main components were (E)-β-Ocimene (24.9%), myristicin (15.7%), terpinolene (14.5%), and α-fenchyl acetate (13.9%) [9].

Accordingly, it is observed that β-Ocimene has been reported as the main constituent of essential oil.

The limonene compound is one of the main monoterpenes in *Chaerophyllum khorassanicum*, and it is found in concentrations as high as 32.1% of the essential oil fraction. Limonene is usually used in the perfume industry, household detergents, foods, and medicines. Many medicinal effects of this compound have been shown by human and animal studies. Limonene is among many plant essential oils that have antioxidant and anti-cancer properties and has been further suggested as a good dietary source for cancer prevention [10].

Likewise, anti-anxiety effects have been reported from this compound, so its effects are comparable to diazepam [11].

Limonene belongs to the cyclic monoterpene hydrocarbon family and is the main component of plant essential oils of *Chaerophyllum khorassanicum* that have antibacterial properties, accumulate in the plasma membrane of bacteria, and cause the destruction of microbial cell membranes [12].

The other major constituent in the essential oil of the studied plant is methyl eugenol. It is found in several plants. The compound has antifungal [13], antibacterial [14], and insect repellent activity [13].

β-Ocimene is one of the most prominent monoterpenes in nature. The biological properties of this compound include anticonvulsant activity, antifungal activity, antitumor activity, and resistance to pests. Fuethermore, β-Ocimene is a volatile pheromone important for the social regulation of bee colonies [15].

Conclusions

The present study is on the chemical content of EO of *Chaerophyllum khorassanicum*, originating from Farizi Village of Khorasan Province, Iran. To the best of my knowledge, the present study is the first one to report the phytochemical characteristics of this plant from this specific geographical area. The essential oil was rich in monoterpene, of which hydrocarbon monoterpenes were the most abundant. In contrast, there was a small amount of oxygenated and hydrocarbon sesquiterpenes. Due to the richness of monoterpene compounds in the essential oil of *Chaerophyllum khorassanicum*, it is suggested to study the antibacterial properties of this plant. Most phytochemical and pharmacological studies of this species are done in our laboratories.

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Disclosure Statement

No potential conflict of interest was reported by the authors.

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Authors' contributions

All authors contributed to data analysis, drafting, and revising of the paper and agreed to be responsible for all the aspects of this work.

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