NATURAL AND PYROLYSIS MOLECULE OF *COTONEASTER ZABELII SCHNEID*

by

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Original scientific paper
https://doi.org/10.2298/TSCI190703035Y

Cotoneaster zabelii Schneid is a unique wood biological resource in China, but its natural ingredients are not used effectively. In this paper, ethanol and phenyl alcohol were used to study the leaves and branches of Cotoneaster zabelii Schneid. Gas chromatographic/mass spectrometry (GC-MS) analysis showed that Cotoneaster zabelii Schneid was rich in chemical constituents that could be used as raw materials for medicine and food. An in-depth study of Cotoneaster zabelii Schneid can provide a more accurate understanding of the value of its internal chemical composition, which can be widely applied in medicine to manufacture new drugs and promote the development of medical technology.

Key words: *Cotoneaster zabelii Schneid, GC-MS, chemical composition*

Introduction

Cotoneaster zabelii Schneid is rosaceae plants of the genus Xun son [1-3], deciduous shrubs, up to 2 m tall. Branches thin open, branchlets cylindrical, deep reddish brown, young dense with yellow pilose, when old glabrous, China's endemic plants. It is distributed in Qinghai, Shaanxi, Gansu, Ningxia, Hebei, Henan, Shandong, Shanxi, Hubei, Hunan and other places in China. Galactitol is used for microbiology [4], biochemical research and pharmaceutical production. Lactose is widely used for producing baby foods, sweets, margarines, *etc.*, it is also used as culture media, chroma absorbents and excipients [5-9]. According to the analysis of the *Cotoneaster zabelii Schneid* by FT-IR and GC-MS, the internal value components were dug out to meet human needs.

Experimental phase

Sample collection

A sample of *Cotoneaster zabelii Schneid* was taken from the forest area of Luanchuan, Henan Province.

Sample preparation

Use a shredder to crush the leaves and their branches, so as to take it as raw material, using ethanol, benzene alcohol, water to extract.

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The GC-MS

The leaves and branches of the Schneid in Cotoneaster zabelii were decomposed by GC-MS.GC: use quartz capillary column of 30 mm × 0.25 mm × 0.25 ms. The carrier gas is high purity helium gas [10], 1 ml/min. MS: the mass range detected by the MS program is 30-600 amu, the voltage is 70 ev, the ion source and four stage temperature are set at 230 ℃ and 150 ℃ [11-21].

The FT-IR

The FT-IR spectrum of the sample was extracted and then determined by FT-IR spectrophotometer. The KBr disc used should contain 1.00% finely crushed samples [22-33].

Results and discussions

The FT-IR analysis results

According to figs. 1 and 2 shows, you can see two kinds of samples in between 3000-2750 peaks, indicates that northwest Xun son leaves and stems are – CH_3, wave peak, there may be an alkyl compounds [34, 35]. The two samples have wave peaks and peaks between 1600 and 1500, indicating that O-H is present and aldehydes may exist. There are peaks, spikes, spikes between 1100 and 1000 that have C-O-C in them, and there may be ethers.

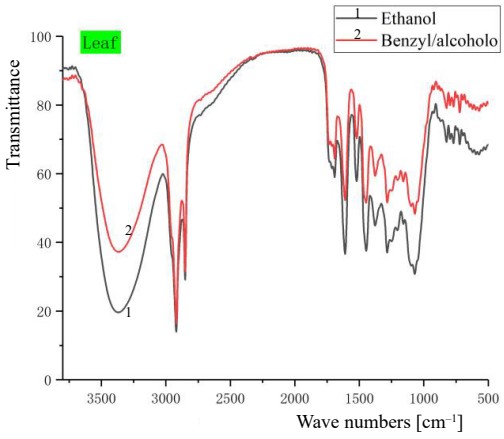

Figure 1. Infrared spectra of leaves

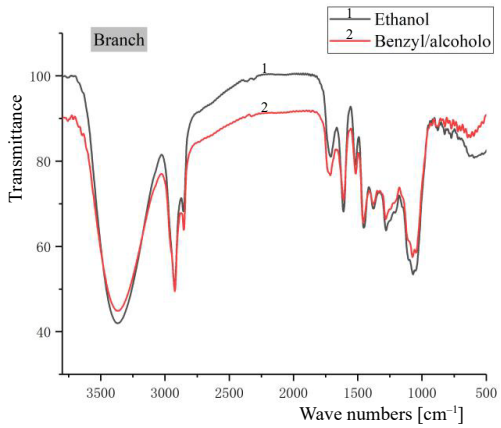

Figure 2. Infrared spectrum of branches

The GC-MS analysis results

Table 1 shows the chemical composition of the *Cotoneaster zabelii Schneid* leaves tested with ethanol by GC-MS. It mainly includes Galactitol (11.31%), which can be used in microbiology, biochemical research and pharmaceuticals. Lactose (0.78%) is used for producing baby food, confectionery, margarine, *etc.* It is also used for culture media, absorbent, exciphers, *etc.* Biochemical studies and the synthesis of vitamin E and vitamin K1 in Phytol (1.94%).

Figure 3 shows the chemical composition of the *Cotoneaster zabelii Schneid* leaves with benzoyl alcohol tested by GC-MS. It mainly consists of 9-octadecenamide (12.55%), it can be used as poly-olefin, PVC, antistatic agent, mold release agent, pigment, dye and other dispersant, printing ink additive. N-hexadecanoic acid (1.05%), to determine the hardness of water and calcium, magnesium, barium, lead, mercury and zinc, to manufacture various metal

Table 1. The GC-MS test results of ethanol extract from the leaves of *Cotoneaster zabelii Schneid*

No.	Retention time	Content [%]	Compound name
1	10.99	0.01	D-Fructose, 1,3,6-trideoxy-3,6-epithio-
2	11.09	0.01	9-[2-Deoxy-.beta.-d-ribohexopyranosyl]purin-6(1H)-one
3	12.30	0.01	Ribitol
4	13.10	0.02	Phytol
5	13.85	0.01	Lactose
6	15.52	0.02	E-11,13-Tetradecadienal
7	15.96	0.00	D-Mannoheptadecane-1,2,3,4,5-pentaol
8	16.54	0.05	Galactitol
9	16.74	0.06	Galactitol
10	18.44	0.00	Isolongifolol
11	19.44	0.01	Benzyl .beta.-d-glucoside
12	23.17	0.01	2H-3,9a-Methano-1-benzoxepin, octahydro-2,2,5a,9-tetramethyl-, [3R-(3.alpha.,5a.alpha.,9.alpha.,9a.alpha.)]-
13	23.66	0.04	Phenol, 4,4'-(tetrahydro-1H,3H-furo[3,4-c]furan-1,4-diyl)bis[2-methoxy-
14	24.41	0.41	Phenol, 4,4'-(tetrahydro-1H,3H-furo[3,4-c]furan-1,4-diyl)bis[2-methoxy-
15	24.54	0.27	Dihydrofuran-2-one, 4-(3,4-dimethoxybenzyl)-3-(4-hydroxy-3-methoxybenzyl)-
16	24.84	0.04	2H-3,9a-Methano-1-benzoxepin, octahydro-2,2,5a,9-tetramethyl-, [3R-(3.alpha.,5a.alpha.,9.alpha.,9a.alpha.)]-
17	25.40	0.02	trans-Geranylgeraniol
18	25.97	0.01	2H-3,9a-Methano-1-benzoxepin, octahydro-2,2,5a,9-tetramethyl-, [3R-(3.alpha.,5a.alpha.,9.alpha.,9a.alpha.)]-
19	26.17	0.01	(2R,3R,4aR,5S,8aS)-2-Hydroxy-4a,5-dimethyl-3-(prop-1-en-2-yl)octahydronaphthalen-1(2H)-one
20	26.66	0.01	2H-3,9a-Methano-1-benzoxepin, octahydro-2,2,5a,9-tetramethyl-, [3R-(3.alpha.,5a.alpha.,9.alpha.,9a.alpha.)]-
21	27.91	0.01	2H-3,9a-Methano-1-benzoxepin, octahydro-2,2,5a,9-tetramethyl-, [3R-(3.alpha.,5a.alpha.,9.alpha.,9a.alpha.)]-

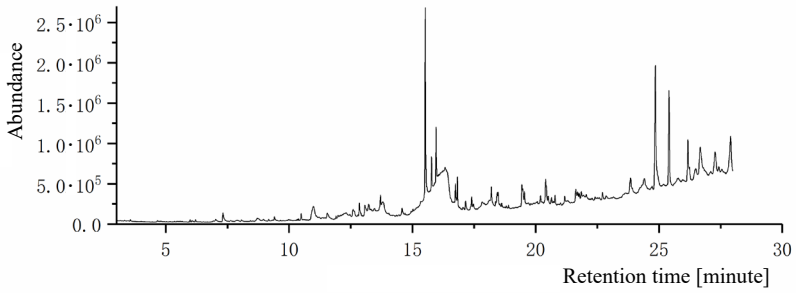

Figure 3. The GC-MS test results of benzenol extract from the leaves of *Cotoneaster zabelii Schneid*

salts of palmitic acid and water-proofing agents. Squalene (7.33%) was prepared as a nutritional drug, which was taken internally for treatment of high and low blood pressure, anemia,

diabetes, cirrhosis, cancer, constipation, and dental insects. External application for tonsillitis, wheezing, bronchitis, cold, tuberculosis, rhinitis, gastric ulcer, duodenal ulcer, gallbladder stones, rheumatism, neuralgia, *etc.*

Table 2 shows the chemical composition of the *Cotoneaster zabelii Schneid* branch mixed with phenyl alcohol by GC-MS. Galactitol (8.97%) is mainly used in microbiology, biochemical research and pharmaceuticals. Vitamin E (2.66%) is used in the prevention of abortion, habitual abortion and threatened abortion caused by vitamin E deficiency, as well as in the treatment of infertility and nutritional giant cell anemia in infants.9-Octadecenamide (10.42%) can be used as poly-olefin, PVC plastic, antistatic agent, mold release agent, pigment, dye and other dispersant, and additive for printing ink.

Table 2. The GC-MS test results of ethanol extract from the trunk of *Cotoneaster zabelii Schneid*

No.	Retention time	Content [%]	Compound name
1	7.32	0.01	Benzoic acid
2	8.72	0.01	Ethylene glycol butyl ether, trimethylsilyl ether
3	10.99	0.04	.alpha.-d-6,3-Furanose, methyl-.beta.-d-glucohexodialdo-1,4-furanoside
4	12.23	0.02	Ribitol
5	13.71	0.01	d-Mannose
6	15.54	0.01	Bicyclo[3.3.0]octan-2-one, 7-trimethylsilylmethylene-
7	15.96	0.03	Silane, (butoxymethyl)trimethyl-
8	16.17	0.09	Galactitol
9	19.99	0.33	6-Tridecanol, 3,9-diethyl-
10	21.27	0.03	Vitamin E
11	21.63	0.01	cis-9-Tetradecenoic acid, heptyl ester
12	21.76	0.02	Cobalt, (.eta.-5-cyclopentadienyl)-[(. eta.-4)-3-ethyl-1,1,2,5-tetramethyl-1-silacyclopentadiene]
13	21.94	0.01	
14	23.64	0.02	2H-3,9a-Methano-1-benzoxepin, octahydro-2,2,5a,9-tetramethyl-, [3R-(3.alpha.,5a.alpha.,9.alpha.,9a.alpha.)]-
15	24.01	0.01	Phenol, 2,4-bis(1,1-dimethylethyl)-, phosphite (3:1)
16	24.23	0.01	Phenol, 4,4'-(tetrahydro-1H,3H-furo[3,4-c]furan-1,4-diyl)bis[2-methoxy-
17	24.40	0.07	Dihydrofuran-2-one, 4-(3,4-dimethoxybenzyl)-3-(4-hydroxy-3-methoxybenzyl)-
18	24.54	0.05	Phenol, 2,6-dimethoxy-4-[tetrahydro-4-(4-hydroxy-3-methoxyphenyl)-1H,3H-furo[3,4-c]furan-1-yl]-
19	24.85	0.10	9-Octadecenamide, (Z)-
20	26.67	0.09	.gamma.-Sitosterol
21	27.27	0.01	(2R,3R,4aR,5S,8aS)-2-Hydroxy-4a,5-dimethyl-3-(prop-1-en-2-yl)octahydronaphthalen-1(2H)-one
22	27.91	0.02	2H-3,9a-Methano-1-benzoxepin, octahydro-2,2,5a,9-tetramethyl-, [3R-(3.alpha.,5a.alpha.,9.alpha.,9a.alpha.)]-

Table 3 describes the use of GC-MS to test the chemical composition of the leaves of *Cotoneaster Zabelii Schneid* mixed with phenyl alcohol. It mainly includes Dibutyl

Table 3. The GC-MS test results of benzenol extract from the trunk of *Cotoneaster zabelii Schneid*

No.	Retention time	Content [%]	Compound name
1	10.99	0.03	.alpha.-D-Xylofuranoside, methyl
2	13.72	0.02	Lactose
3	16.21	0.05	Galactitol
4	16.83	0.02	Dibutyl phthalate
5	18.20	0.03	Lupeol
6	18.38	0.04	Lupeol
7	20.07	0.54	Oxalic acid, cyclohexylmethyl octadecyl ester
8	21.27	0.05	Vitamin E
9	21.77	0.02	Cobalt, (.eta.-5-cyclopentadienyl)-[(. eta.-4)-3-ethyl-1,1,2,5-tetramethyl-1-silacyclopentadiene]
10	24.84	0.06	9-Octadecenamide, (Z)-
11	25.19	0.01	(2R,3R,4aR,5S,8aS)-2-Hydroxy-4a,5-dimethyl-3-(prop-1-en-2-yl)octahydronaphthalen-1(2H)-one
12	26.70	0.12	.gamma.-Sitosterol
13	27.30	0.02	(2R,3R,4aR,5S,8aS)-2-Hydroxy-4a,5-dimethyl-3-(prop-1-en-2-yl)octahydronaphthalen-1(2H)-one

phthalate (1.54%), which is used as plasticizer for nitrates, acetate fibers and polyvinyl chloride. Galactitol (5.00%) was used in microbiology, biochemistry and pharmaceutical research. Lupeol (6.87%) is very helpful in the treatment of leukemia, prostate cancer, melanoma, liver cancer and other tumors. It can be used in the prevention of acute versus host disease after bone marrow transplantation.

Conclusion

In this study, the leaves and stems of the *Cotoneaster zabelii Schneid* were mixed with ethanol and benzenol and decomposed to yield a number of chemical constituents. The mixture of leaves and branches of *Cotoneaster zabelii Schneid* with ethanol and phenylalcohol and the chemical constituents produced by them can be used as raw materials for medicines according to GC-MS. Lupeol (6.87%) is very helpful in the treatment of leukemia, prostate cancer, melanoma, liver cancer and other tumors. It can also be used for the prevention of acute versus host disease after bone marrow transplantation. This research will enhance the development of medicine and better benefit the society.

References

[1] Benjamin, B., *et al.* Dryas as a Model for Studying the Root Symbioses of the Rosaceae, *Frontiers in Plant Science, 10* (2019), June, 661
[2] Prabhakaran, S., *et al.,* Insight on Rosaceae Family with Genome Sequencing and Functional Genomics Perspective, *BioMed Research International, 2019* (2019), ID 7519687
[3] Baohuan, W., *et al.* Taxonomic Reconsideration of Prunusveitchii (Rosaceae), *PhytoKeys, 115* (2019), Jan., pp. 59-71
[4] Mangioni, D., *et al.* Transcriptome Profiling and Fast Microbiology in Sepsis Diagnosis: A Potential Synergy We Cannot Neglect, *Journal of Critical Care, 52* (2019), Aug., pp. 267-268

[5] Vishwanath, H., Soumili, C. S. R. A., High Performance Liquid Chromatography (HPLC) Based Direct and Simultaneous Estimation of Excipients in Biopharmaceutical Products, *Journal of Chromatography. B, Analytical Technologies in the Biomedical and Life Sciences, 1117* (2019), June, pp. 118-126
[6] Harraga, H., Yebdri, M., Attractors for a Nonautonomous Reaction-Diffusion Equation with Delay, *Applied Mathematics & Nonlinear Sciences, 3* (2018), 1, pp. 127-150
[7] Sardar, M. S., *et al.,* Computing Topological Indices of the Line Graphs of Banana Tree Graph and Firecracker Graph, *Applied Mathematics & Nonlinear Sciences, 2* (2017), 1, pp. 83-92
[8] Flanagan, T., Potential for Pharmaceutical Excipients to Impact Absorption: A Mechanistic Review for BCS Class 1 and 3 drugs, *European Journal of Pharmaceutics and Biopharmaceutics, 141* (2019), Aug., pp. 130-138
[9] Song, G., *et al.,* Analysis of Flavor Change in the Industrial Production of Fungal Fermentation Based Mussel (Mytilus Edulis) Cooking Liquor Using a Laser Irradiation Desorption Based GC/MS Method, *LWT-Food Science and Technology, 112* (2019), 108248
[10] Abdel-Naime, W. A., *et al.,* Antibacterial, Antifungal, and GC-MS Studies of Melissa Officinalis, *South African Journal of Botany, 124* (2019), Aug., pp. 228-234
[11] Suppajariyawat, P., *et al.,* Classification of ANFO Samples Based on Their Fuel Composition by GC-MS and FTIR Combined with Chemometrics, *Forensic Science International, 301* (2019, Aug., pp. 419-425
[12] Kusano, M., *et al.,* Development of *Quick-DB Forensic*: A Total Workflow from QuEChERS-dSPE Method to GC-MS/MS Quantification of Forensically Relevant Drugs and Pesticides in Whole Blood, *Forensic Science International, 300* (2019), July, pp. 125-135
[13] Manuel, L., Erik, P., Drying Enhances Signal Intensities for Global GC-MS Metabolomics, *Metabolites, 9* (2019), 68
[14] Morgan, M, A., *et al.,* Evaluating Sub-Lethal Stress from Roundup ® Exposure in Artemia Franciscana Using 1 H NMR and GC-MS, *Aquatic Toxicology, 212* (2019, July, pp. 77-87
[15] Newman, M., *et al.,* Evaluating Urinary Estrogen and Progesterone Metabolites Using Dried Filter Paper Samples and Gas Chromatography with Tandem Mass Spectrometry (GC–MS/MS), *BMC Chemistry, 13* (2019), Feb., 20
[16] Xu, S., Extraction and Quantitative Analysis of Water by GC/MS for Trace-level Dimethylsilanediol (DMSD), *Journal of Chromatography A*, *1600* (2019), Aug., pp. 1-8
[17] Giannetti, V., *et al.,* Flavour Component Analysis by HS-SPME/GC-MS and Chemometric Modeling to Characterize Pilsner-style Lager Craft Beers, *Microchemical Journal, 149* (2019), Sept., 103991
[18] Ncube, E, N., *et al.,* C-MS Based Profiling of Alkanes in the Filamentous Yeast Hyphozyma Roseoniger (Moesziomyces Antarcticus), *Biotechnology Letters, 41* (2019), 6-7, pp. 859-866
[19] Barupal, T., *et al.,* Inhibitory Effects of Leaf Extract of Lawsonia Inermis on Curvularia Lunata and Characterization of Novel Inhibitory Compounds by GC-MS Analysis, *Biotechnology Reports, 23* (2019), Sept., 800335
[20] Mlonka-Mędrala, A., *et al.,* Laboratory Studies on the Influence of Biomass Particle Size on Pyrolysis and Combustion Using TG GC/MS, *Fuel, 252* (2019), Sept., pp. 635-645
[21] Tao, T., *et al.,* GC/MS Analysis of Extracts from Nanzhu by Hot Water, *Journal of Central South University of Forestry and Technology, 29* (2009), 01, pp. 89-91
[22] Smit, G., *et al.,* A Comparative Study of CO Adsorption and Oxidation on Au/Fe_2O_3 Catalysts by FT-IR and in Situ DRIFTS, *Spectroscopies Journal of Molecular Catalysis. A, Chemical, 252* (2006), 1-2, pp. 163-170
[23] Li, Q., *et al.,* Diagnosis of Gastric Endoscopic Biopsies Using Attenuated Total Reflectance (ATR) Fourier Transform Infrared (FT-IR) Spectroscopy with Entropy Weight Local-hyperplane k-nearest Neighbor Based on Frequency Domain Information (EWHFI), *Analytical Letters, 52* (2019), 12, pp. 1914-1925
[24] Singh, J. S., FT-IR and Raman Spectra, AB Initio and Density Functional Computations of the Vibrational Spectra, Molecular Geometries and Atomic Charges of Uracil and 5-halogenated Uracils (5-X-uracils; X<ce:hsp sp="0.25"/>=<ce:hsp sp="0.25"/>F, Cl, Br, I), *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 117* (2014), Jan., pp. 502-518
[25] Squeo, G., *et al.,* FT-IR Extra Virgin Olive Oil Classification Based on Ethyl Ester Content, Food Control, *102* (2019), Aug., pp. 149-156
[26] Jia, Y, Z., *et al.* FT-IR Spectroscopy of Supersaturated Aqueous Solutions of Magnesium Borate, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, *56* (2000), 7, pp. 1291-1297
[27] Svečnjak ,L, *et al.,* Influence of Beeswax Adulteration with Paraffin on the Composition and Quality of Honey Determined by Physico-Chemical Analyses, 1 H NMR, FTIR-ATR and HS-SPME/GC-MS, *Food Chemistry, 291* (2019, Sept., pp. 187-198

[28] Qiao, X., Li, D., Cheng, L., Mechanism of Electrochemical Capture of CO_2 via Redox Cycle of Chlorinated 1,4-naphthoquinone in BMIMBF 4: An in-situ FT-IR Spectroelectrochemical Approach, *Journal of Electroanalytical Chemistry, 845* (2019), July, pp. 126-136
[29] Nageswari, G., *et al.,* Molecular Analyses Using FT-IR, FT-Raman and UV Spectral Investigation; Quantum Chemical Calculations of Dimethyl Phthalate, *Journal of Molecular Structure, 1195* (2019), Nov., pp. 331-343
[30] Vengatesh, G., Sundaravadivelu, M., Non-Toxic Bisacodyl as an Effective Corrosion Inhibitor for Mild Steel in 1 M HCl: Thermodynamic, Electrochemical, SEM, EDX, AFM, FT-IR, DFT and Molecular Dynamics Simulation Studies, *Journal of Molecular Liquids, 287* (2019), Aug., 110906
[31] Jimenez, V. M., *et al.,* Structural Characterization of Partially Amorphous SnO_2 Nanoparticles by Factor Analysis of XAS and FT-IR Spectra, *Solid State Ionics, 116* (1999), 1-2, pp. 117-127
[32] Abosadiya, H. M., *et al.,* Synthesis, X-Ray, Spectroscopic Characterization (FT-IR, NMR, UV-Vis) and Quantum Chemical Calculations of Some Substituted Benzoylthiourea Derivatives, *Journal of Molecular Structure, 1194* (2019), Oct., pp. 48-56
[33] Sathya, B., *et al.,* Vibrational Analysis (FT-IR and FT-Raman Spectra) and Molecular Docking Evaluation of MPTB in GABA Receptor, *Journal of Cluster Science, 30* (2019), 4, pp. 1025-1035
[34] Lim, D., *et al.,* Application of Molecular Dynamics Simulation to Improve the Theoretical Prediction for Collisional cross Section of Aromatic Compounds with Long Alkyl Chains in Crude Oils, *Rapid Communications in Mass Spectrometry, 33* (2019), 7, pp. 650- 656
[35] Quinlivan, P. J., *et al.,* Reactivity of the Carbodiphosphorane, (Ph3P)2C, towards Main Group Metal Alkyl Compounds: Coordination and Cyclometalation, *Dalton Transactions, 48* (2019), 25, pp. 9139-9151

Paper submitted: July, 3, 2019
Paper revised: September 13, 2019
Paper accepted: September 20, 2019