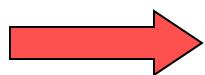


# Study of correlation between volatile carbonyls in cigarette mainstream smoke and chemical constituents in tobacco leaves

**GENG Zhao-liang**

Guizhou Academy of Tobacco Science,  
Guiyang, Guizhou, China

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## ■ Introductions

- Carbonyls
- Main source of Volatile carbonyls
- The impact on people's health
- Resulting thinking

## ■ Experimental Section

- Materials and Dectections

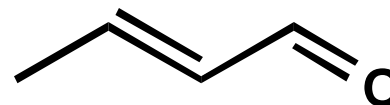
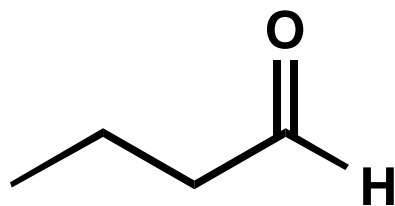
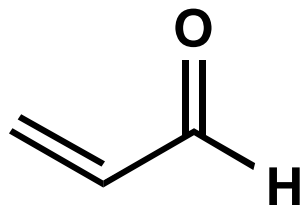
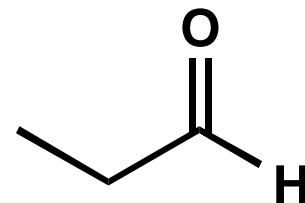
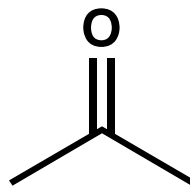
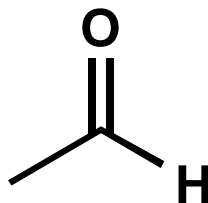
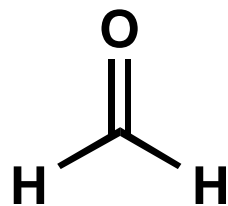
## ■ Results and Analysis

- Different chemical constituents in tobaccl leaves
- The rule of carbonyl compounds emission
- Correlation of carbonyls and chemical constituents

## ■ The Follow-up Consideration

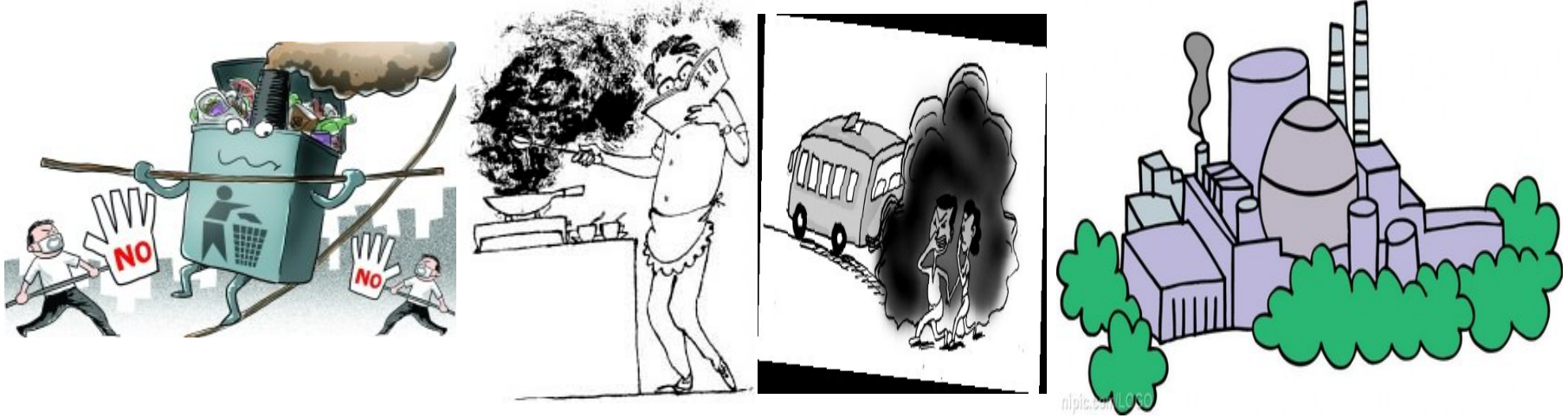
# INTRODUCTIONS

- **Carbonyls (aldehydes and ketones) are an important class of volatile organic pollutants**, including formaldehyde, aldehyde, acetone, acrolein, propionaldehyde, crotonaldehyde, butyl aldehyde.



- People pay more attention as their important role in phytochemistry and for the toxic air contaminants which can cause suspected carcinogens, eye irritants and mutagens to human.

**The main sources of Volatile carbonyls are from waste incineration, cooking oil fume(COF), factory and motobile exhaust, etc.**



**Unfortunately, cigarette smoke also contains many volatile carbonyls.**



# What about the impact of Volatile Carbonyl Compounds on people's health?

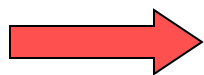
- Compared with nitrosamines, aromatic amines, nitrogen oxides and benzopyrene, Volatile Carbonyl Compounds have higher contents in mainstream cigarette smoke.
- The low molecular aldehydes, such as acrolein, formaldehyde, acetaldehyde and crotonaldehyde in carbonyl compounds, have not only strong pungent odor but also cilia toxicity. That is, they can risk lung irritation.
- The International Agency for Research on Cancer (IARC) clarify formaldehyde as "Group I carcinogen", crotonaldehyde and acetaldehyde as "possibly carcinogenic to humans".
- Therefore, carbonyl compounds are in Hoffmann list and classified by Canadian governments, and it is also regarded by China as one of seven mainstream smoke harmful indicators.

# Resulting Thinking

- How to decrease the content of volatile carbonyls in cigarette smoke become an important challenge in the development of tobacco industry.
- Volatile carbonyls are formed in a combustion and pyrolysis reaction by many different kinds of chemical constituents in tobacco leaf. But what is the interaction of chemical constituents in tobacco leaf and volatile carbonyls in cigarette smoke?
- Through this interrelated analysis, can we put forward a kind of idea for reduction of volatile carbonyls by regulation of chemical constituents in tobacco leaf?

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# ■ The Follow-up Consideration

# Materials and Detections

■ **Tobacco samples:** from 5 flue-cured tobacco producing regions in China in 2010 (10 samples each region)

## ■ Detections I :

**Tobacco leaf**  
(chemical constituents)

- Alkaloids** (nicotine, nornicotine, anabasine, anatabine, nicotyrine, myosmine, 2,3-dihydropyridine, cotinine)
- Polyphenols** (chlorogenic acid, scopoletin, rutin)
- Organic acids** (oxalic acid, malonic acid, acetyl acrylic acid, maleic acid, succinic acid, malic acid, citric acid, myristic acid, palmitic acid, linoleic acid, linolenic acid, etc.)
- Solanesols**
- Soluble sugars** (fructose, glucose, sucrose, maltose)
- Sterols** (cholesterol, campesterol, stigmasterol,  $\beta$ -sitosterol)
- Conventional chemical components** (total sugar, reducing sugar, starch, protein, total nitrogen, potassium, chloride)



# Materials and Dectections

## ■ Dectections II

**Cigarette  
mainstream  
smoke**

(carbonyl compounds)

Formaldehyde  
Acetaldehyde  
Acetone  
Propylene aldehyde  
Propyl aldehyde  
Crotonaldehyde  
Butyraldehyde  
2-butanone

## ■ Data Processing

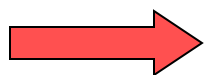
EXCEL 2003 and SPSS 10.0 for data processing and correlation analysis

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# Chemical contents in tobacco leaves from different regions

Sample site	Solanesol	Acides	Alkaloids	Polyphenolics	Sterols
Region 1	12.575	103.807	23.023	37.622	2.917
Region 2	14.788	83.551	22.969	26.162	2.782
Region 3	18.392	89.302	36.840	28.615	2.270
Region 4	13.283	173.918	30.790	37.245	2.344
Region 5	15.667	111.785	36.094	38.608	2.033
Average	14.941	112.473	29.943	33.650	2.469

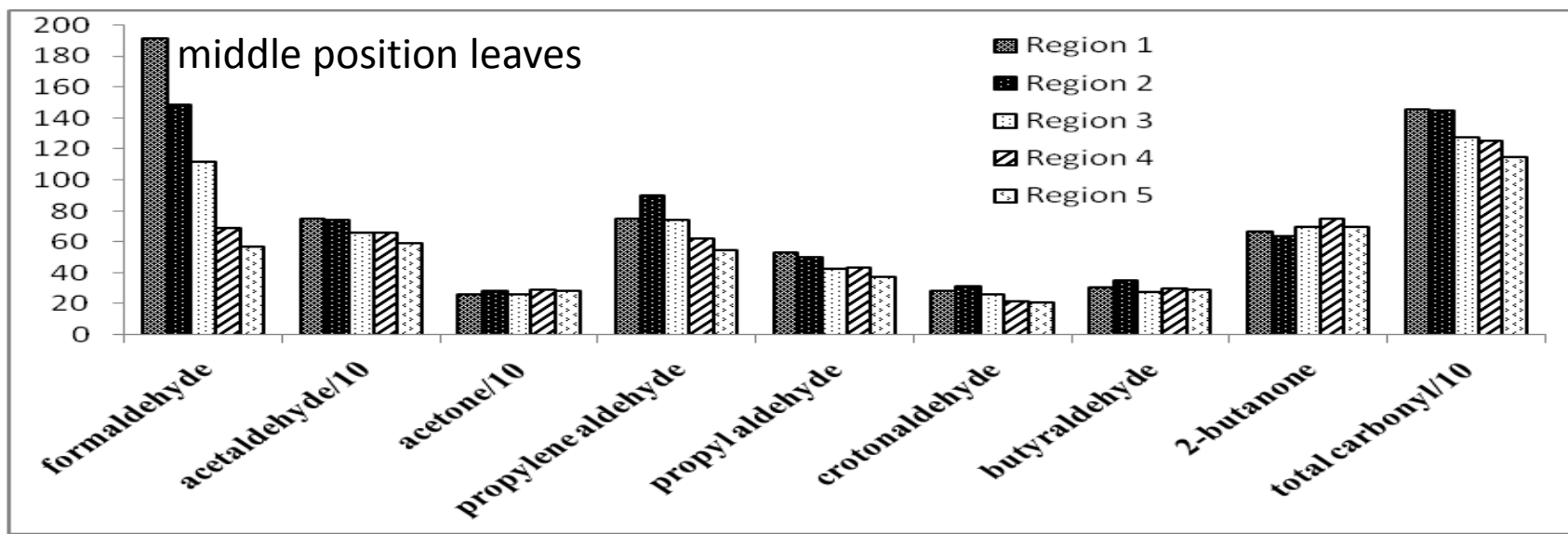
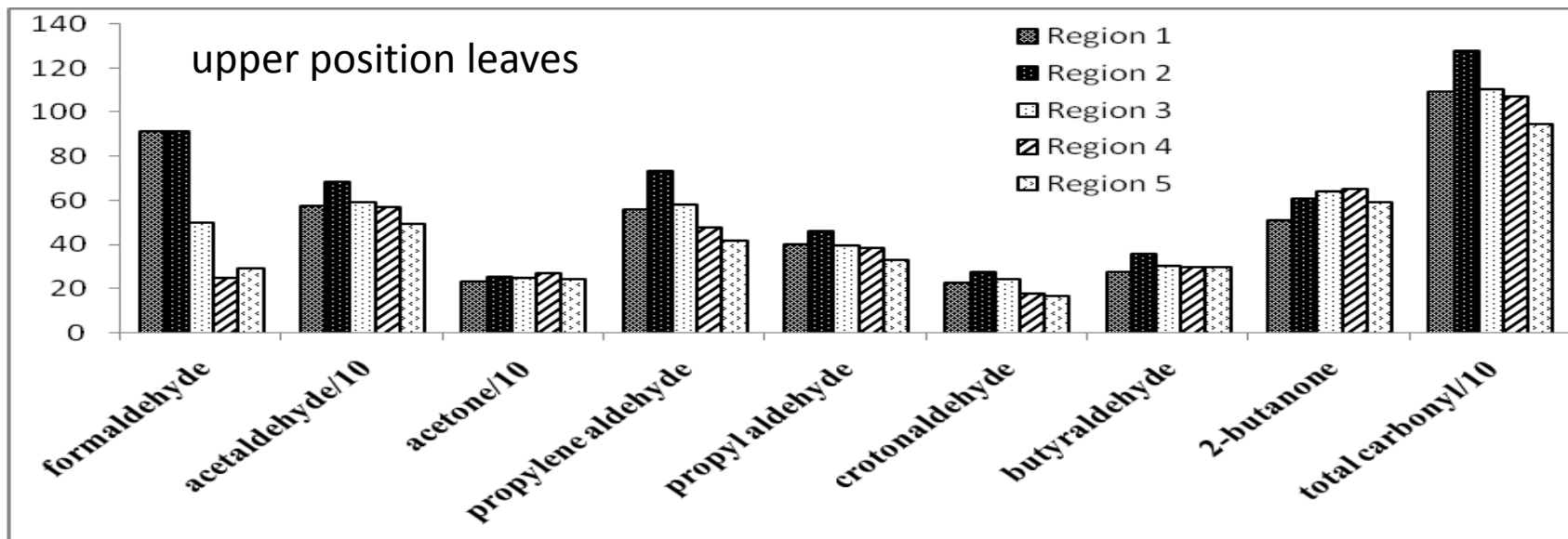
The average contents of major secondary metabolites of tobacco leaves from different regions (mg/g)

	Sample site	TS	RS	T N	Protein	Starch	K	Cl
The average contents of conventional chemical constituents of tobacco leaves from different regions (%)	Region 1	30.877	21.632	1.779	7.037	5.074	1.434	0.106
	Region 2	28.398	20.536	1.962	7.807	3.662	1.853	0.442
	Region 3	28.199	17.396	2.120	7.942	3.554	1.875	0.246
	Region 4	26.284	18.123	2.512	9.130	1.840	1.592	0.328
	Region 5	31.026	20.420	2.462	8.760	2.711	1.374	0.325
	Average	28.957	19.622	2.167	8.135	3.368	1.626	0.289

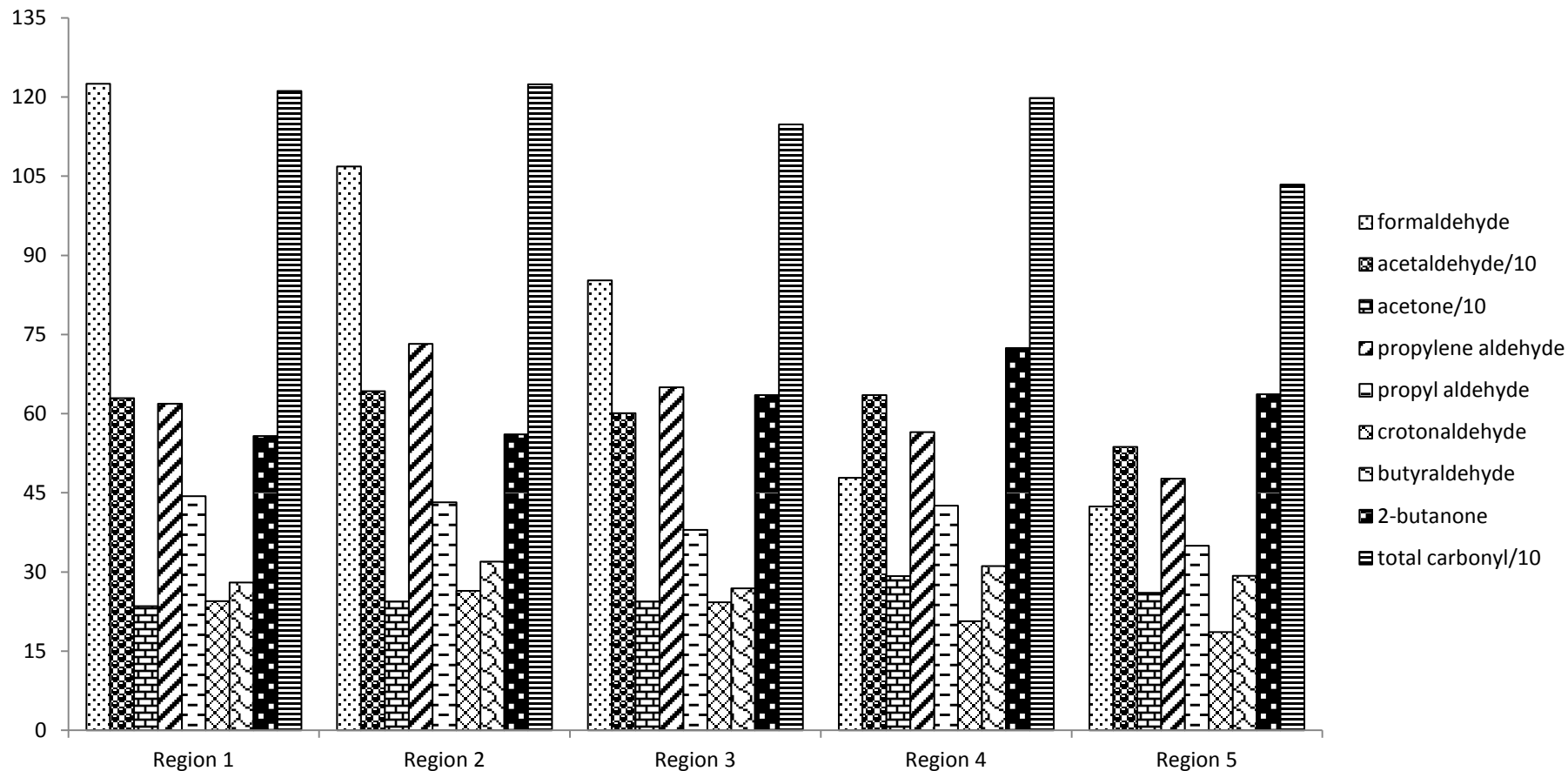
## □ Different chemical constituents in tobacco leaves

- The data of leaf samples from five regions of China southwest demonstrated that leaf secondary metabolites contents of various regions had considerable difference.
- Compared with other regions, the contents of organic acids, polyphenols and alkaloids were high, that of sterol was moderate, and the leaf chemical composition was basically balanced.
- Different regional and ecological conditions produce different tobacco leaves with complex and characteristic chemicals.

# Carbonyl compounds emissions in mainstream smoke of tobacco leaves from different positions



# The carbonyl compounds emission in mainstream smoke of flue-cured tobacco leaves from different regions



The carbonyl compounds emission in mainstream smoke of flue-cured tobacco leaves from different regions ( $\mu\text{g}/\text{cig}$ )

## □ The rule of carbonyl compounds emission

- Carbonyl compounds emission of different leaf positions : in general, the emission of cigarettes made by middle leaf was larger than that of upper leaf cigarette.
- Carbonyl compounds emission in different region Region 1 and 2 leaves were high, region 5 leaf was low, Region 3 and 4 leaf were in the middlens.
- It appeared that the variations of leaf position and structure, chemical composition and producing origins may be the cause of dissimilarity in carbonyl compounds emissions.

# The correlation analysis of major leaf substances with carbonyl compounds emission in mainstream smoke

Inspection items		formaldehyde	acetaldehyde	acraldehyde	crotonaldehyde	Total carbonyl compound
Soluble sugars	Fructose	0.4476**			0.378*	
	Glucose	0.4927**				
	Maltose	0.5092**		0.562**	0.568**	
sterols	Cholesterol	0.669**	0.449**	0.572**	0.708**	0.431**
	Campesterol	0.363*		0.610**	0.396*	
	Stigmasterol	0.675**	0.688**		0.692**	0.671**
	Lanosterol	0.510**			0.363*	0.349**
	β-resinol				0.406*	
	Total sterols	0.515*	0.451**		0.478**	0.407**
Conventional chemical components	Total sugar	0.346*				
	Reducing sugar	0.365*				
	Total nitrogen	-0.757**		-0.635**	-0.656**	-0.408*
	potassium	0.511**	0.568**	0.561**	0.536**	0.570**
	Chlorine	-0.374*				
	Protein	-0.679**		-0.554**	-0.583**	
	Starch	0.502**		0.355*	0.399**	



Inspection items		formaldehyde	acetaldehyde	acraldehyde	crotonaldehyde	Total carbonyl compound
Organic acids	Malonic acid	-0.4606**		-0.459**	-0.459**	
	Acetyl acrylic acid	0.580**		0.466**	0.452**	
	Succinic acid	0.588**	0.529**	0.362*	0.452**	0.540**
	Malic acid				-0.437**	
	Citric acid	-0.511**		-0.452**	-0.497**	
	Myristic acid	-0.378*	-0.409*	-0.435**	-0.406*	-0.464**
	Linoleic acid	-0.606**		-0.496**	-0.508**	
	Linolenic acid	0.425*	0.495**			0.513**
	Maleic acid			-0.356*		
	Total organic acids	-0.340*		-0.357*	-0.454**	
Fatty alcohol	Solanesol	-0.481**	-0.548**	-0.325*		-0.392**
Alkaloids	Nicotine	-0.790**	-0.626**	-0.606**	-0.539**	-0.696**
	Nornicotine	-0.763**	-0.535**	-0.601**	-0.599**	-0.609**
	Anabasine	-0.710**	-0.520**	-0.553**	-0.480**	-0.608**
	Anatabine	-0.767**	-0.531**	-0.596**	-0.589**	-0.595**
	Myosmine	-0.746**	-0.417*	-0.587**	-0.609**	-0.528**
	Nicotyrine	-0.731**	-0.490**	-0.583**	-0.502**	-0.603**
	Isonicotine	-0.588**		-0.448**	-0.389*	-0.371**
	Cotinine	-0.764**	-0.504**	-0.661**	-0.559**	-0.592**
	Total alkaloids	-0.797**	-0.627**	-0.612**	-0.548**	-0.697**
polyphenols	Neochlorogenic acid			-0.344*		
	Scopoletin	-0.612**		-0.472**	-0.558**	
	Rutin	-0.347*	-0.508**	-0.660**	-0.587**	-0.518**
	Total polyphenols			-0.580**	-0.486**	

# □ Correlation of carbonyl compounds(mainstream smoke) and chemical constituents(tobacco leaves)

- Carbonic and nitrogenous compounds in tobacco leaf are all important precursors of carbonyl compounds in mainstream smoke.
- Carbonyl compounds emissions may positively correlated with the contents of soluble sugars, some organic acids, sterols, potassium and starch in tobacco leaf.
- Carbonyl compounds emissions may negatively correlated with the contents of total organic acids, solanesol, polyphenols, alkaloids, proteins and total nitrogen.

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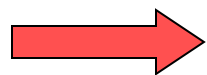
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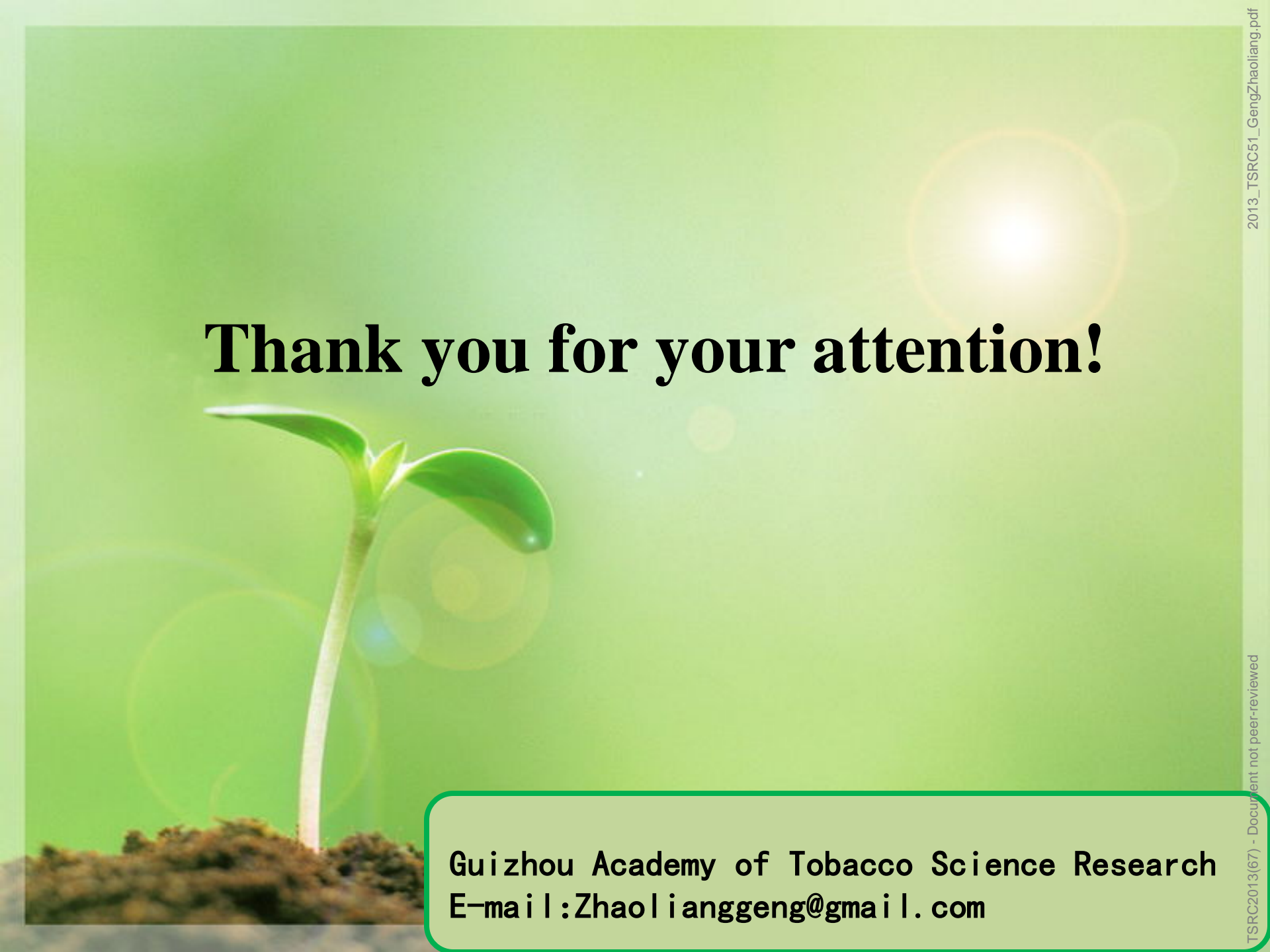
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# ■ The Follow-up Consideration

## ■ The follow-up consideration

- The carbonyl compounds emissions may be affected by local climatic conditions, cultivation and curing techniques, and other factors.
- The results might not be fully and accurately represent the carbonyl compounds emissions of tobacco leaves in different years on the whole area, the carbonyl compound emissions in mainstream smoke of tobacco leaves in different years deserve further study.
- The finding and subsequent studies have great significance in discussing reductions of carbonyl compounds emission in mainstream smoke and smoking and health problems.



**Thank you for your attention!**

Guizhou Academy of Tobacco Science Research  
E-mail: [Zhaolianggeng@gmail.com](mailto:Zhaolianggeng@gmail.com)