Supplementary Information (SI) for RSC Advances.

Supporting Information

Structure-Dependent Pyrolysis Mechanisms of Tobacco Carbohydrates: From Monosaccharides to Polysaccharides under Programmed and Fast Pyrolysis Conditions

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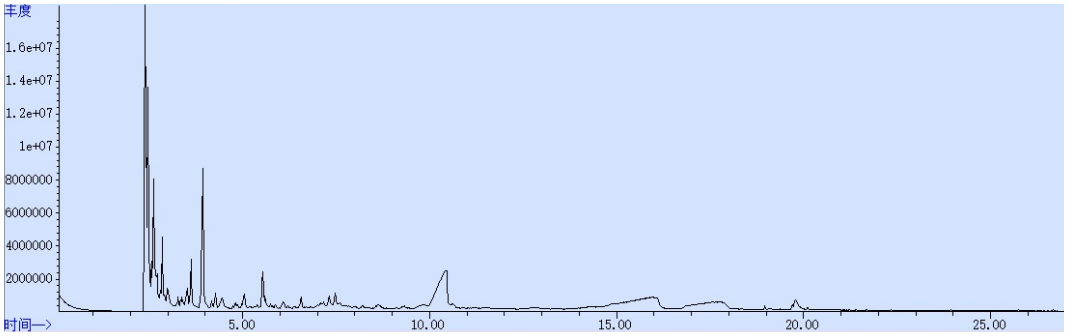

Fig.S1. Glucose fast pyrolysis GC/MS chromatograms

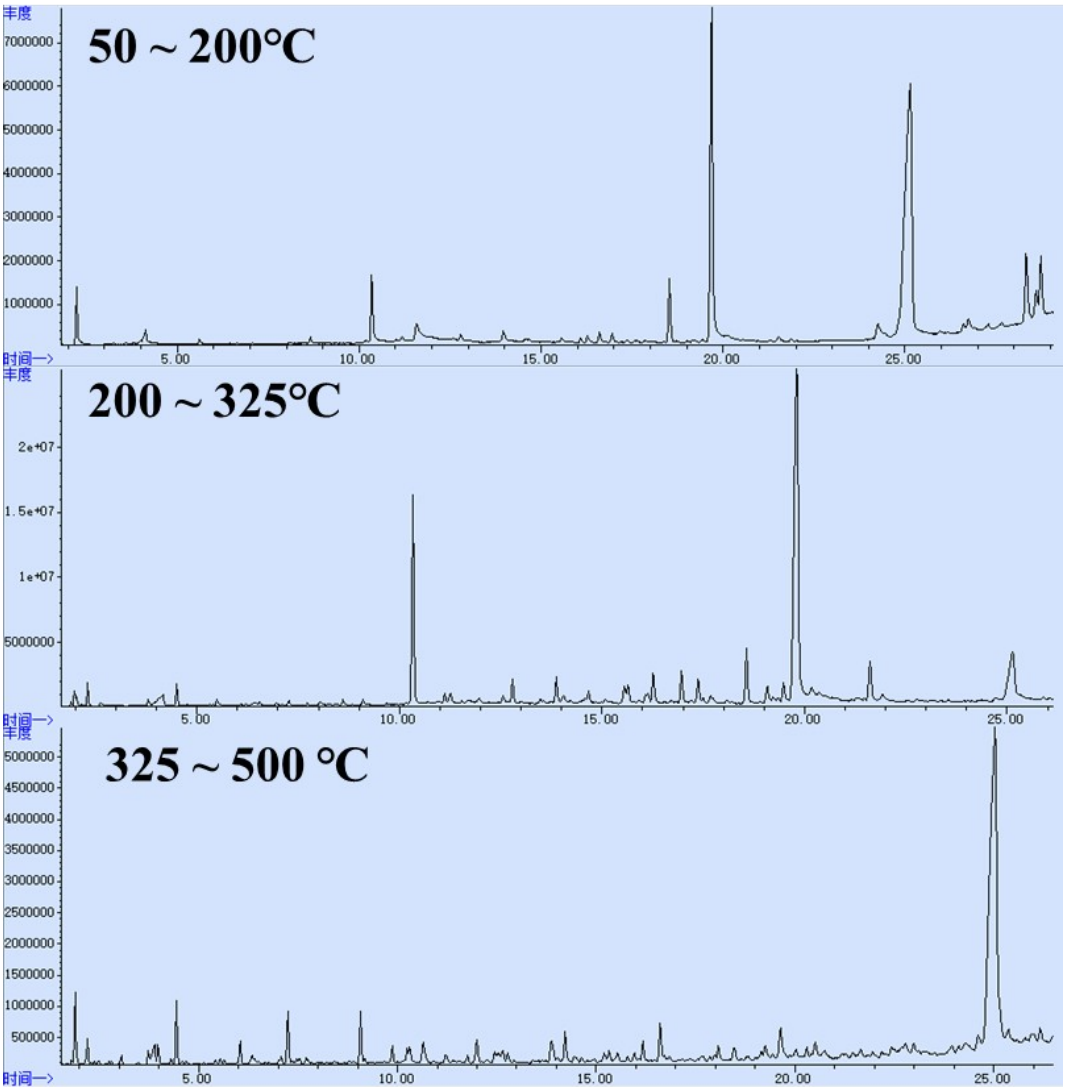

Fig.S2. Glucose temperature-programed pyrolysis GC/MS chromatograms

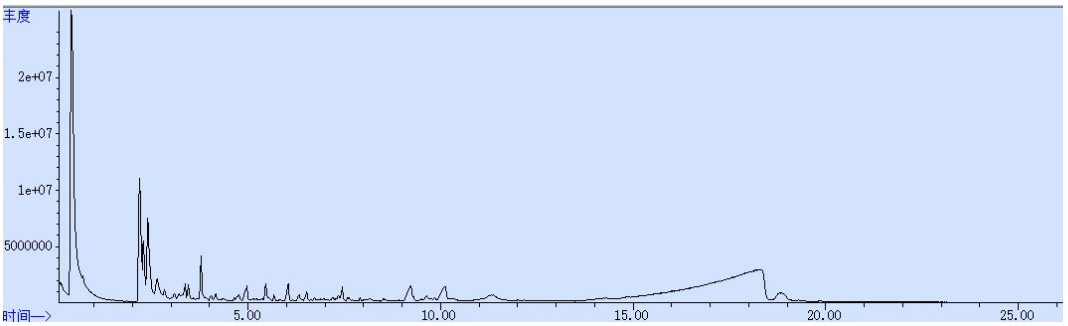

Fig.S3. Cellulose fast pyrolysis GC/MS chromatograms

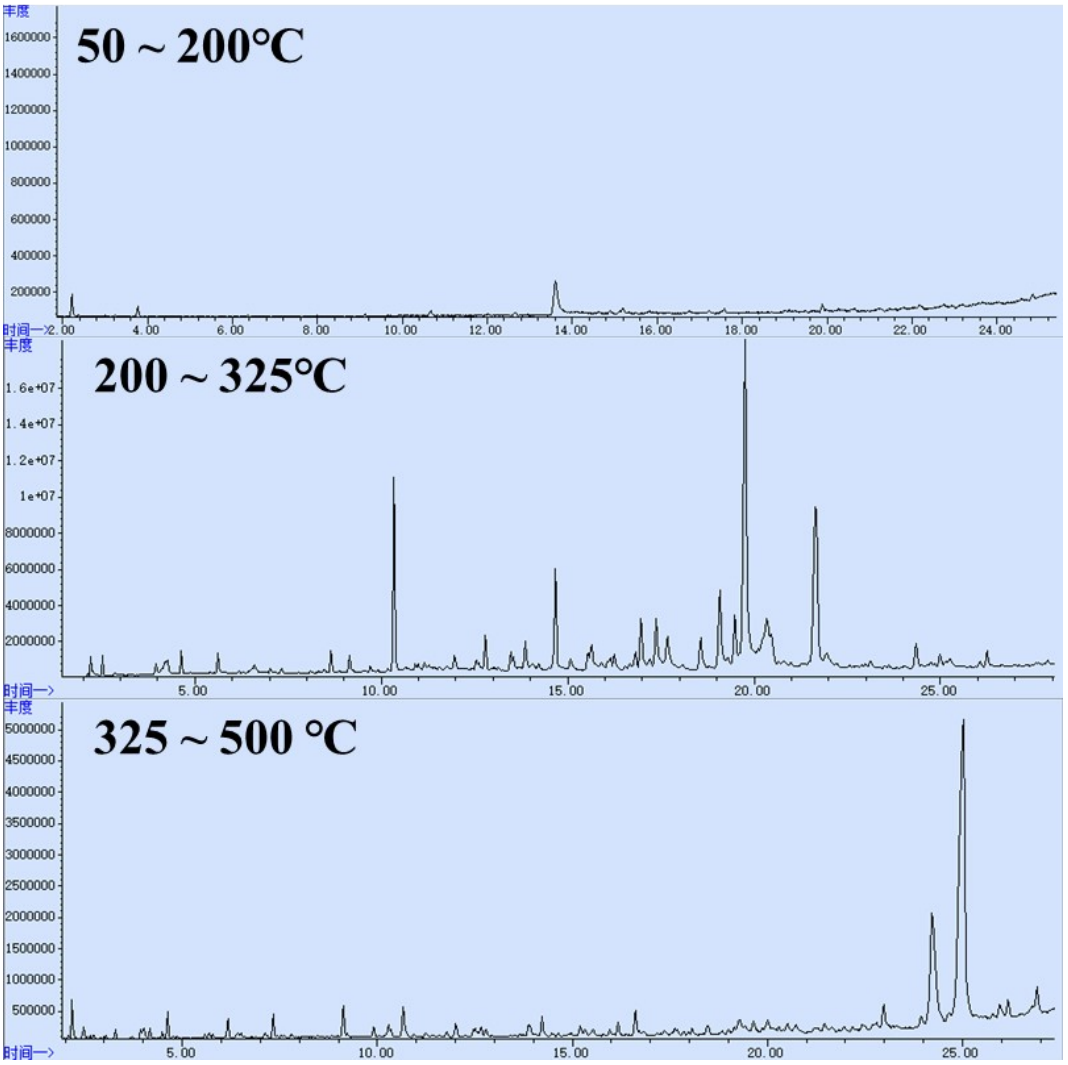

Fig.S4. Cellulose temperature-programed pyrolysis GC/MS chromatograms

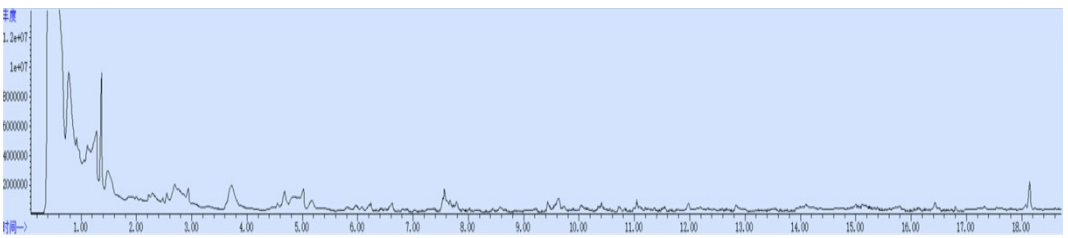

Fig.S5. Cellulose fast pyrolysis GC/MS chromatograms

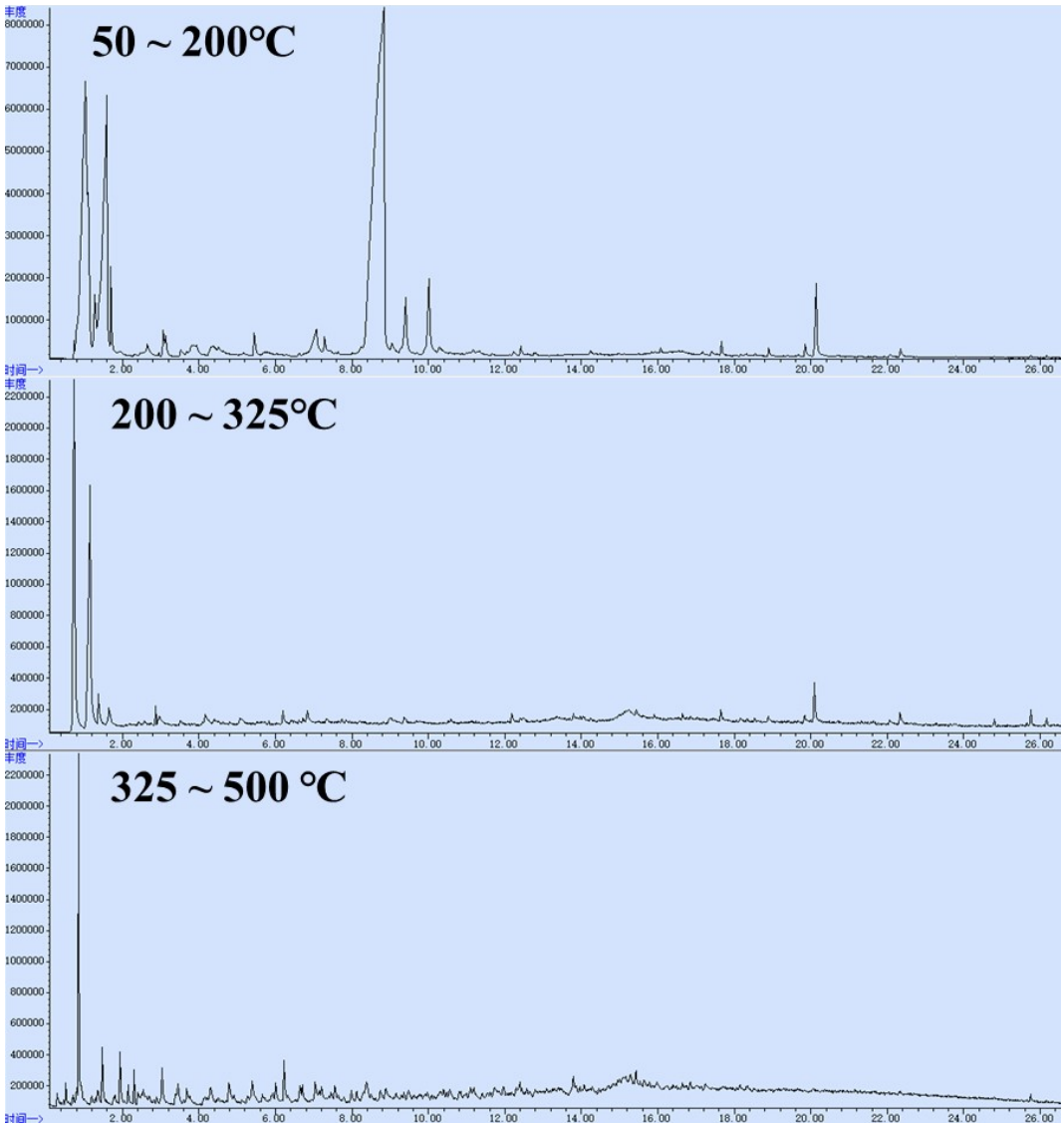

Fig.S6. Cellulose temperature-programed pyrolysis GC/MS chromatograms

Tab.S1. Product distribution of fast pyrolysis for sugar compounds

Compound	Glucose	Fructose	Cellulose	Amylose	Xylan
Anhydrosugars					
Levoglucosan	26.66	24.81	54.53	58.35	14.47
Melezitose	-	-	7.13	9.35	-
1,4-Anhydro-D-xylopyranose	-	-	-	-	19.84
D-Mannose	-	-	-	3.86	-
Furans					
Furfural	16.23	16.07	4.96	3.13	31.66
5-Methylfurfural	3.7	4.21	1.87	1.21	-
2(5H)-Furanone	2.62	1.03	1.78	2.31	1.65
2,5-Dimethylfuran	-	-	-	0.41	-
Furfuryl alcohol	-	-	-	-	1.3
Aldehydes/Ketones					
Methylglyoxal	6.53	8.05	5.64	3.8	5.18
2,3-Butanedione	1.27	0.75	-	-	-
Hydroxyacetone	2.68	2.58	1.26	0.62	2.9
3-Pentanone	1.44	0.32	-	-	0.28
1-Penten-3-one	0.5	0.33	-	-	1.63
Cyclopentenedione	0.48	-	-	-	1.07
1,2-Cyclopentanedione	1.43	-	3.28	2.3	-
Methylcyclopentenolone	-	0.74	1.32	0.58	-
3-Methyl-1,2-cyclopentanedione	-	-	0.99	-	-
Dihydroxyacetone	-	-	-	0.29	-
2-Hydroxy-2-cyclopenten-1-one	-	1.18	-	-	2.79
Esters					

Methyl glyoxylate	1.56	1.7	5.71	3.36	1.51
Methyl pyruvate	0.88	-	1.97	1.16	1.8
Ethyl glycolate	-	-	-	-	-
Methyl 2-oxopropanoate	-	-	-	-	-
1-(Acetoxy)-2-propanone	-	-	-	-	-
Cyclic diketones					
Methylcyclopentenolone	-	0.74	-	-	-
Oxygenated Heterocycles					
5-Hydroxymethylfurfural	30.06	34.27	7.29	6.87	-
DDMP	-	-	0.28	0.8	-
2-Oxobutanoic acid	-	-	-	-	0.44
Carboxylic Acids					
Acetic acid	2.13	1.56	-	-	2.91
Formic acid	-	-	-	-	0.95
Others					
Vinyl ethyl ether	-	0.41	-	-	-
3-Butyn-2-ol	-	-	-	-	1.06
Acetonyl peroxide	-	-	-	-	0.88
Dioxobutadiene diepoxide	-	-	-	-	0.88

Tab.S2. Product distribution of temperature-programmed pyrolysis for small-molecular sugar compounds

Compound	Glucose 50-200	Glucose 200-325	Fructose 50-200	Fructose 200-325
Anhydrosugars				
Levoglucosan	65.12	10.12	-	-
Levoglucosenone	-	2.08	-	-
Furans				
Furfural	4.95	12.55	-	32.9
2,5-Dimethylfuran	-	0.22	-	-
5-Methylfurfural	-	1.8	-	5.54
2(5H)-Furanone	-	0.59	-	-
Aldehydes/Ketones				
Hydroxyacetone	-	0.45	-	-
1,2-Cyclopentanedione	-	1.44	-	-
2,3-Butanedione	-	0.44	-	-
Oxygenated Heterocycles				
5-Hydroxymethylfurfural	29.92	48.74	-	42.35
DDMP	-	3.82	-	3.08
Glycidol	-	0.64	-	-
4H-Pyran-4-one, 3,5-dihydroxy-2-methyl-	-	1.71	-	1.1
Carboxylic Acids				
Acetic acid	-	1.82	-	-
Others				
Isovaleraldehyde propylene glycol acetal	-	3.56	-	-

Tab.S3. Product distribution of temperature-programmed pyrolysis for macromolecular sugar compounds

Compound\Substrate	Cellulose 200-325	Amylose 200-325	Xylan 200-325
Anhydrosugars			
Levoglucosan	0.9	24.06	20.95
Levoglucosenone	3.97	-	-
1,4,3,6-Dianhydro-α-D-glucopyranose	-	6.85	-
Furans			
Furfural	8.12	-	46.6
5-Methylfurfural	2.12	-	-
Furfuryl alcohol	0.73	9.34	-
2(5H)-Furanone	0.99	3.92	-
4-Hydroxy-5-methyl-3(2H)-furanone	-	-	8.35
Aldehydes/Ketones			
Hydroxyacetone	0.81	9.45	3.18
1,2-Cyclopentanedione	1.57	8.54	1.62
Maltol	3.68	-	-
1-Hydroxy-2-butanone	-	-	1.95
Hexane-2,4-dione enol	-	-	3.56
Esters			
Methyl pyruvate	0.86	6.87	0.83
Ethyl butyrate	1.12	-	-
Cyclic diketones			
5-Hydroxymethylfurfural	27.93	3.68	0.92
DDMP	2.26	-	-
4H-Pyran-4-one, 3,5-	3.46	-	-

dihydroxy-2-methyl-			
Carboxylic Acids			
Acetic acid	1.64	-	3.22
Propionic acid	0.79	-	-
Others			
Cyclopropylmethanol	-	23.88	-
1,3-Dioxane	15.76	-	-
n-Butanol	-	3.41	-

Tab.S4. Product distribution of fast pyrolysis for Maillard reaction

Compound	Glucose Maillard(6:1)	Fructose Maillard(6:1)
Furans		
Furfural	5.44	4.15
5-Methylfurfural	4.21	6.15
2,5-Dimethylfuran	6.68	6.32
Furfuryl alcohol	-	7.02
Aldehydes/Ketones		
2,3-Butanedione	34.99	-
Hydroxyacetone	6.6	20.52
1-Hydroxy-2-propanone	-	20.52
Methylcyclopentenolone	2.16	-
Esters		
Methyl pyruvate	7.58	-
Ethyl glycolate	-	12.38
Methyl 2-oxopropanoate	-	7.07
1-(Acetoxy)-2-propanone	-	7.06
Cyclic diketones		
Methylcyclopentenolone	2.16	-
Carboxylic Acids		
Acetic acid	22.54	22.12
Others		
Acetonyl peroxide	7.31	-
Dioxobutadiene diepoxide	-	-
N,N-Diethylaniline	2.48	2.57
1-(1'-Pyrrolidinyl)-2-propanone	-	4.65
Acetylacetone peroxide	7.31	-

Tab.S5. Product distribution of temperature-programmed pyrolysis for Maillard reaction

Compound	Glucose Maillard(6:1) 50-200	Glucose Maillard(6:1) 200-325	Fructose Maillard(6:1)50-200	Fructose Maillard(6:1) 200-325
Furans				
Furfural	1.45	-	6.78	-
2,5-Dimethylfuran	-	73.73	-	28.07
Furfuryl alcohol	-	-	2.74	-
1-(2-Furyl)acetone	-	13.75	-	14.42
Aldehydes/Ketones				
Hydroxyacetone	-	-	3.87	-
Cyclic diketones				
2-Hydroxy-2-cyclopenten-1-one	-	-	-	0.41
Oxygenated Heterocycles				
5-Hydroxymethylfurfural	-	-	4.26	-
DDMP	65.02	-	44.35	-
4H-Pyran-4-one, 3,5-dihydroxy-2-methyl-	3.11	-	3.79	-
Carboxylic Acids				
Acetic acid	23.57	-	27.89	34.01
Formic acid	1.71	-	4.01	-
Others				
Toluene	-	12.51	-	12.29