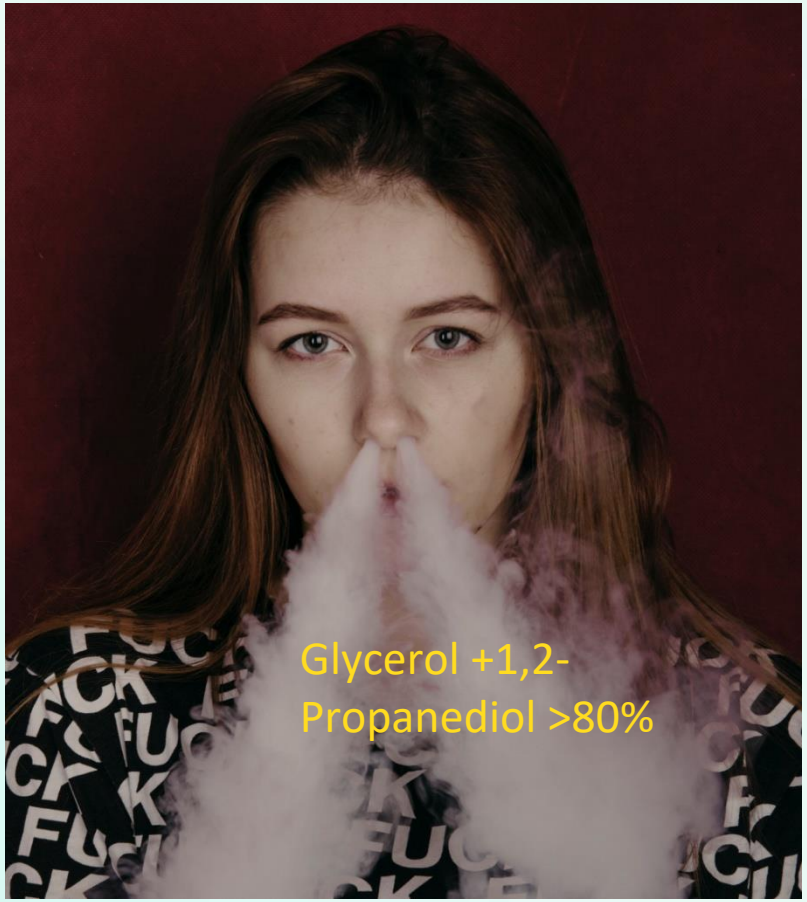
Development of new chemicals for e-cigarette vaporing based on machine learning

Author: HUANG jiaruo

E-mail: huangjr0320@hngytobacco.com

Phone: 86-0731-18507312540

Background



Drawbacks:

1: Toxicity 9-10 times for human endurance;

2: Glycerol has a kind of sweet and soapy feeling;

3: 1,2-Propanediol is full of chemical solvent taste.

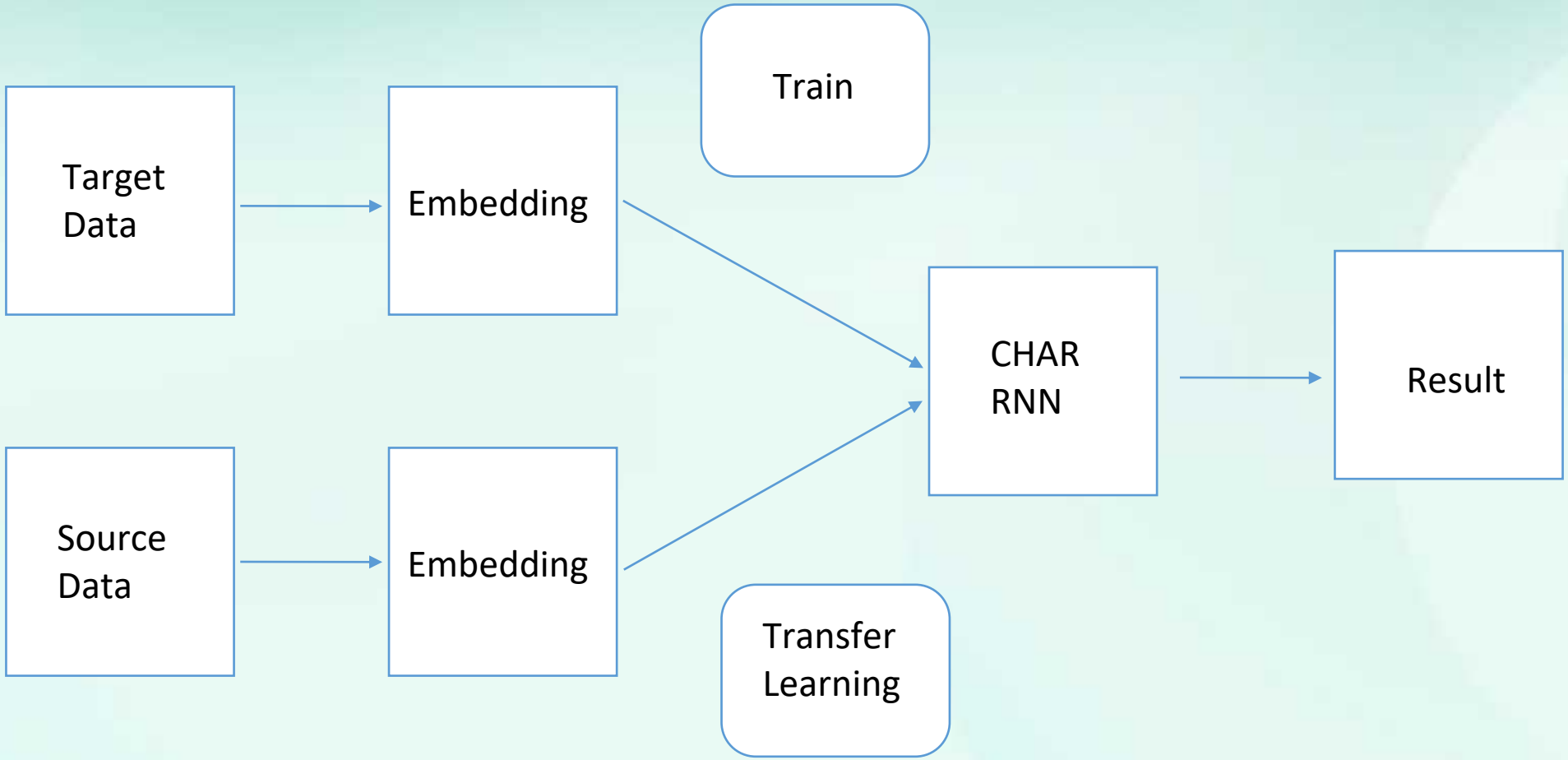


Fig. 1 RNN transfer glycerol and propanediol to atomizing agent by transfer learning

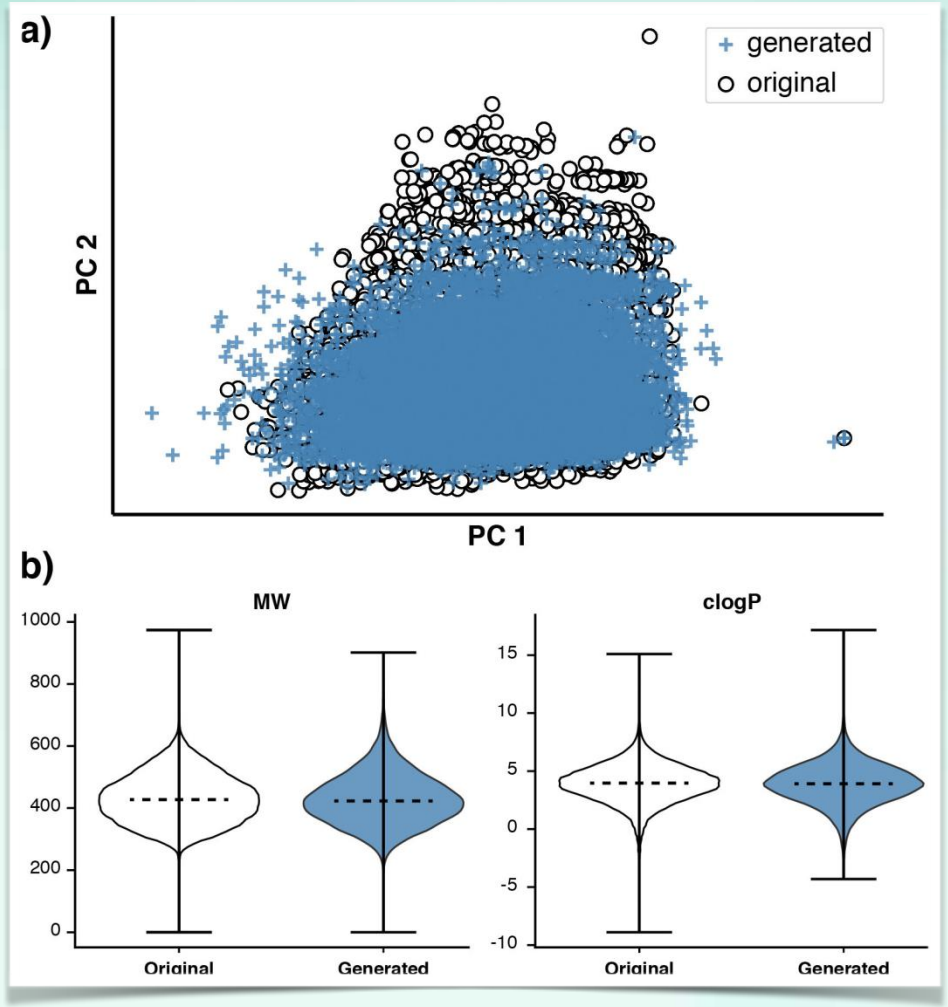
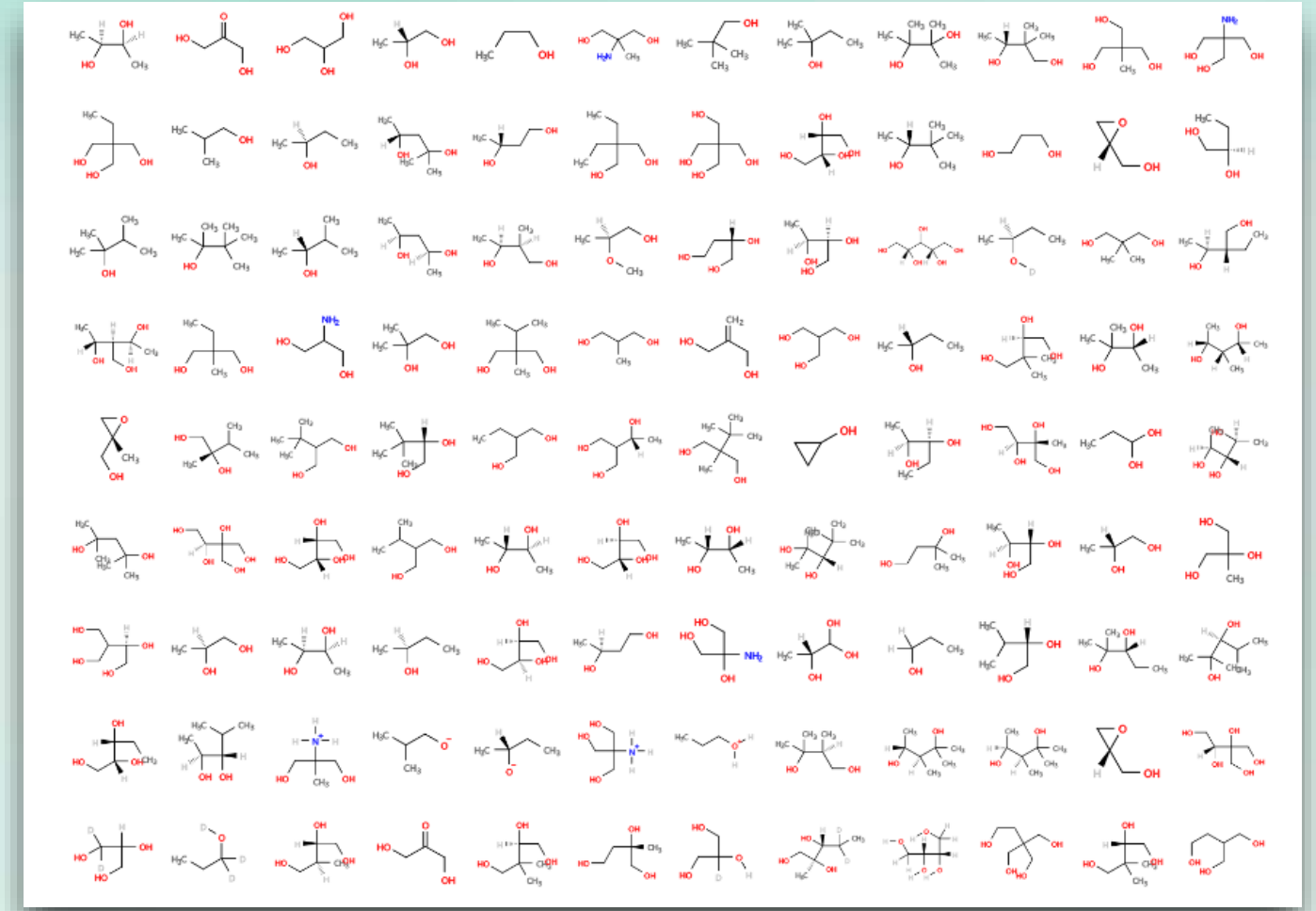


Fig. 2 Comparison of generated data and original data



Molecules to replace Glycerol were found in A week.

The efficiency is more than 100 times that of the traditional Method.

Fig. 3 Atomizer molecules generated by the RNN model

Table 1: Comparison of physical properties between water-based e-cigarette liquid and a traditional oil

Num	Specific Heat Capacity/(J/(g・℃))	Boiling Point/(℃)	Viscosity Coefficient/(mPa・s)
1	3.40	107	9
2	3.50	108	12
3	3.32	108	9
4	2.57	197	250

Xylitol:glycerol:water=40:10:50 in No.1; erythritol:glycerol:water=40:10:50 in No.2; sorbitol:glycerol:water=40:10:50 in No.3; propylene glycol: glycerol:water=28.5:66.5:5 in No.4. the above samples data are obtained by the entrusted testing company according to the method specified in the national standard.

Table 2: Comparison of particles number and diameter of sugar alcohol and glycerol aqueous aerosol

Type of atomizer	Aerosol number(dN/dlogDp[1/cm^3])	Aerosol diameter (dD/ dlogDp[μm/cm^3])
1	663184	0.26
2	409000	0.26
3	586797	0.26
4	356700	0.026

The number and concentration of aerosol particles are measured by electronic low-pressure impactor. The impactor is divided into ten levels, and there is no continuous measurement range from 0.26 μm to 0.026 μm.

Table 3: Taste comparison between water-based e-cigarette liquids and a traditional oil

Num	Smoke volume	Sweet and greasy feeling	Paste flavor	Miscellaneous gas	After taste	Total score
1	4.1	8.8	8.1	8.4	8.2	37.6
2	7.2	8.1	8.1	8.3	8.2	39.9
3	5.1	8.6	7.9	8.1	8.0	37.7
4	7.1	8.0	7.2	8.2	7.9	38.3
5	6.4	8.1	8.1	7.8	8.0	38.4
Contrast sample	8.7	3.2	8.7	3.4	2.7	26.7

The higher the score of each item, the better the performance.

Table 4: Aldehyde release data of propanediol, glycerol and water-based atomizers

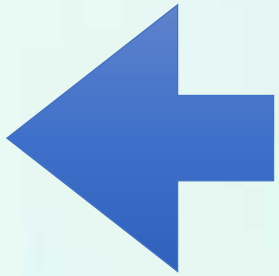
Sample	Formaldehyde	Acetaldehyde	Acetone	Propionaldehyde	Butyraldehyde	Atomization quantity（g）
	Filter catch mass amount（μg）					
Water-based atomizer	4.27	0.88	0.15	0	0	0.1242
Propandediol	13.60	17.16	0.90	0	2.39	0.1134
Glycerol	192.51	28.33	0.49	15.31	4.61	0.0886
	Atomization amount（μg/g）					
Water-based atomizer	34.40	7.08	1.17	0.00	0.00	0.1242
Propanediol	119.92	151.35	7.95	0.00	21.08	0.1134
Glycerol	2172.85	319.76	5.52	172.80	52.03	0.0886
	Amount（μg/mouth）					
Water-based atomizer	0.14	0.03	0.00	0.00	0.00	0.1242
Propanediol	0.45	0.57	0.03	0.00	0.08	0.1134
Glycerol	6.42	0.94	0.02	0.51	0.15	0.0886

Study on inhalation toxicology

- Oral and nasal exposure test to investigate the inhalation toxicity of xylitol.

- SD rats were divided into four groups: control group, low concentration group, medium concentration group and high concentration group.

- The experiments were divided into 28 day and 90 day exposure cycles to investigate acute toxicity and long-term chronic toxicity.
- The rats were dissected, the tissue lesions were observed, the lavage fluid was collected, the contents fo total protein, alkaline phosphatase and lactate dehydrogenase were measured, and the cells were counted.
- SPSS was used to analyze the data, Student's test was used for the comparison between the two groups, and Dunnett's test was used for the three groups and above. $P < 0.05$ indicates significant difference, and $P < 0.01$ indicates very significant difference.



Experimental design and arrangement

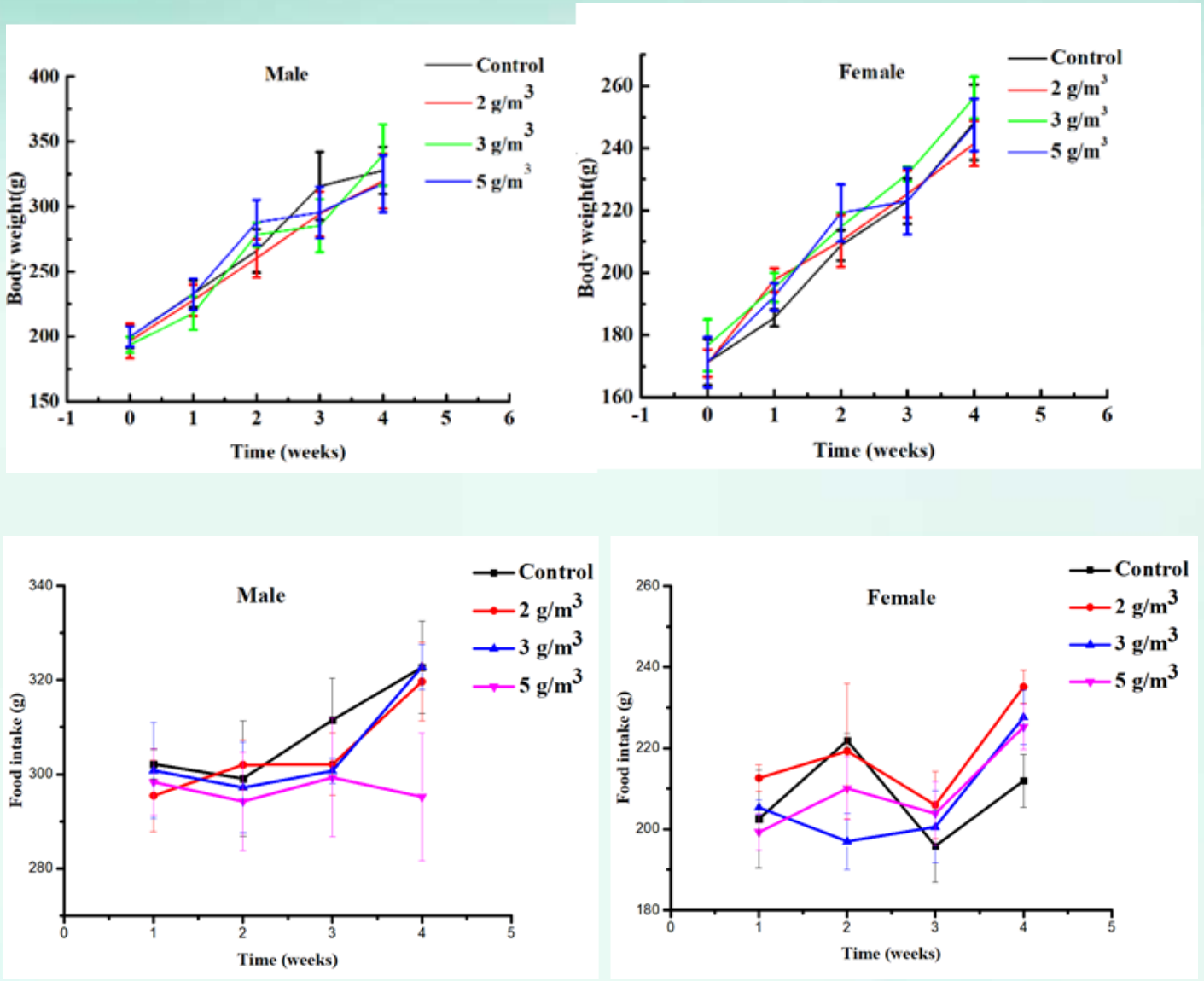


Figure 4: Changes in body weight and food intake of the rats during xylitol exposure

Table 5: Effects of xylitol exposure on blood biochemical indexes

Parameter	Blank Group	Xylitol low dose group (2 g/ m³)	medium dose group (3 g/ m³)	High dose group (5 g/ m³)
Male				
T-Bil-V（μM）	1.67±0.95	1.13±0.67	1.45±0.66	1.52±0.83
D-Bil-V（μM）	0.99±0.62	0.59±0.32	0.88±0.47	0.73±0.35
ALT（U/L）	36.78±2.29	44.88±6.85	41.27±5.51	42.07±5.78
AST（U/L）	67.28±5.40	90.08±20.46*	88.53±16.44*	104.47±21.00*
ALP（U/L）	178.40±78.79	178.46±90.83	142.05±58.13	188.67±29.10
γ-GT（U/L）	0.43±0.22	0.88±0.26	0.87±0.42	0.67±0.35
TP（g/L）	54.73±3.79	52.66±3.15	51.83±3.87	53.80±1.89
ALB II（g/L）	33.18±2.23	32.20±1.94	32.00±2.55	33.12±0.97
TG（mM）	0.41±0.24	0.44±0.18	0.31±0.06	0.37±0.07
LDL-C（mM）	0.34±0.10	1.13±0.67	1.45±0.66	1.52±0.83
HDL-C（mM）	1.28±0.09	1.18±0.23	1.12±0.22	1.17±0.25
TC（mM）	1.82±0.13	1.73±0.32	1.60±0.25	1.77±0.26
CREA-S（μM）	38.53±4.01	39.44±7.43	40.25±3.33	37.38±1.90
UA（μM）	76.40±11.81	80.46±14.42	74.65±15.25	92.33±24.60
UREA（mg/dL）	6.07±0.77	6.86±1.02	6.63±0.80	6.87±1.15
CK-MB（%）	597.78±132.65	657.52±434.25	666.50±339.70	694.27±142.36
CK（U/L）	1011.33±55.26	984.42±264.83	970.50±205.39	986.10±713.53
LDH（mM）	562.90±65.68	531.92±303.45	577.16±337.26	760.95±239.11
AST/ALT（%）	1.80±0.08	2.00±0.27	2.13±0.32	2.47±0.43
IBIL-V（μM）	0.68±0.34	0.56±0.38	0.60±0.21	0.97±0.51
Glo II（μM）	21.55±1.62	20.46±1.28	19.83±1.45	20.68±1.20

Table 5: Continued

Parameter	Blank group	Low dose group (2 g/ m³)	Medium group (3 g/ m³)	High group (5 g/ m³)
Female				
T-Bil-V（μM）	1.13±0.65	0.95±0.13	1.01±0.01	1.22±0.01
D-Bil-V（μM）	0.63±0.29	0.58±0.05	0.54±0.00	0.61±0.24
ALT（U/L）	36.95±3.80	43.23±7.50	41.0±8.71	41.93±9.43
AST（U/L）	69.20±5.49	79.80±9.50	92.47±19.14*	107.17±26.41*
ALP（U/L）	114.90±34.25	139.40±38.94	92.67±17.51	182.20±29.22
γ-GT（U/L）	0.50±0.04	0.83±0.05*	1.04±0.11*	0.60±0.19
TP（g/L）	58.00±0.09	54.20±6.11	55.4±0.31	54.03±2.70
ALB II（g/L）	35.10±0.04	33.2±2.33	34.8±0.41	33.60±0.14
TG（mM）	0.21±0.00	0.41±0.02	0.20±0.01	0.38±0.00
LDL-C（mM）	0.26±0.00	0.28±0.00	0.20±0.01	0.3±0.00
HDL-C（mM）	1.33±0.01	1.34±0.01	1.23±0.01	1.32±0.06
TC（mM）	1.83±0.02	1.95±0.01	1.73±0.01	1.96±0.02
CREA-S（μM）	40.65±4.82	42.63±4.03	38.2±3.31	36.97±1.34
UA（μM）	73.35±14.06	76.83±15.54	68.25±14.11	88.30±27.33
UREA（mg/dL）	6.57±0.38	7.45±0.48	6.10±0.11	5.97±0.47
CK-MB（%）	550.95±132.42	410.17±12.20	605±162.51	641.33±140.38
CK（U/L）	1295.15±243.52	1504.33±145.03	1260±197.21	1138.37±401.10
LDH（mM）	478.35±84.06	606.13±70.14	548±104.11	531.13±100.28
AST/ALT（%）	1.85±0.00	1.87±0.03	2.237±0.14	2.50±0.21
IBIL-V（μM）	0.50±0.09	0.43±0.02	0.50±0.01	0.90±0.13
Glo II（μM）	22.90±0.25	21.00±0.98	21.07±0.14	20.43±1.61

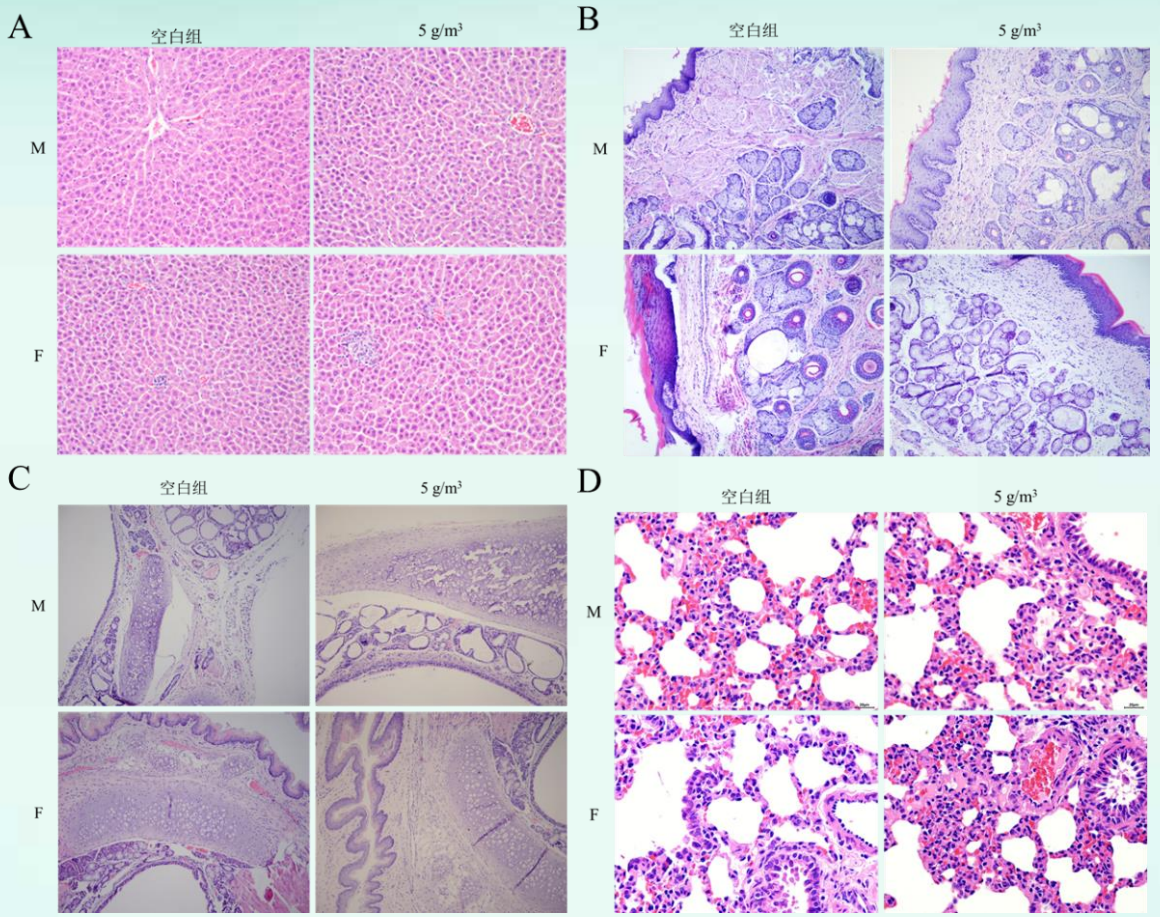


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Figure 5: Effects of xylitol exposure on different tissue morphology in rats: A: liver; B:nose; C:epiglottis; D: lung; M is male, F is female.

Conclusion

- Oral and nasal exposure to xylitol had no significant effect on rats .so xylitol is safe as an aerosol.

- Compared with traditional electronic cigarette oil, the water-based electronic cigarette liquid has better safety and taste.