

Study on the storage stability of three flavors in simulated e-liquid

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OUTLINE

- 1. Background**
- 2. Objective**
- 3. Methods**
- 4. Results**
- 5. Conclusions**

1. Background

- Flavors are common additives in e-liquid.
- During the storage of e-liquid, the flavor ingredients may attenuate, resulting in potential changes of the e-liquid aroma.

2. Objective

- Focus on **the stability of** the simulated e-liquid containing three flavor ingredients under light and high temperature conditions (**acetic acid/octanal/raspberry ketone**).

3. Methods

3.1 Sample preparation

Table1. The formulation of simulated e-liquid

Ingredient	Content (%)
Acetic acid	0.05
Octanal	0.05
Raspberry ketone	0.05
Nicotine	5.00
Benzoic acid	5.00
Propylene glycol (PG)	39.85
Glycerol (VG)	50.00
Total	100.00

3. Methods

3.2 Storage condition setting

Table2. The storage condition of simulated e-liquid

No.	Temp	Environment	Sampling Timepoint
Trial 1	25°C	Darkness	0d / 5d / 10d / 15d / 1M / 3M / 6M
Trial 2	25°C	Light	0d / 5d / 10d / 15d
Trial 3	40°C	Darkness	0d / 1M / 3M / 6M

Note: 3 transparent bottles were randomly taken out from each cabinet at the sampling time for GC-FID and GC-MS analysis.

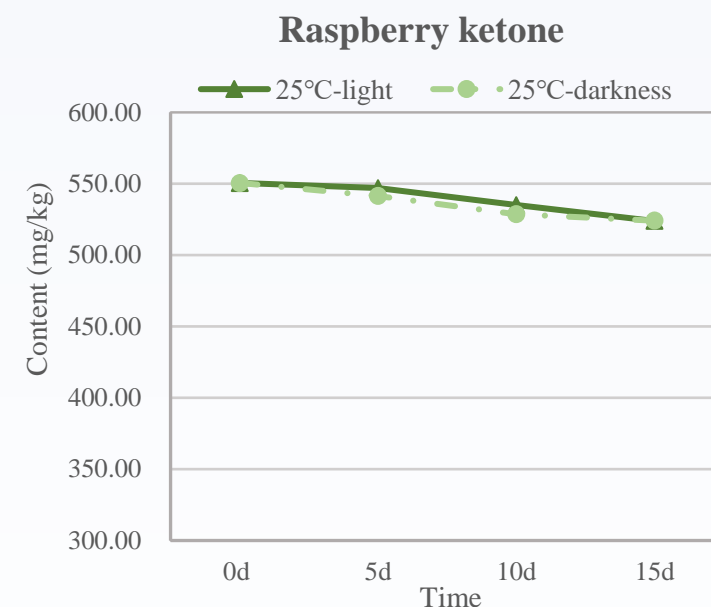
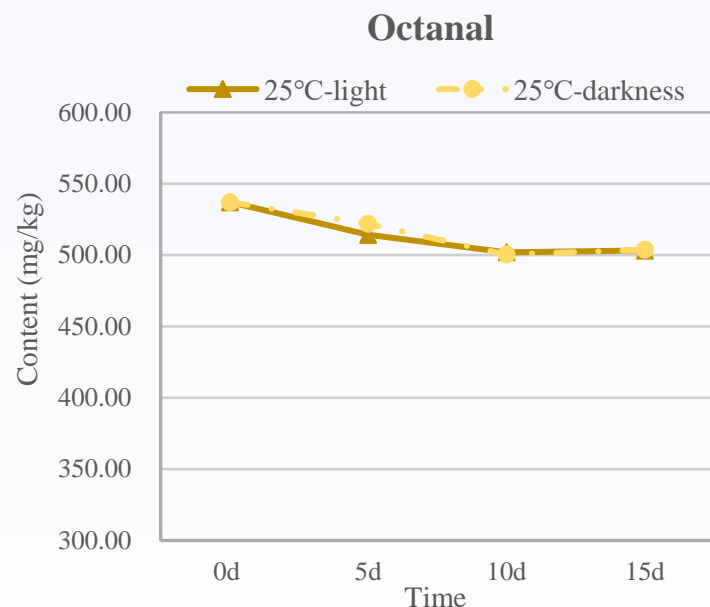
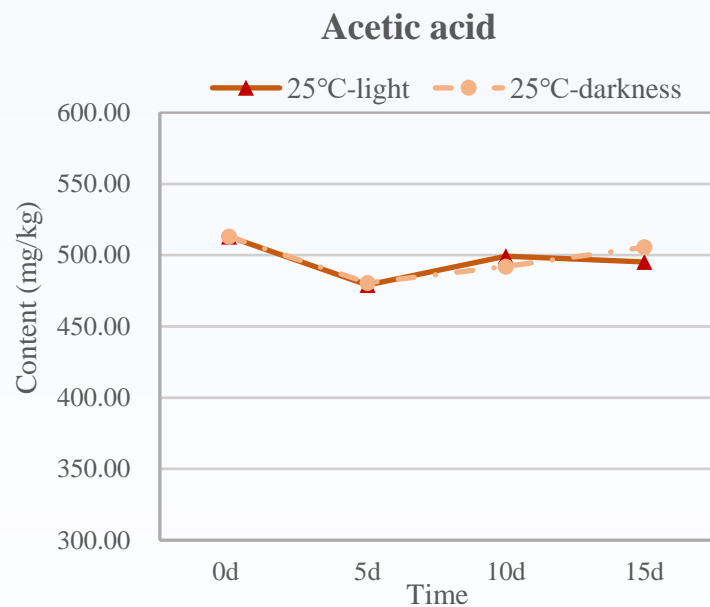
1. Near actual storage condition of e-liquid.
2. As the control of 25°C-light and 40°C-dark.

3. Methods

3.3 Analytical methods

	GC-FID	GC-MS
Pre-treatment	diluting the e-liquid to 0.1 g/mL with ethanol	direct injection
Instrument	Agilent 8860	Agilent 8860 - 5977B
Column	DB-WAX (30 m × 0.25 mm × 0.25 μm)	HP-5MS (30 m × 0.25 mm × 0.25 μm)
Injection temperature	240°C	240°C
programe	80°C (held for 1 min)-10°C/min-to 120°C (held for 1 min)-40°C/min-to 240°C (held for 6 min)	50°C (held for 1 min)-2°C/min-to 150°C-4°C/min-to 250°C (held for 10 min)
Flow rate of carrier gas	N ₂ at 1.2 mL/min	He at 1.2 mL/min
Injection mode	split	split
Split ratio	5:1	40:1
Injection volume	1.0 μL	1.0 μL
Mass range	—	33 - 450 Da
Analyte	acetic acid, octanal, and raspberry ketone	non-targeted analysis

4. Results - light exposure (25°C) in 15d



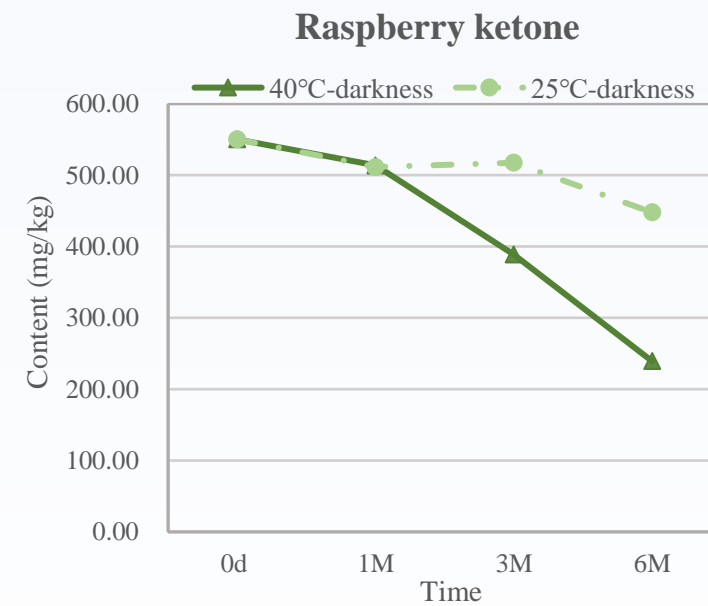
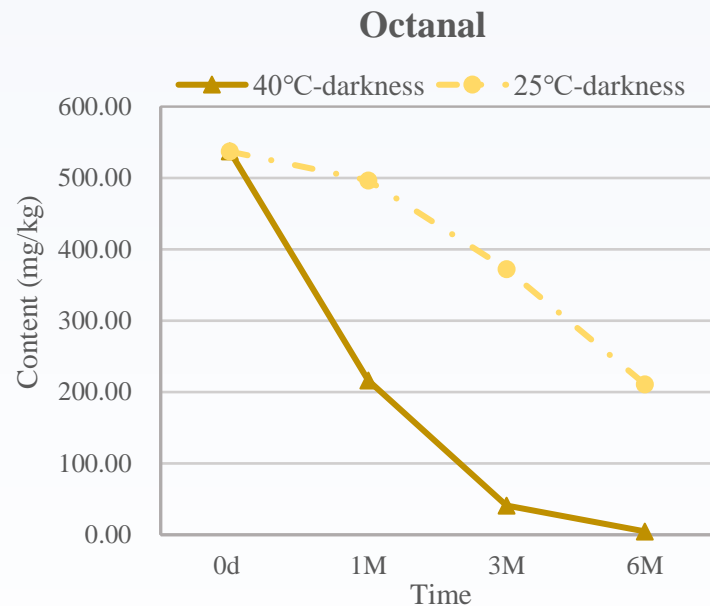
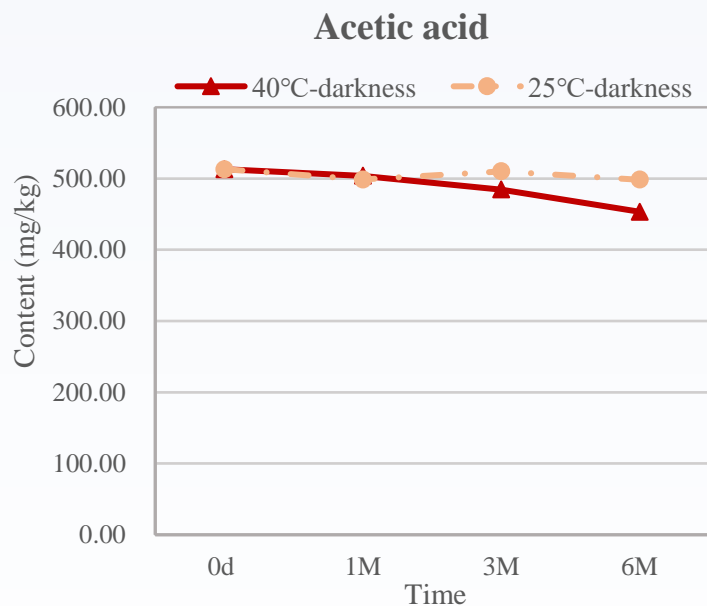
Acetic acid	0d	15d
25°C-light	100%	96.56%
25°C-darkness	100%	98.58%

Octanal	0d	15d
25°C-light	100%	93.70%
25°C-darkness	100%	93.80%

Raspberry ketone	0d	15d
25°C-light	100%	95.18%
25°C-darkness	100%	95.23%

Light has little effect on the three substances.

4. Results - high temperature exposure (darkness) in 6M



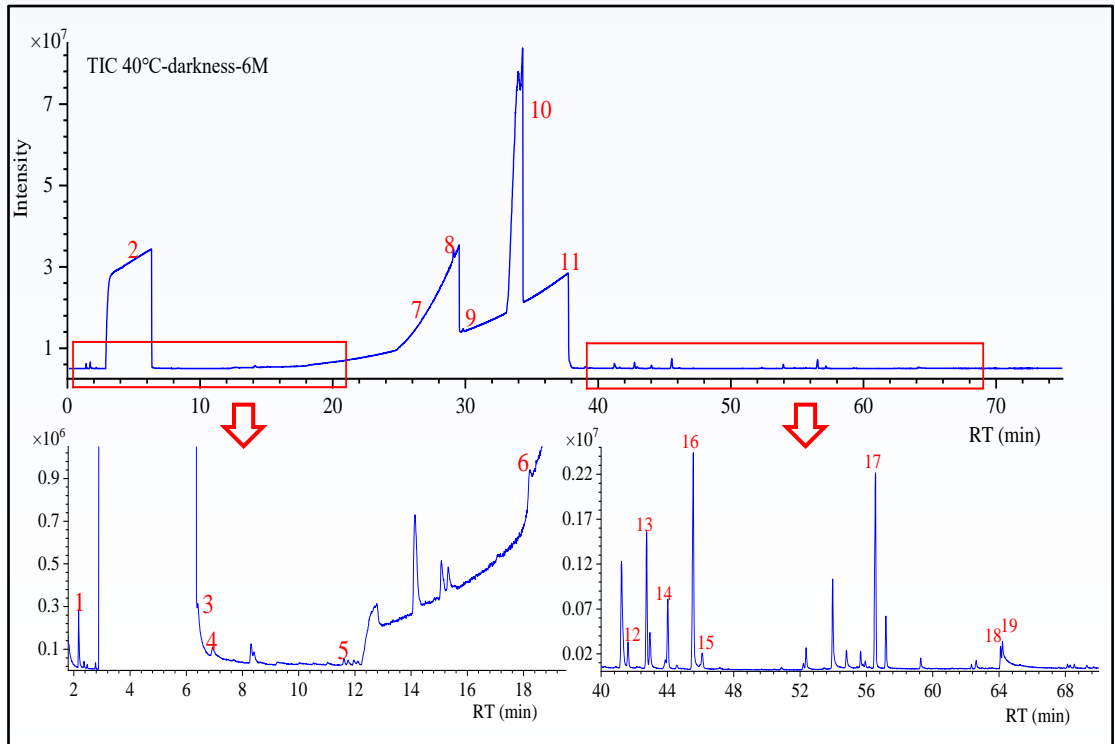
Acetic acid	0d	6M
darkness - 40°C	100%	88.38%
darkness - 25°C	100%	97.17%

Octanal	0d	6M
darkness - 40°C	100%	0.81%
darkness - 25°C	100%	39.26%

Raspberry ketone	0d	6M
darkness - 40°C	100%	43.54%
darkness - 25°C	100%	81.40%

High temperature may accelerate the decay of substances.

4. Results – TIC: 40°C-darkness for 6M



GC-MS analysis after storage for 6M at 40°C

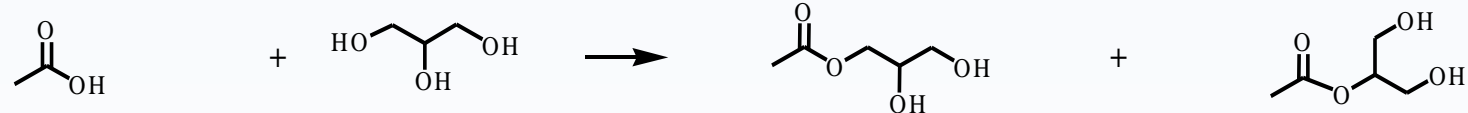
Peak	Substance	0d	6M
1	Acetic acid	0.040%	0.031%
2	PG	18.626%	19.773%
3	PG monoacetate	N	0.016%
5	Octanal	0.123%	0.001%
6	Monoacetin	N	0.034%
7	Benzoic acid	12.542%	12.845%
8	Octanal PG acetal	N	0.087%
9	Nicotine	10.909%	12.429%
10	VG	57.574%	54.526%
11	Octanal VG acetal	N	0.074%
12	Raspberry ketone	0.187%	0.076%
13	Raspberry ketone PG ketal	N	0.063%
14	Raspberry ketone VG ketal	N	0.045%
Total		100%	100%

4. Results – degradation pathways discussions

Acetic acid

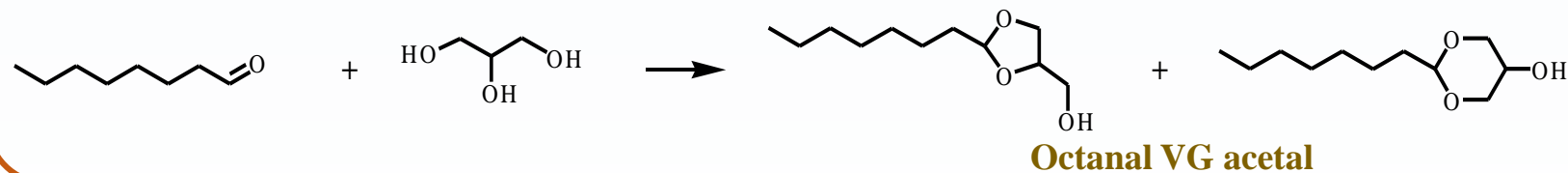


PG monoacetate

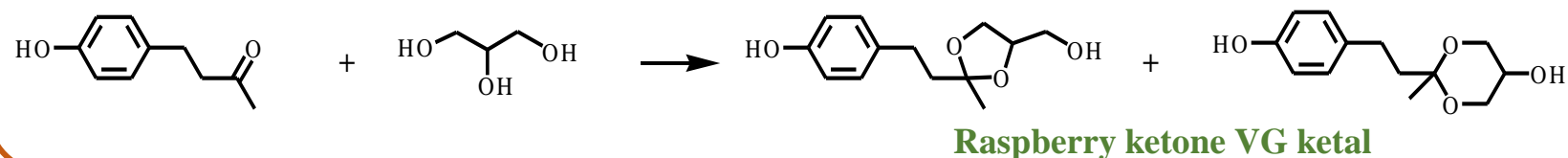
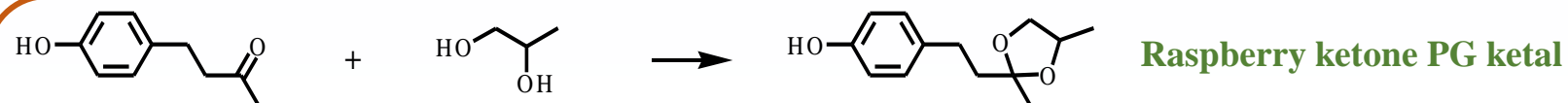


Monoacetin

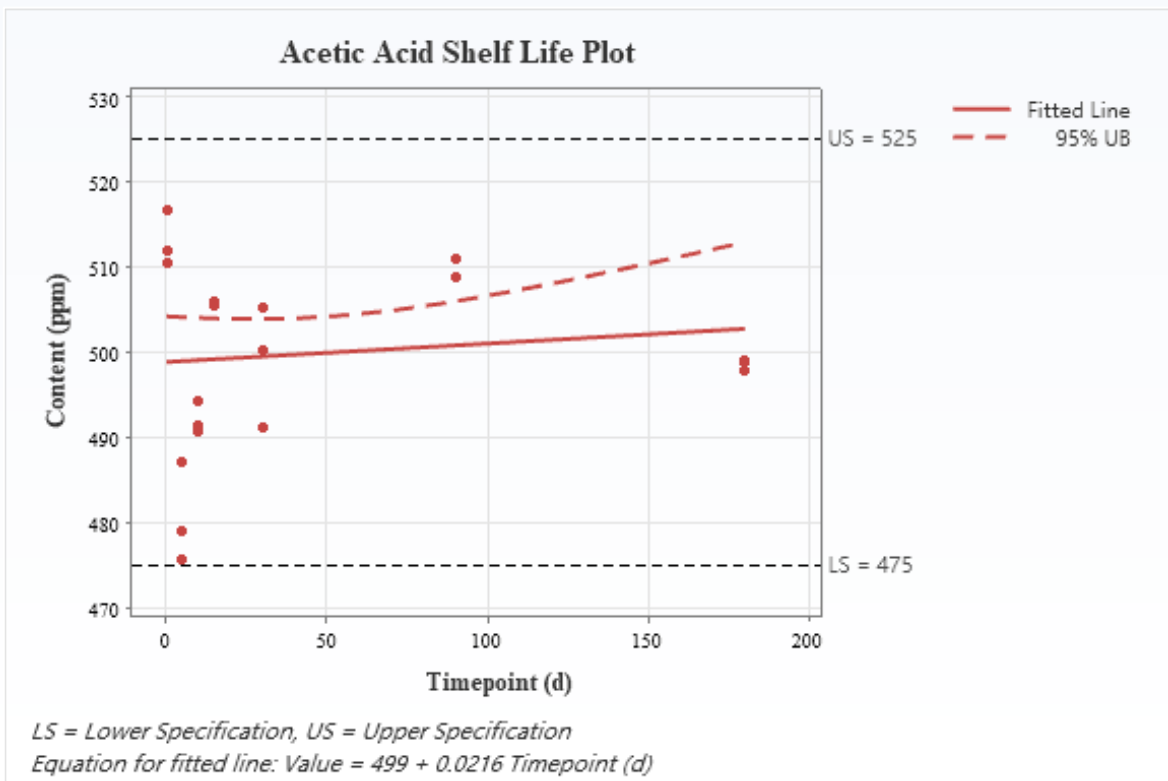
Octanal



Raspberry ketone

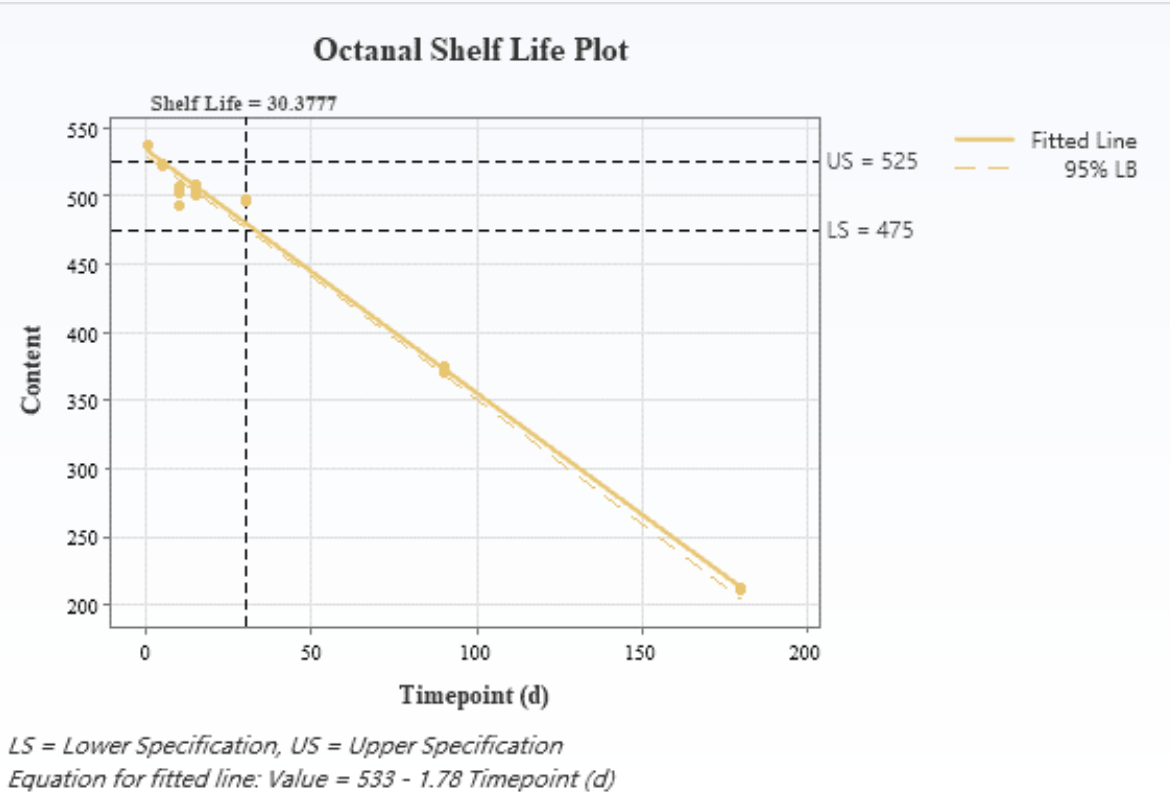


4. Results – linear regression analysis for predicting shelf life



Storage condition	25°C - darkness
Component	Acetic Acid
Fitted line	Content = 499 + 0.0216 Timepoint (d)
Shelf life	> 180 days

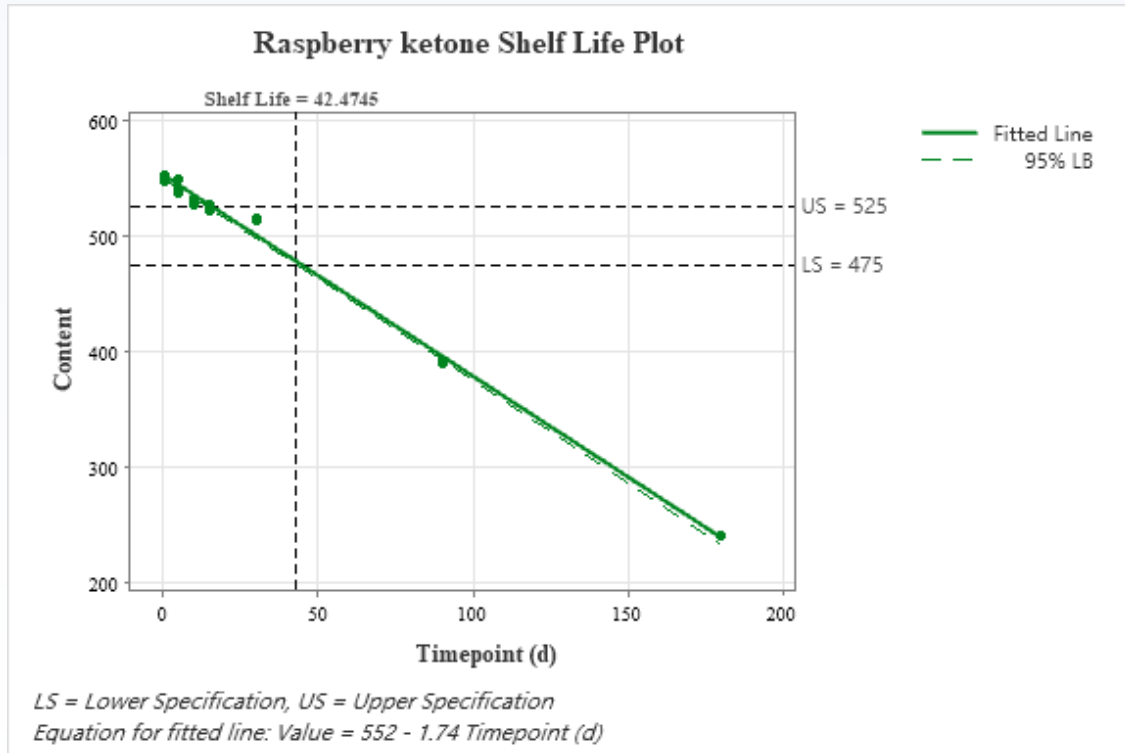
4. Results – linear regression analysis for predicting shelf life



Storage condition	25°C - darkness
Component	Octanal
Fitted line	Content = 533-1.78 Timepoint (d)
Shelf life	30 days

a loss of 1.78 ppm/day

4. Results – linear regression analysis for predicting shelf life



Storage condition	25°C - darkness
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Component	Raspberry ketone
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Fitted line	Content = 552-1.74 Timepoint (d)
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Shelf life	42 days
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a loss of 1.74 ppm/day

5. Conclusions

- The light had no effect on the stability of acetic acid, octanal and raspberry ketone in the simulated e-liquid.
- During the routine storage of simulated e-liquid, all three flavors interact with solvents, and the high temperature could accelerate the process of esterification, acetal, and ketal reaction.
- The results can provide a theoretical basis for the change of flavors in e-liquid, but the shelf life of e-liquid needs to be combined with sensory and component changes.



Thanks

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