Development Support Document
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2-Butene (Cis and Trans)

CAS Registry Number: 107-01-7

Cis-2-Butene

CAS Registry Number: 590-18-1

Trans-2-Butene

CAS Registry Number: 624-64-6

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TEXAS COMMISSION ON ENVIRONMENTAL QUALITY

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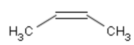
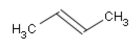
Table 1. Health- and Welfare-Based Values

Short-Term Values	Concentration	Notes
$^{acute}ESL$ [1 h] (HQ = 0.3)	10,000 µg/m^3 (4,500 ppb)	**Critical Effect:** Decreased body weight in female Wistar rats
Acute ReV (HQ = 1)	34,000 µg/m^3 (15,000 ppb) *	
$^{acute}ESL_{odor}$	4,800 µg/m^3 (2,100 ppb) * **Short-Term ESL for Air Permit Reviews**	50% detection threshold, gas-house odor
$^{acute}ESL_{veg}$	---	Insufficient data
Long-Term Values	**Concentration**	**Notes**
$^{chronic}ESL_{nonlinear(nc)}$ $^{chronic}ESL_{linear(nc)}$	---	The minimum database for development of a chronic ReV was not met.
Chronic ReV	---	
$^{chronic}ESL_{linear(c)}$ $^{chronic}ESL_{nonlinear(c)}$	---	No data found
$^{chronic}ESL_{veg}$	---	No data found

* Values that may be used for evaluation of air monitoring data

Abbreviations used: **HQ**, hazard quotient; **ppb**, parts per billion; **µg/m^3**, micrograms per cubic meter; **h**, hour; **ESL**, Effects Screening Level; **ReV**, Reference Value; **$^{acute}ESL$**, acute health-based ESL; **$^{acute}ESL_{odor}$**, acute odor-based ESL; **$^{acute}ESL_{veg}$**, acute vegetation-based ESL; **$^{chronic}ESL_{nonlinear(nc)}$**, chronic health-based ESL for nonlinear dose-response noncancer effects; **$^{chronic}ESL_{linear(nc)}$**, chronic health-based ESL for linear dose-response noncancer effects; **$^{chronic}ESL_{linear(c)}$**, chronic health-based ESL for linear dose-response cancer effect; **$^{chronic}ESL_{nonlinear(c)}$**, chronic health-based ESL for nonlinear dose-response cancer effect and **$^{chronic}ESL_{veg}$**, chronic vegetation-based ESL

Table 2. Chemical and Physical Data				
Parameter	**Value**	**Value**	**Value**	**Reference**
Name of Chemical	2-Butene (cis and trans) *	cis-2-Butene	trans-2-Butene	OECD 2004
Molecular Formula	$CH_3 HC{=}CH CH_3$	$CH_3 HC{=}CH CH_3$	$CH_3 HC{=}CH CH_3$	chemIDplus Lite
Chemical Structure				chemIDplus Lite
Molecular Weight	56.11	56.11	56.11	TRRP 2006
Physical State at 25°C	Gas	Gas	Gas	TRRP 2006
Color	Colorless	Colorless	Colorless	OECD 2004
Odor	Gas-house	Gas-house	Gas-house	Katz and Talbert 1930
CAS Registry Number	107-1-7	590-18-1	624-64-6	OECD 2004
Synonyms	Pseudobutylene; Pseudobutene; beta-Butylene; Butene, mixed -1- and -2- isomers; 1,2-Dimethylethylene; 2-Butylene; Butylene-2; Butylene, -2	cis-beta-Butylene; 2-Butene-cis; cis-Butene; cis-Dimethylethylene; cis-1,2-Dimethylethylene; cis-2-Butylene; cis-Butylene-2; cis-Butylene, -2; (Z)-But-2-ene; 2-Butene, (2Z)-; 2-Butene, (Z)-	trans-beta-Butylene; 2-Butene-trans; trans-Butene; trans-Dimethylethylene; trans-1,2-Dimethylethylene; trans-2-Butylene; trans-Butylene-2; trans-Butylene, -2; 2-Butene, (E)-; 2-Butene, (2E)-; (E)-But-2-ene	OECD 2004
Solubility in water (mg/L)	347.58	347.58	347.58	TRRP 2006
Log K_{ow}	2.37	2.37	2.37	TRRP 2006
Vapor Pressure (mm Hg)	1460.14	1460.14	1460.14	TRRP 2006
Relative Density (g/cm^3)	0.6213 to 0.6042	0.6213	0.6042	OECD 2004
Melting Point°C	-105.5 to -138.9	-138.9	-105.5	OECD 2004
Boiling Point°C	0.8 to 3.7	3.7	0.8	OECD 2004
Conversion Factors	1 ppb = 2.29 $\mu g/m^3$ 1$\mu g/m^3$ = 0.437 ppb	1 ppb = 2.29 $\mu g/m^3$ 1$\mu g/m^3$ = 0.437 ppb	1 ppb = 2.29 $\mu g/m^3$ 1$\mu g/m^3$ = 0.437 ppb	Toxicology Section

* Usually contains cis (70%) and trans (30%) forms

Chapter 2 Major Sources and Uses

The following information was obtained from the Organization for Economic Cooperation and Development (OECD 2004):

> Butenes are a component of natural gas and crude oil. Although butenes have been identified in natural environments, this has traditionally been associated with losses from petrogenic sources resulting from offgassing or venting (e.g. underwater or near-shore oil seepage). Trace levels of butenes can be identified in urban and suburban air arising from combustion of fossil fuels and losses from gas plants and refineries.

Cis- and trans-2-butene are used as solvents and cross-linking agents. They are used in the synthesis of or as a chemical intermediate for butadiene, sec-butanol, C4 and C5 derivatives, gasoline alkylate, and they are a component of liquefied petroleum gas (HSDB 2003). Estimated United States production of 2-butene was 18,990 million pounds (8,600 kilotons) in 2001 (SIAP 2004).

Chapter 3 Acute Evaluation

3.1 Health-Based Acute ReV and ^{acute}ESL

Acute toxicity values were not developed separately for cis- and trans-2-butene because no studies were available on the individual isomers, although there were studies on mixtures of cis- and trans-2-butene.

3.1.1 Physical/Chemical Properties and Key Studies

3.1.1.1 Physical/Chemical Properties

2-Butene is a flammable, colorless gas. The log K_{ow} (2.37), low water solubility (347.58 milligram per liter (mg/L)) and low molecular weight (56.11) indicate the potential for 2-butene to be absorbed via the lungs and widely distributed within the body. The lower explosive limit for the butenes category is greater than 8,000 ppm. Other physical/chemical properties of 2-butene can be found in Table 2.

3.1.1.2 Key Studies

This section is based on information on 2-butene obtained from OECD (2004) as well as a search of the literature since 2000. 2-Butene appears to be somewhat more narcotic than 1-butene; the former also appears to be a mucous membrane irritant and is reported by Drantz (Patty's 1982 in OECD 2004) to be a cardiac sensitizer. The following effects as reported in ACC (2001) have been observed in mice after exposure to cis-butene (96.18% pure) for 10 minutes:

- 172,000 ppm (17.2%) induced surgical anesthesia in mice within 10 minutes (Virtue 1950 in ACC 2001)
- 255,000 ppm (25.5%) produced respiratory arrest in mice (Virtue 1950 in ACC 2001)

The following effects as reported in ACC (2001) have been observed in mice after exposure to trans-butene (98.92% pure) for 10 minutes:

- 187,000 ppm (18.7%) induced surgical anesthesia in mice within 10 minutes (Virtue 1950 in ACC 2001)
- 211,000 ppm (21.1%) produced respiratory arrest in mice (Virtue 1950 in ACC 2001)

3.1.1.2.1 Rat Acute Study

In a study conducted by Arts (1992 in OECD 2004), rats were exposed for 4 hours (h) to 2-butene (approximately 50:50 mixture of cis- and trans- isomers) at a vapor concentration of 23.1 g/m^3 (approximately 10,000 ppm). After exposure, rats were removed from the chambers and returned to their individual living cages for 14 days of observation. Body weight was measured before study initiation and at post-exposure days 7 and 14. Rats were observed for clinical signs during exposure, shortly after exposure, and once daily during the observation period. After the observation period, rats were sacrificed, necropsied, and examined for gross pathological changes. No clinical signs were seen during the 14-day observation period. Normal growth also occurred during this period, and no abnormalities were observed at gross necropsy. The free-standing no observed adverse effect level (NOAEL) was 10,000 ppm. Arts (1992 in OECD 2004) concluded that the 4-h LC_{50} value of 2-butene was higher than 10,000 ppm.

3.1.1.2.2 Rat Repeated Dose Toxicity and Reproductive/Developmental Study

A combined repeated dose toxicity and reproductive/developmental toxicity test conducted in accordance with OECD Guideline 422 was performed by Waalkens-Brendsen and Arts (1992 in OECD 2004 and ACC 2001). Male and female Wistar rats, 12 rats per group, were exposed to concentrations of 0, 2,500, and 5,000 ppm 2-butene (cis and trans 95% purity) via inhalation 6 h/day; 7 days/week. Animals were exposed 2 weeks pre-mating, during mating, and during the gestation period up to and including day 19 for females. Pregnant females were exposed through gestation day (GD) 19; after which they were removed from the inhalation chambers, housed individually in the animal room, and allowed to litter normally and to rear pups to day 4 of lactation, when both dams and pups were sacrificed. Exposure of males was for the entire study (39-46 days).

A number of parameters and health effects were monitored and evaluated: observations of reaction to treatment, ill health or mortality; body weight and food consumption; hematology and clinical chemistry analyses; and microscopic examination of tissues. In addition, total litter size and number of pups of each sex, number of stillbirths, grossly malformed pups, if any, and pup body weight and organ weights were evaluated. Necropsies were performed on stillborns and pups dying during lactation. Macroscopic examinations were performed on these pups and all pups sacrificed on day 4 post-partum and any abnormalities were recorded. All parental (F_0) males and dams were examined macroscopically.

No mortality or treatment-related clinical signs were observed in F_0 animals. Male body weights were comparable in all groups, but mean body weight change was statistically significantly lower in the 1st and 4th week of exposure for the 2,500 ppm group and in the 1st week of exposure for the 5,000 ppm group. Female rats showed statistically significantly decreased mean body weight compared to controls at 7 and 14 days of exposure in the 5,000 ppm group and at 14 days from start of exposure in the 2,500 ppm group.

During gestation, all body weights were comparable in treated and control groups; on lactation day 1, body weight of 5,000 ppm dams was statistically significantly decreased. Body weight changes in dams were comparable to controls throughout the study. Food consumption in males was comparable to controls but food consumption by 5,000 ppm females was decreased during the first week of exposure. No other food consumption differences occurred during the study.

Mating was successful in 11/12 females in the control group and all females (12/12) in each treated group; precoital times were comparable. Female fecundity index was 73% (8/12), 75% (9/12), and 83% (10/12) in control, 2,500 ppm, and 5,000 ppm groups, respectively. Duration of pregnancy was comparable in all groups. One high dose female delivered 1 stillborn pup and 12 live pups while all other dams in all groups delivered live pups. Gestation and live birth indices were approximately 100% in all groups. No treatment-related increase in pre-implantation loss occurred. Post-implantation loss was slightly increased in the 5,000 ppm group but was within historical control limits, and the number of implantation sites in the control group was low. Total number of live births in exposed groups was slightly higher than controls. In the control and 2,500 ppm groups, one pup died between days 1 and 4 of lactation. Viability index was 97-100% and sex ratio of pups was similar in all groups. Mean body weight of pups was slightly but not statistically significantly lower in the 2,500 and 5,000 ppm groups. This might be explained by the higher number of pups in these groups compared to controls. No treatment related effects were noted in pups during lactation or at necropsy.

In conclusion, exposure to 2-butene at concentrations up to 5,000 ppm did not induce significant systemic toxicity in male rats exposed for 39-46 days, or in pregnant female rats exposed for 2 weeks pre-mating, through mating and gestation to day 19 (Waalkens-Brendsen and Arts, 1992 in OECD 2004).

For the first week of exposure, the shortest time period reported in the study, minimal body weight effects in female rats indicate 2,500 ppm was the NOAEL and 5,000 ppm was the lowest observed adverse effect level (LOAEL). There were decreases in mean body weight change in male rats at 2,500 ppm during the 1st week of exposure, but since male body weight was comparable to the control group, this effect in males was not considered adverse. Concentrations of 2-butene were determined with a total carbon analyzer using flame ionization detection chromatography, twice/h in each test atmosphere. Mean actual concentrations of 2-butene in test atmospheres were 0, 2,476 ± 68 ppm, and 5,009 ± 88 ppm. The mean analytical concentration of 2,476 ppm is used as the NOAEL.

3.1.2 Mode-of-Action (MOA) Analysis and Dose Metric

Adverse effects occurring at the lowest concentration are decreases in mean body weight in female rats. The mode of action (MOA) for these effects is unknown. Concentration and duration appear to play a role in 2-butene effects since exposure to 5,000 ppm produced decreased mean body weight at 7 and 14 days of exposure, whereas exposure to 2,500 ppm produced decreased mean body weight at 14 days.

In the toxicity study selected as the key study, data on the exposure concentration of the parent chemical are available. Since the MOA of the toxic response is not fully understood and data on other more specific dose metrics are not available (e.g. blood concentration of parent chemical, area under blood concentration curve of parent chemical, or putative metabolite concentrations in blood or target tissue), the exposure concentration of the parent chemical was used as the default dose metric.

3.1.3 Point of Departure (POD) for Key Study and Dosimetric Adjustments

The health effect that occurs at the earliest time period in the subacute study is a decrease in mean body weight in female rats after the 1st week of exposure (i.e., 7 days). The NOAEL was 2,476 ppm, since female rats showed statistically significantly decreased mean body weight at 7 and 14 days of exposure in the 5,009 ppm group. The rat study conducted by Arts (1992 in OECD 2004) was not used as the key study, because animals were only exposed to one concentration and information on how the study was conducted was not available.

3.1.3.1 Default Exposure Duration Adjustments

The 6-h exposure duration (C_1) was adjusted to a POD_{ADJ} of 1-h exposure duration (C_2) using Haber's Rule as modified by ten Berge (1986) (C_1^n x T_1 = C_2^n x T_2) with n = 3, where both concentration and duration play a role in toxicity:

$$POD_{ADJ} = C_2 = [(C_1)^3 \times (T_1 / T_2)]^{1/3}$$
$$= [(2{,}476\ ppm)^3 \times (6\ h/1\ h)]^{1/3}$$
$$= 4{,}499\ ppm$$

3.1.3.2 Default Dosimetry Adjustments from Animal-to-Human Exposure

2-Butene causes mild body weight changes which are likely to be systemic rather than point-of-entry respiratory effects. In addition, the physical/chemical parameters of 1-butene indicate the potential for 1-butene to be absorbed via the lungs and widely distributed within the body (Section 3.1.1.1). 2-Butene was therefore considered a Category 3 gas (USEPA 1994). For Category 3 gases, the default dosimetric adjustment from animal-to-human exposure is conducted using the following equation:

$$POD_{HEC} = POD_{ADJ} \times [(H_{b/g})_A / (H_{b/g})_H]$$

where:

$H_{b/g}$ = ratio of the blood:gas partition coefficient
A = animal
H = human

For 2-butene, the blood:gas partition coefficients for rat and human are unknown. Therefore, a default value of 1 is used for $(H_{b/g})_A / (H_{b/g})_H$. The $(H_{b/g})_A / (H_{b/g})_H$ is the regional gas dose ratio (RGDR) (USEPA 1994).

$$POD_{HEC} = POD_{ADJ} \times RGDR$$
$$= 4{,}499\ ppm \times 1 = 4{,}499\ ppm$$

3.1.4 Adjustments of the POD_{HEC}

Since the MOA by which 2-butene produces toxicity is not understood, the default for noncarcinogenic effects is to determine a POD and apply uncertainty factors (UFs) to derive a Reference Value (ReV) (i.e., assume a nonlinear MOA). The following UFs were applied to the POD_{HEC} of 4,499 ppm: 10 for intraspecies variability (UF_H), 3 for extrapolation from animals to humans (UF_A), and 10 for database uncertainty (UF_D), for a total UF = 300:

$$\text{acute ReV} = POD_{ADJ} / (UF_H \times UF_A \times UF_D)$$
$$= 4{,}499\ ppm / (10 \times 3 \times 10)$$
$$= 15.00\ ppm$$
$$= 15{,}000\ ppb$$

A UF_H of 10 was used to account for variation in sensitivity among the members of the human population. A UF_A of 3 was used because a default dosimetric adjustment from animal-to-human exposure was conducted which accounts for toxicokinetic differences but not toxicodynamic differences. A UF_D of 10 was used, because toxicity data is available for only one species. The quality of the rat study is high and the confidence in the acute database is medium.

3.1.5 Health-Based Acute ReV and ^{acute}ESL

The acute ReV value was rounded to two significant figures. The resulting 1-h acute ReV is 15,000 ppb (34,000 µg/m^3). The rounded acute ReV was then used to calculate the ^{acute}ESL. At the target hazard quotient (HQ) of 0.3, the ^{acute}ESL is 4,500 ppb (10,000 µg/m^3) (Table 3).

Table 3. Derivation of the Acute ReV and ^{acute}ESL	
Study	OECD Guideline 422 combined repeated-exposure, reproduction and screening study (Waalkens-Brendsen and Arts 1992 in OECD 2004)
Study population	Male and female Wistar rats (12/sex/concentration)
Study quality	High
Exposure methods	Exposures via inhalation at 0, 2,500 and 5,000 ppm (0, 2,476 ± 68 ppm, and 5,009 ± 88 ppm analytical)
Critical effects	NOAEL based on decreased body weight in female rats after 7 days of exposure
POD	2,476 ppm (NOAEL)
Exposure duration	6 h/day for 7 days
Extrapolation to 1 h	6 h to 1 hr (TCEQ 2006 with n = 3)
POD_{ADJ} (1 h)	4,499 ppm
POD_{HEC}	4,499 ppm (gas with systemic effects, based on default RGDR = 1.0)
Total uncertainty factors (UFs)	300
Interspecies UF	3
Intraspecies UF	10
LOAEL UF	Not applicable
Incomplete Database UF *Database Quality*	10 Medium
acute ReV [1 h] (HQ = 1)	**34,000 µg/m^3 (15,000 ppb)**
^{acute}ESL [1 h] (HQ = 0.3)	**10,000 µg/m^3 (4,500 ppb)**

3.1.6 Comparison of ^{acute}ESL to Generic ESL

When a subacute study is used to derive a 1-h ^{acute}ESL, Section 3.2.3 of the ESL guidelines (TCEQ 2006) suggests a generic ESL be derived using approaches in Section 3.6 for comparison to ensure the derived value is not overly conservative. The Threshold of Concern (TOC) approach utilizes the lowest reported inhaled concentrations at which fifty percent of the study specimens die after exposure (LC_{50}). Arts (1992 in OECD 2004) concluded that the 4-h LC_{50} value of 2-butene was higher than 10,000 ppm, which would classify 2-butene as a TOC Category 5 gas and the corresponding generic ESL would be 1000 µg/m^3 (Table 3-3 of the ESL guidelines (TCEQ 2006)). Therefore, the 1-h $^{acute}ESL$ of 10,000 µg/m^3 (4,500 ppb) based on the subacute study is higher than the generic ESL for a Category 5 gas. This provides confidence that the derived value is not overly conservative.

3.2. Welfare-Based Acute ESLs

3.2.1 Odor Perception

Katz and Talbert (1930 as reported in van Gemert 2003) reported 2-butene to have a "gas-house" odor. The 50% odor detection threshold is 4,800 µg/m^3 (2,100 ppb) (Katz and Talbert 1930 in van Gemert 2003). Katz and Talbert (1930) meet the criteria for acceptable odor threshold measurement techniques developed by the American Industrial Hygiene Association and USEPA as discussed in TCEQ (2006), so the $^{acute}ESL_{odor}$ for 2-butene is 4,800 µg/m^3 (2,100 ppb). Since odor is a concentration-dependent effect, the same 1-h $^{acute}ESL_{odor}$ is assigned to all averaging times.

Information on 50% odor detection thresholds for cis- and trans-2-butene individually from an approved odor source is not available, although Mullins (1955 in van Gemert 2003) reported a recognition odor threshold of 28.5 mg/m^3 for cis-2-butene and 2,700 mg/m^3 for trans-2-butene. The $^{acute}ESL_{odor}$ of 4,800 µg/m^3 (2,100 ppb) for 2-butene, a mixture of cis- and trans-2-butene, will be used for both the cis- and trans-2-butene isomers.

3.2.2 Vegetation Effects

Haagen-Smit et al. (1952) conducted a screening study on the effects of cis- and trans-2-butene on spinach (*Spinacia oleracea*), endive (*Cichorium endivia*), beets (*Beta vulgaris*), oats (*Avena sativa*), and alfalfa (*Medicago sativa*). Fumigations in this study were conducted at cis- or trans-butene concentrations of 4 ppm in combination with an "ozone-like" mixture of 0.24 ppm aldehyde, 0.04 ppm acid, and 0.13 ppm peroxide (calculated as O_3) for an exposure duration of 5 h. No damage was observed as a result of exposure to 4 ppm cis-2-butene and an "ozone-like" mixture. No damage was observed as a result of exposure to 4 ppm trans-2-butene and an "ozone-like" mixture. Since the NOAELs for vegetative effects were above odor-based concentrations and the Haagen-Smit et al (1952) study did not identify a threshold effect level or treat plants with pure cis- and trans-2-butene, an $^{acute}ESL_{veg}$ was not developed (TCEQ 2006).

3.3. Short-Term ESL and Values for Air Monitoring Evaluation

The acute evaluation resulted in the derivation of the following values:

- acute ReV = 34,000 µg/m^3 (15,000 ppb)
- $^{acute}ESL$ = 10,000 µg/m^3 (4,500 ppb)
- $^{acute}ESL_{odor}$ = 4,800 µg/m^3 (2,100 ppb)

The short-term ESL for air permit evaluations is the $^{acute}ESL_{odor}$ of 4,800 µg/m^3 (2,100 ppb) as it is lower than the $^{acute}ESL$ of 10,000 µg/m^3 (4,500 ppb) (Table 1). For the evaluation of ambient air monitoring data, the $^{acute}ESL_{odor}$ of 4,800 µg/m^3 (2,100 ppb) is lower than the acute ReV of 34,000 µg/m^3 (15,000 ppb) (Table 1), although both values may be used for the evaluation of air data. The ^{acute}ESL (HQ = 0.3) is not used to evaluate ambient air monitoring data.

Chapter 4 Chronic Evaluation

4.1 Noncarcinogenic Potential

No studies were available describing the potential chronic toxicity of 2-butene. According to the ESL guidelines, if the minimum database requirements are not met, then a chronic ReV and ESL are not developed (TCEQ 2006).

4.2 Carcinogenic Potential

There are no human or animal studies indicating that 2-butene has carcinogenic potential, so a chronic carcinogenic value was not developed. There are data from *in vitro* mutagenity assays which indicate 2-butene is not mutagenic.

4.2.1 *In Vitro* Mutagenicity

The following *in vitro* assays, which indicate that 2-butene is non-mutagenic and non-clastogenic, have been conducted on 2-butene:

- *Salmonella typhimurium* strains TA98, TA100, TA1535 and TA1537 with and without metabolic activation. 2-Butene was found to be non-mutagenic (Thompson 1992 in OECD 2004).
- Mutagenic assays in *E. coli* or in any of the Ames strains tested with or without metabolic activation (Araki et al. 1994 in OECD 2004). 2-Butene was found to be non-mutagenic.
- A chromosome aberration study in accordance with OECD guideline 473 and EC Directive 84/449/EEC, B10 using rat lymphocytes with and without S9 metabolic activation mix. 2-Butene-induced steep dose-related decreases in mitotic indices ± S9; especially toxic to lymphocytes at 80% in +S9 20 h harvest group. However, 2-butene did not induce significant dose-related increases in frequency of structural chromosome aberrations or polyploid cells at any concentration level at any harvest period ± S9. 2-Butene was not clastogenic to rat lymphocytes *in vitro* (Wright 1992 in OECD 2004).

4.2.2 *In Vivo* Mutagenicity

No *in vivo* genetic toxicity studies have been conducted with 2-butene.

4.3. Welfare-Based Chronic ESL

No data were found regarding long-term vegetative effects.

4.4 Long-Term ESL and Values for Air Monitoring Evaluation

No long-term values were derived because no data were found.

Chapter 5. References

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