OFFICE OF CHEMICAL SAFETY AND POLLUTION PREVENTION

WASHINGTON, D.C. 20460

October 22, 2024

MEMORANDUM

SUBJECT: IN-11401; Various Fragrance Components. Human Health Risk Assessment and Ecological Effects Assessment to Support Inert Ingredient Approval for use in Pesticide Formulations

PC Code: Multiple (See Section III)
Decision No.: 560320
Petition No.: IN-11401

CAS No.: Multiple (See Section III)
Registration No.: N/A
Regulatory Action: Addition to inert ingredient list

FROM: David Lieu, Chemist
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TO: Kerry Leifer, Branch Chief
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1. EXECUTIVE SUMMARY

In February 2020, Innovative Reform Group (IRG), on behalf of The Clorox Company, submitted a petition (IN-11401) to the Environmental Protection Agency (EPA or the Agency) requesting an exemption from the requirement of tolerance for various fragrances (CAS Reg. No. multiple) as inert ingredients for use under 40 CFR § 180.940(a) in antimicrobial pesticide formulations used on food contact surfaces in public eating places, dairy processing equipment, and food processing equipment and utensils with end-use concentration not to exceed 33 ppm.

Although there is generally a lack of chemical-specific animal toxicity data for these fragrances, predictive toxicology indicates low potential for carcinogenicity and the expected use concentration is low. Therefore, the Agency assessed these fragrance components via the Threshold of Toxicological Concern (TTC) approach as outlined by the European Food Safety Authority (EFSA) in their 2019 guidance document on the use of TTC in food safety assessment.

TTCs are derived from a conservative and rigorous approach developed by Munro and Kroes to establish generic threshold values for human exposure at which a very low probability of adverse effects is likely. By comparing a range of compounds by Cramer Class (classes I, II, and III) and NOEL (no-observed-effect-level), fifth percentile NOELs were established for each Cramer Class as “Human Exposure Thresholds”. These values were 3, 0.91 and 0.15 mg/kg/day for classes I, II and III, respectively. All fragrances in this document are in Cramer class II; therefore, this assessment uses the NOEL of 0.91 mg/kg/day as the point of departure for all exposure scenarios assessed (chronic dietary, incidental oral, dermal and inhalation exposures).

The dietary assessment for food contact sanitizer solutions calculated the Daily Dietary Dose (DDD) and the Estimated Daily Intake (EDI). The assessment considered: application rates, residual solution or quantity of solution remaining on the treated surface without rinsing with potable water, surface area of the treated surface which comes into contact with food, pesticide migration fraction, and body weight. These assumptions are based on FDA guidelines (1993).

The dietary assessment for food contact sanitizer solutions showed that children 1-2 years old would be the highest exposed subgroup (58% of the cPAD). The general U.S. population resulted in 21% of the cPAD. As these percent cPADs do not exceed 100%, they are not of concern.

Combined short-term aggregated food, water, and residential pesticidal exposures result in MOEs of 455 for both adult males and females and 168 for children. As the level of concern is for MOEs that are lower than 100, these MOEs are not of concern.

Although the proposed use for these fragrances as an inert ingredient in antimicrobial products is expected for residential use, it is possible that these products could be used in commercial

settings. However, exposures in commercial settings have already been incorporated into the FDA model used. Therefore, an additional occupational exposure assessment is not needed.

Environmental fate and ecological effects are expected to be minimal as only indoor exposure scenarios are anticipated.

Taking into consideration all available information for the fragrances listed in this document, EPA has determined that there is a reasonable certainty that no harm to the general population or any population subgroup, including infants and children, will result from aggregate exposure to residues of these fragrances. Therefore, the establishment of an exemption from the requirement of a tolerance under 40 CFR 180.940 for residues of the listed fragrances when used as inert ingredients in pesticide formulations at concentrations not to exceed 33 ppm of the formulation can be considered assessed as safe under section 408 of the FFDCA.

2. BACKGROUND

In February 2020, Innovative Reform Group, on behalf of The Clorox Company, submitted a petition (IN-11401) requesting an exemption from the requirement of a tolerance for various chemicals (CAS Reg. No. multiple, listed in section III) as inert ingredients under 40 CFR § 180.940(a) for use as fragrance components in antimicrobial pesticide formulations for use on food contact surfaces in public eating places, dairy processing equipment, and food processing equipment and utensils at end-use concentrations not to exceed 33 parts per million (ppm). EPA published the notice of filing (NOF) for this petition in the Federal Register on June 2, 2021 (86 FR 29229). No substantive comments were received in response to this notice.

Although there generally is limited animal toxicity data for the listed fragrances, there is a predicted low carcinogenic potential for these substances and these fragrances will be used at low concentrations (≤33ppm) in pesticide formulations. Therefore, the Agency will be assessing these fragrance components via the Threshold of Toxicological Concern (TTC) approach as outlined by the European Food Safety Authority (EFSA) in their 2019 guidance document on the use of TTC in food safety assessment. This approach relies on the most recent evaluation of the literature on TTC as reviewed by EFSA and the World Health Organization (WHO) in 2016. Information regarding the database of studies and chemicals used to derive TTCs are reviewed therein. The TTC approach has been used by the Joint Expert Committee on Food Additives of the U.N.'s Food and Agriculture Organization and the World Health Organization, the former Scientific Committee on Food of the European Commission and by the European Medicines Agency, and EFSA. Details about how the TTC method is applied can be found in section IV of this document.

This document provides an assessment of the risk to human health and the environment for the listed chemicals when used as inert ingredients (fragrance) in food-use antimicrobial

pesticide formulations. Information from the submitter's petition is referenced in this assessment.

3. INERT INGREDIENT PROFILE

The Clorox Company proposes amending the 40 CFR 180.940(a) to include the following fragrance components: For more details, including molecular formulas and simplified molecular-input line-entry system (SMILES) for each of these chemicals, please see Appendix III.

Table 1. List of Inert Ingredients in Petition

Chemical Name in EPA Pesticide Databases	CAS Reg. No.	Chemical name Provided in Petition	Current Inert Ingredient Approval Status
Acetoin	513-86-0	Acetoin	Fragrance Use
4-acetyl-6-t-butyl-1,1-dimethylindan	13171-00-1	4-acetyl-6-t-butyl-1,1-dimethylindan	Fragrance Use
Allyl cinnamate	1866-31-5	Allyl cinnamate	Fragrance Use
Allyl heptanoate	142-19-8	Allyl heptanoate	Fragrance Use
Allyl hexanoate	123-68-2	Allyl hexanoate	Fragrance Use
Allyl propionate	2408-20-0	Allyl propionate	Fragrance Use
Heptanal, 2-(phenlymethylene)-	122-40-7	alpha-Amylcinnamaldehyde	Nonfood Use/Fragrance Use
.alpha.-Butylcinnamaldehyde	7492-44-6	alpha-Butylcinnamaldehyde	Fragrance Use
2-secButylcyclohexanone	14765-30-1	2-sec-butylcyclohexanone	Fragrance Use
Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-, (1R, 4R)-	464-49-3	d-Camphor	Nonfood Use/Fragrance Use
Camphor	21368-68-3	dl-Camphor	Food (180.920) no more than 5%w/w
Cajeput oil (Melaleuca leucadendron L.)	8008-98-8	Cajeput oil (Melaleuca leucadendron L.)	Fragrance Use
Cardamom (Elettaria cardamomum (L.) Maton)	85940-32-5	Cardamom (Elettaria cardamomum (L.) Maton)	Fragrance Use
Cardamom seed oil (Elettaria cardamomum (L.) Maton)	8000-66-6	Cardamom seed oil (Elettaria cardamomum (L.) Maton)	Fragrance Use
7-Oxabicyclo(2.2.1.)heptane, 1-methyl-4-(1-methylethyl)-	470-67-7	1,4-Cineole	Nonfood Use/Fragrance Use
Tetrahydro-6-(3-pentenyl)-2H-pyran-2-one	32764-98-0	8-Decen-5-olide	Fragrance Use
3,4-Dimethyl-1,2-cyclopentadione	13494-06-9	3,4-Dimethyl-1,2-cyclopentadione	Fragrance Use
Diisobutyl ketone	108-83-8	2,6-Dimethyl-4-heptanone	Nonfood Use/Fragrance Use
2,5-Dimethylpyrazine	123-32-0	2,5-Dimethylpyrazine	Fragrance Use
2,6-Dimethylpyrazine	108-50-9	2,6-Dimethylpyrazine	Fragrance Use
6,10-Dimethylundeca-5,9-dien-2-one	689-67-8	6,10-Dimethyl-5,9-undecadien-2-one	Fragrance Use
1-Hexanol, 2-ethyl-	104-76-7	2-Ethyl-1-hexanol	Food (180.910 + 180.920 + 180.930)/Nonfood Use/Fragrance Use

Ethyl maltol	4940-11-8	Ethyl maltol	Food (180.910 + 180.930)/Nonfood Use/Fragrance Use
2-Ethyl-3-methylpyrazine	15707-23-0	2-Ethyl-3-methylpyrazine	Fragrance Use
Ethylvanillin	121-32-4	Ethyl vanillin	Nonfood Use/Fragrance Use
p-Menthane, 1,8-epoxy-	470-82-6	Eucalyptol	Nonfood Use/Fragrance Use
Eucalyptus oil	8000-48-4	Eucalyptus oil (Eucalyptus globulus Labill)	Nonfood Use/Fragrance Use
Fenchone	4695-62-9	d-Fenchone	Fragrance Use
Methyl n-amyl ketone	110-43-0	2-Heptanone	Food (180.910 + 180.930)/Nonfood Use/Fragrance Use
3-Heptanone	106-35-4	3-Heptanone	Fragrance Use
2,3-Hexanedione	3848-24-6	2,3-Hexanedione	Fragrance Use
alpha-Hexylcinnamaldehyde	101-86-0	alpha-Hexylcinnamaldehyde	Nonfood Use/Fragrance Use
4-Hydroxy-2,5-dimethyl-3(2H)-furanone	3658-77-3	4-Hydroxy-2,5-dimethyl-3(2H)-furanone	Fragrance Use
Phenylethyl isoamyl ether	56011-02-0	Isoamyl phenethyl ether	Fragrance Use
2-Isobutyl-3-methoxypyrazine	24683-00-9	2-Isobutyl-3-methoxypyrazine	Fragrance Use
alpha-Isobutylphenethyl alcohol	7779-78-4	alpha-Isobutylphenethyl alcohol	Fragrance Use
Isojasmone	11050-62-7	Isojasmone	Fragrance Use
d,l-Isomenthone	491-07-6	d,l-Isomenthone	Fragrance Use
2-Isopropyl-4-methylthiazole	15679-13-7	2-Isopropyl-4-methylthiazole	Fragrance Use
Linalool oxide	60047-17-8	Linalool oxide	No current pesticide use
(Z)-Linalool oxide	5989-33-3	Linalool oxide	No current pesticide use
(E)-Linalool oxide	34995-77-2	Linalool oxide	No current pesticide use
4H-Pyran-4-one, 3-hydroxy-2-methyl-	118-71-8	Maltol	Nonfood Use/Fragrance Use
Maltyl isobutyrate	65416-14-0	Maltyl isobutyrate	Fragrance Use
p-Mentha-8-thiol-3-one	38462-22-5	p-Mentha-8-thiol-3-one	Fragrance Use
1-p-Menthene-8-thiol	71159-90-5	1-p-Menthene-8-thiol	Fragrance Use
p-Menthan-3-one	10458-14-7	Menthone	No current pesticide use
2-Methoxy-3-(1-methylpropyl)pyrazine	24168-70-5	2-Methoxy-3-(1-methylpropyl)pyrazine	Fragrance Use
3-Methyl-1-cyclopentadecanone	541-91-3	3-Methyl-1-cyclopentadecanone	Fragrance Use
Methylcyclopentenolone	80-71-7	Methylcyclopentenolone	Fragrance Use
Cyclopentaneacetai acid, 3-oxo-2-pentyl-, methyl ester	24851-98-7	Methyl dihydrojasmonate	Nonfood Use/Fragrance Use
6-Methyl-3,5-heptadien-2-one	1604-28-0	6-Methyl-3,5-heptadien-2-one	Fragrance Use
6-Methyl-5-hepten-2-one	110-93-0	6-Methyl-5-hepten-2-one	Fragrance Use
3-Methyl-2-(n-pentanyl)-2-cyclopenten-1-one	1128-08-1	3-Methyl-2-(n-pentanyl)-2-cyclopenten-1-one	Fragrance Use

3-Methyl-2-(2-pentenyl)-2-cyclopenten-1-one, (Z)-	488-10-8	3-Methyl-2-(2-pentenyl)-2-cyclopenten-1-one	Fragrance Use
3-Methyl-2-(2E)-2-penten-1-yl-2-cyclopenten-1-one	6261-18-3	3-Methyl-2-(2-pentenyl)-2-cyclopenten-1-one	No current pesticide use
Methyl phenethyl ether	3558-60-9	Methyl phenethyl ether	Fragrance Use
5-Methyl-2-phenyl-2-hexenal	21834-92-4	5-Methyl-2-phenyl-2-hexenal	Fragrance Use
2-Methyl-4-propyl-1,3-oxathiane	67715-80-4	2-Methyl-4-propyl-1,3-oxathiane	Fragrance Use
2-Methylpyrazine	109-08-0	2-Methylpyrazine	Fragrance Use
5-Methyl-2-thiophenecarboxyaldehyde	13679-70-4	5-Methyl-2-thiophenecarboxyaldehyde	Fragrance Use
Cyclopropanemethanol, 1-methyl-2-[(1,2,2-trimethylbicyclo[3.1.0]hex-3-yl)methyl]-	198404-98-7	(1-Methyl-2-(1,2,2-trimethylbicyclo[3.1.0]hex-3-ylmethyl)cyclopropyl)methanol	Fragrance Use
3-Methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)pent-4-en-2-ol	67801-20-1	3-Methyl-5-(2,2,3-trimethylcyclopent-3-en-1-yl)pent-4-en-2-ol	Fragrance Use
Nerol oxide	1786-08-9	Nerol oxide	Fragrance Use
2-Nonanone	821-55-6	2-Nonanone	Fragrance Use
Nootkatone	4674-50-4	Nootkatone	Fragrance Use
2-Octanone	111-13-7	2-Octanone	Fragrance Use
Ethyl amyl ketone	106-68-3	3-Octanone	Nonfood Use/Fragrance Use
1-Octen-3-ol	3391-86-4	1-Octen-3-ol	Nonfood Use/Fragrance Use
Oils, rosemary	8000-25-7	Rosemary oil (Rosemarinus officinalis L.)	Nonfood Use/Fragrance Use
Oils, sage	8022-56-8	Sage oil, Spanish (Salvia lavandulaefolia Vahl.)	Nonfood Use/Fragrance Use
Origanum oil, Spanish	8007-11-2	Origanum oil	Nonfood Use/Fragrance Use
1,3-Benzodioxole-5-carboxaldehyde	120-57-0	Piperonal	Nonfood Use/Fragrance Use
Piperonyl acetate	326-61-4	Piperonyl acetate	Fragrance Use
Rue oil (Ruta graveolens L.)	8014-29-7	Rue oil (Ruta graveolens L.)	Fragrance Use
Tetrahydro-4-methyl-2-(2-methylpropen-1-yl)pyran	16409-43-1	Tetrahydro-4-methyl-2-(2-methylpropen-1-yl)pyran	Fragrance Use
Theaspirane	36431-72-8	Theaspirane	Fragrance Use
2-Tridecanone	593-08-8	2-Tridecanone	Fragrance Use
2-Undecanone	112-12-9	2-Undecanone	Nonfood Use/Fragrance Use

In the case of the fragrance components listed above, most of these chemicals already have EPA approval for nonfood use in pesticide formulations. Also, many of these substances have been approved for use as a flavoring substance in food under 21 CFR 172.515 or 182.60 by the U.S. Food and Drug Administration (FDA). Additionally, the fragrance components listed above have all been evaluated and approved for use as food flavoring agents by the Joint Food and Agricultural Organization of the United Nations/World Health Organization Expert Committee

on Food Additives (JECFA) as part of their assessment of more than 2,300 food flavoring substances. Toxicological profiles on each are available via the links to the relevant JECFA summary in Appendix II.

4. HAZARD CHARACTERIZATION

4.1. Toxicology Summary

There is limited animal toxicity information available for the fragrances listed in section III. The Joint FAO/WHO Expert Committee on Food Additives (JECFA) reviewed available toxicity information for these chemicals and structurally related compounds in a series of reports, as described in Appendix II. Information from these reports as well as predictive toxicology using the OECD QSAR Toolbox was used to confirm that the fragrances listed in section III have low carcinogenic potential and are thus good candidates for the application of the TTC method. For most chemicals, no alerts were found using the carcinogenicity (genotox and nongenotox) alerts by the ISS tool in the OECD QSAR Toolbox (see Appendix III). For 17 chemicals (CAS Reg. Nos. 120-57-0; 326-61-4; 118-71-8; 3658-77-3; 65416-14-0; 1128-08-1; 488-10-8; 6261-18-3; 11050-62-7; 21834-92-4; 1604-28-0; 4674-50-4; 80-71-7; 13679-70-4; 121-32-4; 67801-20-1; 104-76-7), carcinogenicity alerts were found with the QSAR Toolbox. However, JECFA has concluded in its reports, and EPA concurs, that these 17 chemicals all have a low carcinogenic potential, based on *in vitro* and/or *in vivo* genotoxicity studies available on the chemical or structurally related chemicals (see Appendix II). Therefore, the TTC method can be applied to all fragrances listed in section III.

Munro (1996) developed TTC values for non-cancer effects which were based on analyses of NOAELs from repeated dose toxicity data for chemicals separated into three structural classes using the Cramer (1978) decision scheme. A TTC value was calculated from the respective distribution of NOELs for each of the 3 Cramer structural classes, using a database of 613 chemicals with 2941 NOELs. These substances represent a range of industrial chemicals, pharmaceuticals, food chemicals and environmental, agricultural and consumer chemicals likely to be encountered in commerce with good supporting toxicological data, yielding 137, 28 and 448 chemicals in Cramer class I, II and III, respectively. For each of the 613 chemicals, the most conservative NOEL was selected, based on the most sensitive species, sex and endpoint. The fifth percentile NOEL (in mg/kg bw/day) was calculated for each structural class as “Human Exposure Thresholds”. These values were 3, 0.91 and 0.15 mg/kg/day for classes I, II and III, respectively.

The TTC values for Cramer structural classes derived by Munro in 1996 have been supported by all subsequent analyses of additional databases (providing that the 5th percentile NOEL/NOAEL is converted to a TTC value using the same 100-fold safety factor). Blackburn (2005) analyzed a database of 145 chemicals found in personal and household products; Bernauer (2008) analyzed reproductive and developmental toxicity data for 91 chemicals assessed for oral toxicity under REACH; Brown (2009) analyzed data for 100 active pesticides and 15 pesticide

metabolites and concluded that the TTC values are valid; Pinalli (2011) analyzed the TDIs for 232 food contact materials in relation to the TTC and found that the distribution of recalculated NOAELs was similar to that reported by Munro; Tluczkiewicz (2011) analyzed the RepDose database of 521 chemicals, using dose levels expressed on a molar basis making direct comparison difficult, but the distribution of NOAELs, the overlap between Cramer classes and the TTC values were comparable to Munro; van Ravenzwaay (2011) analyzed data for pre-natal toxicity using NOAELs for maternal and developmental toxicity and found 5th percentile values higher (maternal NOAELs = 4 mg/kg/day, developmental NOAELs = 5 mg/kg/day) than those used by Munro (NOEL = 3 mg/kg/day); Kalkhof (2012) analyzed NOAELs from subacute and subchronic studies (with adjustment for duration of study) on 813 different chemicals and found TTC values for Cramer classes I, II and III similar to those of Munro; Laufersweiler (2012) analyzed reproductive and developmental toxicity data for 283 chemicals and generated TTC values 2-3 times higher than those of Munro. Feigenbaum (2015) assessed the reliability of the TTC approach using 328 pesticides that had been fully evaluated by the EU and by EFSA and concluded that the respective TTC values are protective, even for these biologically active substances.

4.2. Toxicity Endpoint Selection

As outlined in section IV, fifth percentile NOELs established by Munro are 3, 0.91 and 0.15 mg/kg/day for Cramer classes I, II and III, respectively. In the case of the fragrance components listed above, they are all in the Cramer Class II category, which is defined as less innocuous than substances in Class I, but no positive indication of toxic potential. Therefore, the 5th percentile NOEL value of 0.91 mg/kg/day is selected as the point of departure (POD) for all exposure scenarios, as described in Table 2 below.

The OECD Toolbox outputs are provided in Appendix III. Multiple of the OECD Toolbox outputs suggested Cramer classes other than "II". However, all chemicals in this document were ultimately classified as Cramer class II. Please see explanations and justifications in Appendix IV.

Table 2. Summary of Toxicological Doses and Endpoints for Various Fragrances for Use in Human Health Risk Assessments.

Exposure/ Scenario	POD	Uncertainty/FQPA Safety Factors	RfD, PAD, LOC for Risk Assessment	Study and Toxicological Effects
Acute Dietary (All Populations)	Not selected. No appropriate toxicological endpoint attributable to a single exposure was identified.			
Chronic Dietary (All Populations)	5th percentile NOEL = 0.91 mg/kg/day	UFA =10X UFH =10X FQPA= 1X Total UF=100	cRfD = 0.0091 mg/kg/day cPAD = 0.0091 mg/kg/day	Munro et al 1996 TTC method using cumulative distribution of NOELs

Table 2. Summary of Toxicological Doses and Endpoints for Various Fragrances for Use in Human Health Risk Assessments.				
Exposure/ Scenario	**POD**	**Uncertainty/FQPA Safety Factors**	**RfD, PAD, LOC for Risk Assessment**	**Study and Toxicological Effects**
Incidental Oral (Short-Term)	5th percentile NOEL = 0.91 mg/kg/day	UFA =10X UFH =10X FQPA= 1X Total UF=100	LOC for MOE = 100	Munro et al 1996 TTC method using cumulative distribution of NOELs
Dermal and Inhalation (Short-Term and Intermediate-Term)	5th percentile NOEL = 0.91 mg/kg/day	UFA =10X UFH =10X FQPA= 1X Total UF=100	LOC for MOE = 100	Munro et al 1996 TTC method using cumulative distribution of NOELs

Point of departure (POD) = A data point or an estimated point that is derived from observed dose-response data and used to mark the beginning of extrapolation to determine risk associated with lower environmentally relevant human exposures. NOEL = no-observed-effect level. UF = uncertainty factor. UF_A = extrapolation from animal to human (interspecies). UF_H = potential variation in sensitivity among members of the human population (intraspecies).FQPA SF = FQPA Safety Factor. PAD = population-adjusted dose (a = acute, c = chronic). RfD = reference dose. MOE = margin of exposure. LOC = level of concern.

4.3. Special Considerations for Infants and Children

FFDCA Section 408(b)(2)(C) provides that EPA shall retain an additional tenfold (10X) margin of safety for infants and children in the case of threshold effects to account for prenatal and postnatal toxicity and the completeness of the database on toxicity and exposure unless EPA determines based on reliable data that a different margin of safety will be safe for infants and children. This additional margin of safety is commonly referred to as the FQPA safety factor (SF). In applying this provision, EPA either retains the default value of 10X, or uses a different additional safety factor when reliable data available to EPA support the choice of a different factor. The FQPA SF has been reduced to 1X in this risk assessment because clear NOELs and LOELs were established in the studies analyzed by Munro et al 1996 (which included developmental and reproductive toxicity studies), maternal and developmental-specific 5th percentile NOAELs calculated by van Ravenzwaay et al 2011 indicate low potential for offspring susceptibility, and the conservative assumptions made in the exposure assessment are unlikely to underestimate risk.

5. DIETARY EXPOSURE

Dietary exposure (food and drinking water) may occur from the existing and proposed pesticidal uses of these various fragrances (e.g., eating foods placed on surfaces cleaned with pesticide formulations containing these various fragrances, and drinking water exposures). Dietary exposure may also occur from non-pesticidal uses but no reliable information is available for non-pesticidal exposures. Therefore, EPA assessed dietary exposures from pesticidal uses of these various fragrances only.

The FDA food contact surface sanitizing solution dietary exposure assessment model was used to calculate an Estimated Daily Intake (EDI) and Daily Dietary Dose (DDD) using assumptions described in Appendix I. The original FDA model only derived an exposure amount but did not specifically address population subgroups. Therefore, data from the National Health and Nutrition Examination Survey (NHANES) on food consumption (specifically the 2005-2010 survey data) was used to obtain adjustment factors (AFs). Adjusted DDDs for the US population and various population subgroups were obtained by multiplying the DDDs by the AFs, as described in Table 3. The %cPADs were then calculated by comparing the cPAD to the adjusted DDDs.

Acute Dietary Risk Assessment: No acute dietary effects are anticipated from uses at concentrations ≤ 33 ppm. Therefore, a quantitative acute dietary assessment is not necessary.

Chronic Dietary Risk Assessment: The chronic dietary exposure for food and drinking water utilized 21% and 58% of the cPAD for the U.S. population and children 1-2 years old (the most highly exposed population), respectively (see results in Table 3 and assumptions in Appendix II). These risks were not of concern (i.e. values were below 100% of the cPAD).

Cancer Dietary Risk Assessment: These various fragrances are not expected to be carcinogenic, based on their TTC evaluation. Therefore, a cancer dietary exposure assessment was not performed.

Table 3: Chronic Dietary Exposure Assessment for Food-contact Surface Sanitizing Uses

Population Group	Exposure			Risk Estimates
	Exposure (DDD[1] in mg/kg/day)	Adjustment factor[2] (Consumption Ratio)	Total Exposure (Adjusted DDD[3] in mg/kg/day)	% cPAD[4]
General U.S. Population	0.0018803	1.0000000	0.001880	21
Children (1-2 years old)	0.0104762	0.5068493	0.005310	58
Females (13-49 years old)	0.0018107	0.8664384	0.001569	17

[1] DDD = Daily Dietary Dose = Estimated Daily Intake/Body weight
[2] Adjustment factor (AF)= total food consumed by each population/total food consumed by the US population
[3] Adjusted DDD = DDD*AF
[4] %cPAD = (Adjusted DDD/cPAD)*100

6. RESIDENTIAL EXPOSURE ASSESSMENT

The term “residential exposure” is used in this document to refer to non-occupational, non-dietary exposure (e.g., for lawn and garden pest control, indoor pest control, termiticides, and flea and tick control on pets). Although there are non-pesticidal uses for these various fragrances, no reliable exposure information is available to EPA on those uses. These various fragrances may be used as an inert ingredient in pesticide products that are registered for specific uses that may result in residential exposure, such as pesticides used in and around the home. Therefore, screening level residential handler and post-application risk assessments have

been performed for common residential exposure scenarios, using assumptions detailed in the 2012 Residential SOPs[1].

Residential handler exposure: the Agency assumed handlers may receive short-term and intermediate-term dermal and inhalation exposure to these various fragrances from formulations containing the inert ingredient in outdoor and indoor scenarios. Also, homeowners are assumed to complete all elements of an application without use of any protective equipment. Long-term exposures are not calculated because applications are not expected to occur daily for more than 6 months. As shown in tables 4 below, residential handler MOEs range from 13,000 to 230,000 and are not of concern (i.e., MOEs are >100).

Residential post-application exposure: Residential post-application scenarios include short- and intermediate-term dermal (skin contact with treated surfaces) exposure for adults and children as well as short-term incidental oral exposure for children (hand-to-mouth exposure with treated surfaces). As shown in table 5 below, the lowest residential post-application MOE is 16,000 and is not of concern (i.e., MOEs are >100).

[1] Available at https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/standard-operating-procedures-residential-pesticide

Table 4. Short- and Intermediate-Term Residential Handler Exposure and Risk Estimates for Various Fragrances									
Exposure Scenario	Dermal Unit Exposure	Inhalation Unit Exposure	Estimated Application Rate[1]	Area Treated or Amount Handled Daily[2]	Dermal		Inhalation		Total MOE[7]
					Dose[3]	MOE[4]	Dose[5]	MOE[6]	
	mg/lb ai	mg/lb ai			mg/kg/day		mg/kg/day		
Antimicrobial Product Scenarios									
Mopping	71.6	2.38	4.30031E-06	1	3.849E-06	240000	1.279E-07	7100000	230000
Wiping	2870	67.3	4.30031E-06	0.13	2.006E-05	45000	4.703E-07	1900000	44000
Aerosol Spray/Trigger Pump	220	2.4	0.00027522	0.094	7.114E-05	13000	7.761E-07	1200000	13000

1. Based on application assumptions described in D364751 (A. LaMay, 2009)
2. Based on HED's 2012 Residential SOPs (https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/standard-operating-procedure-residential-exposure).
3. Dermal Dose = Dermal Unit Exposure (mg/lb ai) × Application Rate (lb ai/acre or gal) × Area Treated or Amount Handled (A/day or gallons/day) x dermal absorption factor ÷ BW (80 kg).
4. Dermal MOE = Dermal NOAEL (mg/kg/day) ÷ Dermal Dose (mg/kg/day)
5. Inhalation Dose = Inhalation Unit Exposure (mg/lb ai) × Application Rate (lb ai/acre or gal) × Area Treated or Amount Handled (A/day or gallons/day) x inhalation absorption factor ÷ BW (80 kg).
6. Inhalation MOE = Inhalation NOAEL (mg/kg/day) ÷ Inhalation Dose (mg/kg/day)
7. Total MOE = 1/ ((1/dermal MOE)+(1/inhalation MOE))

NA =not applicable due to negligible unit exposure

Table 5. Residential Post-application Exposure and Risk Estimates for Antimicrobial Uses							
Lifestage	**Route of Exposure**	**Transferable residue (ug/cm2)[1]**	**Exposure (mg/day)[2,3]**	**Dose (mg/kg/day)[4]**	**MOEs[5]**	**Combined MOE[6]**	**Combined MOE (rounded)**
Adult	Dermal	0.000	0.00	0.000029	32000	NA	NA
Children 1 to <2 years	Dermal	0.000	0.00	0.000055	16000		
	Hand to mouth	NA	0.000	0.000004	220000	14915	15000

1. Transferable residue = deposited residue*fraction transfered where the deposited residue is the application rate in ug/cm2 and the fraction transfered=0.08
2. Exposure assumptions obtained from 2012 Residential SOPs
3. Dermal Exposure =(Transferable residue)(Weight unit conversion factor in mg/ug)(Transfer coefficient in cm2/hr)(exposure time)
Hand to Mouth Exposure =(HR*(FM*SAH)*(exposure time*N_replen)*(1-(1-SE)^(HtM events per hour/N_replen))
4. Dose (mg/kg/day) = Exposure (mg/day) (dermal absorption factor for dermal route only)/ BW (80 kg for adults or 11 kg for children)
5. MOE = POD (mg/kg/day) ÷ Dose (mg/kg/day).
6. Combined MOE = 1 / ((1/Dermal MOE)+ (1/ hand to mouth M

7. AGGREGATE ASSESSMENT

The Federal Food, Drug, and Cosmetic Act (FFDCA) section 408 directs EPA to consider available information concerning exposure from the pesticide residue in food and other non-occupational exposures to determine that "there is a reasonable certainty that no harm will result from aggregate exposure to the pesticide chemical residue, including all anticipated dietary exposures and all other exposures for which there is reliable information".

In an aggregate assessment, exposures from relevant sources are added together and compared to quantitative estimates of hazard (e.g., a NOAEL or PAD), or the risks themselves can be aggregated. When aggregating exposures and risks from various sources, EPA considers both the route and duration of exposure.

Acute aggregate risk:
There is no acute dietary endpoint therefore an acute aggregate risk is not assessed.

Short-term aggregate risk: Short-term aggregate exposure takes into account short-term residential (dermal and inhalation) exposure plus chronic dietary exposure (food and drinking water). As shown in table 6 below, no short-term aggregate risks of concern were identified (i.e., MOEs are >100).

Table 6. Short-Term and/or Intermediate Term Aggregate Risk Calculations.

Population	Short- or Intermediate-Term Scenario						
	NOEL mg/kg/day	LOC[1]	Max Allowable Exposure[2] mg/kg/day	Average Food and Water Exposure mg/kg/day	Residential Exposure mg/kg/day[3]	Total Exposure mg/kg/day[4]	Aggregate MOE (food, water, and residential)[5]
Adults	0.91	100	0.0091	0.0019	0.0001	0.0020	455
Children	0.91	100	0.0091	0.0053	0.0001	0.0054	168

[1] Indicate in this footnote the basis for the LOC (include the standard inter- and intra- species uncertainty factors totaling 100).
[2] Maximum Allowable Exposure (mg/kg/day) = NOEL/LOC.
[3] Residential Exposure = [Oral exposure + Dermal exposure + Inhalation Exposure]. Residential exposure values used in aggregate assessment (Table # 4 & 5).
[4] Total Exposure = Avg Food & Water Exposure + Residential Exposure.
[5] Aggregate MOE = [NOEL/(Avg Food & Water Exposure + Residential Exposure)].

Intermediate-term aggregate risk: Intermediate-term aggregate exposure takes into account intermediate-term residential (dermal and inhalation) exposure plus chronic dietary exposure (food and drinking water). As the same endpoints were selected for short-term and intermediate-term exposures, intermediate-term aggregate risk is equal to the short-term aggregate risk and it is not of concern (see table 6 above).

Chronic aggregate risk: A chronic aggregate risk assessment considers exposure estimates from chronic dietary consumption of food and drinking water. Therefore, the chronic aggregate risk is equal to the chronic dietary risk, and it is not of concern (see section 5 above).

Aggregate Cancer Risk: The EPA has not identified any concerns for carcinogenicity relating to these various fragrances. Therefore, these various fragrances are not expected to pose a cancer aggregate risk.

8. OCCUPATIONAL EXPOSURE ASSESSMENT

The occupational handler MOEs ranged from 200 to 14,000 (LOC is for MOEs<100) for the assumed maximum applications rates when a double layer of clothing and gloves are worn by workers (see Table 7 below). Therefore, no occupational risks of concern were identified.

Table 7. Occupational Handler Non-Cancer Exposure and Risk Estimates for Various Fragrances.																
Exposure Scenario	**Crop or Target**	**Dermal Unit Exposure (µg/lb ai)**	**Level of PPE or Engineering control (EC)**	**Inhalation Unit Exposure (µg/lb ai)**	**Level of PPE or EC**	**Maximum Application Rate**	**App Rate Unit**	**Area Treated or Amount Handled Daily**	**Area Treated/Amount Handled Unit**	**Dermal**		**Inhalation**		**Total**	
										Dose[1] (mg/kg/day)	**MOE[2]**	**Dose[3] (mg/kg/day)**	**MOE[4]**	**MOE**	**ARI**
Mixer/Loader															
Wettable Powder, Mechanically-pressurized Handgun, Broadcast	Rights-of-way (e.g., utilities, railroad, roadways)	32.8	DL/G	2.75	No-R	0.01	lb ai/gallon solution	1000	gallons solution	0.0041	220	0.000344	2600	200	2
Liquid, Mechanically-pressurized Handgun, Broadcast	Rights-of-way (e.g., utilities, railroad, roadways)	29.1	DL/G	0.219	No-R	0.01	lb ai/gallon solution	1000	gallons solution	0.00364	250	2.74E-05	33000	250	2.5
Liquid, Aerial, Broadcast	Field crop, high-acreage	29.1	DL/G	0.219	No-R	0.01	lb ai/acre	1200	acres	0.00436	210	3.29E-05	28000	210	2.1
Liquid, Airblast, Broadcast	Orchard/Vineyard	29.1	DL/G	0.219	No-R	0.01	lb ai/acre	40	acres	0.000145	6300	1.1E-06	830000	6300	63
Liquid, Groundboom, Broadcast	Golf course (fairways, tees, greens)	29.1	DL/G	0.219	No-R	0.01	lb ai/acre	40	acres	0.000145	6300	1.1E-06	830000	6300	63
Liquid, Groundboom, Broadcast	Field crop, high-acreage	29.1	DL/G	0.219	No-R	0.01	lb ai/acre	200	acres	0.000728	1300	5.48E-06	170000	1300	13
Wettable Powder, Airblast, Broadcast	Orchard/Vineyard	32.8	DL/G	2.75	No-R	0.01	lb ai/acre	40	acres	0.000164	5500	1.38E-05	66000	5100	51
Wettable Powder, Groundboom, Broadcast	Golf course (fairways, tees, greens)	32.8	DL/G	2.75	No-R	0.01	lb ai/acre	40	acres	0.000164	5500	1.38E-05	66000	5100	51
Wettable Powder, Groundboom, Broadcast	Field crop, high-acreage	32.8	DL/G	2.75	No-R	0.01	lb ai/acre	200	acres	0.00082	1100	6.88E-05	13000	1000	10
Applicator															

Spray (all starting formulations), Airblast, Broadcast	Orchard/Vineyard	1480	DL/G	4.71	No-R	0.01	lb ai/acre	40	acres	0.0074	120	2.35E-05	39000	120	1.2
Spray (all starting formulations), Groundboom, Broadcast	Golf course (fairways, tees, greens)	12.6	DL/G	0.34	No-R	0.01	lb ai/acre	40	acres	0.000063	14000	1.7E-06	540000	14000	140
Spray (all starting formulations), Groundboom, Broadcast	Field crop, high-acreage	12.6	DL/G	0.34	No-R	0.01	lb ai/acre	200	acres	0.000315	2900	8.5E-06	110000	2800	28
Flagger															
Spray (all starting formulations), Aerial, Broadcast	Field crop, high-acreage	10.6	DL/G	0.202	No-R	0.01	lb ai/acre	350	acres	0.000464	2000	8.84E-06	100000	2000	20
Mixer/Loader/Applicator															
Liquid, Manually-pressurized Handwand, Broadcast (foliar)	Nursery (ornamentals, vegetables, trees, container stock)	365	DL/G	23.6	No-R	0.01	lb ai/gallon solution	15	gallons solution	0.000685	1300	4.43E-05	21000	1200	12
Wettable Powder, Manually-pressurized Handwand, Broadcast (foliar)	Nursery (ornamentals, vegetables, trees, container stock)	365	DL/G	23.6	No-R	0.01	lb ai/gallon solution	15	gallons solution	0.000685	1300	4.43E-05	21000	1200	12
Wettable Powder, Mechanically-pressurized Handgun, Broadcast	Landscaping, turf (lawns, athletic fields, parks, etc.)	630	DL/G	250	No-R	0.01	lb ai/acre	5	acres	0.000394	2300	0.000156	5800	1600	16

1. Dermal dose = Dermal unit exposure/1000*Application rate*area treated or amount handled daily
2. Dermal MOE = Dermal POD/Dermal dose
3. Inhalation dose = Inhalation unit exposure/1000*Application rate*area treated or amount handled daily
4. Inhalation MOE = Inhalation POD/Dermal dose

9. CUMULATIVE EXPOSURE

Section 408(b)(2)(D)(v) of FFDCA requires that, when considering whether to establish, modify, or revoke a tolerance, the Agency consider “available information” concerning the cumulative effects of a particular pesticide's residues and “other substances that have a common mechanism of toxicity.”

EPA has not found these various fragrances to share a common mechanism of toxicity with any other substances, and these various fragrances do not appear to produce a toxic metabolite produced by other substances. For the purposes of this tolerance exemption, therefore, EPA has assumed that these various fragrances do not have a common mechanism of toxicity with other substances. For information regarding EPA's efforts to determine which chemicals have a common mechanism of toxicity and to evaluate the cumulative effects of such chemicals, see https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/cumulative-assessment-risk-pesticides.

10. ECOTOXICITY AND ENVIRONMENTAL FATE

Environmental fate and effects are expected to be limited and not of concern as the exposure scenarios for 40 CFR 180.940(a) are expected to be on indoor surfaces and a low limitation of 33 ppm is being set for all fragrances listed in this document

11. RISK CHARACTERIZATION

Based on a quantitative human health risk assessment, no risks of concern were identified for the U.S. population, including infants and children following exposure to these various fragrances. Exposures assessed included the oral, dermal and inhalation routes.

Based on the use pattern and anticipated low use concentration, there is low concern for environmental toxicity.

Taking into consideration all available information, EPA concludes that there is a reasonable certainty that no harm to any population subgroup will result from exposure to these various fragrances when considering sources of pesticide exposure for which there is reliable information. Therefore, the use of these various fragrances as inert ingredients under 40 CFR 180.940(a) in antimicrobial pesticide formulations used on food contact surfaces in public eating places, dairy processing equipment, and food processing equipment and utensils with

end-use concentration not to exceed 33 ppm of the finished product can be considered assessed as safe.

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Appendix I.

FDA Food Contact Surface Sanitizing Solution Dietary Exposure Assessment Model

EDI (mg/p/day) = AR x RS x SA x F x 10-6 (1)

DDD (mg/kg/day) = AR x RS x SA x F x 10-6/BW (2)

Where:

AR = Application rate (ppm)
RS = Residual solution (mg/cm2)
SA = Surface area of the treated surface which comes into contact with food (cm2)
F = Fraction of the pesticide transferred or migrated to food (unitless)
BW = Body weight (kg)

Appendix II. Summary of Genotoxicity Information for Chemicals with Carcinogenicity Alerts found Using the OECD QSAR Toolbox (Carcinogenicity Alerts by ISS Profiler)

CAS Number	InertFinder/ ChemID Plus Chemical Name	JECFA Number	JECFA Meeting	21 US CFR	DT Class	JECFA Group/Additional Notes	Links to JECFA Summary	Flavis No.	EFSA/JECFA Opinion on Genotoxicity Concern
120-57-0	1,3-Benzodioxole-5-carboxaldehyde	896	48	21CFR182.60	III	Hydroxy- and alkoxy-substituted benzyl derivatives	Safety evaluation of certain food additives and contaminants prepared by the fifty-seventh meeting of the Joint FAO/WHO Expert Committee on Food Additives (JECFA). WHO Food Additives Series No. 48, 2002 http://www.inchem.org/documents/jecfa/jecmono/v48je15.htm	05.016	Based on combined evidence from *in vitro* assays (including Ames tests, paper disk mutation assay, DNA repair tests, mutation assay, mitotic recombination assay, chromosomal aberration tests, sister chromatid exchange assay, unscheduled DNA synthesis, micronucleus assay, rec assays, and mammalian cell gene mutation tests) as well as *in vivo* genotoxicity studies (including sex-linked recessive lethal mutations (SLRL), micronucleus tests, replicative DNA synthesis tests, sister chromatid exchange assays, chromosomal aberrations tests, micronucleus tests, unscheduled DNA synthesis tests, DNA damage tests, Comet assays, Basc tests, Medium-term rat liver bioassays, spot tests, and dominant lethal assay) for 1,3-benzodioxole-5-carboxaldehyde [Fl-no: 05.016] and materials similar to 1,3-benzodioxole-5-carboxaldehyde [Fl-no: 05.016], the material 1,3-benzodioxole-5-carboxaldehyde [Fl-no: 05.016] was cleared of genotoxicity concern (EFSA, 2008, 2009, 2012). EFSA Panel on Food Additives, Flavourings, Processing Aids and Materials in Contact with Food, 2008. Flavouring Group Evaluation 52 (FGE.52): Consideration of hydroxy- and alkoxy-substituted benzyl derivatives evaluated by JECFA (57th meeting) structurally related to benzyl alcohols, benzaldehydes, a related acetal, benzoic acids, and related esters evaluated by EFSA in FGE.20 (2005) (Commission Regulation (EC) No 1565/2000 of 18 July 2000) - Opinion of the Scientific Panel on Food Additives, Flavourings, Processing Aids and Materials in contact with Food (AFC), EFSA Journal 2008; 6(3):637, 69 pp. doi: 10.2903/j.efsa.2008.637 EFSA Panel on Food Contact Materials, Enzymes, Flavourings and Processing Aids, 2009. Flavouring Group Evaluation 54, Revision 1 (FGE. 54Rev1): Consideration of benzyl derivatives evaluated by JECFA (57th meeting) structurally related to benzyl alcohols, benzaldehydes, a related acetal, benzoic acids and related esters evaluated by EFSA in FGE.

CAS Number	InertFinder/ ChemID Plus Chemical Name	JECFA Number	JECFA Meeting	21 US CFR	DT Class	JECFA Group/Additional Notes	Links to JECFA Summary	Flavis No.	EFSA/JECFA Opinion on Genotoxicity Concern
									20Rev1 (2009). EFSA Journal 2009; 7(5):1025, 73 pp. doi:10.2903/j.efsa.2009.1025 EFSA Panel on Food Contact Materials, Enzymes, Flavourings and Processing Aids (CEF); Scientific Opinion on Flavouring Group Evaluation 20, Revision 4 (FGE.20Rev4): Benzyl alcohols, benzaldehydes, a related acetal, benzoic acids, and related esters from chemical groups 23 and 30. EFSA Journal 2012; 10(12):2994. [140 pp.]. doi:10.2903/j.efsa.2012.2994.
326-61-4	Piperonyl acetate	894	48	21CFR172.515	III	Hydroxy- and alkoxy-substituted benzyl derivatives	Safety evaluation of certain food additives and contaminants prepared by the fifty-seventh meeting of the Joint FAO/WHO Expert Committee on Food Additives (JECFA). WHO Food Additives Series No. 48, 2002 http://www.inchem.org/documents/jecfa/jecmono/v48je15.htm	09.220	Based on combined evidence from *in vitro* assays (including Ames tests, paper disk mutation assay, DNA repair tests, mutation assay, mitotic recombination assay, chromosomal aberration tests, sister chromatid exchange assay, unscheduled DNA synthesis, micronucleus assay, rec assays, and mammalian cell gene mutation tests) as well as *in vivo* genotoxicity studies (including sex-linked recessive lethal mutations (SLRL), micronucleus tests, replicative DNA synthesis tests, sister chromatid exchange assays, chromosomal aberrations tests, micronucleus tests, unscheduled DNA synthesis tests, DNA damage tests, Comet assays, Basc tests, Medium-term rat liver bioassays, spot tests, and dominant lethal assay) for Piperonyl acetate [Fl-no: 09.220] and materials similar to Piperonyl acetate [Fl-no: 09.220], the material Piperonyl acetate [Fl-no: 09.220 was cleared of genotoxicity concern (EFSA, 2008, 2009, 2012). EFSA Panel on Food Additives, Flavourings, Processing Aids and Materials in Contact with Food, 2008. Flavouring Group Evaluation 52 (FGE.52): Consideration of hydroxy- and alkoxy-substituted benzyl derivatives evaluated by JECFA (57th meeting) structurally related to benzyl alcohols, benzaldehydes, a related acetal, benzoic acids, and related esters evaluated by EFSA in FGE.20 (2005) (Commission Regulation (EC) No 1565/2000 of 18 July 2000) - Opinion of the Scientific Panel on Food Additives, Flavourings, Processing Aids and Materials in contact with Food (AFC), EFSA Journal 2008; 6(3):637, 69 pp. doi: 10.2903/j.efsa.2008.637 EFSA Panel on Food Contact Materials, Enzymes, Flavourings and Processing Aids, 2009. Flavouring

CAS Number	InertFinder/ ChemID Plus Chemical Name	JECFA Number	JECFA Meeting	21 US CFR	DT Class	JECFA Group/Additional Notes	Links to JECFA Summary	Flavis No.	EFSA/JECFA Opinion on Genotoxicity Concern
									Group Evaluation 54, Revision 1 (FGE. 54Rev1): Consideration of benzyl derivatives evaluated by JECFA (57th meeting) structurally related to benzyl alcohols, benzaldehydes, a related acetal, benzoic acids and related esters evaluated by EFSA in FGE. 20Rev1 (2009). EFSA Journal 2009; 7(5):1025, 73 pp. doi:10.2903/j.efsa.2009.1025 Suggested citation: EFSA Panel on Food Contact Materials, Enzymes, Flavourings and Processing Aids (CEF); Scientific Opinion on Flavouring Group Evaluation 20, Revision 4 (FGE.20Rev4): Benzyl alcohols, benzaldehydes, a related acetal, benzoic acids, and related esters from chemical groups 23 and 30. EFSA Journal 2012; 10(12):2994. [140 pp.]. doi:10.2903/j.efsa.2012.2994.
118-71-8	4H-Pyran-4-one, 3-hydroxy-2-methyl-	1480	56	21CFR172.515	II	Maltol and related substances	Safety evaluation of certain food additives and contaminants prepared by the sixty-fifth meeting of the Joint FAO/WHO Expert Committee on Food Additives (JECFA). WHO Food Additives Series No. 56, 2006 http://www.inchem.org/documents/jecfa/jecmono/v56je07.pdf	07.014	On the basis of combined evidence from *in vitro* assays (including reverse mutation assay, micronucleus assays, chromosomal aberration tests, sex-linked recessive lethal mutation, DNA damage tests, and sister chromatid exchange) as well as *in vivo* genotoxicity studies (including micronucleus assays, and comment assays) for 4H-Pyran-4-one, 3-hydroxy-2-methyl- [Fl-no: 07.014], the material 4H-Pyran-4-one, 3-hydroxy-2-methyl [Fl-no: 07.014] was cleared of genotoxicity concern (EFSA, 2015). EFSA CEF Panel (EFSA Panel on Food Contact Materials, Enzymes, Flavourings and Processing Aids), 2015. Scientific Opinion on Flavouring Group Evaluation 213, Revision 2 (FGE.213Rev2): Consideration of genotoxic potential for α,β-unsaturated alicyclic ketones and precursors from chemical subgroup 2.7 of FGE.19. EFSA Journal 2015; 13 (9):4244, 49 pp. doi:10.2903/j.efsa.2015.4244
3658-77-3	4-Hydroxy-2,5-dimethyl-3(2H)-furanone	1446	54	N/A	III	Tetrahydrofuran and furanone derivatives	Safety evaluation of certain food additives prepared by the sixty-third meeting of the Joint FAO/WHO Expert Committee on Food Additives (JEFCA). WHO Food Additives Series No.	13.010	Based on combined evidence from *in vitro* assays (reversed mutation assay, DNA damage assays, DNA strand breaks assay, and mouse lymphoma tests), *in vivo* genotoxicity studies (including dominate lethal assay) and a 2-year carcinogenic study for 4-Hydroxy-2,5-dimethyl-3(2H)-furanone [FL-no: 13.010] the material 4-Hydroxy-2,5-dimethyl-3(2H)-furanone

CAS Number	InertFinder/ ChemID Plus Chemical Name	JECFA Number	JECFA Meeting	21 US CFR	DT Class	JECFA Group/Additional Notes	Links to JECFA Summary	Flavis No.	EFSA/JECFA Opinion on Genotoxicity Concern
							54, 2006 http://www.inchem.org/documents/jecfa/jecmono/v54je01.pdf		[Fl-no: 13.010] was cleared of genotoxicity concern (EFSA, 2015a, 2015b). EFSA Panel on Food Contact Materials, Enzymes, Flavourings and Processing Aids, 2015. Scientific Opinion on Flavouring Group Evaluation 99 Revision 1 (FGE.99Rev1): Consideration of furanone derivatives evaluated by the JECFA (63rd, 65th and 69th meetings). EFSA Journal 2015; 13(11):4286, 31 pp. doi:10.2903/j.efsa.2015.4286 EFSA CEF Panel (EFSA Panel on Food Contact Materials, Enzymes, Flavourings and Processing Aids), 2015. Scientific Opinion on Flavouring Group Evaluation 220 Revision 3 (FGE.220Rev3): Consideration of genotoxic potential for $aL,$bT-unsaturated 3(2H)-Furanones from subgroup 4.4 of FGE.19. EFSA Journal 2015; 13(5):4117, 37 pp. doi:10.2903/j.efsa.2015.4117
65416-14-0	Maltyl isobutyrate	1482	56	N/A	III	Maltol and related substances	Safety evaluation of certain food additives and contaminants prepared by the sixty-fifth meeting of the Joint FAO/WHO Expert Committee on Food Additives (JECFA). WHO Food Additives Series No. 56, 2006 http://www.inchem.org/documents/jecfa/jecmono/v56je07.pdf	09.525	On the basis of combined evidence from *in vitro* assays (including reverse mutation assay, micronucleus assays, chromosomal aberration tests, sex-linked recessive lethal mutation, DNA damage tests, and sister chromatid exchange) as well as *in vivo* genotoxicity studies (including micronucleus assays, and comment assays) for 4H-Pyran-4-one, 3-hydroxy-2-methyl- [Fl-no: 07.014], the material Maltyl isobutyrate [Fl-no: 09.525] was cleared of genotoxicity concern (EFSA, 2015). EFSA CEF Panel (EFSA Panel on Food Contact Materials, Enzymes, Flavourings and Processing Aids), 2015. Scientific Opinion on Flavouring Group Evaluation 213, Revision 2 (FGE.213Rev2): Consideration of genotoxic potential for α,β-unsaturated alicyclic ketones and precursors from chemical subgroup 2.7 of FGE.19. EFSA Journal 2015; 13 (9):4244, 49 pp. doi:10.2903/j.efsa.2015.4244
1128-08-1	3-Methyl-2-(n-pentanyl)-2-cyclopenten-1-one	1406	54	N/A	II	Monocyclic and bicyclic secondary alcohols,	Safety evaluation of certain food additives prepared by the sixty-third meeting of the Joint FAO/WHO Expert Committee on Food	07.140	Based on combined evidence from *in vitro* assays (including reverse mutation assays and micronucleus assays) as for the close structural relative 3-methyl-2-cyclopenten-1-one [Fl-no: 07.112], the material 3-Methyl-2-(2-pentenyl)-2-cyclopenten-1-

CAS Number	InertFinder/ ChemID Plus Chemical Name	JECFA Number	JECFA Meeting	21 US CFR	DT Class	JECFA Group/Additional Notes	Links to JECFA Summary	Flavis No.	EFSA/JECFA Opinion on Genotoxicity Concern
						ketones, and related esters	Additives (JEFCA). WHO Food Additives Series No. 54, 2006 http://www.inchem.org/documents/jecfa/jecmono/v54je01.pdf		one [Fl-no: 07.140] was cleared of genotoxicity concern (EFSA, 2015, 2016) EFSA CEF Panel (EFSA Panel on Food Contact Materials, Enzymes, Flavourings and Processing Aids), 2015. Scientific Opinion on Flavouring Group Evaluation 212 Revision 3 (FGE.212Rev3): $aL,$bT-Unsaturated alicyclic ketones and precursors from chemical subgroup 2.6 of FGE.19. EFSA Journal 2015; 13(5):4116, 39 pp. doi:10.2903/j.efsa.2015.4116 EFSA CEF Panel (EFSA Panel on Food Contact Materials, Enzymes, Flavourings and Processing Aids), 2016. Scientific Opinion on Flavouring Group Evaluation 51, Revision 2 (FGE.51Rev2): Consideration of alicyclic ketones and secondary alcohols and related esters evaluated by the JECFA (59th meeting) structurally related to alicyclic ketones secondary alcohols and related esters in FGE.09Rev6 (2015b). EFSA Journal 2016; 14(1):4338, 57 pp. doi:10.2903/j.efsa.2016.4338
488-10-8; 6261-18-3	3-Methyl-2-(2-pentenyl)-2-cyclopenten-1-one	1114	50	21CFR172.515	II	Alicyclic ketones, secondary alcohols and related esters	Safety evaluation of certain food additives and contaminants prepared by the fifty-ninth meeting of the Joint FAO/WHO Expert Committee on Food Additives (JECFA). WHO Food Additives Series No. 50, 2003 http://www.inchem.org/documents/jecfa/jecmono/v50je12.htm	07.094	Based on combined evidence from *in vitro* assays (including reverse mutation assays and micronucleus assays) as for the close structural relative 3-methyl-2-cyclopenten-1-one [Fl-no: 07.112], the material 3-Methyl-2-(2-pentenyl)-2-cyclopenten-1-one [Fl-no: 07.094] was cleared of genotoxicity concern (EFSA, 2015) EFSA CEF Panel (EFSA Panel on Food Contact Materials, Enzymes, Flavourings and Processing Aids), 2015. Scientific Opinion on Flavouring Group Evaluation 212 Revision 3 (FGE.212Rev3): $aL,$bT-Unsaturated alicyclic ketones and precursors from chemical subgroup 2.6 of FGE.19. EFSA Journal 2015; 13(5):4116, 39 pp. doi:10.2903/j.efsa.2015.4116
11050-62-7	Isojasmone	1115	50	21CFR172.515	II	Alicyclic ketones, secondary alcohols and related esters	Safety evaluation of certain food additives and contaminants prepared by the fifty-ninth meeting of the Joint FAO/WHO	07.033	Based on combined evidence from *in vitro* assays (including reverse mutation assays and micronucleus assays) for the close structural relative 3-methyl-2-cyclopenten-1-one [Fl-no: 07.112], the material Isojasmone [Fl-no: 07.033] was cleared of genotoxicity concern (EFSA, 2015)

CAS Number	InertFinder/ ChemID Plus Chemical Name	JECFA Number	JECFA Meeting	21 US CFR	DT Class	JECFA Group/Additional Notes	Links to JECFA Summary	Flavis No.	EFSA/JECFA Opinion on Genotoxicity Concern
							Expert Committee on Food Additives (JECFA). WHO Food Additives Series No. 50, 2003 http://www.inchem.org/documents/jecfa/jecmono/v50je14.htm		EFSA CEF Panel (EFSA Panel on Food Contact Materials, Enzymes, Flavourings and Processing Aids), 2015. Scientific Opinion on Flavouring Group Evaluation 212 Revision 3 (FGE.212Rev3): $aL,$bT-Unsaturated alicyclic ketones and precursors from chemical subgroup 2.6 of FGE.19. EFSA Journal 2015; 13(5):4116, 39 pp. doi:10.2903/j.efsa.2015.4116
21834-92-4	5-Methyl-2-phenyl-2-hexenal	1472	54	N/A	II	Phenyl-substituted aliphatic alcohols and related aldehydes and esters	Safety evaluation of certain food additives prepared by the sixty-third meeting of the Joint FAO/WHO Expert Committee on Food Additives (JEFCA). WHO Food Additives Series No. 54, 2006 http://www.inchem.org/documents/jecfa/jecmono/v54je01.pdf	05.099	Based on combined evidence from *in vitro* assays (including Ames tests, paper disk mutation assay, DNA repair tests, mutation assay, mitotic recombination assay, chromosomal aberration tests, sister chromatid exchange assay, unscheduled DNA synthesis, micronucleus assay, rec assays, and mammalian cell gene mutation tests) as well as *in vivo* genotoxicity studies (including sex-linked recessive lethal mutations (SLRL), micronucleus tests, replicative DNA synthesis tests, sister chromatid exchange assays, chromosomal aberrations tests, micronucleus tests, unscheduled DNA synthesis tests, DNA damage tests, Comet assays, Basc tests, Medium-term rat liver bioassays, spot tests, and dominant lethal assays) for materials similar to 1,3-benzodioxole-5-carboxaldehyde [JECFA no. 1472], the material 1,3-benzodioxole-5-carboxaldehyde [JECFA no. 1472] was cleared of genotoxicity concern (Sips and Hattan, 2006) Sipes, I. G., and D. G. Hattan. "PHENYL-SUBSTITUTED ALIPHATIC ALCOHOLS AND RELATED ALDEHYDES AND ESTERS." Safety evaluation of certain food additives (2006): 525.
1604-28-0	6-Methyl-3,5-heptadien-2-one	1134	50	21CFR172.515	I	Aliphatic secondary alcohols, ketones and related esters	Safety evaluation of certain food additives and contaminants prepared by the fifty-ninth meeting of the Joint FAO/WHO Expert Committee on Food Additives (JECFA). WHO Food Additives Series No. 50, 2003 http://www.inchem.org/documents/jecfa/jecmono/v50je15.htm	07.099	Based on combined evidence from *in vitro* assays (reverse mutation assays and micronucleus induction assays) for 6-Methyl-3,5-heptadien-2-one [Fl-no: 07.099], the material 6-Methyl-3,5-heptadien-2-one [Fl-no: 07.099] was cleared of genotoxicity concern (EFSA, 2011, 2017a, 2017b). EFSA Panel on Food Contact Materials, Enzymes, Flavourings and Processing Aids (CEF); Scientific Opinion on Flavouring Group Evaluation 206 (FGE.206): Consideration of genotoxicity data on representatives for 12 alpha, beta-unsaturated ketones and precursors from chemical subgroup 1.2.3 of

CAS Number	InertFinder/ ChemID Plus Chemical Name	JECFA Number	JECFA Meeting	21 US CFR	DT Class	JECFA Group/Additional Notes	Links to JECFA Summary	Flavis No.	EFSA/JECFA Opinion on Genotoxicity Concern
									FGE.19 by EFSA. EFSA Journal 2011; 9(3):1922. [16 pp.]. doi:10.2903/j.efsa.2011.1922. EFSA CEF Panel (EFSA Panel on Food Contact Materials, Enzymes, Flavourings and Processing Aids), Silano V, Bolognesi C, Castle L, Cravedi J-P, Engel K-H, Fowler P, Franz R, Grob K, Gürtler R, Husøy T, Kärenlampi S, Milana MR, Penninks A, Tavares Poças MF, Smith A, Tlustos C, Wölfle D, Zorn H, Zugravu C-A, Beckman Sundh U, Brimer L, Mulder G, Binderup M-L, Crebelli R, Marcon F, Marzin D, Mosesso P, Kovalkovičová N and Mennes W, 2016. Scientific Opinion on Flavouring Group Evaluation 63, Revision 3 (FGE.63Rev3): aliphatic secondary alcohols, ketones and related esters evaluated by JECFA (59th and 69th meetings) structurally related to saturated and unsaturated aliphatic secondary alcohols, ketones and esters of secondary alcohols and saturated linear or branched-chain carboxylic acids evaluated by EFSA in FGE.07Rev4. EFSA Journal 2017; 15(1):4662, 41 pp. doi:10.2903/j.efsa.2017.4662 EFSA Panel on Food Contact Materials, Enzymes, Flavourings and Processing Aids (CEF), Silano V, Bolognesi C, Castle L, Cravedi J-P, Engel K-H, Fowler P, Franz R, Grob K, Gürtler R, Husøy T, Kärenlampi S, Milana MR, Penninks A, Tavares Poças MF, Smith A, Tlustos C, Wölfle D, Zorn H, Zugravu C-A, Beckman Sundh U, Brimer L, Mosesso P, Mulder G, Anastassiadou M and Mennes W, 2017. Scientific Opinion on Flavouring Group Evaluation 7, Revision 5 (FGE.07Rev5): saturated and unsaturated aliphatic secondary alcohols, ketones and esters of secondary alcohols and saturated linear or branched-chain carboxylic acids from chemical group 5. EFSA Journal 2017; 15(3):4725, 81 pp. doi:10.2903/j.efsa.2017.4725
4674-50-4	Nootkatone	1398	54	21CFR172.515	II	Monocyclic and bicyclic secondary alcohols, ketones, and related esters	Safety evaluation of certain food additives prepared by the sixty-third meeting of the Joint FAO/WHO Expert Committee on Food Additives (JEFCA). WHO	07.089	Based on combined evidence from *in vitro* assays (including reverse mutation assays and micronucleus assays) for Nootkatone [Fl-no: 07.089], the material Nootkatone [Fl-no: 07.089] was cleared of genotoxicity concern (EFSA, 2014, 2015).

CAS Number	InertFinder/ ChemID Plus Chemical Name	JECFA Number	JECFA Meeting	21 US CFR	DT Class	JECFA Group/Additional Notes	Links to JECFA Summary	Flavis No.	EFSA/JECFA Opinion on Genotoxicity Concern
							Food Additives Series No. 54, 2006 http://www.inchem.org/documents/jecfa/jecmono/v54je01.pdf		EFSA CEF Panel (EFSA Panel on Food Contact Materials, Enzymes, Flavourings and Processing Aids), 2014. Scientific Opinion on Flavouring Group Evaluation 87, Revision 2 (FGE.87Rev2): Consideration of bicyclic secondary alcohols, ketones and related esters evaluated by JECFA (63rd meeting) structurally related to bicyclic secondary alcohols, ketones and related esters evaluated by EFSA in FGE.47Rev1 (2008). EFSA Journal 2014; 12(10):3864, 41 pp. doi:10.2903/j.efsa.2014.3864 EFSA CEF Panel (EFSA Panel on Food Contact Materials, Enzymes, Flavourings and Processing Aids), 2015. Scientific Opinion on Flavouring Group Evaluation 213, Revision 2 (FGE.213Rev2): Consideration of genotoxic potential for α,β-unsaturated alicyclic ketones and precursors from chemical subgroup 2.7 of FGE.19. EFSA Journal 2015; 13 (9):4244, 49 pp. doi:10.2903/j.efsa.2015.4244
4940-11-8	Ethyl maltol	1481	56	21CFR172.515	II	Maltol and related substances	Safety evaluation of certain food additives and contaminants prepared by the sixty-fifth meeting of the Joint FAO/WHO Expert Committee on Food Additives (JECFA). WHO Food Additives Series No. 56, 2006 http://www.inchem.org/documents/jecfa/jecmono/v56je07.pdf	07.047	Based on combined evidence from *in vitro* assays (including reverse mutation assays), *in vivo* genotoxicity studies (including micronucleus formation tests and Basc tests), and a 2-year carcinogenicity study for Ethyl maltol [Fl-no: 07.047], the material Ethyl maltol [Fl-no: 07.047] was cleared of genotoxicity concern (EFSA, 2010, 2015). EFSA; Scientific Opinion on Flavouring Group Evaluation 83, Revision 1 (FGE.83Rev1): EFSA Journal 2010; 8(2):1409. [22 pp.]. doi:10.2903/j.efsa.2010.1409. EFSA CEF Panel (EFSA Panel on Food Contact Materials, Enzymes, Flavourings and Processing Aids), 2015. Scientific Opinion on Flavouring Group Evaluation 213, Revision 2 (FGE.213Rev2): Consideration of genotoxic potential for α,β-unsaturated alicyclic ketones and precursors from chemical subgroup 2.7 of FGE.19. EFSA Journal 2015; 13 (9):4244, 49 pp. doi:10.2903/j.efsa.2015.4244
80-71-7	Methylcyclopentenolone	418	42	21CFR172.515	III	Aliphatic acyclic and	Safety evaluation of certain food additives and	07.056	Based on combined evidence from *in vitro* assays (including reverse mutation assays and unscheduled DNA synthesis tests)

CAS Number	InertFinder/ ChemID Plus Chemical Name	JECFA Number	JECFA Meeting	21 US CFR	DT Class	JECFA Group/Additional Notes	Links to JECFA Summary	Flavis No.	EFSA/JECFA Opinion on Genotoxicity Concern
						alicyclic alpha-diketones and related alpha-hydroxyketones	contaminants prepared by the fifty-first meeting of the Joint FAO/WHO Expert Committee on Food Additives (JECFA). WHO Food Additives Series No. 42, 1999 http://www.inchem.org/documents/jecfa/jecmono/v042je20.htm		for Methylcyclopentenolone [Fl-no: 07.056] and a 2-year carcinogenicity study for a related substance, 3-Ethylcyclopentan-1,2-dione [Fl-no: 07.057], the material Methylcyclopentenolone [Fl-no: 07.056] was cleared of genotoxicity concern (EFSA, 2015). EFSA CEF Panel (EFSA Panel on Food Contact Materials, Enzymes, Flavourings and Processing Aids), 2015. Scientific Opinion on Flavouring Group Evaluation 213, Revision 2 (FGE.213Rev2): Consideration of genotoxic potential for α,β-unsaturated alicyclic ketones and precursors from chemical subgroup 2.7 of FGE.19. EFSA Journal 2015; 13 (9):4244, 49 pp. doi:10.2903/j.efsa.2015.4244
13679-70-4	5-Methyl-2-thiophenecarboxaldehyde	1050	50	N/A	III	Sulfur-containing heterocyclic compounds	Safety evaluation of certain food additives and contaminants prepared by the fifty-ninth meeting of the Joint FAO/WHO Expert Committee on Food Additives (JECFA). WHO Food Additives Series No. 50, 2003 http://www.inchem.org/documents/jecfa/jecmono/v50je12.htm	15.004	Based on combined evidence from *in vitro* assays (including Ames assays and micronucleus assays) as well as *in vivo* genotoxicity studies (including micronucleus assay and comet assays) for 5-Methyl-2-thiophenecarboxaldehyde [Fl-no: 15.004], the material Methyl-2-thiophenecarboxaldehyde [Fl-no: 15.004] was cleared of genotoxicity concern (EFSA, 2013a, 2013b) EFSA Panel on Food Contact Materials, Enzymes, Flavourings and Processing Aids (CEF); Scientific Opinion on Flavouring Group Evaluation 224 (FGE.224): Consideration of genotoxic potential for two α,β-unsaturated thiophenes from subgroup 5.2 of FGE.19 by EFSA. EFSA Journal 2013; 11 (2):3093. [18 pp.] doi:10.2903/j.efsa.2013.3093. EFSA CEF Panel (EFSA Panel on Food Contact Materials, Enzymes, Flavourings and Processing Aids), 2013. Scientific Opinion on Flavouring Group Evaluation 76, Revision 1 (FGE.76Rev1): Consideration of sulphur-containing heterocyclic compounds evaluated by JECFA (59th meeting) structurally related to thiazoles, thiophene, thiazoline and thienyl derivatives from chemical group 29 and miscellaneous substances from chemical group 30 evaluated by EFSA in FGE.21Rev3. EFSA Journal 2013; 11(11):3455, 52 pp. doi:10.2903/j.efsa.2013.3455
121-32-4	Ethylvanillin	893	48	21CFR18 2.60;	II	Hydroxy- and alkoxy-	Safety evaluation of certain food additives and	05.019	Based on combined evidence from *in vitro* assays (including Ames tests, paper disk mutation assay, DNA repair tests,

CAS Number	InertFinder/ ChemID Plus Chemical Name	JECFA Number	JECFA Meeting	21 US CFR	DT Class	JECFA Group/Additional Notes	Links to JECFA Summary	Flavis No.	EFSA/JECFA Opinion on Genotoxicity Concern
				21CFR182.90		substituted benzyl derivatives	contaminants prepared by the fifty-seventh meeting of the Joint FAO/WHO Expert Committee on Food Additives (JECFA). WHO Food Additives Series No. 48, 2002 http://www.inchem.org/documents/jecfa/jecmono/v48je15.htm		mutation assay, mitotic recombination assay, chromosomal aberration tests, sister chromatid exchange assay, unscheduled DNA synthesis, micronucleus assay, rec assays, and mammalian cell gene mutation tests) as well as *in vivo* genotoxicity studies (including sex-linked recessive lethal mutations (SLRL), micronucleus tests, replicative DNA synthesis tests, sister chromatid exchange assays, chromosomal aberrations tests, micronucleus tests, unscheduled DNA synthesis tests, DNA damage tests, Comet assays, Basc tests, Medium-term rat liver bioassays, spot tests, and dominant lethal assays) for Ethylvanillin [Fl-no: 05.019] and materials similar to Ethylvanillin [Fl-no: 05.019], the material Ethylvanillin [Fl-no: 05.019] was cleared of genotoxicity concern (EFSA, 2008, 2009). EFSA Panel on Food Contact Materials, Enzymes, Flavourings and Processing Aids, 2009. Flavouring Group Evaluation 54, Revision 1 (FGE. 54Rev1): Consideration of benzyl derivatives evaluated by JECFA (57th meeting) structurally related to benzyl alcohols, benzaldehydes, a related acetal, benzoic acids and related esters evaluated by EFSA in FGE. 20Rev1 (2009). EFSA Journal 2009; 7(5):1025, 73 pp. doi:10.2903/j.efsa.2009.1025 EFSA Panel on Food Additives, Flavourings, Processing Aids and Materials in Contact with Food, 2008. Flavouring Group Evaluation 52 (FGE.52): Consideration of hydroxy- and alkoxy-substituted benzyl derivatives evaluated by JECFA (57th meeting) structurally related to benzyl alcohols, benzaldehydes, a related acetal, benzoic acids, and related esters evaluated by EFSA in FGE.20 (2005) (Commission Regulation (EC) No 1565/2000 of 18 July 2000) - Opinion of the Scientific Panel on Food Additives, Flavourings, Processing Aids and Materials in contact with Food (AFC), EFSA Journal 2008; 6(3):637, 69 pp. doi:10.2903/j.efsa.2008.637
67801-20-1	3-Methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)pent-4-en-2-ol	2220	73	N/A	I	Aliphatic secondary alcohols, ketones and related esters	Safety Evaluation of Certain Food Additives. Prepared by the 82nd meeting of the Joint FAO/WHO Expert Committee on Food	N/A	Based on combined evidence from *in vitro* assays (including reverse mutation assay, forward mutation assay, and chromosome aberration) for 3-Methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)pent-4-en-2-ol [JECFA 2220], the material 3-Methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)pent-4-en-2-ol

CAS Number	InertFinder/ ChemID Plus Chemical Name	JECFA Number	JECFA Meeting	21 US CFR	DT Class	JECFA Group/Additional Notes	Links to JECFA Summary	Flavis No.	EFSA/JECFA Opinion on Genotoxicity Concern
							Additives (JECFA). Who Food Additives Series 73. 2017. http://apps.who.int/iris/bitstream/handle/10665/258934/9789241660730-eng.pdf;jsessionid=3AD1CCCA38A3AEBA4162A4D51490168E?sequence=1		[JECFA 2220] was cleared of genotoxicity concern (WHO, 2017) World Health Organization. "Safety evaluation of certain food additives: prepared by the Eighty-second meeting of the Joint FAO/WHO Expert Committee on Food Additives (JECFA)." (2017).
104-76-7	1-Hexanol, 2-ethyl-	267	40	N/A	I	Saturated aliphatic acyclic branched-chain primary alcohols, aldehydes, and acids	Safety evaluation of certain food additives and contaminants prepared by the forty-ninth meeting of the Joint FAO/WHO Expert Committee on Food Additives (JECFA). WHO Food Additives Series No. 40, 1998 http://www.inchem.org/documents/jecfa/jecmono/v040je11.htm	-02.082	Based on combined evidence from *in vitro* assays (including an Ames assay and a chromosome aberration assay) for 1-hexanol, 2-ethyl- [Fl-no: 02.082], the material 1-hexanol, 2-ethyl- [Fl-no: 02.082], was cleared of genotoxicity concern. (Api et al., 2016). A.M. Api, D. Belsito, S. Bhatia, M. Bruze, P. Calow, M.L. Dagli, W. Dekant, A.D. Fryer, L. Kromidas, S. La Cava, J.F. Lalko, A. Lapczynski, D.C. Liebler, T.M. Penning, V.T. Politano, G. Ritacco, D. Salvito, T.W. Schultz, J. Shen, I.G. Sipes, B. Wall, D.K. Wilcox, RIFM fragrance ingredient safety assessment, 2-ethyl-1-hexanol, CAS registry number 104-76-7, Food and Chemical Toxicology, Volume 97, Supplement, 2016, Pages S147-S156, ISSN 0278-6915, https://doi.org/10.1016/j.fct.2016.09.001. (https://www.sciencedirect.com/science/article/pii/S0278691516303155)

Appendix III. Results from QSAR Toolbox Analysis Using QSAR Toolbox 4.5 (http://www.qsartoolbox.org/home)

InertFinder/ChemID Plus Name	(+)-Fenchone	Camphor	Linalyl oxide	p- Menthan- 3-one	.alpha.-Butylcinnamaldehyde	1,3-Benzodioxole- 5-carboxaldehyde	1- Hexanol, 2-ethyl-	1-Octen-3- ol
CAS	4695-62-9	21368-68-3	60047-17-8; 5989-33-3; 34995-77-2	10458-14-7	7492-44-6	120-57-0	104-76-7	3391-86-4
SMILES	CC1(C)[C@@H]2CC[C@@](C)(C2)C1=O	CC1(C)C2CCC1(C)C(=O)C2	CC1(CCC(O1)C(C)(C)O)C=C	CC(C)C1CCC(C)CC1=O	CCCC\C(C=O)=C/c1ccccc1	O=Cc1ccc2OCOc 2c1	CCCCC(CC)CO	CCCCCC(O)C=C
Ionization at pH = 1	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) No pKb value	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)
Biodegradation ultimate (Biowin 3)	Weeks to months	Weeks to months	Weeks to months	Weeks	Weeks	Weeks	Days to weeks	Days to weeks
Estrogen Receptor Binding	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group	Non binder, non cyclic structure	Non binder, non cyclic structure
Biodeg BioHC half-life (Biowin)	No value	No value	No value	No value	No value	No value	No value	No value
Hydrolysis half-life (pH 6.5-7.4)	No value	No value	No value	No value	No value	No value	No value	No value
Biodegradation probability (Biowin 5)	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast
Toxic hazard classification by Cramer	Intermediate (Class II)	Intermediate (Class II)	High (Class III)	Intermediate (Class II)	Low (Class I)	High (Class III)	Low (Class I)	Intermediate (Class II)

InertFinder/ChemID Plus Name	(+)-Fenchone	Camphor	Linalyl oxide	p- Menthan- 3- one	.alpha.- Butylcinnamaldehyde	1,3-Benzodioxole- 5- carboxaldehyde	1- Hexanol, 2-ethyl-	1-Octen-3- o
Biodegradation probability (Biowin 2)	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast
Ionization at pH = 4	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) No pKb value	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)
Protein binding potency Lys (DPRA 13%)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Non-conjugated mono- and diketones (non reactive)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Non-conjugate d mono- and diketones (non reactive)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Alcohols	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Non-conjugate d mono- and diketones (non reactive)	Out of mechanistic domain	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Vaniline derivatives	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Alcohols	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Alcohols
Protein binding potency Cys (DPRA 13%)	Out of mechanistic domain	Out of mechanistic domain	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Alcohols	Out of mechanistic domain	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> alpha alkyl cinnamaldehydes	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Non- Conjugated monoaldehydes (non reactive) DPRA less than 9% (DPRA 13%) >> Vaniline derivatives	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Alcohols	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Alcohols

InertFinder/ChemID Plus Name	(+)-Fenchone	Camphor	Linalyl oxide	p- Menthan- 3- one	.alpha.- Butylcinnamaldehyde	1,3-Benzodioxole- 5- carboxaldehyde	1- Hexanol, 2-ethyl-	1-Octen-3- o
Hydrolysis half-life (Kb, pH 8) (Hydrowin)	No value	No value	No value	No value	No value	No value	No value	No value
Hydrolysis half-life (Kb, pH 7) (Hydrowin)	No value	No value	No value	No value	No value	No value	No value	No value
Biodegradation probability (Biowin 6)	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast
Protein binding by OECD	No alert found	No alert found	No alert found	No alert found	Michael addition Michael addition >> Polarised Alkenes Michael addition >> Polarised Alkenes >> Polarised alkene - aldehydes Schiff Base Formers Schiff Base Formers >> Direct Acting Schiff Base Formers Schiff Base Formers >> Direct Acting Schiff Base Formers >> Mono-carbonyls	No alert found	No alert found	No alert found
Ultimate biodeg	10 to 100 days	1 to 10 days 10 to 100 days	10 to 100 days	10 to 100 days	No data	1 to 10 days 10 to 100 days	0 to 1 day 1 to 10 days	1 to 10 days 10 to 100 days
Ionization at pH = 9	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000,	Acidic [0.000, 10.000) Basic	Acidic [0.000, 10.000) Basic [0.000,	Acidic [10.000, 20.000) No pKb value	Acidic [90.000, 100.000] Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000,

InertFinder/ChemID Plus Name	(+)-Fenchone	Camphor	Linalyl oxide	p- Menthan- 3- one	.alpha.- Butylcinnamaldehyde	1,3-Benzodioxole- 5- carboxaldehyde	1- Hexanol, 2-ethyl-	1-Octen-3- o
		10.000)	[0.000, 10.000)	10.000)				10.000)
Hydrolysis half-life (Ka, pH 7) (Hydrowin)	No value	No value	No value	No value	No value	No value	No value	No value
Toxic hazard classification by Cramer (extended)	Intermediate (Class II)	Intermediate (Class II)	High (Class III)	Intermediate (Class II)	Low (Class I)	High (Class III)	Low (Class I)	High (Class III)
Biodegradation probability (Biowin 7)	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast
DNA binding by OASIS	No alert found	No alert found	No alert found	No alert found	AN2 AN2 >> Nucleophilic addition to alpha, beta-unsaturated carbonyl compounds AN2 >> Nucleophilic addition to alpha, beta-unsaturated carbonyl compounds >> Alpha, Beta-Unsaturated Aldehydes AN2 >> Schiff base formation AN2 >> Schiff base formation >> Alpha, Beta- Unsaturated Aldehydes	No alert found	No alert found	No alert found
Ionization at pH = 7.4	Acidic [0.000, 10.000)	Acidic [0.000,	Acidic [0.000,	Acidic [0.000,	Acidic [0.000, 10.000)	Acidic [10.000, 20.000)	Acidic [0.000, 10.000)	Acidic [0.000,

InertFinder/ChemID Plus Name	(+)-Fenchone	Camphor	Linalyl oxide	p- Menthan- 3- one	.alpha.- Butylcinnamaldehyde	1,3-Benzodioxole- 5- carboxaldehyde	1- Hexanol, 2-ethyl-	1-Octen-3- o
	Basic [0.000, 10.000)	10.000) Basic [0.000, 10.000)	10.000) Basic [0.000, 10.000)	10.000) Basic [0.000, 10.000)	No pKb value	Basic [0.000, 10.000)	Basic [0.000, 10.000)	10.000) Basic [0.000, 10.000)
Hydrolysis half-life (Ka, pH 8) (Hydrowin)	No value	No value	No value	No value	No value	No value	No value	No value
Protein binding by OASIS	No alert found	No alert found	No alert found	No alert found	Michael addition Michael addition >> Michael addition on alpha, beta- Unsaturated carbonyl compounds Michael addition >> Michael addition on alpha, beta- Unsaturated carbonyl compounds >> alpha, beta- Aldehydes Schiff base formation Schiff base formation >> Schiff base formation with carbonyl compounds Schiff base formation >> Schiff base formation with carbonyl compounds >> Aldehydes	No alert found	No alert found	No alert found
DNA binding by	No alert	No alert	No alert	No alert	No alert found	Michael addition	No alert found	No alert

InertFinder/ChemID Plus Name	(+)-Fenchone	Camphor	Linalyl oxide	p- Menthan- 3- one	.alpha.- Butylcinnamaldehyde	1,3-Benzodioxole- 5- carboxaldehyde	1- Hexanol, 2-ethyl-	1-Octen-3- o
OECD	found	found	found	found		Michael addition >> P450 Mediated Activation to Quinones and Quinone-type Chemicals Michael addition >> P450 Mediated Activation to Quinones and Quinone-type Chemicals >> Methylenedioxyphenyl		found
Biodegradation probability (Biowin 1)	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast
Biodegradation primary (Biowin 4)	Days to weeks	Days to weeks	Days to weeks	Days to weeks	Days	Days	Days	Days
Carcinogenicity (genotox and nongenotox) alerts by ISS	No alert found	No alert found	No alert found	No alert found	No alert found	1,3- Benzodioxoles (Nongenotox) Simple aldehyde (Genotox) Structural alerts for both genotoxic and nongenotoxic carcinogenicity	Structural alert for nongenotoxic carcinogenicity Substitute d n-alkylcarboxylic acids (Nongenotox)	No alert found
in vitro mutagenicity (Ames test) alerts by ISS	No alert found	No alert found	No alert found	No alert found	No alert found	Simple aldehyde	No alert found	No alert found
in vivo	No alert	No alert	H-	No alert	No alert found	H-acceptor-path3 H-	No alert found	No alert

InertFinder/ChemID Plus Name	(+)-Fenchone	Camphor	Linalyl oxide	p- Menthan- 3- one	.alpha.- Butylcinnamaldehyde	1,3-Benzodioxole- 5- carboxaldehyde	1- Hexanol, 2-ethyl-	1-Octen-3- o
mutagenicity (Micronucleus) alerts by ISS	found	found	acceptor-path3-H-acceptor Oxolane	found		acceptor Simple aldehyde		found
Protein Binding Potency h-CLAT	No alert found	No alert found	No alert found	No alert found	alpha, beta-Unsaturated aldehydes	No alert found	No alert found	No alert found
Skin irritation/corrosion Inclusion rules by BfR	Ketones	Ketones	Inclusion rules not met	Ketones	Aldehydes	Aldehydes	Inclusion rules not met	Inclusion rules not met
DNA alerts for AMES, CA and MNT by OASIS	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found
Protein binding alerts for skin sensitization by OASIS	Nucleophilic addition Nucleophilic addition >> Addition to carbon-hetero double bonds Nucleophilic addition >> Addition to carbon-hetero double bonds >> Ketones	Nucleophilic addition Nucleophilic addition >> Addition to carbon-hetero double bonds Nucleophilic addition >> Addition to carbon-hetero double	No alert found	Nucleophilic addition Nucleophilic addition >> Addition to carbon-hetero double bonds Nucleophilic addition >> Addition to carbon-hetero double	Michael Addition Michael Addition >> Michael addition on alpha, beta-Unsaturated carbonyl compounds Michael Addition >> Michael addition on alpha, beta-Unsaturated carbonyl compounds >> alpha, beta-Aldehydes	Schiff base formation Schiff base formation >> Schiff base formation with carbonyl compounds Schiff base formation >> Schiff base formation with carbonyl compounds >> Aldehydes	No alert found	No alert found

InertFinder/ChemID Plus Name	(+)-Fenchone	Camphor	Linalyl oxide	p- Menthan- 3- one	.alpha.- Butylcinnamaldehyde	1,3-Benzodioxole- 5- carboxaldehyde	1- Hexanol, 2-ethyl-	1-Octen-3- o
		bonds >> Ketones		bonds >> Ketones				
rtER Expert System - USEPA	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found
Skin irritation/corrosion Exclusion rules by BfR	Undefined	Undefined	Undefined	Undefined	Undefined	Group C Melting Point > 55 C Undefined	Undefined	Undefined
Protein binding alerts for Chromosomal aberration by OASIS	No alert found	No alert found	No alert found	No alert found	AN2 AN2 >> Michael addition to activated double bonds AN2 >> Michael addition to activated double bonds >> alpha, beta- Unsaturated Carbonyls and Related Compounds	No alert found	No alert found	No alert found

InertFinder/ChemID Plus Name	1-p-Menthene-8 thiol	2,3-Hexanedione	2,5-Dimethyl pyrazine	2,6-Dimethyl pyrazine	2-Ethyl-3-methylpyrazine	2-Isobutyl- 3-methoxypyrazine	2-Isopropyl- 4-methylthiazole	2-Methoxy- 3-(1-methylpropyl) pyrazine	2-Methyl- 4-propyl- 1,3-oxathiane
CAS	71159-90-5	3848-24-6	123-32-0	108-50-9	15707-23-0	24683-00-9	15679-13-7	24168-70-5	67715-80-4
SMILES	CC1=CCC(CC1)C(C)(C)S	CCCC(=O)C(C)=O	Cc1cnc(C) cn1	Cc1cncc(C)n1	CCc1nccn c1C	COc1nccn c1CC(C)C	CC(C)c1sc c(C)n1	CCC(C)c1 nccnc1OC	CCCC1CC OC(C)S1
Ionization at pH = 1	Acidic [0.000, 10.000) No pKb value	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [70.000, 80.000)	Acidic [0.000, 10.000) Basic [90.000, 100.000]	Acidic [0.000, 10.000) Basic [70.000, 80.000)	Acidic [0.000, 10.000) Basic [40.000, 50.000)	Acidic [0.000, 10.000) Basic [90.000, 100.000]	Acidic [0.000, 10.000) Basic [40.000, 50.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)
Biodegradation ultimate (Biowin 3)	Weeks to months	Weeks	Weeks	Weeks	Weeks	Weeks to months	Weeks to months	Weeks to months	Weeks
Estrogen Receptor Binding	Non binder, without OH or NH2 group	Non binder, non cyclic structure	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group
Biodeg BioHC half-life (Biowin)	No value	No value	No value	No value	No value	No value	No value	No value	No value
Hydrolysis half-life (pH 6.5-7.4)	No value	No value	No value	No value	No value	No value	No value	No value	No value
Biodegradation probability (Biowin 5)	Does NOT Biodegrade Fast	Biodegrades Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast
Toxic hazard classification by Cramer	Low (Class I)	High (Class III)	Intermediate (Class II)	High (Class III)	High (Class III)	High (Class III)	High (Class III)	High (Class III)	High (Class III)
Biodegradation	Does NOT	Biodegrades	Biodegrade	Biodegrade	Biodegrades	Biodegrades	Biodegrade	Biodegrade	Does NOT

InertFinder/ChemID Plus Name	1-p-Menthene-8 thiol	2,3-Hexanedione	2,5-Dimethyl pyrazine	2,6-Dimethyl pyrazine	2-Ethyl-3-methylpyrazine	2-Isobutyl- 3-methoxypyrazine	2-Isopropyl- 4-methylthiazole	2-Methoxy- 3-(1-methylpropyl) pyrazine	2-Methyl- 4-propyl- 1,3-oxathiane
probability (Biowin 2)	Biodegrade Fast	Fast	s Fast	s Fast	Fast	Fast	s Fast	s Fast	Biodegrade Fast
Ionization at pH = 4	Acidic [0.000, 10.000) No pKb value	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [10.000, 20.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [30.000, 40.000) Basic [0.000, 10.000)
Protein binding potency Lys (DPRA 13%)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Thiols and disulfides (non reactive)	Out of mechanistic domain	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein binding alert	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein binding alert	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein binding alert	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein binding alert	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein binding alert	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein binding alert	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein binding alert
Protein binding potency Cys (DPRA 13%)	DPRA above 21% (DPRA 13%) DPRA above 21% (DPRA 13%) >> Thiols (reactive)	DPRA above 21% (DPRA 13%) DPRA above 21% (DPRA 13%) >> 1,2- and 1,3-	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >>	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >>	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >>

InertFinder/ChemID Plus Name	1-p-Menthene-8 thiol	2,3-Hexanedione	2,5-Dimethyl pyrazine	2,6-Dimethyl pyrazine	2-Ethyl-3-methylpyrazine	2-Isobutyl- 3-methoxypyrazine	2-Isopropyl- 4-methylthiazole	2-Methoxy- 3-(1-methylpropyl) pyrazine	2-Methyl- 4-propyl- 1,3-oxathiane
		Diketones (reactive)	binding alert	No protein binding alert	binding alert	binding alert	No protein binding alert	binding alert	No protein binding alert
Hydrolysis half-life (Kb, pH 8) (Hydrowin)	No value	No value	No value	No value	No value	No value	No value	No value	No value
Hydrolysis half-life (Kb, pH 7) (Hydrowin)	No value	No value	No value	No value	No value	No value	No value	No value	No value
Biodegradation probability (Biowin 6)	Does NOT Biodegrade Fast	Biodegrades Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast
Protein binding by OECD	SN2 SN2 >> SN2 reaction at a sulphur atom SN2 >> SN2 reaction at a sulphur atom >> Thiols	Schiff Base Formers Schiff Base Formers >> Direct Acting Schiff Base Formers Schiff Base Formers >> Direct Acting Schiff Base Formers >> 1-2-Dicarbonyls	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found

InertFinder/ChemID Plus Name	1-p-Menthene-8 thiol	2,3-Hexanedione	2,5-Dimethyl pyrazine	2,6-Dimethyl pyrazine	2-Ethyl-3-methylpyrazine	2-Isobutyl- 3-methoxypyrazine	2-Isopropyl- 4-methylthiazole	2-Methoxy- 3-(1-methylpropyl) pyrazine	2-Methyl- 4-propyl- 1,3-oxathiane
Ultimate biodeg	No data	No data	No data	No data	> 100 days	No data	No data	No data	No data
Ionization at pH = 9	Acidic [0.000, 10.000) No pKb value	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [60.000, 70.000) Basic [0.000, 10.000)	Acidic [60.000, 70.000) Basic [0.000, 10.000)	Acidic [60.000, 70.000) Basic [0.000, 10.000)	Acidic [60.000, 70.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [60.000, 70.000) Basic [0.000, 10.000)	Acidic [90.000, 100.000] Basic [0.000, 10.000)
Hydrolysis half-life (Ka, pH 7) (Hydrowin)	No value	No value	No value	No value	No value	No value	No value	No value	No value
Toxic hazard classification by Cramer (extended)	Low (Class I)	High (Class III)	Intermediate (Class II)	High (Class III)	High (Class III)	High (Class III)	High (Class III)	High (Class III)	High (Class III)
Biodegradation probability (Biowin 7)	Does NOT Biodegrade Fast	Biodegrades Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Does NOT Biodegrade Fast
DNA binding by OASIS	Radical Radical >> Radical mechanism via ROS formation (indirect) Radical >> Radical mechanism via ROS formation	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found

InertFinder/ChemID Plus Name	1-p-Menthene-8 thiol	2,3-Hexanedione	2,5-Dimethyl pyrazine	2,6-Dimethyl pyrazine	2-Ethyl-3-methylpyrazine	2-Isobutyl- 3-methoxypyrazine	2-Isopropyl- 4-methylthiazole	2-Methoxy- 3-(1-methylpropyl) pyrazine	2-Methyl- 4-propyl- 1,3-oxathiane
	(indirect) >> Thiols								
Ionization at pH = 7.4	Acidic [0.000, 10.000) No pKb value	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [90.000, 100.000] Basic [0.000, 10.000)
Hydrolysis half-life (Ka, pH 8) (Hydrowin)	No value	No value	No value	No value	No value	No value	No value	No value	No value
Protein binding by OASIS	SN2 SN2 >> Interchange reaction with sulphur containing compounds SN2 >> Interchange reaction with sulphur containing compounds >> Thiols	Schiff base formation Schiff base formation >> Direct acting Schiff base formers Schiff base formation >> Direct acting Schiff base formers >> 1,2-Dicarbonyls	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found

InertFinder/ChemID Plus Name	1-p-Menthene-8 thiol	2,3-Hexanedione	2,5-Dimethyl pyrazine	2,6-Dimethyl pyrazine	2-Ethyl-3-methylpyrazine	2-Isobutyl- 3-methoxypyrazine	2-Isopropyl- 4-methylthiazole	2-Methoxy- 3-(1-methylpropyl) pyrazine	2-Methyl- 4-propyl- 1,3-oxathiane
		and 1,3-Dicarbonyls							
DNA binding by OECD	No alert found	Schiff base formers Schiff base formers >> Direct Acting Schiff Base Formers Schiff base formers >> Direct Acting Schiff Base Formers >> Alpha-beta-dicarbonyl	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found
Biodegradation probability (Biowin 1)	Does NOT Biodegrade Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Does NOT Biodegrade Fast
Biodegradation primary (Biowin 4)	Days to weeks	Days to weeks	Days to weeks	Days to weeks	Days to weeks	Days to weeks	Days to weeks	Days to weeks	Days to weeks
Carcinogenicity (genotox and nongenotox) alerts by ISS	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found
in vitro mutagenicity	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found

InertFinder/ChemID Plus Name	1-p-Menthene-8 thiol	2,3-Hexanedione	2,5-Dimethyl pyrazine	2,6-Dimethyl pyrazine	2-Ethyl-3-methylpyrazine	2-Isobutyl- 3-methoxypyrazine	2-Isopropyl- 4-methylthiazole	2-Methoxy- 3-(1-methylpropyl) pyrazine	2-Methyl- 4-propyl- 1,3-oxathiane
(Ames test) alerts by ISS									
in vivo mutagenicity (Micronucleus) alerts by ISS	No alert found	H-acceptor-path3-H-acceptor	H-acceptor-path3-H-acceptor	H-acceptor-path3-H-acceptor	H-acceptor-path3-H-acceptor	H-acceptor-path3-H-acceptor	No alert found	H-acceptor-path3-H-acceptor	No alert found
Protein Binding Potency h-CLAT	Thiols and disulfides	1,2- and 1,3-Dicarbonyls	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found
Skin irritation/corrosion Inclusion rules by BfR	Inclusion rules not met	Ketones	Inclusion rules not met	Inclusion rules not met	Inclusion rules not met	Inclusion rules not met	Inclusion rules not met	Inclusion rules not met	Inclusion rules not met
DNA alerts for AMES, CA and MNT by OASIS	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found
Protein binding alerts for skin sensitization by OASIS	SN2 SN2 >> Interchange reaction with sulphur containing compounds SN2 >> Interchange reaction with sulphur containing compounds >> Thiols and	Schiff base formation Schiff base formation >> Direct acting Schiff base formers Schiff base formation >> Direct acting Schiff base formers >> 1,2-	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found

InertFinder/ChemID Plus Name	1-p-Menthene-8 thiol	2,3-Hexanedione	2,5-Dimethyl pyrazine	2,6-Dimethyl pyrazine	2-Ethyl-3-methylpyrazine	2-Isobutyl- 3-methoxypyrazine	2-Isopropyl- 4-methylthiazole	2-Methoxy- 3-(1-methylpropyl) pyrazine	2-Methyl- 4-propyl- 1,3-oxathiane
	disulfide compounds	Dicarbonyls and 1,3-Dicarbonyls							
rtER Expert System - USEPA	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found
Skin irritation/corrosion Exclusion rules by BfR	Undefined	Undefined	Undefined	Undefined	Undefined	Undefined	Undefined	Undefined	Undefined
Protein binding alerts for Chromosomal aberration by OASIS	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found

InertFinder/ChemID Plus Name	2-Methylpyrazine	2-Nonanone	2-Octanone	2-Tridecanone	2-Undecanone	3,4-Dimethyl-1,2-cyclopentadione	3-Heptanone	3-Methyl-1-cyclopentadecanone	3-Methyl- 2-(2-pentenyl)- 2-cyclopenten-1-one	3-Methyl- 2-(n- pentanyl)- 2- cyclopenten-1-one	3-Methyl- 5-(2,2,3-trimethyl- 3-cyclopenten-1- yl) pent-4-en-2-ol
CAS	109-08-0	821-55-6	111-13-7	593-08-8	112-12-9	13494-06-9	106-35-4	541-91-3	488-10-8; 6261-18-3	1128-08-1	67801-20-1
SMILES	Cc1cnccn 1	CCCCCCCC(C)=O	CCCCCCC(C)=O	CCCCCCCCCCCC(C)=O	CCCCCCCCCC(C)=O	CC1CC(=O)C(=O)C1C	CCCCC(=O)CC	CC1CCCCCCCCCCCC(=O)C1	CCC=CCC1=C(CCC1=O)C	CCCCCC1=C(C)CCC 1=O	CC(O)C(C)\C=C/C1CC=C(C)C1(C)C
Ionization at pH = 1	Acidic [0.000, 10.000) Basic [70.000, 80.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) No pKb value	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)
Biodegradation ultimate (Biowin 3)	Weeks	Weeks	Weeks	Weeks	Weeks	Weeks	Weeks	Weeks to months	Weeks	Weeks	Weeks to months
Estrogen Receptor Binding	Non binder, without OH or NH2 group	Non binder, non cyclic structure	Non binder, non cyclic structure	Non binder, non cyclic structure	Non binder, non cyclic structure	Non binder, without OH or NH2 group	Non binder, non cyclic structure	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group
Biodeg BioHC half-life (Biowin)	No value	No value	No value	No value	No value	No value	No value	No value	No value	No value	No value
Hydrolysis half-life (pH 6.5-7.4)	No value	No value	No value	No value	No value	No value	No value	No value	No value	No value	No value
Biodegradation probability	Does NOT Biodegrad	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Does NOT Biodegrade	Biodegrades Fast	Does NOT Biodegrad	Does NOT Biodegrade	Biodegrades Fast	Does NOT Biodegrade

InertFinder/ChemID Plus Name	2-Methylpyrazine	2-Nonanone	2-Octanone	2-Tridecanone	2-Undecanone	3,4-Dimethyl-1,2-cyclopentadione	3-Heptanone	3-Methyl-1-cyclopentadecanone	3-Methyl- 2-(2-pentenyl)- 2-cyclopenten-1-one	3-Methyl- 2-(n- pentanyl)- 2- cyclopenten-1-one	3-Methyl- 5-(2,2,3-trimethyl- 3-cyclopent en-1- yl) pent-4-en-2-ol
(Biowin 5)	e Fast					Fast		e Fast	Fast		Fast
Toxic hazard classification by Cramer	Intermediate (Class II)	Intermediate (Class II)	Intermediate (Class II)	Intermediate (Class II)	Intermediate (Class II)	Intermediate (Class II)	Intermediate (Class II)	Intermediate (Class II)	Intermediate (Class II)	Intermediate (Class II)	Low (Class I)
Biodegradation probability (Biowin 2)	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Biodegrades Fast	Does NOT Biodegrade Fast
Ionization at pH = 4	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) No pKb value	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)
Protein binding potency Lys (DPRA 13%)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein binding alert	Out of mechanistic domain	Out of mechanistic domain	Out of mechanistic domain	Out of mechanistic domain	Out of mechanistic domain	Out of mechanistic domain	Out of mechanistic domain	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Conjugated alpha, beta-unsaturated ketones (non reactive)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Conjugated alpha, beta-unsaturated ketones (non reactive)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Alcohols
Protein binding	DPRA less	Out of	Out of	Out of	Out of	Out of	Out of	Out of	DPRA less	DPRA less	DPRA less

InertFinder/ChemID Plus Name	2-Methylpyrazine	2-Nonanone	2-Octanone	2-Tridecanone	2-Undecanone	3,4-Dimethyl-1,2-cyclopentadione	3-Heptanone	3-Methyl-1-cyclopentadecanone	3-Methyl- 2-(2-pentenyl)- 2-cyclopenten-1-one	3-Methyl- 2-(n- pentanyl)- 2- cyclopenten-1-one	3-Methyl- 5-(2,2,3-trimethyl- 3-cyclopenten-1- yl) pent-4-en-2-ol
potency Cys (DPRA 13%)	than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein binding alert	mechanistic domain	mechanistic domain	mechanistic domain	mechanistic domain	mechanistic domain	mechanistic domain	mechanistic domain	than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein binding alert	than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein binding alert	than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Alcohols
Hydrolysis half-life (Kb, pH 8) (Hydrowin)	No value	No value	No value	No value	No value	No value	No value	No value	No value	No value	No value
Hydrolysis half-life (Kb, pH 7) (Hydrowin)	No value	No value	No value	No value	No value	No value	No value	No value	No value	No value	No value
Biodegradation probability (Biowin 6)	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Biodegrades Fast	Does NOT Biodegrade Fast
Protein binding by OECD	No alert found	No alert found	No alert found	No alert found	No alert found	Schiff Base Formers Schiff Base Formers >> Direct	No alert found	No alert found	No alert found	No alert found	No alert found

InertFinder/ChemID Plus Name	2-Methylpyrazine	2-Nonanone	2-Octanone	2-Tridecanone	2-Undecanone	3,4-Dimethyl-1,2-cyclopentadione	3-Heptanone	3-Methyl-1-cyclopentadecanone	3-Methyl- 2-(2-pentenyl)- 2-cyclopenten-1-one	3-Methyl- 2-(n- pentanyl)- 2- cyclopent en-1-one	3-Methyl- 5-(2,2,3-trimethyl- 3-cyclopent en-1- yl) pent-4-en-2-ol
						Acting Schiff Base Formers Schiff Base Formers >> Direct Acting Schiff Base Formers >> 1-2-Dicarbonyls					
Ultimate biodeg	No data	No data	1 to 10 days 10 to 100 days > 100 days	No data	10 to 100 days	No data	No data	10 to 100 days	No data	No data	10 to 100 days
Ionization at pH = 9	Acidic [60.000, 70.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) No pKb value	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)
Hydrolysis half-life (Ka, pH7) (Hydrowin)	No value	No value	No value	No value	No value	No value	No value	No value	No value	No value	No value

InertFinder/ChemID Plus Name	2-Methylpyrazine	2-Nonanone	2-Octanone	2-Tridecanone	2-Undecanone	3,4-Dimethyl-1,2-cyclopentadione	3-Heptanone	3-Methyl-1-cyclopentadecanone	3-Methyl- 2-(2-pentenyl)- 2-cyclopenten-1-one	3-Methyl- 2-(n- pentanyl)- 2- cyclopent en-1-one	3-Methyl- 5-(2,2,3-trimethyl- 3-cyclopent en-1- yl) pent-4-en-2-ol
Toxic hazard classification by Cramer (extended)	Intermediate (Class II)	Intermediate (Class II)	Intermediate (Class II)	Intermediate (Class II)	Intermediate (Class II)	Intermediate (Class II)	Intermediate (Class II)	Intermediate (Class II)	Intermediate (Class II)	Intermediate (Class II)	Low (Class I)
Biodegradation probability (Biowin 7)	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast
DNA binding by OASIS	No alert found	No alert found	No alert found	No alert found	No alert found	AN2 AN2 >> Schiff base formation AN2 >> Schiff base formation >> Dicarbonyl compounds	No alert found	No alert found	No alert found	No alert found	No alert found
Ionization at pH = 7.4	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) No pKb value	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)
Hydrolysis half-life (Ka, pH 8) (Hydrowin)	No value	No value	No value	No value	No value	No value	No value	No value	No value	No value	No value

InertFinder/ChemID Plus Name	2-Methylpyrazine	2-Nonanone	2-Octanone	2-Tridecanone	2-Undecanone	3,4-Dimethyl-1,2-cyclopentadione	3-Heptanone	3-Methyl-1-cyclopentadecanone	3-Methyl- 2-(2-pentenyl)- 2-cyclopenten-1-one	3-Methyl- 2-(n- pentanyl)- 2- cyclopent en-1-one	3-Methyl- 5-(2,2,3-trimethyl- 3-cyclopent en-1- yl) pent-4-en-2-ol
Protein binding by OASIS	No alert found	No alert found	No alert found	No alert found	No alert found	Schiff base formation Schiff base formation >> Direct acting Schiff base formers Schiff base formation >> Direct acting Schiff base formers >> 1,2-Dicarbonyls and 1,3-Dicarbonyls	No alert found	No alert found	No alert found	No alert found	No alert found
DNA binding by OECD	No alert found	No alert found	No alert found	No alert found	No alert found	Schiff base formers Schiff base formers >> Direct Acting Schiff Base Formers Schiff base formers >>	No alert found	No alert found	No alert found	No alert found	No alert found

InertFinder/ChemID Plus Name	2-Methylpyrazine	2-Nonanone	2-Octanone	2-Tridecanone	2-Undecanone	3,4-Dimethyl-1,2-cyclopentadione	3-Heptanone	3-Methyl-1-cyclopentadecanone	3-Methyl- 2-(2-pentenyl)- 2-cyclopenten-1-one	3-Methyl- 2-(n- pentanyl)- 2- cyclopenten-1-one	3-Methyl- 5-(2,2,3-trimethyl- 3-cyclopenten-1- yl) pent-4-en-2-ol
						Direct Acting Schiff Base Formers >> Alpha-beta-dicarbonyl					
Biodegradation probability (Biowin 1)	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast
Biodegradation primary (Biowin 4)	Days to weeks	Days	Days	Days	Days	Days to weeks	Days	Days to weeks	Days	Days	Days to weeks
Carcinogenicity (genotox and nongenotox) alerts by ISS	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	alpha, beta-unsaturated carbonyls (Genotox) Structural alert for genotoxic carcinogenicity	alpha, beta-unsaturated carbonyls (Genotox) Structural alert for genotoxic carcinogenicity	Structural alert for nongenotoxic carcinogenicity Substituted n-alkylcarboxylic acids (Nongenotox)
in vitro mutagenicity (Ames test)	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	alpha, beta-unsaturate	alpha, beta-unsaturate	No alert found

InertFinder/ChemID Plus Name	2-Methylpyrazine	2-Nonanone	2-Octanone	2-Tridecanone	2-Undecanone	3,4-Dimethyl-1,2-cyclopentadione	3-Heptanone	3-Methyl-1-cyclopentadecanone	3-Methyl- 2-(2-pentenyl)- 2-cyclopenten-1-one	3-Methyl- 2-(n- pentanyl)- 2- cyclopent en-1-one	3-Methyl- 5-(2,2,3-trimethyl- 3-cyclopent en-1- yl) pent-4-en-2-ol
alerts by ISS									d carbonyls	d carbonyls	
in vivo mutagenicity (Micronucleus) alerts by ISS	H-acceptor-path3-H-acceptor	No alert found	No alert found	No alert found	No alert found	H-acceptor-path3-H-acceptor	No alert found	No alert found	alpha, beta-unsaturated carbonyls	alpha, beta-unsaturated carbonyls	No alert found
Protein Binding Potency h-CLAT	No alert found	No alert found	No alert found	No alert found	No alert found	1,2- and 1,3-Dicarbonyls	No alert found	No alert found	alpha, beta-Unsaturted ketones	alpha, beta-Unsaturted ketones	No alert found
Skin irritation/corrosion Inclusion rules by BfR	Inclusion rules not met	Ketones	Ketones	Ketones	Ketones	Ketones	Ketones	Ketones	Ketones	Ketones	Inclusion rules not met
DNA alerts for AMES, CA and MNT by OASIS	No alert found	No alert found	No alert found	No alert found	No alert found	AN2 AN2 >> Schiff base formation AN2 >> Schiff base formation >> Dicarbonyl compounds	No alert found	No alert found	No alert found	No alert found	No alert found

InertFinder/ChemID Plus Name	2-Methylpyrazine	2-Nonanone	2-Octanone	2-Tridecanone	2-Undecanone	3,4-Dimethyl-1,2-cyclopentadione	3-Heptanone	3-Methyl-1-cyclopentadecanone	3-Methyl- 2-(2-pentenyl)- 2-cyclopenten-1-one	3-Methyl- 2-(n- pentanyl)- 2- cyclopent en-1-one	3-Methyl- 5-(2,2,3-trimethyl- 3-cyclopent en-1- yl) pent-4-en-2-ol
Protein binding alerts for skin sensitization by OASIS	No alert found	Nucleophilic addition Nucleophilic addition >> Addition to carbon-hetero double bonds Nucleophilic addition >> Addition to carbon-hetero double bonds >> Ketones	Nucleophilic addition Nucleophilic addition >> Addition to carbon-hetero double bonds Nucleophilic addition >> Addition to carbon-hetero double bonds >> Ketones	Nucleophilic addition Nucleophilic addition >> Addition to carbon-hetero double bonds Nucleophilic addition >> Addition to carbon-hetero double bonds >> Ketones	Nucleophilic addition Nucleophilic addition >> Addition to carbon-hetero double bonds Nucleophilic addition >> Addition to carbon-hetero double bonds >> Ketones	Schiff base formation Schiff base formation >> Direct acting Schiff base formers Schiff base formation >> Direct acting Schiff base formers >> 1,2-Dicarbonyls and 1,3-Dicarbonyls	Nucleophilic addition Nucleophilic addition >> Addition to carbon-hetero double bonds Nucleophilic addition >> Addition to carbon-hetero double bonds >> Ketones	Nucleophilic addition Nucleophilic addition >> Addition to carbon-hetero double bonds Nucleophilic addition >> Addition to carbon-hetero double bonds >> Ketones	No alert found	No alert found	No alert found
rtER Expert System - USEPA	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found
Skin irritation/corrosion Exclusion rules by BfR	Undefined	Undefined	Undefined	Undefined	Undefined	Undefined	Undefined	Group C Melting Point > 55 C	Undefined	Undefined	Undefined

InertFinder/ChemID Plus Name	2-Methylpyrazine	2-Nonanone	2-Octanone	2-Tridecanone	2-Undecanone	3,4-Dimethyl-1,2-cyclopentadione	3-Heptanone	3-Methyl-1-cyclopentadecanone	3-Methyl- 2-(2-pentenyl)- 2-cyclopenten-1-one	3-Methyl- 2-(n- pentanyl)- 2- cyclopent en-1-one	3-Methyl- 5-(2,2,3-trimethyl- 3-cyclopent en-1- yl) pent-4-en-2-ol
								Undefined			
Protein binding alerts for Chromosomal aberration by OASIS	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found

InertFinder/ChemID Plus Name	4-Acetyl-6 t-butyl- 1,1-dimethylindan	4H-Pyran-4-one, 3- hydroxy-2-methyl-	4-Hydroxy-2,5-dimethyl-3(2H)-furanone	5-Methyl-2-phenyl-2- hexenal	5-Methyl-2-thiophenecarboxaldehyde	6,10-Dimethyl undeca-5,9-dien- 2-one
CAS	13171-00-1	118-71-8	3658-77-3	21834-92-4	13679-70-4	689-67-8
SMILES	CC(=O)c1 cc(cc2c1C CC2(C)C)C (C)(C)C	CC1=C(O)C(=O)C=CO1	CC1OC(=C(O)C1= O)C	CC(C)C\C=C(C=O)/c1ccccc1	Cc1sc(C=O)cc1	CC(C)=CC C\C(C)=C\ CCC(C)=O
Ionization at pH = 1	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)
Biodegradation ultimate (Biowin 3)	Months	Weeks	Weeks	Weeks	Weeks	Weeks to months
Estrogen Receptor Binding	Non binder, without OH or NH2 group	Non binder, impaired OH or NH2 group	Non binder, impaired OH or NH2 group	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group	Non binder, non cyclic structure
Biodeg BioHC half-life (Biowin)	No value	No value	No value	No value	No value	No value
Hydrolysis half-life (pH 6.5-7.4)	No value	No value	No value	No value	No value	No value
Biodegradation probability (Biowin 5)	Does NOT Biodegrade Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast
Toxic hazard classification by Cramer	Intermediate (Class II)	Intermediate (Class II)	High (Class III)	Intermediate (Class II)	High (Class III)	Low (Class I)
Biodegradation	Does NOT	Does NOT Biodegrade	Does NOT	Biodegrades Fast	Biodegrades Fast	Does NOT

InertFinder/ChemID Plus Name	4-Acetyl-6 t-butyl- 1,1-dimethylindan	4H-Pyran-4-one, 3- hydroxy-2-methyl-	4-Hydroxy-2,5-dimethyl-3(2H)-furanone	5-Methyl-2-phenyl-2- hexenal	5-Methyl-2-thiophenecarboxaldehyde	6,10-Dimethyl undeca-5,9-dien- 2-one
probability (Biowin 2)	Biodegrade Fast	Fast	Biodegrade Fast			Biodegrade Fast
Ionization at pH = 4	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)
Protein binding potency Lys (DPRA 13%)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Non-conjugate d mono- and diketones (non reactive)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Conjugated alpha, beta-unsaturated ketones (non reactive)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Conjugated alpha, beta-unsaturated ketones (non reactive)	Out of mechanistic domain	Out of mechanistic domain	Out of mechanistic domain
Protein binding potency Cys (DPRA 13%)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein	Out of mechanistic domain	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein binding alert	Out of mechanistic domain	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Non-Conjugated monoaldehydes (non reactive)	Out of mechanistic domain

InertFinder/ChemID Plus Name	4-Acetyl-6 t-butyl- 1,1-dimethylindan	4H-Pyran-4-one, 3- hydroxy-2-methyl-	4-Hydroxy-2,5-dimethyl-3(2H)-furanone	5-Methyl-2-phenyl-2- hexenal	5-Methyl-2-thiophenecarboxaldehyde	6,10-Dimethyl undeca-5,9-dien- 2-one
	binding alert					
Hydrolysis half-life (Kb, pH 8) (Hydrowin)	No value	No value	No value	No value	No value	No value
Hydrolysis half-life (Kb, pH 7) (Hydrowin)	No value	No value	No value	No value	No value	No value
Biodegradation probability (Biowin 6)	Does NOT Biodegrad e Fast	Biodegrades Fast	Biodegrades Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Biodegrades Fast
Protein binding by OECD	No alert found	Michael addition Michael addition >> Quinones and Quinone-type Chemicals Michael addition >> Quinones and Quinone-type Chemicals >> Pyranones (and related nitrogen chemicals)	No alert found	Michael addition Michael addition >> Polarised Alkenes Michael addition >> Polarised Alkenes >> Polarised alkene - aldehydes Schiff Base Formers Schiff Base Formers >> Direct Acting Schiff Base Formers Schiff Base Formers >> Direct Acting Schiff Base Formers >> Mono-carbonyls	No alert found	No alert found
Ultimate biodeg	> 100 days	(N/A)	No data	No data	No data	No data

InertFinder/ChemID Plus Name	4-Acetyl-6 t-butyl- 1,1-dimethylindan	4H-Pyran-4-one, 3- hydroxy-2-methyl-	4-Hydroxy-2,5-dimethyl-3(2H)-furanone	5-Methyl-2-phenyl-2- hexenal	5-Methyl-2-thiophenecarboxaldehyde	6,10-Dimethyl undeca-5,9-dien- 2-one
Ionization at pH = 9	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [90.000, 100.000] Basic [0.000, 10.000)	Acidic [90.000, 100.000] Basic [0.000, 10.000)	Acidic [30.000, 40.000) Basic [0.000, 10.000)	Acidic [90.000, 100.000] Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)
Hydrolysis half-life (Ka, pH 7) (Hydrowin)	No value	No value	No value	No value	No value	No value
Toxic hazard classification by Cramer (extended)	Intermediate (Class II)	Intermediate (Class II)	High (Class III)	Intermediate (Class II)	High (Class III)	Low (Class I)
Biodegradation probability (Biowin 7)	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast
DNA binding by OASIS	No alert found	No alert found	No alert found	AN2 AN2 >> Nucleophilic addition to alpha, beta-unsaturated carbonyl compounds AN2 >> Nucleophilic addition to alpha, beta-unsaturated carbonyl compounds >> Alpha, Beta-Unsaturated Aldehydes AN2 >> Schiff base formation AN2 >> Schiff base formation >> Alpha, Beta- Unsaturated Aldehydes	No alert found	No alert found

InertFinder/ChemID Plus Name	4-Acetyl-6 t-butyl- 1,1-dimethylindan	4H-Pyran-4-one, 3- hydroxy-2-methyl-	4-Hydroxy-2,5-dimethyl-3(2H)-furanone	5-Methyl-2-phenyl-2- hexenal	5-Methyl-2-thiophenecarboxaldehyde	6,10-Dimethyl undeca-5,9-dien- 2-one
Ionization at pH = 7.4	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [90.000, 100.000] Basic [0.000, 10.000)	Acidic [90.000, 100.000] Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [30.000, 40.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)
Hydrolysis half-life (Ka, pH 8)(Hydrowin)	No value	No value	No value	No value	No value	No value
Protein binding by OASIS	No alert found	Michael addition Michael addition >> Michael addition on quinoid type compounds Michael addition >> Michael addition on quinoid type compounds >> Pyranones, Pyridones (and related nitrogen chemicals)	No alert found	Michael addition Michael addition >> Michael addition on alpha, beta-Unsaturated carbonyl compounds Michael addition >> Michael addition on alpha, beta-Unsaturated carbonyl compounds >> alpha, beta-Aldehydes Schiff base formation Schiff base formation >> Schiff base formation with carbonyl compounds Schiff base formation >> Schiff base formation with carbonyl compounds >> Aldehydes	Schiff base formation Schiff base formation >> Schiff base formation with carbonyl compounds Schiff base formation >> Schiff base formation with carbonyl compounds >> Aldehydes	No alert found
DNA binding by OECD	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found

InertFinder/ChemID Plus Name	4-Acetyl-6 t-butyl- 1,1-dimethylindan	4H-Pyran-4-one, 3- hydroxy-2-methyl-	4-Hydroxy-2,5-dimethyl-3(2H)-furanone	5-Methyl-2-phenyl-2- hexenal	5-Methyl-2-thiophenecarboxaldehyde	6,10-Dimethyl undeca-5,9-dien- 2-one
Biodegradation probability (Biowin 1)	Does NOT Biodegrade Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast
Biodegradation primary (Biowin 4)	Weeks	Days	Days	Days	Days	Days to weeks
Carcinogenicity (genotox and nongenotox) alerts by ISS	No alert found	alpha, beta-unsaturated carbonyls (Genotox) Structural alert for genotoxic carcinogenicity	alpha, beta-unsaturated carbonyls (Genotox) Structural alert for genotoxic carcinogenicity	alpha, beta-unsaturated carbonyls (Genotox) Structural alert for genotoxic carcinogenicity	Simple aldehyde (Genotox) Structural alert for genotoxic carcinogenicity	No alert found
in vitro mutagenicity (Ames test) alerts by ISS	No alert found	alpha, beta-unsaturated carbonyls	alpha, beta-unsaturated carbonyls	alpha, beta-unsaturated carbonyls	Simple aldehyde	No alert found
in vivo mutagenicity (Micronucleus) alerts by ISS	No alert found	alpha, beta-unsaturated carbonyls H-acceptor-path3-H-acceptor	alpha, beta-unsaturated carbonyls H-acceptor-path3-H-acceptor	alpha, beta-unsaturated carbonyls	Simple aldehyde	No alert found
Protein Binding Potency h-CLAT	No alert found	Pyranones, Pyridones and related chemicals	No alert found	alpha, beta-Unsaturated aldehydes	No alert found	No alert found
Skin irritation/corrosion Inclusion rules by BfR	Ketones	Ketones	Ketones	Aldehydes	Aldehydes	Ketones
DNA alerts for	No alert	No alert found	No alert found	No alert found	No alert found	No alert

InertFinder/ChemID Plus Name	4-Acetyl-6 t-butyl- 1,1-dimethylindan	4H-Pyran-4-one, 3- hydroxy-2-methyl-	4-Hydroxy-2,5-dimethyl-3(2H)-furanone	5-Methyl-2-phenyl-2- hexenal	5-Methyl-2-thiophenecarboxaldehyde	6,10-Dimethyl undeca-5,9-dien- 2-one
AMES, CA and MNT by OASIS	found					found
Protein binding alerts for skin sensitization by OASIS	No alert found	Michael Addition Michael Addition >> Michael addition on quinoid type compounds Michael Addition >> Michael addition on quinoid type compounds >> Pyranones, Pyridones (and related nitrogen chemicals)	No alert found	Michael Addition Michael Addition >> Michael addition on alpha, beta-Unsaturated carbonyl compounds Michael Addition >> Michael addition on alpha, beta-Unsaturated carbonyl compounds >> alpha, beta-Aldehydes	Schiff base formation Schiff base formation >> Schiff base formation with carbonyl compounds Schiff base formation >> Schiff base formation with carbonyl compounds >> Aldehydes	Nucleophilic addition Nucleophilic addition >> Addition to carbon-hetero double bonds Nucleophilic addition >> Addition to carbon-hetero double bonds >> Ketones
rtER Expert System - USEPA	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found
Skin irritation/corrosion Exclusion rules by BfR	Group C Melting Point > 55 C Undefine d	Group C Melting Point > 55 C Undefined	Group C Melting Point > 55 C Group C Surface Tension > 62 mN/m Undefined	Undefined	Undefined	Undefined

InertFinder/ChemID Plus Name	4-Acetyl-6 t-butyl- 1,1-dimethylindan	4H-Pyran-4-one, 3- hydroxy-2-methyl-	4-Hydroxy-2,5-dimethyl-3(2H)-furanone	5-Methyl-2-phenyl-2- hexenal	5-Methyl-2-thiophenecarboxaldehyde	6,10-Dimethyl undeca-5,9-dien- 2-one
Protein binding alerts for Chromosomal aberration by OASIS	No alert found	AN2 AN2 >> Michael addition to activated double bonds AN2 >> Michael addition to activated double bonds >> alpha, beta-Unsaturated Carbonyls and Related Compounds	No alert found	No alert found	No alert found	No alert found

InertFinder/ChemID Plus Name	6-Methyl-3,5-heptadien-2-one	6-Methyl-5-hepten-2-one	7-Oxabicyclo(2.2.1.)heptane, 1-methyl-4- (1-methylethyl)-	Acetoin	Allyl cinnamate	Allyl heptanoate	Allyl hexanoate	Allyl propionate
CAS	1604-28-0	110-93-0	470-67-7	513-86-0	1866-31-5	142-19-8	123-68-2	2408-20-0
SMILES	CC(C)=C/C=C/C(C)= O	CC(C)=CC CC(C)=O	CC(C)C12 CCC(C)(CC 1)O2	CC(O)C(C) =O	C=CCOC(=O)\C=C \c1ccccc1	CCCCCCC(=O)OCC= C	CCCCCC(= O)OCC=C	CCC(=O)O CC=C
Ionization at pH = 1	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)
Biodegradation ultimate (Biowin 3)	Weeks	Weeks	Weeks to months	Weeks	Weeks	Days to weeks	Days to weeks	Weeks
Estrogen Receptor Binding	Non binder, non cyclic structure	Non binder, non cyclic structure	Non binder, without OH or NH2 group	Non binder, non cyclic structure	Non binder, without OH or NH2 group	Non binder, non cyclic structure	Non binder, non cyclic structure	Non binder, non cyclic structure
Biodeg BioHC half-life (Biowin)	No value	No value	No value	No value	No value	No value	No value	No value
Hydrolysis half-life (pH 6.5-7.4)	No value	No value	No value	No value	Very slow	Moderate	Moderate	Moderate
Biodegradation probability (Biowin 5)	Biodegrades Fast	Biodegrades Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast
Toxic hazard classification by Cramer	Low (Class I)	Low (Class I)	High (Class III)	Low (Class I)	High (Class III) Intermediate (Class II)	Intermediate (Class II)	Intermediate (Class II)	Intermediate (Class II)
Biodegradation probability (Biowin 2)	Biodegrades Fast	Biodegrades Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast

InertFinder/ChemID Plus Name	6-Methyl-3,5-heptadien-2-one	6-Methyl-5-hepten-2-one	7-Oxabicyclo(2.2.1.)heptane, 1-methyl-4-(1-methylethyl)-	Acetoin	Allyl cinnamate	Allyl heptanoate	Allyl hexanoate	Allyl propionate
Ionization at pH = 4	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)
Protein binding potency Lys (DPRA 13%)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Conjugated alpha, beta- unsaturated ketones (non reactive)	Out of mechanistic domain	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein binding alert	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Alcohols	Out of mechanistic domain	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Non-Conjugate d carboxylic acids and esters (non reactive)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Non-Conjugate d carboxylic acids and esters (non reactive)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Non-Conjugate d carboxylic acids and esters (non reactive)
Protein binding potency Cys (DPRA 13%)	Grey zone 9-21% (DPRA 13%) Grey zone 9-21% (DPRA 13%) >> Conjugated alpha, beta-unsaturated ketones (Grey zone)	Out of mechanistic domain	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein binding alert	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Alcohols	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Other alpha, beta-unsaturated compounds with polarized double bonds (non reactive)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Non-Conjugate d carboxylic	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Non-Conjugate d carboxylic	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Non-Conjugate d carboxylic

InertFinder/ChemID Plus Name	6-Methyl-3,5-heptadien-2-one	6-Methyl-5-hepten-2-one	7-Oxabicyclo(2.2.1.)heptane, 1-methyl-4- (1-methylethyl)-	Acetoin	Allyl cinnamate	Allyl heptanoate	Allyl hexanoate	Allyl propionate
						acids and esters (non reactive)	acids and esters (non reactive)	acids and esters (non reactive)
Hydrolysis half-life (Kb, pH 8) (Hydrowin)	No value	No value	No value	No value	> 100 days	10 to 100 days	10 to 100 days	10 to 100 days
Hydrolysis half-life (Kb, pH 7) (Hydrowin)	No value	No value	No value	No value	> 100 days	> 100 days	> 100 days	> 100 days
Biodegradation probability (Biowin 6)	Biodegrades Fast	Biodegrades Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast
Protein binding by OECD	Michael addition Michael addition >> Polarised Alkenes Michael addition >> Polarised Alkenes >> Polarised alkene - ketones	No alert found	No alert found	No alert found	Michael addition Michael addition >> Polarised Alkenes Michael addition >> Polarised Alkenes >> Polarised alkene - esters SN2 SN2 >> SN2 reaction at sp3 carbon atom SN2 >> SN2 reaction at sp3 carbon atom >>	SN2 SN2 >> SN2 reaction at sp3 carbon atom SN2 >> SN2 reaction at sp3 carbon atom >> Allyl acetates and related chemicals	SN2 SN2 >> SN2 reaction at sp3 carbon atom SN2 >> SN2 reaction at sp3 carbon atom >> Allyl acetates and related chemicals	SN2 SN2 >> SN2 reaction at sp3 carbon atom SN2 >> SN2 reaction at sp3 carbon atom >> Allyl acetates and related chemicals

InertFinder/ChemID Plus Name	6-Methyl-3,5-heptadien-2-one	6-Methyl-5-hepten-2-one	7-Oxabicyclo(2.2.1.)heptane, 1-methyl-4-(1-methylethyl)-	Acetoin	Allyl cinnamate	Allyl heptanoate	Allyl hexanoate	Allyl propionate
					Allyl acetates and related chemicals			
Ultimate biodeg	No data	1 to 10 days 10 to 100 days	No data	10 to 100 days	1 to 10 days	1 to 10 days 10 to 100 days	1 to 10 days 10 to 100 days	0 to 1 day 1 to 10 days 10 to 100 days
Ionization at pH = 9	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)
Hydrolysis half-life (Ka, pH 7) (Hydrowin)	No value	No value	No value	No value	No value	No value	No value	No value
Toxic hazard classification by Cramer (extended)	Low (Class I)	Low (Class I)	High (Class III)	Low (Class I)	High (Class III) Intermediate (Class II)	High (Class III)	High (Class III)	High (Class III)
Biodegradation probability (Biowin 7)	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast
DNA binding by OASIS	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found

InertFinder/ChemID Plus Name	6-Methyl-3,5-heptadien-2-one	6-Methyl-5-hepten-2-one	7-Oxabicyclo(2.2.1.)heptane, 1-methyl-4- (1-methylethyl)-	Acetoin	Allyl cinnamate	Allyl heptanoate	Allyl hexanoate	Allyl propionate
Ionization at pH = 7.4	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)
Hydrolysis half-life (Ka, pH 8) (Hydrowin)	No value	No value	No value	No value	No value	No value	No value	No value
Protein binding by OASIS	Michael addition Michael addition >> Michael addition on conjugated systems with electron withdrawing group Michael addition >> Michael addition on conjugated systems with electron withdrawing group >> alpha, beta-Carbonyl compounds with polarized double bonds	No alert found	No alert found	No alert found	Michael addition Michael addition >> Michael addition on conjugated systems with electron withdrawing group Michael addition >> Michael addition on conjugated systems with electron withdrawing group >> alpha, beta-Carbonyl compounds with polarized double bonds	SN2 SN2 >> SN2 Reaction at a sp3 carbon atom SN2 >> SN2 Reaction at a sp3 carbon atom >> Activated alkyl esters and thioesters	SN2 SN2 >> SN2 Reaction at a sp3 carbon atom SN2 >> SN2 Reaction at a sp3 carbon atom >> Activated alkyl esters and thioesters	SN2 SN2 >> SN2 Reaction at a sp3 carbon atom SN2 >> SN2 Reaction at a sp3 carbon atom >> Activated alkyl esters and thioesters

InertFinder/ChemID Plus Name	6-Methyl-3,5-heptadien-2-one	6-Methyl-5-hepten-2-one	7-Oxabicyclo(2.2.1.)heptane, 1-methyl-4- (1-methylethyl)-	Acetoin	Allyl cinnamate	Allyl heptanoate	Allyl hexanoate	Allyl propionate
DNA binding by OECD	Michael addition Michael addition >> Polarised Alkenes- Michael addition Michael addition >> Polarised Alkenes-Michael addition >> Alpha, beta-unsaturated ketones	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found
Biodegradation probability (Biowin 1)	Biodegrades Fast	Biodegrades Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast
Biodegradation primary (Biowin 4)	Days to weeks	Days to weeks	Days to weeks	Days	Days	Days	Days	Days
Carcinogenicity (genotox and nongenotox) alerts by ISS	alpha, beta-unsaturated carbonyls (Genotox) Structural alert for genotoxic carcinogenicity	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found
in vitro mutagenicity (Ames test) alerts by ISS	alpha, beta-unsaturated carbonyls	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found
in vivo mutagenicity (Micronucleus)	alpha, beta-unsaturated	No alert found	Oxolane	H-acceptor-	No alert found	No alert found	No alert found	No alert found

InertFinder/ChemID Plus Name	6-Methyl-3,5-heptadien-2-one	6-Methyl-5-hepten-2-one	7-Oxabicyclo(2.2.1.)heptane, 1-methyl-4- (1-methylethyl)-	Acetoin	Allyl cinnamate	Allyl heptanoate	Allyl hexanoate	Allyl propionate
alerts by ISS	carbonyls			path3-H-acceptor				
Protein Binding Potency h-CLAT	alpha, beta-Unsaturated ketones	No alert found	No alert found	No alert found	alpha, beta-Unsaturated esters	No alert found	No alert found	No alert found
Skin irritation/corrosion Inclusion rules by BfR	Ketones	Ketones	Inclusion rules not met	Ketones	Inclusion rules not met	Inclusion rules not met	Inclusion rules not met	Inclusion rules not met
DNA alerts for AMES, CA and MNT by OASIS	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found
Protein binding alerts for skin sensitization by OASIS	Michael Addition Michael Addition >> Michael addition on conjugated systems with electron withdrawing group Michael Addition >> Michael addition on conjugated systems with electron withdrawing group >> alpha, beta-Carbonyl compounds with	Nucleophilic addition Nucleophilic addition >> Addition to carbon-hetero double bonds Nucleophilic addition >> Addition to carbon-hetero	No alert found	Nucleophilic addition Nucleophilic addition >> Addition to carbon-hetero double bonds Nucleophilic addition >> Addition to carbon-hetero	Michael Addition Michael Addition >> Michael addition on conjugated systems with electron withdrawing group Michael Addition >> Michael addition on conjugated systems with electron withdrawing group >> alpha, beta-	SN2 SN2 >> SN2 Reaction at a sp3 carbon atom SN2 >> SN2 Reaction at a sp3 carbon atom >> Activated alkyl esters and thioesters	SN2 SN2 >> SN2 Reaction at a sp3 carbon atom SN2 >> SN2 Reaction at a sp3 carbon atom >> Activated alkyl esters and thioesters	No alert found

InertFinder/ChemID Plus Name	6-Methyl-3,5-heptadien-2-one	6-Methyl-5-hepten-2-one	7-Oxabicyclo(2.2.1.)heptane, 1-methyl-4- (1-methylethyl)-	Acetoin	Allyl cinnamate	Allyl heptanoate	Allyl hexanoate	Allyl propionate
	polarized double bonds	double bonds >> Ketones		double bonds >> Ketones	Carbonyl compounds with polarized double bonds			
rtER Expert System - USEPA	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found
Skin irritation/corrosion Exclusion rules by BfR	Undefined	Undefined	Undefined	Undefined	Undefined	Undefined	Undefined	Undefined
Protein binding alerts for Chromosomal aberration by OASIS	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found

InertFinder/ChemID Plus Name	alpha-Hexylcinnamaldehyde	alpha-Isobutylphenethyl alcohol	Bicyclo[2.2.1]hepta n-2-one, 1,7,7-trimethyl-, (1R,4R)-	Cyclohexanone, 2-(1-methylpropyl)-	Cyclopentane acetai acid, 3- oxo-2-pentyl-, methyl ester	Cycloprop anemethanol, 1- methyl-2- [(1,2,2-trimethyl bicyclo[3.1.0]hex-3-yl)methyl]	d,l-Isomenthone	Diisobutyl ketone	Ethyl amyl ketone
CAS	101-86-0	7779-78-4	464-49-3	14765-30-1	24851-98-7	198404-98-7	491-07-6	108-83-8	106-68-3
SMILES	CCCCCC\C(C=O)=C/c1ccc ccc1	CC(C)CC(O)Cc1ccc cc1	CC1(C)[C@H]2CC[C@@]1(C)C(=O)C2	CCC(C)C1CCCCC1= O	CCCCCC1C(CC C1=O)CC(=O) OC	CC1(C(CC2C1(C2)C)CC3CC3(C)CO)C	CC(C)C1CCC(C)CC1=O	CC(C)CC(=O)CC(C)C	CCCCCC(=O)CC
Ionization at pH = 1	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)
Biodegradation ultimate (Biowin 3)	Weeks	Weeks	Weeks to months	Weeks	Weeks	Months	Weeks	Weeks	Weeks
Estrogen Receptor Binding	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group	Non binder, non cyclic structure	Non binder, non cyclic structure
Biodeg BioHC half-life (Biowin)	No value	No value	No value	No value	No value	No value	No value	No value	No value
Hydrolysis half-life (pH 6.5-7.4)	No value	No value	No value	No value	Slow	No value	No value	No value	No value
Biodegradation	Biodegrades Fast	Does NOT	Does NOT	Does NOT	Biodegrade	Does NOT	Does NOT	Does NOT	Biodegrade

InertFinder/ChemID Plus Name	alpha-Hexylcinnamaldehyde	alpha-Isobutylphenethyl alcohol	Bicyclo[2.2.1]hepta n-2-one, 1,7,7-trimethyl-, (1R,4R)-	Cyclohexanone, 2-(1-methylpropyl)-	Cyclopentane acetai acid, 3- oxo-2-pentyl-, methyl ester	Cycloprop anemethanol, 1- methyl-2- [(1,2,2-trimethyl bicyclo[3.1.0]hex-3-yl)methyl]	d,l-Isomenthone	Diisobutyl ketone	Ethyl amyl ketone
probability (Biowin 5)		Biodegrade Fast	Biodegrade Fast	Biodegrade Fast	s Fast	Biodegrade Fast	Biodegrade Fast	Biodegrade Fast	s Fast
Toxic hazard classification by Cramer	Intermediate (Class II)	Intermediate (Class II)	Intermediate (Class II)	Intermediate (Class II)	High (Class III)	Low (Class I)	Intermediate (Class II)	Intermediate (Class II)	Intermediate (Class II)
Biodegradation probability (Biowin 2)	Biodegrades Fast	Biodegrades Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Biodegrades Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast
Ionization at pH = 4	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)
Protein binding potency Lys (DPRA 13%)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Conjugated alpha, beta- unsaturated aldehydes (non reactive)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Alcohols	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Non-conjugate d mono- and diketones	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Non-conjugate d mono- and diketones	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Non-Conjugated carboxylic acids and esters (non	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Alcohols	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Non-conjugate d mono- and diketones	Out of mechanistic domain	Out of mechanistic domain

InertFinder/ChemID Plus Name	alpha-Hexylcinnamaldehyde	alpha-Isobutylphenethyl alcohol	Bicyclo[2.2.1]hepta n-2-one, 1,7,7-trimethyl-, (1R,4R)-	Cyclohexanone, 2-(1-methylpropyl)-	Cyclopentane acetai acid, 3- oxo-2-pentyl-, methyl ester	Cycloprop anemethanol, 1- methyl-2- [(1,2,2-trimethyl bicyclo[3.1.0]hex-3-yl)methyl]	d,l-Isomenthone	Diisobutyl ketone	Ethyl amyl ketone
			(non reactive)	(non reactive)	reactive) DPRA less than 9% (DPRA 13%) >> Non-conjugated mono- and diketones (non reactive)		(non reactive)		
Protein binding potency Cys (DPRA 13%)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> alpha alkyl cinnamaldehydes	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Alcohols	Out of mechanistic domain	Out of mechanistic domain	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Non-Conjugated carboxylic acids and esters (non reactive)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Alcohols	Out of mechanistic domain	Out of mechanistic domain	Out of mechanistic domain
Hydrolysis half-life (Kb, pH 8) (Hydrowin)	No value	No value	No value	No value	> 100 days	No value	No value	No value	No value

InertFinder/ChemID Plus Name	alpha-Hexylcinnamaldehyde	alpha-Isobutylphenethyl alcohol	Bicyclo[2.2.1]hepta n-2-one, 1,7,7-trimethyl-, (1R,4R)-	Cyclohexanone, 2-(1-methylpropyl)-	Cyclopentane acetai acid, 3- oxo-2-pentyl-, methyl ester	Cycloprop anemethanol, 1- methyl-2- [(1,2,2-trimethyl bicyclo[3.1.0]hex-3-yl)methyl]	d,l-Isomenthone	Diisobutyl ketone	Ethyl amyl ketone
Hydrolysis half-life (Kb, pH 7) (Hydrowin)	No value	No value	No value	No value	> 100 days	No value	No value	No value	No value
Biodegradation probability (Biowin 6)	Biodegrades Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Biodegrades Fast	Does NOT Biodegrde Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast
Protein binding by OECD	Michael addition Michael addition >> Polarised Alkenes Michael addition >> Polarised Alkenes >> Polarised alkene - aldehydes Schiff Base Formers Schiff Base Formers >> Direct Acting Schiff Base Formers Schiff Base Formers >> Direct Acting Schiff Base Formers >> Mono- carbonyls	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found
Ultimate biodeg	No data	No data	1 to 10 days 10 to 100 days	10 to 100 days	1 to 10 days 10 to 100 days	> 100 days	10 to 100 days	1 to 10 days 10 to 100 days	1 to 10 days 10 to 100 days

InertFinder/ChemID Plus Name	alpha-Hexylcinnamaldehyde	alpha-Isobutylphenethyl alcohol	Bicyclo[2.2.1]hepta n-2-one, 1,7,7-trimethyl-, (1R,4R)-	Cyclohexanone, 2-(1-methylpropyl)-	Cyclopentane acetai acid, 3- oxo-2-pentyl-, methyl ester	Cycloprop anemethanol, 1- methyl-2- [(1,2,2-trimethyl bicyclo[3.1.0]hex-3-yl)methyl]	d,l-Isomenthone	Diisobutyl ketone	Ethyl amyl ketone
Ionization at pH = 9	Acidic [40.000, 50.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)
Hydrolysis half-life (Ka, pH 7) (Hydrowin)	No value	No value	No value	No value	No value	No value	No value	No value	No value
Toxic hazard classification by Cramer (extended)	Intermediate (Class II)	Intermediate (Class II)	Intermediate (Class II)	Intermediate (Class II)	High (Class III)	Low (Class I)	Intermediate (Class II)	Intermediate (Class II)	Intermediate (Class II)
Biodegradation probability (Biowin 7)	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrde Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast
DNA binding by OASIS	AN2 AN2 >> Nucleophilic addition to alpha, beta- unsaturated carbonyl compounds AN2 >> Nucleophilic addition to alpha, beta- unsaturated carbonyl compounds	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found

InertFinder/ChemID Plus Name	alpha-Hexylcinnamaldehyde	alpha-Isobutylphenethyl alcohol	Bicyclo[2.2.1]hepta n-2-one, 1,7,7-trimethyl-, (1R,4R)-	Cyclohexanone, 2-(1-methylpropyl)-	Cyclopentane acetai acid, 3- oxo-2-pentyl-, methyl ester	Cycloprop anemethanol, 1- methyl-2- [(1,2,2-trimethyl bicyclo[3.1.0]hex-3-yl)methyl]	d,l-Isomenthone	Diisobutyl ketone	Ethyl amyl ketone
	>> Alpha, Beta-Unsaturated Aldehydes AN2 >> Schiff base formation AN2 >> Schiff base formation >> Alpha, Beta-Unsaturated Aldehydes								
Ionization at pH = 7.4	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)
Hydrolysis half-life (Ka, pH 8) (Hydrowin)	No value	No value	No value	No value	No value	No value	No value	No value	No value
Protein binding by OASIS	Michael addition Michael addition >> Michael addition on alpha, beta-Unsaturated carbonyl compounds Michael addition >>	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found

InertFinder/ChemID Plus Name	alpha-Hexylcinnamaldehyde	alpha-Isobutylphenethyl alcohol	Bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-, (1R,4R)-	Cyclohexanone, 2-(1-methylpropyl)-	Cyclopentane acetaic acid, 3-oxo-2-pentyl-, methyl ester	Cyclopropanemethanol, 1-methyl-2-[(1,2,2-trimethylbicyclo[3.1.0]hex-3-yl)methyl]	d,l-Isomenthone	Diisobutyl ketone	Ethyl amyl ketone
	Michael addition on alpha, beta-Unsaturated carbonyl compounds >> alpha, beta-Aldehydes Schiff base formation Schiff base formation >> Schiff base formation with carbonyl compounds Schiff base formation >> Schiff base formation with carbonyl compounds >> Aldehydes								
DNA binding by OECD	No alert found	Michael addition Michael addition >> P450 Mediated Activation to Quinones and Quinone-type Chemicals Michael addition >> P450	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found

InertFinder/ChemID Plus Name	alpha-Hexylcinnamaldehyde	alpha-Isobutylphenethyl alcohol	Bicyclo[2.2.1]hepta n-2-one, 1,7,7-trimethyl-, (1R,4R)-	Cyclohexanone, 2-(1-methylpropyl)-	Cyclopentane acetai acid, 3- oxo-2-pentyl-, methyl ester	Cycloprop anemethanol, 1- methyl-2- [(1,2,2-trimethyl bicyclo[3.1.0]hex-3-yl)methyl]	d,l-Isomenthone	Diisobutyl ketone	Ethyl amyl ketone
		Mediated Activation to Quinones and Quinone-type Chemicals >> Arenes							
Biodegradation probability (Biowin 1)	Biodegrades Fast	Biodegrades Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Biodegrades Fast	Does NOT Biodegrde Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast
Biodegradation primary (Biowin 4)	Days	Days to weeks	Days to weeks	Days to weeks	Days	Weeks	Days to weeks	Days to weeks	Days
Carcinogenicity (genotox and nongenotox) alerts by ISS	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found
in vitro mutagenicity (Ames test) alerts by ISS	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found
in vivo mutagenicity (Micronucleus) alerts by ISS	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found
Protein Binding	No alert found	No alert found	No alert	No alert	No alert	No alert	No alert	No alert	No alert

InertFinder/ChemID Plus Name	alpha-Hexylcinnamaldehyde	alpha-Isobutylphenethyl alcohol	Bicyclo[2.2.1]hepta n-2-one, 1,7,7-trimethyl-, (1R,4R)-	Cyclohexanone, 2-(1-methylpropyl)-	Cyclopentane acetai acid, 3- oxo-2-pentyl-, methyl ester	Cycloprop anemethanol, 1- methyl-2- [(1,2,2-trimethyl bicyclo[3.1.0]hex-3-yl)methyl]	d,l-Isomenthone	Diisobutyl ketone	Ethyl amyl ketone
Potency h-CLAT			found	found	found	found	found	found	found
Skin irritation/corrosion Inclusion rules by BfR	Aldehydes	Inclusion rules not met	Ketones	Ketones	Ketones	Inclusion rules not met	Ketones	Ketones	Ketones
DNA alerts for AMES, CA and MNT by OASIS	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found
Protein binding alerts for skin sensitization by OASIS	Michael Addition Michael Addition >> Michael addition on alpha, beta-Unsaturated carbonyl compounds Michael Addition >> Michael addition on alpha, beta-Unsaturated carbonyl compounds >> alpha, beta-Aldehydes	No alert found	Nucleophilic addition Nucleophilic addition >> Addition to carbon-hetero double bonds Nucleophilic addition >> Addition to carbon-hetero double	Nucleophilic addition Nucleophilic addition >> Addition to carbon-hetero double bonds Nucleophilic addition >> Addition to carbon-hetero double	Nucleophilic addition Nucleophilic addition >> Addition to carbon-hetero double bonds Nucleophilic addition >> Addition to carbon-hetero double bonds >> Ketones	No alert found	Nucleophilic addition Nucleophilic addition >> Addition to carbon-hetero double bonds Nucleophilic addition >> Addition to carbon-hetero double	Nucleophilic addition Nucleophilic addition >> Addition to carbon-hetero double bonds Nucleophilic addition >> Addition to carbon-hetero double	Nucleophilic addition Nucleophilic addition >> Addition to carbon-hetero double bonds Nucleophilic addition >> Addition to carbon-hetero double

InertFinder/ChemID Plus Name	alpha-Hexylcinnamaldehyde	alpha-Isobutylphenethyl alcohol	Bicyclo[2.2.1]hepta n-2-one, 1,7,7-trimethyl-, (1R,4R)-	Cyclohexanone, 2-(1-methylpropyl)-	Cyclopentane acetai acid, 3- oxo-2-pentyl-, methyl ester	Cycloprop anemethanol, 1- methyl-2- [(1,2,2-trimethyl bicyclo[3.1.0]hex-3-yl)methyl]	d,l-Isomenthone	Diisobutyl ketone	Ethyl amyl ketone
			bonds >> Ketones	bonds >> Ketones			bonds >> Ketones	bonds >> Ketones	bonds >> Ketones
rtER Expert System - USEPA	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found
Skin irritation/corrosion Exclusion rules by BfR	Undefined	Undefined	Undefined	Undefined	Group C Melting Point > 55 C Undefined	Group C Melting Point > 55 C Undefined	Undefined	Undefined	Undefined
Protein binding alerts for Chromosomal aberration by OASIS	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found

InertFinder/ChemID Plus Name	Ethyl maltol	Ethyl vanillin	Heptanal, 2-(phenylmethylene)-	Isojasmone	Maltyl isobutyrate	Methyl n-amyl ketone	Methyl phenethyl ether	Methylcyclopentenolone
CAS	4940-11-8	121-32-4	122-40-7	11050-62-7	65416-14-0	110-43-0	3558-60-9	80-71-7
SMILES	CCC1=C(O)C(=O)C =CO1	CCOc1cc(C=O)ccc1O	CCCCC/C(C=O)=C/c1cc ccc1	CC/C=C/C C1=C(C)C(=O)CC1	CC(C)C(=O)OC1 =C(C)OC=CC1=O	CCCCCC(C)=O	COCCc1ccccc1	CC1=C(O) C(=O)CC1
Ionization at pH = 1	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) No pKb value	Acidic [0.000, 10.000) No pKb value	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)
Biodegradation ultimate (Biowin 3)	Weeks	Weeks	Weeks	Weeks	Weeks	Weeks	Weeks	Weeks
Estrogen Receptor Binding	Non binder, impaired OH or NH2 group	Weak binder, OH group	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group	Non binder, non cyclic structure	Non binder, without OH or NH2 group	Non binder, impaired OH or NH2 group
Biodeg BioHC half-life (Biowin)	No value	No value	No value	No value	No value	No value	No value	No value
Hydrolysis half-life (pH 6.5-7.4)	No value	No value	No value	No value	Fast	No value	No value	No value
Biodegradation probability (Biowin 5)	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Biodegrades Fast	Does NOT Biodegrade Fast	Biodegrades Fast
Toxic hazard classification by Cramer	Intermediate (Class II)	Intermediate (Class II)	Intermediate (Class II)	Intermediate (Class II)	High (Class III)	Intermediate (Class II)	Intermediate (Class II)	High (Class III)
Biodegradation probability (Biowin 2)	Does NOT Biodegrade Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast

InertFinder/ChemID Plus Name	Ethyl maltol	Ethyl vanillin	Heptanal, 2-(phenylmethylene)-	Isojasmone	Maltyl isobutyrate	Methyl n-amyl ketone	Methyl phenethyl ether	Methylcyclopentenolone
Ionization at pH = 4	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) No pKb value	Acidic [0.000, 10.000) No pKb value	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)
Protein binding potency Lys (DPRA 13%)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Conjugated alpha, beta-unsaturated ketones (non reactive)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Vaniline derivatives Grey zone 9-21% (DPRA 13%) Grey zone 9-21% (DPRA 13%) >> Non- alpha, beta-conjugated monoaldehydes (Grey zone)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Conjugated alpha, beta- unsaturated aldehydes (non reactive)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Conjugate d alpha, beta-unsaturated ketones (non reactive)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Conjugated alpha, beta-unsaturated ketones (non reactive)	Out of mechanistic domain	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein binding alert	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Conjugate d alpha, beta- unsaturated ketones (non reactive)
Protein binding potency Cys (DPRA 13%)	Out of mechanistic domain	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> alpha alkyl cinnamaldehydes	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%)	Out of mechanistic domain	Out of mechanistic domain	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein binding alert

InertFinder/ChemID Plus Name	Ethyl maltol	Ethyl vanillin	Heptanal, 2-(phenylmethylene)-	Isojasmone	Maltyl isobutyrate	Methyl n-amyl ketone	Methyl phenethyl ether	Methylcyclopentenolone
		>> Non-Conjugated monoaldehydes (non reactive) DPRA less than 9% (DPRA 13%) >> Vaniline derivatives		>> No protein binding alert			>> No protein binding alert	
Hydrolysis half-life (Kb, pH 8) (Hydrowin)	No value	No value	No value	No value	> 100 days	No value	No value	No value
Hydrolysis half-life (Kb, pH 7) (Hydrowin)	No value	No value	No value	No value	> 100 days	No value	No value	No value
Biodegradation probability (Biowin 6)	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Does NOT Biodegrade Fast	Biodegrades Fast
Protein binding by OECD	Michael addition Michael addition >> Quinones and Quinone-type Chemicals Michael addition >> Quinones and Quinone-	No alert found	Michael addition Michael addition >> Polarised Alkenes Michael addition >> Polarised Alkenes >> Polarised alkene - aldehydes Schiff Base Formers Schiff Base Formers >> Direct Acting Schiff Base Formers	No alert found	Acylation Acylation >> Direct Acylation Involving a Leaving group Acylation >> Direct Acylation Involving a Leaving group	No alert found	No alert found	No alert found

InertFinder/ChemID Plus Name	Ethyl maltol	Ethyl vanillin	Heptanal, 2-(phenylmethylene)-	Isojasmone	Maltyl isobutyrate	Methyl n-amyl ketone	Methyl phenethyl ether	Methylcyclopentenolone
	type Chemicals >> Pyranones (and related nitrogen chemicals)		Schiff Base Formers >> Direct Acting Schiff Base Formers >> Mono-carbonyls		>> Acetates Michael addition Michael addition >> Quinones and Quinone-type Chemicals Michael addition >> Quinones and Quinone-type Chemicals >> Pyranones (and			
Ultimate biodeg	(N/A)	0 to 1 day 1 to 10 days	10 to 100 days	No data	No data	10 to 100 days	10 to 100 days	10 to 100 days
Ionization at pH = 9	Acidic [90.000, 100.000] Basic [0.000, 10.000)	Acidic [80.000, 90.000) Basic [0.000, 10.000)	Acidic [40.000, 50.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) No pKb value	Acidic [0.000, 10.000) No pKb value	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)
Hydrolysis half-life (Ka, pH 7) (Hydrowin)	No value	No value	No value	No value	No value	No value	No value	No value
Toxic hazard classification by Cramer (extended)	Intermediate (Class II)	Intermediate (Class II)	Intermediate (Class II)	Intermediate (Class II)	High (Class III)	Intermediate (Class II)	Intermediate (Class II)	High (Class III)

InertFinder/ChemID Plus Name	Ethyl maltol	Ethyl vanillin	Heptanal, 2-(phenylmethylene)-	Isojasmone	Maltyl isobutyrate	Methyl n-amyl ketone	Methyl phenethyl ether	Methylcyclopentenolone
Biodegradation probability (Biowin 7)	Does NOT Biodegrade Fast	Biodegrades Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast
DNA binding by OASIS	No alert found	No alert found	AN2 AN2 >> Nucleophilic addition to alpha, beta-unsaturated carbonyl compounds AN2 >> Nucleophilic addition to alpha, beta-unsaturated carbonyl compounds >> Alpha, Beta-Unsaturated Aldehydes AN2 >> Schiff base formation AN2 >> Schiff base formation >> Alpha, Beta- Unsaturated Aldehydes	No alert found	No alert found	No alert found	No alert found	No alert found
Ionization at pH = 7.4	Acidic [90.000, 100.000] Basic [0.000, 10.000)	Acidic [10.000, 20.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) No pKb value	Acidic [0.000, 10.000) No pKb value	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)
Hydrolysis half-	No value	No value	No value	No value	No value	No value	No value	No value

InertFinder/ChemID Plus Name	Ethyl maltol	Ethyl vanillin	Heptanal, 2-(phenylmethylene)-	Isojasmone	Maltyl isobutyrate	Methyl n-amyl ketone	Methyl phenethyl ether	Methylcyclopentenolone
life (Ka, pH 8) (Hydrowin)								
Protein binding by OASIS	Michael addition Michael addition >> Michael addition on quinoid type compounds Michael addition >> Michael addition on quinoid type compounds >> Pyranones, Pyridones (and related nitrogen chemicals)	No alert found	Michael addition Michael addition >> Michael addition on alpha, beta-Unsaturated carbonyl compounds Michael addition >> Michael addition on alpha, beta-Unsaturated carbonyl compounds >> alpha, beta-Aldehydes Schiff base formation Schiff base formation >> Schiff base formation with carbonyl compounds Schiff base formation >> Schiff base formation with carbonyl compounds >> Aldehydes	No alert found	Michael addition Michael addition >> Michael addition on quinoid type compounds Michael addition >> Michael addition on quinoid type compounds >> Pyranones, Pyridones (and related nitrogen chemicals)	No alert found	No alert found	No alert found

InertFinder/ChemID Plus Name	Ethyl maltol	Ethyl vanillin	Heptanal, 2-(phenylmethylene)-	Isojasmone	Maltyl isobutyrate	Methyl n-amyl ketone	Methyl phenethyl ether	Methylcyclopentenolone
DNA binding by OECD	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	Michael addition Michael addition >> P450 Mediated Activation to Quinones and Quinone-type Chemicals Michael addition >> P450 Mediated Activation to Quinones and Quinone-type Chemicals >> Arenes	No alert found
Biodegradation probability (Biowin 1)	Does NOT Biodegrade Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Biodegrades Fast	Biodegrades Fast
Biodegradation primary (Biowin 4)	Days to weeks	Days	Days	Days	Days	Days	Days to weeks	Days

InertFinder/ChemID Plus Name	Ethyl maltol	Ethyl vanillin	Heptanal, 2-(phenylmethylene)-	Isojasmone	Maltyl isobutyrate	Methyl n-amyl ketone	Methyl phenethyl ether	Methylcyclopentenolone
Carcinogenicity (genotox and nongenotox) alerts by ISS	alpha, beta-unsaturated carbonyls (Genotox) Structural alert for genotoxic carcinogenicity	Simple aldehyde (Genotox) Structural alert for genotoxic carcinogenicity	No alert found	alpha, beta-unsaturated carbonyls (Genotox) Structural alert for genotoxic carcinogenicity	alpha, beta-unsaturated carbonyls (Genotox) Structural alert for genotoxic carcinogenicity	No alert found	No alert found	alpha, beta-unsaturated carbonyls (Genotox) Structural alert for genotoxic carcinogeniciy
in vitro mutagenicity (Ames test) alerts by ISS	alpha, beta-unsaturated carbonyls	Simple aldehyde	No alert found	alpha, beta-unsaturated carbonyls	alpha, beta-unsaturated carbonyls	No alert found	No alert found	alpha, beta-unsaturated carbonyls
in vivo mutagenicity (Micronucleus) alerts by ISS	alpha, beta-unsaturated carbonyls H-acceptor-path3- H-acceptor	H-acceptor-path3-H-acceptor Simple aldehyde	No alert found	alpha, beta-unsaturated carbonyls	alpha, beta-unsaturated carbonyls H-acceptor-path3-H-acceptor	No alert found	No alert found	alpha, beta-unsaturated carbonyls H-acceptor- path3-H-acceptor
Protein Binding Potency h-CLAT	Pyranones, Pyridones and related chemicals	No alert found	alpha, beta-Unsaturated aldehydes	alpha, beta-Unsaturated ketones	Pyranones, Pyridones and related chemicals	No alert found	No alert found	No alert found
Skin irritation/corrosion Inclusion rules by BfR	Ketones	Aldehydes Phenols	Aldehydes	Ketones	Ketones	Ketones	Inclusion rules not met	Ketones
DNA alerts for AMES, CA and MNT by OASIS	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found

InertFinder/ChemID Plus Name	Ethyl maltol	Ethyl vanillin	Heptanal, 2-(phenylmethylene)-	Isojasmone	Maltyl isobutyrate	Methyl n-amyl ketone	Methyl phenethyl ether	Methylcyclopentenolone
Protein binding alerts for skin sensitization by OASIS	Michael Addition Michael Addition >> Michael addition on quinoid type compounds Michael Addition >> Michael addition on quinoid type compounds >> Pyranones, Pyridones (and related nitrogen chemicals)	Schiff base formation Schiff base formation >> Schiff base formation with carbonyl compounds Schiff base formation >> Schiff base formation with carbonyl compounds >> Aldehydes	Michael Addition Michael Addition >> Michael addition on alpha, beta-Unsaturated carbonyl compounds Michael Addition >> Michael addition on alpha, beta-Unsaturated carbonyl compounds >> alpha, beta-Aldehydes	No alert found	Michael Addition Michael Addition >> Michael addition on quinoid type compounds Michael Addition >> Michael addition on quinoid type compounds >> Pyranones, Pyridones (and related nitrogen chemicals)	Nucleophilic addition Nucleophilic addition >> Addition to carbon-hetero double bonds Nucleophilic addition >> Addition to carbon-hetero double bonds >> Ketones	No alert found	No alert found
rtER Expert System - USEPA	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found
Skin irritation/corrosion Exclusion rules by BfR	Group C Melting Point > 55 C Undefined	Group C Melting Point > 55 C Undefined	Undefined	Undefined	Group C Melting Point > 55 C Undefined	Undefined	Undefined	Undefined
Protein binding alerts for Chromosomal aberration by OASIS	AN2 AN2 >> Michael addition to activated double bonds	No alert found	No alert found	No alert found	AN2 AN2 >> Michael addition to activated	No alert found	No alert found	No alert found

InertFinder/ChemID Plus Name	Ethyl maltol	Ethyl vanillin	Heptanal, 2-(phenylmethylene)-	Isojasmone	Maltyl isobutyrate	Methyl n-amyl ketone	Methyl phenethyl ether	Methylcyclopentenolone
	AN2 >> Michael addition to activated double bonds >> alpha, beta-Unsaturated Carbonyls and Related Compounds				double bonds AN2 >> Michael addition to activated double bonds >> alpha, beta-Unsaturated Carbonyls and Related Compounds			

InertFinder/ChemID Plus Name	Nerol oxide	Nootkatone	Phenylethyl isoamyl ether	Piperonyl acetate	p-Mentha-8-thiol-3-one	p- Menthane, 1,8-epoxy-	Tetrahydr o-4-methyl-2- (2-methylpropen-1yl) pyran
CAS	1786-08-9	4674-50-4	56011-02-0	326-61-4	38462-22-5	470-82-6	16409-43-1
SMILES	CC(C)=CC 1CC(=CCO 1)C	CC1CC(=O)C=C2CCC (CC12C)C(C)=C	CC(C)CCOCCc1ccccc 1	CC(=O)OCc1ccc2OCOc2c 1	CC1CCC(C(=O)C1)C(C)(C)S	CC12CCC(CC1)C(C)(C)O2	CC1CCOC(C1)C=C(C) C
Ionization at pH = 1	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) No pKb value	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) No pKb value	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)
Biodegradation ultimate (Biowin 3)	Weeks	Weeks to months	Weeks to months	Weeks	Weeks to months	Weeks to months	Weeks
Estrogen Receptor Binding	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group
Biodeg BioHC half-life (Biowin)	No value	No value	No value	No value	No value	No value	No value
Hydrolysis half-life (pH 6.5-7.4)	No value	No value	No value	Very slow	No value	No value	No value
Biodegradation probability (Biowin 5)	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast
Toxic hazard classification by Cramer	High (Class III)	Intermediate (Class II)	Intermediate (Class II)	High (Class III)	High (Class III)	High (Class III)	High (Class III)
Biodegradation probability (Biowin 2)	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast

Ionization at pH = 4	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) No pKb value	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) No pKb value	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)
Protein binding potency Lys (DPRA 13%)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein binding alert	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Conjugated alpha, beta-unsaturated ketones (non reactive)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein binding alert	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Non-Conjugated carboxylic acids and esters (non reactive)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Non-conjugated mono- and diketones (non reactive) DPRA less than 9% (DPRA 13%) >> Thiols and disulfides (non reactive)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein binding alert	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein binding alert
Protein binding potency Cys (DPRA 13%)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein binding alert	Out of mechanistic domain	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein binding alert	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Non-Conjugated carboxylic acids and esters (non reactive)	DPRA above 21% (DPRA 13%) DPRA above 21% (DPRA 13%) >> Thiols (reactive)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein binding alert	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein binding alert
Hydrolysis half-life (Kb, pH 8) (Hydrowin)	No value	No value	No value	10 to 100 days	No value	No value	No value
Hydrolysis half-life (Kb, pH 7)	No value	No value	No value	> 100 days	No value	No value	No value

(Hydrowin)							
Biodegradation probability (Biowin 6)	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast
Protein binding by OECD	No alert found	No alert found	No alert found	SN2 SN2 >> SN2 reaction at sp3 carbon atom SN2 >> SN2 reaction at sp3 carbon atom >> Allyl acetates and related chemicals	SN2 SN2 >> SN2 reaction at a sulphur atom SN2 >> SN2 reaction at a sulphur atom >> Thiols	No alert found	No alert found
Ultimate biodeg	No data	No data	10 to 100 days	No data	No data	10 to 100 days	No data
Ionization at pH = 9	Acidic [70.000, 80.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) No pKb value	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [80.000, 90.000) Basic [0.000, 10.000)	Acidic [20.000, 30.000) No pKb value	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [20.000, 30.000) Basic [0.000, 10.000)
Hydrolysis half-life (Ka, pH 7) (Hydrowin)	No value	No value	No value	No value	No value	No value	No value
Toxic hazard classification by Cramer (extended)	High (Class III)	Intermediate (Class II)	Intermediate (Class II)	High (Class III)	High (Class III)	High (Class III)	High (Class III)
Biodegradation probability (Biowin 7)	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast

DNA binding by OASIS	No alert found	No alert found	No alert found	SN1 SN1 >> Nucleophilic attack after carbenium ion formation SN1 >> Nucleophilic attack after carbenium ion formation >> Specific Acetate Esters SN2 SN2 >> Nucleophilic substitution at sp3 Carbon atom SN2 >> Nucleophilic substitution at sp3 Carbon atom >> Specific Acetate Esters	Radical Radical >> Radical mechanism via ROS formation (indirect) Radical >> Radical mechanism via ROS formation (indirect) >> Thiols	No alert found	No alert found
Ionization at pH = 7.4	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) No pKb value	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [10.000, 20.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) No pKb value	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) Basic [0.000, 10.000)
Hydrolysis half-life (Ka, pH 8) (Hydrowin)	No value	No value	No value	No value	No value	No value	No value
Protein binding by OASIS	No alert found	Nucleophilic addition Nucleophilic addition >> Addition to carbon- hetero double bonds Nucleophilic addition >>	No alert found	SN2 SN2 >> SN2 Reaction at a sp3 carbon atom SN2 >> SN2 Reaction at a sp3 carbon atom >> Activated alkyl esters and thioesters	SN2 SN2 >> Interchange reaction with sulphur containing compounds SN2 >> Interchange reaction with sulphur containing compounds >> Thiols	No alert found	No alert found

		Addition to carbon- hetero double bonds >> Ketones					
DNA binding by OECD	No alert found	No alert found	Michael addition Michael addition >> P450 Mediated Activation to Quinones and Quinone-type Chemicals Michael addition >> P450 Mediated Activation to Quinones and Quinone-type Chemicals >> Arenes	Michael addition Michael addition >> P450 Mediated Activation to Quinones and Quinone-type Chemicals Michael addition >> P450 Mediated Activation to Quinones and Quinone-type Chemicals >> Methylenedioxyphenyl	No alert found	No alert found	No alert found
Biodegradation probability (Biowin 1)	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Biodegrades Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast
Biodegradation primary (Biowin 4)	Days to weeks	Days to weeks	Days to weeks	Days	Days to weeks	Days to weeks	Days to weeks
Carcinogenicity (genotox and nongenotox) alerts by ISS	No alert found	alpha,beta-unsaturated carbonyls (Genotox) Structural alert for genotoxic carcinogenicity	No alert found	1,3-Benzodioxoles (Nongenotox) Structural alert for nongenotoxic carcinogenicity	No alert found	No alert found	No alert found
in vitro mutagenicity	No alert found	alpha,beta-unsaturated	No alert found	No alert found	No alert found	No alert found	No alert found

(Ames test) alerts by ISS		carbonyls					
in vivo mutagenicity (Micronucleus) alerts by ISS	No alert found	alpha,beta-unsaturated carbonyls	No alert found	H-acceptor-path3-H-acceptor	No alert found	No alert found	No alert found
Protein Binding Potency h-CLAT	No alert found	alpha, beta-Unsaturated ketones	No alert found	No alert found	Thiols and disulfides	No alert found	No alert found
Skin irritation/corrosion Inclusion rules by BfR	Inclusion rules not met	Ketones	Inclusion rules not met	Inclusion rules not met	Ketones	Inclusion rules not met	Inclusion rules not met
DNA alerts for AMES, CA and MNT by OASIS	No alert found	No alert found	No alert found	SN1 SN1 >> Nucleophilic attack after carbenium ion formation SN1 >> Nucleophilic attack after carbenium ion formation >> Specific Acetate Esters SN2 SN2 >> Nucleophilic substitution at sp3 Carbon atom SN2 >> Nucleophilic substitution at sp3 Carbon atom >> Specific Acetate Esters	No alert found	No alert found	No alert found

Protein binding alerts for skin sensitization by OASIS	No alert found	Nucleophilic addition Nucleophilic addition >> Addition to carbon- hetero double bonds Nucleophilic addition >> Addition to carbon- hetero double bonds >> Ketones	No alert found	SN2 SN2 >> SN2 Reaction at a sp3 carbon atom SN2 >> SN2 Reaction at a sp3 carbon atom >> Activated alkyl esters and thioesters	Nucleophilic addition Nucleophilic addition >> Addition to carbon-hetero double bonds Nucleophilic addition >> Addition to carbon-hetero double bonds >> Ketones SN2 SN2 >> Interchange reaction with sulphur containing compounds SN2 >> Interchange reaction with sulphur containing compounds >> Thiols and disulfide compounds	No alert found	No alert found
rtER Expert System - USEPA	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found
Skin irritation/corrosion Exclusion rules by BfR	Undefined	Group C Melting Point > 55 C Undefined	Group C Surface Tension > 62 mN/m Undefined	Group C Melting Point > 55 C Undefined	Undefined	Undefined	Undefined
Protein binding alerts for Chromosomal aberration by OASIS	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found	No alert found

InertFinder/ChemID Plus Name	Tetrahydr o-6-(3- pentenyl)- 2H-pyran- 2-one	Theaspira ne
CAS	32764-98-0	36431-72-8
SMILES	C/C=C/CC C1CCCC(= O)O1	CC1CCC2(O1)C(=CC CC2(C)C)C
Ionization at pH = 1	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) No pKb value
Biodegradation ultimate (Biowin 3)	Days to weeks	Weeks to months
Estrogen Receptor Binding	Non binder, without OH or NH2 group	Non binder, without OH or NH2 group
Biodeg BioHC half-life (Biowin)	No value	No value
Hydrolysis half-life (pH 6.5-7.4)	Moderate	No value
Biodegradation probability (Biowin 5)	Biodegrades Fast	Does NOT Biodegrade Fast
Toxic hazard classification by Cramer	Low (Class I)	High (Class III)
Biodegradation probability (Biowin 2)	Biodegrades Fast	Does NOT Biodegrade Fast
Ionization at pH = 4	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) No pKb value
Protein binding potency Lys (DPRA 13%)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Non- Conjugate d carboxylic acids and esters (non reactive)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein binding alert
Protein binding potency Cys (DPRA 13%)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> Non- Conjugate d carboxylic acids and esters (non reactive)	DPRA less than 9% (DPRA 13%) DPRA less than 9% (DPRA 13%) >> No protein binding alert
Hydrolysis half-life (Kb, pH 8)(Hydrowin)	No value	No value
Hydrolysis half-life (Kb, pH 7)(Hydrowin)	No value	No value
Biodegradation probability (Biowin 6)	Biodegrad es Fast	Does NOT Biodegrad e Fast
Protein binding by OECD	Acylation Acylation >> Direct Acylation Involving a Leaving group Acylation >> Direct Acylation Involving a Leaving group >> Acetates	No alert found

InertFinder/ChemID Plus Name	Tetrahydr o-6-(3- pentenyl)- 2H-pyran- 2-one	Theaspira ne
Ultimate biodeg	10 to 100 days	No data
Ionization at pH = 9	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) No pKb value
Hydrolysis half-life (Ka, pH 7)(Hydrowin)	No value	No value
Toxic hazard classification by Cramer (extended)	Low (Class I)	High (Class III)
Biodegradation probability (Biowin 7)	Does NOT Biodegrade Fast	Does NOT Biodegrade Fast
DNA binding by OASIS	No alert found	No alert found
Ionization at pH = 7.4	Acidic [0.000, 10.000) Basic [0.000, 10.000)	Acidic [0.000, 10.000) No pKb value
Hydrolysis half-life (Ka, pH 8)(Hydrowin)	No value	No value
Protein binding by OASIS	Acylation Acylation >> Ring opening acylation Acylation >> Ring opening acylation >> Active cyclic agents	No alert found
DNA binding by OECD	No alert found	No alert found
Biodegradation probability (Biowin 1)	Biodegrades Fast	Does NOT Biodegrade Fast
Biodegradation primary (Biowin 4)	Days	Days to weeks
Carcinogenicity (genotox and nongenotox) alerts by ISS	No alert found	No alert found
in vitro mutagenicity (Ames test) alerts by ISS	No alert found	No alert found
in vivo mutagenicity (Micronucleus) alerts by ISS	No alert found	Oxolane
Protein Binding Potency h-CLAT	Lactones	No alert found
Skin irritation/corrosion Inclusion rules by BfR	Inclusion rules not met	Inclusion rules not met
DNA alerts for AMES, CA and MNT by OASIS	No alert found	No alert found
Protein binding alerts for skin sensitization by OASIS	Acylation Acylation >> Ring opening acylation Acylation >> Ring opening acylation >> Active cyclic agents	No alert found
rtER Expert System - USEPA	No alert found	No alert found
Skin irritation/corrosion Exclusion rules by BfR	Undefined	Undefined
Protein binding alerts for Chromosomal aberration by OASIS	No alert found	No alert found

Appendix IV. Explanation and Justification for OCED Toolbox outputs indicating Cramer classification other than II.

Two outputs regarding Cramer decision tree classification are provided from the OECD Toolbox (Appendix II):
A. Toxic hazard classification by Cramer (original)
B. Toxic hazard classification by Cramer (extension)

Outputs (A) and (B) are from the QSAR toolbox (TB) algorithms. Output A represents a programming of the original steps outlined by Cramer and associates based on the scheme published in 1978 (Cramer et al., 1978). The extended algorithm contains 5 additional questions. The QSAR toolbox offers datasheets on each algorithm (see QSAR toxtree accessed 20230905 and QSAR toxtree_extended assessed 20230905).
The Cramer scheme requires expert knowledge or databases on “normal constituents of the body” (Q1), “common terpenes” (Q16) and “common component of food” (Q22). The manner in which these questions, as well as questions regarding hydrolysis of esters and acetals and the interpretation of other questions of the Cramer tree for the purpose of programming the algorithms have differed among the programmers involved (Lapenna and Worth, 2011; Bhatia et al., 2015). The OECD QSAR V.4 Application Manual is using external files with 440 compounds in "Common component of food" and 107 compounds in "Normal constituents of body" from ToxTree v.2.1.0 (https://toxtree.sourceforge.net/).

The approach used by JECFA relied on expert judgement for each compound, following the original Cramer et al., 1978 publication. JECFA experts examined peer-reviewed literature and currated databases (such as Volatile Compounds in Food) to answer questions 16 and 22 on normal constituents of the body, common terpenes and common components in food. In addition, metabolism data was used to predict the hydrolysis of esters and acetals. As the petition cites the JECFA safety determinations, we used the Cramer classifications as assigned by JECFA.

For some materials, the OECD Toolbox output classifies the material as a common terpene based on database knowledge. However, some materials have natural occurrence data relevant to question 22 (common components in food) that have been evaluated by JECFA, but not considered by the OECD QSAR Toolbox. A summary table of the substances with discrepancies between the JECFA assigned decision tree class and the OECD Toolbox “Toxic hazard classification by Cramer (original)” field is listed below.

CAS	Chemical name in InertFinder/ChemID Plus	JECFA assigned DT Class	OECD Toolbox Toxic hazard classification by Cramer (original)	Cramer Path for JECFA Assignment	Resolution
19840 4-98-7	Cyclopropanemethanol, 1-methyl-2-[(1,2,2-trimethylbicyclo[3.1.0]hex-3-yl)methyl]-	II	I - 1N,2N,3N,5N,6N,7N,16Y	1N,2N,3N,5N,6N,7N,16N,17N,19N,23N,24N,25N,26Y	JECFA Class II

71159-90-5	1-p-Menthene-8-thiol	II	I - 1N,2N,3N,5N,6N,7N,16Y	Class II - 1N,2N,3N,5N,6N,7N,16N,17N,19N,23N,24N,25Y	JECFA Class II
104-76-7	1-Hexanol, 2-ethyl-	II	I - 1N,2N,3N,5N,6N,7N,16N,17N,19Y,20Y,21N,18N	Class II - 1N,2N,3N,5N,6N,7N,16N,17N,19Y,20Y,21N,18Y	JECFA Class II
67801-20-1	3-Methyl-5-(2,2,3-trimethyl-3-cyclopenten-1-yl)pent-4-en-2-ol	II	I – 1N,2N,3N,5N,6N,7N,16Y	1N,2N,3N,5N,6N,7N,16N,17N,19N,23N,24Y,18N	JECFA Class II
689-67-8	6,10-Dimethylundeca-5,9-dien-2-one	II	I - 1N,2N,3N,5N,6N,7N,16N,17N,19Y,20Y,21N,18N	Class II - 1N,2N,3N,5N,6N,7N,16N,17N,19Y,20Y,21N,18Y	JECFA Class II
1604-28-0	6-Methyl-3,5-heptadien-2-one	II	I - 1N,2N,3N,5N,6N,7N,16N,17N,19Y,20Y,21N,18N	Class II - 1N,2N,3N,5N,6N,7N,16N,17N,19Y,20Y,21N,18Y	JECFA Class II
110-93-0	6-Methyl-5-hepten-2-one	II	I - 1N,2N,3N,5N,6N,7N,16N,17N,19Y,20Y,21N,18N	Class II - 1N,2N,3N,5N,6N,7N,16N,17N,19Y,20Y,21N,18Y	JECFA Class II
32764-98-0	Tetrahydro-6-(3-pentenyl)-2H-pyran-2-one	II	I – 1N,2N,3N,5N,6N,7Y,8Y,9N,20Y,21N,18N	Class II – 1N,2N,3N,5N,6N,7Y,8Y,9N,20Y,21N,18Y	JECFA Class II
513-86-0	Acetoin	II	I - 1N,2N,3N,5N,6N,7N,16N,17N,19Y,20Y,21N,18N	1N,2N,3N,5N,6N,7N,16N,17N,19Y,20Y,21N,18Y	JECFA Class II
7492-44-6	.alpha.-Butylcinnamaldehyde	II	I - 1N,2N,3N,5N,6N,7N,16N,17N,19N,23Y,27Y,28N,30N,18N	Step 30 – Yes, material contains a ring bearing substituents other than 1-5 carbon aliphatic groups. Class II - 1N,2N,3N,5N,6N,7N,16N,17N,19N,23Y,27Y,28N,30Y,31N, 32Y	JECFA Class II
60047-17-8; 5989-33-3; 34995-77-2	Linalyl oxide	II	III - 1N,2N,3N,5N,6N,7Y,8N, 10N,11Y,33N	Step 11 – No, other than the heteroatom within the heterocyclic ring, the material does not contain substituents other than simply branched hydrocarbons and an alkyl alcohol. Step 22 – Yes, the material is a common component of food. A consumption ratio of 57 was calculated by JECFA for this material, indicating the natural occurrence of this substance in a variety of foods (JECFA 1454). Class II – 1N,2N,3N,5N,6N,7Y,8N, 10N,11N,12N,22Y	JECFA Class II
3848-24-6	2,3-Hexanedione	II	III - 1N,2N,3N,5N,6N,7N,16N,17N,19Y,20N,22N,33N	Material occurs naturally in beer (<0.01 ppm); clams (0.02 ppm); and coffee (0.3-3.2 ppm) (VCF, 2024).	JECFA Class II

				Class II - 1N,2N,3N,5N,6N,7N,16N,17N,19Y,20N,22Y	
108-50-9	2,6-Dimethylpyrazine	II	III - 1N,2N,3N,5N,6N,7Y,8N, 10N,11N,12Y,13Y,14N, 22N,33N	Step 22 – Yes, the material is a common component of food. A consumption ratio of 2,600 was calculated by JECFA for this material in the U.S., indicating the natural occurrence of this substance in a variety of foods (JECFA 767). Class II - 1N,2N,3N,5N,6N,7Y,8N, 10N,11N,12Y,13Y,14N,22Y	JECFA Class II
15707-23-0	2-Ethyl-3-methylpyrazine	II	III - 1N,2N,3N,5N,6N,7Y,8N, 10N,11N,12Y,13Y,14N, 22N,33N	Step 22 – Yes, the material is a common component of food. A consumption ratio of 250 was calculated by JECFA for this material in the U.S., indicating the natural occurrence of this substance in a variety of foods (JECFA 768). Class II - 1N,2N,3N,5N,6N,7Y,8N, 10N,11N,12Y,13Y,14N,22Y	JECFA Class II
24683-00-9	2-Isobutyl-3-methoxypyrazine	II	III - 1N,2N,3N,5N,6N,7Y,8N, 10N,11N,12Y,13Y,14N, 22N,33N	Step 22 – Yes, the material is a common component of food. A consumption ratio of 250 was calculated by JECFA for this material in the U.S., indicating the natural occurrence of this substance in a variety of foods (JECFA 792). Class II - 1N,2N,3N,5N,6N,7Y,8N, 10N,11N,12Y,13Y,14N,22Y	JECFA Class II
15679-13-7	2-Isopropyl-4-methylthiazole	II	III - 1N,2N,3N,5N,6N,7Y,8N,10N,11N,12Y,13Y,14N,22N,33N	Step 22 – Yes, JECFA considers this material to be structurally closely related to common constituents of food. Class II – 1N,2N,3N,5N,6N,7Y,8N, 10N,11N,12Y,13Y,14N,22Y	JECFA Class II
24168-70-5	2-Methoxy-3-(1-methylpropyl)pyrazine	II	III - 1N,2N,3N,5N,6N,7Y,8N, 10N,11N,12Y,13Y,14N, 22N,33N	Step 22 – Yes, the material is structurally related to other substances that are common components of foods (see other JECFA materials in group). Class II - 1N,2N,3N,5N,6N,7Y,8N, 10N,11N,12Y,13Y,14N,22Y	JECFA Class II

67715-80-4	2-Methyl-4-propyl-1,3-oxathiane	II	III - 1N,2N,3N,5N,6N,7Y,8N, 10N,11N,12N,22N,33N	Step 22 – Yes, the material occurs naturally in food (common component in food) but quantitative data not avaialble for a consumption ratio calculation by JECFA (JECFA 464) Class II – 1N,2N,3N,5N,6N,7Y,8N, 10N,11N,12N,22Y	JECFA Class II
3658-77-3	4-Hydroxy-2,5-dimethyl-3(2H)-furanone	II	III - 1N,2N,3N,5N,6N,7Y,8N,10N,11N,12N,22N,33N	Step 22 – Yes, the material is a common component of food. A consumption ratio of 1 was calculated by JECFA for this material in the U.S., indicating the natural occurrence of this substance in a variety of foods (JECFA 1446). Class II – 1N,2N,3N,5N,6N,7Y,8N, 10N,11N,12N,22Y	JECFA Class II
13679-70-4	5-Methyl-2-thiophenecarboxaldehyde	II	III - 1N,2N,3N,5N,6N,7Y,8N, 10N,11N,12Y,13Y,14N,22N,33N	Step 22 – Yes, the material is a common component of food. A consumption ratio of 9,100 was calculated by JECFA for this material in the U.S., indicating the natural occurrence of this substance in a variety of foods (JECFA 1050). Class II – 1N,2N,3N,5N,6N,7Y,8N, 10N,11N,12Y,13Y,14N,22Y	JECFA Class II
65416-14-0	Maltyl isobutyrate	II	III - 1N,2N,3N,5N,6N,7Y,8N, 10N,11N,12N,22N,33N	Step 22 – Yes, this material is structurally closely related to common constituents of food (see JECFA 1480, maltol). Class II – 1N,2N,3N,5N,6N,7Y,8N, 10N,11N,12N,22Y	JECFA Class II
80-71-7	Methylcyclopentenolone	II	III - 1N,2N,3N,5N,6N,7N,16N,17N,19N,23N,24N,25N,26N,22N,33N	Class II - 1N,2N,3N,5N,6N,7N,16N,17N,19N,23N,24N,25N,26Y	JECFA Class II
1786-08-9	Nerol oxide	II	III - 1N,2N,3N,5N,6N,7Y,8N,10N,11N,12N,22N,33N	Step 22 – Yes, this material is a common component of food (JECFA 1235). Class II – 1N,2N,3N,5N,6N,7Y,8N,10N,11N, 12N,22Y	JECFA Class II
326-61-4	Piperonyl acetate	II	III - 1N,2N,3N,5N,6N,7Y,8N,10N,11N,12N,22N,33N	Step 22 – Yes, this material is structurally closely related to common constituents of food.	JECFA Class II

				Class II – 1N,2N,3N,5N,6N,7Y,8N,10N,11N,12N,22Y	
38462-22-5	p-Mentha-8-thiol-3-one	II	III - 1N,2N,3N,5N,6N,7N,16N,17N,19N,23N,24N,25N,26N,22N,33N	Step 22 – Yes, this material is a common component of food (JECFA 561). Class II – 1N,2N,3N,5N,6N,7N,16N,17N,19N,23N,24N,25N,26N,22Y	JECFA Class II
16409-43-1	Tetrahydro-4-methyl-2-(2-methylpropen-1-yl)pyran	II	III - 1N,2N,3N,5N,6N,7Y,8N,10N,11N,12N,22N,33N	Step 22 – Yes, this material is a common component of food (JECFA 1237). Class II – 1N,2N,3N,5N,6N,7Y,8N,10N,11N,12N,22Y	JECFA Class II
36431-72-8	Theaspirane	II	III - 1N,2N,3N,5N,6N,7Y,8N,10N,11N,12N,22N,33N	Step 22 – Yes, this material is a common component of food (JECFA 1238). Class II – 1N,2N,3N,5N,6N,7Y,8N,10N,11N,12N,22Y	JECFA Class II
470-67-7	7-Oxabicyclo(2.2.1.)heptane, 1-methyl-4-(1-methylethyl)-	II	III - 1N,2N,3N,5N,6N,7Y,8N,10N,11N,12N,22N,33N	Step 22 – Yes, this material is a common component of food (JECFA 1233). Class II – 1N,2N,3N,5N,6N,7Y,8N,10N,11N,12N,22Y	JECFA Class II
470-82-6	p-Menthane, 1,8-epoxy-	II	III - 1N,2N,3N,5N,6N,7Y,8N,10N,11N,12N,22N,33N	Step 22 – Yes, the material is a common component of food. A consumption ratio of 23 was calculated by JECFA for this material in the U.S., indicating the natural occurrence of this substance in a variety of foods (JECFA 1234). Class II – 1N,2N,3N,5N,6N,7Y,8N,10N,11N,12N,22Y	JECFA Class II
24851-98-7	Cyclopentaneacetai acid, 3-oxo-2-pentyl-, methyl ester	II	III – 1N,2N,3N,5N,6N,7N,16N,17N,19N,23N,24N,25N,26N,22N,33N	Step 22 – Yes, this material is a common component of food (JECFA 1898). Class II – 1N,2N,3N,5N,6N,7N,16N,17N,19N,23N,24N,25N,26N,22Y 1N,2N,3N,5N,6N,7N,16N,17N,19N,23N,24N,25N,26Y	JECFA Class II

120-57-0	1,3-Benzodioxole-5-carboxaldehyde	II	III - 1N,2N,3N,5N,6N,7Y,8N,10N,11N,12N,22N,33N	Step 22 – Yes, this material is structurally closely related to common constituents of food. Class II – 1N,2N,3N,5N,6N,7Y,8N,10N,11N,12N,22Y	JECFA Class II
1866-31-5	Allyl cinnamate	II	II & III – Pathway unavailable	OECD Toolbox provides two outputs for two different predicted metabolic products. Toolbox uses the more conservative class. Class II - 1N,2N,3N,5N,6N,7N,16N,17N,19N,23Y,27Y,28N,30N,18Y	JECFA Class II

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