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3 February 1998

**NATIONAL INDUSTRIAL CHEMICALS NOTIFICATION  
AND ASSESSMENT SCHEME**

**FULL PUBLIC REPORT**

**Habanolide**

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Director  
Chemicals Notification and Assessment

**FULL PUBLIC REPORT****Habanolide****1. APPLICANT**

Firmenich Ltd of 73 Kenneth Rd Balgowlah NSW 2093. has submitted a limited notification statement in support of their application for an assessment certificate for Habanolide

**2. IDENTITY OF THE CHEMICAL**

Habanolide is considered not to be hazardous based on the nature of the chemical and the data provided. Therefore the chemical name, CAS number, molecular and structural formulae, molecular weight, spectral data, details of the polymer composition and details of exact import volume and customers have been exempted from publication in the Full Public Report and the Summary Report.

**Trade Name:** Habanolide

**3. PHYSICAL AND CHEMICAL PROPERTIES**

<b>Appearance at 20°C and 101.3 kPa:</b>	colourless liquid
<b>Boiling Point:</b>	283.5 -331.3°C at 94.84 kPa
<b>Specific Gravity:</b>	0.964 at 20°C
<b>Vapour Pressure:</b>	$1.6 \times 10^{-4}$ kPa at 25°C
<b>Water Solubility:</b>	$< 0.203 \text{ mg L}^{-1}$ at 20°C
<b>Partition Co-efficient (n-octanol/water):</b>	$\log P_{ow} > 3.94$ at 22°C
<b>Hydrolysis as a Function of pH:</b>	not determined, insoluble in H <sub>2</sub> O (see comments)
<b>Adsorption/Desorption:</b>	$\log K_{OC} > 3.55$ (calculated)

<b>Dissociation Constant:</b>	not soluble in H <sub>2</sub> O, no ionisable groups
<b>Flash Point:</b>	157°C
<b>Flammability Limits:</b>	test not conducted
<b>Autoignition Temperature:</b>	252°C
<b>Explosive Properties:</b>	none found
<b>Reactivity/Stability:</b>	chemical structure indicates relatively stable, non-oxidising

### Comments on Physico-Chemical Properties

It has not been possible to determine the exact solubility of the chemical as it is below the quantification limit of 0.203 mg.L<sup>-1</sup> for the shake flask method used.

Hydrolysis has not been tested due to the low solubility of the chemical. This is acceptable. Some hydrolysis at the ester linkage is possible but unlikely in the environmental pH range and conditions.

A preliminary assessment of the octanol/water Log P<sub>ow</sub> from the ratio of the solubilities of the test material in pure solvents has indicated it to be greater than 6.41. Although this result suggests that the HPLC method (OECD Test Guideline 117) would be more applicable for the main determination, the shake flask method (OECD Test Guideline 107) was used on the basis of the test material being more suited to gas chromatographic detection than an ultraviolet detection technique. However, in the main test the concentration of the chemical in the water phase could not be measured accurately as it remained below the detection limit (0.25 mg.L<sup>-1</sup>). Hence Log P<sub>ow</sub> was considered to be greater than 3.94.

Log K<sub>oc</sub> has been calculated, using solubility and/or Log P<sub>ow</sub> values. As the latter parameters have been estimated to be greater than particular values, the Log K<sub>oc</sub> has also been given as greater than 3.55.

The high Log K<sub>ow</sub> value and low solubility indicate that the chemical would bind strongly to sediment and have a low tendency to be associated with the aqueous phase.

The chemical does not contain any dissociable functionalities.

#### 4. PURITY OF THE CHEMICAL

Degree of Purity: >90%

Hazardous Impurities: nil

Additives/Adjuvants: nil

Exact details are confidential, not disclosed in the full public report.

#### 5. USE, VOLUME AND FORMULATION

Habanolide is a synthetic musk like perfume which will be imported as a minor ingredient (less than 1%) of mixtures of concentrated fragrance preparations. It will be imported into Australia from Europe, in lacquered drums (size between 12 and 215 L) or tightly closed aluminium containers (size 1.25, 6.25, 12.5 or 31 L).

The final products will incorporate the concentrates at a maximum of 20% in perfumes and 0.5% in cosmetics (shampoos, soaps, air fresheners, etc.) and household cleaning products. The maximum concentration of the notified chemical will therefore be 0.2% in perfumes and 0.005% in cosmetics and household cleaning products.

Import volumes for the notified chemical are as follows:

Year	1	2	3	4	5
Import Volume (kg)	400	600	800	825	850

#### 6. OCCUPATIONAL EXPOSURE

Transport workers and store personnel will only be exposed to the notified chemical in the event of an accidental spill. The maximum concentration of Habanolide in the imported preparations is less than one per cent, so that in the event of a spill, exposure will be minor.

Workers at Firmenich Australia and customer sites will be involved in quality control checking and blending Habanolide into final consumer products. Blending is carried out in closed systems so the opportunity for respiratory or dermal exposure is low.

Manufacturers of consumer products use batch processes to add the aroma concentrate containing Habanolide, but the fragrance perfumes are kept in their drums and added sequentially (ie they are not pumped to and from reservoirs as are some of the major ingredients of these products). The concentration of the notified chemical in the final consumer products ranges from 0.005 to 0.2%, sufficiently low that exposure of workers to Habanolide in the final products is

negligible. In any event automated packaging and handling systems are used for most consumer products containing the notified chemical thus limiting the potential for occupational exposure.

## **7. PUBLIC EXPOSURE**

Widespread public exposure will occur from using perfumes, cosmetics and household cleaning products containing the notified chemical, although the exposure level is expected to be low. Minor public exposure may result from disposal of unused fragrance containing the notified chemical, accidental spillage of the fragrance during transport and storage, or during reformulation. However, adequate measures are described by the notifier to minimise the risk of public exposure during disposal, reformulation or in the event of accidental spillage.

## **8. ENVIRONMENTAL EXPOSURE**

### **Release**

The formulation of the fragrance preparations into consumer products is done in closed systems and the filling/packaging to final products is done using fully automated technology. The notifier states that the water and aqueous solutions used to clean the formulation equipment are re-used for other purposes. Hence the environmental release of the chemical during the above processes is expected to be minimal. Small amounts will be wasted as residues in empty containers. The notifier estimates that the total waste from all sources may not exceed 2%. For a maximum import volume of 850 kg this equates to 17 kg per annum. Part of this will reach the landfill (eg empty containers) and the other the sewer.

Consumer products containing the chemical will gain wide distribution across the country. Through the use of cosmetics and cleaning products in bathrooms and kitchens, almost the entire import volume of the chemical will be released to the sewer in a dispersive manner.

### **Fate**

Due to its low solubility and high partition coefficient the chemical discharged into the sewer is expected to be initially trapped with the solids in the sludge. Ready biodegradability of the chemical has been investigated using a Manometric Respirometry Test and the CO<sub>2</sub> Production (Modified Sturm) test according to OECD Guidelines 301F and 301B respectively. The former showed 61% and 95% degradation within 10 and 28 days respectively. The latter showed 72% and 86% CO<sub>2</sub> yield within 10 and 28 days respectively. These results indicate that the notified chemical is readily biodegradable. Although not required from the results of the ready biodegradability tests, an inherent biodegradability has also been carried out by measuring the Soluble Organic Carbon (SOC) removal in a Semi-Continuous Activated Sludge (SCAS) system (OECD Test Guideline No 302A).

This showed 99% removal confirming the ultimate biodegradable nature of the chemical. This test however is specific for water soluble organic compounds and the low solubility of the present chemical casts some doubt on the validity of the results. Strong binding to the sludge and high biodegradability will minimise amounts left in the water discharged from the sewer (see below).

To estimate the fate of the chemical in a Waste Water Treatment Plant (WWTP) the notifier applied the SIMPLETREAT model (1) considering the substance to be readily biodegradable with Log H greater than 2.27 and Log K<sub>oc</sub> greater than 3.55. The model predicted the chemical to partition as follows in the WWTP; to water 5.5%, to air 11.7%, to sludge 28.7% and degradation 54.1%.

Low solubility and high Log P<sub>ow</sub> suggest a potential for bioaccumulation. However the readily biodegradable nature of the chemical and its low concentration in the water compartment should prevent this.

## 9. EVALUATION OF TOXICOLOGICAL DATA

No toxicological data are required, for notified chemicals whose use is less than 1 000kg per annum according to the Act. However test reports produced by the notifier in support of claims in the Material Safety Data Sheet (MSDS) for the notified chemical are summarised below.

### Summary of the toxicity of Habanolide.

<b>Test*</b>	<b>Species</b>	<b>Outcome</b>	<b>Reference</b>
acute oral toxicity	rat	LD <sub>50</sub> > 2 000 mg.kg <sup>-1</sup>	(2)
acute dermal toxicity	rat	LD <sub>50</sub> > 2 000 mg.kg <sup>-1</sup>	(3)
skin irritation	rabbit	slight irritant	(4)
eye irritation	rabbit	non irritant	(5)
skin sensitisation	guinea pig	non sensitising	(6)
4 week oral	rat	no measurable effect up to 1 000 mg.kg <sup>-1</sup> .day <sup>-1</sup>	(7)
reverse mutation	<i>S. typhimurium</i>	not mutagenic	(8)
chromosome aberration	human lymphocytes	non-clastogenic	(9)

\*All tests were performed according to OECD protocols (10)

## 9.4 Overall Assessment of Toxicological Data

The results of the toxicological tests do indicate a minimal hazard from exposure to Habanolide. Habanolide is not classified as hazardous according to National Occupational Health and Safety Commission criteria (11).

## 10. ASSESSMENT OF ENVIRONMENTAL EFFECTS

While not required by the Act for substances imported in quantities less than 1 tonne per annum, the following ecotoxicity studies have been supplied by the notifier. The tests followed OECD Test Guidelines (10).

Test	Species	Results
Acute Toxicity	Rainbow Trout ( <i>Oncorhynchus mykiss</i> )	LC <sub>50</sub> = 2.4 mg.L <sup>-1</sup> 96 h # NOEC = 1.0 mg.L <sup>-1</sup> # LC <sub>50</sub> = 2.0 mg.L <sup>-1</sup> 96 h * NOEC = 0.52 mg.L <sup>-1</sup> *
Acute Immobilisation	Water Flea ( <i>Daphnia magna</i> )	LC <sub>50</sub> = 0.88 mg.L <sup>-1</sup> 48 h # NOEC = 0.32 mg.L <sup>-1</sup> # LC <sub>50</sub> = 0.48 mg.L <sup>-1</sup> 48 h * NOEC = 0.24 mg.L <sup>-1</sup> *
Growth Inhibition	Algae ( <i>Scenedesmus subspicatus</i> )	E <sub>b</sub> C <sub>50</sub> = 2.4 mg.L <sup>-1</sup> 72 h # 24-48 h E <sub>r</sub> C <sub>50</sub> = 5.0 mg.L <sup>-1</sup> # NOEC = 0.625 mg.L <sup>-1</sup> #

# Based on nominal concentrations. \* Based on measured concentrations. Results at measured concentrations are not available for the algal test as the chemical was not detected after 72 hours.

The ecotoxicity data for the notified chemical indicate that it is highly toxic to daphnia and moderately toxic to fish and algae.

In all three tests 5% v/v Tween 80-dimethylformamide was used to prepare stock solutions and there were marked decreases in the test concentration with time. The fish test used nominal concentrations of 1.0, 1.8, 3.2, 5.6, and 10 mg.L<sup>-1</sup> and the measured concentrations were between 75 to 96% after 24 hours, 44 to 62% after 48 hours and 0 to 25% after 72 hours. In the water flea test with nominal concentrations of 0.10, 0.18, 0.32, 0.56, 1.0, 1.8, 3.2, 5.6 and 10 mg.L<sup>-1</sup> the measured concentrations were between 24 to 98% of nominal after 48 hours. In the algal test done with nominal concentrations of 0.625, 1.25, 2.5, 5.0 and 10 mg.L<sup>-1</sup> no test material was detectable after 72 hours for any of the initial concentrations.

The rapid decrease in test concentrations can question the validity of toxicity limits expressed using nominal concentrations and underestimate the real toxicities. The notifier has attempted to examine the cause of the marked

decrease in the concentration of the chemical in test solutions. In spite of low solubility of the chemical the tests did not report any signs of precipitation. The loss of the test substance was generally greater at lower test concentrations which was thought to indicate an adsorption of the test material to the glassware. However, recovery and stability analysis did not reveal whether the material adsorbed to the glassware. Further, the pre-study stability analysis during daphnia and algal tests found the test substance to be stable over the 72 hour test period.

In all three tests the measured concentrations at 0 hours were very close to nominal. In the Rainbow Trout test a marked decrease was observed after the initial addition of the test organisms but over 24 hours there was no significant decrease in the absence of test organisms. Based on these observations notifier suggested that the decrease may be due to an accumulation in the fish. Low water solubility and high partition coefficient (Log Pow greater than 3.94) of the chemical also indicate potential for bioaccumulation. Further support for the above explanation comes from the fact that the large decrease in the test concentrations soon after introduction of the fish was paralleled by a greater death of fish in the early stages, especially seen at the higher levels of the test concentrations (5.6 & 10 mg.L<sup>-1</sup>). For example, at 5.6 mg.L<sup>-1</sup> four fish out of 10 died after 3 hours and all 10 were dead by 6 hours. At 10 mg.L<sup>-1</sup> concentration 8 fish died after 3 hours and all were dead by 6 hours. A similar pattern is seen in the daphnia test. At the highest concentration of 10 mg.L<sup>-1</sup> used, out of 10 individuals per replicate 8 (replicate 1) and 9 (replicate 2) were immobilised within the first 24 hours and all were immobilised by 48 hours. These observations suggest that the toxicity limits calculated on nominal concentrations may in fact be quite acceptable.

Overall the indication is that the decrease in the concentrations may be due to accumulation and/or sticking of the chemical to test organisms. No further conclusions could be made without information on the build up of the chemical in the bodies/tissues of the test organisms.

In the algal test there was a considerable change in pH of test solutions. The pH of control and test solutions increased from the range of 7.9-8.1 at 0 h to the range of 8.3 to 10.3 at 72 hours. The notifier attributed this to a production of carbonates and bicarbonates during photosynthesis/respiration equilibrium. The increase in pH over the 72 hour period was also dependent on the concentration of the test material, with low concentrations exhibiting greater increases in pH. This was considered to be due to there being greater numbers of viable cells in the lower concentrations and hence greater production of carbonates and bicarbonates. This explanation is acceptable as the 24 to 48 hour growth inhibitions for the nominal concentrations of 0.625, 1.25, 2.5, 5.0, and 10 mg.L<sup>-1</sup> were respectively 8%, 6%, 16%, 58%, and 72%.



## **11. ASSESSMENT OF ENVIRONMENTAL HAZARD**

With almost the entire import volume of the chemical expected to go into the sewer, the notifier has predicted the environmental concentration in surface water. For a large city such as Melbourne or Sydney, assuming a usage of 0.3 tonnes per year, 5 million households, 200 L of waste water per household per day, 5.5% of the chemical in the WWTP to be in the water phase (see above), and a dilution factor of 10 by surface water, the concentration of the chemical in surface water can be estimated to be  $4.6 \text{ ng.L}^{-1}$ . This is about six orders of magnitude lower than the toxicity limits of sensitive aquatic organisms.

The sludge containing the chemical after removal from WWTP will either be landfilled or incinerated. In landfill the chemical will remain associated with the soil and undergo slow hydrolysis and degradation. Incineration will destroy the chemical.

The environmental hazard from the notified chemical is therefore expected to be low.

## **12. ASSESSMENT OF PUBLIC AND OCCUPATIONAL HEALTH AND SAFETY EFFECTS**

The toxicological test results indicate minimal hazard from exposure to the notified chemical in its pure state. Since the imported fragrance concentrates contain Habanolide at less than 1% concentration, this dilution coupled with the non-hazardous nature of the notified chemical, minimise the possible potential for occupational health risk.

The incorporation of the fragrance concentrate into final consumer products will generally occur in automated processes at industrial sites. The blending process is carried out in closed systems and personal protective equipment is expected to be used to minimise exposure during mixing. Cleaning of lines and vessels is also automated and exposure to the compound during connection and disconnection of lines will be minimal. Many of these controls exist to prevent exposure to solvent vapours in perfume concentrate preparations. The wearing of protective clothing and the use of ventilation or respiratory protection as recommended in the MSDS, will further prevent any likely exposure to the notified chemical and its formulation.

The fragrance is a minor component (0.005 to 0.2%) of the ultimate consumer products which are expected to be manufactured on a large industrial scale using fully automated technology including the final stages of filling the containers, cartons or wrappings in which it is commercialised. No identifiable risk is expected to exposed workers.

The chemical will be incorporated (as part of fragrance preparations) into products such as cosmetics and household cleaners, which will contain the notified chemical at concentrations ranging from 0.2% to 0.005%. Use of the products which incorporate the notified chemical results in considerable dermal exposure. Given that the concentration of the chemical in the products, and its irritancy

potential are low, the chemical poses a negligible public health risk. The potential for minor public exposure exists during transport, disposal and reformulation of the notified chemical. The low concentration and toxicity of Habanolide limit the hazard of public exposure in the unlikely event of a spill.

### **13. RECOMMENDATIONS**

To minimise occupational exposure to Habanolide the following guidelines and precautions should be observed:

- Industrial clothing should conform to the specifications detailed in AS 2919 and AS 3765.1 (12);
- All occupational footwear should conform to AS/NZS 2210 (13);
- Spillage of the notified chemical should be avoided, spillages should be cleaned up promptly with absorbents which should then be put into containers for disposal;
- Good personal hygiene should be practised to minimise the potential for ingestion;
- A copy of the MSDS should be easily accessible to employees.

### **14. MATERIAL SAFETY DATA SHEET**

The MSDS for the notified chemical was provided in accordance with the *National Code of Practice for the Preparation of Material Safety Data Sheets* (14).

This MSDS was provided by the applicant as part of the notification statement. It is reproduced here as a matter of public record. The accuracy of this information remains the responsibility of the applicant.

### **15. REQUIREMENTS FOR SECONDARY NOTIFICATION**

Under the Act, secondary notification of the notified chemical shall be required if any of the circumstances stipulated under subsection 64(2) of the Act arise. No other specific conditions are prescribed.

## 16. REFERENCES

1. European Commission 1996, *Technical Guidance Document in Support of Commission Directive 93/67/EEC on Risk Assessment for New Notified Substances and Commission Regulation (EC) No 1488/94 on Risk Assessment for Existing Substances. Part IV*, ECSC-EC-EAEC, Brussels, 672-673.
2. Chubb, D. 1992a, *Acute Oral Toxicity Study in the Rat-ST 11 C 91*, Project no., A/O/33096, Toxicol Laboratories Limited, Ledbury, Herefordshire.
3. Chubb, D. 1992b, *Acute Dermal Toxicity Study in the Rat-ST 11 C 91*, Project no., A/O/33097, Toxicol Laboratories Limited, Ledbury, Herefordshire.
4. Chubb, D. 1992c, *Acute Dermal Irritation Study in the Rabbit-ST 11 C 91*, Project no., A/S/33152, Toxicol Laboratories Limited, Ledbury, Herefordshire.
5. Chubb, D. 1992d, *Acute Eye Irritation Study in the Rabbit-ST 11 C 91*, Project no., A/E/33098, Toxicol Laboratories Limited, Ledbury, Herefordshire.
6. Teale, H. 1992, *Skin sensitisation in the guinea pig, Magnusson-Kligman maximisation*, Project no., A/K/33099, Toxicol Laboratories Limited, Ledbury Herefordshire.
7. Brownlie, S.-A. 1996, *4 week oral (gavage) toxicity study in the rat followed by a 2 week treatment-free period*, Project no., FCH/16/96, Toxicol Laboratories Limited, Ledbury Herefordshire.
8. Kelly, M. 1992, *Bacterial Reverse Mutation Assay ST 11 C 91*, Project no., FCH/16/96, Toxicol Laboratories Limited, Ledbury Herefordshire.
9. Durward, R. 1995, *Chromosome aberration Test in human lymphocytes in vitro ST 11 C91*, Project no., 161/063, Safeparm Laboratories Limited, Derby.
10. Organisation for Economic and Co-operation and Development. 1995-1996. *OECD Guidelines for the Testing of Chemicals on CD-Rom*, OECD, Paris.
11. National Occupational Health and Safety Commission 1994, *Approved Criteria for Classifying Hazardous Substances [NOHSC:1008(1994)]*, Australian Government Publishing Service, Canberra.
- 11 Standards Australia 1987, *Australian Standard 2919-1987, Industrial Clothing*, Standards Association of Australia, Sydney.
12. Standards Australia/Standards New Zealand 1994a, *Australian/New Zealand Standard 2210-1994, Occupational Protective Footwear*, Standards Association of Australia/Standards Association of New Zealand, Sydney/Wellington.

13. National Occupational Health and Safety Commission 1994d, *National Code of Practice for the Preparation of Material Safety Data Sheets [NOHSC:2011(1994)]*, Australian Government Publishing Service, Canberra.