



IDEA
Hydroperoxide task force

Brussels, December 3rd 2015

A. Chaintreau

Agenda

- › Antitrust statement
 - › No discussions of agreements or concerted actions that may restrain competition
- › Adoption of the agenda

The members of the IDEA Hydroperoxides TF

Name	Email	Affiliation
Jean-Marie Aubry	jean-marie.aubry@univ-lille1.fr;	U.Lille
Annabelle Besson	annabelle.besson@iff.com	IFF
Anna Börje	aborje@chem.gu.se	U. Gothenburg
Hugues Brevard	hugues.brevard@robertet.com	Robertet
Michael Calandra	michael.calandra@firmenich.com	Firmenich
Alain Chaintreau	alain.chaintreau@firmenich.com	Firmenich
Elise Corbi	elise.corbi@chanel-corp.com	Chanel
André Düsterloh	andre.duesterloh@dsm.com	DSM
Cécile Gonzalez	cgonzalez@ifraorg.org	IDEA Management Team
Elena Gimenez Arnau	egimenez@unistra.fr	U. Strasbourg
Ann-Therese Karlberg	karlberg@chem.gu.se	U. Gothenburg
Hans Leijs	hans.leijs@iff.com	IFF
Clémentine Marteau	clementine.marteau@iff.com	IFF
Andreas Natsch	andreas.natsch@givaudan.com	Givaudan
Ulrika Nilsson	ulrika.nilsson@anchem.su.se	U. Stockholm
Neil Owen	neil.owen@givaudan.com	Givaudan
Christophe Peres	christophe.peres@chanel-corp.com	Chanel
Veronique Rataj	veronique.rataj@univ-lille1.fr	U. Lille
David W. Roberts	d.w.roberts@ljmu.ac.u	U. Liverpool
Matthias Vey	mvey@ifraorg.org	IDEA Management Team

December 2015

Objectives of this meeting

- › Synthesizing last results
- › Defining next steps
- › Drawing conclusions for the meeting with the Commission

01

Results

See presentations by:

- [M. Calandra](#)
- A. Natsch
- [A. Chaintreau](#)
- Others ?

02

Outlooks & new questions

Achievements

- › Synthesis of pure standards
- › Purity measurement
- › Quantification method
 - › →Next slide
- › New compound found
 - › Unknown role in allergy
 - › Major impact on quantification



Methods: Conclusions & assumptions to check

› NMR

- › Exact composition, low sensitivity

› GC-FID & GC-MS of underivatized ROOHs

- › Unsuitable

› GC & derivatization

- › Free ROOH + reversible fraction from the adduct ?
- › FID → non alcoholic products. No standard needed

› HPLC

- › Exact ROOH concentration ?
 - › Depends on the dissociation kinetics in mobile phase
- › But: frequent and major overestimations in LC-MS/MS (ring test)

Methods

- › GC & LC methods to be rechecked taking the amount of adduct into account
 - › Requires the devt of a quantification method for the adduct
- › Alcoholic perfumery and aqueous cosmetics
 - › Possibly no adduct (can be easily checked)
 - › If true
 - PPh₃ reduction applicable
 - LC-MS if the cause of overestimation is solved
 - LC-CL applicable



**Key points to answer the Workshop's request
on the analysis of consumer products**

Next steps

- › Variability of TPP method in the same consumer products (fine fragrances)
 - › Greenpharma will prepare the samples and standards ready to be analyzed (only one batch)
- › Some people might want to apply other methods on the same samples.
- › Look at the role of the adduct in more complex samples

Questions on the adduct

- › To what extent does it revert into ROOH ?
- › Is it stable ?
 - › Stability differences = $f(\text{RCHO}, \text{ROOH})$?
 - › Degradation products ?
- › Is it more/less allergenic than the free ROOH ?
 - › Impact on patch tests
 - › Petrolatum → adduct favored
 - not representative of perfumes & cosmetics
 - representative of e.g. massage applications ?
 - › Impact on fragrances
 - › EtOH or water → adduct disfavored

03

Election

Election of a new Chairman

- › A. Chaintreau
 - › End of December
 - Retirement from Firmenich
 - Resignation from my role of Chairman
 - Corresponding member ?
 - › Still participates in the review by the Commission
 - › Starting from January 15th → Email: firm.alc@sfr.fr
- › New Chairman to be elected

Volunteers ?

Firmenich

inspiring!



INNOVATIVE CRAFTSMANSHIP IN FRAGRANCES AND FLAVORS SINCE 1895