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Article

Bio-based HSP Determination for Cosmetic Applications

Sander van Loon & Beverley Fricker – May 28, 2020

TAGS: Science-based Formulation Natural/ Organic

Consumer preference and awareness about the environmental impact of the cosmetic industry means that there is a big drive towards replacing raw materials with bio-based alternatives. In addition to this, there are also tighter regulations and sustainability targets being introduced.

Some of the new claims and labels being sought after by consumers are:

- Bio-degradable
- Bio-based
- Carbon-neutral
- Eco-cert
- Natural and fair trade

Whether you are looking for green, plant based or just a different ingredient, HSP will remove the trial and error of the process.

To learn more about the theory behind HSP, see **Professor Steven Abbott's Tutorial Here!**

Now, let's discover the bio-based alternatives with VLCI's existing HSP workflow using traditional solvents.

Selecting Bio-based & Green Solvents Using HSP

VLCI has been a **certified center for performing HSP determinations** since 2011, via a very efficient workflow. Now, this HSP workflow can be offered by using bio-based solvents.

VLCI has collaborated with many companies to obtain a **range of bio-based solvents** that are spread across the HSP space to perform the determination. These solvents will also be

supplemented with few green solvents, that are found in the extremities of the HSP space, where no bio-based solvents currently lie to achieve the highest accuracy in our determinations until suitable bio-based solvents can be sourced to replace them.

With that, it is possible to practically determine the HSP of products using only these solvents and then based upon this, **recommend suitable replacements** or **predict their compatibility**. This selection of **bio-based solvents** is constantly expanding as more bio-based solvents are being released into the market.

So, what do we mean by these terms?

Plant-based products are a subgroup of bio-based products which, in turn, refers to **products wholly** or **partly derived from biomass**, such as:

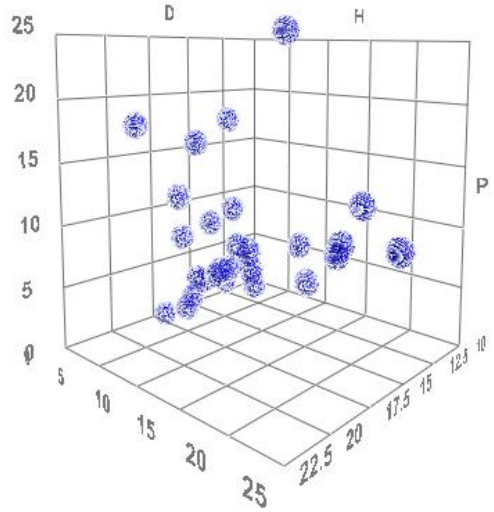
- Plants
- Trees or
- Animals

The biomass can have undergone physical, chemical or biological treatment[3].

There is no universal definition of a "**Green Solvent**", but usually the term refers to a solvent that has:

- Minimal health hazards (e.g. non-carcinogenic)
- Minimal safety hazards (e.g. non-flammable)
- Minimal environmental concerns based upon CLP/GHS analysis

…and then an analysis of the impact/efficiency of the manufacturing process is also taken into consideration.[1, 2]



The Bio-based Solvents in HSP Space

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Validation of the Bio-based Test Method

HSP Determination of Selected Ingredients

To validate our bio-based HSP workflow, we performed an HSP determination of **Baycusan® C 1003** and **Escalol™ 557 UV filter** using both the standard HSP solvent selection and the bio-based solvent selection.

- The HSP determination of Baycusan® C 1003 was performed at a concentration of **0.5 g in 5 ml of solvent**.
- The recommended use of Escalol™ 557 UV filter is between 2-7.5%, so the HSP was determined at a concentration of **0.375 g in 5 ml of solvent**.

Baycusan® C 1003 by Covestro, is a colloidal system of a high molecular weight polyurethane polymer dispersed in water. An internal emulsifier is incorporated into the polymer backbone to ensure the stability of the dispersion. Therefore, the use of external surfactants is not required. This polymer performs exceptionally well as a **film former in face mask applications**.

Escalol™ 557 UV filter by Ashland, is a UV filter containing **Ethylhexyl Methoxycinnamate**. It shows a broad UV-B absorbency profile and is water-insoluble. Escalol™ 557 UV filter finds application in formulating:

- Sun-care (after-sun, self-tanning and sunscreen application)
- Body- & facial-care formulas
- Color cosmetics

Validating the Solvents

The test materials were added to the samples, shaken and left to dissolve. The samples were then visually assessed with a **qualitative rank**.

- **Baycusan® C 1003** was assessed from 1-6, where -
  - A 1 means the product is completely dissolved.
  - A 6 means there has been no interaction between the solvent and the product.
  - The other scores indicating various stages of dissolution.

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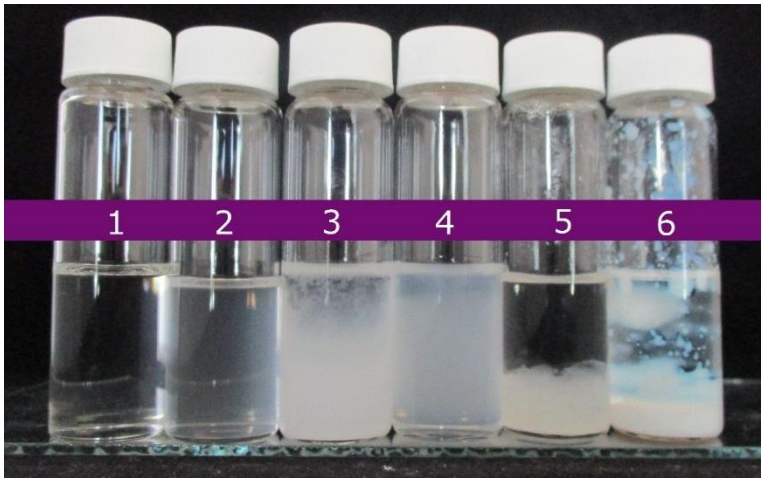
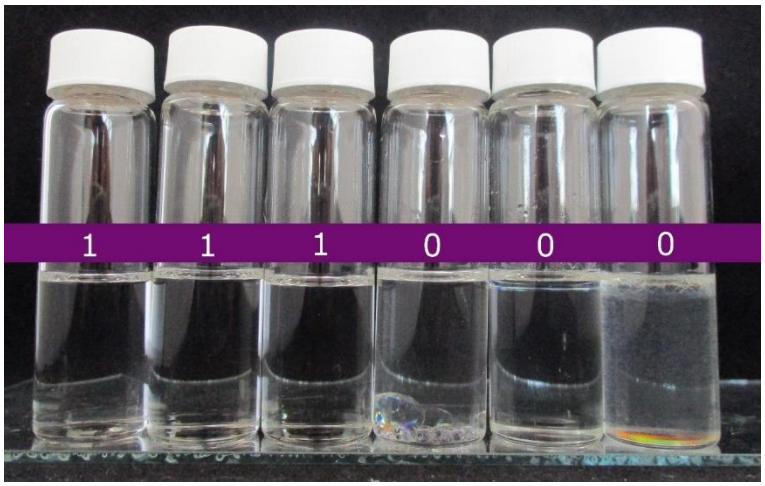
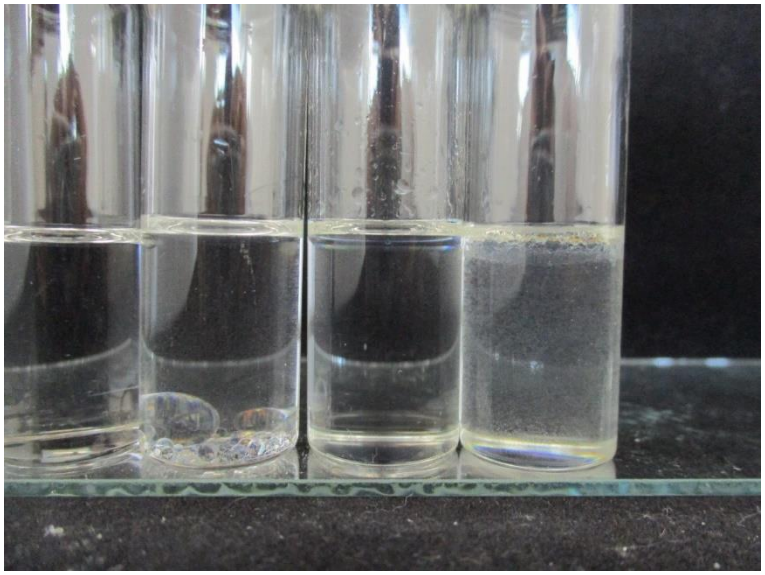


Visual differences and scores of Baycusan® C 1003

- In the case of **Escalol™ 557 UV filter**, only 2 clear differences were present, so this was assessed with the scores of 1 and 0.



Visual differences and scores of Escalol™ 557 UV filter



Immiscibility seen in samples with Escalol™ 557 UV filter

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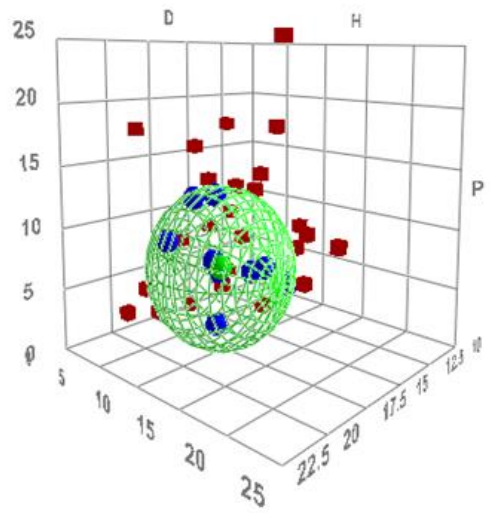
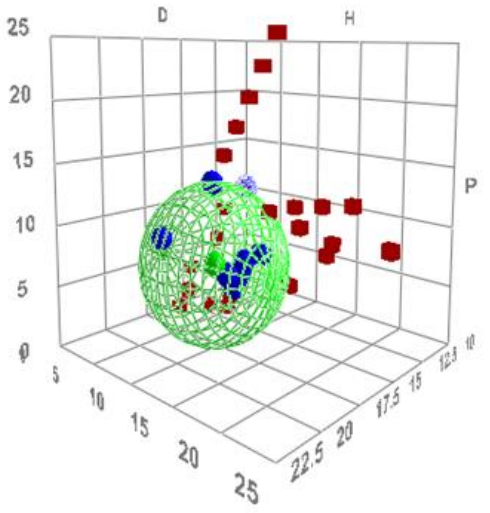
This data is then entered into the **HSPiP Software**, which defines a spheroidal cluster of the solvents that dissolved the test material. This cluster is called the **Hansen Solubility Sphere**, and its central coordinates (δD, δP and δH) define the core solubility parameters of the test material.

The software also performs an analysis of the "**fit**" of the data to the parameters it has determined, highlighting the validity of the result, which can indicate if more experimental data is needed.

Classic HSP – Baycusan® C 1003	Bio-based HSP – Baycusan® C 1003
	
In = 10, Out = 26, Total = 36 D = 18.37, P = 7.49, H = 11.33 Tot = 22.8, R = 6.4	GA Fit In = 10, Out = 23, Total = 33 D = 18.33, P =7.52, H = 11.23
Fit = 1.000 Core = ±[0.10, 0.25, 0.30]	Tot = 22.8, R = 6.5 Fit = 0.970

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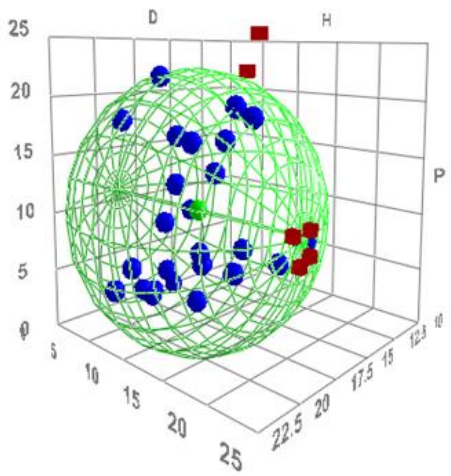
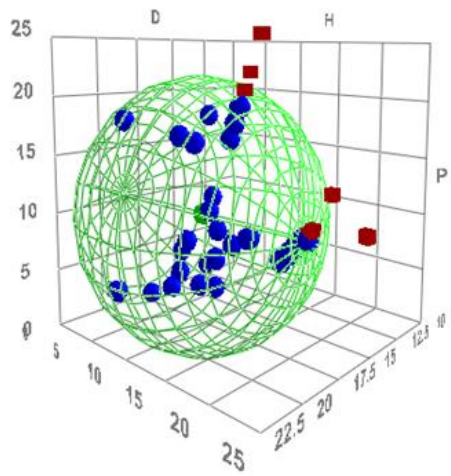
Classic HSP – Escalol™ 557 UV filter	Bio-based HSP – Escalol™ 557 UV filter
	
GA Fit In = 30, Out = 7, Total = 37 D = 16.54, P = 9.21, H = 7.61 Tot = 20.4, R = 12.6 Fit = 1.000	GA Fit In = 30, Out = 7, Total = 37 D = 16.42, P = 8.98, H = 7.39 Tot = 20.1, R = 12.9 Fit = 1.000
Fit = 1.000 Core = ±[0.10, 0.25, 0.30]	Tot = 22.8, R = 6.5 Fit = 0.970

From both the tables above, it can be seen that **all four HSP determinations were successful** and that the bio-based solvents are suitable for determining HSP.

For more details on how to practically determine an HSP, see our article **Predicting Ingredient Compatibility Using HSP in Cosmetic Formulations**.

Conclusion

Bio-based alternatives are in demand across the formulation industry. In this article, the HSP's of Escalol™ 557 UV filter (by Ashland) and Baycusan® C 1003 (by Covestro), were determined using only bio-based and green solvents. These determinations were then successfully validated against **VLCI's existing HSP workflow using traditional solvents**.

- This demonstrates that the bio-based solvents are suitable for determining Hansen solubility parameters.
- And, in addition to this, it allows for immediate recommendations of bio-based solvents and oils that are compatible with the test material.

Knowing the HSP's of your materials allow for smart and efficient formulating and material replacement.

To learn more about how to implement HSP's, see our **other articles here!**

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References

1. Adrien Benazzouz, Laurianne Moity, Christel Pierlot, Michelle Sergent, Valérie Molinier and Jean-Marie Aubry. 2013. “Selection of a Greener Set of Solvents Evenly Spread in the Hansen Space by Space-Filling Design.” Ind. Eng. Chem. Res. 52: 16585-16597.
2. Denis Prat, Andy Wells, John Hayler, Helen Sneddon, C. Robert McElroy, Abou-Shehadad and Peter J. Dunne. 2016. “CHEM21 selection guide of classical- and less.” Green Chemistry 18: 228.
3. European Committee for Standardization CEN. 2014. “EN 16575:2014 ‘Bio-based products – Vocabulary’.”