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ViridisChem's Chemical Analyzer For Sustainable Product Development

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Goal of the case-study

This case-study will show how ViridisChem's Chemical Analyzer can be used to identify toxicity implications of the chemicals being used during product development; and how less toxic alternatives that satisfy specific product requirements can be found within seconds to help scientists optimize and adopt sustainable product development.

For the case-study, we have chosen a real production issue faced by the Textile industry to illustrate how ViridisChem product can be used to find less toxic alternatives.

Company Background

ViridisChem has built a highly performant, scalable and secure SaaS infrastructure that offers toxicity evaluation of every known or proprietary chemical, including new or postulated molecules. In addition to this platform, ViridisChem has built one of the largest toxicity databases available in the market and offers on-demand execution of AI-driven toxicity prediction models. Combining the power of all these capabilities into its product Chemical analyzer, it can provide comprehensive toxicity profile of any known/proprietary or even new molecules, identify most US and international regulatory implications, and provide detailed ecological, health and safety impact. Chemical analyzer also offers advanced search capabilities that allow scientists to find less toxic alternatives based on their specific application needs (needing specific functional/leaving groups, oxidizing/reducing agents, specific physical properties, or needing to find chemicals that do not have specific acute or chronic health issues) during product development or process optimization efforts.

Case Study

Formaldehyde[1,2,3] made into a resin has been used for a long time in **textile finishing after manufacturing** to give fabrics certain characteristics like increasing wrinkles, making them crease resistant, and avoiding mold during transport. It also allows some dyes and inks to better penetrate fabrics. However, it has many health and safety issues. For example, it is highly flammable in liquid, and in solid form causes severe skin and eye irritation. It is also carcinogenic and genotoxic. It was believed that the chemical would wash away after washing. But in recent years, number of studies have shown that this is not the case. Since 2015 State of California, Japan, Vietnam, and many countries in Europe have defined strict restrictions on the use of this chemical in most clothes (specially children clothes).

Today, Formaldehyde is on the "Manufacturing Restricted Substance List" (MRSL), a published list by ZDHC (Zero Discharge of Hazardous Chemicals), an international association of textile and shoe manufacturers, with input from key stakeholders from its member brands and chemical companies. ZDHC strongly recommends that Formaldehyde should not be used for textile finishing and must be replaced by

Zinc formaldehyde sulfoxylate (ZFS). This case study will explore if ZFS is the best alternative, or if other more suitable chemicals are available.

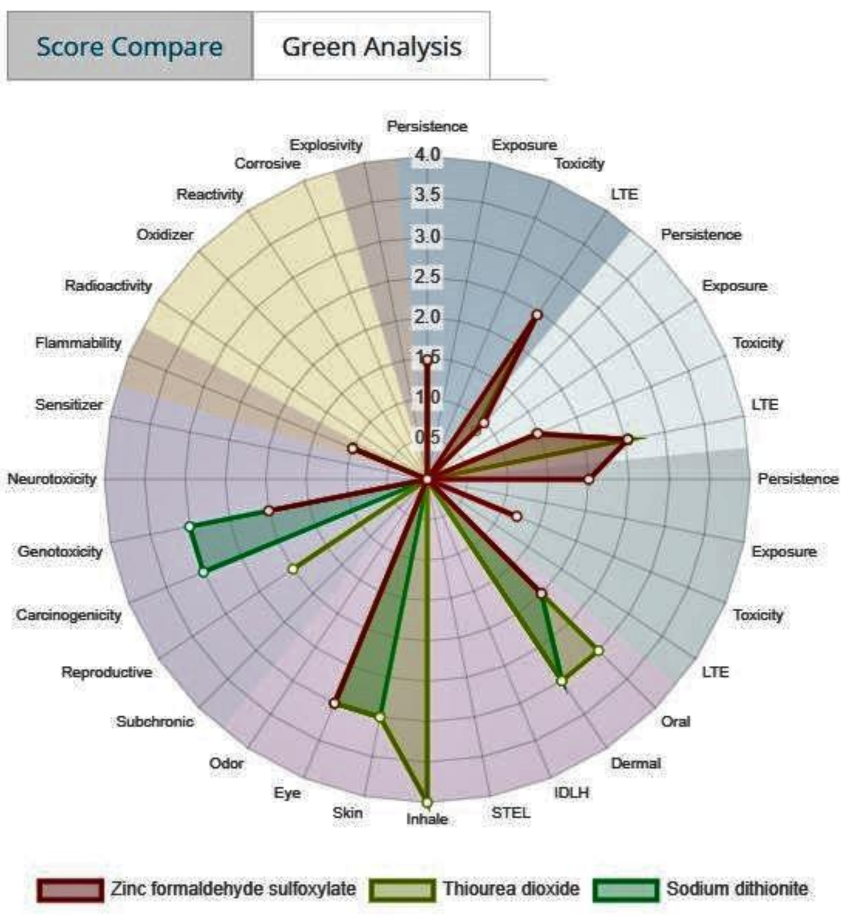
Study Approach

It was understood that to achieve the required textile finishing effect for which formaldehyde was originally used, a strong reducing agent like sulfinic acid was needed. Based on this requirement, the following alternative chemicals were considered that have marginally better toxicity footprint:

- Zinc formaldehyde sulfoxylate (ZFS: CAS# 24887-06-7)
- Thiourea dioxide (CAS# 1758-73-2)
- Sodium dithionite (CAS# 7775-14-6)

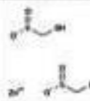
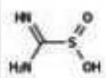
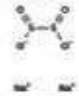
ViridisChem's Chemical Analyzer visually shows the differentiation between these chemicals in terms of various toxicity endpoints in order to judge the suitability of each of these chemicals.

FIGURE 1: Detailed toxicity profiles of 3 chemical options using Chemical analyzer



Name	Zinc formaldehyde sulfoxylate	Thiourea dioxide	Sodium dithionite
Final Score	1.54	1.61	1.69
–Ecological Score	1.66	1.67	N/A
–Water Score	1.90	1.89	N/A
Persistence	1.48	1.46	N/A
Exposure	N/A	N/A	N/A
Toxicity	N/A	N/A	N/A
Long Term Effect	2.45	2.45	N/A
+Air Score	1.55	1.47	N/A
+Soil Score	1.55	N/A	N/A
–Health Score	2.21	2.52	2.85
–Acute Health Score	2.45	3.18	2.71
Oral LD50	2.00	3.00	2.00
Dermal LD50	N/A	3.00	3.00
Inhalation LC50	N/A	4.00	N/A
Skin Irritation	N/A	3.00	3.00
Eye Irritation	3.00	3.00	3.00
–Chronic Health Score	2.00	2.00	3.00
Subchronic Toxicity	N/A	N/A	N/A
Reproductive Effect	N/A	2.00	N/A
Endocrine Disruptor	N/A	N/A	N/A
Carcinogenicity	N/A	N/A	3.00
Genotoxicity	2.00	N/A	3.00
Neurotoxicity	N/A	N/A	N/A
Sensitizer	N/A	N/A	N/A
–Safety Score	1.00	1.00	1.00
+Fire Score	1.00	1.00	1.00
+Special Score	N/A	N/A	N/A
+Reactivity Score	N/A	N/A	N/A

FIGURE 2: Physical-toxicological properties of the chemical options using Chemical analyzer

Name	Zinc formaldehyde sulfoxylate	Thiourea dioxide	Sodium dithionite
Structure			
Customizations	View	View	View
Functional Groups	Alcohol, Sulfinic Acid	Amine, Sulfinic Acid	Sulfinic Acid
+Identifications			
+Rule of 5	true	true	true
+Health & Safety	Warning	Danger	Danger
MW	255.56	108.12	176.11
BP	364.63 deg C	300.33 deg C	
MP	168.00 deg C	127.00 ° C	52.00 ° C
VP	0.00 mm Hg	0.20 mm Hg	
LogP	0.00	0.00	
FlashPt	268.26 celsius	168.70 celsius	100.00 ° C

Name	Zinc formaldehyde sulfoxylate	Thiourea dioxide	Sodium dithionite
-Lethal Dose			
LC50 Air	0.00	0.00	0.00
LC50 Water			
LC50 Soil	989.63 mg/L		
LD50 (Oral)		1120.00 mg/kg	2500.00 mg/kg
RfC			
RfD			
TLV			
logKow (log P)	0.00	0.00	
BAF		0.89 L/kg wet-wt	
logBAF	-0.05	-0.05	
BCF	3.16 L/kg wet-wt	3.16 L/kg wet-wt	0.46 L/kg wet-wt
logBCF	0.50	0.50	-0.33
BTF		0.00 days	
logBTF		-2.85	
Henry's Const	0.00 atm-m3/mole	0.00 atm-m3/mole	
KP	0.00 cm/hr	0.00 cm/hr	-3.77 cm/hr
KOA	4954501908.05	33728730865.89	
logKOA	9.70	10.53	
KOC	1.00 L/kg	1.00 L/kg	
logKOC	0.00	0.00	
OH k	0.00 cm3/molecule-sec	0.00 cm3/molecule-sec	
OZ k	0.00 cm3/molecule-sec	0.00 cm3/molecule-sec	
WS	387000.00 mg/L	0.00 mg/L	0.37 mg/L

Each of the chemicals in the study were selected because they are less toxic than formaldehyde. As you can see in Figure 1 and 2, they are all genotoxic and eye irritant, although the severity of Zinc Formaldehyde sulfoxylate is lower. Both Thiourea dioxide and sodium dithionite have other chronic and acute health issues (skin, inhalation and oral irritation, carcinogenicity, reprotoxicity, and organ-related toxicity through prolonged exposure), are self-heating and pose a serious fire hazard. They also have expensive storage restrictions and must be monitored. As such Zinc Formaldehyde Sulfoxylate seems to be a better choice than the other two chemicals.

However, it is worthwhile to note that Zinc Formaldehyde Sulfoxylate genotoxic, has moderate ecological toxicity issues and is persistent in air, water, and soil. Care must be taken during disposal of the waste. Some researchers are also worried that since formaldehyde is highly soluble in water and other solvents, there is a possibility of zinc formaldehyde sulfoxylate carrying residual formaldehyde.

Using the ViridisChem's Chemical Analyzer, we decided to explore other better and greener alternative(s) to Zinc formaldehyde sulfoxylate that may satisfy the textile processing requirements. We decided to find chemicals that match following criteria:

- Functional groups: Sulfinic acids and alcohol
- Avoid chronic health issues: genotoxicity, carcinogenicity
- Avoid acute health issues: Eye irritation, skin irritation
- Has overall smallest toxicity score

Utilizing the Chemical Analyzer's "Advanced Search" feature that offers the list of chemicals and their toxicity scores that match the given comprehensive set of criteria we were able to get following results:

FIGURE 3: Advanced Search based on multiple criteria within ViridisChem's Chemical Analyzer

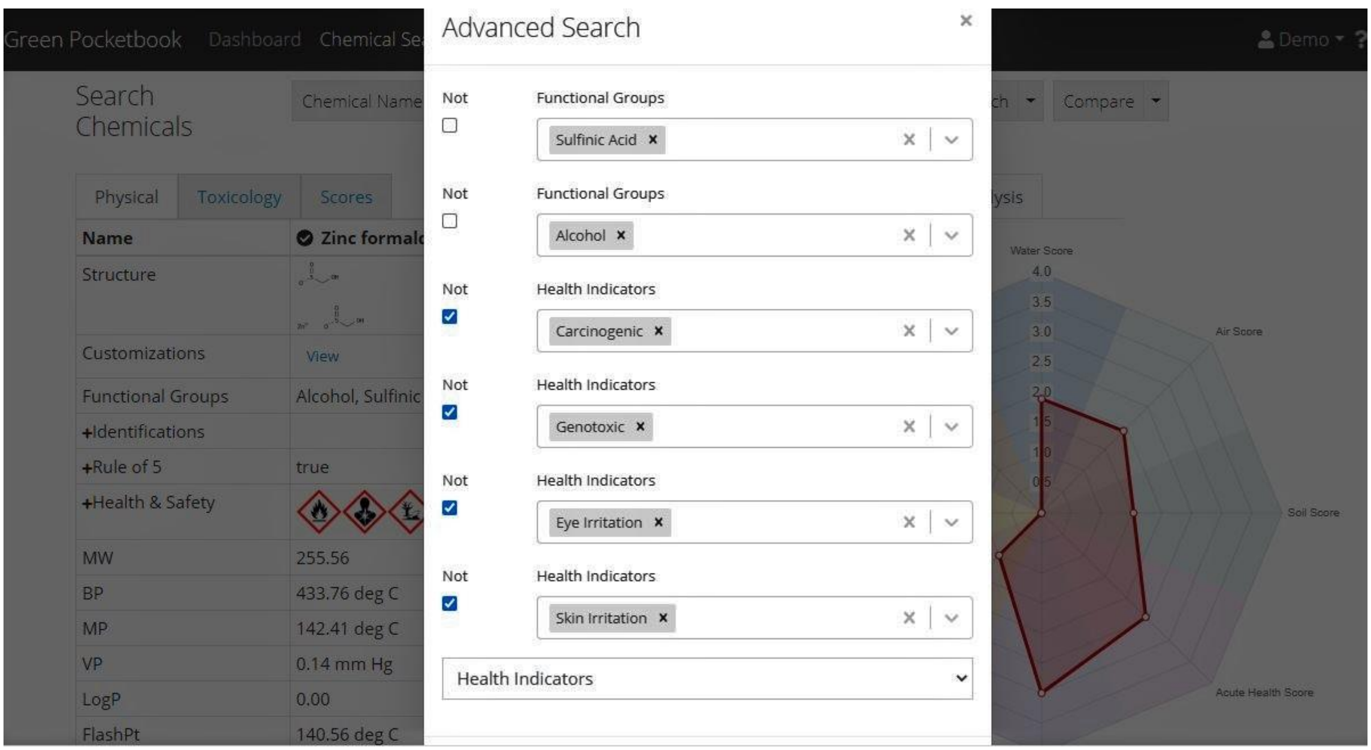
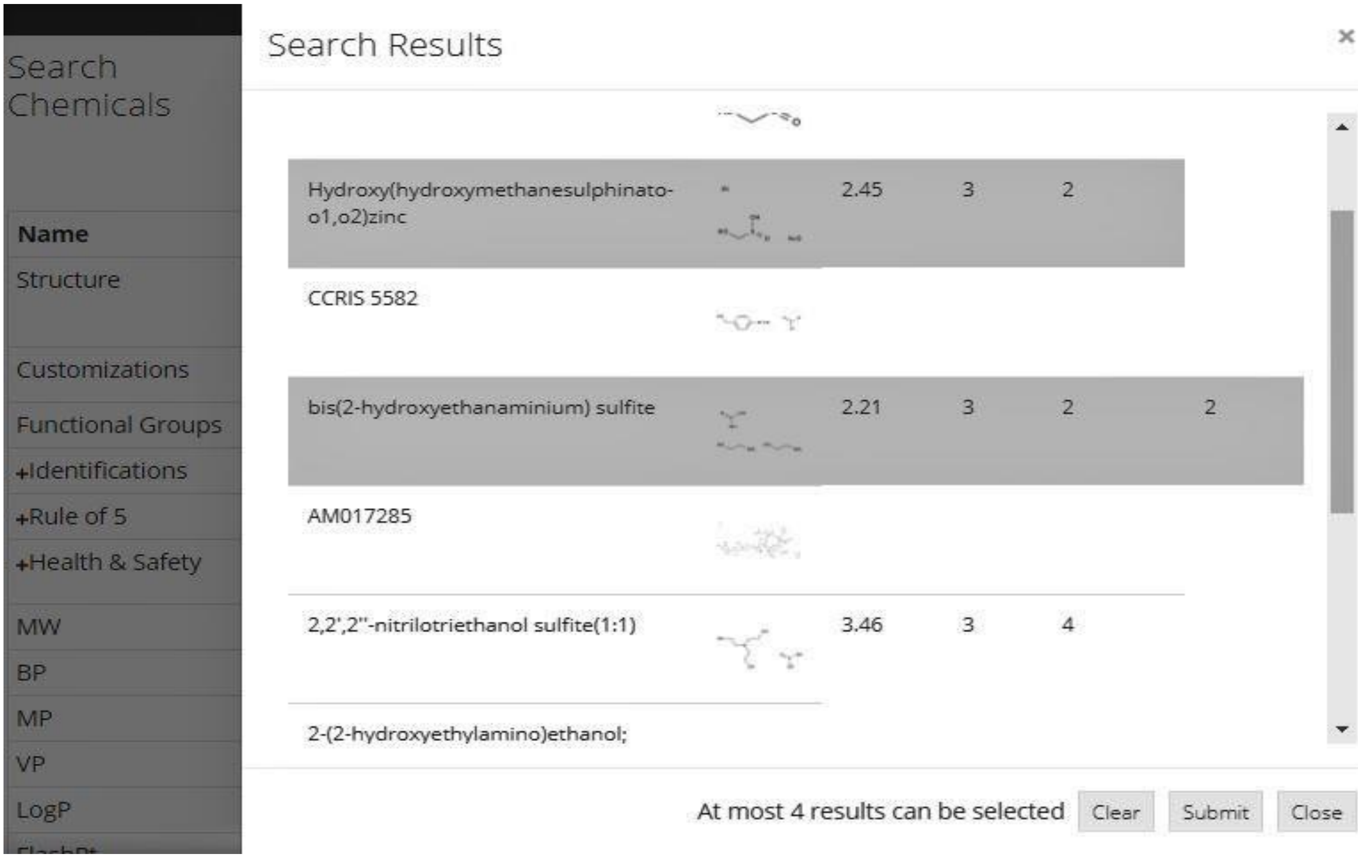


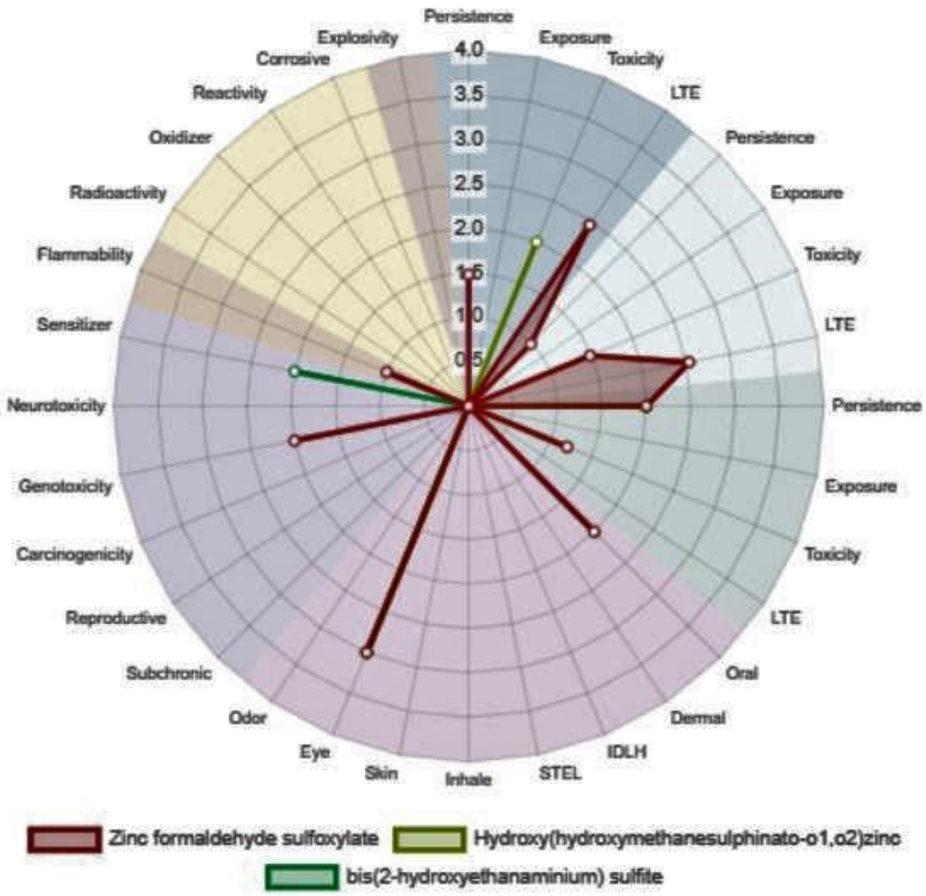
FIGURE 4: Advanced Search Results



Based on the toxicity scores, two chemical alternatives were selected:

1. Hydroxy(hydroxymethanesulphinato-o1,o2)zinc (CAS# 56329-30-7)
2. bis(2-hydroxyethanaminium) sulfite (CAS# 15535-29-2)

FIGURE 5: Toxicity profiles of the selected alternatives (detailed view)



Name	Zinc formaldehyde sulfoxylate	Hydroxy(hydroxy o1,o2)zinc	bis(2-hydroxyethanaminium) sulfite
Final Score	1.54	2.45	2.21
-Ecological Score	1.66	2.00	2.00
-Water Score	1.90	2.00	N/A
Persistence	1.48	N/A	N/A
Exposure	N/A	N/A	N/A
Toxicity	N/A	2.00	N/A
Long Term Effect	2.45	N/A	N/A
-Air Score	1.55	N/A	N/A
Persistence	0.99	N/A	N/A
Exposure	N/A	N/A	N/A
Toxicity	1.48	N/A	N/A
Long Term Effect	2.53	N/A	N/A
-Soil Score	1.55	2.00	2.00
Persistence	2.00	2.00	2.00
Exposure	N/A	N/A	N/A
Toxicity	1.20	N/A	N/A
Long Term Effect	N/A	N/A	N/A
-Health Score	2.21	3.00	2.45
-Acute Health Score	2.45	3.00	3.00
Oral LD50	2.00	N/A	N/A
Dermal LD50	N/A	N/A	N/A
Inhalation LC50	N/A	N/A	N/A
Skin Irritation	N/A	N/A	N/A
Eye Irritation	3.00	3.00	3.00
-Chronic Health Score	2.00	N/A	2.00
Subchronic Toxicity	N/A	N/A	N/A
Reproductive Effect	N/A	N/A	N/A
Endocrine Disruptor	N/A	N/A	N/A
Carcinogenicity	N/A	N/A	N/A
Genotoxicity	2.00	N/A	N/A
Neurotoxicity	N/A	N/A	N/A
Sensitizer	N/A	N/A	2.00
-Safety Score	1.00	N/A	N/A
+Fire Score	1.00	N/A	N/A
+Special Score	N/A	N/A	N/A
+Reactivity Score	N/A	N/A	N/A

As you can see from the Figure 5, all 3 chemicals cause moderate eye irritation and have low soil persistence. And although Zinc formaldehyde sulfoxylate seems to have higher overall toxicity and the 2 alternative candidates do not have genotoxicity issues, little experimental data is available for those 2 chemicals. Therefore we recommend that if Hydroxy(hydroxymethanesulphinato-o1,o2)zinc and/or bis(2-hydroxyethanaminium) sulfite are commercially viable (low cost and easy commercial availability), they should be studied further to ensure that one or both of them are less toxic alternatives for commercial use.

We also recommend that by changing the "Advanced search" criteria further to include some of the physical or toxicological properties, structural classification (oxidizing/reducing agent, strong or weak acid, specific pH, specific functional or leaving groups, etc.), a more focused set of chemicals can be found as candidates for optimum product development.

While optimizing the complex product development processes, scientists know that in most cases, there is no clear indication of one chemical being more or less toxic in all aspects, but rather, you need to select the better alternative based on

- Which acute and chronic health problems are critical to be avoided (cosmetics for face cannot have skin and eye irritation),
- Target user of the finished product (children, pregnant female, etc.)
- Potential lab-safety issues during the production
- Amount of the chemical needed
- Toxicity footprint during product development and its end-of-life disposal
- Disposal options and long-term impact

Being able to narrow the selection of process optimization candidates earlier in the process without having to do experimental work can save lot of R&D efforts and allow scientists to focus on other critical process optimization aspects.

ViridisChem's Chemical Analyzer allows you to define specific criteria based on your product's requirements and offer you 2-3 alternate candidates that you can focus on during process optimization.

For more detailed information, please go to the company's website: https://www.viridischem.com or contact us by email at: support@viridischem.com

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