

CASE STUDY

What's Really in Our Sunscreens?

Project by Anaya Khanzode,
Summer intern at Covalent Metrology

Introduction

Every summer, we reach for sunscreen to protect our skin from harmful UV rays. But how often do we stop and think about what's actually inside the bottle—or how those ingredients behave once they're on our skin?

Those questions are what drove Anaya Khanzode, Covalent summer intern, to perform a full characterization of two different kinds of sunscreen. Well, that and the fact that one kind irritated her skin and the other didn't.

Sunscreens generally fall into two categories:

- **Mineral sunscreens** (using titanium dioxide [TiO₂] and zinc oxide [ZnO]) scatter UV light, creating a physical barrier.
- **Chemical sunscreens** (with ingredients like octocrylene, homosalate, octisalate, and avobenzone) absorb UV light before it can damage skin.

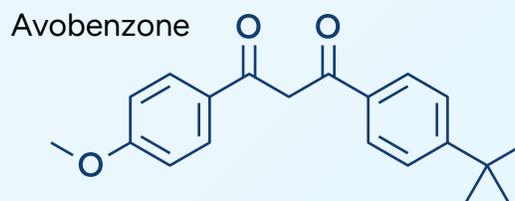
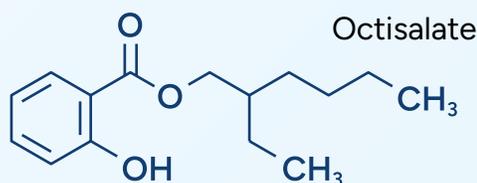
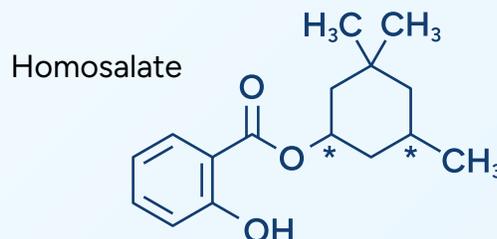
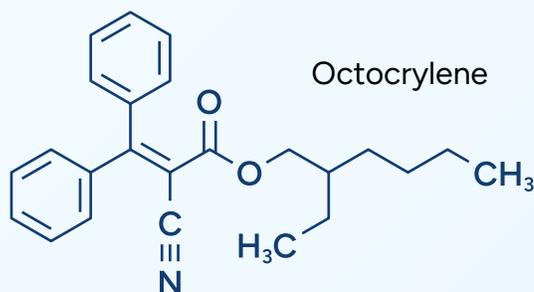
For many people, chemical sunscreens work just fine. But others experience irritation or eczema flare-ups after applying them. That led Anaya to the question, what's actually causing those reactions?



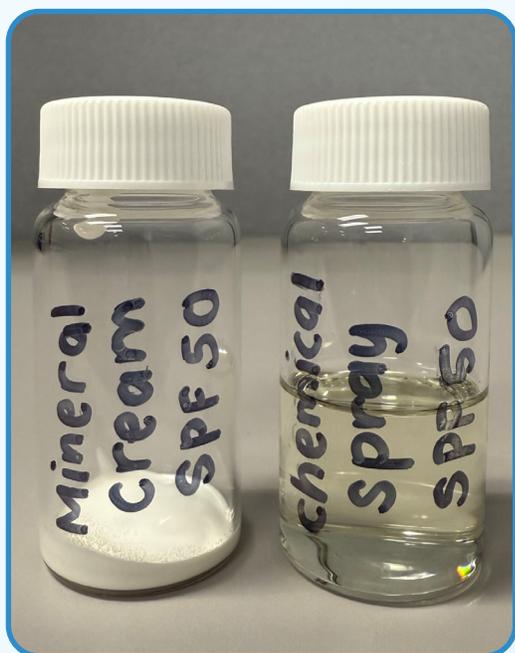
TiO₂



ZnO



To better understand sunscreen safety and performance, Anaya used Covalent Metrology tools to evaluate two commercially available sunscreens—one mineral-based and one chemical-based—using advanced analytical techniques.



Statement of Work

The project set out to investigate three key questions:

1. **Chemical composition** – What volatile compounds are present in chemical sunscreens, and do they change after UV exposure? (Analyzed by GC-MS)
2. **Trace metals** – Are there harmful levels of heavy metals present? (Analyzed by ICP-MS)
3. **Particle size and distribution** – How do mineral nanoparticles scatter or absorb UV radiation? (Analyzed by SEM-EDS)

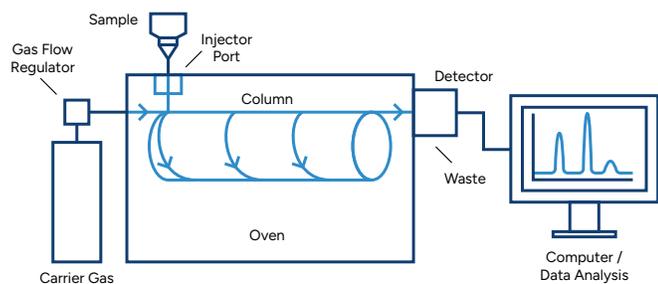
Methods and Findings

1. Volatile Compounds

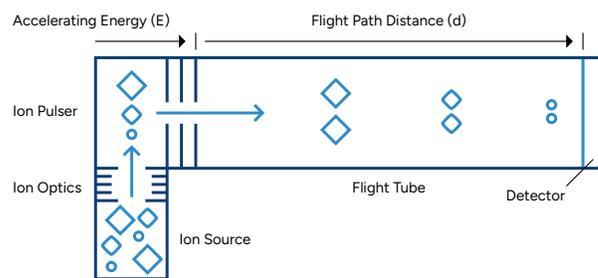
The chemical sunscreen contained vague label ingredients such as “acrylates,” “fragrance,” and “denatured alcohol.” The label also suggests re-application every two hours, so Anaya wondered if the sunscreen was chemically degrading after being exposed to UV radiation.

Gas Chromatography and Time of Flight Mass Spectrometry (GC-MS) were used to investigate the exact chemical identity of these ingredients. In GC-MS, the mixture is first separated into its individual components as it travels through a chromatography column (gas chromatography), then each compound is ionized, fragmented, and measured by its mass-to-charge ratio (mass spectrometry). This allows researchers to identify even trace chemicals with high precision.

Gas Chromatography



Time of Flight Mass Spectrometry



One sample was tested immediately after coming out of the bottle and the other after it was left in a petri dish in the sun for 2 hours. GC-MS analysis revealed multiple volatile organic compounds that could contribute to skin irritation. UV exposure altered the chemical profile, suggesting possible breakdown or reaction of ingredients over time.

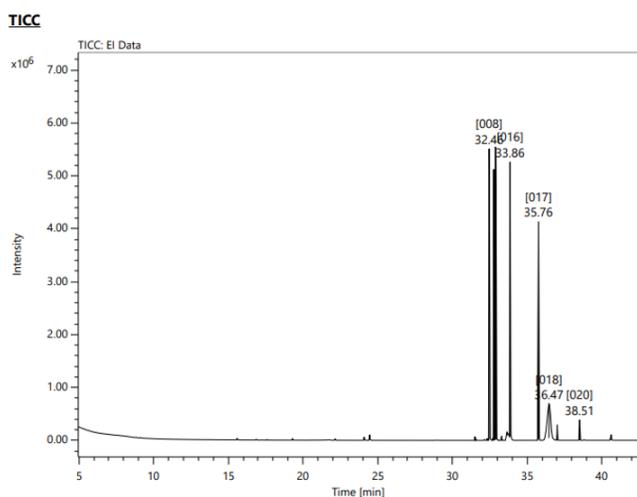


Figure 1: Pre UV Exposure

ID	Compound Name	Match Factor	Formula	Description
001	1,6-Octadiene, 7-methyl-3-methylene-	936	C10 H16	
002	1,6-Octadien-3-ol, 3,7-dimethyl-	865	C10 H18 O	solvent
003	α -Terpineol [α , α , 4-trimethyl-3-cyclohexene-1-methanol]	888	C10 H18 O	
004	Propanoic acid, phenylmethyl ester	927	C10 H12 O2	anti-fungal
005	Ethyl salicylate	969	C9 H10 O3	emollient
006	Cinnamaldehyde, α -pentyl-	895	C14 H18 O	fragrance
007	1-Hexadecene	913	C16 H32	solvent
008	Octisalate	963	C15 H22 O3	active ingredient
009	Benzoic acid, 2-hydroxy-, 3-methyl-2-butenyl ester	710	C12 H14 O3	fragrance
010-012	Homosalate	956	C16 H22 O3	active ingredient
013	<i>o</i> -Anisic acid, 3-pentadecyl ester	-	C23 H38 O3	fragrance
014	1-Octodecanol	-	C18 H38 O	solvent
015-016	Octisalate	762	C15 H22 O3	
017	Octocrylene	950	C24 H27 N O2	active ingredient
018	Avobenzone	871	C20 H22 O3	
019	Glycerol tricaprylate	844	C27 H50 O6	emollient/fragrance
020	2-(Decanoyloxy)propane-1,3-diyl dioctanoate	829	C29 H54 O6	
021	3-(Octanoyloxy)propane-1,2-diyl bis(decanoate)	755	C31 H58 O6	emollient

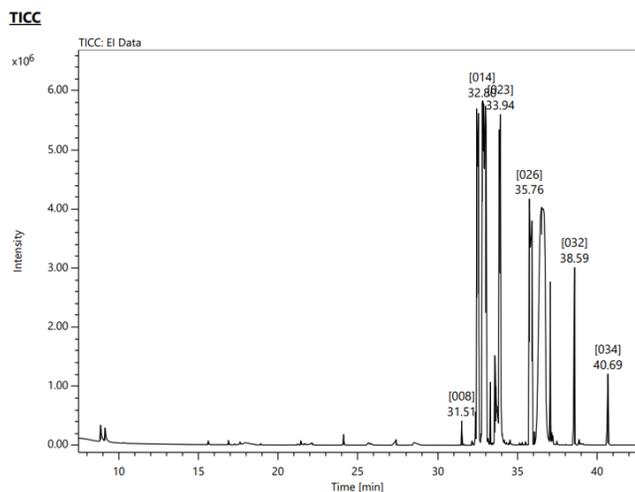


Figure 2: Post UV Exposure

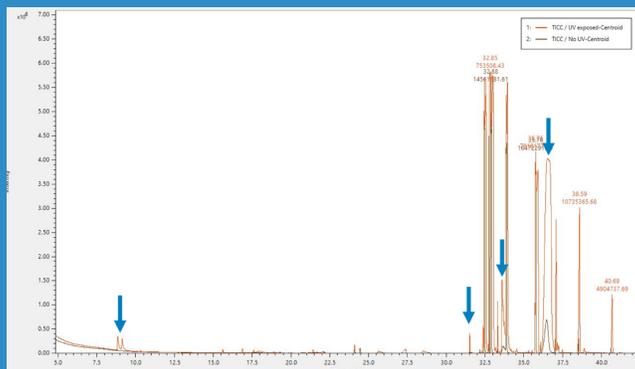


Figure 3: Shown above are the overlain chromatograms of both the UV exposed and non-exposed samples. The peaks highlighted with blue arrows are ones that only appear after UV exposure, and are likely photodegradation products.

ID	Compound Name	Match Factor	Formula	Description
001-002	Cyclohexene, 3,3,5-trimethyl-	908	C9 H16	solvent
003	1,6-Octadiene, 7-methyl-3-methylene-	892	C10 H16	
004	Limonene	933	C10 H16	fragrance
005	1-Hexene, 5-methyl-	810	C7 H14	solvent
006	Propanoic acid, phenylmethyl ester	945	C10 H12 O2	anti-fungal
007	Decanoic acid	892	C10 H20 O2	emollient
008	Heptanal, 2-(phenylmethylene)-	942	C14 H18 O	fragrance
009	Octanal, 2-(phenylmethylene)-	857	C15 H20 O	
010	1-Hexadecanol	801	C16 H34 O	solvent
011-012	Octisalate	952	C15 H22 O3	active ingredient
013-017	Homosalate	893	C16 H22 O3	
018	o-Anisic acid, 2-pentadecyl ester	788	C23 H38 O3	fragrance
019	1-Hexadecene	904	C16 H32	solvent
020	1-Nonadecene	801	C19 H38	
021-023	Octisalate	791	C15 H22 O3	active ingredient
024	Vinyl caprylate	700	C10 H18 O2	fragrance
025-027	Octocrylene	900	C24 H27 N O2	active ingredient
028	Octanoic acid, heptadecyl ester	898	C25 H50 O2	anti-fungal
029	Avobenzone	935	C20 H22 O3	active ingredient
030	Glycerol tricaprylate	878	C27 H50 O6	emollient/fragrance
031	Decanoic acid, tetradecyl ester	827	C24 H48 O2	emollient
032	2-(Decanoyloxy)propane-1,3-diyl dioctanoate	885	C29 H54 O6	
033	dl- α -Tocopherol	933	C29 H50 O2	vitamin E
034	3-(Octanoyloxy)propane-1,2-diyl bis(decanoate)	898	C31 H58 O6	emollient

2. Trace Metals (ICP-MS)

Next up, Anaya looked at trace metals using Inductively Coupled Plasma Mass Spectrometry (ICP-MS). This technique works by ionizing a sample in a super-heated plasma, then separating and detecting the resulting ions by their mass-to-charge ratio. The method is incredibly sensitive, capable of spotting elements at parts-per-billion or even parts-per-trillion levels.

Both the mineral and chemical sunscreens contained detectable metals, but none exceeded toxicity thresholds for topical use. The panel included vanadium, chromium, manganese, cobalt, arsenic, selenium, molybdenum, antimony, barium, mercury, and lead. The mineral sunscreen showed trace amounts of nearly every element tested, while the chemical sunscreen lacked detectable cobalt, copper, and silver.

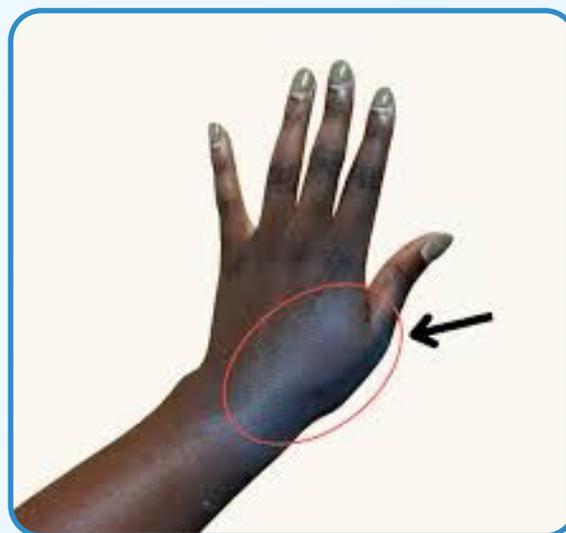
At first glance, seeing names like mercury, lead, and arsenic might raise alarms. But it's important to note that while these elements were present, they were measured at concentrations far below levels considered harmful when applied to skin.

3. Nanoparticle Characterization (SEM-EDS)

If you've ever noticed that mineral sunscreens sometimes leaves your skin looking a little ghostly, the reason comes down to particle size. Titanium dioxide (TiO_2) and zinc oxide (ZnO) work in two ways: nanoparticles (smaller than 100 nm) absorb UV light and go on clear, while larger particles scatter UV light—and that scattering is what creates the whitish cast. Anaya noticed that the mineral sunscreen left a white cast on her skin, so she hypothesized that the nanoparticles were agglomerating.

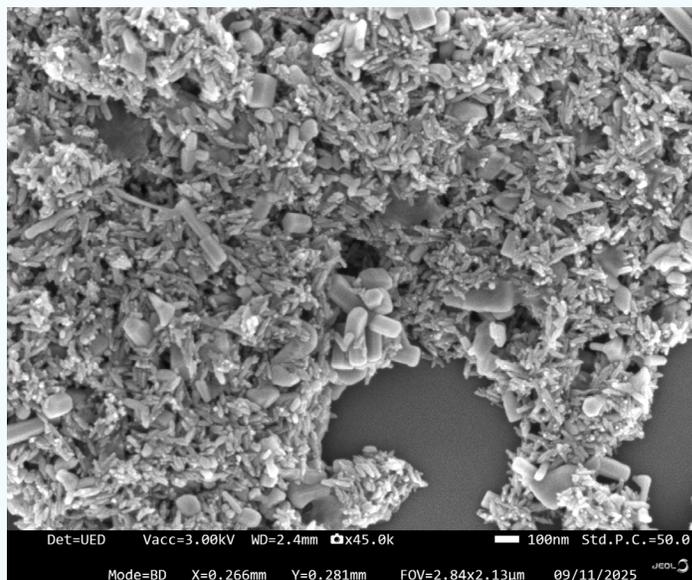
Element	Chemical Spray (ppb)	Mineral Cream (ppb)	Toxic Levels?
V	6	300	No
Cr	2,000	500	No
Mn	2	300	No
Fe	1,000	2,000	No
Co	<1	20	No
Ni	4	2,000	No
Cu	<20	4,000	No
As	1	100	No
Se	4	7	No
Mo	35	200	No
Ag	<300	10,000	No
Sb	2	200	No
Ba	6	100	No
Hg	1	7	No
Pb	1	300	No

Figure 4: Trace metals analysis



To confirm her hypothesis, she imaged a sample of the mineral sunscreen into a Scanning Electron Microscope (SEM).

Here is an SEM image that Anaya captured while zooming in on a chunk of sunscreen. The image revealed two distinct kinds of nanoparticles: larger, hexagonal prism-shaped rods and smaller, globular particles. Anaya predicted that these corresponded to ZnO and TiO₂, though she did not yet know which was which. The non-uniform, larger globs visible in the background are likely residual solvents and emollients that could not be fully extracted prior to SEM analysis.



To determine which nanoparticles corresponded to which minerals, Anaya used **Energy Dispersive Spectroscopy (EDS)**. In this technique, when a sample is struck by an electron beam inside the microscope, the atoms in the material are excited and then release characteristic X-rays as they relax back to their ground state. By detecting those X-rays and converting their wavelengths into energy values, EDS produces a spectrum—or in this case, a map—that shows which elements are present in the sample.

Using the same SEM image as before, Anaya generated an elemental map for titanium (Ti) and zinc (Zn). The results showed that Ti was evenly distributed throughout the sunscreen, while Zn appeared in concentrated clumps that lined up with the large hexagonal nanoparticles. From this data, she was able to confidently assign the smaller spherical particles to TiO₂ and the larger hexagonal rods to ZnO.

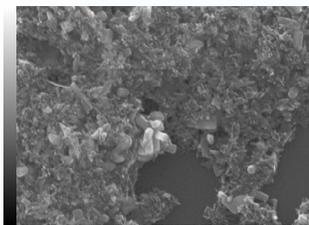


Figure 5: SEM Image

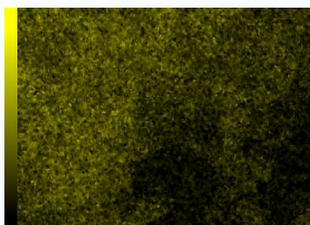


Figure 6: Ti EDS Map

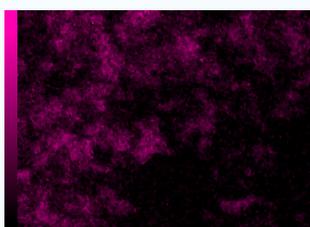


Figure 7: Zn EDS Map

To confirm her observations about the nanoparticles, Anaya collected EDS spectra from two different areas of the SEM image. She focused the analysis on the hexagonal nanoparticles (marked in lime green) and the smaller spherical nanoparticles (marked in pink). The spectra revealed that the pink region had a much stronger signal for titanium, while the lime green region showed a much stronger signal for zinc. Combined with the elemental maps, this evidence allowed Anaya to confidently identify the smaller spherical particles as TiO_2 and the larger hexagonal rods as ZnO .

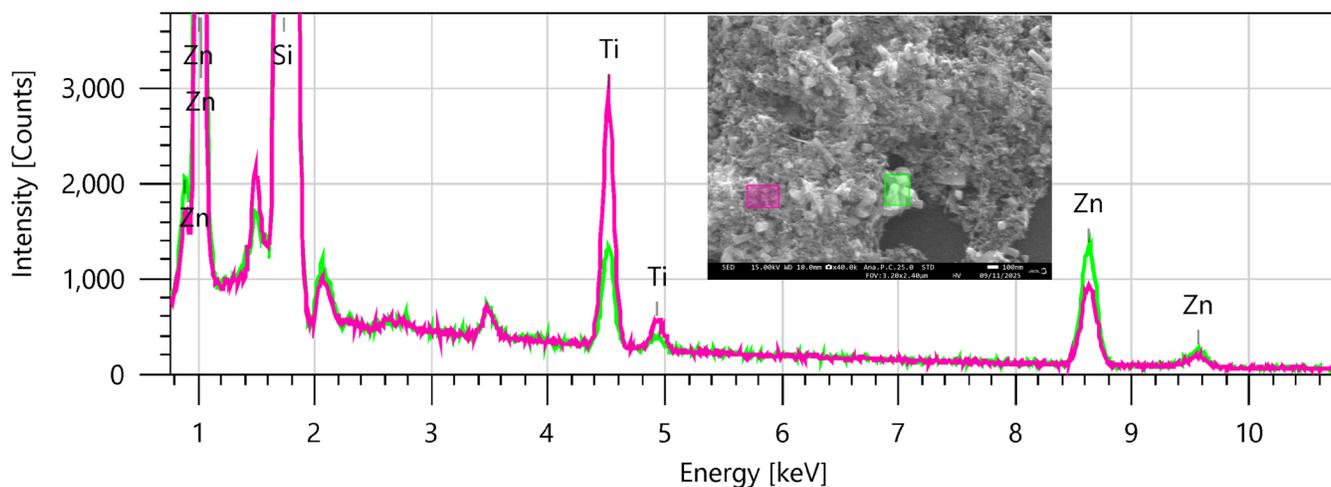


Figure 8: EDS Spectra

Conclusion

While Anaya may not have fully uncovered the exact reason why chemical sunscreens irritate her skin, her project gave her valuable insights into how these products behave under real-world conditions. Along the way, she learned to apply a wide range of analytical techniques—GC-MS for tracking volatile compounds, ICP-MS for detecting trace metals, and SEM-EDS for visualizing and identifying nanoparticles. Her careful work revealed how chemical formulas can shift under UV light, how even safe products can contain measurable heavy metals, and how particle size drives the look and feel of mineral sunscreens. Most importantly, Anaya demonstrated curiosity, persistence, and skill in using advanced materials characterization to investigate a question that mattered personally to her.



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Sunscreen Case Study

Inductively Coupled Plasma Mass Spectrometry (ICP-MS)

Gas Chromatography-Mass Spectrometry (GC-MS)

Scanning Electron Microscopy + Energy Dispersed X-ray Spectroscopy (SEM-EDS)

Authors Anaya Khanzode, Valerie Brogden

Reviewer Adlai Katzenberg, Ph.D.

February 12th, 2026

Statement of Work

Goal

- Covalent evaluated two commercially available sunscreens—one mineral-based (TiO_2/ZnO) and one chemical-based (e.g., octocrylene, homosalate, octisalate, avobenzone)—to better understand what's in these products and how they behave under real-world use, including potential links to skin irritation and ingredient changes under UV exposure.
- The goal of the investigation was to compare the two sunscreen types across (1) volatile/organic chemistry, (2) trace metals, and (3) particle morphology/elemental distribution, including whether the chemical sunscreen's composition changes after UV exposure.

Methods

The objective of this work was to:

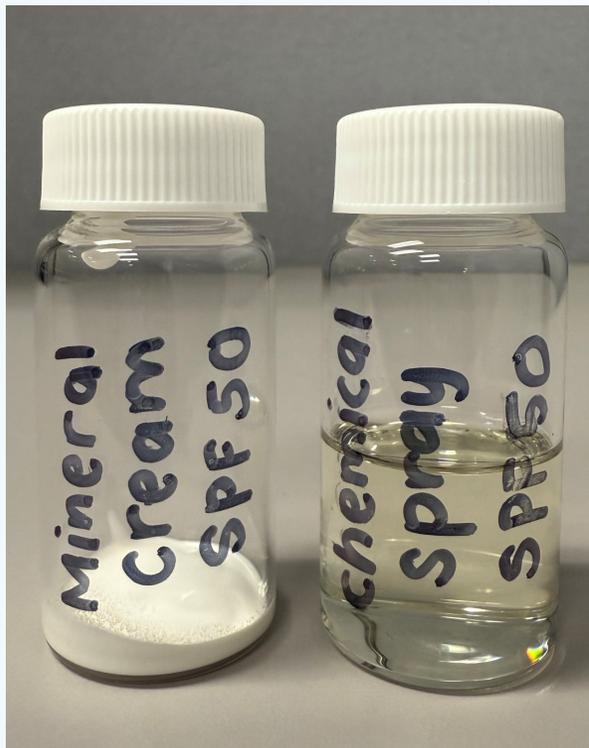
- Identify volatile compounds present in the chemical sunscreen and evaluate whether the volatile profile changes after UV exposure.
- Measure trace metals in both sunscreens to check for the presence of metals of concern (heavy metals panel).
- Characterize mineral sunscreen particles (size/shape/distribution) and determine how TiO_2 vs ZnO are distributed within the formulation using microscopy + elemental analysis.



Samples as-received

***See Appendix I for additional test parameters**

Statement of Work



Sample Handling

For the chemical sunscreen GC-MS work, one sample was analyzed as-dispensed, and a second sample was analyzed after being placed in a petri dish in sunlight for ~2 hours to simulate UV exposure effects.

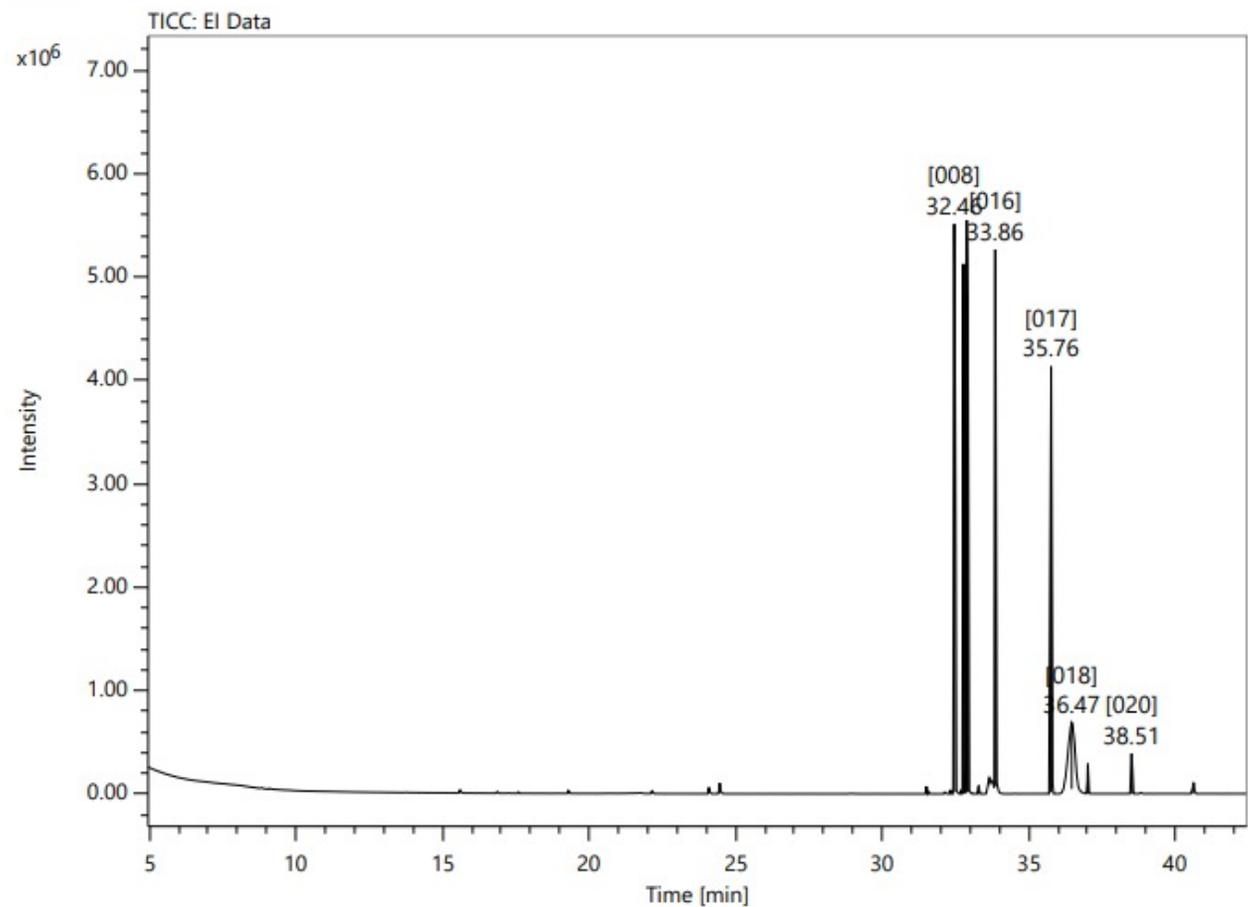
Techniques Used

- GC-MS (Gas Chromatography–Mass Spectrometry):** Separate and identify volatile/semi-volatile organic compounds; compare pre- vs post-UV exposure profiles for evidence of change/photodegradation.
- ICP-MS (Inductively Coupled Plasma–Mass Spectrometry):** Quantify trace metals in each sunscreen at very low concentration levels (ppb/ppt sensitivity).
- SEM-EDS (Scanning Electron Microscopy + Energy Dispersive X-ray Spectroscopy):** Image mineral sunscreen particulates and map/confirm elemental composition to assign particles to TiO_2 vs ZnO and assess distribution/agglomeration.

Summary of Results: GC-MS

No UV Exposure

TICC



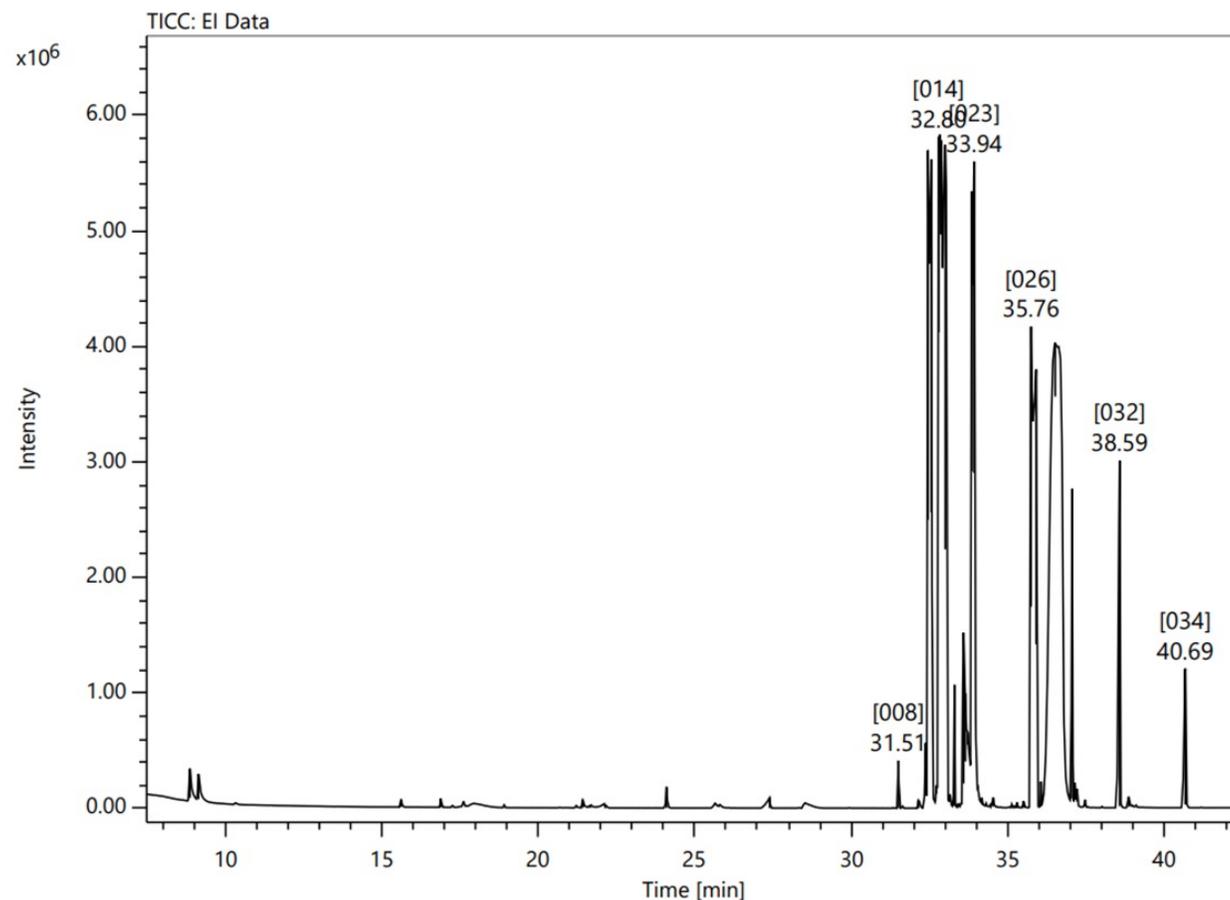
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004	Propanoic acid, phenylmethyl ester	927	C10 H12 O2	anti-fungal
005	Ethyl salicylate	969	C9 H10 O3	emollient
006	Cinnamaldehyde, α-pentyl-	895	C14 H18 O	fragrance
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020	2-(Decanoyloxy)propane-1,3-diyl dioctanoate	829	C29 H54 O6	emollient
021	3-(Octanoyloxy)propane-1,2-diyl bis(decanoate)	755	C31 H58 O6	

***See Appendix I for additional test parameters**

Summary of Results: GC-MS

2hr UV Exposure

TICC



ID	Compound Name	Match Factor	Formula	Description
001-002	Cyclohexene, 3,3,5-trimethyl-	908	C9 H16	solvent
003	1,6-Octadiene, 7-methyl-3-methylene-	892	C10 H16	
004	Limonene	933	C10 H16	fragrance
005	1-Hexene, 5-methyl-	810	C7 H14	solvent
006	Propanoic acid, phenylmethyl ester	945	C10 H12 O2	anti-fungal
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011-012	Octisalate	952	C15 H22 O3	active ingredient
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020	1-Nonadecene	801	C19 H38	
021-023	Octisalate	791	C15 H22 O3	active ingredient
024	Vinyl caprylate	700	C10 H18 O2	fragrance
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034	3-(Octanoyloxy)propane-1,2-diyl bis(decanoate)	898	C31 H58 O6	emollient

***See Appendix I for additional test parameters**

Conclusions: GC-MS

- For the control sample that was not exposed to any UV radiation, we observe all four active ingredients, as well as some fragrance, like cinnamaldehyde and other fragrant esters. The other ingredients are various kinds of alcohols and glycerols that act as solvents and emollients to improve skin-feel of the sunscreen.
- As can be seen in the experimental sample, all of the active ingredients in the sunscreen are still present. We do see other kinds of fragrance, like limonene and various aldehydes, which might be photodegradation products of the fragrances observed in the previous sample. We also observe Vitamin E, which is on the ingredient list, but not observed in the previous samples. We observe the same emollients and solvents, indicating that they do not degrade after UV exposure.

***See Appendix I for additional test parameters**

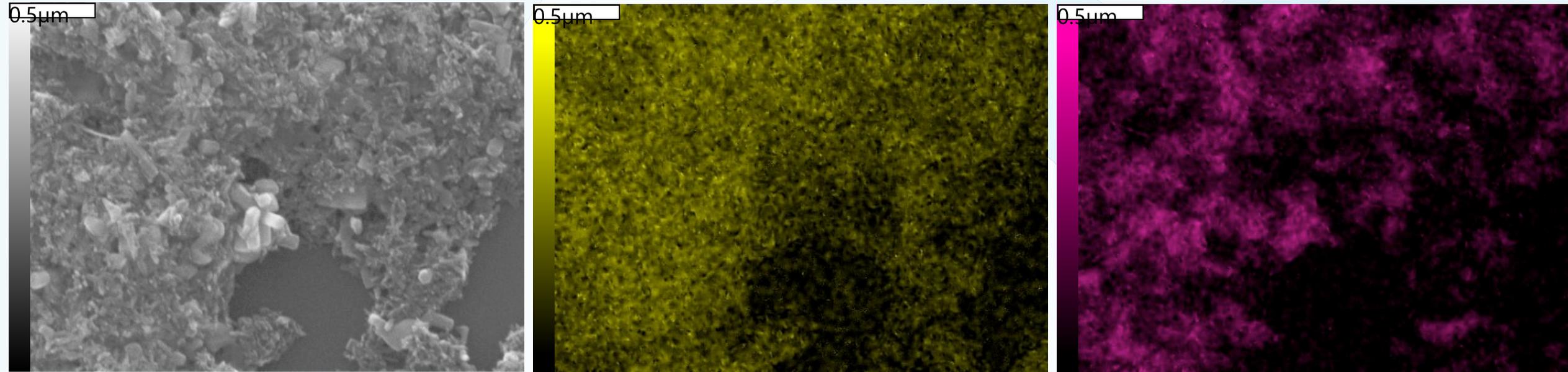
Summary of Results: ICP-MS

- Every element that was analyzed was detected above the instrument's detection limit detection limit in mineral cream
 - despite this, none of the levels are considered toxic to humans when applied on skin
- Only Co, Cu, and Ag were not detected in the chemical spray

Element	Chemical Spray(ppb)	Mineral Cream (ppb)	Toxic Levels?
V	6	300	No
Cr	2,000	500	No
Mn	2	300	No
Fe	1,000	2,000	No
Co	< 1	20	No
Ni	4	2,000	No
Cu	< 20	4,000	No
As	1	100	No
Se	4	7	No
Mo	35	200	No
Ag	< 300	10,000	No
Sb	2	200	No
Ba	6	100	No
Hg	1	7	No
Pb	1	300	No

***See Appendix I for additional test parameters**

Summary of Results: SEM and EDS



SEM image

Ti EDS map

Zn EDS map

- Smaller, spherical nanoparticles are TiO₂ (more even distribution across sunscreen)
- Larger, hexagonal prism nanoparticles are ZnO (concentrated in clumps where larger nanoparticles can be seen)

***See Appendix I for
additional test parameters**

Appendix I

Sample Preparation

ICP-MS: microwave digestion

Sample	Recipe	Mass	Volume
PRB	HNO3	-	24.99 mL
Chemical Spray	HNO3	200.3 mg	
PRB	HNO3 + HF	-	
Mineral Cream	HNO3 + HF	200.2 mg	

GCMS: sample dilution

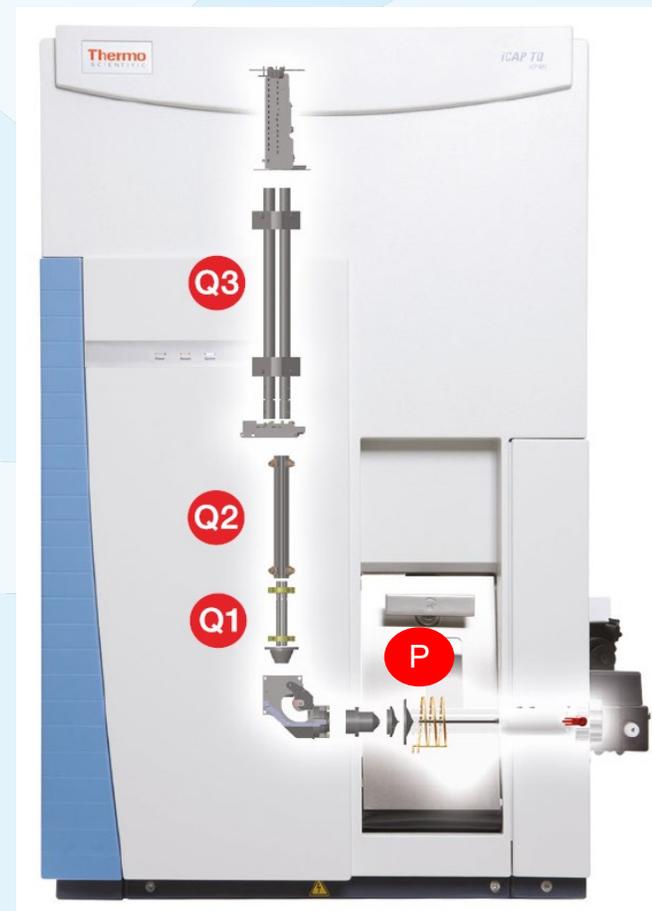
Sample	Solvent	Solvent Ratio
Chemical Spray	DCM	10:1
Chemical Spray (2hr UV exposure)	DCM	10:1

- SEM-EDS

- Mineral Cream sample was extracted 2x in dichloromethane and 2x in isopropanol
- White powder was collected and diluted heavily in isopropanol
- Solution was drop-cast onto clean Si wafers and coated in Pt
- Pt-coated wafers were loaded onto stage using copper tape and analyzed

ICP-MS

- Analytical work was performed on a Thermo Scientific iCAP triple quadrupole inductively coupled plasma mass spectrometer – TQ-ICP-MS.
- To remove interferences from analysis matrix, instrument can use a variety of instrument modes as described below and on next page.
 - After ionization in plasma (P), quadrupole 1 (Q1) works as a selective mass filter for ions entering instrument.
 - Using hydrogen, helium, oxygen or ammonia gas, selective reaction chemistry- or collision interference removal takes place in Q2. When no gases are used, cell is in pass-through mode.
 - Q3 is the final mass filter after collisions/reactions in Q2 before the product (analyte) ions are counted by detector.
 - Reactive gases either form a product ion with the analyte that is interference free (mass shift mode) or reacts with the interference to remove the interference signal from the analyte (on mass mode).
 - The mass analyzer quadrupole (Q3) is either set to the original analyte mass (on-mass analysis) or the product ion mass (mass shift mode).



The Thermo Scientific
iCAP TQ ICP-MS System

GCMS

GC Oven Program

Step	Rate [°C/min]	Temperature [°C]	Hold Time [min]
Initial	0	35	6
Step 1	5	150	0
Step 2	30	300	10

Analysis was performed on a JEOL JMS-T2000GC AccuTOF™ GC-Alpha with 18.7 fg instrument detection limit and <100 μDa mass resolution. This system is equipped with electron, chemical, and field ionization modes and liquid, headspace, SPME, thermal desorption, and pyrolysis injection modes.



Thank You

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