FORMULAITE

Simulaite Stability Report

Curcumin Antioxidant-Excipient Benchmark

Generated: May 12, 2026 at 8:25 PM

Executive Summary

This report benchmarks Formulaite stability predictions against Kharat et al. 2020, which measured curcumin retention in oil-in-water emulsions containing different antioxidant excipients. The focus is on ranking antioxidant excipient strategies and explaining the pathway-level chemistry behind the observed stability differences.

Key Result

The predicted primary antioxidant order from Formulaite simulations is identical to the ordering found in the scientific literature: Trolox > Ascorbic acid > Ascorbyl palmitate > No antioxidant. Pairwise agreement on this claim set: 6/6.

Benchmark Setup

Formulaite predicts stability using quantum chemistry-informed pathway models. Degradation pathways include radical chain autoxidation, direct molecular oxidation, photodegradation, and hydrolysis if detected. Pathway kinetics are integrated with Arrhenius temperature scaling and environment corrections such as oxygen exposure, water activity, pH, packaging permeability, UV attenuation, and phase accessibility. For this benchmark, the differentiating signal is BDE-informed antioxidant protection depending on its radical-quenching chemistry and its availability in the emulsion environment.

Parameter	Value
Literature source	Enhancement of chemical stability of curcumin-enriched oil-in-water emulsions: Impact of antioxidant type and concentration. doi:10.1016/j.foodchem.2020.126653
Modeled formulation	0.01 wt% curcumin, 10 wt% MCT oil, 1 wt% QS liquid extract, phosphate buffer context
Antioxidant dose	600 μM for antioxidant type comparison
Aqueous phase	5 mM phosphate buffer, pH 7.0, matching the paper method; buffered pH is retained for primary kinetics.
Model endpoint	Predicted total degradation rate constant K_total (s^{-1}), then relative ranking
Modeled pathways	Direct oxidation, radical autoxidation, photodegradation, hydrolysis if detected

Antioxidant Ranking

Lower K means slower degradation and better stability. Primary claim order: Trolox > Ascorbic acid > Ascorbyl palmitate > No antioxidant.

	Literature benchmark		Formulaite prediction		
Scenario	Literature Retention	Literature K vs Control	Predicted K vs Control	Dominant Pathway	Interpretation
No antioxidant	57.9%	1.00×	1.00×	Radical Autoxidation	Unprotected reference.
Trolox	82.6%	**0.35×**	**0.39×**	Photodegradation	BDE-informed antioxidant protection lowers predicted degradation rate.
Ascorbic acid	82.2%	**0.36×**	**0.41×**	Photodegradation	BDE-informed antioxidant protection lowers predicted degradation rate.
Ascorbyl palmitate	79.5%	**0.42×**	**0.46×**	Photodegradation	BDE-informed antioxidant protection lowers predicted degradation rate.

Literature K vs Control is derived from reported endpoint retention using first-order degradation: K ratio = -ln(retention fraction) / -ln(control retention fraction). Storage time cancels because all rows are compared at the same endpoint.

Primary ranking accuracy

Primary claim set: 6/6 pairwise comparisons. Alpha-tocopherol is handled separately as an exclusion case and is not included in this score.

What Was Calculated

Calculation Layer	Engine Signal	Why It Matters Here
Antioxidant reactivity	Relative H-donor and radical-quenching strength of each antioxidant	Explains why Trolox and ascorbate reduce curcumin degradation compared with control.
Radical degradation	Oxygen- and antioxidant-sensitive radical pathway terms	Captures the main protective effect of antioxidant excipients.
Emulsion availability	Whether each antioxidant is more available to the curcumin degradation environment	Separates hydrophilic ascorbic acid from more oil-preferring ascorbyl palmitate without fitted ranking multipliers.
Photodegradation	Light-sensitive curcumin degradation pathway	Curcumin is chromophoric, so residual light can remain a competing pathway.
Total degradation rate	Combined degradation rate across modeled pathways	Used for relative K ranking against the literature-derived K ratios.

Pathway Breakdown

The table below shows each scenario's pathway contribution to K_total. For the primary claim set, antioxidant protection suppresses radical pathways and shifts the limiting pathway balance.

Scenario	Direct Ox.	Autoxid.	Photo.	Hydro.	Dominant
No antioxidant	10.9%	51.1%	38.0%	0.0%	Radical Autoxidation
Trolox	1.4%	0.1%	98.5%	0.0%	Photodegradation
Ascorbic acid	1.3%	6.9%	91.8%	0.0%	Photodegradation
Ascorbyl palmitate	1.2%	17.1%	81.8%	0.0%	Photodegradation

Mechanistic Insights

The pathway table becomes more useful when read as a mechanism shift: the unprotected formulation is co-limited by radical autoxidation and residual photodegradation, while strong antioxidant protection pushes the remaining risk toward light-driven chemistry.

Pathway-level readout

- Baseline is mixed-risk: autoxidation contributes 51.1% and photodegradation contributes 38.0% of K_total.
- Trolox changes the limiting pathway: autoxidation is suppressed 2,234× vs control, so photodegradation becomes 98.5% of the residual risk.
- Ascorbic acid and ascorbyl palmitate share the same ascorbate enediol chemistry, but the phase screen gives different aqueous accessibility: 1.118× vs 0.384× bulk. Relative K: 0.41× vs 0.46× control.
- Formulator takeaway: ask which pathway remains limiting after the excipient is added, not only which antioxidant ranks highest.

Model Scope Note

Exclusion case: alpha-tocopherol is treated outside the primary 6/6 ranking claim. Its behavior in this emulsion depends on oil/interfacial localization and tocopheroxyl radical fate, while the current model uses generic chain-breaking antioxidant chemistry and a bulk oil/water phase screen..