

# Simulaite Stability Report

## Carrier-Differentiated Curcumin Stability Analysis

Generated: March 27, 2026 at 12:31 AM

Formulaite predicts solid-state stability using quantum chemistry-informed models. Degradation pathways include radical chain autoxidation (Bolland-Gee kinetics), direct molecular oxidation, photodegradation (UV-driven isomerization), and hydrolysis. Pathway kinetics are integrated using the Arrhenius equation to predict shelf-life across ICH steady-state conditions – accounting for packaging permeability, UV attenuation, carrier physical state, and antioxidant excipients. All formulation compositions are derived from published patent examples.

## Formulation Compositions

Product	Type	Carrier	Antioxidant	Source
C3+BioPerine	Crystalline	None (crystalline powder)	None	Sabinsa Corp (C3 = 95% extract, BioPerine® = US5536506)
BCM-95	Crystalline	None (crystalline + essential oil)	None	US7736679B2 (DolCas Biotech)
Meriva	ASD	Soy PC (phytosome) + MCC (filler)	None	EP1991244B1 (Indena SpA)
Longvida	ASD	Stearic acid SLN + soy PC	Ascorbic acid (4.5%)	US9192644B2 (Verdure Sciences)
CurcuWIN	ASD	HPMC + Mannitol (filler) + Lipid	$\alpha$ -Tocopherol (2.5%) + Ascorbyl palmitate (1.9%)	US20130274343A1 Example 2 (OmniActive Health)

### C3+BioPerine

Ingredient	w/w %	Role
Curcumin	76.2%	active
DMC	16.8%	active
BDMC	5.9%	active
Piperine	1%	active

### BCM-95

Ingredient	w/w %	Role
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Ingredient	w/w %	Role
Curcumin	86.4%	active
DMC	4.5%	active
ar-Turmerone	4.1%	active

## Meriva

Ingredient	w/w %	Role
Curcumin	13.2%	active
DMC	3.7%	active
Soy phosphatidylcholine	40%	carrier
MCC	40%	filler

## Longvida

Ingredient	w/w %	Role
Curcumin	35%	active
DMC	7.7%	active
BDMC	2.7%	active
Ascorbic acid	4.5%	antioxidant
Stearic acid	28.2%	carrier
Soy phosphatidylcholine	16.7%	carrier

## CurcuWIN

Ingredient	w/w %	Role
Curcumin	16.6%	active
DMC	3.7%	active
BDMC	1.3%	active
α-Tocopherol	2.5%	antioxidant
Ascorbyl palmitate	1.9%	antioxidant
Mannitol	63.1%	filler
HPMC	5.7%	carrier
Hydrogenated soybean oil	4.7%	carrier

## Shelf-Life Predictions

All values are relative stability ratios vs the baseline (C3+BioPerine = unprotected crystalline curcumin extract = 1.00×). Ratios >1.0× indicate improved stability; <1.0× indicates increased degradation vulnerability. The model predicts relative rankings, not absolute shelf-life.

### ICH Long-Term (25°C/60%RH)

Formulation	HDPE Bottle	Capsule + HDPE	Capsule + Alu-Alu	HDPE+N <sub>2</sub>	Risk
C3+BioPerine	1.00×	1.00×	1.00×	1.00×	Baseline
BCM-95	1.01×	1.01×	1.00×	1.01×	Comparable
Meriva	0.22×	0.94×	1.52×	0.20×	Reduced
Longvida	1.98×	3.49×	3.02×	1.78×	Enhanced
CurcuWIN	2.28×	>5.00×	>5.00×	2.06×	Enhanced

### ICH Intermediate (30°C/65%RH)

Formulation	HDPE Bottle	Capsule + HDPE	Capsule + Alu-Alu	HDPE+N <sub>2</sub>	Risk
C3+BioPerine	1.00×	1.00×	1.00×	1.00×	Baseline
BCM-95	1.02×	1.01×	1.01×	1.01×	Comparable
Meriva	0.37×	0.98×	0.91×	0.31×	Reduced
Longvida	2.64×	2.79×	2.03×	2.22×	Enhanced
CurcuWIN	3.52×	>5.00×	>5.00×	3.06×	Enhanced

### ICH Accelerated (40°C/75%RH)

Formulation	HDPE Bottle	Capsule + HDPE	Capsule + Alu-Alu	HDPE+N <sub>2</sub>	Risk
C3+BioPerine	1.00×	1.00×	1.00×	1.00×	Baseline
BCM-95	1.01×	1.02×	1.01×	1.01×	Comparable
Meriva	0.20×	0.35×	0.33×	0.17×	At Risk
Longvida	1.81×	1.42×	0.93×	1.49×	Comparable
CurcuWIN	2.12×	3.35×	>5.00×	1.78×	Enhanced

Baseline: C3+BioPerine = 1.00×. **Green** ≥ 1.5× **Amber** 0.8–1.5× **Orange** 0.4–0.8× **Red** < 0.4×

## Degradation Pathway Analysis

For each formulation, the engine computes how the dominant degradation pathway shifts based on packaging. Notice how removing the opaque capsule shell exposes amorphous formulations to catastrophic photodegradation, instantly changing their failure kinetics compared to crystalline solids.

### C3+BioPerine

Type: Crystalline | Limiting compound: Curcumin | Dominant (Capsule): **Radical Autoxidation**

Pathway	Contrib. (No Capsule, HDPE)	Contrib. (Capsule, HDPE)
<b>Radical Autoxidation</b>	18.8%	53.4%
<b>Direct Oxidation</b>	36.6%	40.1%
<b>Photodegradation</b>	44.6%	6.4%
<b>Hydrolysis</b>	0.0%	0.0%

### BCM-95

Type: Crystalline | Limiting compound: Curcumin | Dominant (Capsule): **Radical Autoxidation**

Pathway	Contrib. (No Capsule, HDPE)	Contrib. (Capsule, HDPE)
<b>Radical Autoxidation</b>	19.0%	54.1%
<b>Direct Oxidation</b>	35.8%	39.4%
<b>Photodegradation</b>	45.1%	6.5%
<b>Hydrolysis</b>	0.0%	0.0%

### Meriva

Type: ASD | Limiting compound: Curcumin | Dominant (Capsule): **Photodegradation**

Pathway	Contrib. (No Capsule, HDPE)	Contrib. (Capsule, HDPE)
<b>Photodegradation</b>	95.8%	58.2%
<b>Radical Autoxidation</b>	3.3%	38.0%
<b>Direct Oxidation</b>	0.9%	3.9%
<b>Hydrolysis</b>	0.0%	0.0%

### Longvida

Type: ASD | Limiting compound: Curcumin | Dominant (Capsule): **Radical Autoxidation**

Pathway	Contrib. (No Capsule, HDPE)	Contrib. (Capsule, HDPE)
<b>Radical Autoxidation</b>	14.3%	76.2%
<b>Photodegradation</b>	85.5%	23.3%
<b>Direct Oxidation</b>	0.2%	0.5%
<b>Hydrolysis</b>	0.0%	0.0%

### CurcuWIN

Type: ASD | Limiting compound: Curcumin | Dominant (Capsule): **Photodegradation**

Pathway	Contrib. (No Capsule, HDPE)	Contrib. (Capsule, HDPE)
<b>Photodegradation</b>	99.6%	97.4%
<b>Direct Oxidation</b>	0.4%	2.6%
<b>Hydrolysis</b>	0.0%	0.0%
<b>Radical Autoxidation</b>	0.0%	0.0%

## Packaging Impact: O<sub>2</sub>, UV, and N<sub>2</sub> Blanketing

Packaging controls two key environmental drivers: oxygen permeation (oxidation) and UV transmission (photodegradation). The table below shows how each packaging tier affects the internal environment at 25°C/60%RH.

Packaging	O <sub>2</sub> (atm)	UV Transmission	RH eff. (%)	Key Benefit
HDPE Bottle (No Capsule)	0.0293	2.5%	31%	Basic: minimal UV barrier
Capsule + HDPE	0.0053	0.1%	31%	Capsule shell adds UV/O <sub>2</sub> barrier
Capsule + Alu-Alu	0.0010	0.0%	30%	Near-hermetic: eliminates O <sub>2</sub> & moisture ingress
HDPE+N <sub>2</sub> (No Capsule)	0.0141	2.5%	31%	N <sub>2</sub> purge: initial O <sub>2</sub> reduced to near zero

### Nitrogen Blanketing Impact (HDPE Bottle, 25°C/60%RH)

Formulation	Without N <sub>2</sub>	With N <sub>2</sub>	Δ
C3+BioPerine	1.00×	1.00×	+11%

Formulation	Without N <sub>2</sub>	With N <sub>2</sub>	Δ
BCM-95	1.01×	1.01×	+11%
Meriva	0.22×	0.20×	+0%
Longvida	1.98×	1.78×	+0%
CurcuWIN	2.28×	2.06×	+0%

## Physics Engine: Solid-State Carrier Modeling

The engine leverages fundamental thermodynamic principles to model how the physical state of the carrier matrix restricts molecular mobility and suppresses degradation:

- Hancock-Shamblin Rotational Mobility:** For glassy polymers, mobility scales with the temperature gap below the glass transition. The further storage temperature is below the glass transition, the stronger the geometric cage, suppressing degradation rates.
- Gordon-Taylor Plasticization:** The engine calculates how moisture ingress lowers the carrier's glass transition. If moisture drops it below storage temperature, the matrix melts into a rubbery state, unlocking massive mobility and catastrophic degradation.
- Crystalline / Lipid Modeling:** Crystalline API and solid lipids (stored below melting point) provide a rigid lattice cage. Conversely, liquid lipids (stored above melting point) have high free-volume, removing the cage effect and increasing vulnerability to photoisomerization.

Carrier Type	Example	Physical State	Stability Effect
Glassy polymer	HPMC (CurcuWIN)	Rigid glass, deeply below T <sub>g</sub>	Strongly restricts molecular motion, suppressing radical propagation
Crystalline lipid	Stearic acid (Longvida)	Solid below T <sub>m</sub> (70°C)	Geometric cage limits photoisomerization, comparable to crystalline API
Liquid lipid	Soy PC (Meriva)	Liquid above T <sub>m</sub> (-15°C)	High molecular mobility increases photodegradation vulnerability
No carrier	C3+BioPerine, BCM-95	Crystalline powder	Crystal lattice provides geometric cage; baseline stability reference

## Formulation Recommendations

**For maximum chemical stability:**

Use a glassy polymer carrier (HPMC, PVP-VA) with dual antioxidant system (α-tocopherol + ascorbyl palmitate) in HPMC

capsules + HDPE bottles. This is the CurcuWIN approach. N<sub>2</sub> blanketing provides additional margin.

**For phytosome/lipid formulations (e.g., Meriva):**

Liquid lipid carriers increase photodegradation vulnerability. Mitigate with: (1) opaque Alu-Alu blister packaging for UV/O<sub>2</sub> barrier, (2) addition of a sacrificial antioxidant (the Meriva patent does not include one), (3) nitrogen blanketing if using bottles.

**For cost-sensitive formulations:**

Crystalline curcumin extract in HPMC capsules + HDPE bottles provides robust baseline stability. BCM-95 performs equivalently. No antioxidant is required for the crystalline physical form.

*Disclaimer: These predictions represent relative stability rankings based on first-principles degradation kinetics. Absolute shelf-life values should be validated with ICH stability studies. Real-world stability also depends on manufacturing process controls (N<sub>2</sub> purging, blend uniformity, residual solvents) not modeled here.*