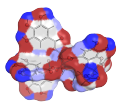
FORMULAITE

Simulaite Report



Formulaite Metabolic Support vs Market Reference Formula

Asian-population PK/PD comparison using target-site exposure, IC50/EC50 activity modeling, and docking de-risked modeled target scoring

June 27, 2026

Executive Summary

This methodology demo compares Formulaite Metabolic Support against a market reference formula by asking which modeled active markers reach the right biological sites, at meaningful concentrations, with enough potency and structural support to count. The score is intentionally conservative: a marker-target pair contributes only when activity, exposure, and structural evidence all support the same mechanism.

The workflow combines active-marker dose modeling, Asian-population oral PBPK, target-site concentration-time profiles, IC50/EC50 activity prediction from molecular descriptors and graph neural network models, quantum-chemistry-supported ligand preparation, docking against concrete target pockets, pose de-risking, and ingredient contribution analysis.

Bottom Line: Formulaite Shows Broader Support, Including GLP-1/GIP Release Signaling

- Formulaite Metabolic Support shows the stronger double-gated signal for carb absorption support and GLP-1/GIP release & satiety signaling support.
- Market Reference shows one clear tradeoff advantage: stronger GLP-1/GIP incretin preservation support, mainly through the HCA-DPP4 mechanism.
- The final comparison therefore favors Formulaite for broader modeled metabolic-support coverage.
- The model highlights a practical formulation principle: ingredient names are not enough; dose must be sufficient for target-site exposure that is meaningful relative to predicted potency.

Table 1. Final Double-Gated Modeled Scores

Endpoint	Formulaite	Market Reference	Winner	Direction
Carb absorption support	0.002	0.001	Formulaite Metabolic Support	Higher Is Better
GLP-1/GIP incretin preservation support	0.002	0.015	Market Reference Formula	Higher Is Better
GLP-1/GIP release & satiety signaling support	7.70e-5	1.10e-5	Formulaite Metabolic Support	Higher Is Better
Modeled mechanism-area wins	2 of 3	1 of 3	Formulaite Metabolic Support	Breadth summary

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Study Design: PK, PD, and Strict Scoring

Oral PK outputs provide plasma, gut-local, and target-site concentration-time curves. Activity models estimate target-specific IC50 or EC50 potency. Docking is then used as a structural de-risking layer rather than as potency by itself.

Molecular layer	Records	Interpretation
Ligand geometry optimization	**38**	Quantum-informed conformer-quality and geometry provenance. Not binding strength.
Quantum chemistry descriptor	**38**	Electronic-structure descriptor support. Not potency.
Molecular docking	**342**	Direct pocket-fit signal against concrete target pockets and controls.
IC50/EC50 activity models	**20**	Target-specific potency estimates from curated activity data, molecular descriptors, and graph neural network models.

How the Score Is Built

- First, each extract is converted into modeled active-marker doses from the daily extract dose, standardization percentage, and marker split.
- The PBPK layer estimates how much of each marker reaches the target-relevant site over time. Intracellular, mucosal, lumen, and plasma-facing targets use the appropriate concentration-time profile.
- The activity layer predicts target-specific IC50 or EC50 potency. Engagement is computed directly from C(t)/(C(t)+potency), so exposure below potency contributes little or nothing.
- The docking layer compares each marker against the same target pocket and acts as structural evidence. The pair must clear the docking floor and pose check, then its activity score is scaled by the de-risked docking score.
- Each molecular target contributes to one primary endpoint only. DPP4 counts in GLP-1/GIP preservation, MGAM in carb absorption, and GPR119 in GLP-1/GIP release and satiety signaling.
- A zero in this modeled lane means no marker-target pair survived all evidence gates for that endpoint; it does not mean the biology is impossible.

Formulation Profiles

The PK simulation uses the declared daily serving regimen as scheduled oral dose events rather than collapsing the day into one bolus dose. This matters because target-site exposure is time-dependent.

Formula	Daily regimen	Simulated schedule	Dose model
Formulaite Metabolic Support	1 capsule x 3 dose events/day (3 capsules/day)	0 h, 8.0 h, 16.0 h	Single Per Dose Event For Scheduled Superposition
Market Reference Formula	2 capsules x 2 dose events/day (4 capsules/day)	0 h, 12.0 h	Single Per Dose Event For Scheduled Superposition

Formulaite Metabolic Support

Fenugreek, gymnema, Triphala, bitter melon, and black pepper.

Ingredient	Dose	Active	Modeled markers
Fenugreek seed extract, std. 50% saponins	450.0 mg/day	50.00%	Diosgenin: 225.000 mg
Black pepper extract, std. 95% piperine	15.0 mg/day	95.00%	Piperine: 14.250 mg
Gymnema sylvestre leaf	399.0 mg/day	25.00%	Gymnemic acid I: 69.825 mg Gymnemagenin: 29.925 mg

Market Reference Formula

Garcinia cambogia, Terminalia chebula, Fenugreek, Gymnema sylvestre, and Guggul resin. Unknown standardizations are modeled using explicit comparator assumptions.

Ingredient	Dose	Active	Modeled markers
Garcinia cambogia fruit rind extract, assumed 50% HCA	1200.0 mg/day	50.00%	Hydroxycitric acid: 600.000 mg
Terminalia	40.0	45.00%	Chebulinic acid: 7.200 mg Chebulagic acid: 7.200 mg

Ingredient	Dose	Active	Modeled markers
extract, std. 25% gymnemic acids			
Triphala extract, std. 45% tannins/ polyphenols	150.0 mg/day	45.00%	Chebulinic acid: 23.625 mg Chebulagic acid: 23.625 mg Gallic acid: 10.125 mg Ellagic acid: 10.125 mg
Bitter melon fruit extract, std. 10% charantin	300.0 mg/day	10.00%	Stigmasteryl glucoside: 15.000 mg Beta-sitosteryl glucoside: 15.000 mg

Ingredient	Dose	Active	Modeled markers
chebula fruit extract, assumed 45% tannins/ polyphenols	mg/day		Gallic acid: 1.800 mg Ellagic acid: 1.800 mg
Fenugreek seed extract, assumed 50% saponins	40.0 mg/day	50.00%	Diosgenin: 20.000 mg
Gymnema sylvestre leaf extract, assumed 25% gymnemic acids	40.0 mg/day	25.00%	Gymnemic acid I: 7.000 mg Gymnemagenin: 3.000 mg
Guggul resin powder, assumed 2.5% guggulsterones	280.0 mg/day	2.50%	E-guggulsterone: 3.500 mg Z-guggulsterone: 3.500 mg

Modeled marker dose is based on extract dose, active percentage, and marker split, not full extract mass. Triphala is modeled as 45% tannins/polyphenols. These modeled marker doses feed the PK layer directly, so low marker dose can limit target-site exposure even before potency or docking evidence is considered.

PK Results: Systemic and Gut-Local Exposure Inputs

The PK layer uses a PBPK-style virtual-cohort simulation to estimate plasma, gut-local, and tissue-adjacent exposure for each modeled active marker after oral dosing. The same population and meal context are used for both products.

Virtual Population and PBPK Conditions

Parameter	Value
Population	Asian adults
Population type	Asian
Sample size (n)	100
Age range	35-65 years (mean 51)
Female %	50%
Weight	57-105 kg (mean 70 kg)
Height	141-179 cm (mean 159 cm)
BMI	25-35 kg/m² (mean 27)
BMI categories	Underweight 0; normal 3; overweight 83; obese 14
Prandial state	Fed
Meal fat	10.0 g
Simulation duration	24.0 h

The same virtual cohort is used across formula conditions. F% is computed as oral AUC divided by matched IV AUC for the same population cohort.

Table 2A. Formulaite Metabolic Support PK Metrics

Marker	Dose mg	F %	F CV %	Cmax ng/mL	AUC ng*h/mL	Tmax h
Beta-sitosteryl glucoside	5.000	9.95e-4	72.3	0	0.0442	3.12
Chebulagic acid	7.875	1.1014	58.6	1.1456	8.4981	3.24
Chebulinic acid	7.875	0.5910	58.9	0.6697	4.6654	2.88
Diosgenin	75.000	0.0024	64.6	0.0829	1.9128	4.32
Ellagic acid	3.375	30.2442	37.8	16.1069	165.6350	5.40

Marker	Dose mg	F %	F CV %	Cmax ng/mL	AUC ng*h/mL	Tmax h
Gallic acid	3.375	61.0426	21.0	70.9911	573.0027	2.40
Gymnemagenin	9.975	0.0769	70.9	0.4054	6.4574	3.12
Gymnemic acid I	23.275	0.0477	72.5	0.4842	3.6637	2.40
Piperine	4.750	5.3478	57.0	3.3956	53.6778	9.12
Stigmasteryl glucoside	5.000	0.0023	71.9	0	0.0996	3.12

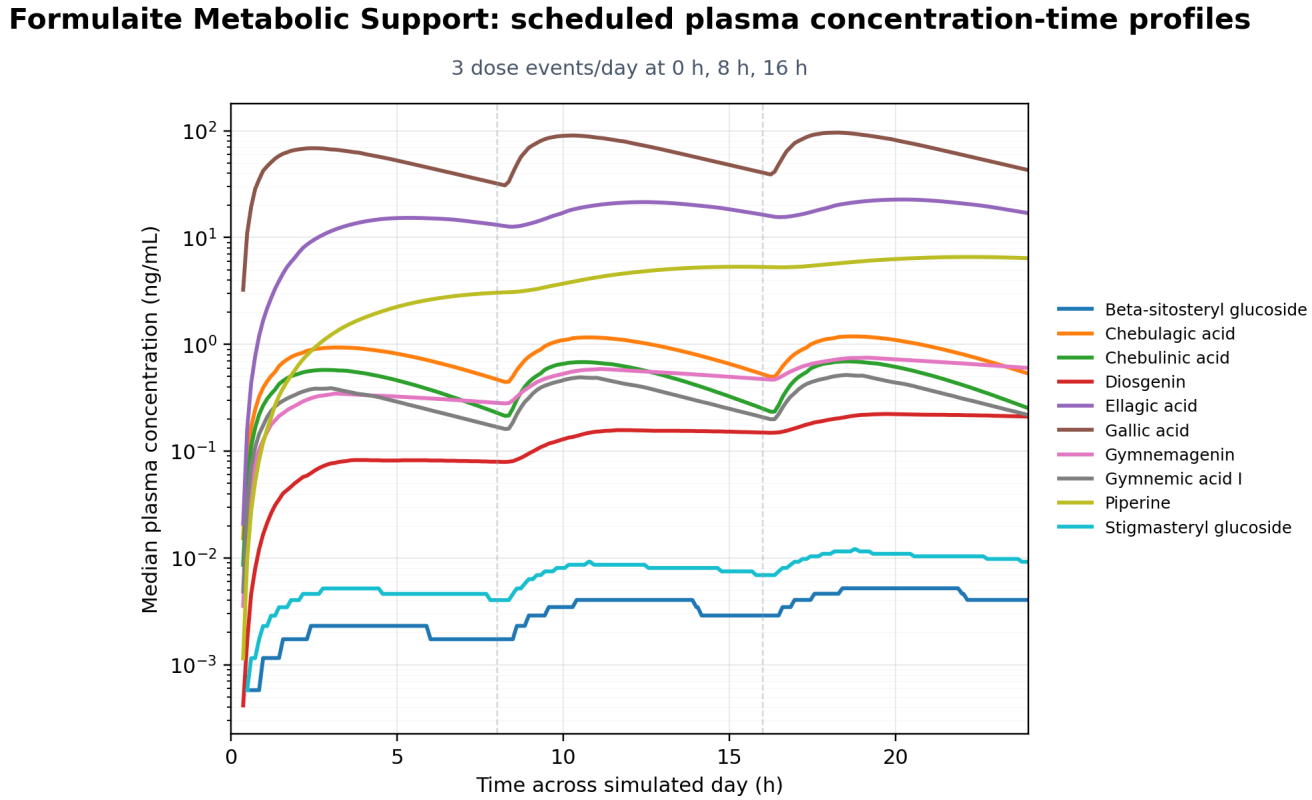

Figure 1A. Scheduled median plasma concentration-time curves for modeled active markers in Formulaite Metabolic Support using 1 capsule x 3 daily dose events. Curves are shown on a log concentration scale so lower-exposure markers remain visible.

Table 2B. Market Reference Formula PK Metrics

Marker	Dose mg	F %	F CV %	Cmax ng/mL	AUC ng*h/mL	Tmax h
Chebulagic Acid	3.600	0.8489	58.6	0.4773	2.9945	2.88
Chebulinic Acid	3.600	0.2565	58.7	0.1913	0.9264	2.04
Diosgenin	10.000	9.11e-4	65.0	0	0.0974	3.96
E Guggulsterone	1.750	0.0074	72.5	0	0.0354	6.00
Ellagic Acid	0.900	20.0914	44.4	3.0219	29.2811	4.56
Gallic Acid	0.900	55.1479	23.9	17.4543	137.9616	2.28
Gymnemagenin	1.500	0.0257	72.2	0	0.3243	3.00
Gymnemic Acid I	3.500	0.0140	72.7	0	0.1614	2.40
Hydroxycitric Acid	300.000	34.6793	33.9	3132.9437	26743.7863	2.16
Z Guggulsterone	1.750	0.0092	72.3	0	0.0526	6.84

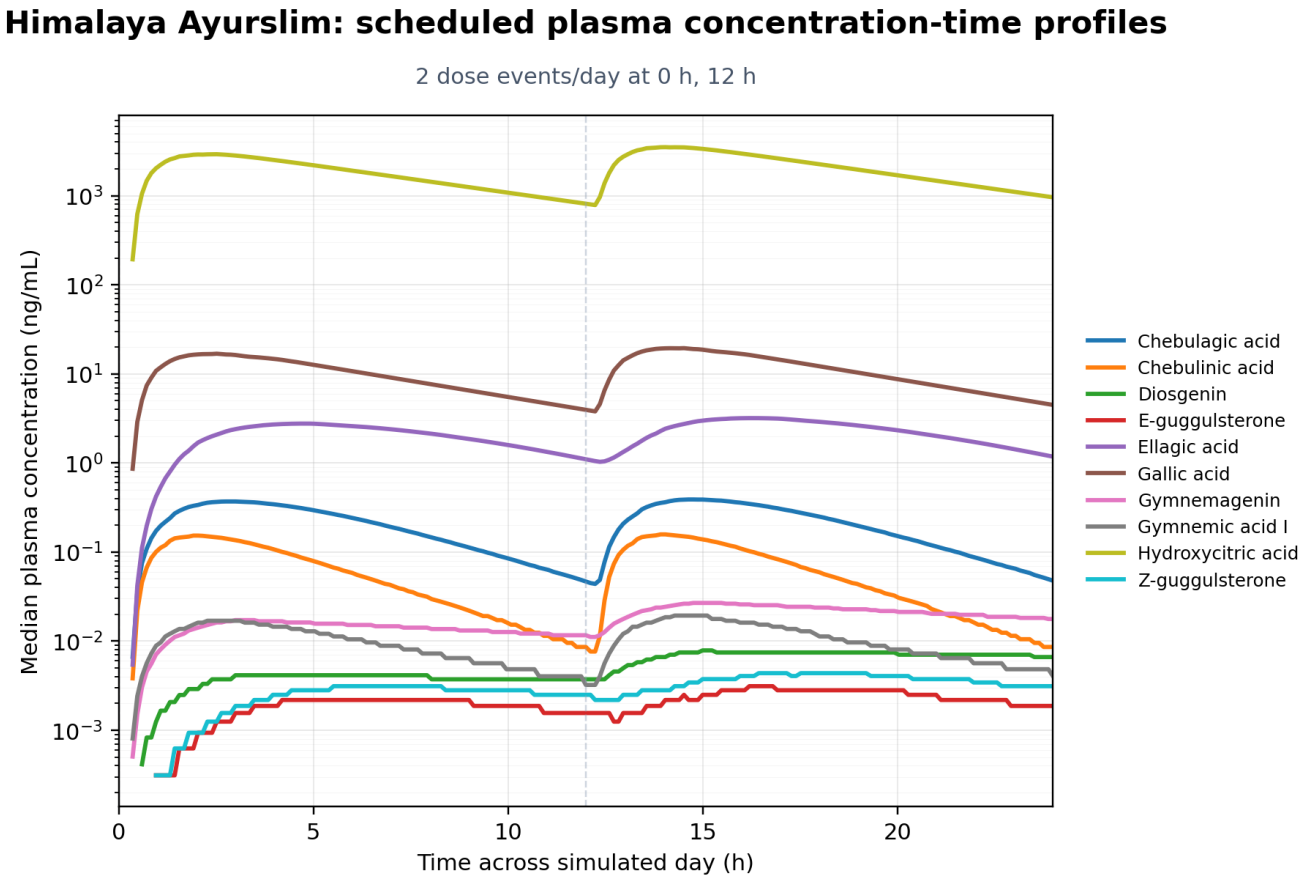

Figure 1B. Scheduled median plasma concentration-time curves for modeled active markers in Market Reference Formula using 2 capsules x 2 daily dose events, with the same virtual population and meal context.

Target-Site PK/PD Inputs Used in Scoring

The headline scores are not based on one generic plasma exposure number. Each target uses the exposure site that matches the biology: DPP4 uses systemic plasma, MGAM uses gut lumen exposure, and GPR119 uses small-intestine mucosa interstitial exposure.

Engagement is the PK/PD bridge: engagement(t) = C(t) / (C(t) + IC50 or EC50). If target-site exposure is far below predicted potency, engagement stays near zero even when docking looks acceptable. Passing pairs are then scaled by the de-risked docking weight.

Table 3. All Modeled Pair Contributions, Ranked by Score

Product	Marker-target	Mechanism area	Scoring site	Cmax uM	AUC uM*h	IC50/ EC50 uM	Engage ment	Docki ng wt	Score
Market Reference Formula	**Hydroxycitric Acid to DPP4**	GLP-1/GIP incretin preservation support	Systemic plasma	20.134	263.550	11.795	0.4585	0.323	**0.0740**
Formulaite Metabolic Support	**Chebulinic acid to MGAM**	Carb absorption support	Gut lumen	35.691	43.348	29.444	0.0779	1.000	**0.0389**
Market Reference Formula	**Chebulinic Acid to MGAM**	Carb absorption support	Gut lumen	15.762	13.363	29.444	0.0438	1.000	**0.0219**
Formulaite Metabolic Support	**Gallic acid to DPP4**	GLP-1/GIP incretin preservation support	Systemic plasma	0.667	10.219	4.900	0.0793	0.376	**0.0149**
Formulaite Metabolic	**Gymnemagenin to DPP4**	GLP-1/GIP incretin preservation support	Systemic plasma	0.002	0.026	0.063	0.0171	0.953	**0.0082**

Product	Marker-target	Mechanism area	Scoring site	Cmax uM	AUC uM*h	IC50/ EC50 uM	Engagement	Docking wt	Score
Support									
Formulaite Metabolic Support	Gymnemic acid I to DPP4	GLP-1/GIP incretin preservation support	Systemic plasma	7.55e-4	0.011	0.047	0.0098	0.728	0.0036
Formulaite Metabolic Support	Piperine to DPP4	GLP-1/GIP incretin preservation support	Systemic plasma	0.025	0.368	3.269	0.0047	0.842	0.0020
Formulaite Metabolic Support	Gallic acid to GPR119	GLP-1/GIP release & satiety signaling support	Small-intestine mucosa interstitial	0.009	0.077	0.530	0.0119	0.209	8.29e-4
Formulaite Metabolic Support	Chebulagic acid to DPP4	GLP-1/GIP incretin preservation support	Systemic plasma	0.001	0.024	0.624	0.0016	1.000	8.09e-4
Formulaite Metabolic Support	Ellagic acid to MGAM	Carb absorption support	Gut lumen	0.112	0.365	21.320	0.0014	0.814	5.78e-4
Formulaite Metabolic Support	Chebulinic acid to DPP4	GLP-1/GIP incretin preservation support	Systemic plasma	8.57e-4	0.014	0.669	8.45e-4	1.000	4.23e-4
Market Reference Formula	Gymnemagenin to DPP4	GLP-1/GIP incretin preservation support	Systemic plasma	6.20e-5	9.71e-4	0.063	6.45e-4	0.956	3.08e-4
Formulaite Metabolic Support	Ellagic acid to GPR119	GLP-1/GIP release & satiety signaling support	Small-intestine mucosa interstitial	0.001	0.011	0.471	0.0020	0.399	2.63e-4
Market Reference Formula	Chebulagic Acid to DPP4	GLP-1/GIP incretin preservation support	Systemic plasma	4.84e-4	0.006	0.624	4.07e-4	1.000	2.04e-4
Market Reference Formula	Gallic Acid to GPR119	GLP-1/GIP release & satiety signaling support	Small-intestine mucosa interstitial	0.002	0.011	0.530	0.0026	0.208	1.78e-4
Market Reference Formula	Ellagic Acid to MGAM	Carb absorption support	Gut lumen	0.030	0.069	21.320	4.03e-4	0.803	1.62e-4
Market Reference Formula	Gymnemic Acid I to DPP4	GLP-1/GIP incretin preservation support	Systemic plasma	2.80e-5	3.51e-4	0.047	3.11e-4	0.726	1.13e-4
Formulaite Metabolic Support	Piperine to GPR119	GLP-1/GIP release & satiety signaling support	Small-intestine mucosa interstitial	1.99e-4	0.001	0.234	4.74e-4	0.711	1.12e-4
Formulaite Metabolic Support	Piperine to MGAM	Carb absorption support	Gut lumen	0.013	0.040	16.146	2.04e-4	1.000	1.02e-4
Formulaite Metabolic Support	Gymnemagenin to MGAM	Carb absorption support	Gut lumen	0.013	0.040	18.026	1.87e-4	1.000	9.30e-5
Market Reference Formula	Chebulinic Acid to DPP4	GLP-1/GIP incretin preservation support	Systemic plasma	1.92e-4	0.002	0.669	1.19e-4	1.000	6.00e-5
Market Reference Formula	Ellagic Acid to GPR119	GLP-1/GIP release & satiety signaling support	Small-intestine mucosa interstitial	1.94e-4	0.001	0.471	2.81e-4	0.399	3.70e-5
Market Reference Formula	Z Guggulsterone to DPP4	GLP-1/GIP incretin preservation support	Systemic plasma	1.70e-5	2.61e-4	0.232	4.70e-5	0.891	2.10e-5
Market Reference Formula	E Guggulsterone to DPP4	GLP-1/GIP incretin preservation support	Systemic plasma	1.10e-5	1.80e-4	0.232	3.20e-5	0.928	1.50e-5
Formulaite Metabolic Support	Diosgenin to DPP4	GLP-1/GIP incretin preservation support	Systemic plasma	6.05e-4	0.009	13.063	2.90e-5	0.985	1.40e-5
Market	Gymnemagenin to	Carb absorption	Gut lumen	0.002	0.004	18.026	2.70e-5	1.000	1.30e-5

Product	Marker-target	Mechanism area	Scoring site	Cmax uM	AUC uM*h	IC50/ EC50 uM	Engage ment	Docki ng wt	Score
Reference Formula	MGAM	support							
Market Reference Formula	Z Guggulsterone to MGAM	Carb absorption support	Gut lumen	0.001	0.003	55.566	6.00e-6	1.000	**3.00e-6**
Formulaite Metabolic Support	Diosgenin to GPR119	GLP-1/GIP release & satiety signaling support	Small-intestine mucosa interstitial	5.00e-6	3.60e-5	0.448	7.00e-6	0.906	**2.00e-6**
Formulaite Metabolic Support	Stigmasteryl glucoside to DPP4	GLP-1/GIP incretin preservation support	Systemic plasma	2.30e-5	3.54e-4	9.046	2.00e-6	1.000	**1.00e-6**

This table includes every nonzero modeled pair that passed the activity, target-site exposure, and same-pair docking gates, ranked by final pair contribution. Failed pairs are excluded from this table. Cmax and AUC are shown in the target-site compartment actually used for the pair score, not necessarily plasma. Engagement is the average C(t)/(C(t)+potency) over the scoring window.

Endpoint Results and Ingredient Contributions

The tables below show the final double-gated modeled scores. A pair must have target-site exposure, an IC50/EC50 activity estimate, and same-pair docking support that clears the structural floor. Passing pairs are scaled by the de-risked docking score, so weaker structural support contributes less even after passing the gate.

Why Some Familiar Ingredients Contribute Little Here

- Ingredient contribution is driven by modeled marker dose, target-site exposure, predicted IC50/EC50 potency, and same-pair docking support together; high extract mass alone does not guarantee a modeled score.
- The same ingredient marker can contribute in one formula but drop to zero in another if the lower-dose formula does not reach target-site concentrations that are meaningful relative to predicted potency, as seen for some lower-dosed Market Reference ingredients.

Carb absorption support

Gut-local carbohydrate enzyme biology, driven here by MGAM. A higher score means stronger modeled modeled support for slowing carbohydrate breakdown or absorption at the intestinal target site.

Formulaite	Market Reference	Winner	Delta	Direction
0.002	0.001	Formulaite Metabolic Support	9.02e-4	Higher Is Better

Formulaite contributors

Ingredient	Contribution
Fenugreek extract	0%
Black pepper extract	1.0%
Gymnema extract	0.5%
Triphala extract	98.5%
Bitter melon extract	0%

Market Reference contributors

Ingredient	Contribution
Garcinia cambogia extract	0%
Terminalia chebula extract	99.9%
Fenugreek extract	0%
Gymnema sylvestre extract	0.1%
Guggul resin powder	0.0%

MGAM Mechanism Spotlight

The strongest carb absorption support signal in Formulaite Metabolic Support is chebulinic acid from Triphala on MGAM. The panel pairs a quantum electrostatic surface with a locked-view docking comparison against the MGAM acarbose reference pocket.

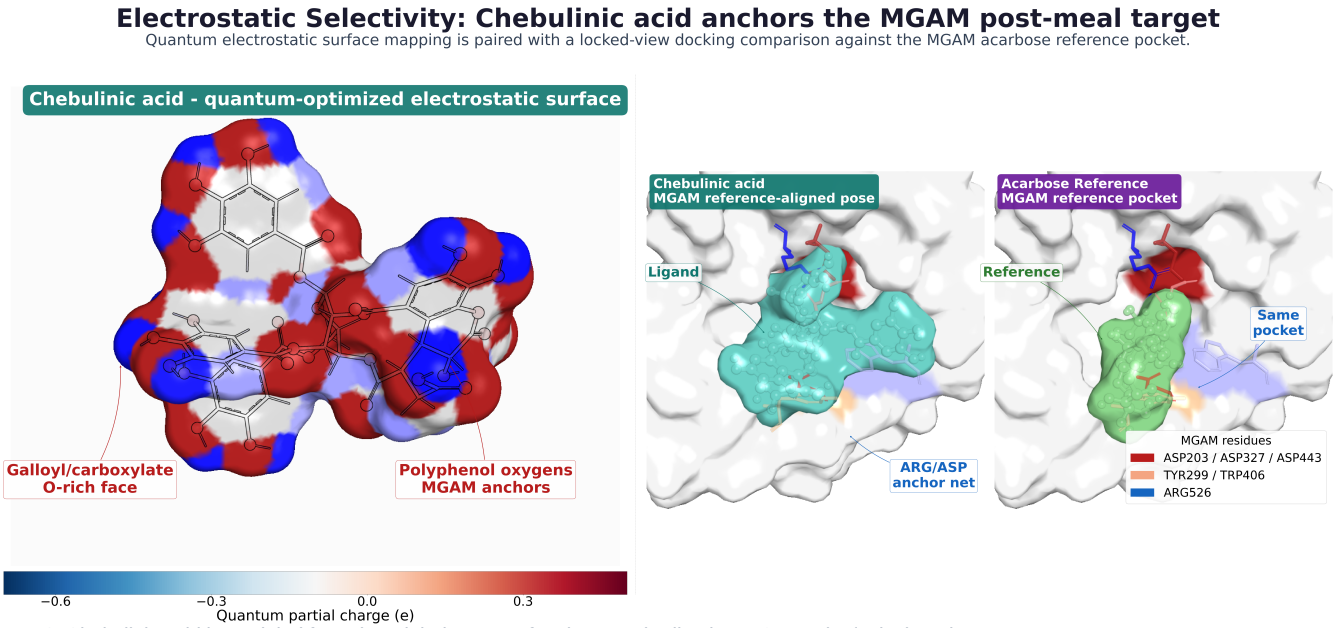

Figure 2. Chebulinic acid is modeled from the Triphala extract fraction standardized to 45% tannins/polyphenols.

GLP-1/GIP incretin preservation support

DPP4-linked preservation of GLP-1/GIP incretin signaling. A higher score means stronger modeled modeled support for reducing incretin breakdown after release.

Formulaite	Market Reference	Winner	Delta	Direction
0.002	0.015	Market Reference Formula	-0.012	Higher Is Better

Formulaite contributors

Ingredient	Contribution
Fenugreek extract	0.1%
Black pepper extract	16.5%
Gymnema extract	49.4%
Triphala extract	34.0%
Bitter melon extract	0%

Market Reference contributors

Ingredient	Contribution
Garcinia cambogia extract	99.6%
Terminalia chebula extract	0.1%
Fenugreek extract	0%
Gymnema sylvestre extract	0.3%
Guggul resin powder	0.0%

GLP-1/GIP release & satiety signaling support

GPR119-linked gut-hormone release and satiety signaling. A higher score means stronger modeled modeled support for GLP-1/GIP release-adjacent gut hormone signaling.

Formulaite	Market Reference	Winner	Delta	Direction
7.70e-5	1.10e-5	Formulaite Metabolic Support	6.60e-5	Higher Is Better

Formulaite contributors

Ingredient	Contribution
Fenugreek extract	0.5%
Black pepper extract	28.9%
Gymnema extract	0%
Triphala extract	70.5%
Bitter melon extract	0%

Market Reference contributors

Ingredient	Contribution
Garcinia cambogia extract	0%
Terminalia chebula extract	100.0%
Fenugreek extract	0%
Gymnema sylvestre extract	0%
Guggul resin powder	0%

Tracked but Not Supported in This Run

The workflow also tracked additional mechanistic areas. They are reported as zero in the modeled lane because the available marker-target evidence did not pass the full activity, target-site exposure, and same-pair docking gate.

Area	Modeled score interpretation
Insulin-sensitivity metabolic support	PPARG and PTP1B were routed here as their primary area; available docked pairs had negligible target-site engagement after IC50/EC50 and C(t) integration.
Lipid metabolism support	Lipid metabolism targets were tracked, but did not have modeled same-pair structural support in this report.
Insulin secretion support	Beta-cell insulin secretion targets were tracked, but did not have modeled same-pair structural support in this report.
Appetite sensory signaling support	Taste and sensory-receptor biology was tracked as exploratory context, but no marker-target pair passed all modeled gates in this run.
Safety interaction target index	Interaction-liability targets were screened. The modeled score remains zero because modeled engagement was negligible after potency and exposure integration. Lower is better.

Suggested Validation Next Steps

The computational benchmark is best used to prioritize a small set of confirmatory assays. These follow-ups focus on the modeled mechanisms that survived the IC50/EC50, target-site exposure, and docking de-risking workflow.

Priority	Question	Recommended assay
1	Does the carb absorption support signal translate into enzyme activity?	MGAM enzymatic assay using chebulinic acid, Triphala extract, HCA, and final capsule extracts.
2	Does the GLP-1/GIP preservation signal hold in a direct assay?	DPP4 enzymatic assay for HCA, gallic acid, piperine, gymnemagenin, and final product extracts.
3	Does the GLP-1/GIP release and satiety signaling hypothesis translate in cells?	GPR119 functional assay and enteroendocrine GLP-1/GIP release assay for gallic acid, ellagic acid, piperine, and product extracts.