

Simulaite Report — Women's Libido Boost

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4 formulation(s) compared · 5 molecule(s) · 3 extract(s)

Bioavailability Results

Extract Breakdown

Formulation	Extract	Target Dose	Dose-Weighted F	Effective Dose	n
Blend Capsule (All Three Extracts)	Fenugreek Extract	80.00 mg	28.19%	~22.55 mg	89
Blend Capsule (All Three Extracts)	Shatavari Root Extract	10.00 mg	1.09%	~0.11 mg	89
Blend Capsule (All Three Extracts)	Damiana Extract	4.50 mg	1.45%	~0.07 mg	89
Fenugreek Capsule	Fenugreek Extract	80.00 mg	26.71%	~21.36 mg	89
Shatavari Capsule	Shatavari Root Extract	10.00 mg	0.64%	~0.06 mg	89
Damiana Capsule	Damiana Extract	4.50 mg	1.30%	~0.06 mg	89

Compound Breakdown

4-Hydroxyisoleucine

Formulation	F%	CV%	Effective Dose	Onset (T _{1/2} -rise)	Tmax (h)	n
Blend Capsule (All Three Extracts)	92.79% ± 5.13%	6%	~13.92 mg	42 min	1.8	89
Fenugreek Capsule	92.79% ± 5.13%	6%	~13.92 mg	42 min	1.8	89

Apigenin

Formulation	F%	CV%	Effective Dose	Onset (T _½ -rise)	Tmax (h)	n
Blend Capsule (All Three Extracts)	1.45% ± 0.73%	50%	~0.07 mg	35 min	2.0	89
Damiana Capsule	1.30% ± 0.72%	55%	~0.06 mg	34 min	1.8	89

Protodioscin

Formulation	F%	CV%	Effective Dose	Onset (T _½ -rise)	Tmax (h)	n
Blend Capsule (All Three Extracts)	1.42% ± 0.77%	54%	~0.71 mg	1.8 h	4.2	89
Fenugreek Capsule	0.90% ± 0.49%	54%	~0.45 mg	1.5 h	3.6	89

Shatavarin IV

Formulation	F%	CV%	Effective Dose	Onset (T _½ -rise)	Tmax (h)	n
Blend Capsule (All Three Extracts)	1.09% ± 0.61%	56%	~0.11 mg	2.5 h	8.6	89
Shatavari Capsule	0.64% ± 0.36%	56%	~0.06 mg	2.1 h	8.4	89

Trigonelline

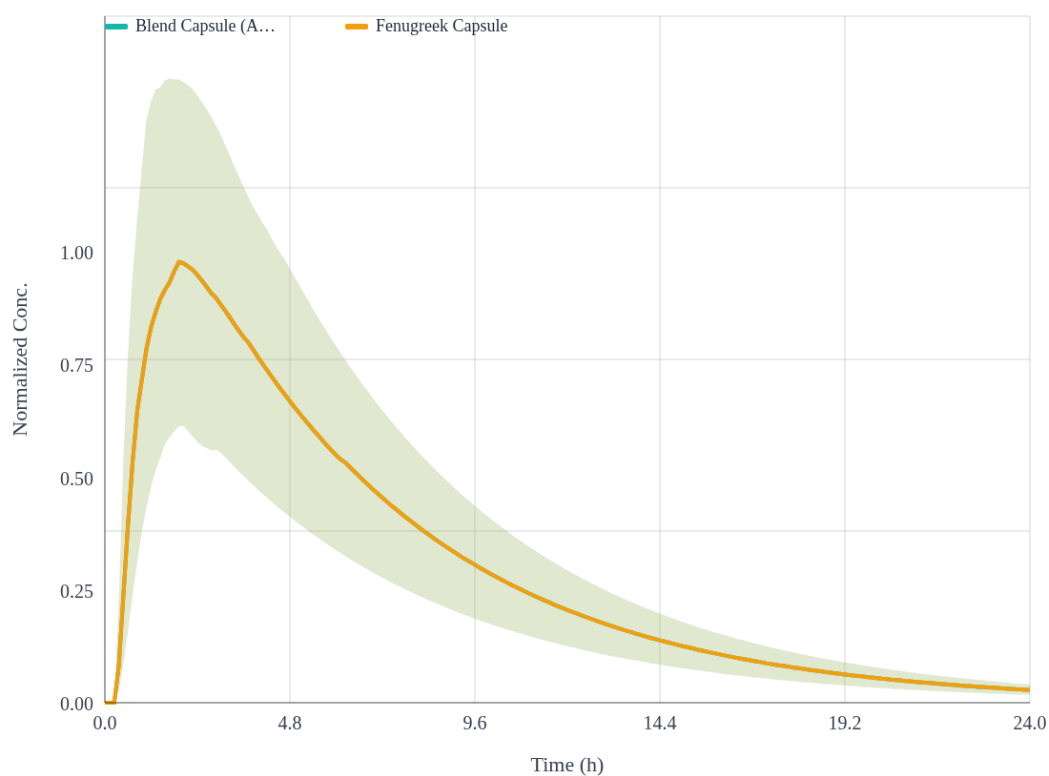
Formulation	F%	CV%	Effective Dose	Onset (T _½ -rise)	Tmax (h)	n
Blend Capsule (All Three Extracts)	52.84% ± 14.52%	27%	~7.93 mg	25 min	0.8	89
Fenugreek Capsule	46.64% ± 14.09%	30%	~7.00 mg	25 min	0.8	89

Extract dose-weighted $F = \Sigma(\text{compound dose} \times F\%) / \Sigma(\text{compound dose})$. Extract effective dose = $\Sigma(\text{compound effective doses})$, using each compound's own F%. T_½-rise = time from dose to 50% of peak. Tmax = time to peak.

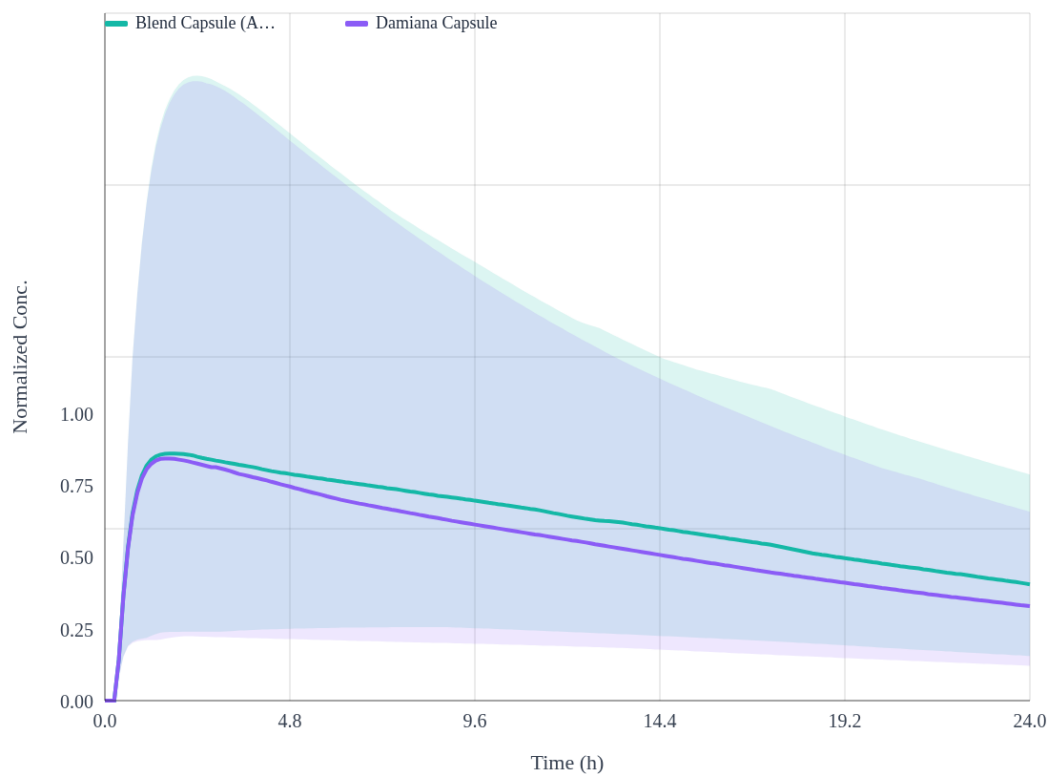
PK Concentration-Time Curves (normalized)

Y-axis normalized to peak C_{max}. Shaded band = P5-P95 population range.

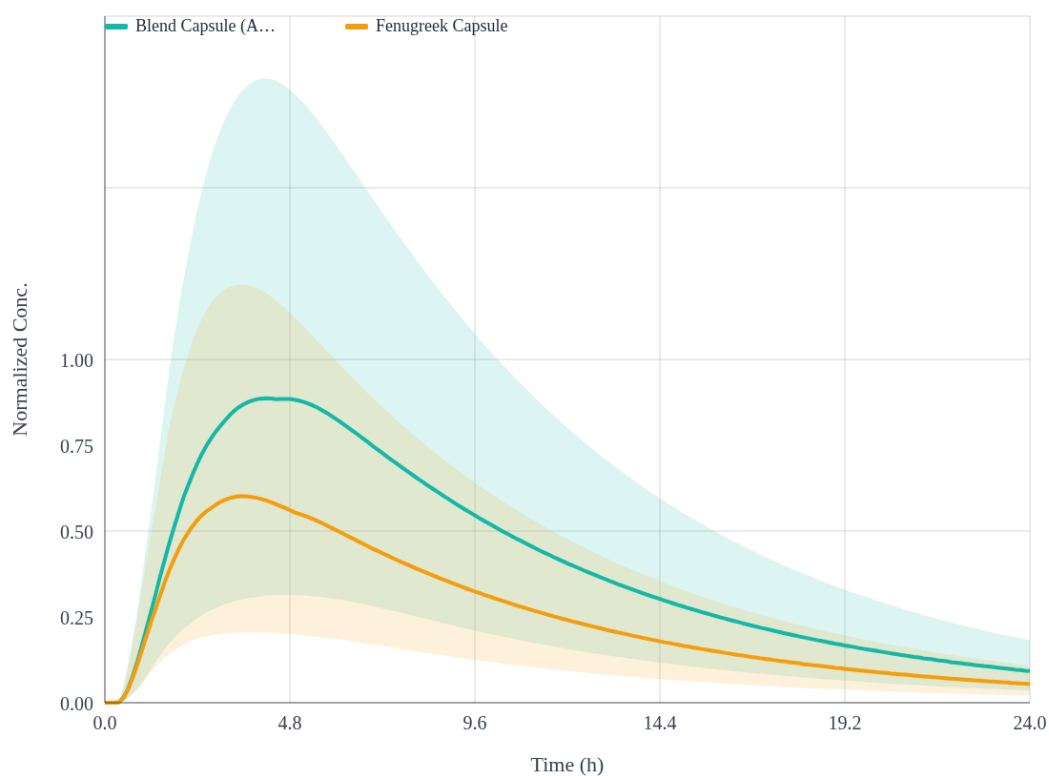
4-Hydroxyisoleucine



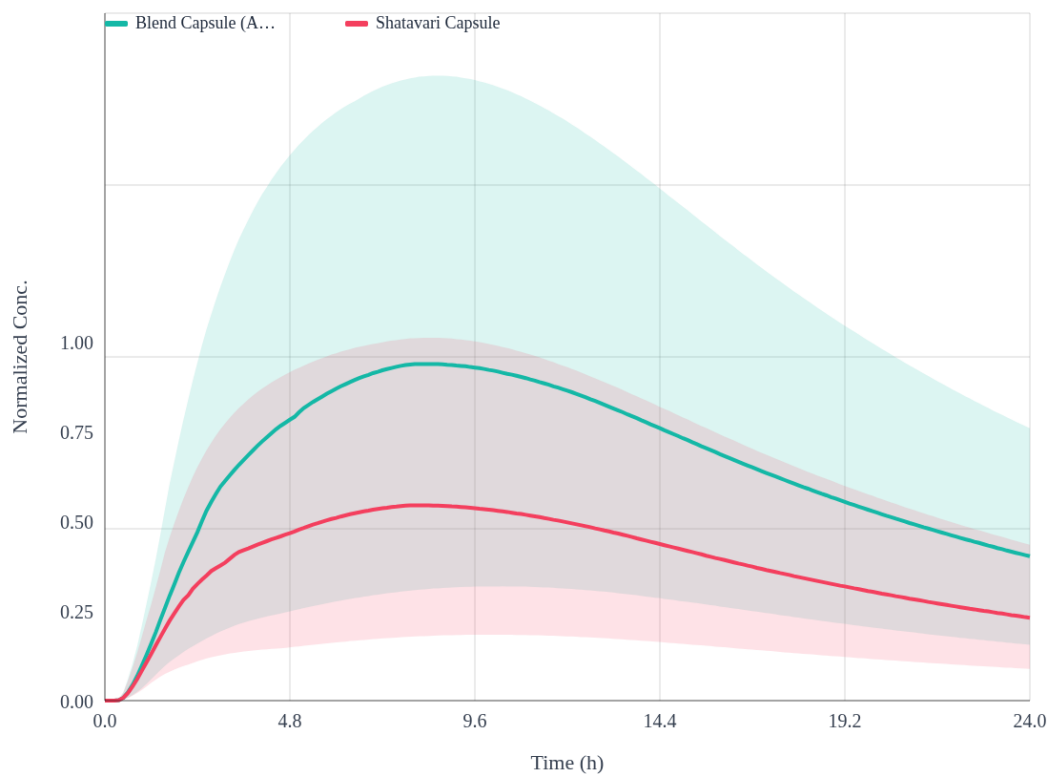
Apigenin



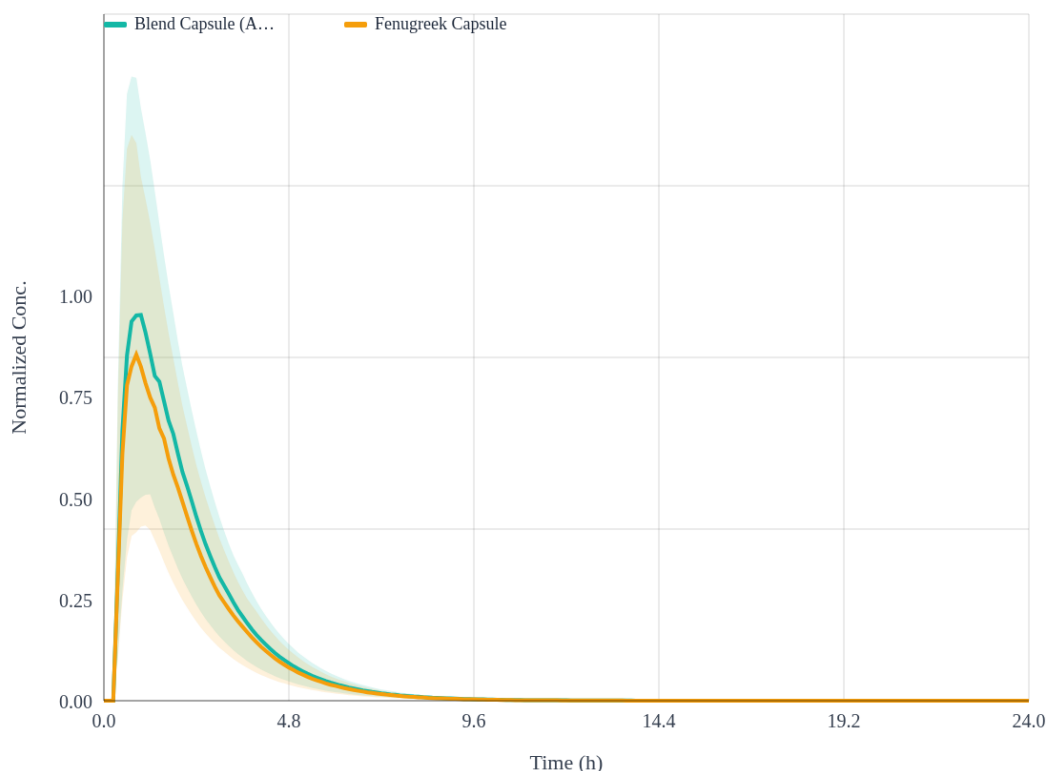
Protodioscin



Shatavarin IV



Trigonelline



Molecules

Name	SMILES
Protodioscin	<chem>C[C@H]1[C@H]2[C@H](C[C@@H]3[C@@]2(CC[C@H]4[C@H]3CC=C5[C@@H]1C[C@@H](C4=O)C5)O</chem>
Trigonelline	<chem>C[N+]1=CC=CC(=C1)C(=O)[O-]</chem>
4-Hydroxyisoleucine	<chem>C[C@H]([C@@H](C(=O)O)N)C(C)O</chem>
Shatavarin IV	<chem>C[C@H]1CC[C@@]2([C@H]([C@H]3[C@@H](O2)C[C@@H]4[C@@]3(CC[C@@H]1C4)O)C</chem>
Apigenin	<chem>C1=CC(=CC(=C1)C2=CC(=O)C3=C(C(=C(C=C3O)O)O)O</chem>

We use our suite of graph neural networks to predict relevant molecular properties and interactions with liver enzymes, plasma proteins, and the gut wall to inform the simulations.

Extracts

Fenugreek Extract — 500 mg / 500 mg

Molecule	%	Dose (mg)
Protodioscin	10%	50.0 / 50.0 mg
Trigonelline	3%	15.0 / 15.0 mg
4-Hydroxyisoleucine	3%	15.0 / 15.0 mg

Shatavari Root Extract — 100 mg / 100 mg

Molecule	%	Dose (mg)
Shatavarin IV	10%	10.0 / 10.0 mg

Damiana Extract — 300 mg / 300 mg

Molecule	%	Dose (mg)
Apigenin	1.5%	4.5 / 4.5 mg

Recipes

Blend Capsule

Ingredient	Type	Dose (mg)
Fenugreek Extract	Extract	500 mg
Shatavari Root Extract	Extract	100 mg
Damiana Extract	Extract	300 mg

Fenugreek Only

Ingredient	Type	Dose (mg)
Fenugreek Extract	Extract	500 mg

Shatavari Only

Ingredient	Type	Dose (mg)
Shatavari Root Extract	Extract	100 mg

Damiana Only

Ingredient	Type	Dose (mg)
Damiana Extract	Extract	300 mg

Formulations

1. Blend Capsule (All Three Extracts)

Delivery Type	Capsule
Capsule Shell Lag Time	15 min
Time to 50% Dissolved	15 min
Compound	Fenugreek Extract
Dose	500 mg
Formulation Type	Powder
Particle Radius (Lognormal Mean)	80 µm
Particle Radius (Lognormal GSD)	2
Compound	Shatavari Root Extract
Dose	100 mg
Formulation Type	Powder
Particle Radius (Lognormal Mean)	80 µm
Particle Radius (Lognormal GSD)	2
Compound	Damiana Extract
Dose	300 mg
Formulation Type	Powder
Particle Radius (Lognormal Mean)	80 µm
Particle Radius (Lognormal GSD)	2

2. Fenugreek Capsule

Delivery Type	Capsule
Capsule Shell Lag Time	15 min
Time to 50% Dissolved	15 min
Compound	Fenugreek Extract
Dose	500 mg

Formulation Type	Powder
Particle Radius (Lognormal Mean)	80 µm
Particle Radius (Lognormal GSD)	2

3. Shatavari Capsule

Delivery Type	Capsule
Capsule Shell Lag Time	15 min
Time to 50% Dissolved	15 min
Compound	Shatavari Root Extract
Dose	100 mg
Formulation Type	Powder
Particle Radius (Lognormal Mean)	80 µm
Particle Radius (Lognormal GSD)	2

4. Damiana Capsule

Delivery Type	Capsule
Capsule Shell Lag Time	15 min
Time to 50% Dissolved	15 min
Compound	Damiana Extract
Dose	300 mg
Formulation Type	Powder
Particle Radius (Lognormal Mean)	80 µm
Particle Radius (Lognormal GSD)	2

Advanced Details (Predicted)

Enzyme contributions, P-gp substrate probability, and inhibition flags are ADMET model predictions — not clinically validated values.

Metabolic Clearance — Enzyme Contributions

Compound	CYP1A2	CYP3A4	CYP2D6	CYP2C9	CYP2C19	UGT1A1	P-gp sub.
4-Hydroxyisoleucine	—	—	—	—	—	—	—
Apigenin	—	0.9%	0.6%	0.5%	—	49.8% *	—
Protodioscin	—	41.5%	5.9%	—	—	52.6% *	Yes
Shatavarin IV	—	35.1%	7.4%	—	—	57.4% *	Yes

Compound	CYP1A2	CYP3A4	CYP2D6	CYP2C9	CYP2C19	UGT1A1	P-gp sub.
Trigonelline	—	29.7% *	22.2%	20.8%	—	27.3%	—

Enzyme Inhibition Profile

Compound	CYP1A2	CYP3A4	CYP2D6	CYP2C9	CYP2C19	UGT1A1	P-gp inh.
4-Hydroxyisoleucine	—	—	—	—	—	—	—
Apigenin	Yes	Yes	—	—	—	Yes	—
Protodioscin	—	—	—	—	—	—	—
Shatavarin IV	—	—	—	—	—	—	—
Trigonelline	Yes	—	—	—	—	—	—

Inhibition probability ≥50% = inhibitor. Relevant for co-administration with CYP substrates.

Bioavailability Targets

Protodioscin, Trigonelline, 4-Hydroxyisoleucine, Shatavarin IV, Apigenin

Population & Conditions

Population	American (with Census Demographics)
Sample Size (n)	100
Age Range	26–60 years
Female %	100%
Weight	44–124 kg (mean 70 kg)
Height	143–178 cm (mean 161 cm)
BMI	18–45 kg/m² (mean 27)
Race/Ethnicity	White 61% · Latino 19% · African American 13% · Asian 6%
BMI Breakdown	Normal 46% · Overweight 31% · Obese 22% · Underweight 1%
Prandial State	Fasted
Simulation Duration	24h