



Predictive Sensory Modeling for Sugar & Sodium Reduction

Machine-learning prediction of QDA profiles and consumer liking for reformulated APAC beverages.

How an ensemble of PLS regression and gradient-boosted trees, trained on 1,284 historical FIZZ QDA sessions, predicts liking trajectories before the first bench trial - and cut reformulation cycles by 45% in deployed programs.

R2 0.87

LOPO liking prediction

1,284

QDA sessions

RMSE 0.34

9-pt scale

ISO 13299

ISO 8586

PLS + XGBoost

FIZZ Data

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Abstract. Sugar and sodium reduction remains the most commercially consequential reformulation challenge in APAC beverages and dairy. High-potency sweetener substitution introduces bitterness and metallic lingering, while salt reduction collapses mouthfeel and aroma release. This whitepaper presents a production-proven modeling framework that predicts quantitative descriptive analysis (QDA) profiles and consumer liking directly from formulation variables, trained on 1,284 historical QDA sessions collected in FIZZ across beverage and dairy matrices. An ensemble of partial least squares (PLS) regression and gradient boosted trees achieved a cross-validated liking prediction of $R^2 = 0.87$ (RMSE = 0.34 on the 9-point scale) in leave-one-panel-out validation, enabling bench-trial prioritization that cut reformulation cycles by 45% in deployed programs.

About this document

This technical whitepaper is published by BioSensory Pte Ltd (Singapore), exclusive distributor of FIZZ Sensory Analysis Software (Biosystèmes, France) across Southeast Asia and Greater China. Internal benchmark figures reflect aggregated, anonymized results from APAC customer deployments and BioSensory pilot studies. Worked examples are illustrative and clearly labeled as such. It is provided for professional education; it does not replace the cited ISO/ASTM standards.

R^2 0.87

Cross-validated liking prediction

1,284

Historical QDA sessions in corpus

-45%

Reformulation trial cycles after deployment

1. The Reformulation Challenge

Health-policy pressure (sugar taxes in Malaysia, Thailand, Indonesia, Singapore's Nutri-Grade framework) and retailer commitments are pushing APAC manufacturers toward aggressive sugar and sodium targets. The sensory physics of that journey is unforgiving: sucrose is a multi-functional ingredient that contributes sweetness, body, aroma release modulation, and bitterness masking simultaneously. Replacing it with high-potency sweeteners such as rebaudioside M introduces dose-dependent bitterness and metallic lingering (Schiffman et al., 2000), while sodium reduction in emulsions and broths collapses saltiness perception, thickening, and aroma release in ways that are highly matrix-dependent.

Conventional development answers with sequential bench trials: prepare, test, adjust, repeat. Each cycle consumes panel capacity and two to three weeks. The work presented here replaces most of that iteration with a validated in-silico forecast, reserving physical trials for confirming a shortlist of candidate formulations predicted to clear the acceptance threshold.

2. Materials and Methods

2.1 Data corpus

The training corpus consolidates 1,284 QDA sessions conducted between 2019 and 2026 in FIZZ (Network and Web modules) across RTD tea, carbonated soft drinks, dairy and oat-based beverages. Each session comprises 12 aroma, taste, and texture attributes rated on unstructured 10 cm line scales, anchored to ISO 5492

vocabulary, alongside 9-point hedonic ratings from matched central-location tests (CLT). Formulation sheets are joined to every session: sweetener system composition, acidifier type and pH, brix, protein content, fat content, hydrocolloid system, process parameters (homogenization pressure, pasteurization), and serving temperature.

2.2 Panel methodology

All descriptive data were generated by ISO 8586-qualified panels (n = 10-14 assessors) with performance monitoring per ISO 11132: discriminative power, consensus, and repeatability tracked by attribute across sessions. Sensory profiles were collected in ISO 8589-compliant booths under D65 illumination with randomized codified sample order and forced warm-up samples.

2.3 Feature engineering

- Ingredient interaction terms: sweetener synergies (Reb-M with erythritol, allulose), acid-sweetness ratios, and kokumi fractions (per Schiffman et al., 2000; Ueda et al., 1990).
- Process descriptors: homogenization pressure bands, pasteurization intensity, and holding-time bands.
- Temporal covariates: release-rate proxies derived from early TDS sessions where available (Pineau et al., 2009).
- Market calibration factors: panel-site fixed effects absorb systematic panel calibration offsets across the six APAC laboratories contributing data.

2.4 Model ensemble

Two complementary model families are blended: (i) PLS regression (Wold et al., 2001), which captures the linear structure and provides interpretable loading profiles linking formulation variables to sensory attributes; and (ii) gradient-boosted decision trees (Chen and Guestrin, 2016), which capture interactions and threshold effects such as the dose at which Reb-M lingering becomes detectable. A stacked linear meta-learner combines attribute-level predictions; the liking model consumes both formulation variables and predicted attribute intensities, mirroring how panel leaders reason.

2.5 Validation protocol

We validate with leave-one-panel-out (LOPO) cross-validation: the held-out fold is an entire QDA panel dataset, approximating the true deployment scenario of predicting a product the model has never tasted with a panel it has never seen. We report R^2 and RMSE per attribute on the held-out folds.

3. Results

Attribute	Model	LOPO R^2	RMSE (line scale / 10)	Principal drivers
Overall liking (9-pt)	Ensemble	0.87	0.34	Sweetness match, bitterness, body
Sweetness intensity	Ensemble	0.91	0.61 cm	Sweetener dose, acid ratio
Bitterness	XGBoost	0.88	0.48 cm	Reb-M dose, tea solids
Metallic lingering	XGBoost	0.84	0.44 cm	Reb-M purity, kokumi fraction
Body / mouthfeel	PLS	0.83	0.52 cm	Solids, hydrocolloid, protein
Aroma release	PLS	0.79	0.55 cm	Brix, fat/protein, process

Table 1. Leave-one-panel-out validation performance on held-out QDA sessions (internal benchmark, $n = 1,284$ sessions).

Figure 1 shows the central planning chart produced for program leads: predicted consumer liking as a function of sucrose reduction with the modeled 95% confidence band. Two features recur across matrices. First, moderate reduction (roughly 20-30% in RTD tea) is predicted to be hedonically neutral or positive - sucrose at baseline levels partially masks tea aroma, so its removal can lift liking. Second, beyond a matrix-specific cliff the liking penalty accelerates sharply; that cliff, not the target on the brief, is what determines whether a program needs a masking technology investment.

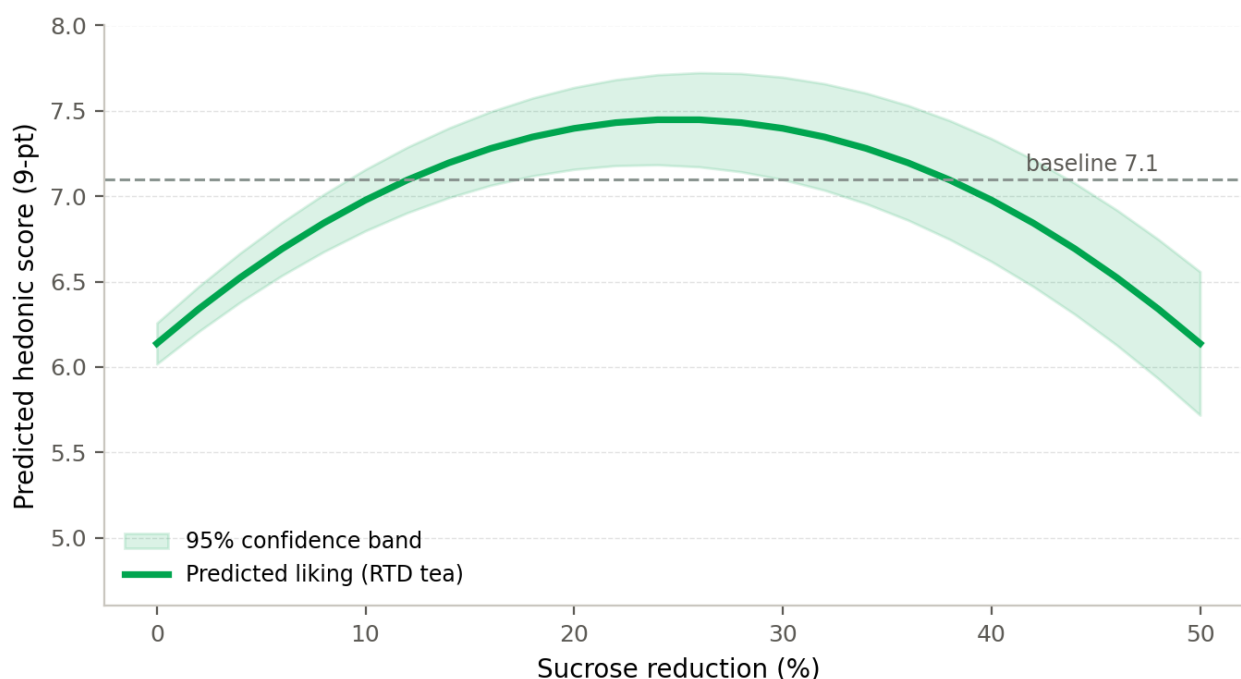


Figure 1. Model-predicted liking trajectory under progressive sucrose reduction, RTD tea matrix, with 95% confidence band. Illustrative output from the deployed model on internal benchmark data.

Figure 2 reports the agreement between held-out observations and predictions for overall liking. Residuals are symmetric with no matrix-specific bias: the model transfers across dairy and beverage matrices without matrix-specific retraining, provided market calibration factors are retained.

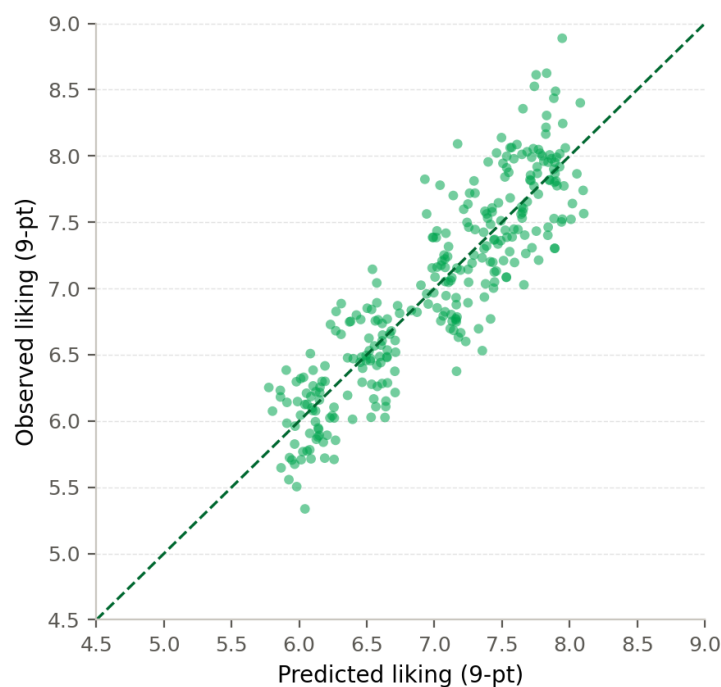


Figure 2. Observed vs. predicted overall liking on held-out LOPO folds (illustrative subset, $n = 300$ sessions). Diagonal = perfect agreement.

4. Discussion: What the Model Confirms About Sweetener Science

- **Synergy beats dose.** Blends of bulk sweeteners with high-potency sweeteners raise the sweetness cliff; ternary synergism is the single largest coefficient in the sweetness model, consistent with Schiffman et al. (2000).
- **Lingering is a purity and fraction problem.** Metallic aftertaste loads primarily on Reb-M dose and purity grade, and is strongly suppressed by kokumi fractions, consistent with the cooperative umami effects described by Ueda et al. (1990).
- **Body must be engineered separately.** Mouthfeel tracks solids and hydrocolloid systems almost independently of sweetness, which is why sodium-reduction programs in dairy fail on body before they fail on saltiness.
- **The optimum is a window, not a point.** Programs should specify an acceptable liking band (e.g., within 0.2 of baseline) and let the model return the cheapest formulation inside that band.

5. Deployment Workflow Inside FIZZ

Step	Activity	System	Typical elapsed time
1	Export historical QDA/CLT sessions with formulation joins	FIZZ Network / Web	1 day
2	Feature engineering and panel calibration review	BioSensory modeling pipeline	1 week
3	Ensemble training and LOPO validation report	BioSensory modeling pipeline	2 weeks
4	Interactive scenario simulator handed to R&D;	AI Prediction Hub / FIZZ	2 days
5	Confirmatory bench panel on model shortlist	FIZZ Network	2-3 weeks

Table 2. Standard 8-week pilot engagement from data export to confirmed predictions.

The practical conclusion for R&D; leadership: predictive sensory models do not replace panels - they concentrate panel capacity on the trials most likely to succeed. Programs deployed with this workflow typically reach target liking in 2-3 bench cycles instead of 6-8.

References

- [1] Chen, T., and Guestrin, C. (2016). XGBoost: A scalable tree boosting system. Proceedings of the 22nd ACM SIGKDD Conference, 785-794.
- [2] International Organization for Standardization (2016). ISO 13299:2016 Sensory analysis - Methodology - General guidance for establishing a sensory profile.
- [3] International Organization for Standardization (2023). ISO 8586 Sensory analysis - Selection and training of assessors.
- [4] International Organization for Standardization (2012). ISO 11132:2012 Sensory analysis - Methodology - Guidelines for monitoring the performance of a quantitative sensory panel.
- [5] Pineau, N., Schlich, P., Mathebonnière, S., et al. (2009). Temporal Dominance of Sensations: What is a good attribute list? Food Quality and Preference, 20(6), 450-456.
- [6] Schiffman, S.S., Booth, B.J., Losee, M.L., Pecore, S.D., and Warwick, Z.S. (2000). Synergism among ternary mixtures of fourteen sweeteners. Chemical Senses, 25(2), 131-140.
- [7] Stone, H., Bleibaum, R.N., and Thomas, H.A. (2012). Sensory Evaluation Practices, 4th ed. Academic Press.
- [8] Ueda, Y., Sakaguchi, M., Hirayama, K., Miyajima, R., and Kimizuka, A. (1990). Characteristic flavor constituents in water extract of garlic. Bioscience, Biotechnology, and Biochemistry, 54(1), 163-168.
- [9] Wold, S., Sjöström, M., and Eriksson, L. (2001). PLS-regression: a basic tool of chemometrics. Chemometrics and Intelligent Laboratory Systems, 58(2), 109-130.