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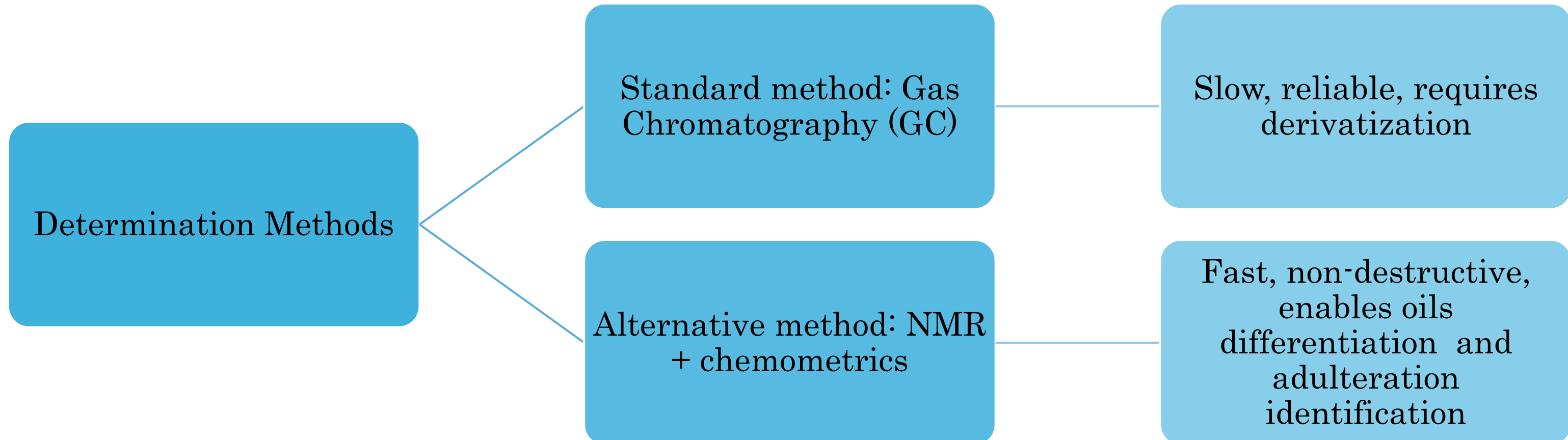
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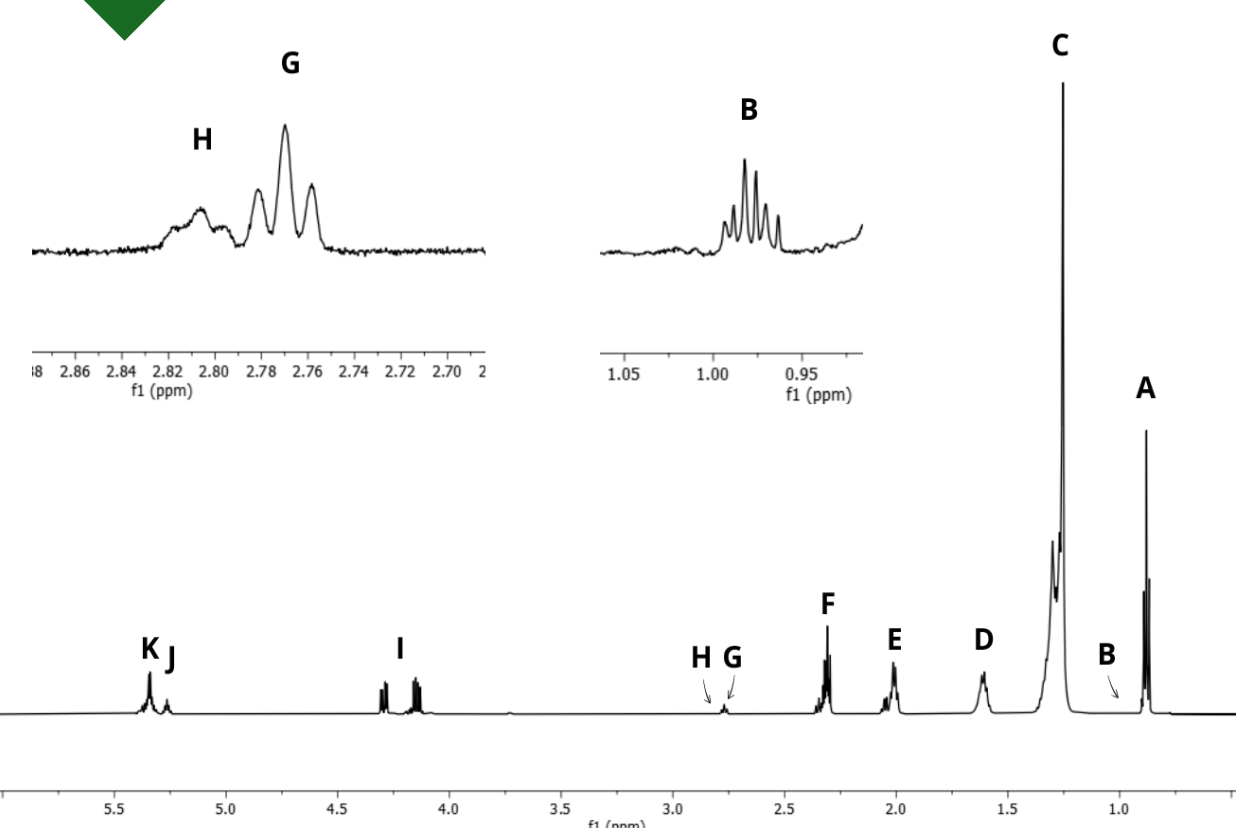
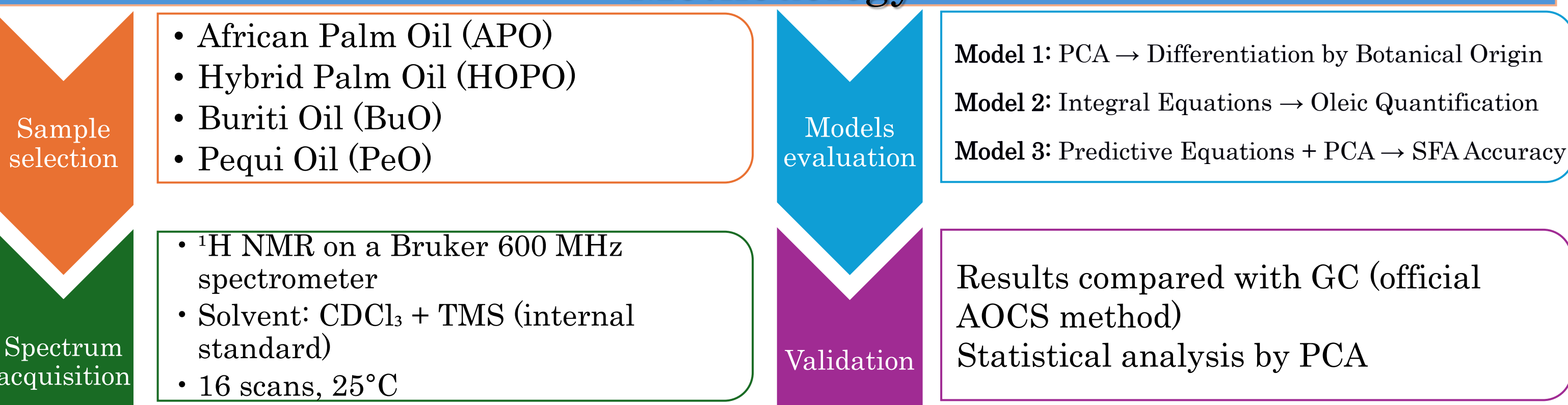
Introduction

Vegetable oils are essential raw materials in the food, cosmetic, pharmaceutical, and biofuel industries. Their quality is directly related to their fatty acid composition, which influences their nutritional, technological, and stability properties.



Evaluation and comparison of the effectiveness of three predictive models based on ¹H NMR analyses for the quantification of fatty acids in vegetable oils.

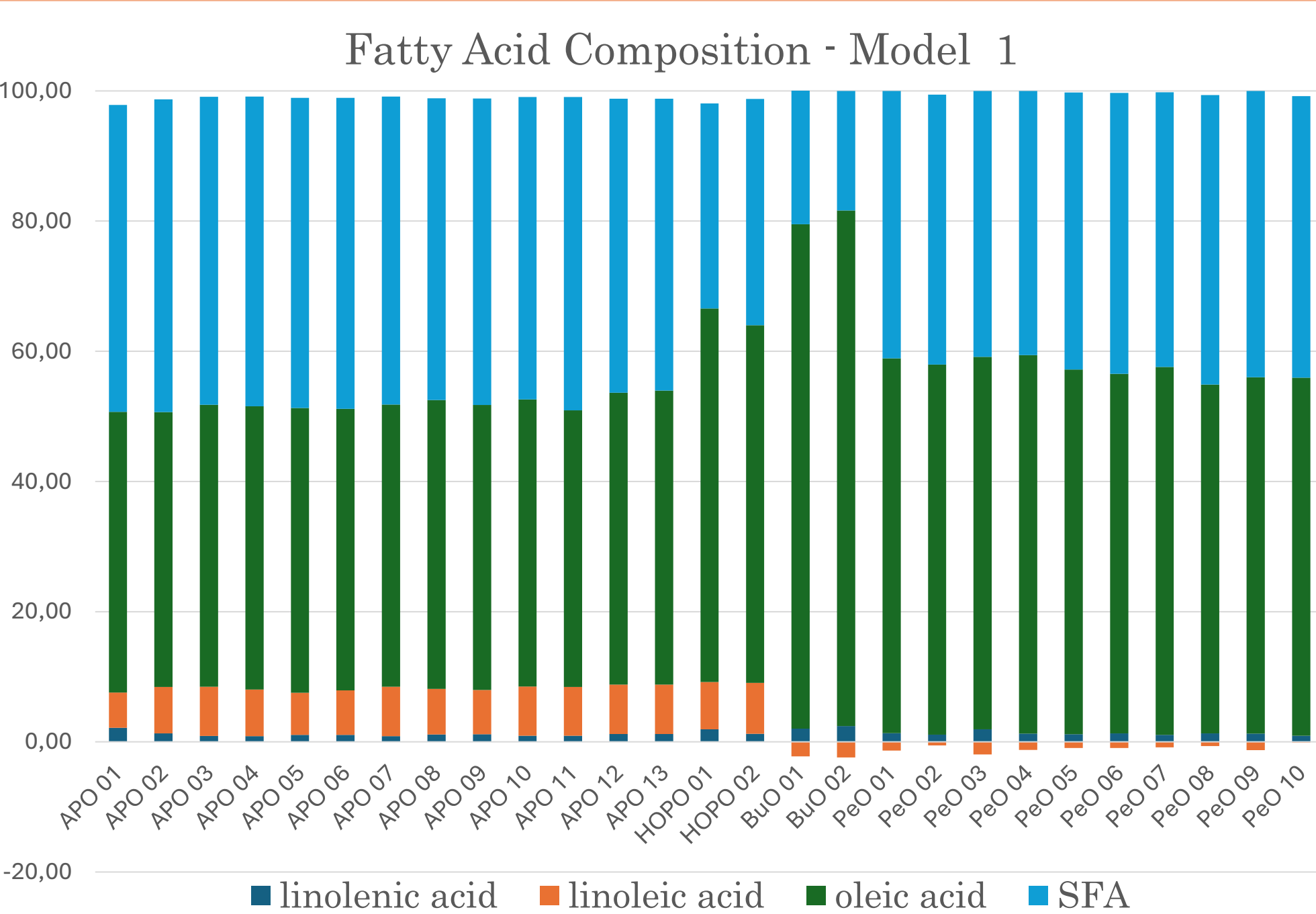
Methodology



	Linolenic Acid	Linoleic Acid	Oleic Acid	SFA
Model 1	$\frac{B}{B+A} \times 100$	$\frac{3G-4B}{2(A+B)} \times 100$	$\frac{3E}{4(G+H) - Ln \times 100}$	$\frac{A}{B+A} - L - Ln - O$
Model 2	$\frac{B}{B+A}$	$\frac{G}{6} - 2Ln$	$\frac{E}{12} - \frac{G}{6} + Ln$	$100 - (L + Ln + O)$
Model 3	$\frac{H}{3I} \times 100$	$\frac{2G}{3I} \times 100$	$\frac{E-2G-H}{3I} \times 100$	$100 - (L + Ln + O)$

Table 01 - Percentage of variance explained by PCA analysis

Results



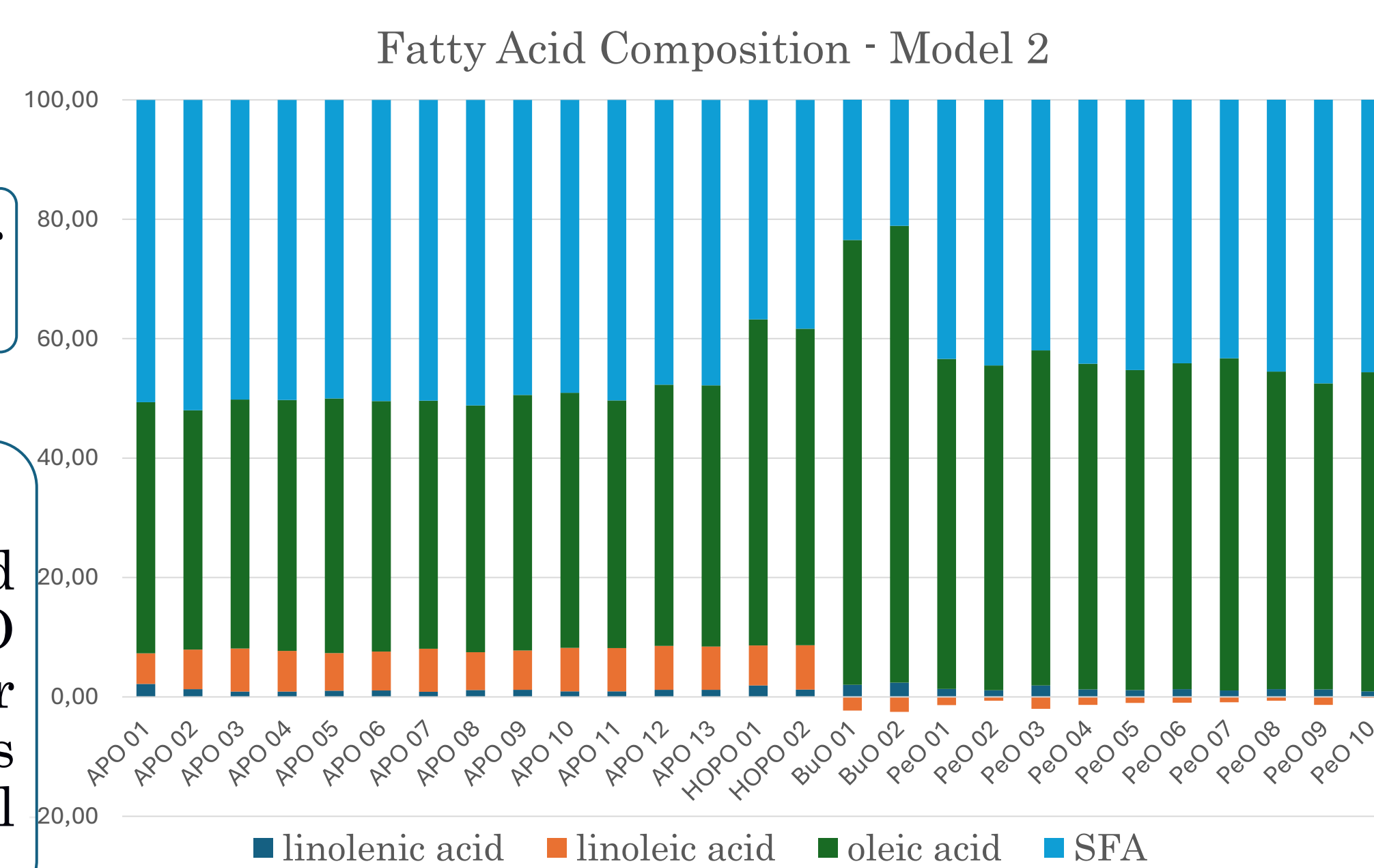
Model 1

Good distinction between oils with different profiles (palm X buriti/pequi).

Drawbacks:

Negative values for linoleic acid in some samples (especially BuO and PeO).

Model 2

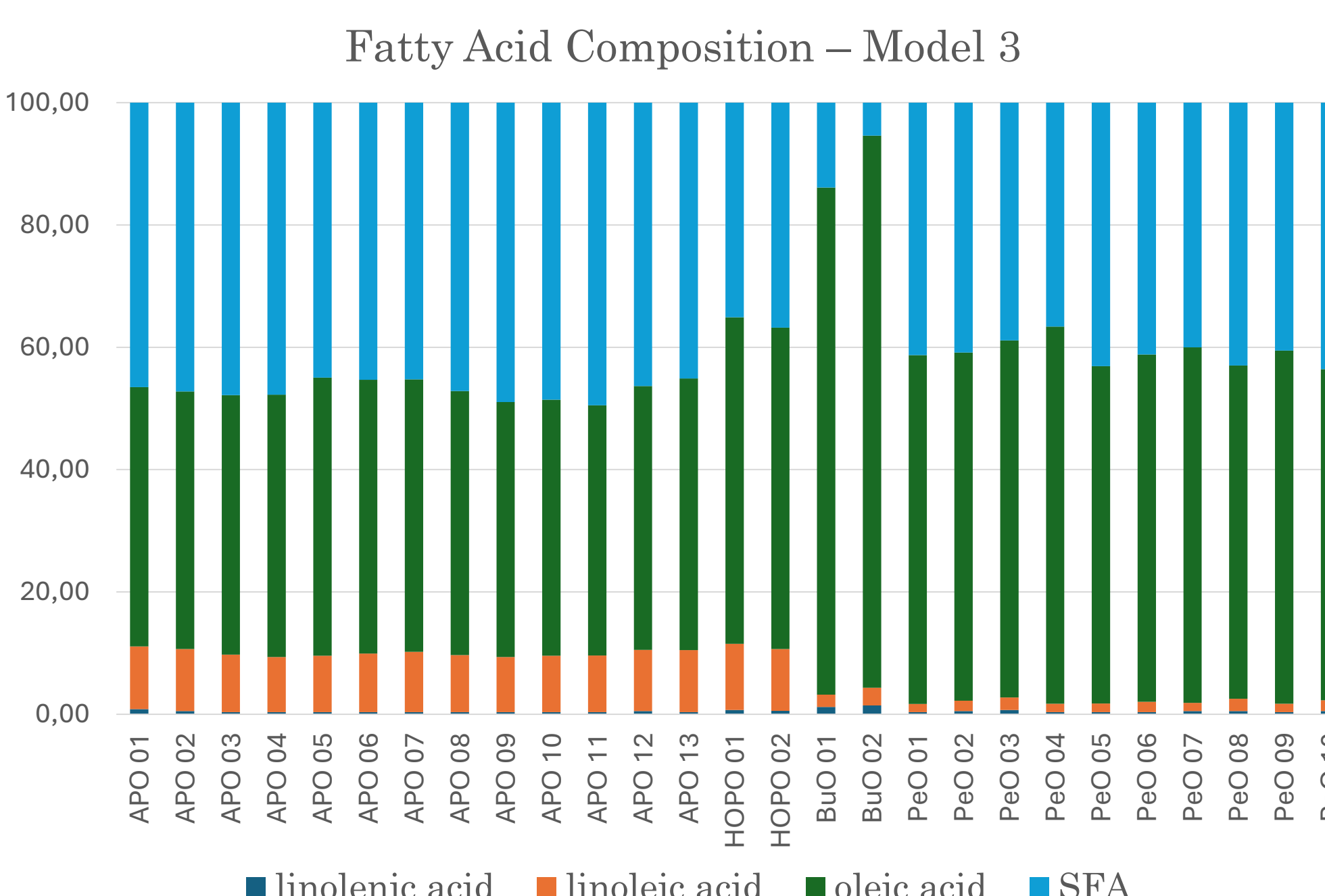


Best model tested for oleic acid quantification.

Drawbacks:

Negative linoleic acid values occurred in BuO and PeO, with poor results in samples unlike the model's oil profiles.

Model 3

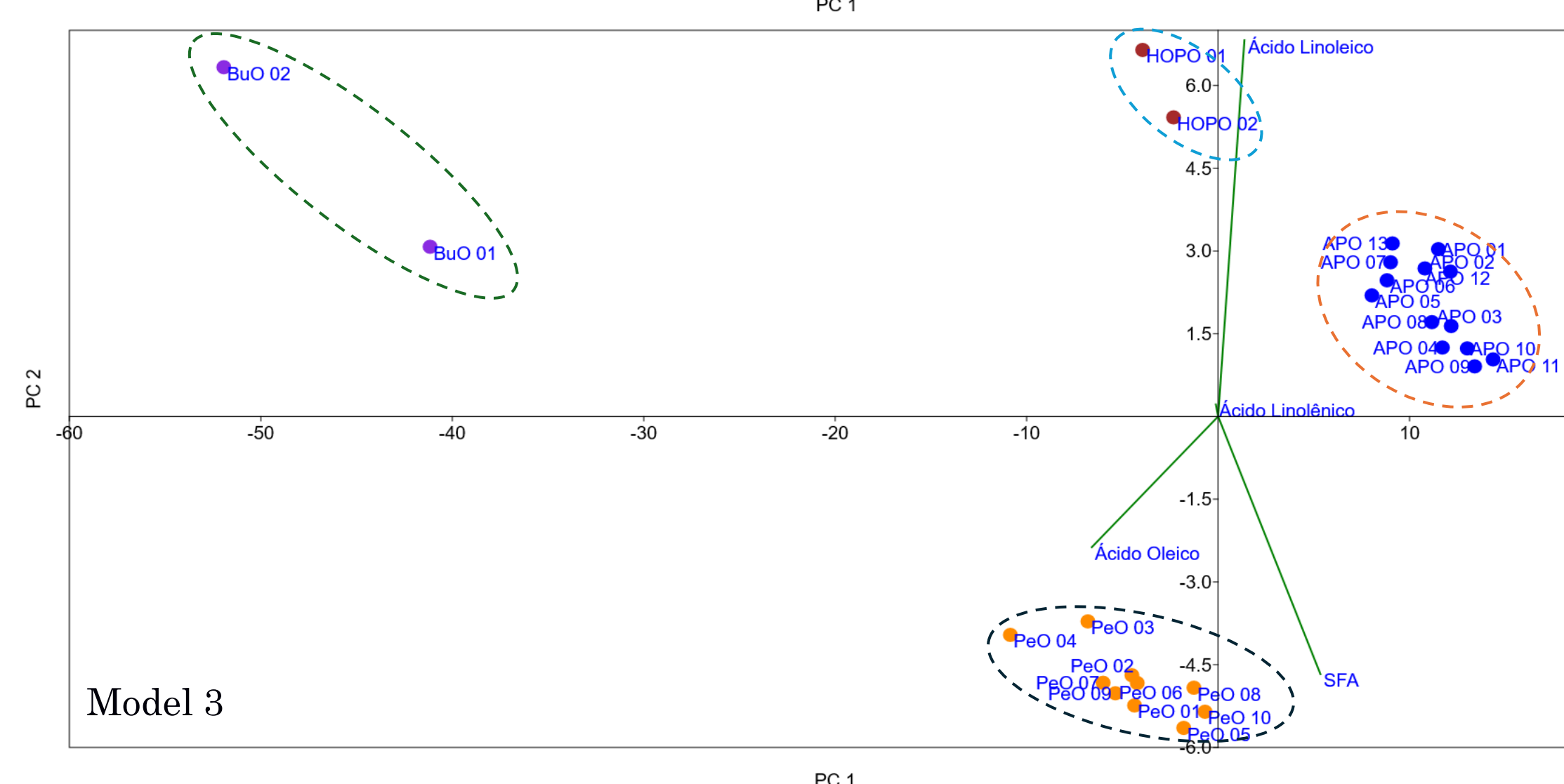
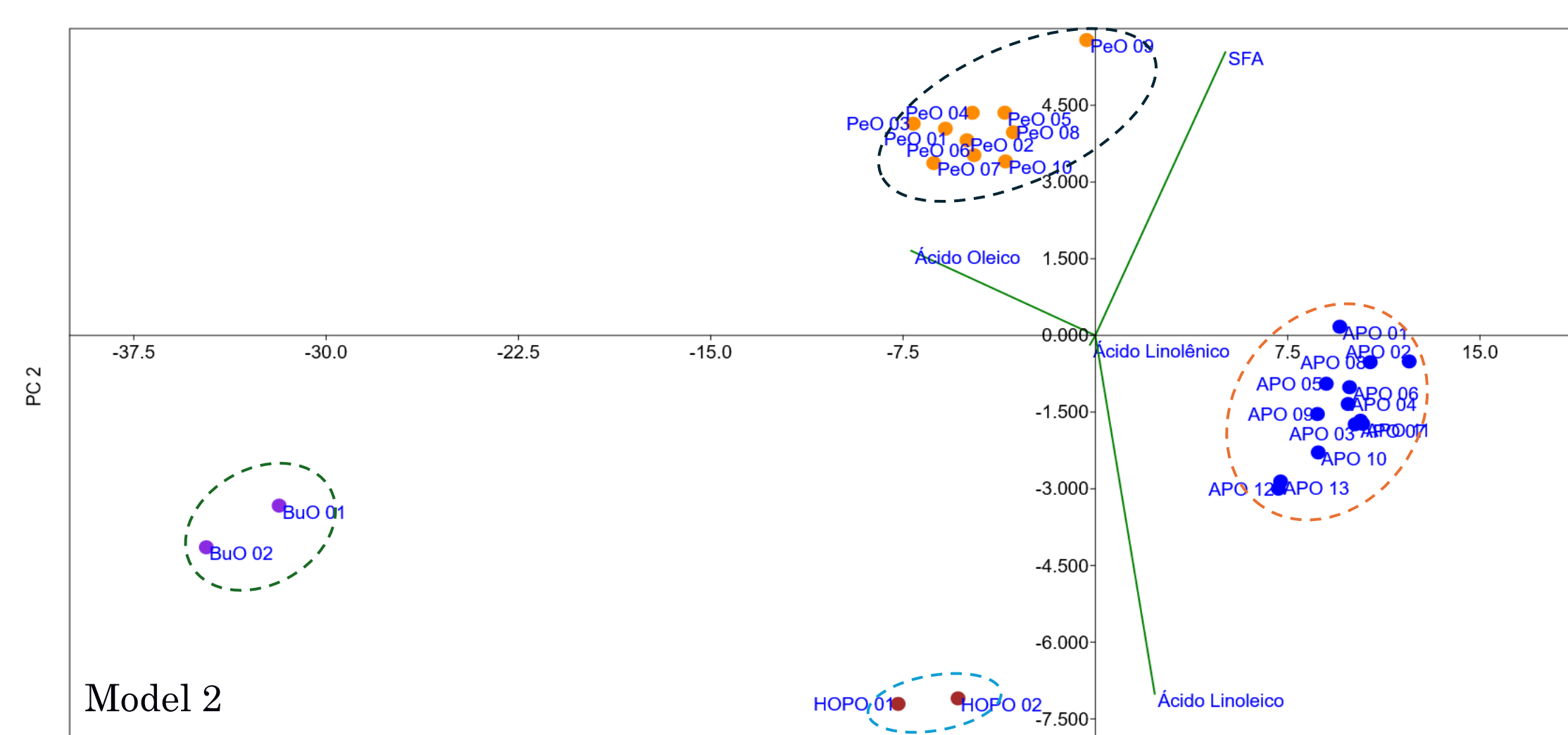
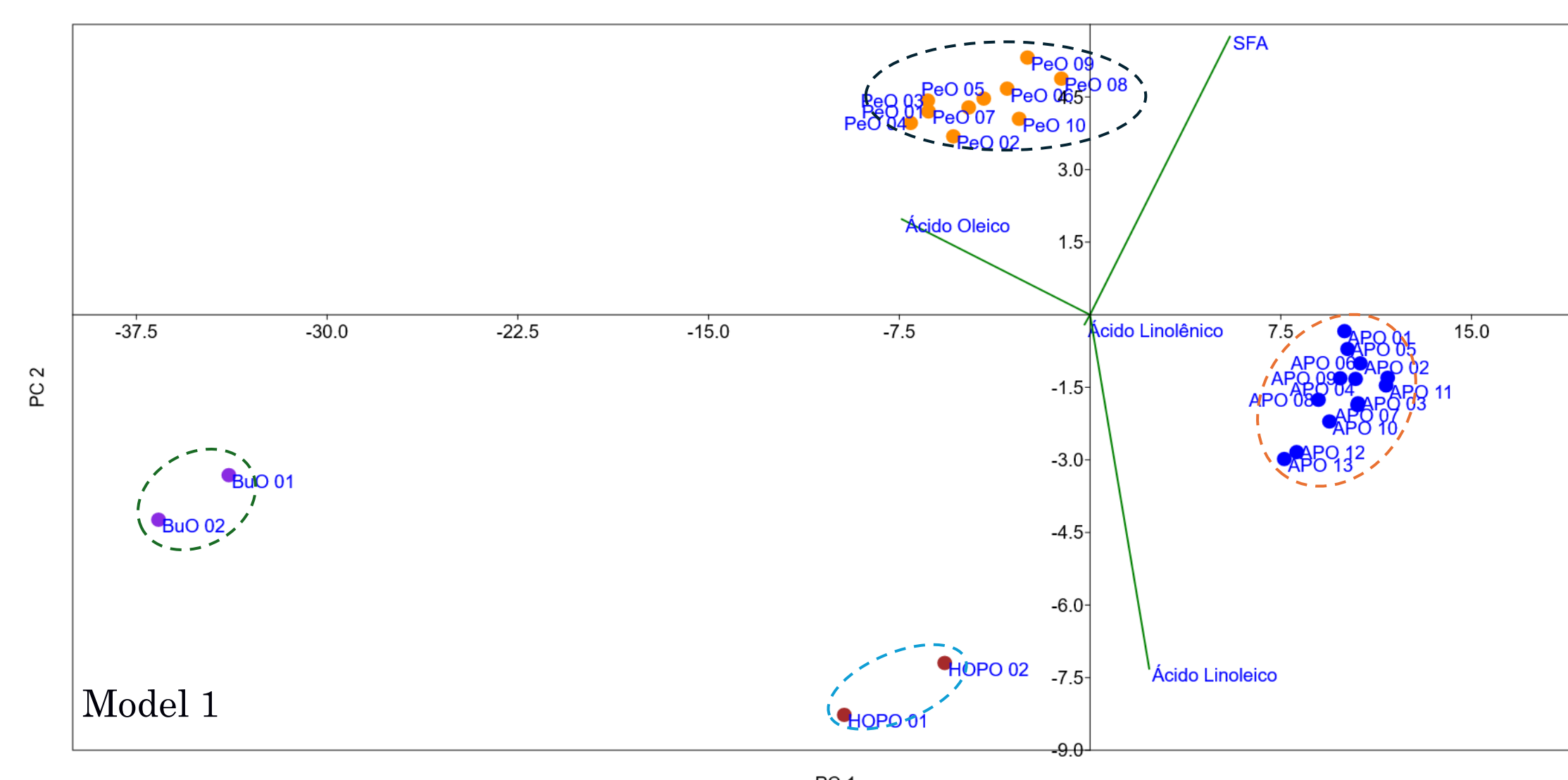


Good GC agreement for oleic and SFA, with no negatives and balanced PCA quantification and clustering.

Drawbacks:

More robust but dependent on external calibration, with accuracy loss in samples unlike the model's oil profiles.

- APO samples clustered consistently, associated with linoleic and linolenic acids.
- PeO samples grouped in the region correlated with oleic acid and SFA.
- HOPO samples showed a distinct pattern, positively related to linoleic acid.
- BuO remained isolated, highlighting its unique fatty acid profile.



- PCA confirmed the discriminatory power of ¹H NMR for oil differentiation.
- PC1 explained variance mainly through oleic acid and SFA, while PC2 was influenced by linoleic and linolenic acids.
- The first two PCs together explained more than 90% of the total variance.

% Variance	Model 1	Model 2	Model 3
PC 1	91,40	91,61	93,79
PC 2	8,48	8,31	6,20
PC 3	0,12	0,08	0,01

Table 02 - Percentage of variance explained by PCA analysis

Conclusion

- ¹H NMR analysis was an effective technique for differentiating vegetable oils with distinct compositions: palm oil (APO and HOPO) – richer in saturated compounds from buriti(BuO) and pequi (PeO) oils –richer in unsaturated compounds
- Consistent correlation with GC data, assessing the robustness of the technique
- Model 1:** good for clustering with poor quantification results
- Model 2:** greater precision for oleic and SFA quantification with some limitation
- Model 3:** good balance between quantification and clustering with good agreement with CG data
- Combination between ¹H NMR and chemometric tools represents a promising alternative for the characterization, authentication and monitoring of vegetable oils.

Acknowledgement