Comparison of Collection Strategies for the Analysis of Targeted Compounds in ENDS Aerosol

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Goal

Assess the effect of aerosol collection methodology on estimated whole pod yields for primary constituents, metals, and carbonyl compounds in closed system ENDS products

Analytes

- **Primary Constituents**: Glycerol, Menthol, **Nicotine**, Propylene glycol, Water
- **Metals**: Arsenic, Beryllium, Cadmium, Chromium, Cobalt, Copper, Iron, Lead, **Nickel**, Selenium, Silver, Tin, Zinc
- **Carbonyls and Glycidol**: Acetaldehyde, Acrolein, Butyraldehyde, Crotonaldehyde, Diacetyl (2,3-Butanedione), **Formaldehyde**, Glycidol, 2,3-Pentanedione (Acetyl propionyl)

Background

Background

- Analyzed the effect of puffing regime on ENDS aerosol yield
- Analyses were performed from the beginning of aerosol generation until full pod depletion
- ACM yields decrease over the duration of testing, until pod depletion

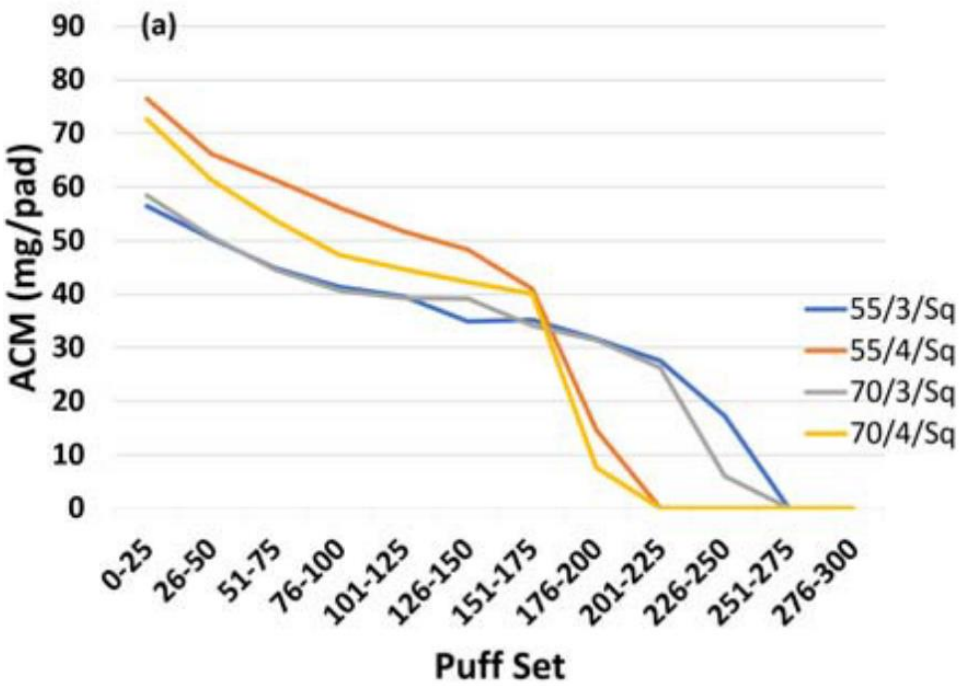


Figure 2. Puff profile diagram. Puff block results example shown as (a) puff block to puff block yield trending

Gupta, A., Tayyarah, R., Gillman, G., Garner, C., & Stevens, R. (2021). Machine Vaping of Electronic Cigarettes - A Comparison of Puffing Regimes #. *Contributions to Tobacco & Nicotine Research*, *30*(3), 127–136. https://doi.org/10.2478/CTTR-2021-0009

Background

- Studied product performance of a range of e-cigarettes
- Analyses were performed from the beginning of aerosol generation until full pod depletion
- Majority of 16 closed systems tested increased formaldehyde production after 50% pod depletion

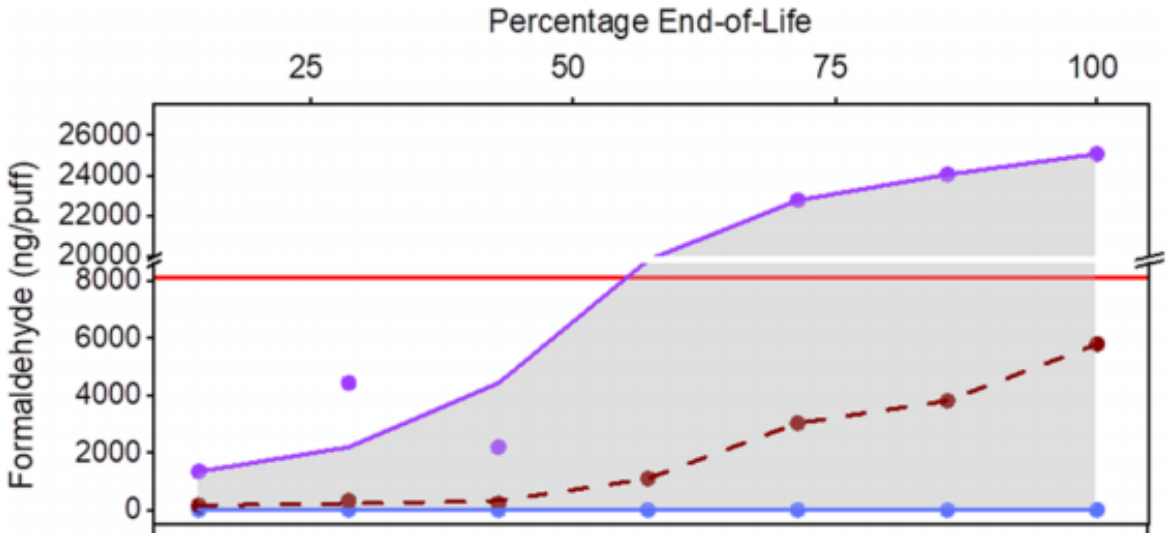


Figure 3. End-of-life of formaldehyde in aerosol for 16 closed systems (excluding disposable systems). The horizontal line shows the 3R4F level as a reference with an intense smoking regime ISO 20778. The upper solid, middle dashed, and bottom solid lines illustrate the max, average, and min yield, respectively, across all products. These are the best polynomial fit to the raw data.

Belushkin, M., Tafin Djoko, D., Esposito, M., Korneliou, A., Jeannet, C., Lazzerini, M., & Jaccard, G. (2019). Selected Harmful and Potentially Harmful Constituents Levels in Commercial e-Cigarettes. https://doi.org/10.1021/acs.chemrestox.9b00470

Background

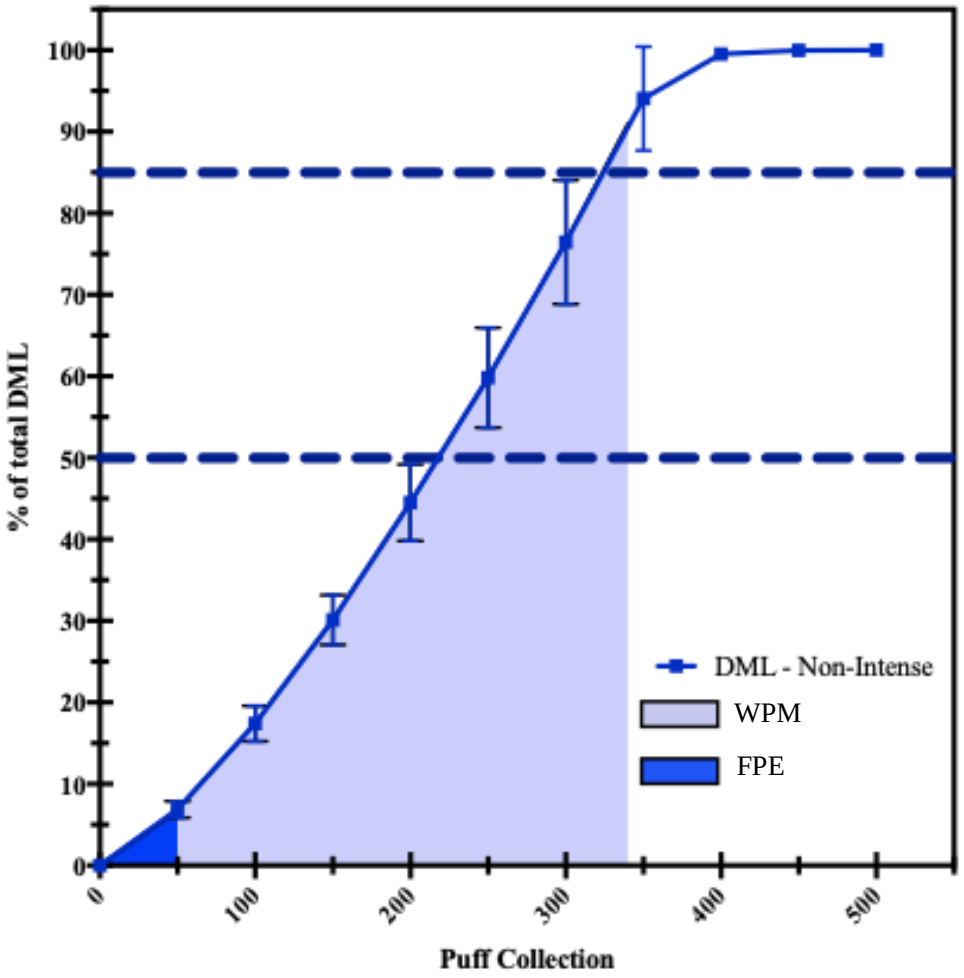
Three collection strategies were compared to determine the effect of model projections on reported whole pod HPHC yields

Collection Strategies

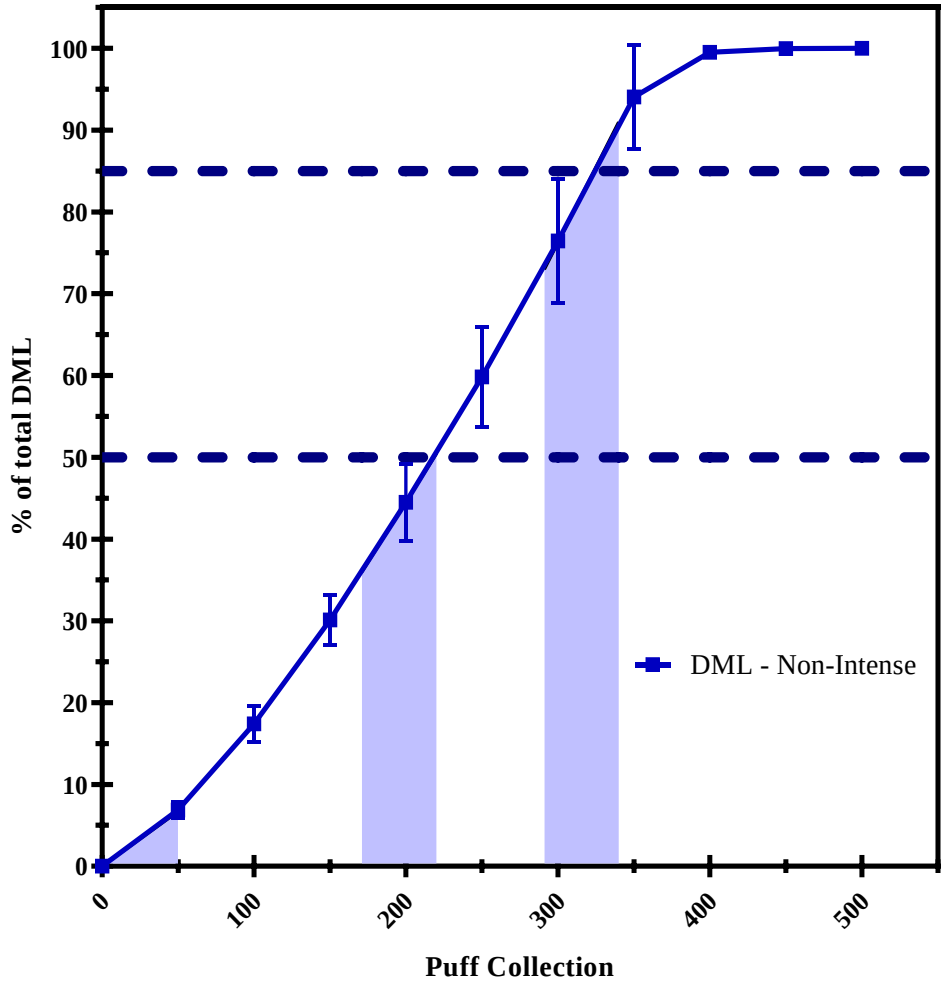
- **Whole Pod Measurement (WPM)**: All puffs were collected and analyzed from one to end of pod life
- **Whole Pod Extrapolation (WPE)**: Three 50-puff blocks were collected and analyzed from the beginning, middle, and end of pod life. Whole pod yield was projected by assuming linear yields over the pod life
- **Fifty Puff Extrapolation (FPE)**: A single 50-puff blocks was collected and analyzed from the beginning of pod life. Whole pod yield was projected by assuming a flat linear yield from puff one through the end of pod life

Collection Strategies

FPE and WPM Collections



WPE Collection



End-of-Life Determination

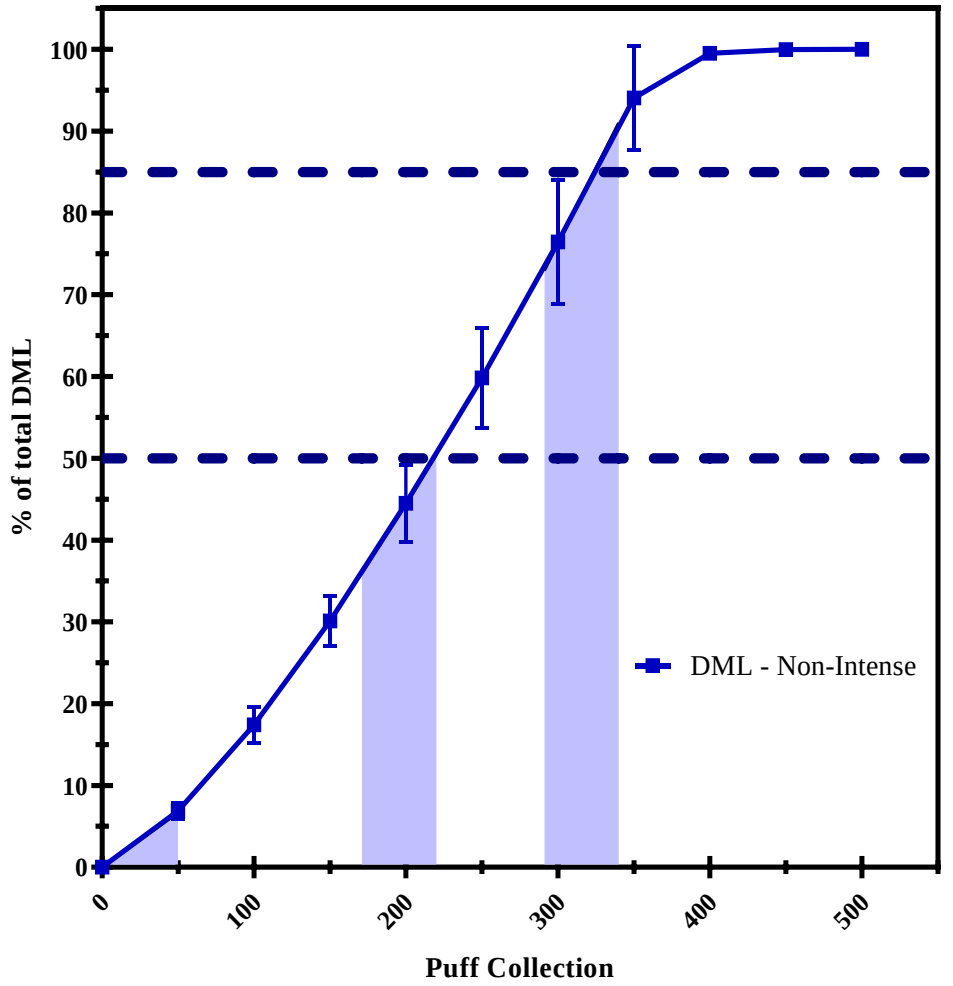
Target End-of-Life (EOL) is 85~90% of total DML

- Device is puffed to total depletion in 50-puff segments
- EOL is set at ~90% of total liquid depletion

Representative Product EOL Measurement

- 90% depletion at 340 puffs

Representative ENDS Product - CORESTA Puff Regime



End-of-Life and Average Collected Mass

Brand	Flavor	Puffs to EOL	DML to EOL (mg)	% of WP in FPE	% of WP in WPE
Brand A	Tobacco	371	433	11%	45%
	Mint/Menthol	455	525	9%	36%
Brand B	Tobacco	262	1577	19%	58%
	Mint/Menthol	323	1626	18%	45%
Brand C	Tobacco	360	1744	16%	42%
	Mint/Menthol	405	1719	16%	34%
Brand D	Tobacco	363	1489	17%	46%
	Mint/Menthol	260	1527	18%	56%

WP: Whole Pod
FPE: Fifty Puff Extrapolated
WPE: Whole Pod Extrapolated
DML: Device Mass Loss
EOL: End-of-Life

Preliminary Data

Results

Nicotine

- Four Brands

-Tobacco and Menthol

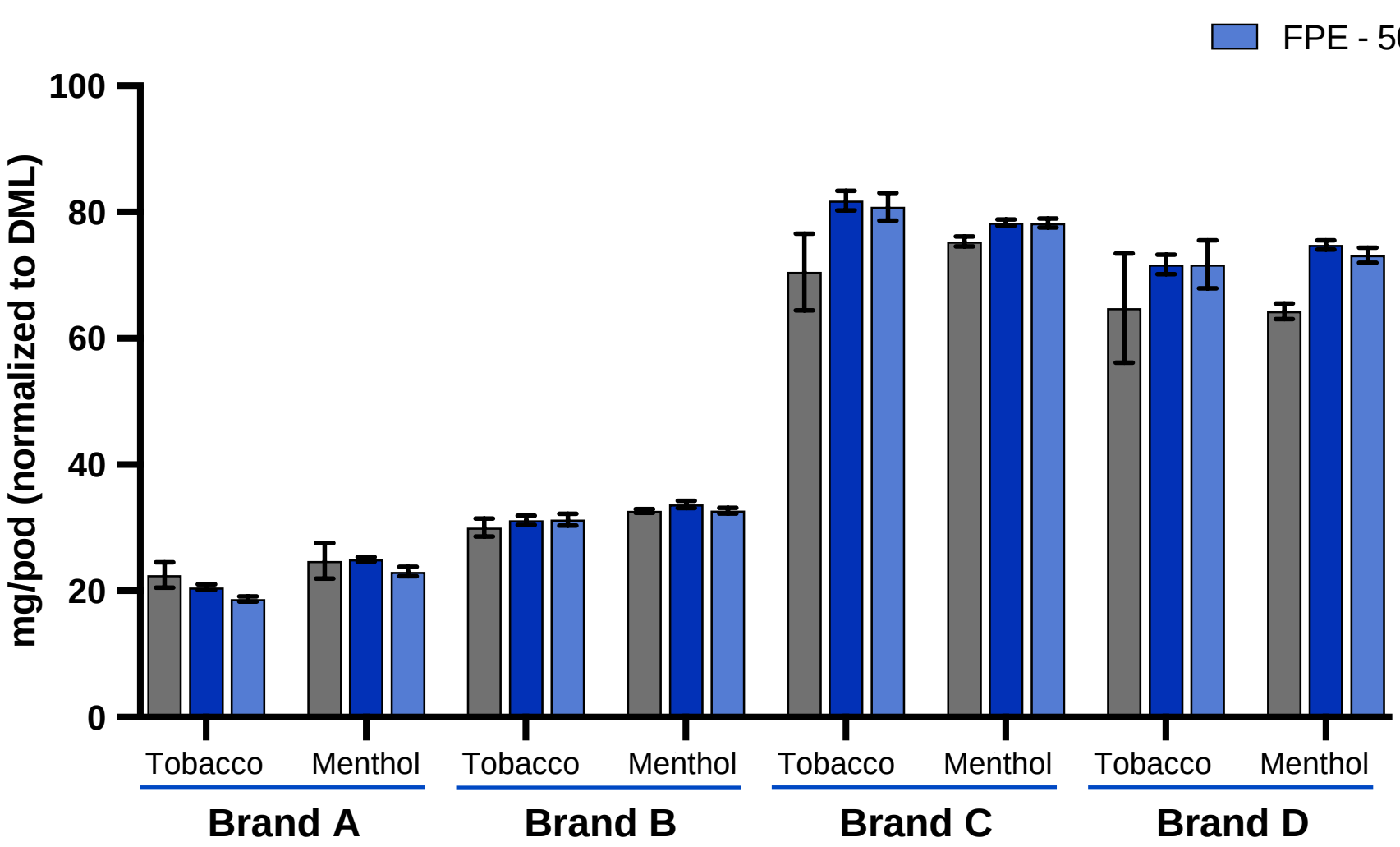
- Five replicates per collection

- 55/3/30 and 110/6/30 puff regimes (only 55/3/30 shown here)

- Data normalized to device mass loss, bars represent yield of analyte from a single pod

- Nicotine yield is expected to be linear over whole pod life

- FPE and WPE align well with WPM



Preliminary Data

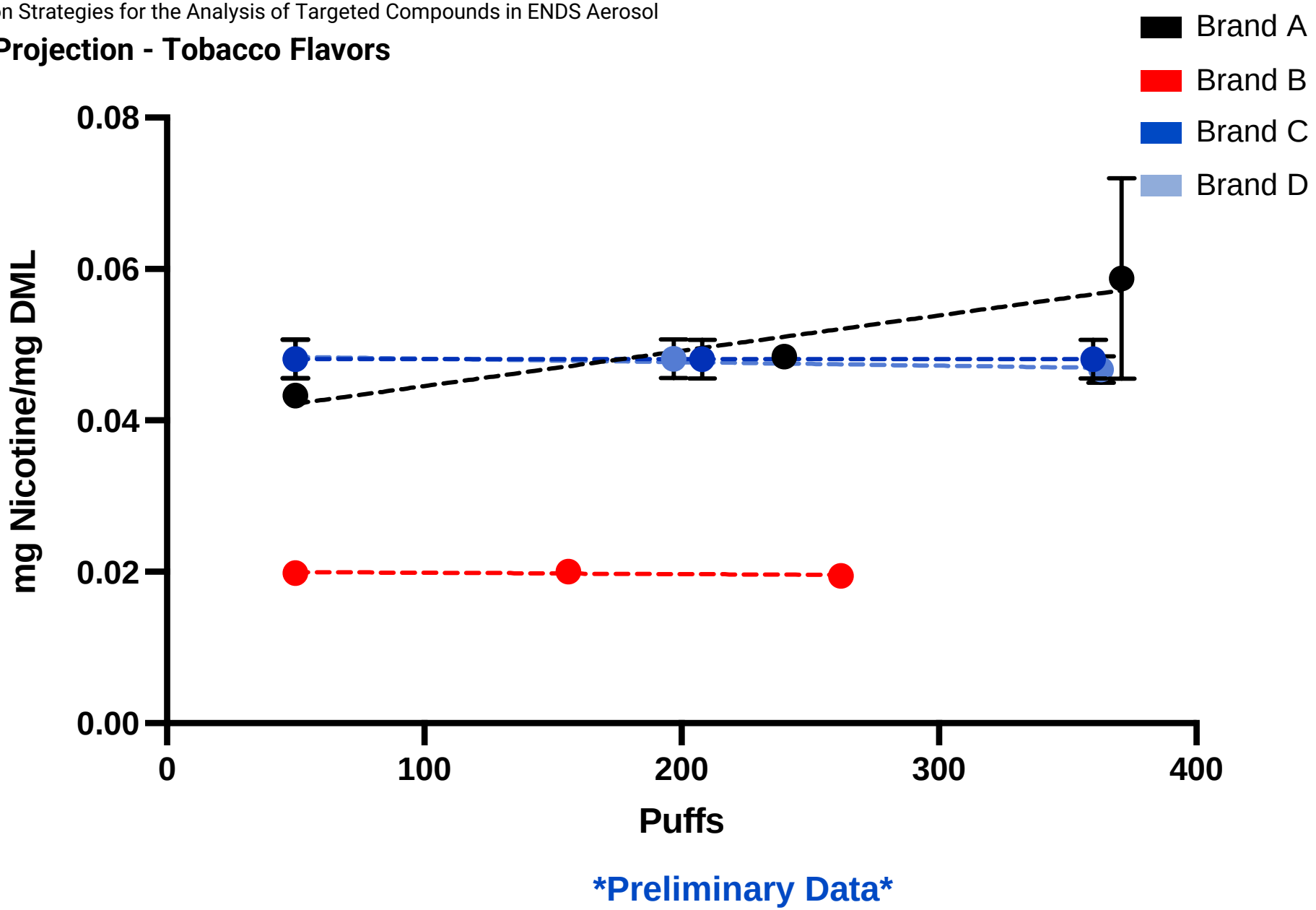
Nicotine Model Projection - Tobacco Flavors

- For WPE, linear fit is applied to determine the "slope" of change to yield over whole pod life

-For FPE, yield is assumed to be linear with slope = 0

- Beginning, middle and end puff blocks are linear, WPE is a good approximation

- Slopes are close to zero, FPE is a decent approximation

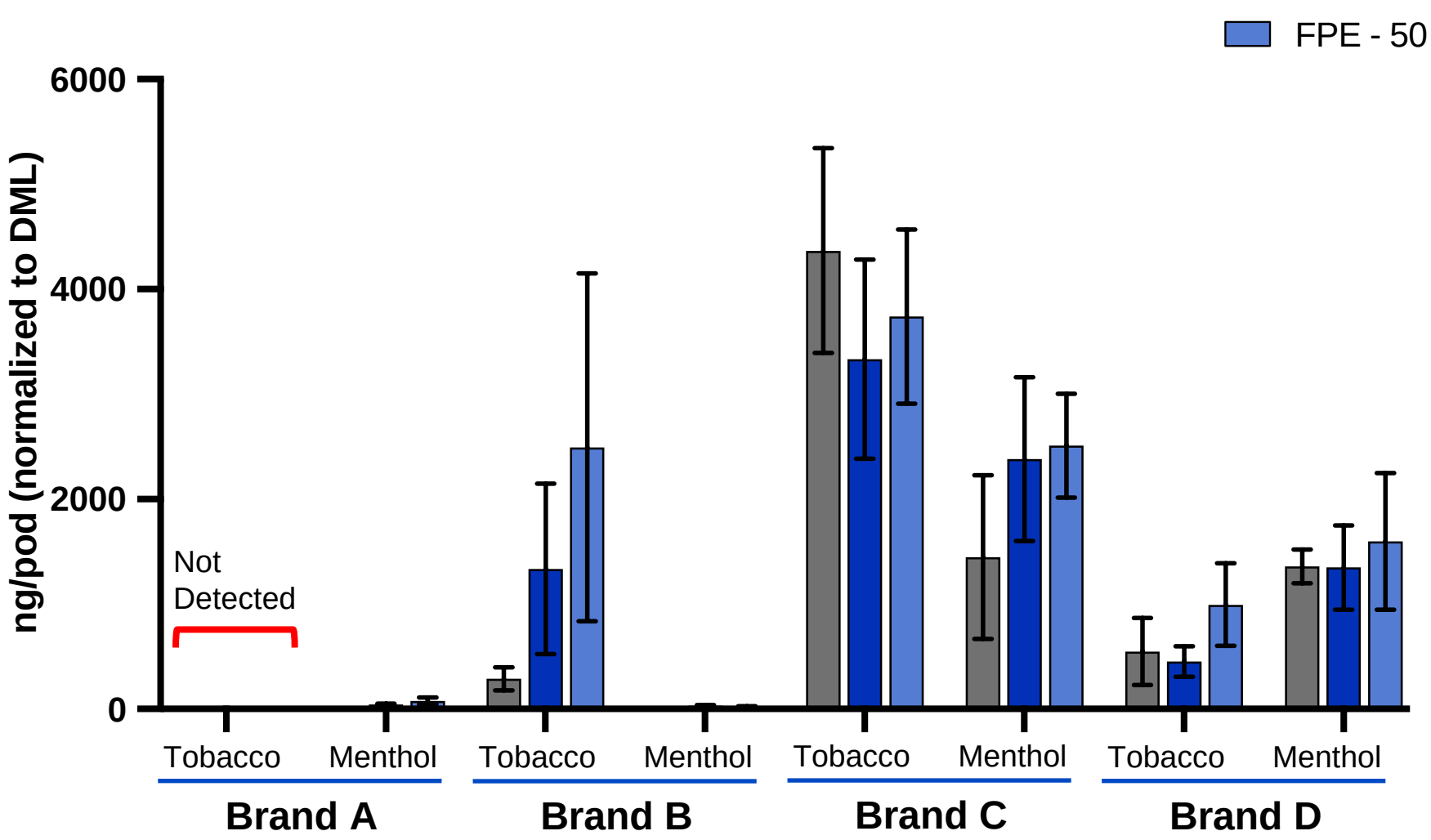


Preliminary Data

Nickel

- Nickel yields may decrease over pod life, depending on product

- FPE often over-estimates total exposure

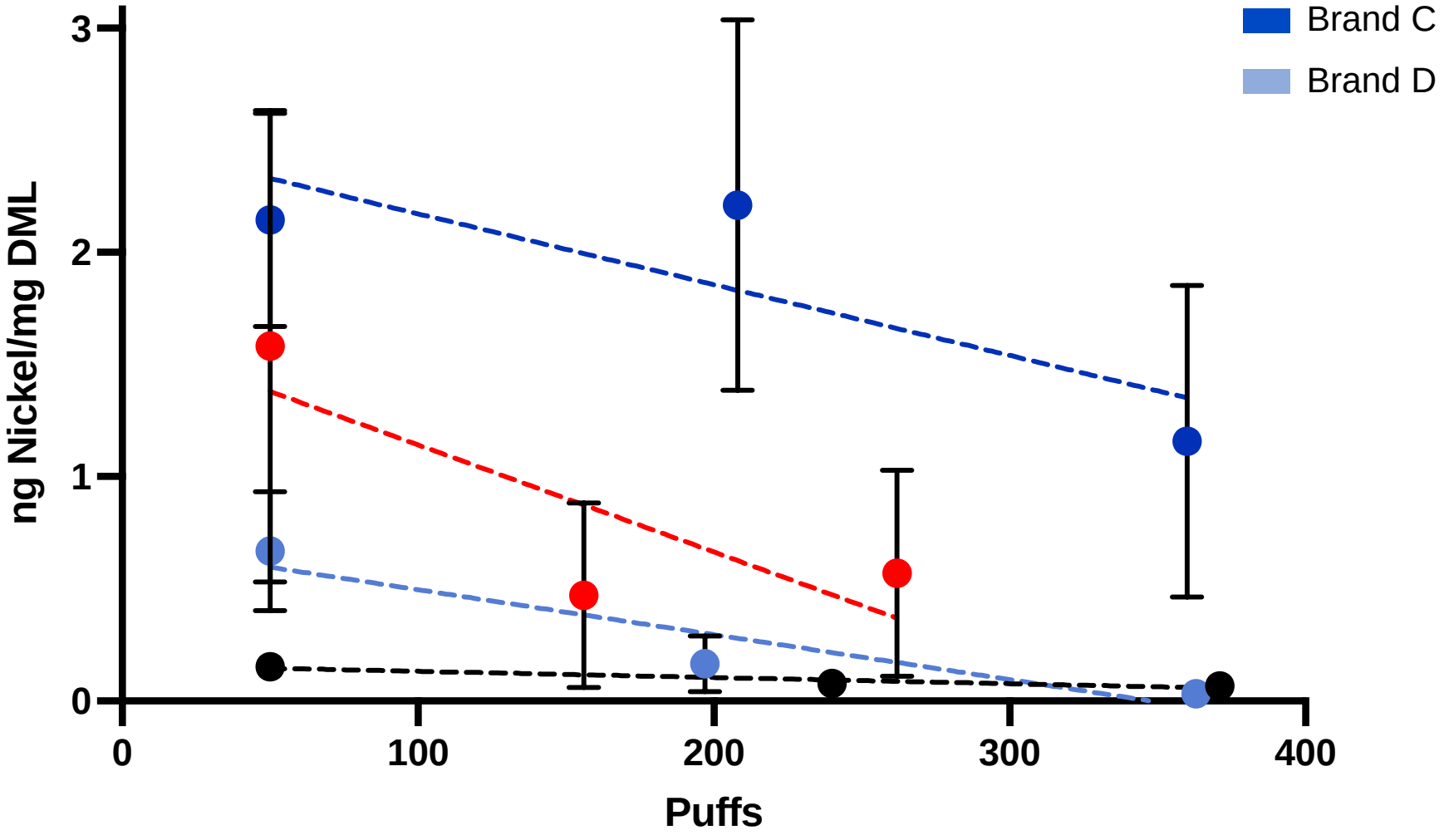


Preliminary Data

Nickel Model Projection - Tobacco Flavors

- Beginning, middle and end puff blocks are mostly within 1 standard deviation of linear, WPE can be a reasonable approximation

- Slopes are non-zero, FPE is often a poor approximation

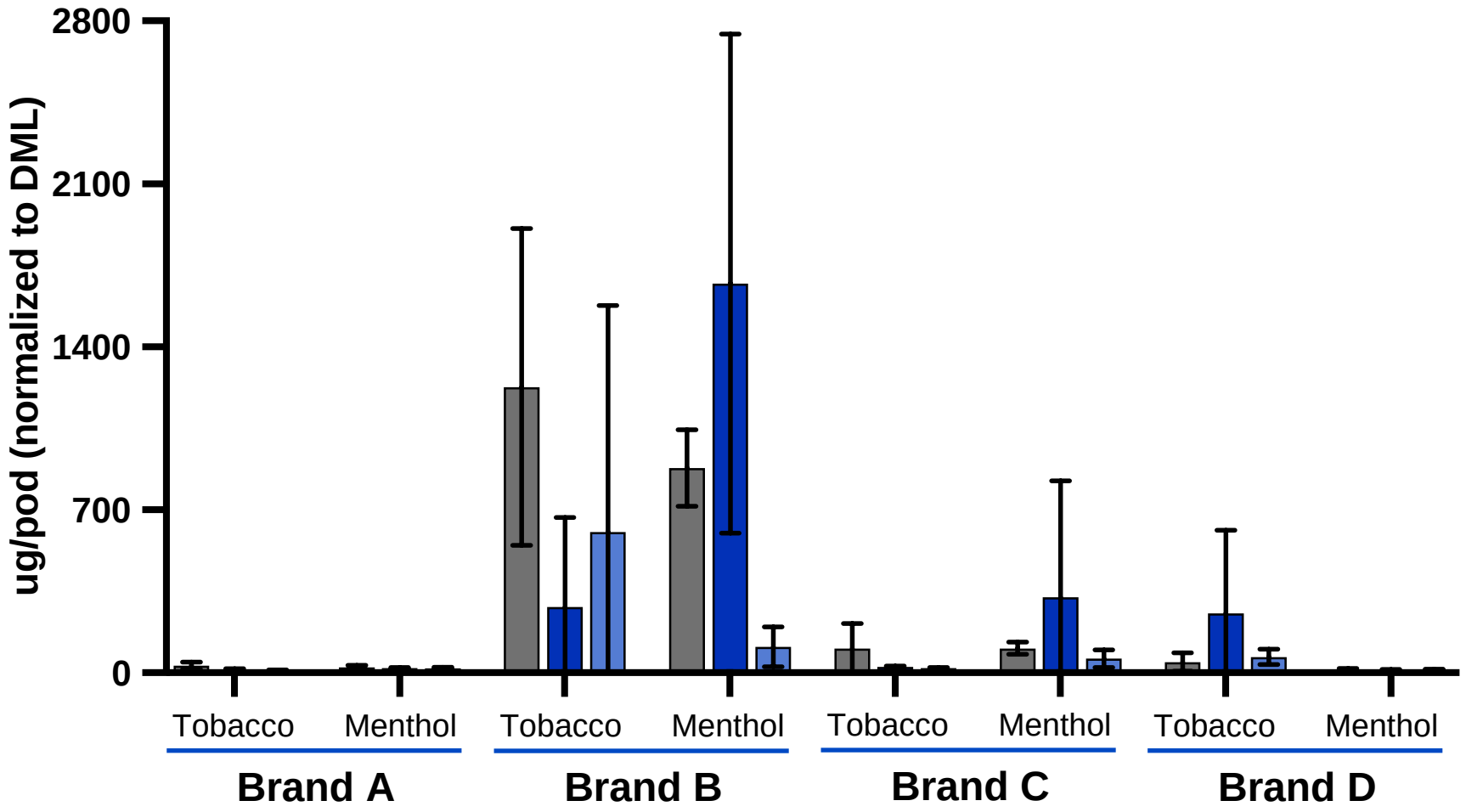


Preliminary Data

Formaldehyde

- Formaldehyde yield is not expected to be linear over whole pod life

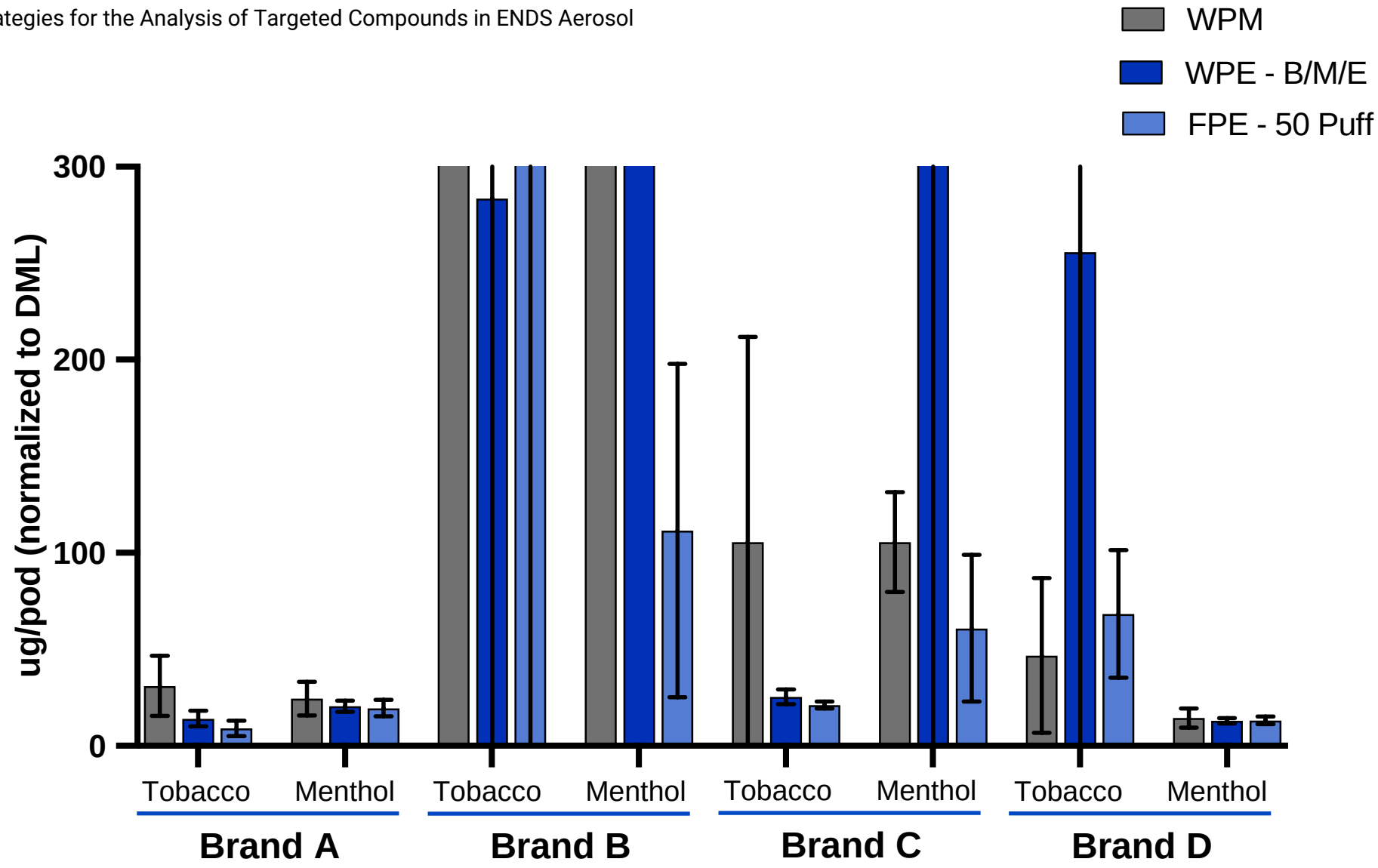
- High measurement SD was observed for several products, likely due to pod-to-pod variability



Preliminary Data

Formaldehyde

- Formaldehyde yield is not expected to be linear over whole pod life
- High measurement SD was observed for several products, likely due to pod-to-pod variability
- FPE is superior to WPE in several cases, due to very non-linear formaldehyde yield

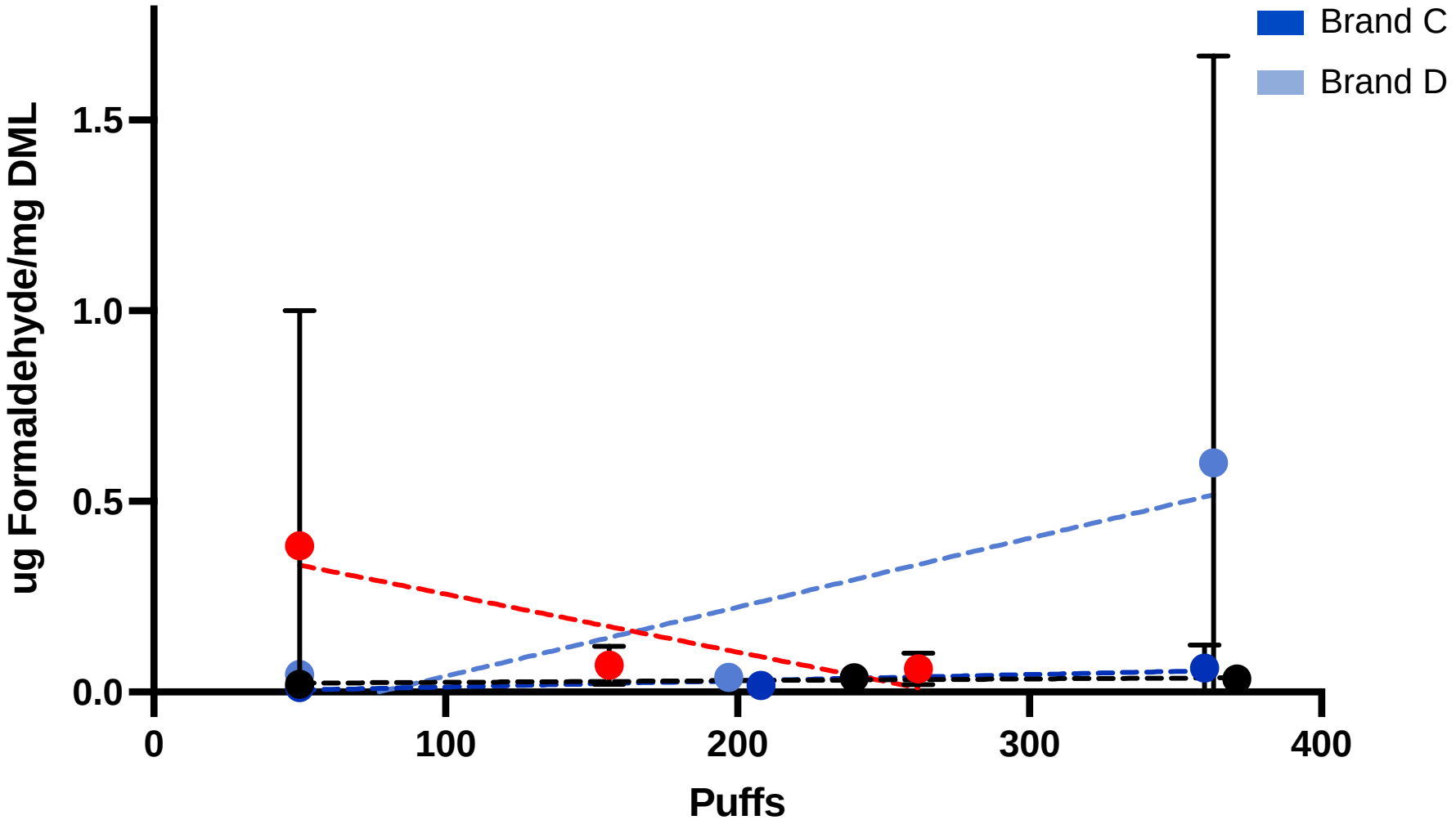


Preliminary Data

Formaldehyde Model Projection - Tobacco Flavors

- Beginning, middle and end puff blocks are not linear, WPE is a poor approximation

- Slope is ≠ 0, FPE is a poor approximation



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Formaldehyde Model Projection - Tobacco Flavors

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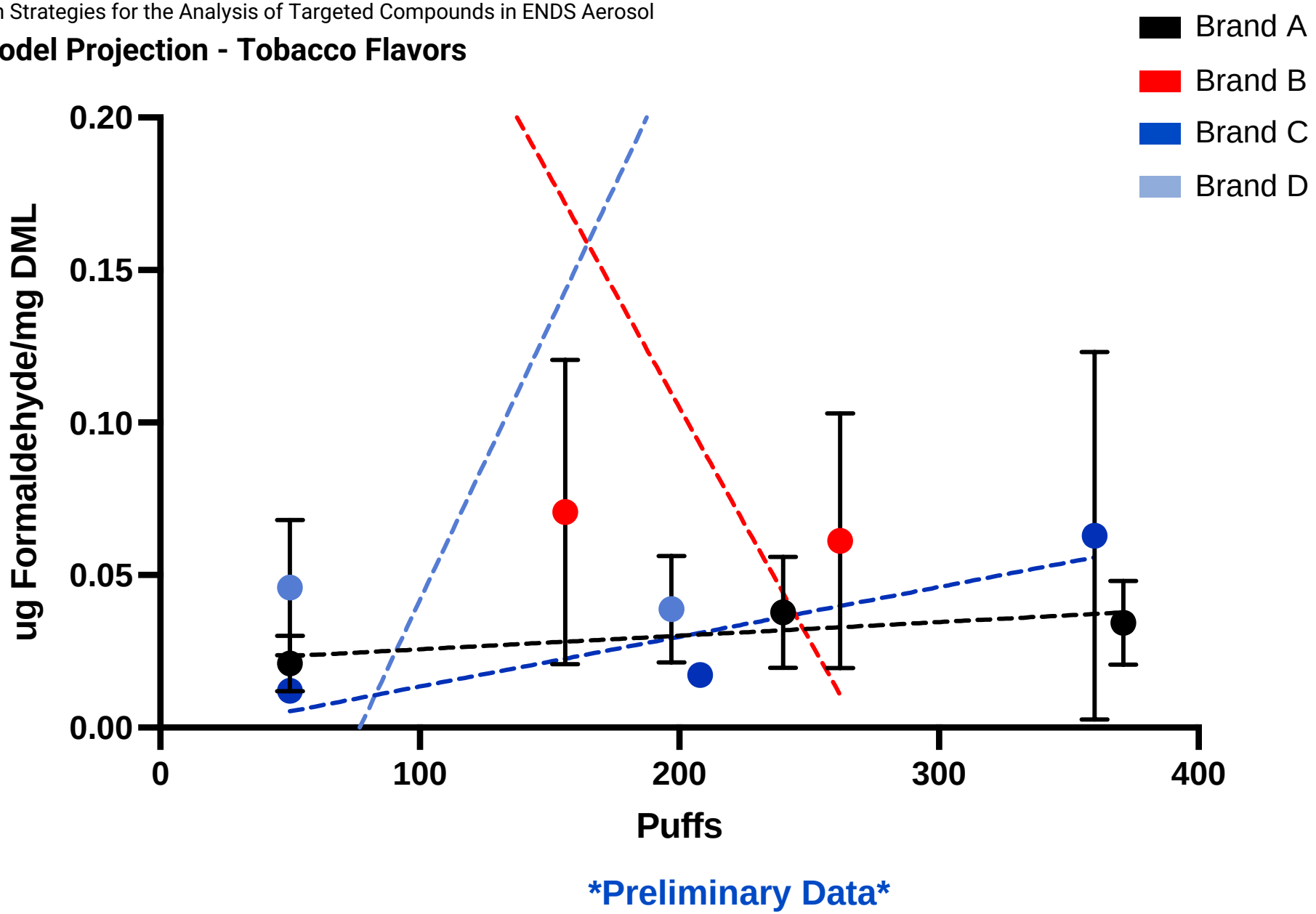
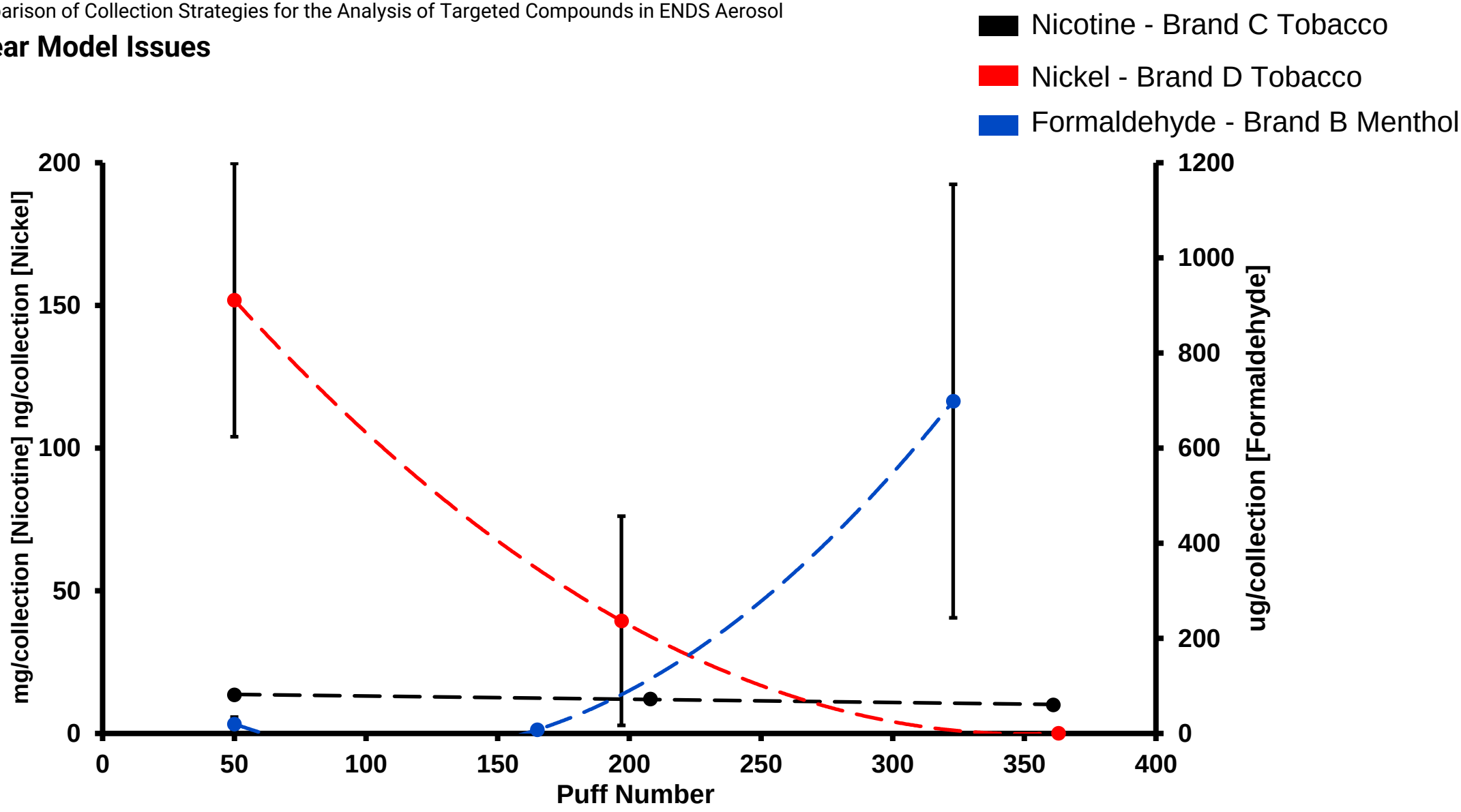


Preliminary Data

Linear Model Issues



Preliminary Data

Conclusions

FPE and WPE provide reasonable approximations for analytes whose yields are linear over pod life. However, only WPM is sufficient for determining user exposure to some non-linear or very low concentration analytes

Collection Strategies by Analyte Type

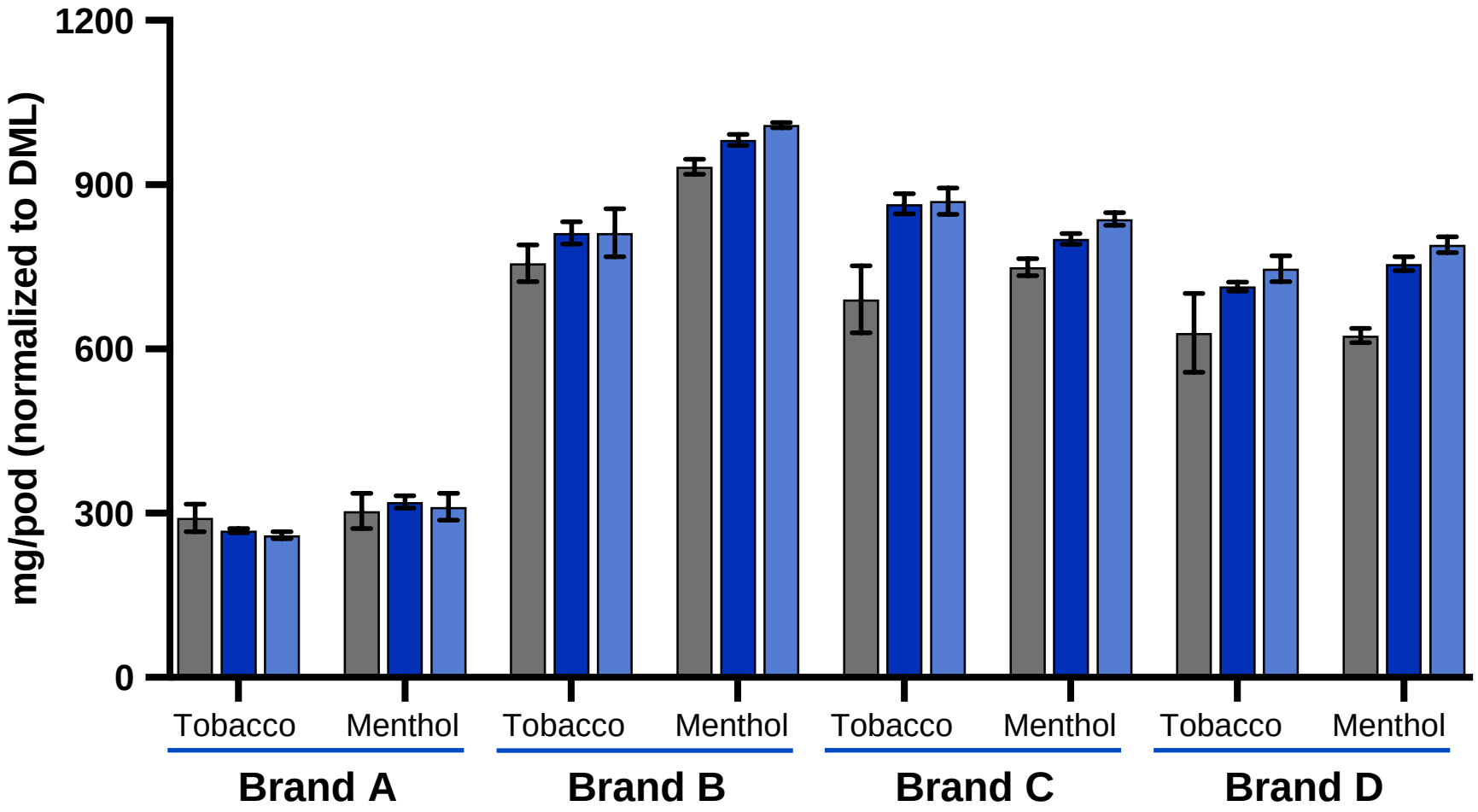
- **Primary Constituents**: Yields are linear with pod life, WPE, and often FPE, match well with WPM.
- **Metals**: Relationship of yield to pod life varies by analyte and product. Fifty puff model projections often overestimate whole pod yield.
- **Carbonyls**: Yields are not linear with pod life. Linear model projections generally underestimate true whole pod yield.

Supplementary Slides

Glycerol

- Glycerol yield is expected to be linear over whole pod life

- FPE and WPE align well with WPM



Preliminary Data

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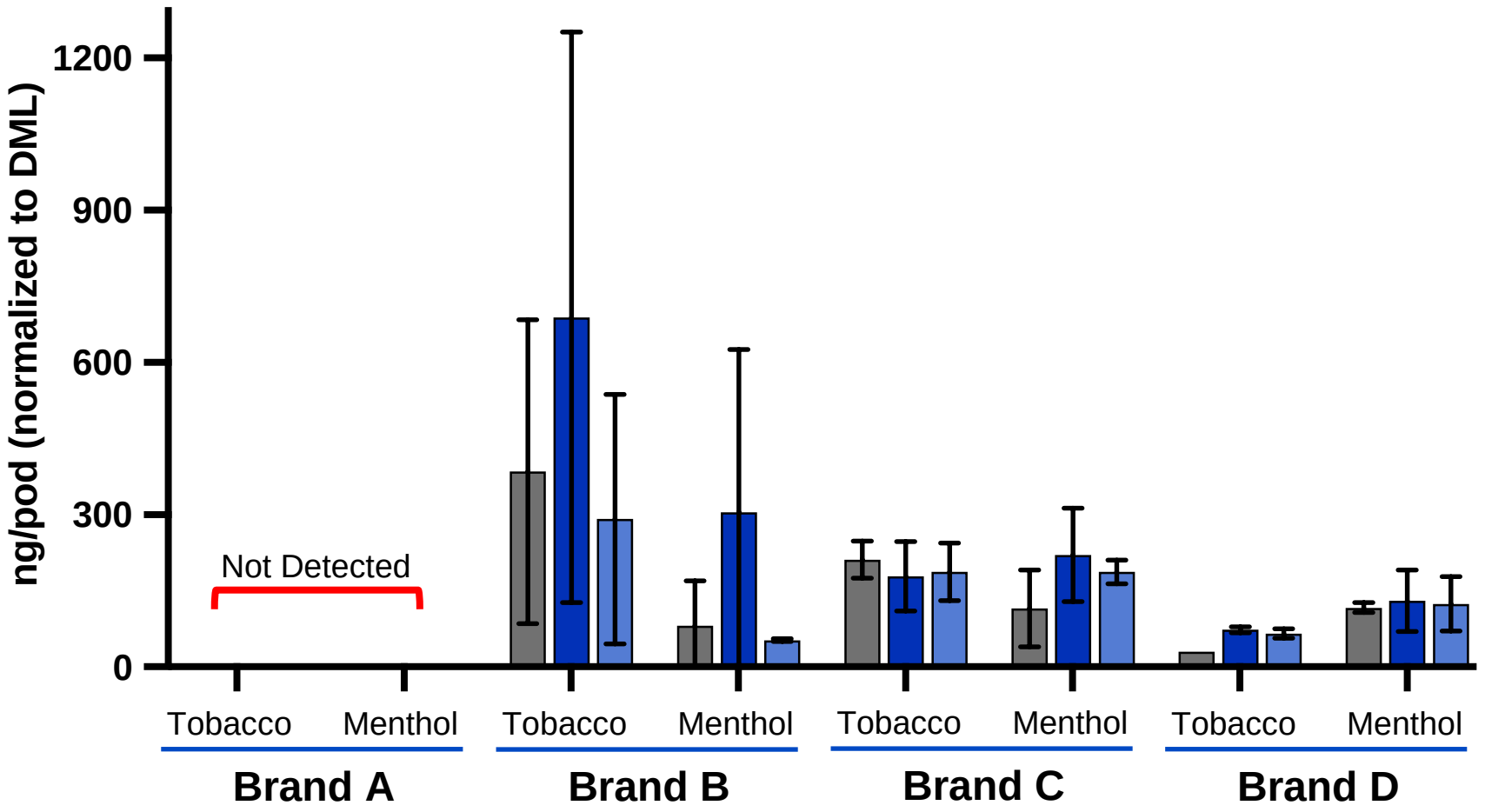
Chromium

- Chromium yields can obscured by method detection limits
- All 50 puff collections for Brands C and D were BLOQ
- Only Brand D Tobacco was BLOQ for whole pod collection

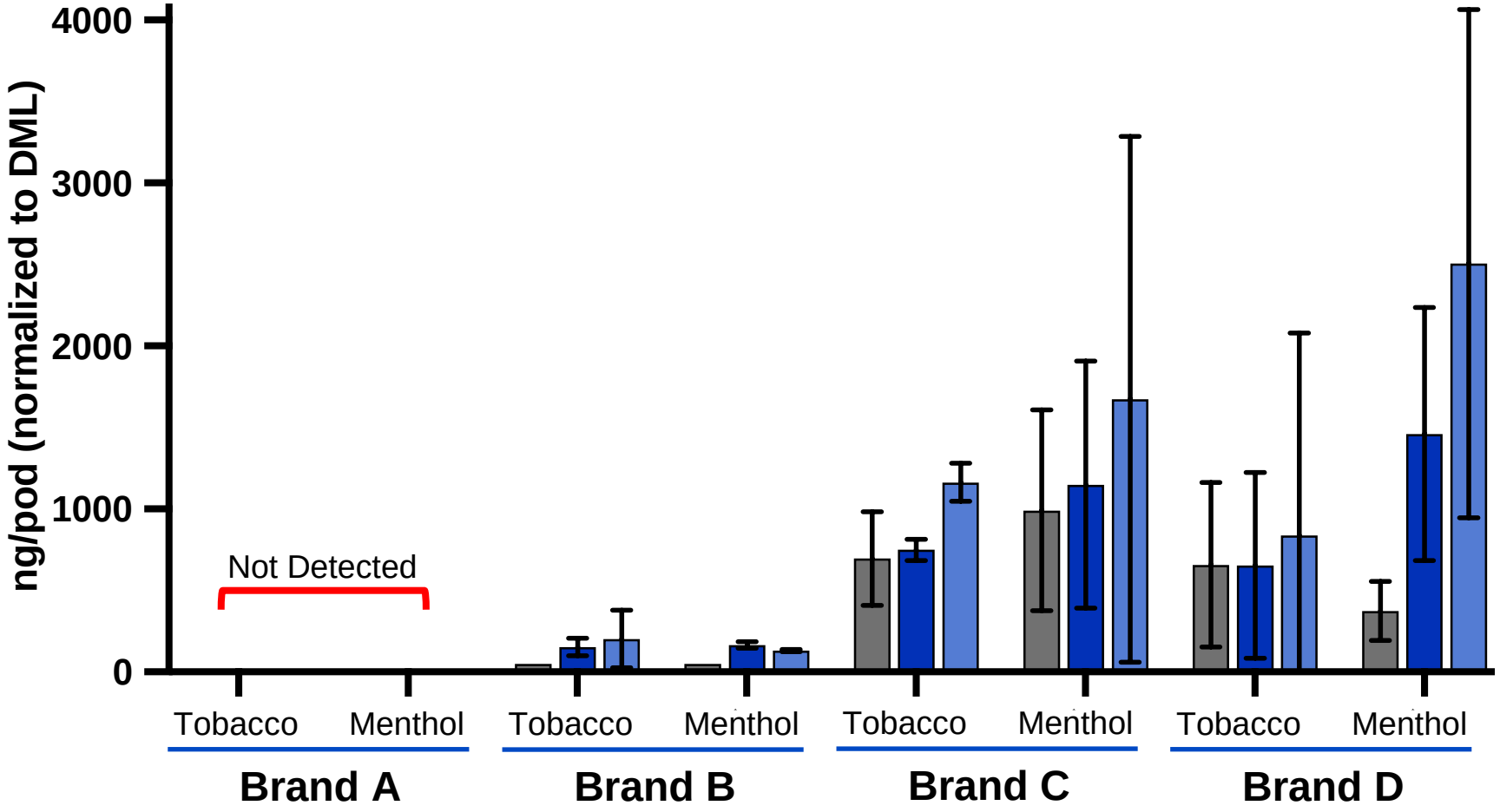


Preliminary Data

Copper

- Copper yields decrease over pod life

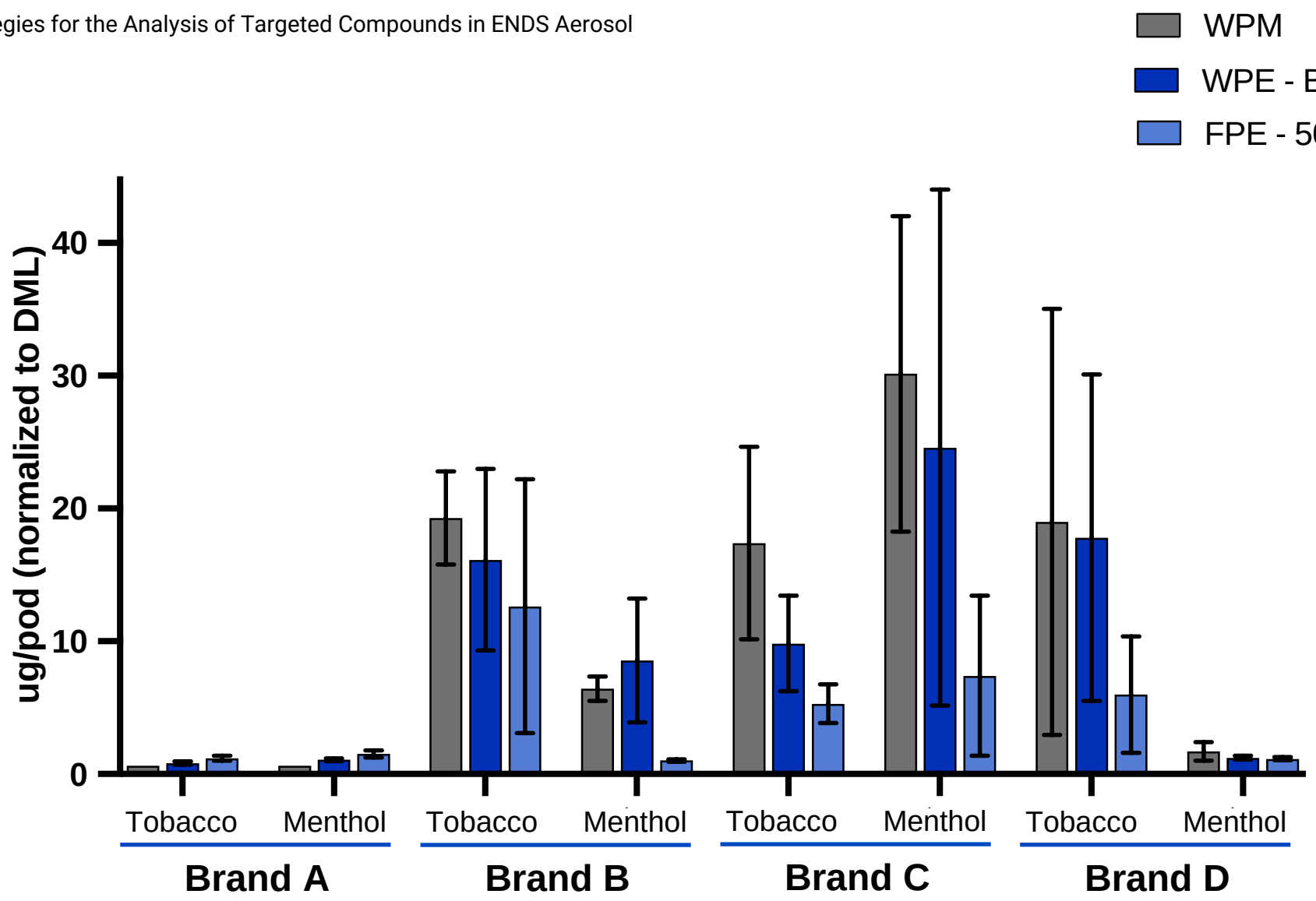
- WPE is superior to FPE for analytes that decrease linearly over pod life



Preliminary Data

Diacetyl

- Diacetyl yield is not linear over whole pod life
- First 50 puffs often BLOQ
- FPE underestimates diacetyl yield for most products
-WPE is generally below, but not statistically different from WPM



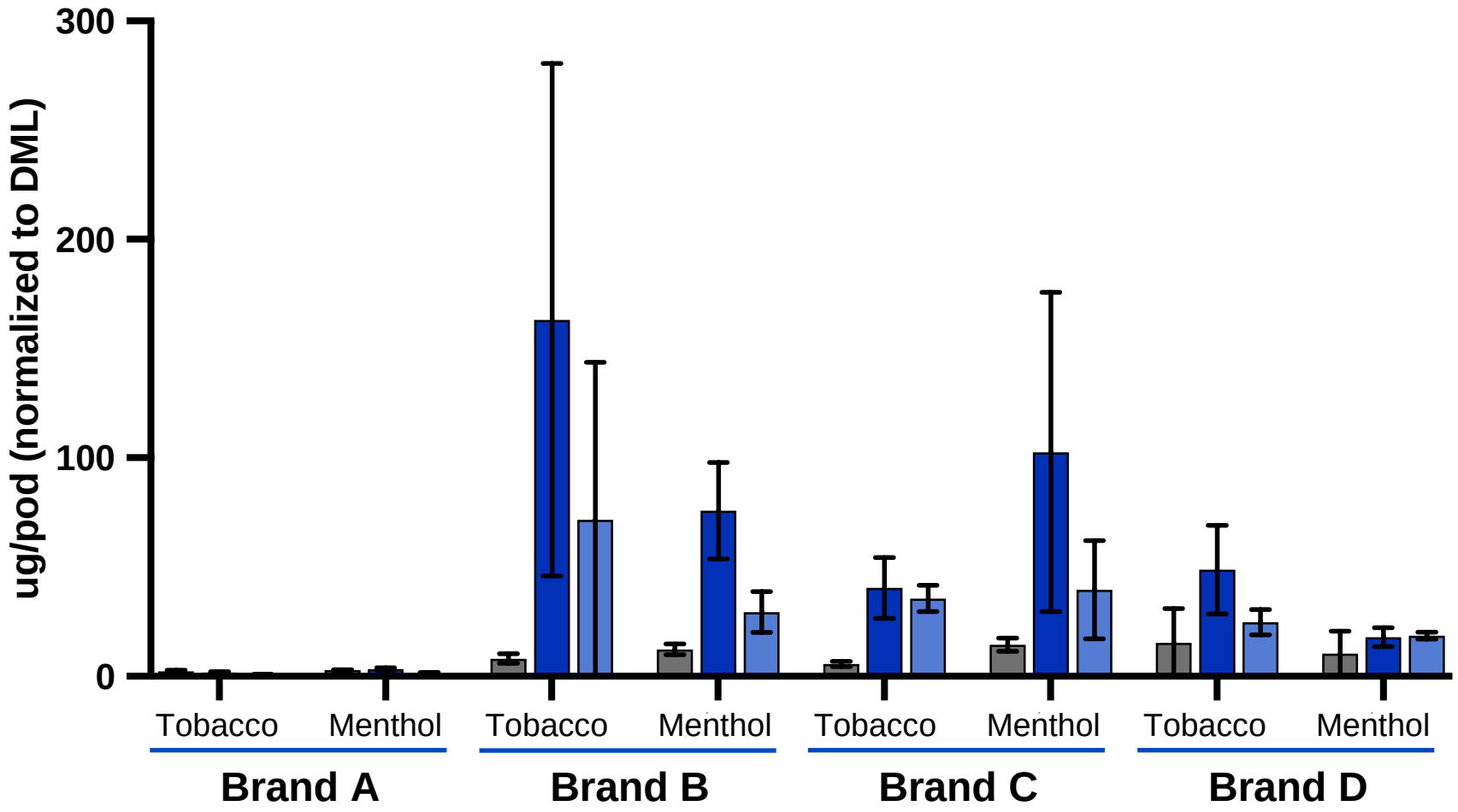
Preliminary Data

Glycidol

- FPE and WPE extrapolations give estimates greater than WPM

- Greater variability in FPE and WPE compared to WPM

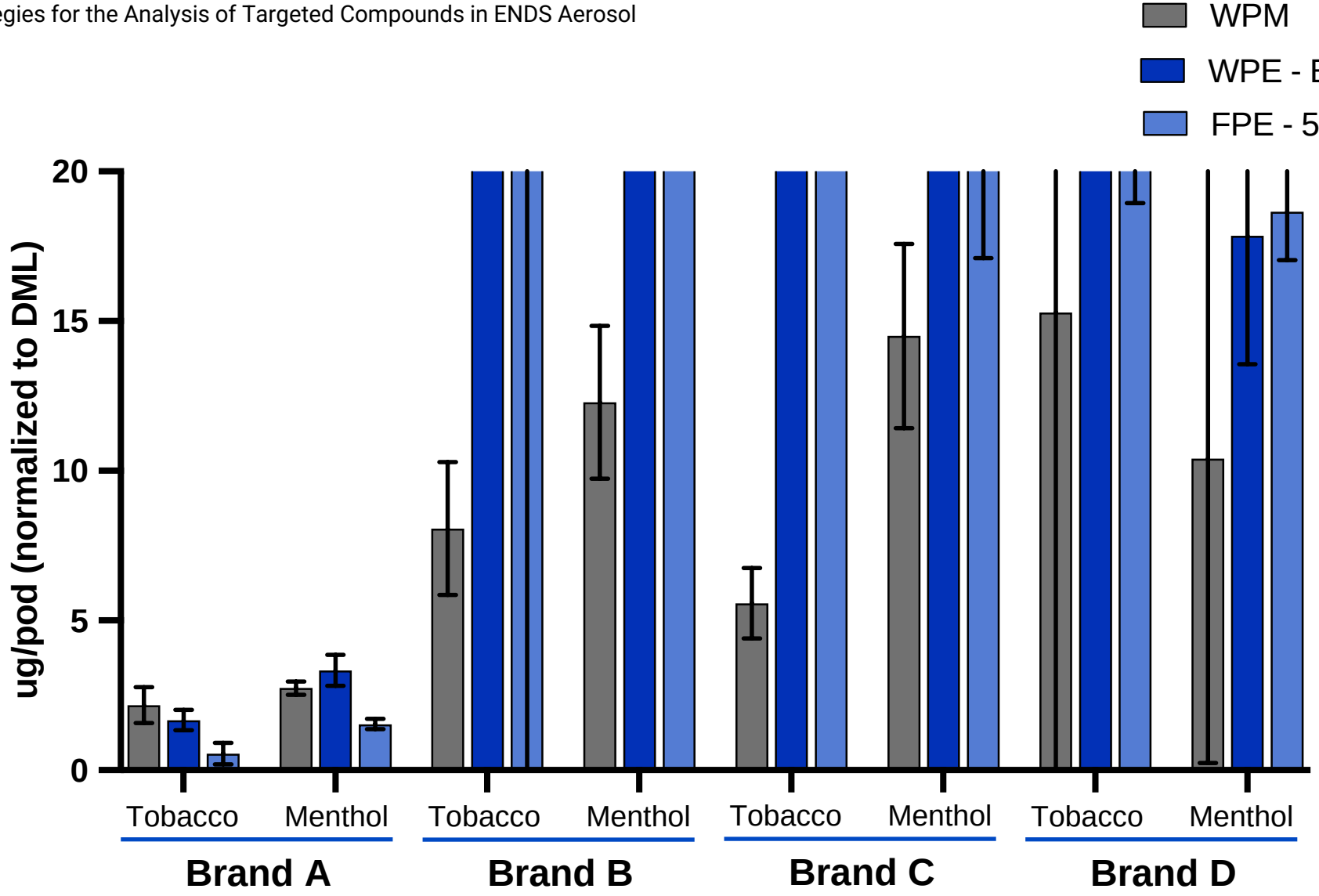
- More glycidol generated early in pod life for the majority of products



Preliminary Data

Glycidol

- FPE and WPE extrapolations give estimates greater than WPM
- Greater variability in FPE and WPE compared to WPM
- More glycidol generated early in pod life for the majority of products
- Brand A uniquely generates more glycidol later in pod life
- WPE is a good approximation for Brand A only

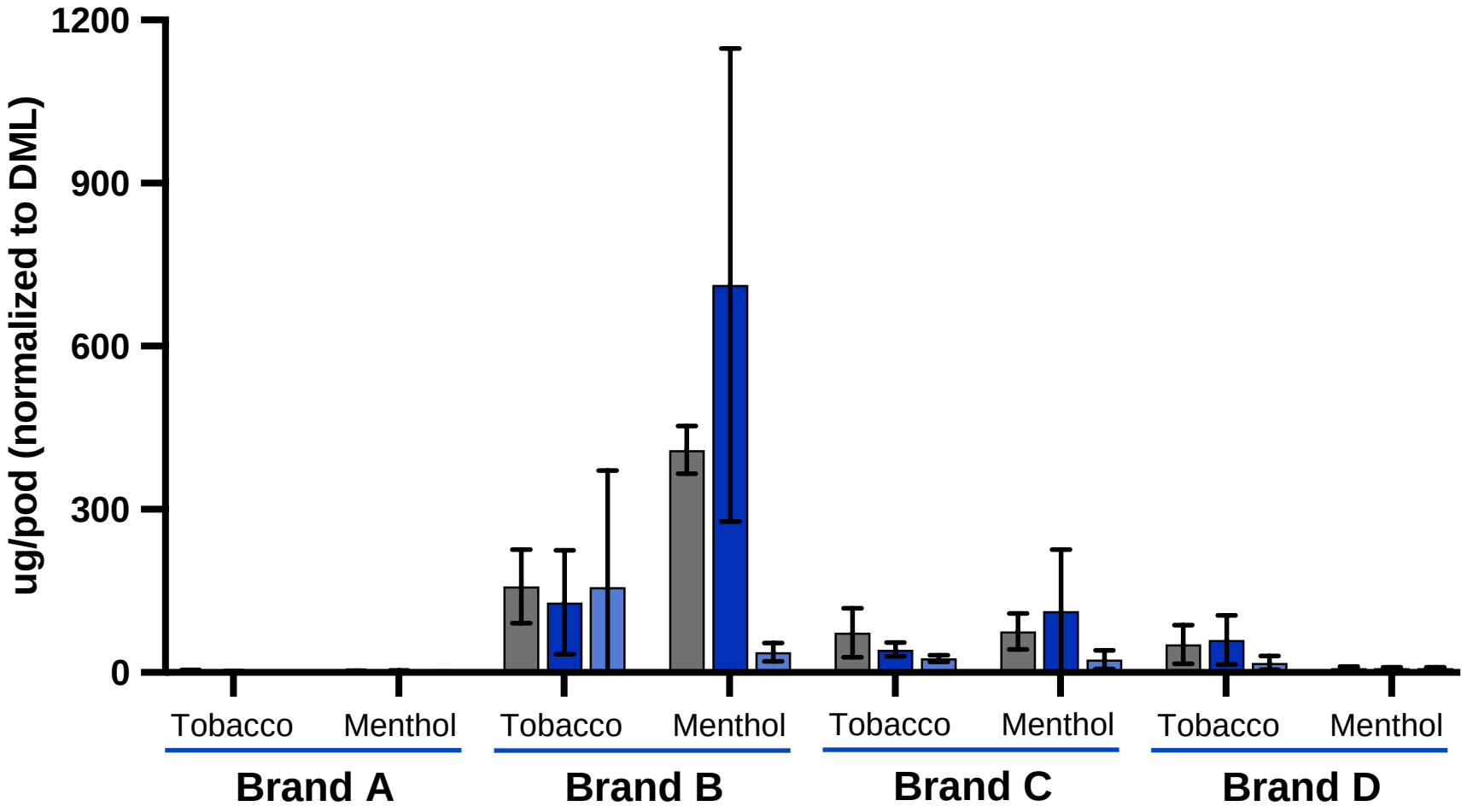


Preliminary Data

Acrolein

- Acrolein yield is not linear over whole pod life

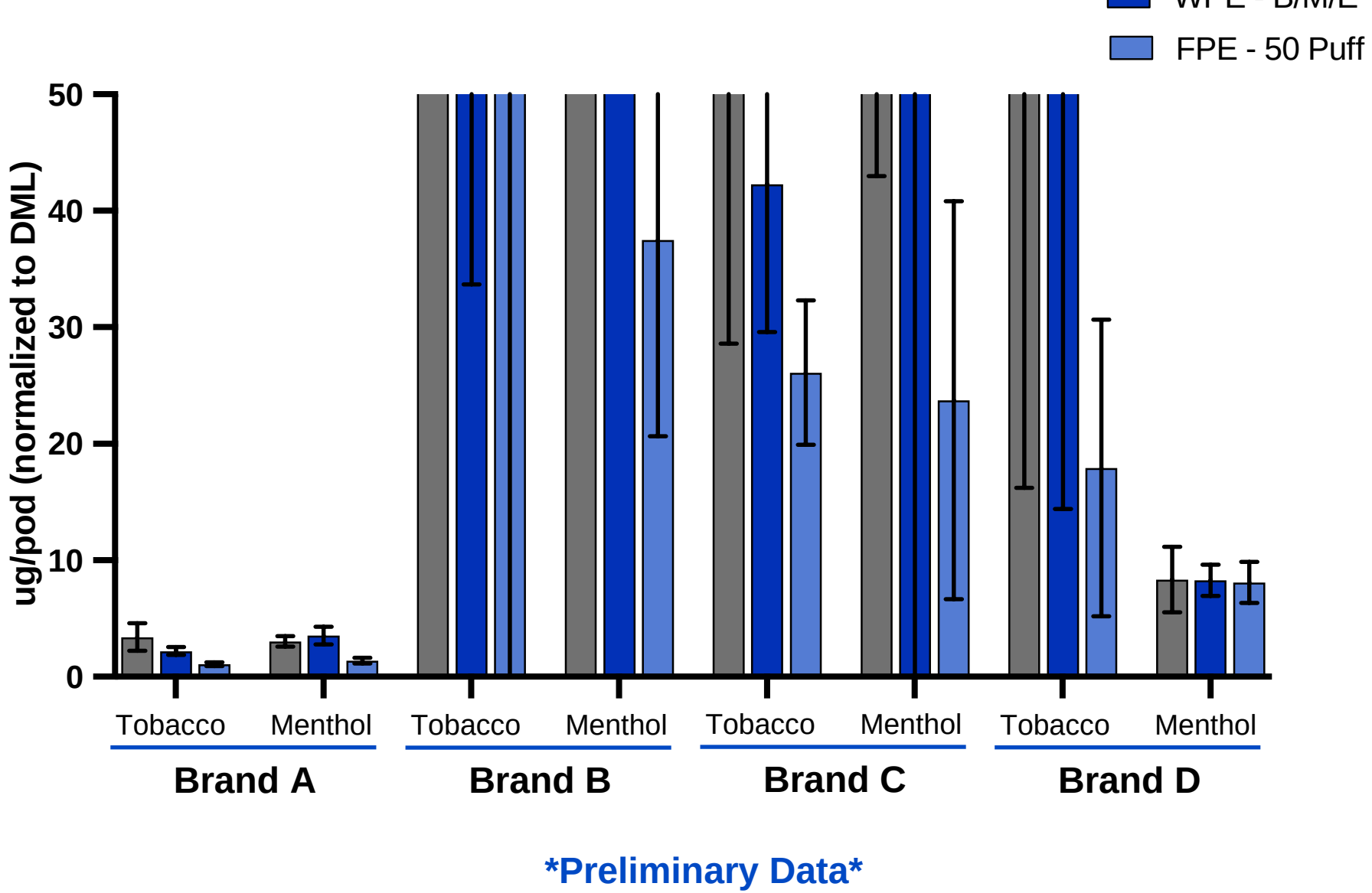
- FPE underestimates Acrolein yield for most products



Preliminary Data

Acrolein

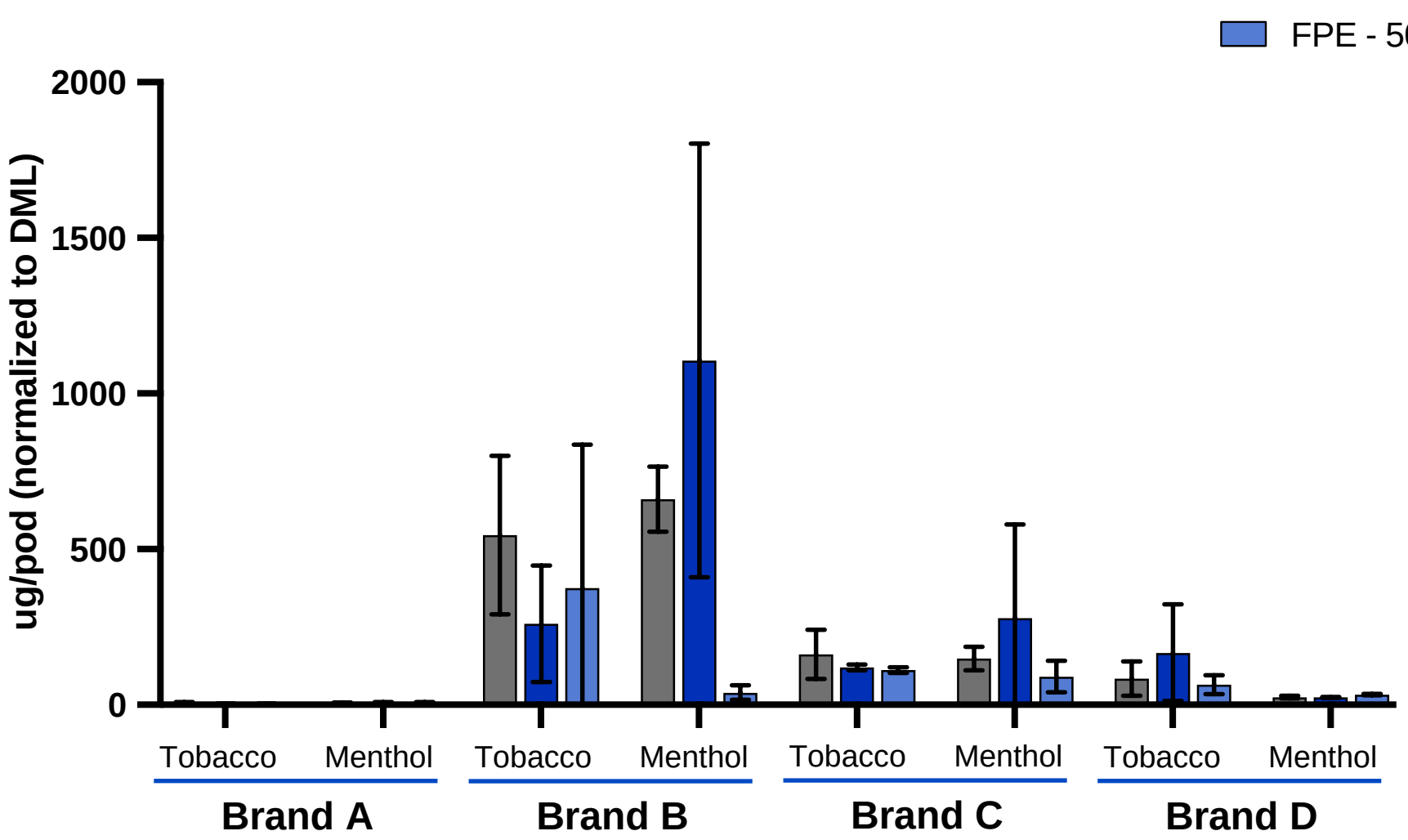
- Acrolein yield is not linear over whole pod life
- FPE underestimates acrolein yield for most products
- Brand A acrolein yield is BLOD for first 50-puff collection



Preliminary Data

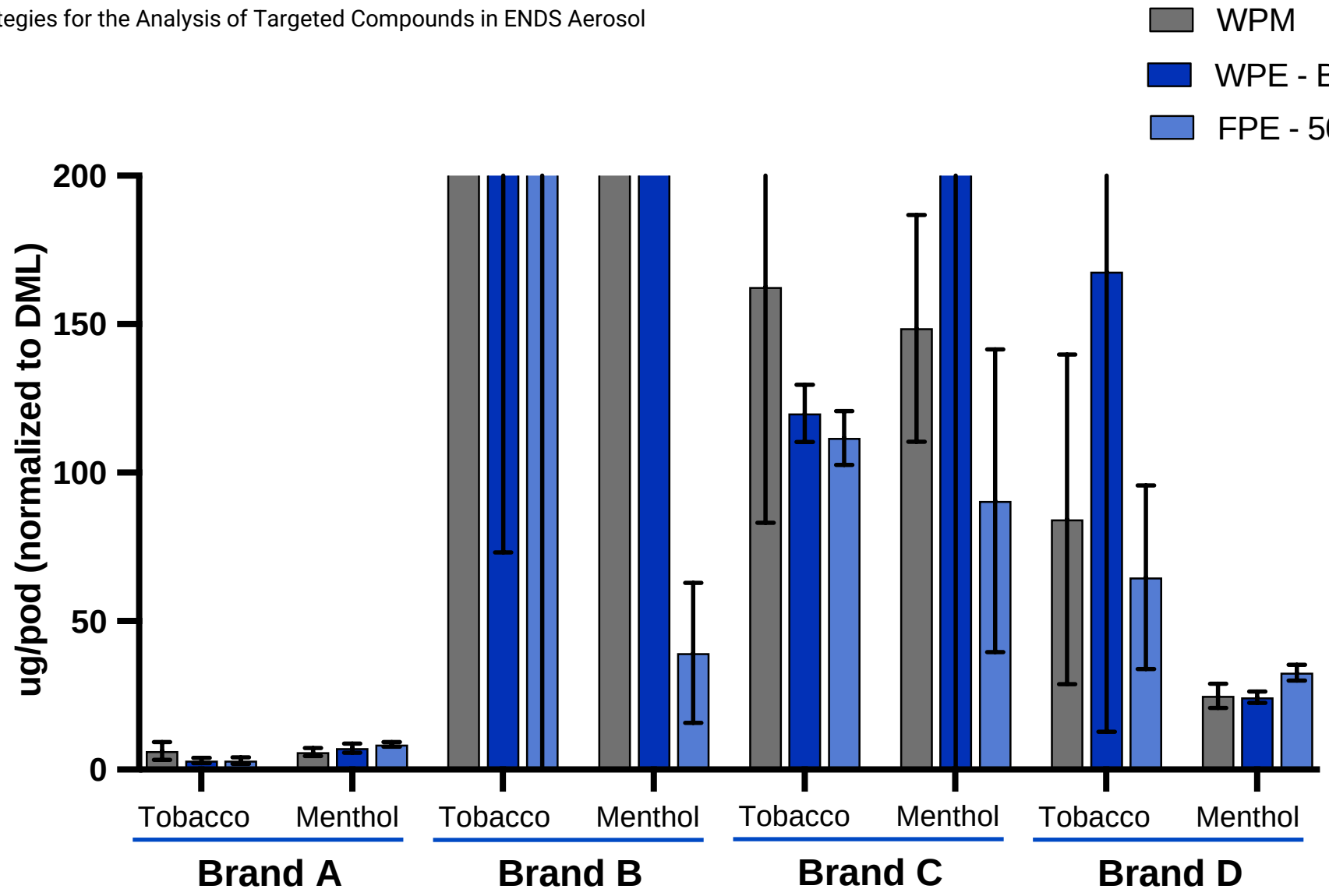
Acetaldehyde

- Brand B Menthol model projections for acetaldehyde whole pod yield are particularly poor



Preliminary Data

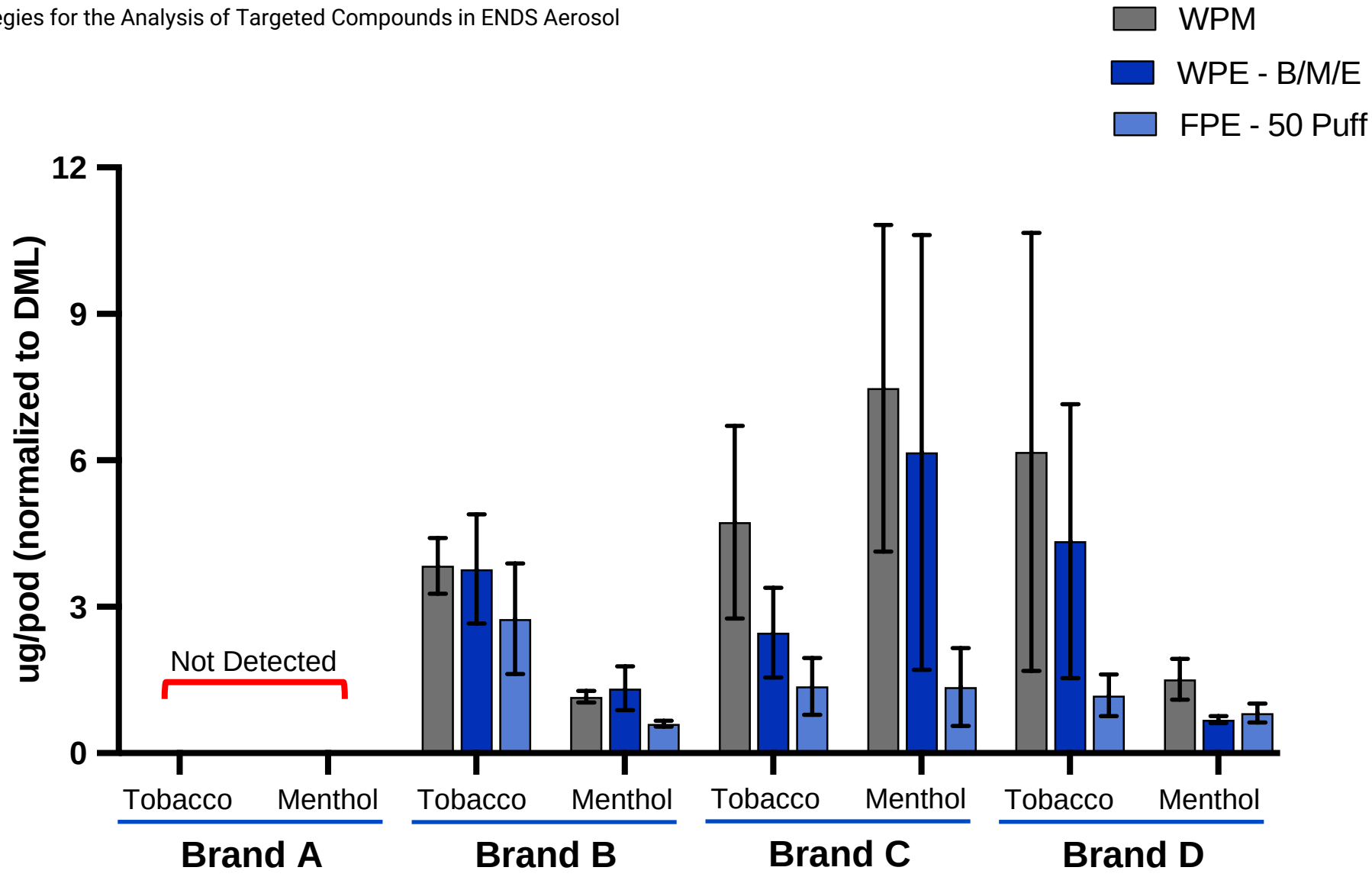
Acetaldehyde



Preliminary Data

Acetyl Propionyl

- WPE is superior to FPE in most cases
- Acetyl propionyl yields are frequently BLOD or BLOQ in 50 puff measurements
- WPM increases method sensitivity for low concentration analytes



Preliminary Data