

Comment on "Cocktail Chromatography: Enabling the Migration of HPLC to Nonlaboratory Environments"

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Welch et al.¹ recently described the use of distilled alcohol spirits as an economical and green alternative to

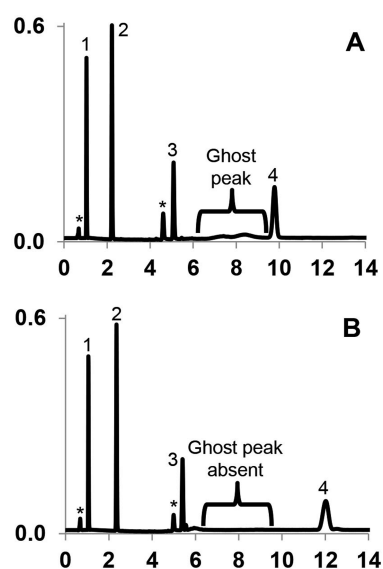


Figure 1. Comparison of the gradient separation of four analytes (A) before and (B) after Brita filtration. Chromatographic conditions: column, Zorbax Eclipse XDB C8 (4.6 mm × 150 mm, 5 μ m); eluents, A = deionized water, B = Smirnoff vodka, or 3× Brita filtered Smirnoff vodka, 20% to 100% B in 5 min then hold 9 min; 1.5 mL/min; analytes, 0.1 mg/mL of (1) uracil, (2) caffeine, (3) 1-phenylethanol, and (4) butyl paraben in 20% EtOH; 65 °C; 215 nm. * indicates analyte impurities.

traditional HPLC solvents. While the authors demonstrated the effectiveness of this approach, there are several factors related to chromatographic performance that the authors undersold or did not adequately address.

(1) **Gradient Peak Widths of Separation with Grain Alcohol vs HPLC Grade Ethanol:** In Figure 3 of the paper,¹ it appears that use of grain alcohol caused an increased peak width. We replicated their separation and found that the peak widths were actually equivalent for grain alcohol vs HPLC grade ethanol.

(2) **Backpressure Penalty of Ethanol:** Aqueous ethanol mixtures have significantly higher viscosity than traditional HPLC solvents.² Under the authors' conditions,¹ the backpressure was 3700–4200 psi for the HPLC ethanol and grain alcohol eluents. These pressures are within the maximum operating limits of most HPLC instruments but above the typical 3000 psi method development target.

(3) **Choice of Vodka Brand and Ghost Peaks:** The authors evaluated one brand of each type of spirit.¹ We evaluated seven brands of vodka and found the Smirnoff used by the authors had the highest ultraviolet absorbance (i.e., more impurities). The presence of such impurities increase the likelihood of solvent ghost peaks appearing in a gradient separation.³ These ghost peaks can confound chromatographers due to their variable nature (size depends on equilibration time).³ Such a peak was observed in Figure 3 of the original paper¹ (baseline hump at 7.7 min for vodka at 60 °C). When we replicated this separation, we observed two ghost peaks (Figure 1A).

The quality of "cheaper" vodka may be improved by filtration through several Brita filters.⁴ Hence, we sequentially filtered the Smirnoff (\$24.68/L) through three Brita filters (\$8 each). The Brita filtrations eliminated the ghost peaks (Figure 1B). However, the retention of all compounds in Figure 1B increased, suggesting the filters may adsorb some ethanol from the vodka.

Alternatively, one could use a more premium brand of vodka. We found that unfiltered Absolut (\$28.43/L) and Ketel One (\$36.53/L) vodka, with reasonable cost and less manual preparation, yielded chromatograms without any ghost peak.

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Notes

The authors declare no competing financial interest.

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REFERENCES

- (1) Welch, C. J.; Nowak, T.; Joyce, L. A.; Regalado, E. L. Cocktail chromatography: enabling the migration of HPLC to nonlaboratory environments. *ACS Sustainable Chem. Eng.* 2015, 3 (5), 1000–1009.
- (2) Sandra, P.; Sandra, K.; Pereira, A.; Vanhoenacker, G.; David, F. Green chromatography. Part 1: introduction and liquid chromatography. *LC-GC Eur.* 2010, 23 (5), 242–259.
- (3) Sadikin, S.; Zhang, D. D.; Inloes, R.; Redkar, S. Ghost peak investigation in a reversed-phase gradient LC system. *LC-GC North Am.* 2011, 29 (5), 394–400.
- (4) Mythbusters. Top Shelf Vodka Myth. Originally aired April 29, 2006.

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