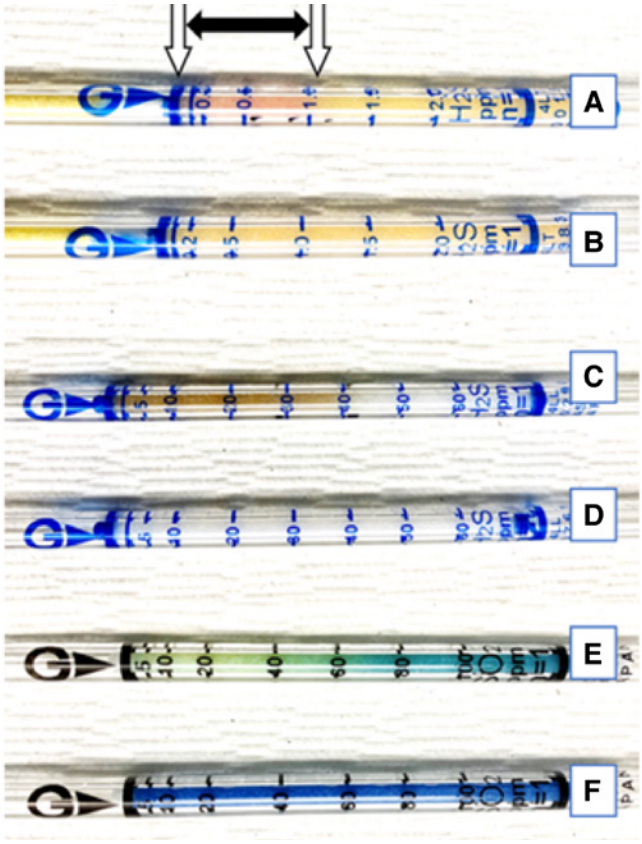
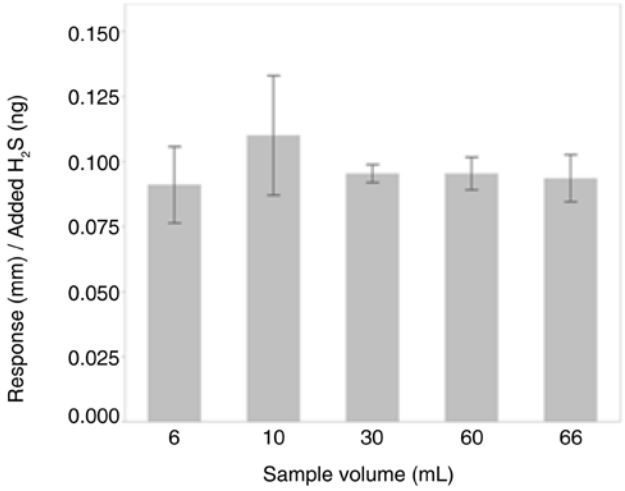
catalyst discovery into practice

Supplemental Data for:

Allison RB, Montgomery A and Sacks GL. 2021. Analysis of free hydrogen sulfide in wines using gas detection tubes. Catalyst 6:1-8. doi: 10.5344/catalyst.2021.21003.



Supplemental Figure 1 Color change in Gastec 4LT (**A**, **B**), 4LL (**C**, **D**), and 5L (**E**, **F**) gas detection tubes, showing tubes before (**B**, **D**, **F**) and after (**A**, **C**, **E**) use.



Supplemental Figure 2 The response of the gas detection tube method (mm stain/ng hydrogen sulfide [H_2S]) with changing sample volume. Measurements were performed by the N_2 Method, and samples are prepared in both model wine and water. The response did not differ significantly (analysis of variance, $p > 0.05$) as a function of sample volume.

Supplemental Video 1 Analysis of Free Hydrogen Sulfide in Wines Using Gas Detection Tubes

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Supplemental Calculation

Theoretical mass of hydrogen sulfide (H_2S), as determined from 4LT gas detection tube (GDT) concentration markings (length of color change in mm to ng).

4LT mm markings	4LT concentration markings (ppm)	4LT markings (mol equivalent)	4LT (ng)
7	0.5	2.1E-09	69.9
14	1.0	4.1E-09	139.9
21	1.5	6.2E-09	209.8
28	2.0	8.2E-09	279.8
35	-	1.0E-08	349.7

Conversion from "ppm" to "ng" for the manufacturer calibrated quantity of gas on the 4LT GDT, using the Ideal Gas Law, $PV = nRT$.

Volume (V) = 0.1 L, Pressure (P) = 1 bar, Ideal gas constant (R) = 0.083144598 L bar/mol K, Temperature (T) = 293 K, Moles in 0.1 L of gas (n) = 0.004105 mol

Definition of "ppm" = moles of H_2S/1,000,000 moles of gas.

(a)	1 ppm =	1 mol H_2S/1,000,000 moles gas
(b)	1 ppm =	4.10E-09 mol H_2S/0.004105 mol gas
(c)	1 ppm =	139.9 ng H_2S

The concentration markings in ppm on the GDT were reported with their corresponding length of color change in mm. Then, the ppm markings were converted into moles and mass of H_2S because the tubes are calibrated to measure concentration in 100-mL gas samples. Moles of gas corresponding to a 100-mL gas sample were calculated assuming the Ideal Gas Law under the indicated conditions.

A sample containing 1 mol H_2S in 1,000,000 mol gas should correspond to the "1 ppm" mark on the GDT (a). Therefore, a 100-mL sample containing 0.004105 mol gas and producing "1 ppm" on the GDT would contain 0.004105/1,000,000 = 4.10E-0.9 mol of H_2S (b).

Finally, moles of H_2S required to get a "1 ppm" mark on the GDT is converted to mass using the molecular weight of H_2S (34.076 g/mol); this is the total mass of H_2S that has been measured on the tube up to that mark (c). Using the amount of H_2S calculated for "1 ppm", the value is scaled to get the mass of H_2S for all ppm markings and their corresponding mm measurements, giving the theoretical relationship

$$H_2S\ (ng) = 10.0 \times mm\ on\ 4LT.$$