

SUPPORTING INFORMATION



FIGURE S 1: PASSIVE SAMPLER

SHS	
Incubation	10 min, 65°C, with agitation
Injection volume	0.8 ml
TD	
Dry purge	N ₂ , 3 min, 50 ml.min ⁻¹
Primary desorption	10 min, 280°C, 80 ml.min ⁻¹ , 30 ml.min ⁻¹ split
Secondary desorption	1 min purge, 50 ml.min ⁻¹ , 40°C–300°C, >40°C.s ⁻¹ , 5 min
GC	
Inlet	Split 1/10, 250°C
Column	TR-V1, 60 m x 0.25 mm x 1.4 μm
Gas	He, 1 ml.min ⁻¹
Oven	50°C to 150°C, 10°C.min ⁻¹
MS transfer line	230°C
MS	
Source temperature	230°C
Scan	50–250 m/z
SRM	62 > 27; 64 > 27; 65 > 30; 10 eV

FIGURE S 2: PARAMETERS FOR ANALYSIS OF VCM

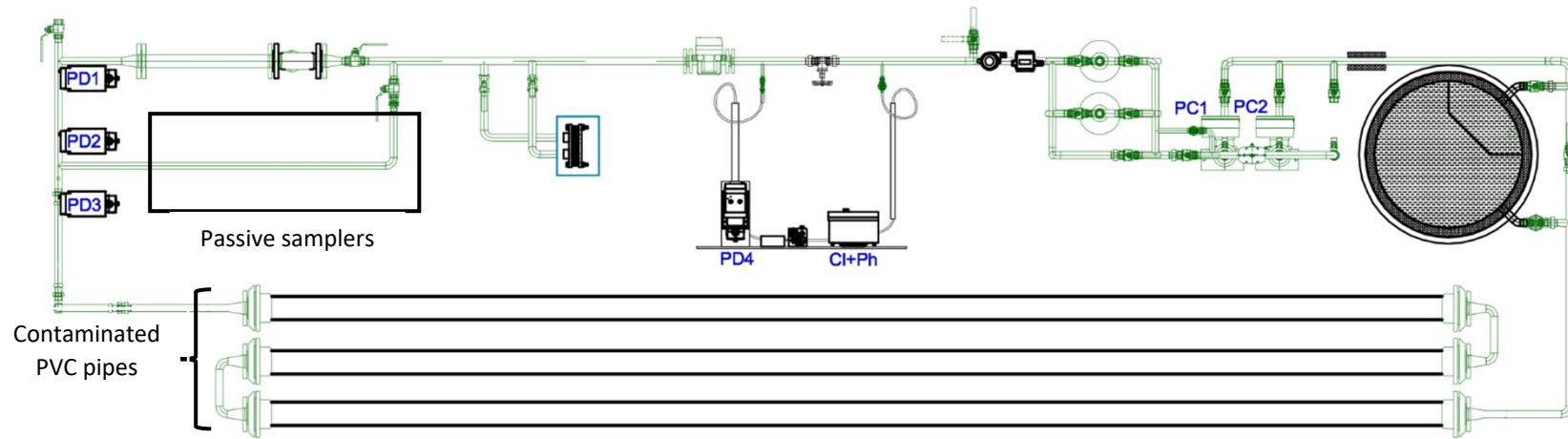


FIG. S 3: HYDRAULIC PILOT USED FOR CALIBRATION OF PASSIVE SAMPLERS

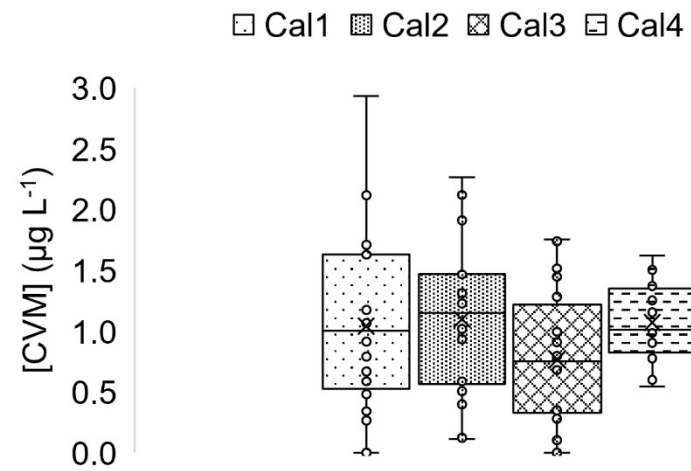


FIG. S 4: VCM CONCENTRATIONS IN WATER FOR THE FOUR CALIBRATION REPLICATES

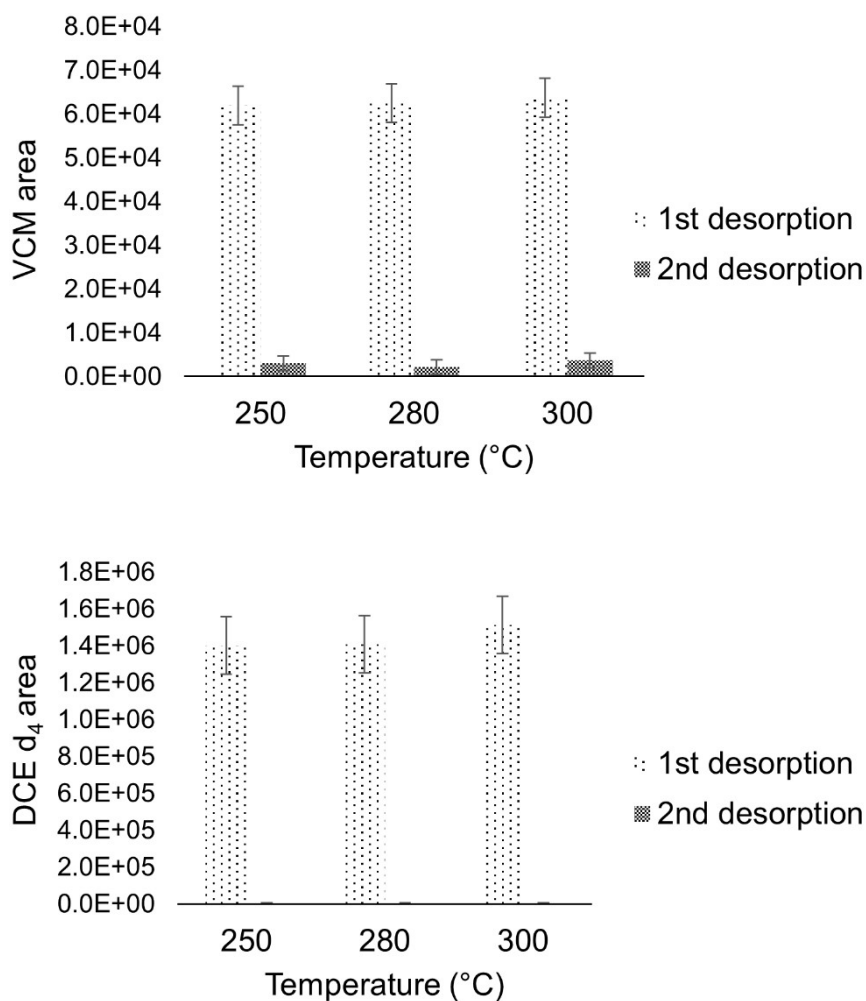


FIG. S 5: THERMAL DESORPTION TEMPERATURE COMPARISON FOR VCM AND ITS INTERNAL STANDARD AT A FIXED DESORPTION TIME OF 5 MIN AND DESORPTION FLOW OF 50 ML.MIN⁻¹

Desorption temperature °C	VCM response area				Internal standard area			
	1st desorption	standard deviation	2nd desorption	standard deviation	1st desorption	standard deviation	2nd desorption	standard deviation
250	61956	981	3046	1971	1400236	78022	4171	419
280	62397	5426	2101	1064	1407659	104057	3871	671
300	63684	6880	3657	1993	1511295	283920	4115	1002

FIG. S 6: ANALYTE AND INTERNAL STANDARD RESPONSE AREAS FOR 3 TEMPERATURES AND 2 DESORPTIONS

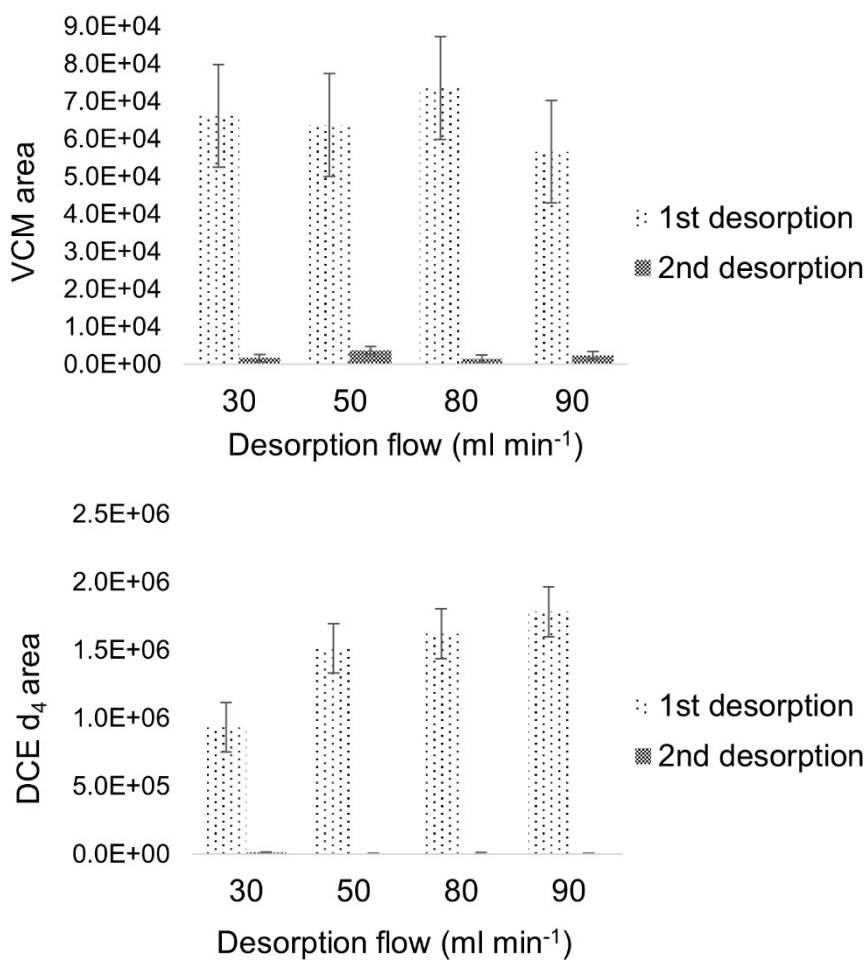


FIG. S 7: THERMAL DESORPTION FLOW COMPARISON FOR VCM AND ITS INTERNAL STANDARD AT A FIXED DESORPTION TEMPERATURE OF 300°C AND DESORPTION FLOW OF 50 ML.MIN⁻¹

Desorption flow ml/min	VCM area				Internal standard area			
	1st desorption	standard deviation	2nd desorption	standard deviation	1st desorption	standard deviation	2nd desorption	standard deviation
30	66044	19794	1651	274	932135	118291	11314	11638
50	63684	6880	3657	1993	1511295	283920	4115	1002
80	73513	17841	1471	452	1618296	133704	5468	2087
90	56614	10207	2303	1233	1780637	195266	2377	1787

FIG. S 8: ANALYTE AND INTERNAL STANDARD RESPONSE AREAS FOR 4 FLOWS AND 2 DESORPTIONS

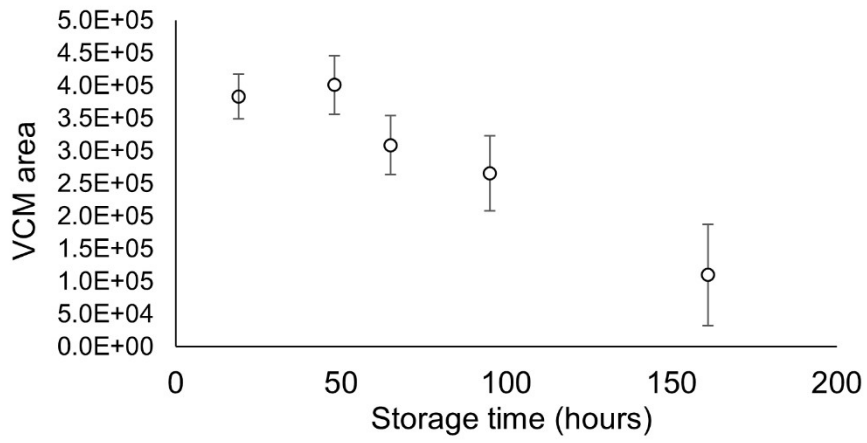


FIG. S 9: ANALYTE STABILITY IN THE DESORPTION TUBES DURING STORAGE

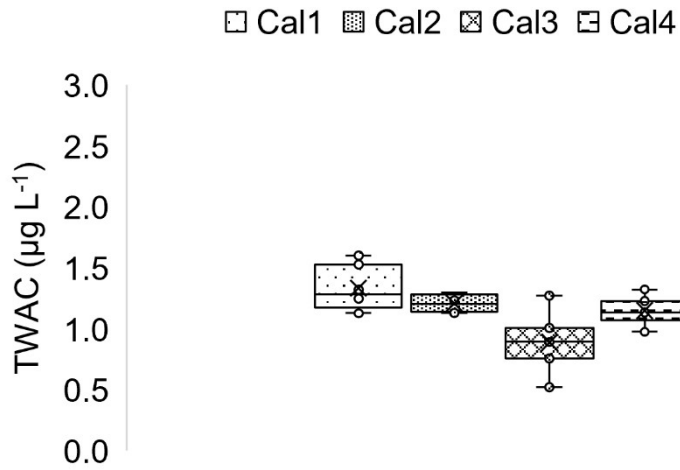


FIG. S 10: AVERAGE CONCENTRATIONS OF VCM MEASURED BY SPOT SAMPLING DURING CALIBRATION

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Call:
lm(formula = lnFC ~ lnt)

Residuals:
    Min       1Q   Median       3Q      Max
-0.26613 -0.12148 -0.00769  0.07342  0.47402

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) -7.41012    0.13617  -54.42  <2e-16 ***
lnt          1.00985    0.03004   33.61  <2e-16 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.1646 on 29 degrees of freedom
Multiple R-squared:  0.975,    Adjusted R-squared:  0.9741
F-statistic: 1130 on 1 and 29 DF,  p-value: < 2.2e-16

Analysis of Variance Table

Response: lnFC
            Df Sum Sq Mean Sq F value    Pr(>F)
lnt          1 30.6281 30.6281  1129.9 < 2.2e-16 ***
Residuals  29  0.7861  0.0271
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

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FIG. S 11: RESULTS OF THE ANOVA PERFORMED FOR THE PS CALIBRATION

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Call:
lm(formula = lnk ~ invtemp, data = donnees_rs_all_temp)

Residuals:
    1      2      3
-0.03789  0.01959  0.01830

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  12.7914    0.9615   13.30  0.0478 *
invtemp     -5885.1830  281.4057  -20.91  0.0304 *
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.04642 on 1 degrees of freedom
Multiple R-squared:  0.9977,    Adjusted R-squared:  0.9954
F-statistic: 437.4 on 1 and 1 DF,  p-value: 0.03042

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FIG. S 12: RESULTS PERFORMED TO ESTIMATE THE INFLUENCE OF TEMPERATURE ON RS

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Call:
lm(formula = rs ~ debit, data = donnees_rs_all_deb)

Residuals:
    1      2      3      4      5 
2.723e-05 -1.977e-05 -5.770e-06 -1.689e-05  1.520e-05

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  2.518e-04  1.761e-05  14.295 0.000742 ***
debit       -1.177e-07  2.960e-07  -0.398 0.717540
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 2.368e-05 on 3 degrees of freedom
(1 observation effacée parce que manquante)
Multiple R-squared:  0.05005, Adjusted R-squared:  -0.2666
F-statistic: 0.1581 on 1 and 3 DF, p-value: 0.7175

> anova(reg_rs_deb)
Analysis of Variance Table

Response: rs
          Df      Sum Sq   Mean Sq F value Pr(>F)
debit      1  8.8630e-11  8.8630e-11  0.1581 0.7175
Residuals  3  1.6822e-09  5.6072e-10

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FIG. S 13: RESULTS OF THE ANOVA PERFORMED TO ESTIMATE THE INFLUENCE OF FLOW VELOCITY ON RS

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Call:
lm(formula = rs ~ temperature + debit, data = donnees_rs_all)

Residuals:
    1      2      3      4      5      6      7      8 
3.490e-06 -4.351e-05 -2.961e-05  1.539e-05 -1.838e-05  2.804e-05  1.654e-05  2.804e-05

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept) -1.008e-04  5.154e-05  -1.957 0.107763
temperature  1.756e-05  2.281e-06  7.701 0.000589 ***
debit        2.139e-07  3.641e-07  0.587 0.582498
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 3.226e-05 on 5 degrees of freedom
Multiple R-squared:  0.9227, Adjusted R-squared:  0.8917
F-statistic: 29.82 on 2 and 5 DF, p-value: 0.001664

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FIG. S 14: RESULTS OF THE MULTILINEAR REGRESSION $RS = F(\text{TEMPERATURE, FLOW VELOCITY})$