A novel graphene wool gas adsorbent for volatile and semi volatile organic compounds

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Supporting Information

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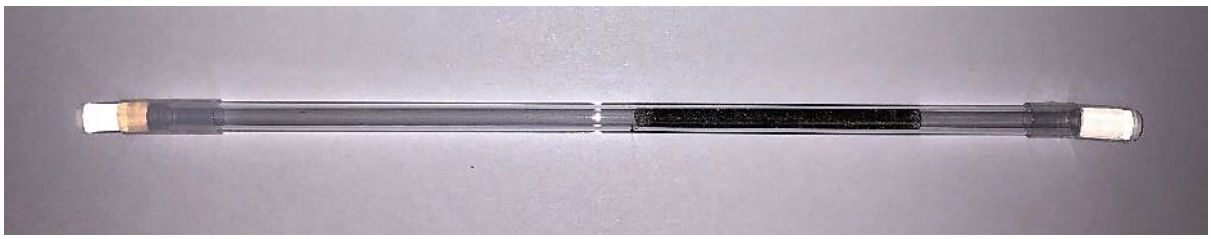

Figure S1: Optimized graphene wool (GW) sampler assembly.

Table S1: Concentration of individual deuterated alkane standards in the Internal Standards mix.

Internal Standard	**Concentration in mix [µg µl]**
n-Heptane d16	0.0664
n-Dodecane d26	0.0693
n-Hexadecane d34	0.0387

Table S2: Average retention times (min) used for the calculation of the breakthrough volume for the analytes at isothermal temperatures 25 – 200 °C for the QW sampler. (-) represents temperatures at which the analyte was not run. N=2.

Temp (°C)	Average retention times (min) at isothermal temperatures reported with SD. % RSD is reported in brackets underneath each stated average.								
	MeOH	Hex	Prop	Tol	But	Oct	Cycl	Dode	Hexd
25	0.51 ± 0.00 (0.11)	0.35 ± 0.01 (1.80)	1.03 ± 0.00 (0.23)	1.11 ± 0.06 (5.60)	4.76 ± 0.15 (3.09)	1.59 ± 0.02 (1.41)	6.74 ± 0.25 (3.74)	-	-
30	0.47 ± 0.05 (11.29)	0.33 ± 0.00 (1.11)	0.94 ± 0.03 (3.11)	1.02 ± 0.03 (2.51)	3.59 ± 0.18 (5.11)	1.23 ± 0.11 (8.75)	4.55 ± 0.12 (2.69)	-	-
40	0.41 ± 0.00 (0.54)	0.32 ± 0.01 (2.26)	0.53 ± 0.03 (5.92)	0.74 ± 0.03 (3.67)	2.03 ± 0.09 (4.29)	0.84 ± 0.00 (0.16)	2.61 ± 0.10 (3.89)	-	-
50	0.36 ± 0.00 (1.19)	-	0.42 ± 0.02 (3.59)	0.51 ± 0.00 (0.24)	1.25 ± 0.22 (17.24)	0.6 ± 0.02 (3.90)	1.55 ± 0.07 (4.66)	-	-
60	0.36 ± 0.00 (1.06)	-	0.36 ± 0.01 (2.89)	0.44 ± 0.01 (2.69)	0.79 ± 0.04 (5.40)	0.49 ± 0.03 (5.10)	-	-	-
70	0.36 ± 0.00 (0.54)	-	0.35 ± 0.01 (1.56)	-	-	-	0.89 ± 0.01 (0.95)	5.42 ± 0.08 (1.51)	-
80	-	-	-	0.35 ± 0.01 (3.90)	0.48 ± 0.04 (8.89)	0.37 ± 0.02 (4.23)	-	-	-
90	-	-	-	-	-	-	0.51 ± 0.01 (1.27)	2.12 ± 0.03 (1.22)	-
110	-	-	-	-	-	-	-	1.05 ± 0.09 (9.02)	-
120	-	-	-	-	-	-	-	-	5.99 ± 0.14 (2.26)
130	-	-	-	-	-	-	-	0.54 ± 0.00 (0.69)	4.19 ± 0.15 (3.65)
140	-	-	-	-	-	-	-	-	2.79 ± 0.27 (9.81)
150	-	-	-	-	-	-	-	0.41 ± 0.02 (4.08)	-
160	-	-	-	-	-	-	-	-	1.35 ± 0.10 (7.71)
180	-	-	-	-	-	-	-	0.35 ± 0.01 (3.50)	0.76 ± 0.07 (9.83)
200	-	-	-	-	-	-	-	-	0.46 ± 0.00 (1.04)

Table S3: Average retention times used for the calculation of the breakthrough volume for the analytes at isothermal temperatures 25 – 190 °C for the GW sampler. (-) represents temperatures at which the analyte was not run. N=2.

Temp (°C)	Average retention times (min) at isothermal temperatures reported with SD. % RSD is reported in brackets underneath each stated average.								
	MeOH	Hex	Prop	Tol	But	Oct	Cycl	Dode	Hexd
25	0.82 ± 0.01 (1.03)	0.41 ± 0.01 (1.53)	1.32 ± 0.04 (3.21)	1.39 ± 0.06 (3.98)	5.57 ± 0.05 (0.88)	1.84 ± 0.07 (3.57)	8.02 ± 0.20 (2.48)	-	-
30	0.68 ± 0.01 (0.76)	0.40 ± 0.00 (0.10)	1.09 ± 0.08 (6.89)	1.14 ± 0.01 (0.54)	4.22 ± 0.06 (1.39)	1.47 ± 0.04 (2.97)	6.19 ± 0.4 (6.38)	-	-
35	0.58 ± 0.01 (1.46)	-	0.9 ± 0.03 (3.49)	0.93 ± 0.03 (3.43)	3.16 ± 0.03 (1.00)	1.2 ± 0.00 (0.18)	4.32 ± 0.29 (6.63)	-	-
40	0.52 ± 0.00 (0.52)	0.36 ± 0.01 (2.40)	0.72 ± 0.03 (4.44)	0.79 ± 0.02 (2.28)	2.33 ± 0.00 (0.01)	0.87 ± 0.07 (8.05)	3.3 ± 0.21 (6.32)	-	-
45	0.46 ± 0.00 (0.25)	-	0.66 ± 0.03 (4.10)	0.68 ± 0.00 (0.31)	1.81 ± 0.01 (0.45)	0.8 ± 0.00 (0.25)	2.46 ± 0.08 (3.36)	-	-
50	0.44 ± 0.00 (0.09)	0.36 ± 0.00 (0.03)	0.59 ± 0.02 (4.10)	0.57 ± 0.03 (5.39)	1.44 ± 0.05 (3.62)	0.69 ± 0.02 (2.26)	2.16 ± 0.01 (0.60)	-	-
60	0.43 ± 0.00 (0.37)	-	0.46 ± 0.02 (4.66)	0.48 ± 0.02 (3.85)	0.91 ± 0.06) (6.10	0.5 ± 0.02 (3.76)	1.45 ± 0.11 (7.62)	-	-
70	0.43 ± 0.00 (0.30)	-	0.42 ± 0.01 (1.95)	0.41 ± 0.01 (3.26)	0.66 ± 0.05 (7.68)	0.43 ± 0.01 (1.21)	1.06 ± 0.01 (0.49)	6.26 ± 0.09 (1.42)	-
80	-	-	-	0.38 ± 0.00 (0.81)	0.49 ± 0.03 (7.03)	0.38 ± 0.01 (3.41)	0.85 ± 0.08 (9.62)	3.83 ± 0.08 (1.98)	-
90	-	-	-	-	-	-	0.64 ± 0.05 (8.37)	2.39 ± 0.06 (2.60)	-
100	-	-	-	-	-	-	-	1.53 ± 0.00 (0.13)	-
110	-	-	-	-	-	-	-	1.06 ± 0.02 (1.85)	-
120	-	-	-	-	-	-	-	0.82 ± 0.03 (3.43)	8.18 ± 0.47 (5.81)
130	-	-	-	-	-	-	-	0.62 ± 0.02 (3.65)	4.71 ± 0.18 (3.90)
140	-	-	-	-	-	-	-	0.49 ± 0.01	3.11 ± 0.1

								(1.02)	(3.11)
150	-	-	-	-	-	-	-	-	2.14 ± 0.05 (2.33)
160	-	-	-	-	-	-	-	-	1.49 ± 0.02 (1.03)
170	-	-	-	-	-	-	-	-	1.07 ± 0.01 (0.67)
180	-	-	-	-	-	-	-	-	0.79 ± 0.03 (3.19)
190	-	-	-	-	-	-	-	-	0.62 ± 0.01 (0.87)

Table S4: Average retention times used for the calculation of the breakthrough volume for the analytes at isothermal temperatures 25 – 340 °C for the PDMS sampler. (-) represents temperatures at which the analyte was not run. N=2.

Temp (°C)	Average retention times (min) at isothermal temperatures reported with SD. % RSD is reported in brackets underneath each stated average.								
	MeOH	Hex	Prop	Tol	But	Oct	Cycl	Dode	Hexd
25	1.61 ± 0.02 (0.99)	9.41 ± 0.07 (0.71)	4.37 ± 0.16 (3.55)	-	-	-	-	-	-
30	1.35 ± 0.01 (0.67)	-	3.57 ± 0.11 (2.96)	-	-	-	-	-	-
35	1.22 ± 0.01 (1.13)	-	-	-	-	-	-	-	-
40	1.03 ± 0.02 (1.53)	5.43 ± 0.03 (0.52)	2.54 ± 0.07 (2.63)	-	-	-	-	-	-
45	0.91 ± 0.00 (0.24)	-	-	-	-	-	-	-	-
50	0.82 ± 0.01 (1.04)	-	1.9 ± 0.02 (0.02)	-	-	-	-	-	-
60	0.72 ± 0.01 (0.80)	3.07 ± 0.05 (1.69)	1.47 ± 0.00 (0.13)	-	-	-	-	-	-
70	0.64 ± 0.01 (1.16)	-	1.21 ± 0.01 (1.94)	-	-	-	-	-	-
80	-	1.96 ± 0.00 (0.23)	-	6.12 ± 0.12 (1.92)	-	-	-	-	-
100	-	1.37 ± 0.00 (0.27)	-	3.64 ± 0.02 (0.50)	1.81 ± 0.06 (3.12)	4.54 ± 0.07 (1.47)	-	-	-

120	-	1.03 ± 0.00 (0.25)	-	2.36 ± 0.01 (0.60)	1.29 ± 0.02 (1.18)	2.83 ± 0.05 (1.71)	4.52 ± 0.06 (1.43)	-	-
140	-	-	-	1.71 ± 0.03 (1.88)	0.98 ± 0.04 (3.58)	1.89 ± 0.02 (0.90)	2.86 ± 0.03 (0.94)	-	-
160	-	-	-	1.31 ± 0.01 (0.62)	0.87 ± 0.04 (4.20)	1.39 ± 0.01 (0.72)	2.06 ± 0.04 (2.09)	7.25 ± 0.06 (0.76)	-
180	-	-	-	1.08 ± 0.03 (2.46)	0.74 ± 0.00 (0.44)	1.08 ± 0.02 (2.04)	1.55 ± 0.01 (0.53)	4.51 ± 0.00 (0.09)	-
200	-	-	-	-	0.68 ± 0.01 (1.96)	0.91 ± 0.02 (2.22)	1.26 ± 0.01 (1.16)	2.94 ± 0.03 (0.92)	-
220	-	-	-	-	-	-	1.04 ± 0.03 (2.57)	2.07 ± 0.02 (0.98)	-
240	-	-	-	-	-	-	-	1.55 ± 0.03 (1.86)	4.49 ± 0.02 (038)
260	-	-	-	-	-	-	-	1.25 ± 0.01 (0.48)	3.05 ± 0.03 (0.85)
280	-	-	-	-	-	-	-	-	2.2 ± 0.02 (1.06)
300	-	-	-	-	-	-	-	-	1.66 ± 0.06 (3.64)
320	-	-	-	-	-	-	-	-	1.34 ± 0.01 (0.99)
340	-	-	-	-	-	-	-	-	1.12 ± 0.02 (2.05)

Table S5: Exponential equations and corresponding correlation coefficients calculated from the BV curves shown in Figure 7.

Analyte (BP °C)	Abbr.	QW	R^2	GW	R^2	PDMS	R^2
Methanol (64.7°C)	MeOH	$y = 47.704e^{-0.007x}$	0.8170	$y = 69.311e^{-0.014x}$	0.7570	$y = 66.873e^{-0.02x}$	0.9603
Hexane (68°C)	Hex	$y = 32.774e^{-0.006x}$	0.8542	$y = 32.775e^{-0.006x}$	0.9422	$y = 385.37e^{-0.023x}$	0.9722
Propanol-2 (82.5°C)	Prop	$y = 146.19e^{-0.025x}$	0.8753	$y = 155.92e^{-0.025x}$	0.9535	$y = 231.2e^{-0.029x}$	0.9884
Toluene (110.6°C)	Tol	$y = 158.73e^{-0.023x}$	0.9176	$y = 148.8e^{-0.023x}$	0.9457	$y = 576.36e^{-0.017x}$	0.9734
Butan-1-ol (117.7°C)	But	$y = 1016.6e^{-0.043x}$	0.9629	$y = 1069.8e^{-0.045x}$	0.9832	$y = 113.26e^{-0.009x}$	0.9430
Octane (125.6°C)	Oct	$y = 212.28e^{-0.026x}$	0.9519	$y = 226.61e^{-0.029x}$	0.9559	$y = 553.3e^{-0.016x}$	0.9728
Cyclohexanone (155.6°C)	Cyclo	$y = 1132.2e^{-0.038x}$	0.9667	$y = 1179.6e^{-0.038x}$	0.9727	$y = 598.31e^{-0.014x}$	0.9723
Dodecane (216.2°C)	Dode	$y = 1756.2e^{-0.025x}$	0.8940	$y = 4870e^{-0.037x}$	0.9801	$y = 2983.8e^{-0.018x}$	0.9817
Hexadecane (286.8°C)	Hexd	$y = 22133e^{-0.032x}$	0.9902	$y = 35767e^{-0.036x}$	0.9872	$y = 3207.5e^{-0.014x}$	0.9835

Table S6: LODs and LOQs ($ng.m^{-3}$) of target analytes on GW samplers that were directly thermally desorbed

Target analyte	Abbr.	LOD ($ng.m^{-3}$)	LOQ ($ng.m^{-3}$)
n-Octane	n-Oct	4874	16244
n-Nonane	n-Non	820	2730
n-Decane	n-Dec	336	1122
n-Undecane	n-Und	424	1412
n-Dodecane	n-Dod	664	2216
n-Tridecane	n-Tri	668	2226
n-Tetradecane	n-Tet	740	2466
n-Pentadecane	n-Pent	638	2130
n-Hexadecane	n-Hex	806	2684
n-Heptadecane	n-Hept	698	2328
n-Octadecane	n-Oct	672	2240
n-Nonadecane	n-Non	798	2664
n-Eicosane	n-Eic	690	2300

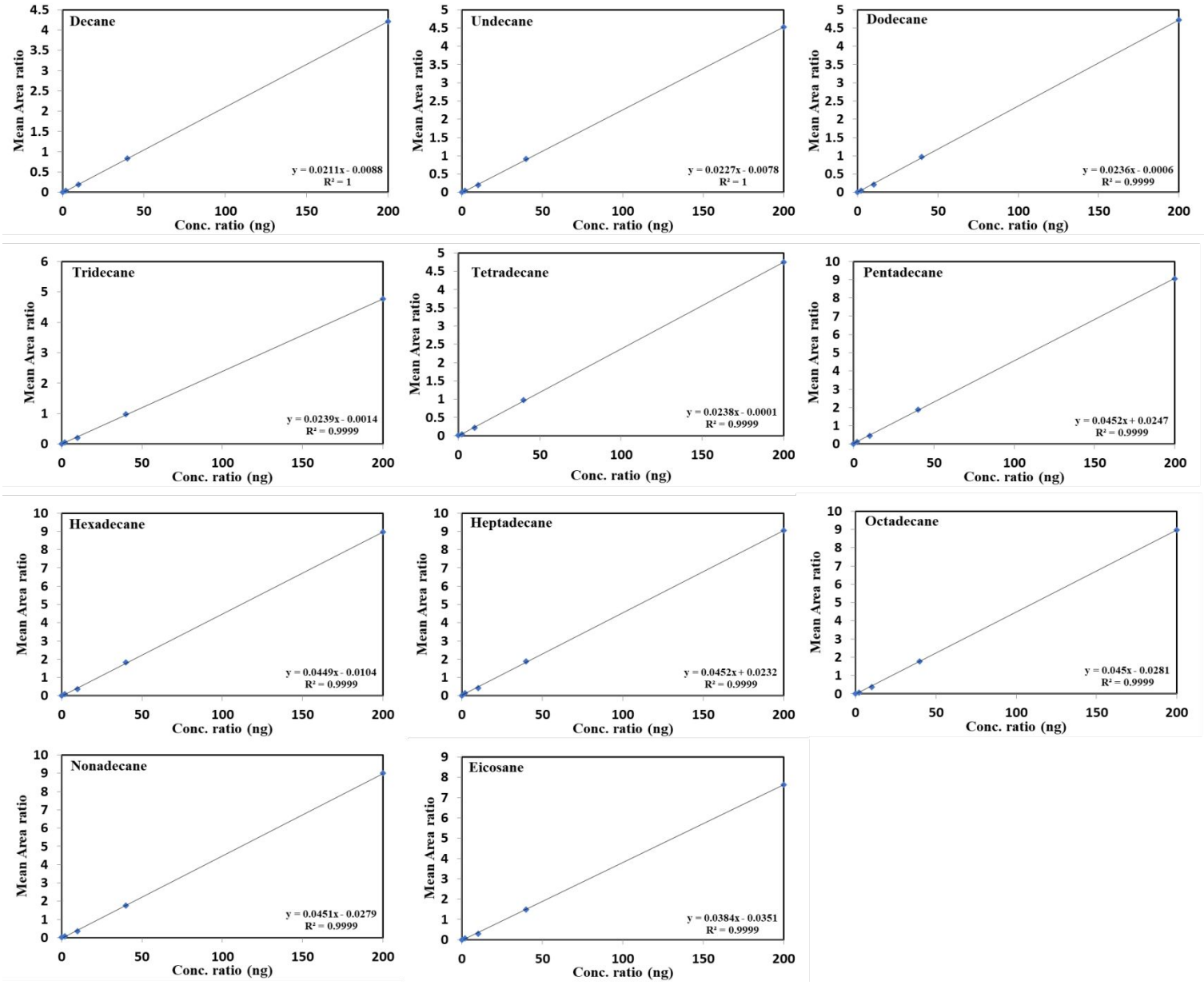

Figure S*2*: Calibration curves of C_{10}-C_{20} alkanes in RME biodiesel combustion emissions on GW samplers that were thermally desorbed and analysed by GC-MS.