Feasibility of high-resolution continuum source molecular absorption spectrometry for vanadium determination

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Table 1S Optimization of sensitivity and detectability. HR-CS FMAS technique.

Wavelength, nm		Number of pixels taken for analyte signal evaluation	Pixels taken for analyte signal evaluation	Characteristic concentration, mg L^{-1}	For solution, mg L^{-1}		For catalyst, % (1:83 m:v dilution ratio)	
of central pixel	range				DL*	DTL*	DL	DTL
546.9331	546.6221-547.2421	14	99-105,123-129	550	44	150	0.4	1.2
573.7642	573.4612-574.0642	15	73-81,98-103	660	20	66	0.2	0.6
		23	73-81,98-103, 119-121,131-132,143-144,156	520	22	73	0.3	0.7
		39	73-81,98-103, 109-111,119-121,130-132, 142-145,155-157,187-190	400	26	87	0.2	0.6
550.6230	550.3440-550.8992	15	44-49,99-103,156-159	560	22	72	0.2	0.6
		28	23-25,31-33,44-49,77-79,86-87,99-103,142-143,156-159	380	15	50	0.1	0.4
550.5593	550.2803-550.8355	15	15-18,68-70,101,123-125,180-183	440	23	76	0.2	0.6
		23	14-18,68-71,100-102,123-126,179-183	340	18	62	0.2	0.5
		34	14-18,46-48,54-56,67-71,100-102,109,122-126,165-166,179-183	270	17	56	0.1	0.5
		50	13-19,45-49,53-57,66-72,99-103,1-8-110,121-126,164-167,177-184	230	19	64	0.2	0.5

Table 2S Particular data concerning experiments carried out using HR- CS GF MAS option and illustrated in Figs. 5-6.

Figure	Initial analyte form	Sample form l-liquid s-solid	Measured analyte form	Pyrolysis 3 / molecule formation temperature, °C	Air (O_2) step +: yes -: no	Ar purging step after air step +: yes -: no	Heating rate up to molecule formation temperature, °C s^{-1}	Pd modifier	Absorbance (3 pixels)
8a	V_2O_5	s	VO	500/2200	+	+	1500	no	0.050
8b	V_2O_5	s	VO	500/2500	+	+	1500	no	0.10
8c	V_2O_5	s	VO	700/2500	+	-	1500	no	0.20
8d	Empty platform	no sample	VO	500/2500	+	+	500	no	0.015
8e	V_2O_5	s	VO	500/2500	+	+	500	no	0.090
8f	V_2O_5	s	VO	500/2500	-	+	500	no	0.030
9b	V_2O_5	s	VO	500/2500	+	+	1500	Pd	0.130
9a	V_2O_5	s	VO	500/2500	-	+	1500	Pd	0.070
9c	Empty platform	no sample	V	1200/2550	-	+	1500	no	>10

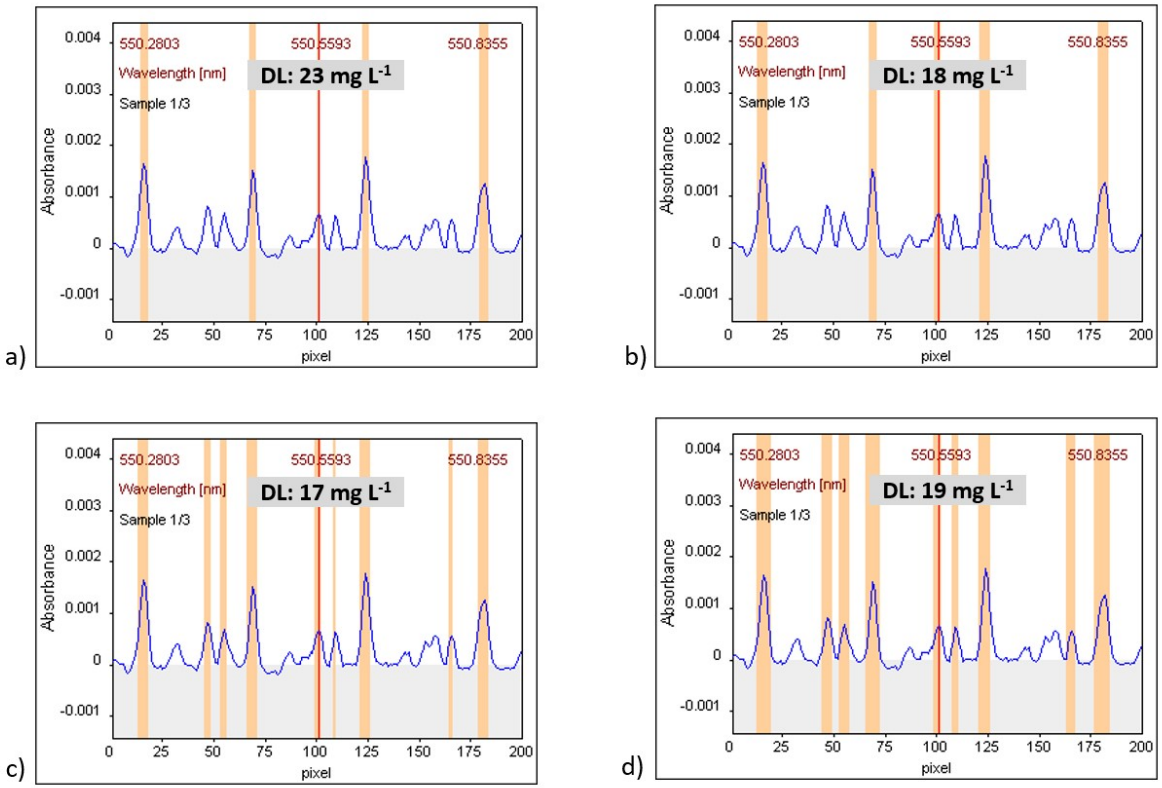

Fig. 1S View of a spectrum acquired using contrAA 700 spectrometer (FMAS technique), centred at 550.5593 nm with various sets of pixels used for VO molecule signal evaluation: 15 (a), 23 (b), 34 (c) and 50 (d). The pixels are marked as vertical bars.

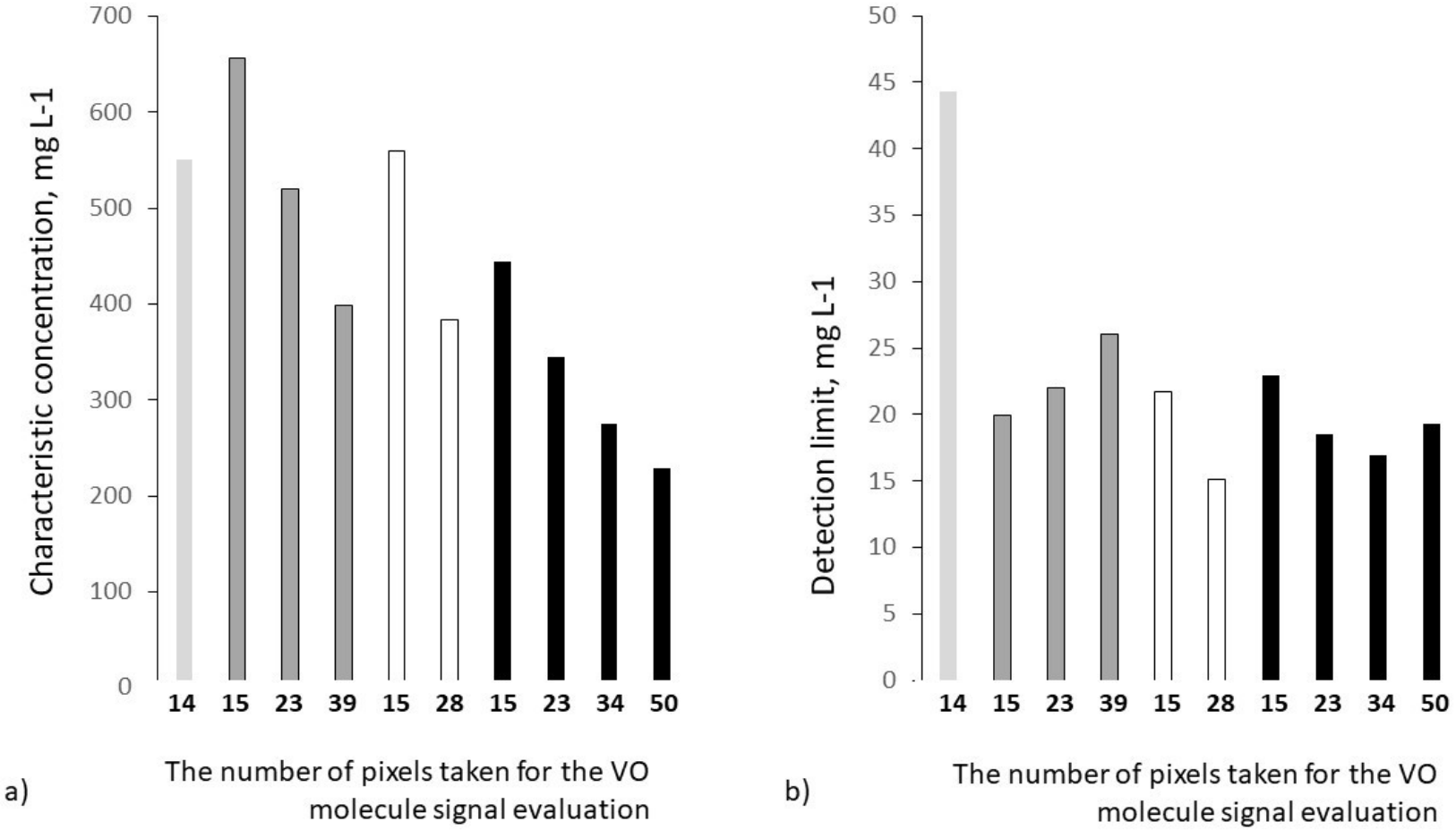

Fig. 2S Comparison of: characteristic concentration (a) and detection limit (b) for various spectral conditions. Spectrum centred at: 546.9331 nm (light grey bar), 573.7642 (dark grey bars), 550.6230 (white bars) and 550,5593 nm (black bars). The numbers under bars indicate the numbers of pixels in sets used for the VO molecule signal evaluation.

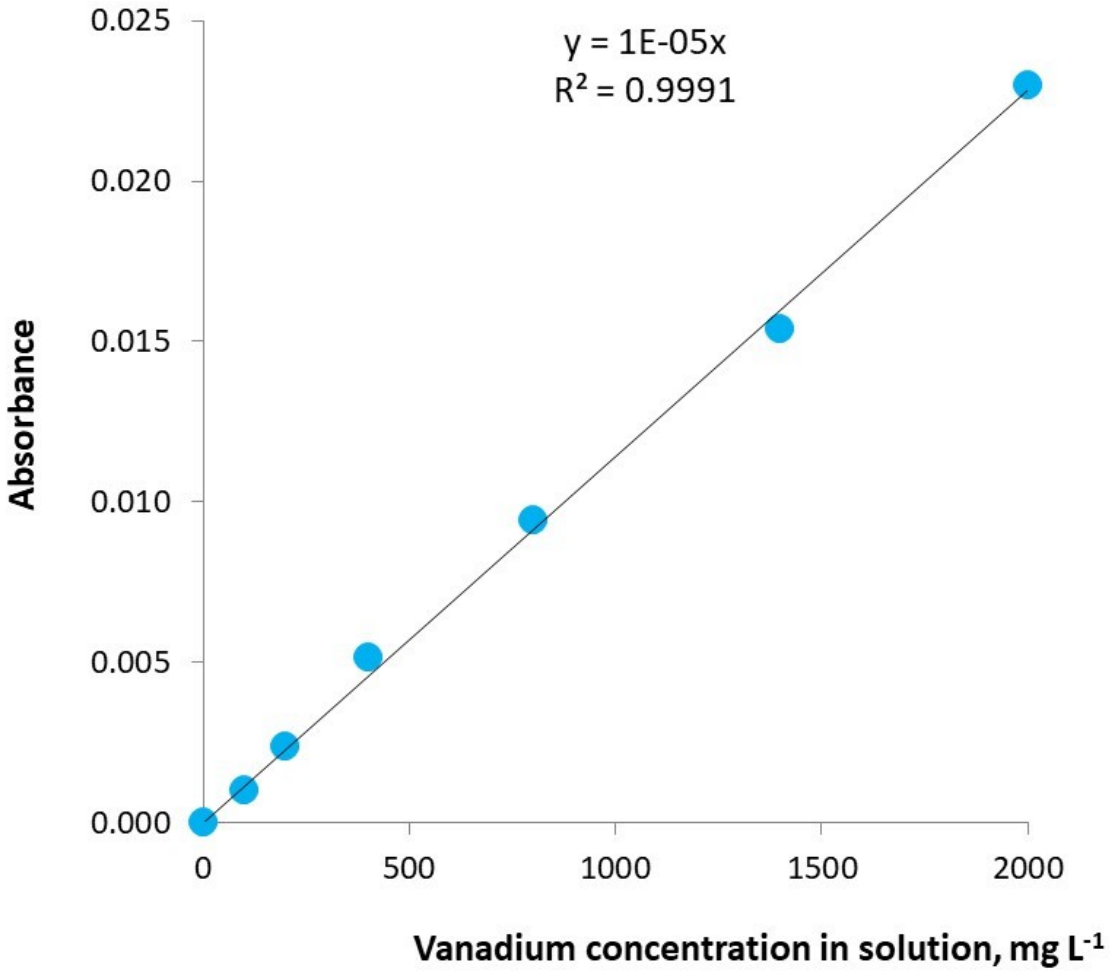

Fig. 3S A calibration curve for the determination of V using the HR-CS FMAS technique.

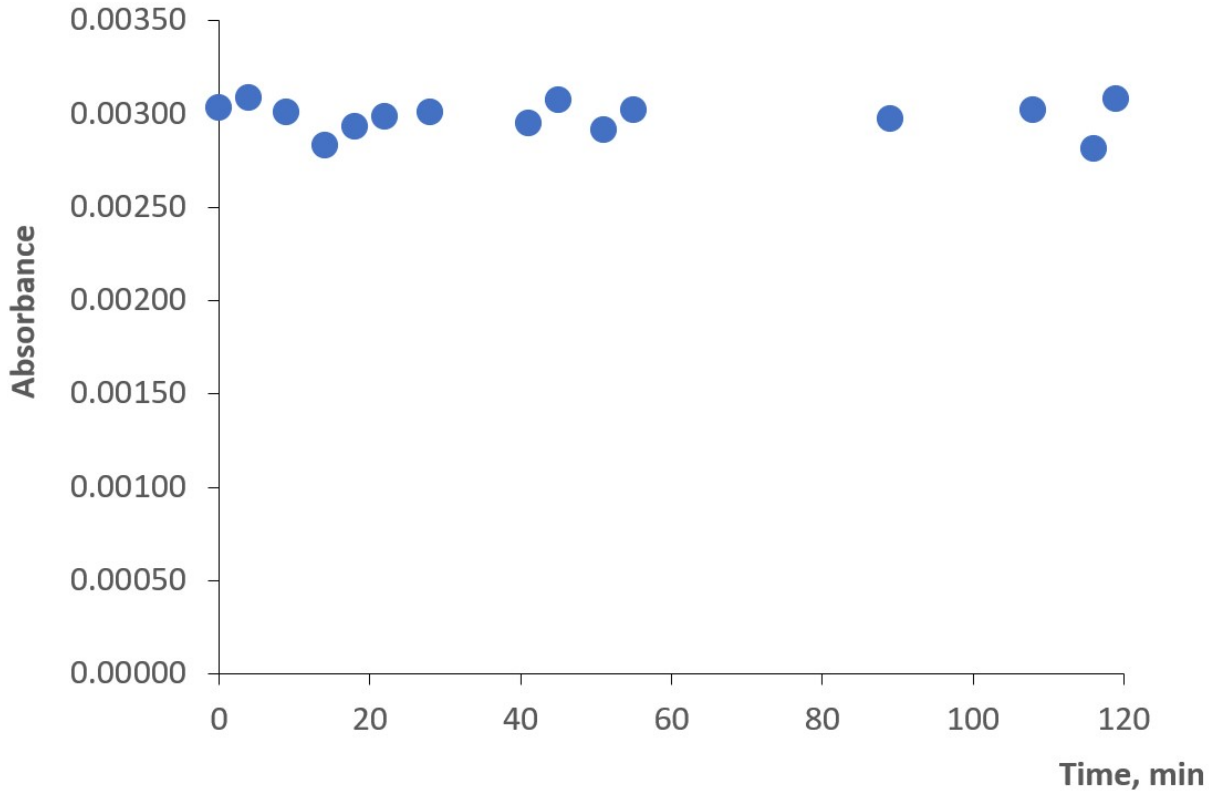

Fig. 4S Stability of measurements of a solution containing 280 mg L^{-1} of V, 5000 mg L^{-1} of Al and HCl 1:5 v:v in 120 minutes time.