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SUPPLEMENTARY MATERIAL TO

Comparison of non-destructive techniques and conventionally used spectrometric techniques for determination of elements in plant samples (coniferous leaves)

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TABLE S-I. Analytical lines and parameters of analysed elements

Element	Line	Wavelength, Å	Crystal	Detector	Count time, s	Filter
Na	Ka 1,2	11.9101	AX03	FPC	40	None
Mg	Ka 1,2	9.89	AX03	FPC	40	None
Al	Ka 1,2	8.3401	PET	FPC	24	None
K	Ka 1,2	3.7424	LiF200	FPC	24	None
Ca	Ka 1,2	3.3595	LiF200	FPC	24	None
Cr	Ka 1,2	2.291	LiF200	FPC	24	None
Mn	Ka 1,2	2.1031	LiF200	FPC	24	None
Fe	Ka 1,2	1.9374	LiF200	FPC	24	None
Co	Ka 1,2	1.7903	LiF200	FPC	24	None
Ni	Ka 1,2	1.6592	LiF200	SC	24	None
Cu	Ka 1,2	1.5418	LiF200	SC	24	None
Zn	Ka 1,2	1.4364	LiF200	SC	24	None
Ga	Ka 1,2	1.3414	LiF200	SC	24	None
Sr	Ka 1,2	0.8766	LiF200	SC	16	None
Ag	Ka 1,2	0.5609	LiF200	SC	40	Cu 0.27 mm
Cd	Ka 1,2	0.5365	LiF200	SC	40	Cu 0.27 mm
In	Ka 1,2	0.5136	LiF200	SC	24	Cu 0.27 mm
Tl	La 1	1.2074	LiF200	SC	24	None
Pb	La 1	1.175	LiF200	SC	24	None
Bi	La 1	1.1439	LiF200	SC	24	None

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TABLE S-II. Certified and measured (using ICP-MS, ICP-OES, INAA, UQ, and WD-XRF) values with the relative standard deviation (RSD) of the three repeated measurements and uncertainties values (SD) for the reference material

Element	Certified		ICP-MS		ICP-OES		INAA		UQ		WD-XRF	
	c / mg L^{-1}	RSD, %	c / mg L^{-1}	RSD, %	c / mg L^{-1}	RSD, %	c / mg L^{-1}	RSD, %	c / mg L^{-1}	RSD, %	c / mg L^{-1}	RSD, %
Na	63	1	53	3	112	115			343	44	15	7
Mg	1060	170	854	33	945	18	1067	105	1267	6	923	52
Al	580	30	489	28	539	8	681	155	710	11	574	34
P	1070	80	1054	79					1367	15		
K	4170	70	3733	158	3120	49			4727	124	3849	128
Ca	2500	100	2269	97	2421	41	2667	115	2707	64	2542	71
Mn	488	12	472	30	462	10	496	48	595	19	500	10
Fe	45	2	45	3	50	13			46	4	47	1
Ni	1.47	0.1	1.2	0.1	1.5	0.2						
Zn	38	2	41	3	35	2			100	4	20	25
Rb	16.5	0.9	16	1					5	9		
Ba	6	0.2	5.4	0.2	5.6	0.1					2	1

TABLE S-III. Descriptive statistics of all investigated elements measured using different analytical techniques: minimum, maximum, median, arithmetic mean (AR), and standard deviation (SD), median relative ratio (RR) of content and number of analysed samples (n)

		ICP-MS	ICP-OES	INAA	UQ	WD-XRF	ICP-MS	ICP-OES	INAA	UQ	WD-XRF
		Na					Mg				
Content, mg kg^{-1}	Minimum	1.8	2.4	18.3	229.5	0.5	527.7	414.1	185.0	528.5	304.4
	Maximum	1840.6	1633.5	2160.0	1815.0	216.5	1812.4	1494.5	1740.0	1770.0	914.9
	Median	13.6	83.8	39.3	384.3	91.3	1030.2	854.2	1120.0	1055.0	509.4
	AR	83.7	144.5	135.9	434.8	87.3	1051.1	872.1	1084.5	1022.7	524.9
	SD	266.8	252.3	359.6	245.9	45.8	256.7	219.0	282.9	303.0	116.2
	RR[a], %	100	359	322	2210	473	100	84	105	96	50
	n	49	41	36	46	46	49	35	39	48	49
		Al					K				
Content, mg kg^{-1}	Minimum	3.9	2.4	12.2	16.5	6.6	3334	1591	2700	3285	2475
	Maximum	256.0	324.7	297.0	545.5	416.1	20011	5722	20800	29500	16901
	Median	30.8	30.5	38.9	77.3	47.1	9896	3555	8300	13100	7488
	AR	51.0	46.9	62.6	129.3	90.1	10089	3673	8549	13175	7809
	SD	54.2	54.7	63.7	121.2	91.7	4434	1117	3970	6134	3790
	RR[a], %	100	90	130	308	174	100	36	84	135	81
	n	49	47	39	46	49	49	40	39	48	49
		Ca					P				
Content, mg kg^{-1}	Minimum	618	425	370	806	636	876	/	/	681	/
	Maximum	17690	13093	16200	22200	16348	5646	/	/	5540	/
	Median	3620	2513	3100	4548	3347	2977	/	/	2418	/
	AR	4297	3266	4231	6319	3894	2948	/	/	2635	/
	SD	3448	2904	3458	5196	3172	1405	/	/	1321	/
	RR[a], %	100	74	101	167	97	100	/	/	92	/
	n	49	49	39	48	49	49	/	/	48	/

		ICP-MS	ICP-OES	INAA	UQ	WD-XRF	ICP-MS	ICP-OES	INAA	UQ	WD-XRF
		S					Mn				
Content, mg kg^{-1}	Minimum	667	/	/	446	/	14	7	11	25	7
	Maximum	2145	/	/	2100	/	1300	533	600	1740	810
	Median	1288	/	/	893	/	85	36	56	123	52
	AR	1319	/	/	1007	/	157	78	89	227	101
	SD	372	/	/	414	/	230	105	116	308	149
	RR[a], %	100	/	/	76	/	100	56	77	158	64
	n	49	/	/	48	/	49	48	38	48	49
		Fe					Ni				
Content, mg kg^{-1}	Minimum	21	4	38	24	10	0	0	1	9	/
	Maximum	146	136	359	251	95	10	35	6	13	/
	Median	55	20	98	81	27	2	2	2	11	/
	AR	62	26	111	83	34	2	3	3	11	/
	SD	35	23	67	49	21	2	6	1	2	/
	RR[a], %	100	38	173	146	56	100	82	120	187	/
	n	49	46	35	48	49	49	36	30	2	/
		Zn					Rb				
Content, mg kg^{-1}	Minimum	10	7	9	35	1	0.4	/	0.4	11.0	/
	Maximum	84	271	81	337	215	36.2	/	41.0	45.5	/
	Median	36	24	44	127	55	4.3	/	5.2	16.5	/
	AR	40	32	44	135	63	6.5	/	7.7	20.8	/
	SD	17	37	17	62	36	6.6	/	8.1	10.4	/
	RR[a], %	100	68	102	367	161	100	/	116	192	/
	n	49	49	39	44	44	49	/	39	17	/
		Sr					Ba				
Content, mg kg^{-1}	Minimum	0.5	0.1	3.4	10.0	/	0.1	0.02	3	104	/
	Maximum	59.8	32.7	91.0	67.5	/	100	18	103	139	/
	Median	6.5	2.1	14.4	28.5	/	4	3	10	131	/
	AR	11.9	3.9	19.6	30.5	/	12	5	25	125	/
	SD	13.2	5.7	18.5	15.0	/	22	6	30	18	/
	RR[a], %	100	42	111	149	/	100	44	136	143	/
	n	49.0	40.0	26.0	23.0	/	49	18	23	3	/

[a]The median relative ratio (%) values calculated by dividing the element concentration measured using different techniques with ICP-MS concentration of the same plant sample

TABLE S-IV. Minimum, maximum, median, arithmetic mean (AR), and standard deviations (SD) of relative ratios of elements content

	ICP-OES	INAA	UQ	WD-XRF	ICP-OES	INAA	UQ	WD-XRF
				Content, %				
		Na				Mg		
Minimum	9	117	99	1	64	20	46	31
Maximum	5888	1826	15424	4367	116	214	196	74
Median	359	322	2210	473	84	105	96	50
AR	925	468	4169	869	86	107	100	51
SD	1445	384	4503	1055	11	26	31	9
		Al				K		
Minimum	23	0	26	12	18	0	57	24
Maximum	285	314	831	514	51	135	299	143
Median	90	130	308	174	36	84	135	81
AR	99	133	319	197	35	82	138	79
SD	56	67	172	103	7	20	48	18
		Ca				P		
Minimum	7	17	14	11	/	/	17	/
Maximum	281	447	542	300	/	/	229	/
Median	74	101	167	97	/	/	92	/
AR	79	110	171	100	/	/	98	/
SD	39	61	98	47	/	/	39	/
		S				Mn		
Minimum	/	/	27	/	3	0	5	2
Maximum	/	/	178	/	418	111	964	524
Median	/	/	76	/	56	77	158	64
AR	/	/	79	/	66	71	183	76
SD	/	/	32	/	67	21	148	80
		Fe				Ni		
Minimum	0	99	26	12	1	45	156	/
Maximum	139	638	336	78	962	604	218	/
Median	38	173	146	56	82	120	187	/
AR	43	219	143	56	188	139	187	/
SD	25	126	59	12	226	95	43	/
		Zn				Rb		
Minimum	32	62	97	4	/	16	82	/
Maximum	455	236	838	529	/	558	843	/
Median	68	102	367	161	/	116	192	/
AR	78	119	363	177	/	126	292	/
SD	58	44	175	111	/	83	242	/
		Sr				Ba		
Minimum	7	66	84	/	0,5	74	131	/
Maximum	162	175	326	/	380	305	251	/
Median	42	111	149	/	44	136	143	/
AR	47	112	160	/	62	142	175	/
SD	27	26	59	/	83	52	66	/

TABLE S-V. Minimum, maximum, median, arithmetic mean (AR) of relative standard deviation (RSD) of repeated measurements of elements content

	ICP-MS	ICP-OES	INAA	UQ	WD-XRF	ICP-MS	ICP-OES	INAA	UQ	WD-XRF
					RSD, %					
			Na					Mg		
Minimum	0.8	0.6	3	0.8	0	0.8	0.2	9.8	0	0
Maximum	23	95	7	38	18	12	9	41	11	3
Median	5	25	5	10	4	3	2	10	1	2
AR	7	34	5	10	4	3	2	11	2	2
			Al					K		
Minimum	0.5	1.2	4	0	0	0.4	0.0	11	0	0.5
Maximum	19	94	23	65	7	15	1	12	69	1
Median	4	8	5	6	1	3	0	11	0.4	0.8
AR	5	12	6	11	1	4	0	11	2	0.8
			Ca					P		
Minimum	0.3	0.3	11	0	0.4	0.9	/	/	0	/
Maximum	9	23	15	118	1	16	/	/	101	/
Median	3	3	11	0.4	0.6	5	/	/	0.6	/
AR	3	5	11	3	0.7	5	/	/	3	/
			S					Mn		
Minimum	1	/	/	0	/	0.5	0.1	6	0	0
Maximum	12	/	/	54	/	12	3	8	109	7
Median	5	/	/	0.8	/	3	1	6	1	0.3
AR	5	/	/	4	/	4	1	6	5	1
			Fe					Ni		
Minimum	0.5	1.1	6	0	0	1	0	8	17	0
Maximum	17	38	18	17	7	533	35	18	33	13
Median	4	7	9	3	0	8	1	11	25	0
AR	4	10	9	4	1	30	4	12	25	1
			Zn					Rb		
Minimum	0.3	0.04	4	0	3	0.6	/	17	0	/
Maximum	15	1	11	14	47	19	/	18	44	/
Median	3	0	5	2	1	3	/	17	10	/
AR	4	0	7	3	0.4	4	/	17	15	/
			Sr					Ba		
Minimum	0.3	0.4	8	1	/	0.2	0.4	13	15	/
Maximum	11	17	13	44	/	14	32	17	47	/
Median	3	2	9	7	/	3	3	15	38	/
AR	4	3	9	9	/	4	7	15	35	/