Article:
Zhai, J, Burke, IT orcid.org/0000-0002-0484-568X, Mayes, WM et al. (1 more author) (2021) New insights into biomass combustion ash categorisation: a phylogenetic analysis. Fuel, 287. 119469. ISSN 0016-2361

https://doi.org/10.1016/j.fuel.2020.119469

Supporting information for:

New insights into biomass combustion ash categorisation: a phylogenetic analysis

Jihua Zhai [1], Ian T. Burke [2], William M. Mayes [3], Douglas I. Stewart [1,*]

[1] School of Civil Engineering, University of Leeds, Leeds LS2 9JT, UK

[2] School of Earth and Environment, University of Leeds, Leeds LS2 9JT, UK

[3] Department of Geography, Geology and Environment, University of Hull, Cottingham Road, Hull HU6 7RX, UK

[*] Corresponding Author: d.i.stewart@leeds.ac.uk

Consisting of 18 pages with 9 Tables and 5 Figures.

Table S1. Chemical composition (wt. %) dataset of four different ash categories (black font for hardwood ash; red font for softwood ash; blue font for eudicot straw ash; green font for grass straw ash).

ID-number	CaO	MgO	MnO	K_2O	P_2O_5	SO_3	Cl_2O	SiO_2	Al_2O_3	Fe_2O_3	Na_2O	TiO_2
#2142	26.1	9.2		23.5				20	7	1.4	1.8	
#77	45	10.8		11.4	17	2.2		2.8	1.4	0.7	1.3	0.1
#91	65	8.3		9.9	7.5	2.2		2.3	0.9	0.5	0.8	0.1
#92	40.02	0.13	0.1	4.64					0.58	0.22	0.47	
#803	10.9	4.15		22.4	1.33	2.69		20.97	2.99	2.94	1.4	0.27
#2894	15.76	11.96		14.46				2.5	11.14	1.25	0.65	
#288	29.24	0.12	0.1	10.72					0.51	0.31	0.4	
#700	47.28	11.58		24.37	14.81			9.22	3.26		0.1	
#845	44.4	4.32		20.08	0.15	3.95		0.88	0.31	0.57	0.23	0.16
#806	49.92	18.4		9.64	1.34	2.04		5.9	0.84	1.4	0.13	0.3
#1998	38.5	3.6		15.2	9.3			22.7	0.6	0.4	0.8	0.1
#719	45.62	1.16		13.2	10.04	1.15		8.08	1.39	0.84	2.47	0.06
#947	32	3		17	9.3	1.5	0.27	15	1.6	0.92	2.6	
#1305	37.2	4.8		12.1	10.2	3.2	1.84	2.3	0.35	0.33	2.8	0.03
#1306	25.1	4.1		10.1	7.3	2.6	0.98	27.4	2.6	1.4	2.5	0.15
#1307	37.5	5.1		12.8	10.8	3.6	1.72	2	0.3	0.2	2.9	0.02
#851	34.86	2.46		12.2	10.36	1.7		16.76	3.01	0.85	3.05	0.07
#852	36.51	1.54		19.9	12.9	1.94		2.83	0.12	0.42	1.97	0.06
#867	40.48	3.04		13.9	8.16	1.7		1.11	0.09	0.21	0.77	0
#868	32	7.67		22.1	11.68	3.09		1.89	0.16	0.3	0.65	0.04
#869	41.2	2.47		15	7.4	1.83		2.35	1.41	0.73	0.94	0.05
#870	44.68	2.16		15.3	7.18	2.33		1.82	1.48	0.49	0.86	0.05
#3159	30.78	5.14		26.5	11.46	3		0.43	0.3	0.19	0.24	0.02
#720	34.18	2.98		18.4	7.1	2.92		2.05	1.97	0.35	2.67	0.03
#1267	42	11.8		12.3				8.3	2.1	1.9	0.24	0.12
#3160	41.84	11.81		12.29	5.25	1.95		8.34	2	1.84	0.24	0.12
#765	37.08	5.86		17	1.86	11.2	0.02	12.26	2.83	4.24	3.16	0.08
#3154	33.58	5.14		12.05	4.81	1.62		23.53	5.1	2.14	0.19	0.06
#122	32.9	1.55	1.2	6.75					2.52	2	0.94	
#123	32	1.02	0.8	6.57					1.76	2.07	0.74	
#151	25.5	6.5		6				39	14	3	1.3	
#1786	29.05	4.73		13.06	5.27			46.06	10.91	4.48	0.62	0.17
#1996	12.3	0.6		1	0.1						0.2	
#1808	49.27	13.53		10.03	2.82	13.46		6.15	0.92	1.53	1.28	1.2
#163	42.2	2.4		7.3	2.84	1.29	0.42	8.5	1.03	0.78	0.23	
#166	31.9	3.55		10.3	3.39	1.46	0.32	21.9	0.56	0.83	0.24	
#167	32	3.94		13.5	4.22	0.97	0.12	18.2	0.42	0.74	0.28	
#177	39.6	5		6.8	2.2			25.3	4	2.8	0.8	
#2134	37.08	5.86		17	1.86	11.2		12.26	2.83	4.24	3.16	
#3155	15.39	3.98		8.31	3.21	1.62		38.51	4.72	3.72	0.31	0.5
#3156	11.89	1.82		4.1	1.76	1.35		27.81	5.67	2	1.44	0.35
#2801	48.05	7.39		16.06	4.69			14.01	4.68	1.71	0.58	0.19
#804	11.9	4.59		7	2.87	2.93		15.17	3.96	6.58	23.5	0.27
#880	51.6	5.5		4.1				16	6.3	5		
#2895	48.05	7.39		16.06	4.69			14.01	4.68	1.71	0.58	0.19
#2770	8.75	3.35		4.94	1.44	0.05		57.2	13.4	5.94	1.38	1.16
#2912	21.09	5.69	0.16		6.24				9.38	7.49		

Continued from Table S1

ID-number	CaO	MgO	MnO	K_2O	P_2O_5	SO_3	Cl_2O	SiO_2	Al_2O_3	Fe_2O_3	Na_2O	TiO_2
#299	32	4.4		8.5	4.8	1.7		36.3	4.7	1.5	2.3	0.3
#1995	28.6	6.7		23.9	11.6			2.77	0.7	0.4	0.9	0.1
#2929	23	4.9		7.5	0.9	1.8		37.2	8.7	6.2	6.3	0.3
#847	9.5	2.52		7.86	2.4	11.36		38.89	14.74	9.3	0.53	0.36
#2030	39.95	4.84		9.81	2.06	1.86		23.7	4.1	1.65	2.25	0.36
#408	8.88	2.58		13.1	8.92	4.05	6	1.4	0.06	0.12	2.6	
#409	24.9	3.14		25.4	7.86	14	14.6	4.1	0.28	0.75	1.37	
#410	14.5	16		24.1	40.9			1.3	0.2	0.6	0.1	
#538	22.9	2.5		21.6	5.1	12.7	22.54	7.8	1.57	0.78	6.8	
#539	39.97	5.41		16.86	3.76	2.65		8.49	0.09	0.56	2.7	0.1
#540	46.63	4.51		7.95	5.93	3.37		12.49	2.8	4.43	0.96	0.68
#541	66	1.9		13.6	3.2	9.3		0.9	0.2	0.2	2.6	0.01
#542	50.3	2.5		21	5.9	10.9		1.3	0.4	0.2	3.8	0.02
#543	33.1	1.4		16.4	4.8	5.4		30.5	3.8	2.2	0.8	0.23
#544	26.5	1		30.7	3	6.6	12.99	0.3	0.1	0.1	5.6	0.01
#3162	29.38	0.63		16.86	8.94	10.74		3.21	0.47	0.94	0.35	0.07
#419	6.6	4.27		27.5	18.5	3.22	3.06	3.1	0.11	0.18	0.04	
#420	10.6	5.25		33.5	13.1	3.77	3.45	8.1	0.29	0.28	0.08	
#553	14.9	1.85		43.7	2.7	2.55	15.8	4.5	0.12	1.02	0.03	
#554	8.82	1.17		19.5	3.36	1.81	9.65	4.4	0.1	0.05	0.1	
#555	13.1	1.82		13.9	0.89	0.81	8.45	6.4	0.28	0.12	0.32	
#556	13.2	2.76		40.6	0.66	1.12	16.15	3.9	0.34	0.24	0.35	
#624	14	2.21		44.2	8.79	3.59	11.71	6.2	0.45	0.36	0.2	
#625	22	2.23		38	5.27	6.3	11.54	13.1	1.11	0.41	0.35	
#626	18.2	2.5		36.7	5.13	2.8	8.33	2.1	0.21	0.17	0.19	
#627	15.6	1.96		41.1	5	2.87	6.59	2.3	0.24	0.19	0.2	
#628	22.6	2.65		35.6	7.01	3.88	6.93	4.5	0.32	0.24	0.14	
#629	17	3.42		40.6	6.99	4.2	12.64	4.3	0.3	0.25	0.24	
#630	11.2	2.87		33.97	10.46	4.64		7.96		51	3.64	
#1902	27.7	3.1		28.4	8.2	1.9	10.78	3.3	0.3	0.3	0.7	
#1993	27.7	3.1		28.4	7.6			3.3	0.3	0.3	0.7	
#432	5.1	0.77		5.6	1.22	0.91	5.51	59.4	0.38	0.22	0.26	
#433	8.3	2.22		26.1	2.73	4.43	29.16	33.8	0.28	0.28	4.11	
#434	5.6	1.81		14.54	1.88	2.57		67.93	0.09	0.16	0.38	0.1
#435	11.6	1.79		14.5	4.06	2.9		50.92	0.09	0.4	1.01	0.1
#436	8	1.1		33	4.2	3.1	32.34	35.4	0.1	0.1	1.5	0.01
#437	8	1.6		21.6	2.6	2.4		59.3	0.2	2	2.3	0.02
#438	3.22	4.84		8.01	11.56	1.8		44.7		2.6	5.25	
#439	14.7	2		24.4	4.1	4.8		47.1	0.2	0.1	1.5	0.01
#440	5.2	1.6		8.8	3.4	2		69.8	2.1	6.3	0.3	0.17
#441	8.1	1.6		26	5	2.8	7.84	47.6	0.3	0.2	1	0.02
#946	18	2.1		41	4.9	4.3	11.03	22	0.64	0.67	1.9	
#3169	4.48	2.16		19.27	2.52	1.42		62.04	0.19	0.17	0.44	0.02
#517	0.46	2.7		10.28	0.66	2.2		71.7		7.1	0.33	
#518	3.9	3.08		10.3	10	11.08		50.7		3.14	0.53	
#519	0.56	4.78		8.37	2.06	7.2		63.3		4.72	0.47	
#704	8.66	6.11		20.67	8.68			54.04	1.99		0.15	
#401	4	0.59		18.5	4.7	1.3	27.93	61.7	0.72	0.17	0.23	
#533	3.5	3		38.7	9.2	1.8	9.07	31.2	0.38	0.56	0.73	

Continued from Table S1

ID-number	CaO	MgO	MnO	K_2O	P_2O_5	SO_3	Cl_2O	SiO_2	Al_2O_3	Fe_2O_3	Na_2O	TiO_2
#534	9.9	4.25		21.8	2.18	2.03	10.71	36.4	0.51	0.59	0.08	
#516	1.05	3.32		9.59	2.98	3.48		55.3		2.4	0.73	
#444	1.9	1.8		13.5	1.4	0.7		73	1.4	0.6	0.4	
#448	0.72	0.83		11.9	8.87	1.51		75.2		0.58	0.28	
#449	0.88	2		14.5	0.9	1.83		78.6		0.44	0.44	
#450	0.7	2		13	0.8	1.69		78.3		0.36	0.43	
#451	1.1	2.5		15.85	1.1	1		75		0.47	0.54	
#702	1.97	2.05		5.72	1.67			80.68	1.49	0.88	0.74	
#994	3.01	1.75		12.3	1.41	1.24		74.67	1.04	0.85	0.96	0.09
#2001				16.6				72.2	0.1		0.4	
#2802	1.74	1.79		13.02	0.66			82.13	0.1	0.11	0.15	0.01
#2896	1.74	1.79		13.02	0.66			82.13	0.1	0.11	0.15	0.01
#2002				2				82.2	4.4		0.6	
#737	2.09	1.32		2.21	0.63	0.36		91.6	0.82	0.5	0.19	0.02
#736	2.12	0.86		2.03	0.39	0.32		93.13	0.98	0.46	0.18	0.05
#735	2.36	2.17		7.45	1.68	0.86		81.3	0.59	0.74	1.57	0.07
#766	1.61	1.89		11.3	2.65	0.84		74.31	1.4	0.73	1.85	0.02
#547	9.7	1.87		28.9	4.85	4.19	17.52	23.2	0.23	0.22	0.12	
#548	2.96	1		2.1	0.64	0.55	0.32	67.9	0.26	0.18	0.04	
#558	9.9	3.36		33.6	7.8	2.93	12.5	30.1	0.86	0.41	0.22	
#559	26.5	3.42		11.4	0.89	1.23	5.41	44.3	3.42	2.03	0.51	
#560	11.8	3.69		18.2	5.2	3.64	4.29	43	1.83	1.5	0.17	
#561	8.8	3.6		24	6.5	3.4	4.66	45.1	1.19	0.71	0.45	
#562	8.1	4		28.6	6.2	3.6	5.39	46	0.53	0.39	0.48	
#563	23.8	4.43		20.4	4.19	1.04	9.82	16.2	0.52	0.34	0.12	
#564	8	2.87		13.5	4.59	4.29	4.09	52.7	3.51	1.82	0.32	
#3166	8.95	2.65		8.19	2.98	3		57.76	0.66	0.53	1.31	0.05
#424	4.1	1.96		11.2	6.42	1.12	4.8	35.3	0.35	0.25	0.08	
#425	2.7	1.56		12.2	5.68	1.15	6.1	38.6	0.26	0.19	0.06	
#426	4.1	1.04		17.4	2.16	1.56	9.41	61.5	0.57	0.28	0.1	
#427	4.3	2.65		15.1	7.86	1.49	7.03	45.5	0.33	0.22	0.15	
#454	4.03	0.75		5.9	2.75	0.83	0.42	62.5	0.48	0.29	0.21	
#455	8.7	2.27		26.2	2.18	4.56	15.61	39.2	0.2	0.19	0.16	
#456	5.1	2.22		23.9	2.05	1.47	17.71	59.3	0.16	0.11	0.11	
#457	4.4	0.81		20.1	2.74	1.55	10.14	66	0.17	0.09	0.14	
#459	12.03	3.7		24.1	3.02	6.02		42.79	0.09	0.39	1.54	0.1
#460	9.18	1.92		12.3	3.07	2.55		69.41	0.09	0.4	0.3	0.1
#462	4	1.2		16.3	2	2.5		72.5	0.2	0.1	0.1	0.02
#463	7.6	1.3		22	2.9	3.5		61.1	0.3	0.2	0.3	0.01
#464	3.7	1.4		16.8	3.6	2.1		71.1	0.5	0.2	0.2	0.02
#465	5.9	1.3		16.7	1.9	2.4		70.8	0.1	0.1	0.2	0.01
#466	17	2.6		22	7.4	6.6		42.6	0.4	0.2	0.4	0.02
#467	7.3	1.8		19.1	3.4	3.9		63	0.2	0.3	0.5	0.02
#468	11.4	1.2		16.3	2.6	3.2		60.6	1.5	2.2	0.3	0.11
#470	10	2.1		21.4	2.8	6.4		55.4	0.3	0.3	0.6	0.02
#472	5.97	2.53		19.3	1.72	4.43		40.58	2.66	0.98	9.77	0.12
#475	2.6	2.4		22.8	1.2	1.7		55.7	1.8	0.7	0.9	
#476	4.91	2.55		21.7	2.04	4.44		37.06	2.23	0.84	9.74	0.17
#703	2.79	2.62		11.4	1.35			65.49	1.94	1.03	1.85	

Continued from Table S1

ID-number	CaO	MgO	MnO	K_2O	P_2O_5	SO_3	Cl_2O	SiO_2	Al_2O_3	Fe_2O_3	Na_2O	TiO_2
#712	9.33	1.58		7.96	3.49			63.15	2.16	1.36	0.91	
#713	12.2	2.58		9.63	4.28			54.64	0.59	0.89	1.49	
#760	10.79	4.19		36.15	6.5	2.47		27.26	0.73	0.76	0.97	
#945	8.1	1.8		14	2.4	2.6	1.35	62	1.7	2	0.36	
#990	12.27	2.48		12.9	4.3	2.49		55.32	0.84	1.05	1.51	0.22
#991	9.95	2.45		25.2	3.32	4.92		46.07	1.69	1.85	1.18	0.09
#992	6.14	1.06		25.6	1.26	4.4		55.32	1.88	0.73	1.71	0.08
#1271	8.1	2		20.2				58.2	0.8	0.7	0.5	0.03
#1903	7.9	2.4		25.3	4.7	4	9.07	30.6	0.5	0.4	0.7	
#1965	14.4	4.3		14.06		5.27	6.69	39.2	3.85		4.3	
#2141	10.2	2.5		36.7				36.6	0.8	0.6	2.3	
#3161	7.28	1.82		16.86	2.27	1.1		59.9	0.81	0.54	0.42	0.04
#1302	6.3	2		21.3	2.3	3.5	8.58	54	0.12	0.06	0.23	0.01
#1308	6.5	2		19	2.6	3.9	7.11	55	0.1	0.9	0.2	0.01
#1310	6.4	2		22	2.4	5.6	5.88	54	0.14	0.08	0.4	0.01
#1303	14	2.6		21	4.2	5	1.59	42	0.4	0.2	0.3	0.02
#1309	15	3		24	4	5.4	1.72	43	0.4	0.2	0.4	0.02
#1311	14	2.6		22	4	5	1.96	38	0.4	0.2	0.3	0.02
#2804	9.2	1.8		21.9	3.2	4	13.72	52	0.6	1.1	0.3	
#714	7.62	1.67		11.73	2.77			57.79	0.38	0.58	0.72	
#1966	4.43	0.92		13.12		5.9	7.3	38.5	1.73		3.3	
#739	5.84	2.37		5.81	3.35	1.68		61.79	2.85	1.62	3.48	0.04
#767	4.66	2.51		18.4	1.47	5.46	36.02	35.84	2.46	0.97	10.5	0.15

Table S2. Ash fusion behaviour (IDT, SOT, HT and FT; °C for all) dataset of four different ash categories (black font for hardwood ash; red font for softwood ash; blue font for eudicot straw ash; green font for grass straw ash).

ID-number	IDT	SOT	HT	FT
#77	1365			1380
#91	1360			1380
#947	1110		1470	1500
#3159	1490			
#3160	1150	1180	1200	1225
#3154	1210	1225	1250	1275
#151	1193		1277	1266
#1786	1198	1219	1228	1235
#1808	1343	1354	1360	1377
#163	1110	1640	1700	1750
#166	1140	1580	1630	1660
#167	1340	1410	1750	1800
#177	1340	1410	1700	1700
#3155	1175	1205	1230	1250
#3156	1180	1190	1205	1235
#2801	1236	1244	1246	1249
#880	1343		1400	1400
#299	1170		1180	1200
#408	1380	1590	1640	1660
#409	900	1420	1660	1750
#410	1000	1120	1140	1140
#538	920	1380	1460	1530
#539	1380		1400	1420
#3162	1500			1600
#419	1100	1180	1300	1340
#420	1020	1100	1750	1800
#553	600	620	650	680
#554	820	920	1640	1650
#555	700	780	1750	1800
#556	620	630	670	700
#624	820	840	1560	1590
#625	1130	1500	1650	1670
#626	650	680	760	1680
#627	660	680	710	710
#628	650	680	1620	1750
#629	800	820	1640	1650
#630	700			1550
#1902	1550	1580		
#432	900	1000	1110	1180
#433	720	760	1010	1080
#435	1120		1180	1230
#438	925			1100
#946	1160		1230	1250
#3169	750			1050
#517	980			1140
#518	820			1091
#519	1120			1235
#401	920	1040	1140	1200

Continued from Table S2

ID-number	IDT	SOT	HT	FT
#533	830	960	1050	1130
#534	930	1050	1120	1140
#516	1010			1180
#448	823			1190
#449	850			1280
#450	1060			1250
#451	985			1200
#2802	1240	1378	1429	1470
#547	840	850	1030	1100
#548	880	1120	1270	1320
#558	920	950	1040	1040
#559	1140	1220	1250	1250
#560	850	1060	1120	1140
#561	900	1000	1080	1130
#562	950	1050	1070	1130
#563	1260	1350	1440	1490
#564	1120	1150	1200	1250
#3166	975	1090	1257	1340
#424	970	1020	1120	1180
#425	980	1020	1130	1190
#426	780	800	1140	1260
#427	1010	1020	1170	1220
#454	900	1110	1270	1330
#455	860	900	1040	1080
#456	820	880	1050	1210
#457	800	860	1130	1220
#459	1080		1280	1500
#945	790		1120	1320
#1903	900	1040	1170	1190
#3161	860	1030	1045	1365
#1302	850		1090	1200
#1303	870		1050	1240

Table S3. Proximate and ultimate analysis (wt. % of biomass) dataset of four different biomass categories (black font for hardwood; red font for softwood; blue font for eudicot straw; green font for grass straw).

ID-number	Carbon	Hydrogen	Nitrogen	Sulphur	Oxygen	Ash content	Volatile matter	Fixed carbon
#2142	49.8	6.3	0.1	0.1	43.7	0.6	84	15.4
#803	50.12	5.94	0.03	0.01	43.9	0.31	86.22	13.47
#2894	51.01	8.12	0.58	0.02	40.26	3.71	83.64	12.65
#700	50.03	6.07	0.23	0.05	43.6	1.22	85.07	13.71
#845	51.65	5.99	0.6	0.02	41.71	1.6	86.14	12.26
#806	51.57	6.23	0.62	0.02	41.55	2.7	84.81	12.49
#1998	49.54	6.32	0.51	0	44.14	1.9	82.6	15.5
#719	49.56	5.95	0.36	0.03	44.1	0.95	85.24	13.81
#947	50.36	6.74	1.12	0.1	41.64	2.1	78.6	19.3
#1305						4.59		
#1306						4.01		
#851	48.47	5.9	0.64	0.06	44.91	1.1	84.91	13.99
#852	50.9	6.08	0.51	0.07	42.43	1.2	83.05	15.75
#867	49.69	6.14	0.72	0.06	43.37	1.7	82.16	16.14
#868	50.51	6.09	0.66	0.09	42.64	1.5	81.83	16.67
#869	50.77	6	0.62	0.07	42.53	1.71	82.22	16.07
#870	49.47	6.11	0.36	0.04	44	1.06	84.13	14.81
#3159	50.29	6.17	0.4	0.03	43.1	1.18	79.9	18.92
#720	50.61	6.04	0.98	0.13	42.24	2.34	79.66	18
#1267	51.05	6.01	0.1		42.83	0.1	83.1	16.8
#3160	51.04	5.99	0.08	0	42.85	0.08	83.1	16.82
#3154	52.11	6.14	0.3	0.01	41.44	0.6	80	19.4
#151	55	5.8	0.1	0.1	39	3	73	24
#1786	52.88	4.84	0.53	0.15	41.6	3.03	75.56	21.41
#1996	52.77	5.85	0.2		41.27	0.9	81.9	17.2
#1808	51.31	6.36	0.25	0.01	42.07	0.22	83.15	16.63
#163	51.59	5.59	0.12	0.01	42.68	0.96		
#166	50.74	5.7	0.11	0.01	43.43	0.28		
#167	50.81	5.68	0.11	0.01	43.38	0.32		
#177	50.85	5.68	0.11	0.01	43.34	0.3		
#2134	50.97	6.02	0.3		42.7	0.5	83.69	15.81
#3155	51.99	6.18	0.41	0.02	41.4	1.33	79.3	19.37
#3156	53.15	6.04	0.94	0.04	39.82	4.05	74.1	21.85
#2801	54.83	5.9	0.08	0.02	41.29	1.2		
#804	51.44	6	0.06	0.03	42.27	0.41	82.11	17.48
#880	53.4	5.9	0.1		40.6	2.17	74.33	23.5
#2895	53.64	5.77	0.1	0	40.49	1.2		
#2770	49.15	6.41	0.2	0.2	44.04	0.1	84.7	15.2
#2912	49	6.4	0.14	0.01	44.45	1.59	87.5	10.91
#1995	48.79	6.07	0.71		45.14	1.2	75.9	22.9
#2929	53.3	6.2	0.1	0.01	40.4	1.03	81.85	17.12
#847	54.43	5.89	0.55	0.42	38.72	5.21	73.99	20.8
#2030	49.8	6	0.4	0.02	43.76	1.06	84.57	14.37
#408	54.07	6.82	2.43	0.42	35.98	5.54		
#409	53.97	6.57	1.99	0.71	36.06	7.66		
#410	53.58	7.32	5.39	0.82	32.86	6.3		
#538	49.47	5.68	1.55	0.33	41.87	9.73		

Continued from Table S3

ID-number	Carbon	Hydrogen	Nitrogen	Sulphur	Oxygen	Ash content	Volatile matter	Fixed carbon
#539	43.22	5.27	0.87		50.59	3.85	76.5	19.65
#540	40.39	4.61	0.8		54.12	3.8	78.8	17.4
#3162	49.52	6.07	0.08	0.22		2.86	79.2	17.94
#419	62.52	7.39	2.07	0.12	27.77	3.51		
#420	56.45	6.01	1.34	0.13	35.99	2.95		
#553	49.87	5.56	1.38	0.11	42.04	12.9		
#554	53.12	6.26	2.15	0.24	37.65	11.95		
#555	48.1	5.66	1.11	0.12	44.13	11.14		
#556	49.91	5.52	0.34	0.03	43.45	8.82		
#624	50.26	5.54	3.68	0.18	39.69	10.28		
#625	50.95	5.77	3.68	0.34	38.66	10.71		
#626	49.77	5.68	1.86	0.13	42.23	6.92		
#627	50.3	5.72	3.24	0.26	40.14	10.1		
#628	51.03	5.91	3.18	0.29	39.25	9.17		
#629	51.74	5.73	2.33	0.16	39.5	10.71		
#1902	51.04	6.45	3.39	0.17	38.91	8.5		
#1993	49.67	6.62	2.76	2.21	40.73	9.4	73.9	16.7
#432	49.18	5.81	0.43	0.06	44.08	4.86		
#433	49.79	5.64	0.78	0.13	42.63	5.88		
#434	47.9	6.18	0.45	0.21	44.89	4.26	76.8	18.94
#435	49.25	6.34	0.83	0.36	42.81	6.4	75.4	18.2
#946	48.54	6.32	0.82	0.15	43.87	2.73	79.9	17.37
#3169	49.09	6.06	0.64	0.08	44.14	5.88	76.1	18.02
#704	49.31	6.04	0.7	0.11	43.56	5.06	80.86	14.08
#401	48.77	5.87	0.45	0.05	43.25	8.5		
#533	49.57	5.65	0.8	0.04	43.58	2.69		
#534	48.13	5.73	0.36	0.04	45.57	5.29		
#444	48.09	5.86	1.69	0.14	43.64	19.09		
#702	49.15	6.23	1.59	0.13	42.13	20.15	65.62	14.23
#994	47.02	6.39	1.07	0.22	44.58	18.67	65.47	15.86
#2001	48.47	5.63	0.86	0.13	44.55	18.3		
#2802	53.43	4.94	0.76	0.08	50.38	22.1		
#2896	49.42	4.62	0.77	0.13	44.42	22.1		
#2002	48.72	6.03	0.77	0.15	44.36	22		
#737	48.14	6.27	0.73	0.07	44.72	17.84		
#736	48.32	6.27	0.58	0.07	44.68	17.1		
#735	47.87	6.2	0.57	0.08	44.81	17.59		
#766	46.64	5.9	0.64	0.11	45.8	18.63		
#547	49.76	5.54	0.48	0.06	43.73	4.57		
#548	49.64	5.85	0.25	0.04	44.16	3.98		
#558	50.19	5.17	1.45	0.08	42.7	6.79		
#559	49.45	4.85	0.36	0.02	44.97	7.34		
#560	48.52	6	0.8	0.05	44.49	6.96		
#561	48.78	5.87	1.17	0.08	43.81	5.48		
#562	49.08	5.9	1.18	0.07	43.38	5.42		
#563	47.7	6.1	1.34	0.06	44.37	7.44		
#564	51.46	5.71	1.01	0.08	41.42	10.18		
#3166	49.65	6.09	0.42	0.09	43.74	4.74	77.2	18.06
#424	48.46	5.79	1.74	0.11	43.64	5.04		

Continued from Table S3

ID-number	Carbon	Hydrogen	Nitrogen	Sulphur	Oxygen	Ash content	Volatile matter	Fixed carbon
#425	48.83	5.7	1.32	0.09	43.67	4.58		
#426	52.12	5.48	0.51	0.08	41.36	7.36		
#427	48.46	5.8	1.62	0.12	43.73	5.16		
#454	49.71	5.83	0.29	0.03	44.09	3.22		
#455	49.99	5.53	0.49	0.08	43.48	4.35		
#456	50.34	5.57	0.4	0.06	42.94	7.17		
#457	49.74	5.61	0.55	0.06	43.53	6.63		
#459	48.24	6.07	0.8	0.25	44.36	8.95	73.4	17.65
#460	49.74	6.33	1.06	0.17	42.55	7	75.8	17.2
#472	47.42	5.76	0.63	0.39	43.56	9.44		
#475	48.84	5.83	0.96	0.21	43.92	7.35		
#476	47.43	5.65	0.59	0.32	43.74	9.55	71.11	19.34
#703	49.06	6.17	1	0.2	43.29	8.24	75.54	16.22
#712	49.63	6.08	0.75	0.12	43.15	5.82	78.72	15.47
#713	49.47	6.1	0.6	0.1	43.55	3.89	81.23	14.88
#760	47.59	5.98	0.57	0.12	45.71	3.41	78.8	17.79
#945	50.43	6.2	0.75	0.18	42.26	6.4	77.3	16.3
#990	49.47	6.1	0.61	0.09	43.54	3.89	81.24	14.87
#991	49.08	5.95	0.45	0.2	44.18	4.32	78.62	17.06
#992	48.31	5.87	0.47	0.17	44.92	7.02	75.27	17.71
#1271	49.09	5.96	0.53	0.09	44.01	6.1	75.8	18.1
#1903	47.61	6.06	0.85	0.1	45.27	5.9		
#1965	47.24	5.49	0.85	0.46	45.51	7.5	76	16.5
#2141	49.7	6.1	0.5	0.2	42.4	5.2	77.8	17
#3161	49.64	6.16	0.61	0.07	43.54	4.71	77.7	17.59
#1302	49.3	6.42	0.48	0.17	43.2	7.1	74.9	18
#1308	49.35	6.42	0.48	0.17	43.14	7.2	74.9	17.9
#1310	49.09	6.39	0.48	0.17	43.44	6.7	74.9	18.4
#1303						3.3		
#1309						2.94		
#1311						3.3		
#2804	49.33	6.63	0.57	0.14	43.33	7.79		
#714	49.32	6.02	0.73	0.1	43.36	5.89	78.93	15.18
#1966	50.34	6.34	0.66	0.26	42.07	5.04	77.23	17.73
#739	48.82	6.1	0.68	0.1	44.07	6.45		
#767	48.72	5.87	0.78	0.45	41.87	12.78		

Table S4. Heavy metal concentration (mg/kg) dataset of four different ash categories (black font for hardwood; red font for softwood; blue font for eudicot straw; green font for grass straw).

ID-number	Pb	Cd	Cu	Cr	Hg
#92	220	10	120		
#288	50	10	60		
#122	330	10	400		
#123	350	10	210		
#1786	22		115	70	
#163	29	1.7	148		1.8
#166	18	1.1	1290		1.7
#167	40	0.7	333		0.1
#177	13	0	324	127	
#2912			3879		
#408	3	0	33		0
#409	3	0.1	36		0
#410	0	0	75	7	
#538	27	0.1	82		0
#419	2	0.3	253		0
#420	13	0.1	340		0
#553	6	0	62		0
#554	5	0.1	84		0
#555	1	0	53		0
#556	1	0	38		0
#624	4	0	59		0
#625	9	0.1	98		0
#626	1	0.1	55		0
#627	1	0	89		0
#628	2	0	68		0
#629	4	0	81		0
#432	8	0	57		0
#433	2	0.2	36		0
#401	3	3	5.3		0
#533	255	0	270		0
#534	3	0.1	67		0
#547	3	0.1	34		0
#548	5	0	25		0
#558	25	0.4	138		0
#559	60	0.1	49		0
#560	22	0.3	84		0
#561	41	0.1	114		0
#562	33	0.4	95		0
#563	3	0.1	83		0
#564	40	0.1	57		0
#424	2	0.1	33		0
#425	2	0.2	37		0
#426	2	0	17		0
#427	4	0.2	46		0
#454	20	0	23		0
#455	3	0.1	28		0
#456	1	0	16		0
#457	2	0	13		0

Table S5. Median and range of biomass feedstock properties (wt. % of biomass). K-W *H* shows the Kruskal-Wallis *H* statistic with level of significance (** denotes p <0.001; * denotes p <0.05: degrees of freedom = 3 for all tested items in the left-hand column). Different superscript letters in a row indicate a significant difference in median value between sample populations based on post-hoc pairwise comparisons (Dunn's Test with Bonferroni correction, p <0.05).

Item	Hardwood	Softwood	Eudicot Straw	Grass Straw	K-W *H*
Volatile matter	83.6 (78.6-86.2)^{a}	81.9 (73.0-87.5)^{ab}	77.7 (73.9-79.2)^{bc}	76.5 (65.7-81.2)^{c}	28.7**
Fixed Carbon	15.4 (12.3-19.3)^{a}	17.3 (10.9-24.0)^{b}	17.7 (16.7-19.7)^{ab}	17.5 (14.1-19.3)^{b}	13.3*
Carbon	50.3 (48.5-51.7)^{a}	51.5 (48.8-55.0)^{a}	50.3 (40.4-62.5)^{a}	49.1 (46.6-53.4)^{b}	49.8**
Hydrogen	6.1 (5.9-8.1)^{a}	6.0 (4.8-6.4)^{a}	5.8 (4.6-7.4)^{a}	6.0 (4.6-6.6)^{a}	6.6
Nitrogen	0.58 (0.03-1.12)^{ab}	0.13 (0.06-0.94)^{a}	2.07 (0.08-5.39)^{c}	0.68 (0.25-1.74)^{b}	59.3**
Sulphur	0.05 (0.01-0.13)^{a}	0.01 (0.01-0.42)^{a}	0.22 (0.03-2.21)^{b}	0.11 (0.02-0.46)^{c}	46.8**
Oxygen	43.1 (40.3-44.9)^{ab}	42.2 (38.7-45.1)^{a}	39.6 (27.8-54.2)^{a}	43.7 (41.4-50.4)^{b}	36.7**

Table S6. Median and range of contaminant trace metal concentrations (mg/kg) for ashes derived from different types of biomass. K-W *H* shows the Kruskal-Wallis *H* statistic with level of significance (** denotes p <0.001; * denotes p <0.05: degrees of freedom = 3 for all tested items in the left-hand column). Different superscript letters in a row indicate a significant difference in median value between sample populations based on post-hoc pairwise comparisons (Dunn's Test with Bonferroni correction, p <0.05).

Item	Hardwood	Softwood	Eudicot Straw	Grass Straw	K-W *H*
Cu	90 (60-120)^{ab}	329 (115-3879)^{b}	72 (33-340)^{a}	42 (5-270)^{a}	20.5**
Pb	135 (50-220)^{ab}	29 (13-350)^{a}	3 (0-27)^{b}	4 (1-255)^{ab}	16.1*
Cd	10.0 (10.0-10.0)^{a}	1.4 (0-10)^{a}	0.0 (0.0-0.3)^{b}	0.1 (0.0-3.0)^{ab}	16.1**
Cr	No data	99 (70-127)	7 (7-7)	No data	1.5
Hg	No data	1.7 (0.1-1.8)^{a}	0.0 (0.0-0.0)^{b}	0.0 (0.0-0.0)^{b}	38.9**

Table S7. Median and range of the initial deformation temperature (IDT), softening temperature (SOT), hemispherical temperature (HT), fluid temperature (FT), for ashes derived from different types of biomass (all °C). K-W *H* shows the Kruskal-Wallis *H* statistic with level of significance (** denotes p <0.001; * denotes p <0.05: degrees of freedom = 3 for all tested items in the left-hand column). Different superscript letters in a row indicate a significant difference in median value between sample populations based on post-hoc pairwise comparisons (Dunn's Test with Bonferroni correction, p <0.05).

Item	Hardwood	Softwood	Eudicot Straw	Grass Straw	K-W *H*
IDT	1363 (1110-1490)^{a}	1196 (1110-1343)^{a}	860 (600-1550)^{b}	910 (720-1260)^{b}	27.3**
SOT	No data	1244 (1180-1640)^{a}	920 (620-1590)^{b}	1025 (760-1378)^{b}	14.1*
HT	1470 (1470-1470)^{ab}	1264 (1180-1750)^{b}	1560 (650-1750)^{b}	1125 (1010-1440)^{a}	17.2*
FT	1380 (1380-1500)^{ab}	1271 (1200-1800)^{a}	1600 (680-1800)^{a}	1200 (1040-1500)^{b}	22.3**

Correlation of available trace metals concentration against ash CaO content

As for Cu, two samples with over 1000 mg/kg were excluded for the correlation analysis because both samples were obviously abnormal to others. The same applied to Pb (deleting three obviously higher values) during correlation analysis. The results are shown in Fig. S1 and Table S8.

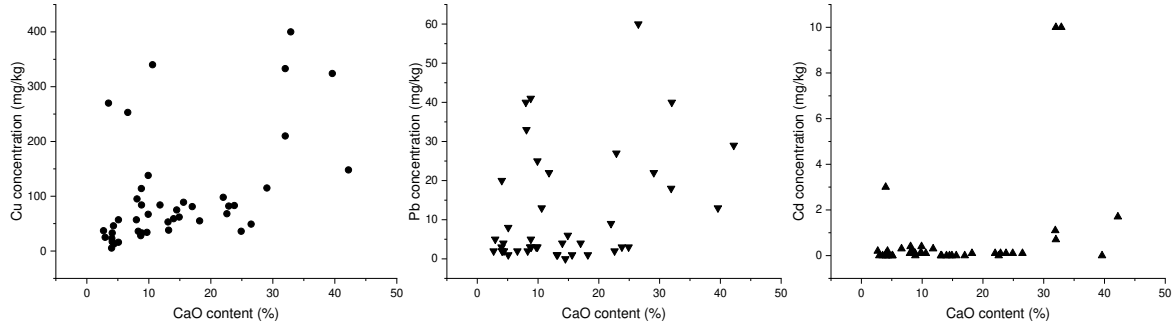

Fig. S1. Scatterplots showing Cu, Pb and Cd concentration against CaO content.

Table S8. Spearman rank correlation analysis results of Cu, Pb and Cd concentration against CaO content.

Trace metal	Spearman Rank correlation coefficient	P value	Confidence level
Cu	0.59	<0.001	99%
Pb	0.35	0.016	95%
Cd	0.30	0.046	95%

Correlation of ash melting behavior and ash chemical compositions

IDT, SOT, HT and FT are commonly used to describe ash fusion behaviour, but less was centred on their relationship with ash chemical compositions. The study by *Niu et al.* pointed that "Initial deformation temperature (IDT) increases with decreased K_2O and went up with increased MgO, CaO, Fe_2O_3 and Al_2O_3. Softening temperature (ST), hemispherical temperature (HT) and fluid temperature (FT) were not affected by the elemental concentrations as strongly [1]. One limit is that the authors just used three studied samples. However, the study by *Wile´n et al.* did not find significant correlations between the IDT and the contents of inorganic elements in biomass ash [2]. Further, SOT is generally used as the index of coal ash fusion behaviour (AFC). For biomass ash, there is no strong basis for which one of IDT, SOT, HT and FT could be a better choice to describe its AFC.

Therefore, the correlation analyses between ash melting behaviour and ash chemical compositions were carried out through SPSS software. Some significant correlation for IDT, SOT, HT and FT with ash chemical compositions was found and shown in Figs. S2-S5 and Table S9.

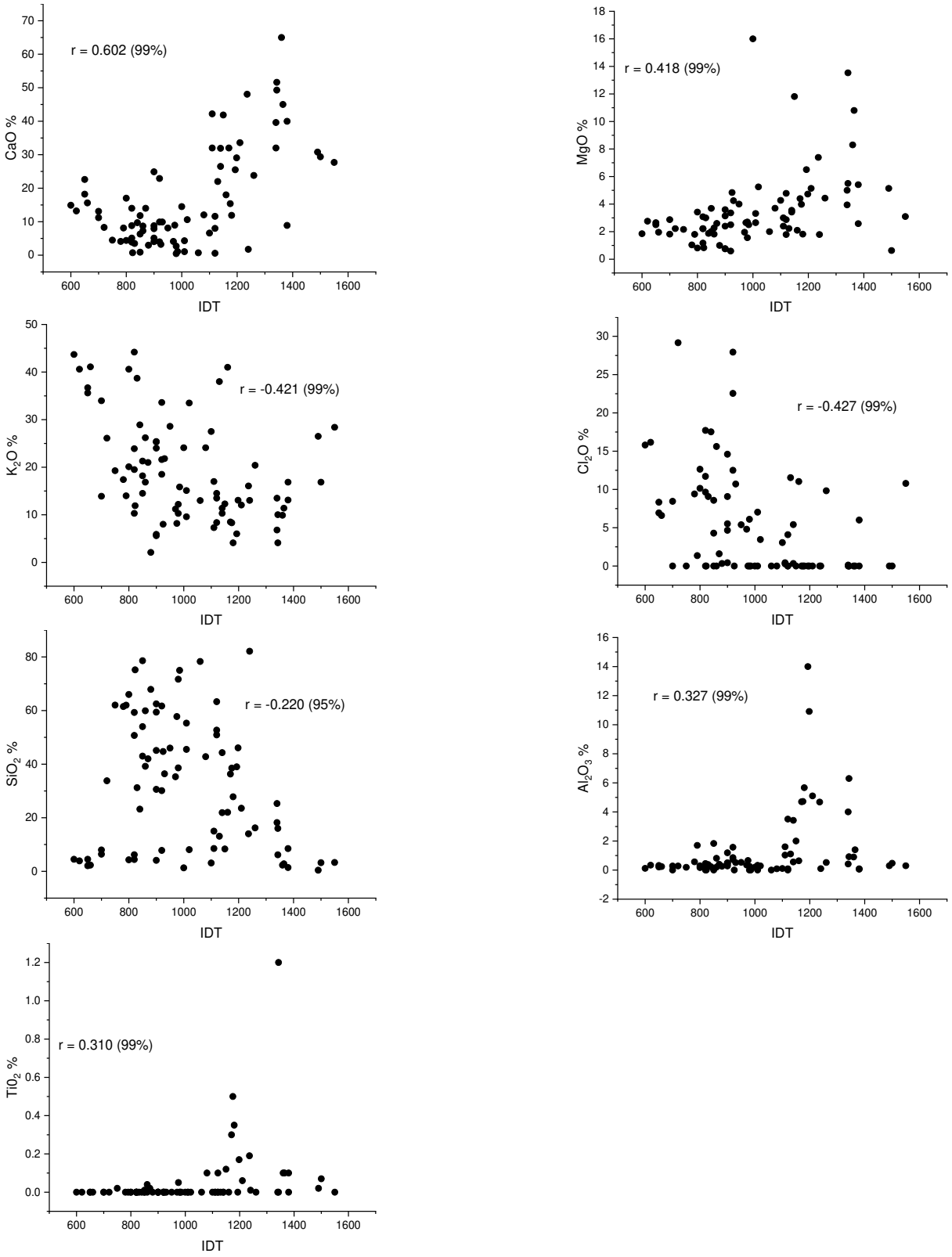

Fig. S2. Some significant correlations of ash chemical compositions against IDT (80 samples).

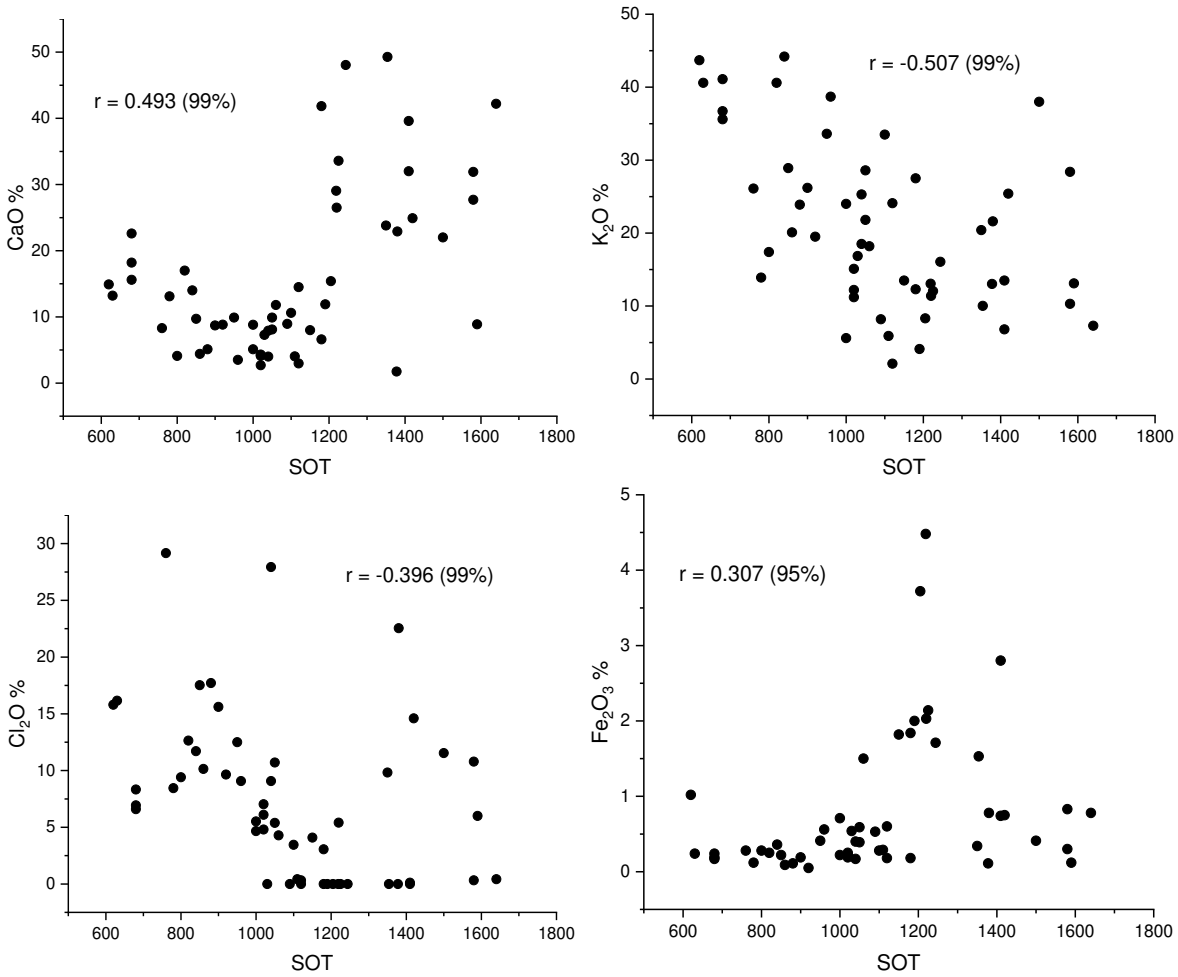

Fig. S3. Some significant correlations of ash chemical compositions against SOT (54 samples).

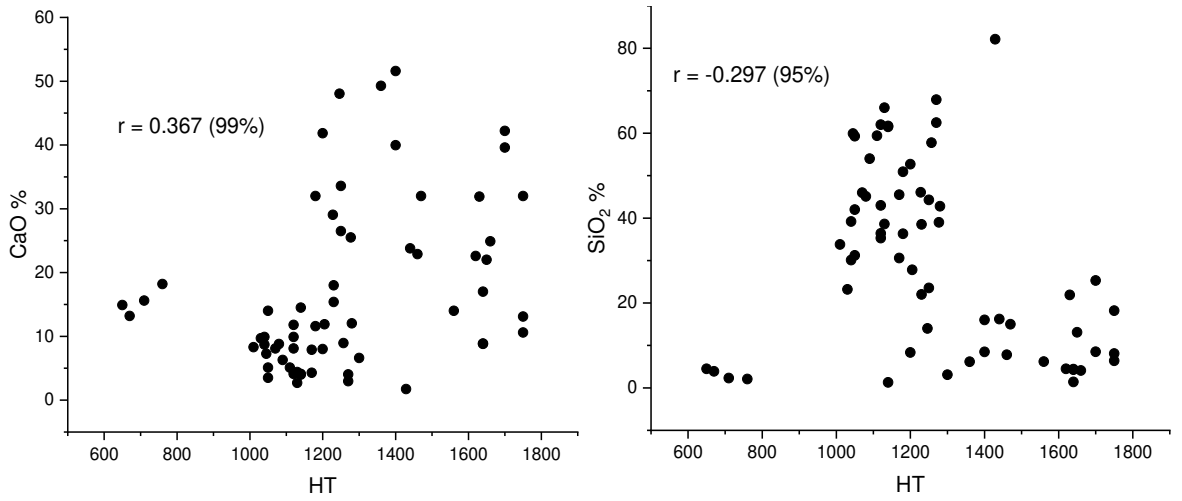

Fig. S4. Some significant correlations of ash chemical compositions against HT (64 samples).

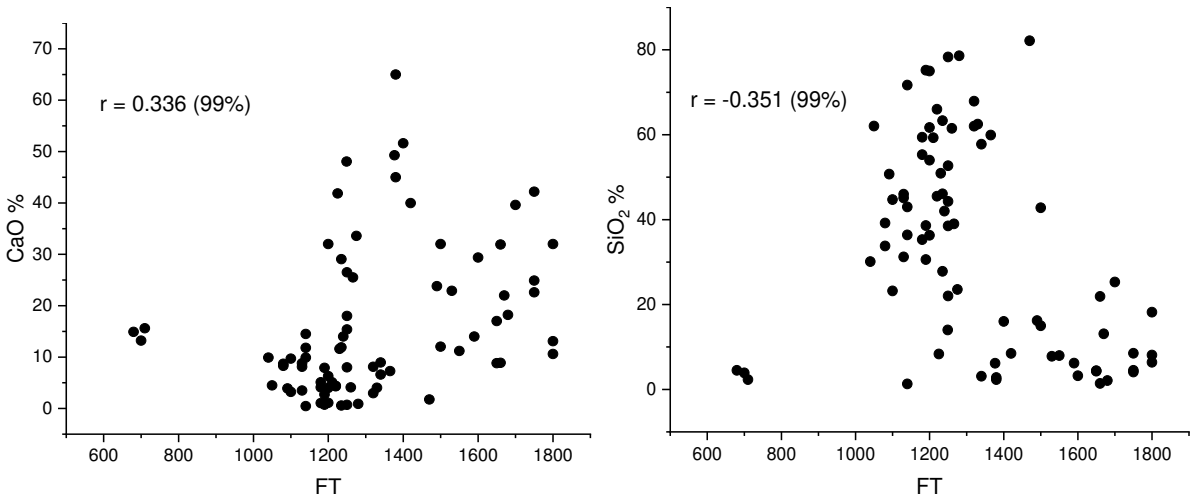

Fig. S5. Some significant correlations of ash chemical compositions against HT (78 samples).

Table S9. Some significant correlation coefficient values (r) at 99% confidence level (80 samples for IDT, 54 samples for SOT, 64 samples for HT and 78 samples for FT; * at 95% confidence level).

Item	CaO	MgO	MnO	K_2O	P_2O_5	SO_3	Cl_2O	SiO_2	Al_2O_3	Fe_2O_3	Na_2O	TiO_2
IDT	0.60	0.42	n.c.	-0.42	n.c.	n.c.	-0.43	-0.22*	0.33	n.c.	n.c.	0.31
SOT	0.49	n.c.	n.c.	-0.51	n.c.	n.c.	-0.40	n.c.	n.c.	0.31*	n.c.	n.c.
HT	0.37	n.c.	n.c.	n.c.	n.c.	n.c.	n.c.	-0.30*	n.c.	n.c.	n.c.	n.c.
FT	0.34	n.c.	n.c.	n.c.	n.c.	n.c.	n.c.	-0.35	n.c.	n.c.	n.c.	n.c.

n.c.: no significant correlation.

Based on the results shown in Figs. S2-S5 and Table S9, it could be seen that IDT has significant correlation with 7 chemical compositions including IDT-SiO_2 correlation at 95% confidence level. In general, IDT showed a positive relationship with element concentrations of CaO, MgO Al_2O_3 and TiO_2. Meanwhile, a negative correlation between IDT and K_2O, Cl_2O and SiO_2 was found. Comparatively, SOT has significant correlation with 4 chemical compositions, including 2 positive correlation with CaO and Fe_2O_3 and 2 negative correlations with K_2O and Cl_2O. With regard to HT and FT, significant correlation with only 2 chemical compositions was found. By comparison, IDT, as the index of ash melting behavior, showed the closest correlation with ash chemical compositions. Therefore, these results provided firm support to use IDT as the better index for describing ash fusion characteristics.

S.I. References

[1] Y. Niu, H. Tan, X. Wang, Z. Liu, H. Liu, Y. Liu, T. Xu, Study on fusion characteristics of biomass ash, Bioresource technology 101 (2010) 9373-9381.
[2] C. Wilén, A. Moilanen, E. Kurkela, Biomass feedstock analyses, Technical Research Centre of Finland1996.