Lodging Variability in Sorghum Stalks Is Dependent on the Biomechanical and Chemical Composition of the Stalk Rinds

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Supplementary Material

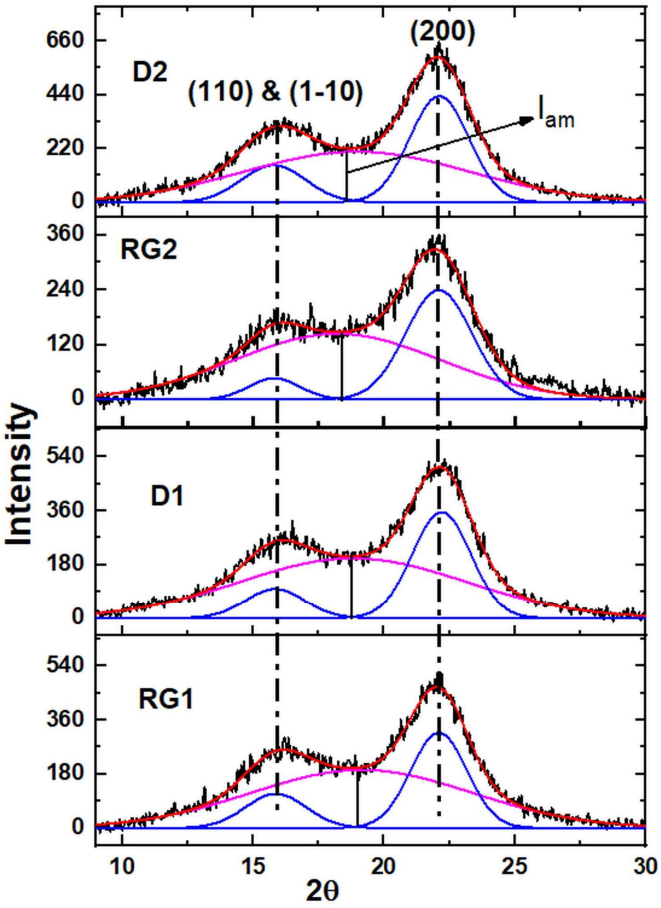

Figure S1. XRD diffractograms of powdered sorghum rinds from D2, RG2, D1 and RG1. The diffraction was performed on the powder samples of rinds. The diffractogram shown was obtained after subtracting the baseline and deconvolution of the amorphous and crystalline regions using Gaussian curve-fitting. The peaks (110) and (1-10) were not detected as separate peaks.

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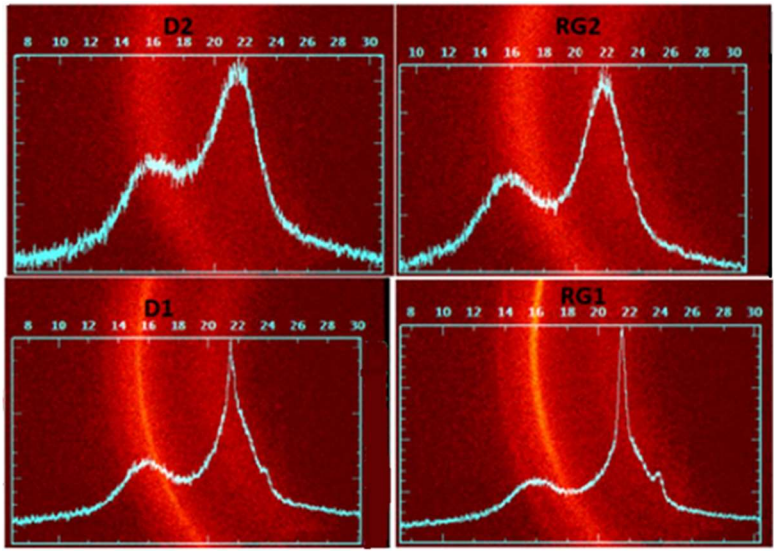

Figure S2. X-ray diffraction patterns of intact D2, RG2, D1 and RG1 rinds.

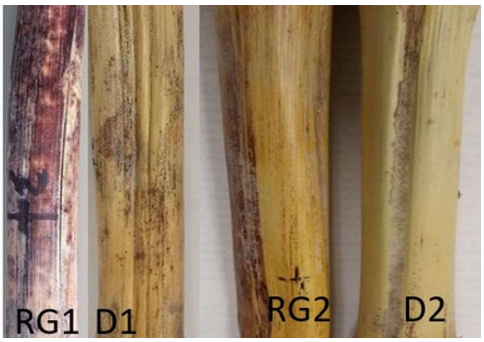

Figure S3. Representative samples for RG1, D1, RG2 and D2 stalks at Internode 2.

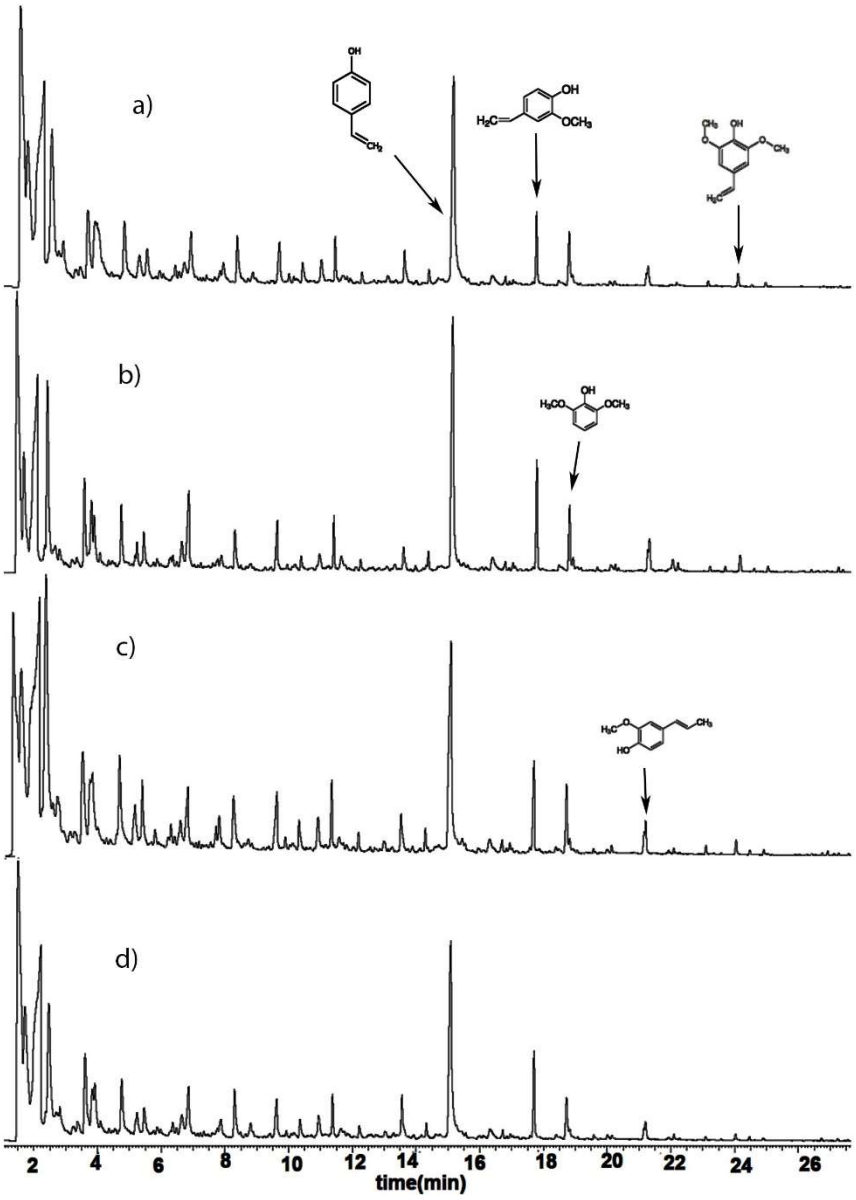

Figure S4. Py-GCMS pyrograms of rinds from a) D2, b) RG2, c) D1 and d) RG1.

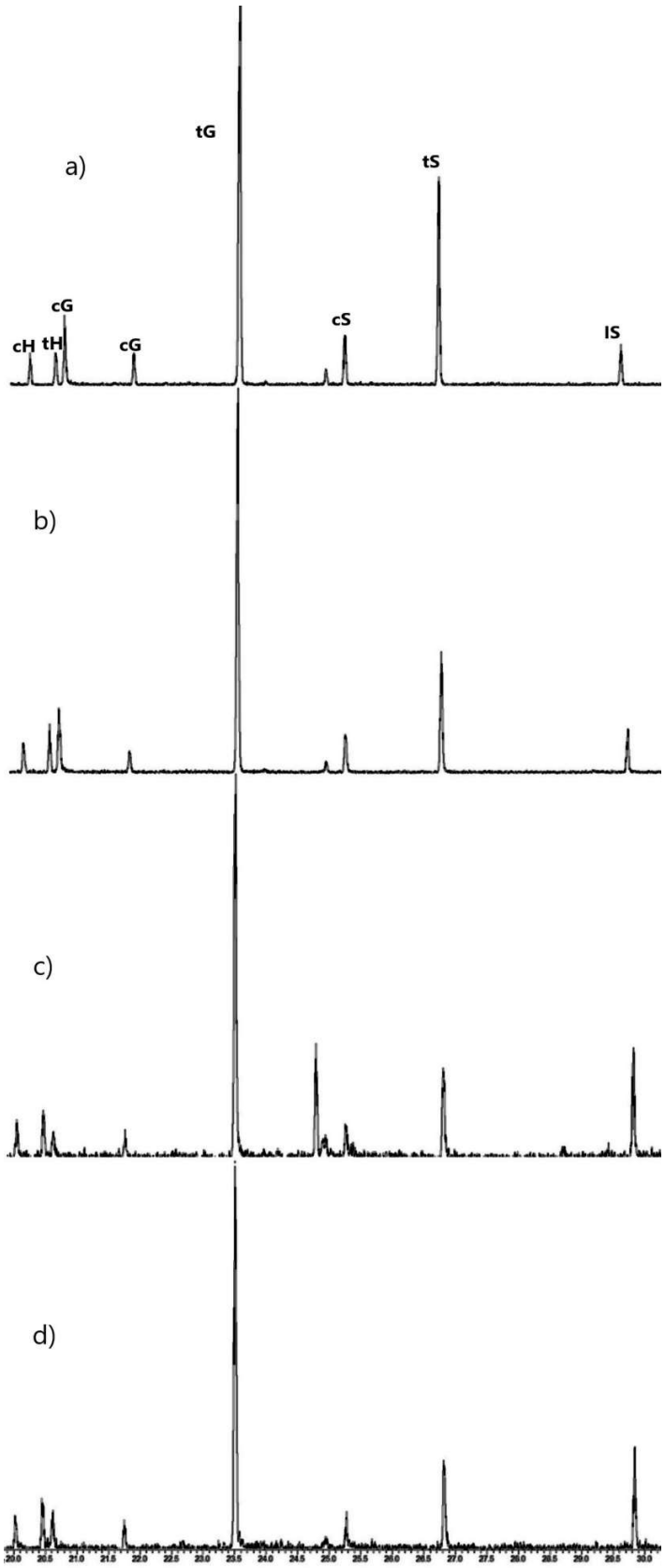

Figure S5. Chromatograms (GC-TIC) of the DFRC degradation products from the MWL isolated from sorghum stalks of: (a) D2, b) RG2, c) D1 and d) RG1. The monomers cH, tH, cG, tG, cS, represents cis- and trans- *p*-hydroxyphenyl, guaiacyl and syringyl.

Table S1. FTIR Assignments for functional groups in sorghum rinds of WT1, RG1, WT2 and RG2 assigned based on [71,93].

Wavenumber (cm^{-1})	Assignments
3340	O–H stretching from cellulose, hemicellulose, and lignin (phenolic and CH_2OH)
2900;2853	Asymmetric and symmetric C—H stretching respectively; from OCH_3 & CH_3 and CH_2 groups of the side chains of lignin and aliphatic waxes.
1730	Unconjugated C═O stretching in ketones, aldehydes, and ester groups.
1630	Conjugated carbonyl-carboxyl stretching from ketone groups
1605-1600	C=C vibrations in S and G lignin, coupled with C═O stretch
1520-1510	Aromatic skeletal (C═C) vibrations of S and G
1460	Asymmetric bending of C—H from CH_2 in cellulose, CH_3 in CH_3O and hemicelluloses (CH_3-(C=O)-)
1425-1430	Skeletal vibrations (C=C) coupled with C—H in plane deformation
1375	C—H bending of CH_3 in cellulose and hemicelluloses
1325	Syringyl ring breathing with C—O stretching
1235	C—C, C—O and C═O stretching in Guacyl
1160	Typical for HGS; C═O stretching from conjugated ketone and ester groups
1120	Aromatic C—H bending in-plane (typical for S units)
1035	Mainly C–O–C glycosidic linkage from hemicellulose and cellulose
898	C–H deformation in cellulose
865	Aromatic out-of-plane deformation vibration in G
835	C-H out-of-plane in position 2 and 6 of S, and in all positions of H units
820	Aromatic out-of-plane deformation vibration in S

Table S2. Pyrolysis products identified in the rinds of D2, RG2, D1 and RG1 sorghum variety.

RT	Compound	MW	Formula	D2	RG2	D1	RG1
1.43	Carbon dioxide	44	CO_2	19.29±1.61	14.90±0.78	12.86±1.50	17.42±0.97
1.72	Methyl glyoxal	72	$C_3H_4O_2$	8.04±0.24	6.53±0.15	9.28±0.345	7.55±0.60
2.24	Acetic acid	60	$C_2H_4O_2$	15.23±1.13	13.49±1.01	12.21±0.52	15.67±0.56
2.49	1-hydroxy-2-Propanone	74	$C_3H_6O_2$	7.54±0.07	6.96±0.04	9.96±0.62	7.33±0.28
2.84	Dianhydromannitol	146	$C_6H_{10}O_4$	1.29±0.04	0.88±0.11	1.01±0.11	0.75±0.19
3.21	Butanal, 3-hydroxy-	88	$C_4H_8O_2$	0.44±0.04	0.34±0.01	0.4±0.04	0.39±0.01
3.36	3-Cyclopentene-1,2-diol, cis-	100	$C_5H_8O_2$	0.48±0.01	0.42±0.01	0.45±0.01	0.73±0.02
3.61	2-Butanone, 1-(acetyloxy)-	130	$C_6H_{10}O_3$	2.39±0.26	2.93±0.06	3.07±0.18	2.89±0.03
3.84	Succindialdehyde	86	$C_4H_6O_2$	4.21±0.04	4.18±0.07	3.88±0.4	4.18±0.06
4.76	Furfural	96	$C_5H_4O_2$	2.54±0.01	2.45±0.04	2.43±0.41	2.55±0.01
5.23	2-Furanmethanol	98	$C_5H_6O_2$	1.11±0.02	1.02±0.02	1.35±0.02	1.02±0.01
5.44	2-Propanone, 1-(acetyloxy)-	116	$C_5H_8O_3$	1.33±0.07	1.23±0.02	1.64±0.04	1.34±0.01
5.83	Cyclohexanone, 3-hydroxy-	114	$C_6H_{10}O_2$	0.26±0.01	0.38±0.01	0.44±0.06	0.26±0.03
6.32	2-Cyclopenten-1-one, 2-methyl-	96	C_6H_8O	0.56±0.01	0.68±0.01	0.54±0.06	0.72±0.08
6.47	Ethanone, 1-(2-furanyl)-	110	$C_6H_6O_2$	0.15±0.01	0.14±0.00	0.14±0.03	0.21±0.00
6.63	Dihydropyran	84	C_5H_8O	0.91±0.04	1.11±0.00	0.92±0.07	1.00±0.04
6.86	1,2-Cyclopentanedione	98	$C_5H_6O_2$	2.14±0.11	2.66±0.01	1.86±0.09	2.43±0.06
7.85	2-Furancarboxaldehyde, 5-methyl-	110	$C_6H_6O_2$	0.94±0.07	0.67±0.01	0.91±0.04	0.71±0.04
8.26	Phenol	94	C_6H_6O	1.79±0.01	1.67±0.01	1.75±0.01	1.98±0.08
8.79	3,4-Dihydro-2-methoxy-2H-pyran	114	$C_6H_{10}O_2$	0.41±0.10	0.40±0.01	0.28±0.00	0.36±0.00
9.57	3-Methyl-1,2-cyclopentanedione	112	$C_6H_8O_2$	1.69±0.19	1.66±0.01	1.7±0.01	1.85±0.13
9.89	2,3-Dimethyl-2-cyclopenten-1-one	110	$C_7H_{10}O$	0.30±0.02	0.25±0.01	0.27±0.05	0.24±0.00
10.4	Phenol, 3-methyl-	108	C_7H_8O	0.75±0.01	0.62±0.02	0.76±0.02	0.69±0.04
10.9	Phenol, 3-methyl-	108	C_7H_8O	1.00±0.04	0.89±0.09	1.089±0.04	1.05±0.05
11.4	Phenol, 2-methoxy-	124	$C_7H_8O_2$	1.04±0.01	1.28±0.04	1.18±0.03	1.20±0.02
11.7	Cyclopropyl carbinol	72	C_4H_8O	0.14±0.00	0.825±0.02	0.22±0.11	0.61±0.04
12.2	2-Cyclopenten-1-one, 3-ethyl-2-hydroxy-	126	$C_7H_{10}O_2$	0.32±0.02	0.32±0.01	0.36±0.00	0.47±0.04
13.0	Phenol, 2,5-dimethyl-	122	$C_8H_{10}O$	0.31±0.03	0.29±0.00	0.33±0.03	0.31±0.00
13.5	Phenol, 4-ethyl-	122	$C_8H_{10}O$	1.27±0.1	1.65±0.35	1.47±0.25	1.35±0.07
14.3	Creosol	138	$C_8H_{10}O_2$	0.43±0.06	0.68±0.06	0.49±0.01	0.52±0.04
15.0	4-vinylphenol	120	C_8H_8O	9.74±0.1	10.73±0.06	8.08±0.62	11.50±0.04
16.3	1,2-Benzenediol, 3-methoxy-	140	$C_7H_8O_3$	0.85±0.02	0.74±0.04	1.45±0.27	2.95±0.98
16.7	Phenol, 4-ethyl-2-methoxy-	152	$C_9H_{12}O_2$	0.22±0.01	0.30±0.02	0.24±0.01	0.25±0.01
16.9	p-Isobutylbenzaldehyde	162	$C_{11}H_{14}O$	0.26±0.04	0.31±0.00	0.26±0.00	0.26±0.03
17.7	2-Methoxy-4-vinylphenol	150	$C_9H_{10}O_2$	1.82±0.00	2.70±0.16	1.90±0.05	2.57±0.04
18.7	Phenol, 2,6-dimethoxy-	154	$C_8H_{10}O_3$	1.82±0.05	2.23±0.05	1.68±0.08	2.12±0.11
20.0	Benzaldehyde, 3-hydroxy-4-methoxy-	152	$C_8H_8O_3$	0.13±0.01	0.20±0.02	0.16±0.05	0.05±0.00
20.1	Phenol, 4-methoxy-3-(methoxymethyl)-	168	$C_9H_{12}O_3$	0.20±.06	0.21±0.00	0.88±0.04	0.16±0.00
21.2	Phenol, 2-methoxy-4-(1-propenyl)-	164	$C_{10}H_{12}O_2$	0.84±0.08	1.36±0.00	0.86±0.05	0.99±0.08
22.0	Benzene, 3-ethyl-1,2,4,5-tetramethyl-	162	$C_{12}H_{18}$	0.21±0.1	0.25±0.03	0.25±0.03	0.08±0.00
23.0	2,5-Dimethoxybenzoic acid	182	$C_9H_{10}O_4$	0.19±0.02	0.21±0.01	0.16±0.00	0.08±0.00
24.0	Phenol, 4-ethenyl-2,6-dimethoxy-	180	$C_{10}H_{12}O_3$	0.60±0.07	0.53±0.03	0.61±0.10	0.20±0.11
24.8	Phenol, 2,6-dimethoxy-4-(2-propenyl)-	194	$C_{11}H_{14}O_3$	0.14±0.03	0.14±0.01	0.13±0.02	0.08±0.01
26.2	Benzaldehyde, 4-hydroxy-3,5-dimethoxy-	182	$C_9H_{10}O_4$	-	0.07±0.01	-	-
27.0	(E)-2,6-Dimethoxy-4-(prop-1-en-1-yl) phenol	194	$C_{11}H_{14}O_3$	-	0.27±0.16	-	-
27.8	Benzaldehyde, 2,3,4-trimethoxy-	196	$C_{10}H_{12}O_4$	-	0.185±0.08	-	-

Note: RT=retention time (min); MW= Molecular weight, the errors are standard error from duplicates