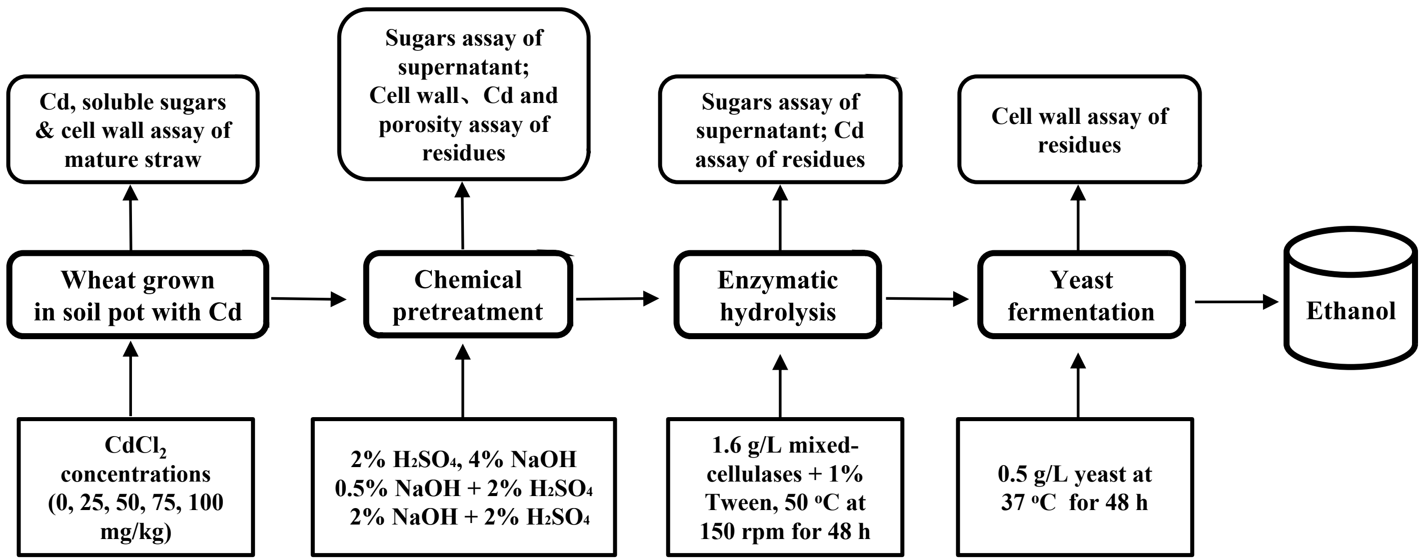

Fig. S1 General experimental procedure of Cd release and bioethanol conversion

Table S1 Cd content of wheat mutant and wild type grown in soil pots supplied with $CdCl_2$

Sample	$CdCl_2$ supply in pot (mg/kg soil)	Cd content of wheat (ug/g dry matter)#	
		Straw	Seed
Wild Type (WT) (ZM9023)	0	0.06 ± 0.01^{e}	0.03 ± 0.01^{e}
	25	4.25 ± 0.12^{c}	3.51 ± 0.34^{c}
	50	5.11 ± 0.75^{b}	4.19 ± 0.39^{b}
	75	6.43 ± 0.56^{a}	4.84 ± 0.45^{a}
	100	2.32 ± 0.09^{d}	2.20 ± 0.02^{d}
Mutant (*ZT*5)	0	0.05 ± 0.01^{d}	0.02 ± 0.00^{d}
	25	4.63 ± 0.80^{c}	3.23 ± 0.28^{c}
	50	5.03 ± 0.40^{c}	4.36 ± 0.32^{b}
	75	8.29 ± 0.51^{a}	4.99 ± 0.39^{a}
	100	6.59 ± 0.90^{b}	4.49 ± 0.35^{b}

Data as means ± SD (N = 3) with LSD-test for significant differences among all values marked as a, b, c, d, e, respectively.

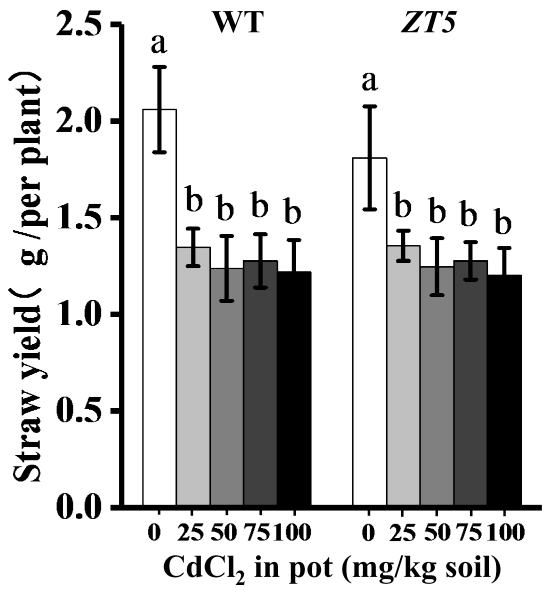

Fig. S2 Dry weight (g/per plant) of mature straws in wheat mutant (*ZT5*) and wild type (WT/ZM9023) grown in soil pots supplied with different concentrations of $CdCl_2$. Data as means ± SD (N = 3), and letters (a, b, c, d, e) as mean values for significant difference each others by LSD-test, respectively.

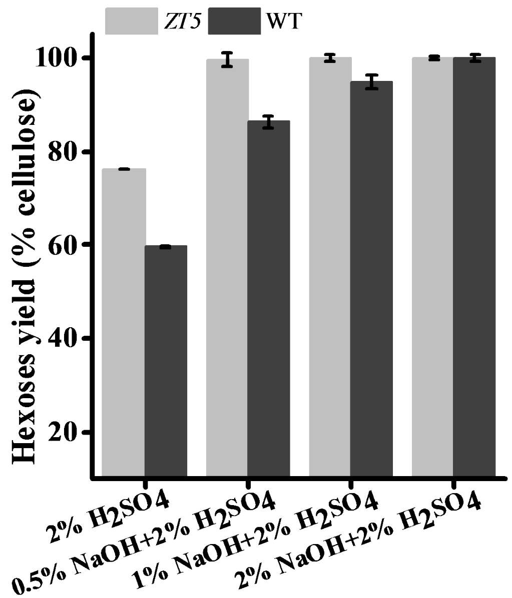

Fig. S3 Hexoses yields in wheat mutant (*ZT5*) and WT. Hexoses yields (% cellulose) released from enzymatic hydrolysis after two-step pretreatment (NaOH + H_2SO_4) at a series of concentrations.

Table S2 Hexoses yield (% cellulose) released from enzymatic hydrolysis after chemical pretreatments

sample	$CdCl_2$ supply (mg/kg soil)	2%H_2SO_4	4%NaOH	0.5%NaOH+2%H_2SO_4	2%NaOH+2%H_2SO_4
WT	**0**	63.99±1.47	100±1.00	84.43±2.11	100±2.58
	75	63.58±0.97	100±1.83	86.91±0.71	100±2.26
ZT5	**0**	81.05±2.83	100±2.24	92.66±3.00	100±1.95
	75	75.89±1.45	100±3.11	91.33±2.31	100±3.15

Data as means ± SD (N = 3).

Table S3 Total sugars (% dry matter) released from enzymatic hydrolysis after chemical pretreatments

Sample	$CdCl_2$ supply (mg/kg soil)	2%H_2SO_4	4%NaOH	0.5%NaOH+2%H_2SO_4	2%NaOH+2%H_2SO_4
WT	**0**	26.44±0.57	48.08±0.68	35.23±0.18	43.09±0.86
	75	23.66±0.39	45.64±0.82	33.75±0.18	40.86±1.20
ZT5	**0**	23.61±0.82	36.64±1.40	27.21±0.85	30.71±0.62
	75	21.25±0.40	35.60±0.99	25.84±0.34	30.05±0.97

Data as means ± SD (N = 3).

Table S4 Bioethanol yield (% dry matter) from yeast fermentation using total hexoses from enzymatic hydrolyses of soluble sugars and pretreated biomass residues

sample	$CdCl_2$ supply (mg/kg soil)	2%H_2SO_4	4%NaOH	0.5%NaOH+2%H_2SO_4	2%NaOH+2%H_2SO_4
WT	**0**	10.19±0.46	14.46±0.11	13.34±0.41**	15.15±0.19
	75	11.90±0.50	15.43±0.10	14.52±0.11**	15.75±0.19
ZT5	**0**	9.52±0.30	11.24±0.20	11.17±0.11**	11.63±0.19
	75	11.04±0.19	12.22±0.20	11.83±0.19**	12.29±0.31

Data as means ± SD (N = 3). ** As significant difference between 0.5%NaOH + 2%H_2SO_4 and 2%H_2SO_4 by t-test at $P < 0.01$.

Table S5 Monosaccharide composition of total soluble sugars (% of total) extracted from mature wheat straw

Sample	$CdCl_2$ supply (mg/kg soil)	Rha	Fuc	Ara	Xyl	Man	Glc	Gal
WT	**0**	1.95	1.19	19.14	14.65	4.96	49.47	8.63
	75	0.54	0.69	5.03	2.95	2.47	84.60	3.72
ZT5	**0**	1.29	1.20	14.67	10.86	7.31	57.26	7.41
	75	0.57	0.59	6.13	4.09	3.19	81.47	3.97

Table S6 Cellulose features (DP, CrI) in wheat mutant and WT straws

Cellulose features	$CdCl_2$ supply (mg/kg soil)	Sample	Raw material	$0.5\%NaOH+2\%H_2SO_4$	
DP	0	WT	1272±3.19	809±0.95	**-36%****
		ZT5	863±0.69	597±1.59	**-31%****
			-32%**	**-26%****	
	75	WT	972±1.56	756±1.63	**-22%****
		ZT5	794±0.00	606±0.90	**-24%****
			-18%**	**-20%****	
CrI	0	WT	46.53	55.72	**20%**
		ZT5	36.19	47.84	**32%**
			-22%	**-14%**	
	75	WT	47.61	54.98	**16%**
		ZT5	37.21	49.55	**33%**
			-22%	**-12%**	

Data as means ± SD (N = 3). ** As significant difference between two samples by t-test at $P < 0.01$ (N = 3).

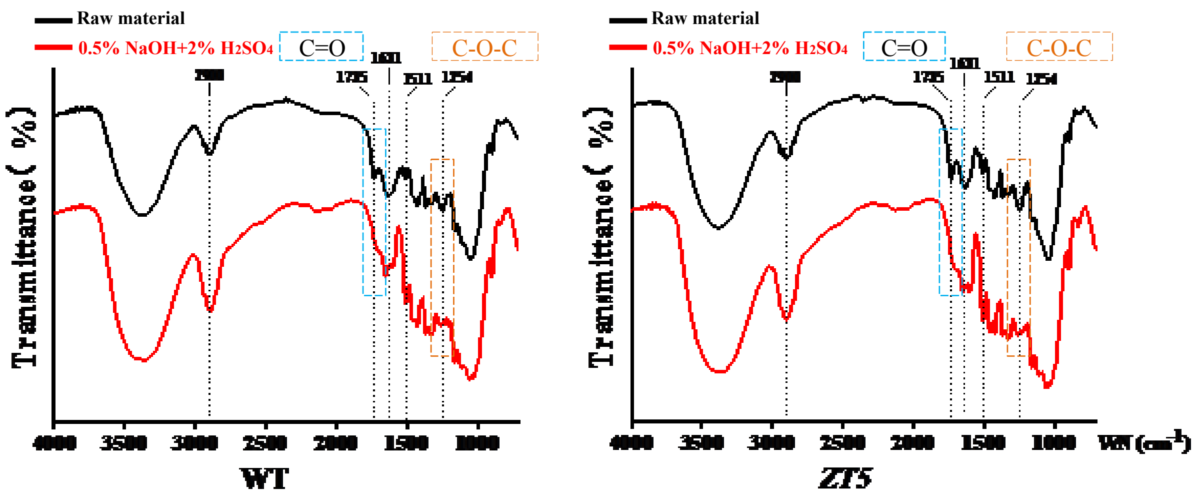

Fig. S4 Fourier transform infrared spectroscopic profiling among the raw materials (black) and two-step pretreated residues (red) in wheat mutant and WT straws.

Table S7 Characteristic peaks of the FTIR spectra in wheat biomass residues as referred from previous studies

Reported wave number (cm^{-1})	**Observed wave number (cm^{-1})**	**Functional group**	**Assignment**	**Reference**
898	898	C─H vibration	Cellulose	3
1051	1051	C─O─C ring skeletal vibration	Hemicelluloses	3
1163	1164	C─O─C asymmetric stretching	Cellulose	2
1247	1254	C─O─C stretching of aryl-alkyl ether	Lignin	5
1373	1371	C─H_2 scissoring	Cellulose	4
1430	1430	C─H_2 bending	Cellulose	8
1460	1460	C─H_3 asymmetric bending	Lignin	7
1515	1511	C=C stretching of the aromatic ring	Lignin	3
1603	1631	C=C stretching	Lignin	8
1735	1735	C=O stretching of acetyl or carboxylic acid	Hemicelluloses & lignin	9
2900	2900	C─H stretching	Cellulose	10