Supporting Information

Pyrolysis and Combustion Behavior of Flax Straw as Biomass: Evaluation of Kinetic, Thermodynamic Parameters, and Qualitative Analysis of Degradation Products

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Table S1: list of elements presents in ash of flax straw biomass

Type of Elements	wt%
Mg	4.9
Al	0.9
Si	37.2
P	3.8
S	1.3
Cl	3.6
Cu	0.1
Fe	1.6
Mn	0.3
Ti	0.1
K	26.1
Ca	19.9
Sr	0.1

Table S2: Intercept and slope of pyrolysis and combustion of flax straw biomass from Friedman, KAS, and OFW methods

Kinetic Method	Conversion (α)	Pyrolysis		Combustion	
		intercept	slope	intercept	slope
Freidman	0.1	32.6	-19972	94.6	-53042
	0.2	36.4	-22595	102.9	-60071
	0.3	41.5	-26268	62.5	-40285
	0.4	31.4	-20691	71.9	-44539
	0.5	22.2	-15510	52.9	-33829
	0.6	14.4	-10938	135.2	-85262
KAS	0.1	6.8	-9640	38.0	-26193
	0.2	14.6	-14569	50.0	-34315
	0.3	20.2	-18339	26.5	-22515
	0.4	14.9	-15587	35.3	-27349
	0.5	17.3	-17526	29.6	-24476
	0.6	10.2	-13383	36.8	-29303
OFW	0.1	22.2	-11117	66.2	-34564
	0.2	30.1	-16149	86.7	-47809
	0.3	33.8	-18803	70.8	-39741
	0.4	29.8	-16834	66.1	-38073
	0.5	31.3	-18262	64.9	-38052
	0.6	24.8	-14416	70.7	-42225

Table S3: Differential and integral forms of kinetic models used in solid-state kinetic.

Model Code	Differential Form, f(α)	Integral Form, g(α)
F_1	$(1- \alpha)$	$-\ln (1- \alpha)$
F_2	$(1- \alpha)^2$	$(1- \alpha)^{-1} -1$
G_1	$1-\{2 (1- \alpha)\}$	$1- (1- \alpha)^2$
G_2	$1/[3(1 - \alpha)^{2}]$	$1 - (1 - \alpha)^3$
P_2	$2\alpha^{1/2}$	$\alpha^{1/2}$
P_3	$3\alpha^{2/3}$	$\alpha^{1/3}$
P_4	$4\alpha^{3/4}$	$\alpha^{1/4}$
$A_1(F_1)$	$(1- \alpha)$	$-\ln(1- \alpha)$
Avarami–Erofeev A_2	$2(1 - \alpha)[-\ln(1 - \alpha)]^{1/2}$	$[-\ln(1 - \alpha)]^{1/2}$
Avarami–Erofeev A_3	$3(1 - \alpha)[-\ln(1 - \alpha)]^{2/3}$	$[-\ln(1 - \alpha)]^{1/3}$
Avarami–Erofeev A_4	$4(1 - \alpha)[-\ln(1 - \alpha)]^{3/4}$	$[-\ln(1 - \alpha)]^{1/4}$
$A_{3/2}$	$3/2(1 - \alpha)[-\ln(1 - \alpha)]^{1/3}$	$-\ln(1 - \alpha)]^{2/3}$
$A_{1/2}$	$1/2(1 - \alpha)[-\ln(1 - \alpha)]^{(-1)}$	$[-\ln(1 - \alpha)]^2$
$A_{1/3}$	$1/3(1 - \alpha)[-\ln(1 - \alpha)]^{(-2)}$	$[-\ln(1 - \alpha)]^3$
D_1	$1/(2 \alpha)$	α^2
D_2	$[-\ln(1 - \alpha)]^{-1}$	$[(1 - \alpha)\ln(1 - \alpha)]+ \alpha$
R_1	1	α
R_2	$2(1 - \alpha)^{1/2}$	$[1 - (1 - \alpha)^{1/2}]$
R_3	$3(1 - \alpha)^{2/3}$	$[1 - (1 - \alpha)^{1/3}]$

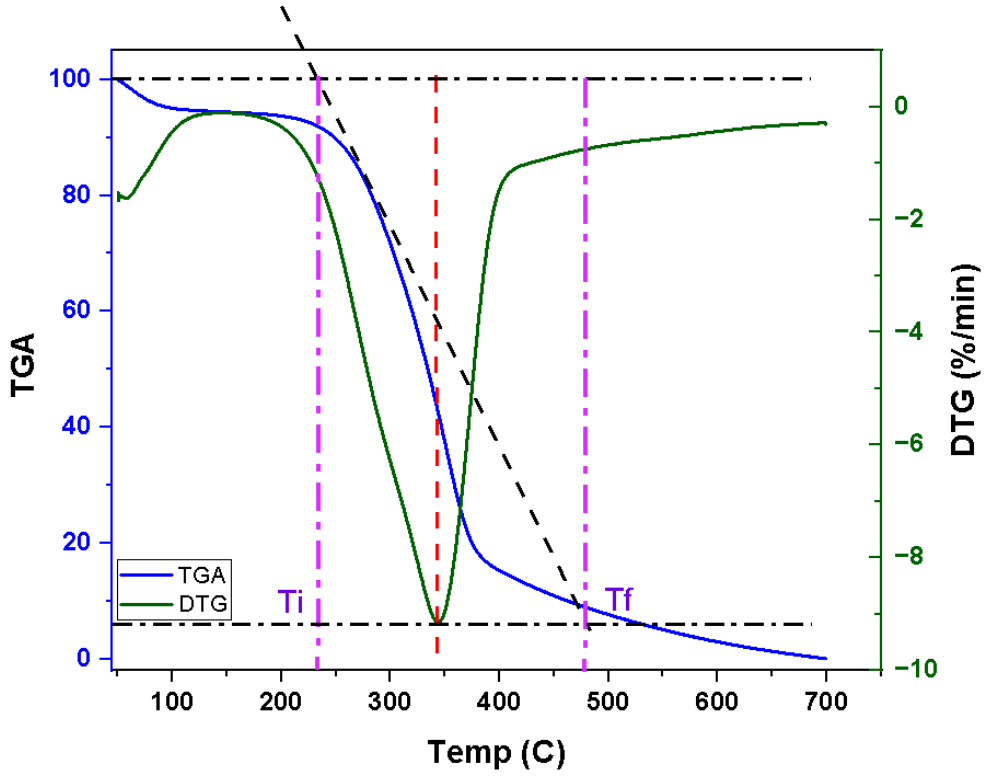
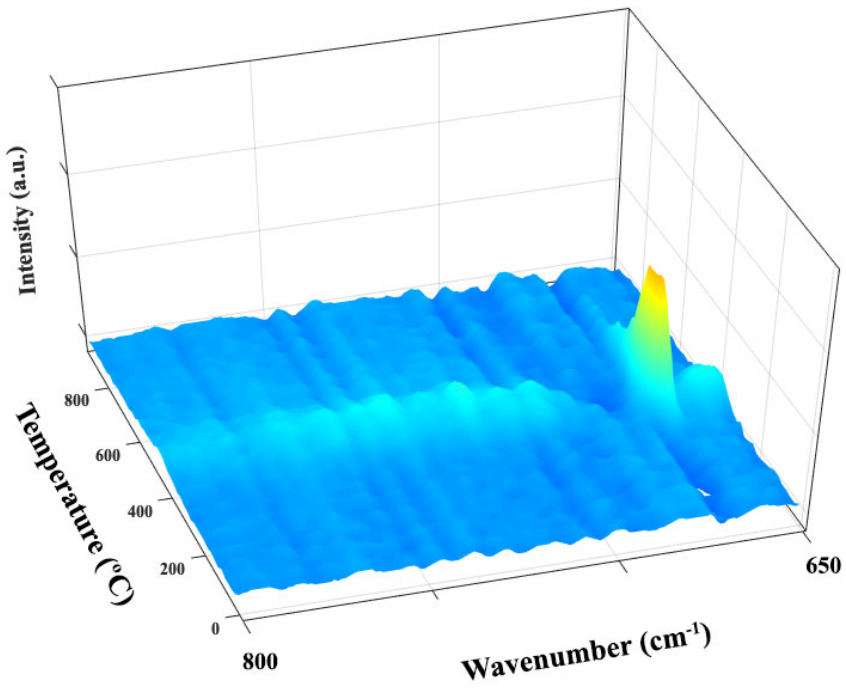
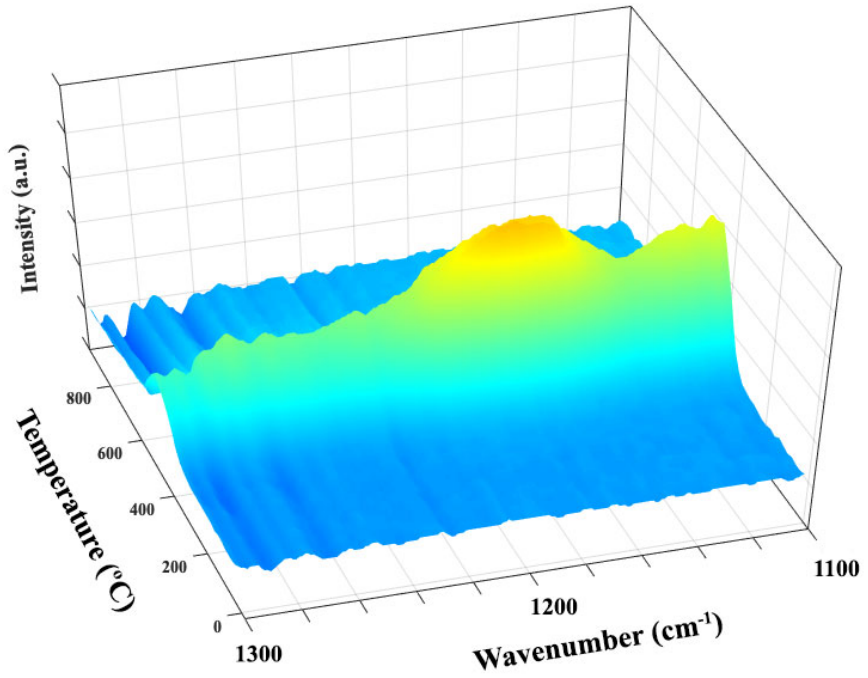


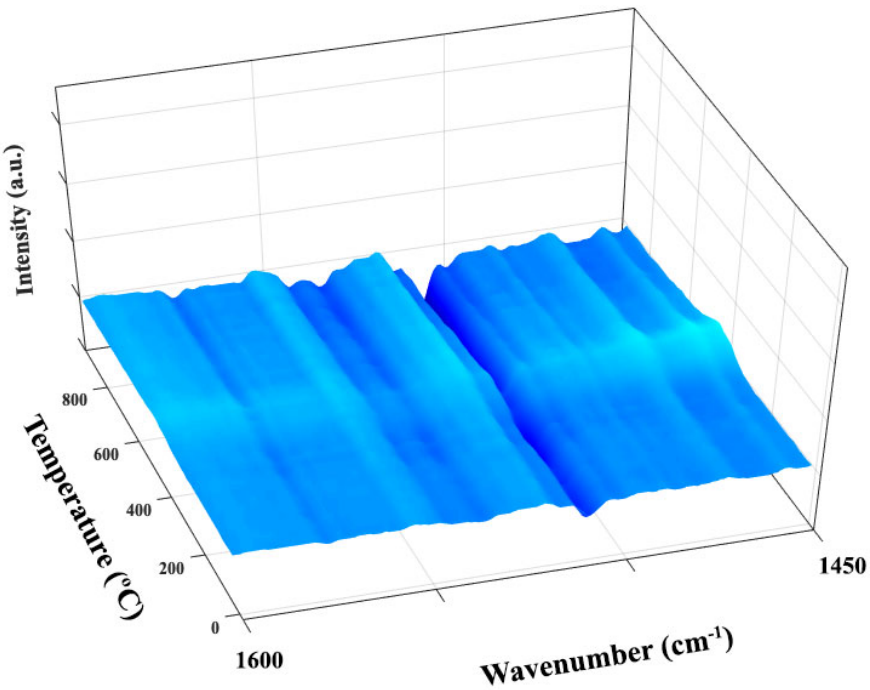
Figure S1: Calculation of T_i and T_f (Black Line: Tangent line)



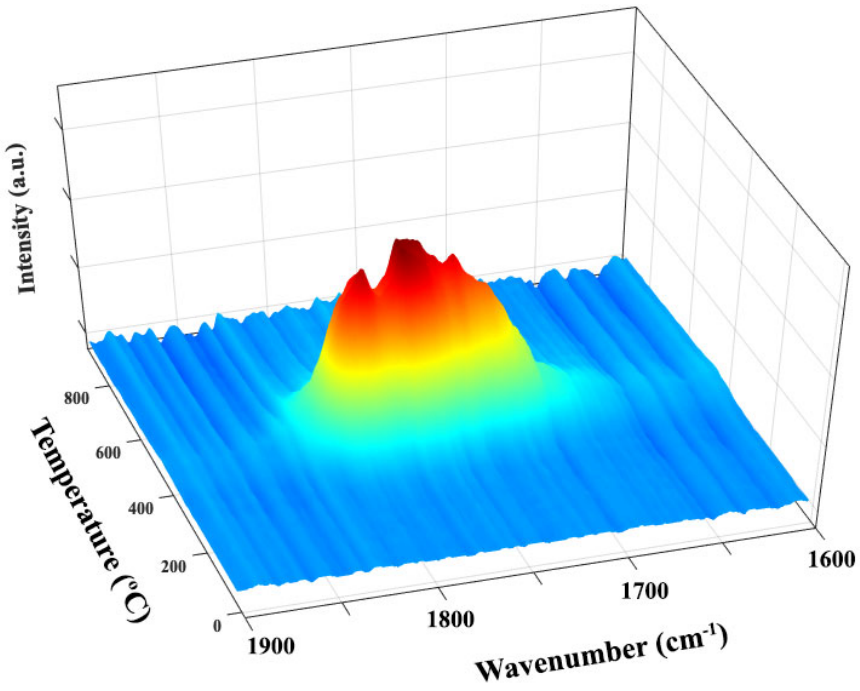
(a) 650-800 cm^{-1} aromatic Region



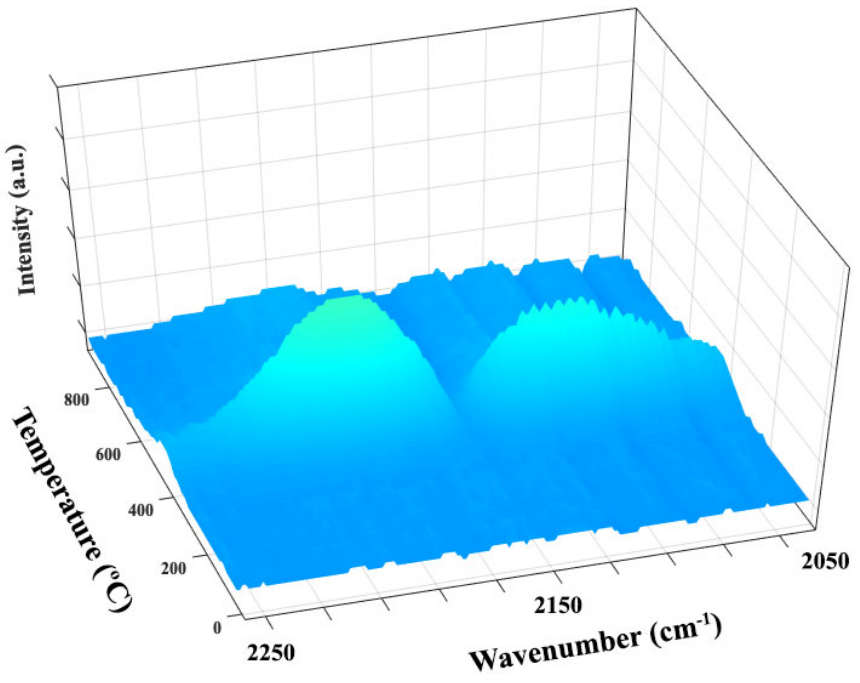
(b) 1100-1300 cm^{-1} Ethers and Alcohols



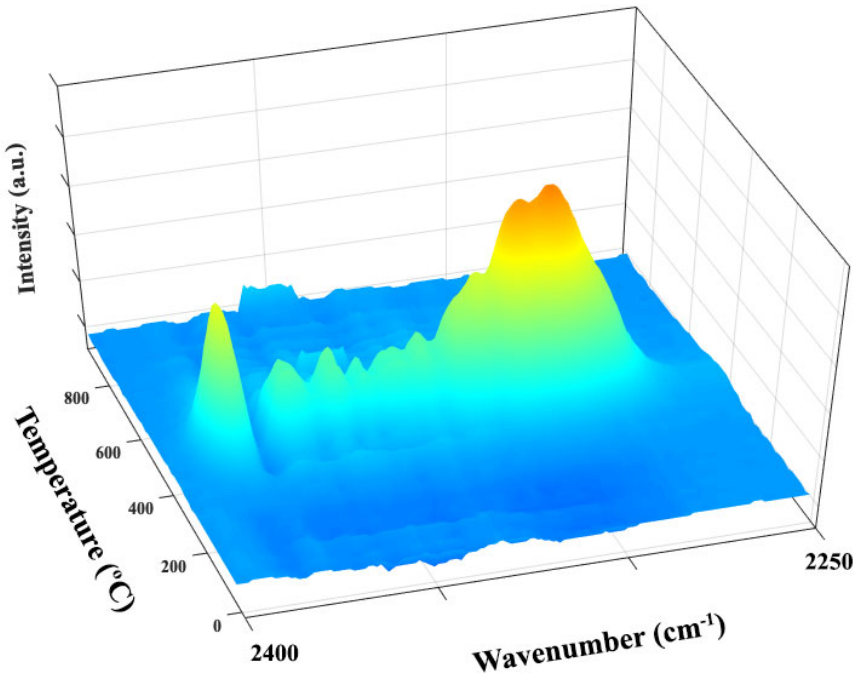
(c) 1450-1600 cm^{-1} Aromatics



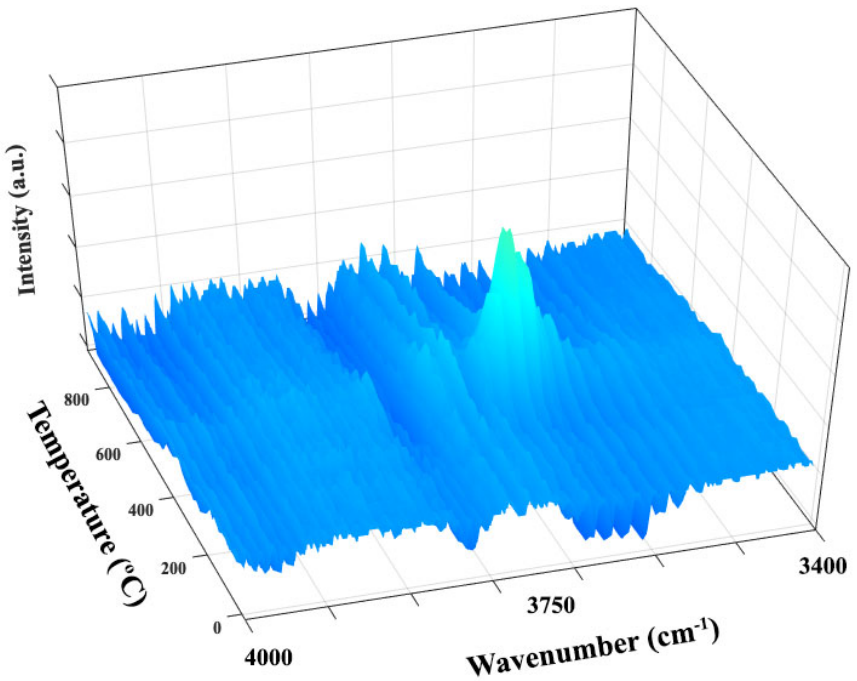
(d) 1600-1900 cm^{-1} Carboxylic acids



(e) 2050-2250 cm^{-1} CO



(f) 2250-2400 cm^{-1} CO_2



(g) 3400-4000 cm^{-1} Hydrogen bond

Figure S2: 3D FT-IR profiles of the evolved gases released from flax straw during pyrolysis focused spectra in each region.

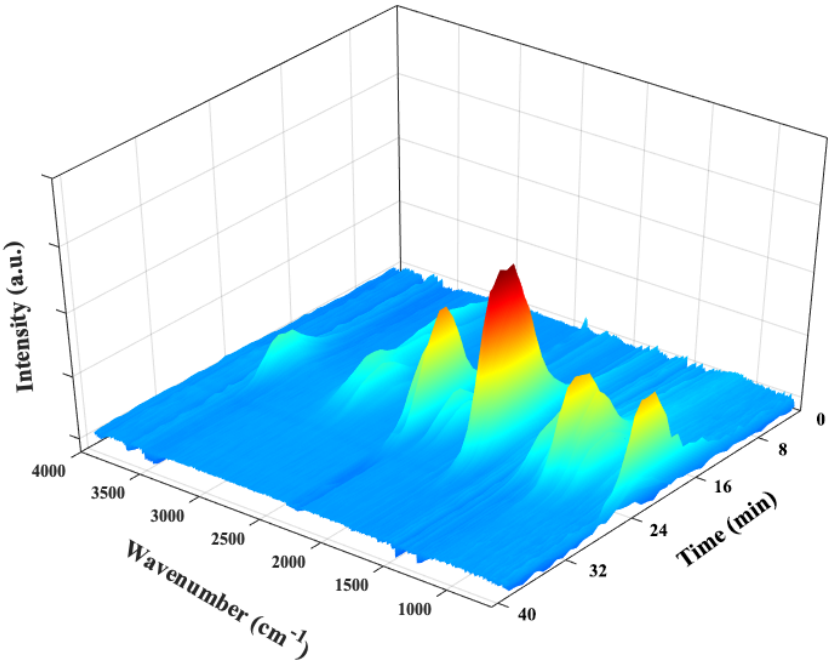
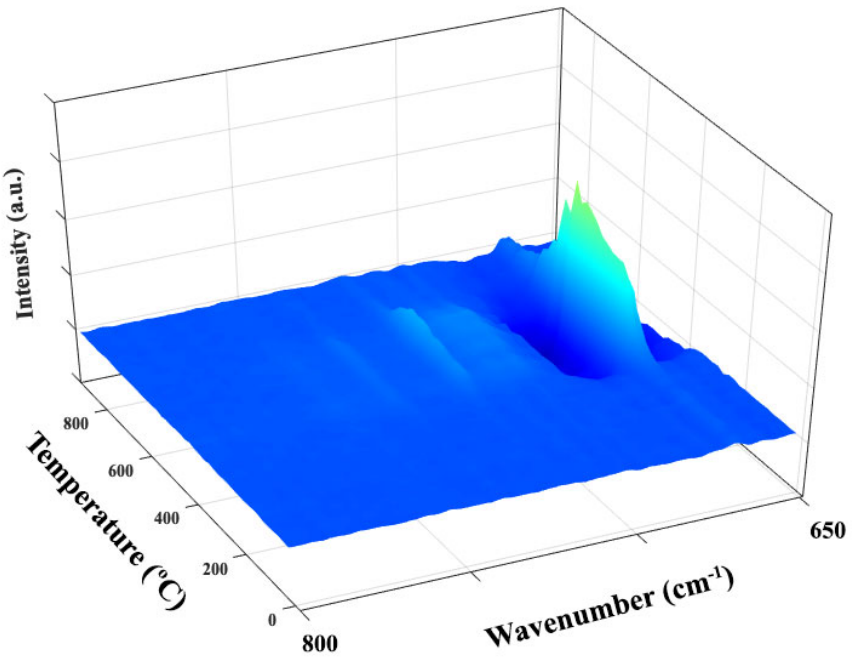
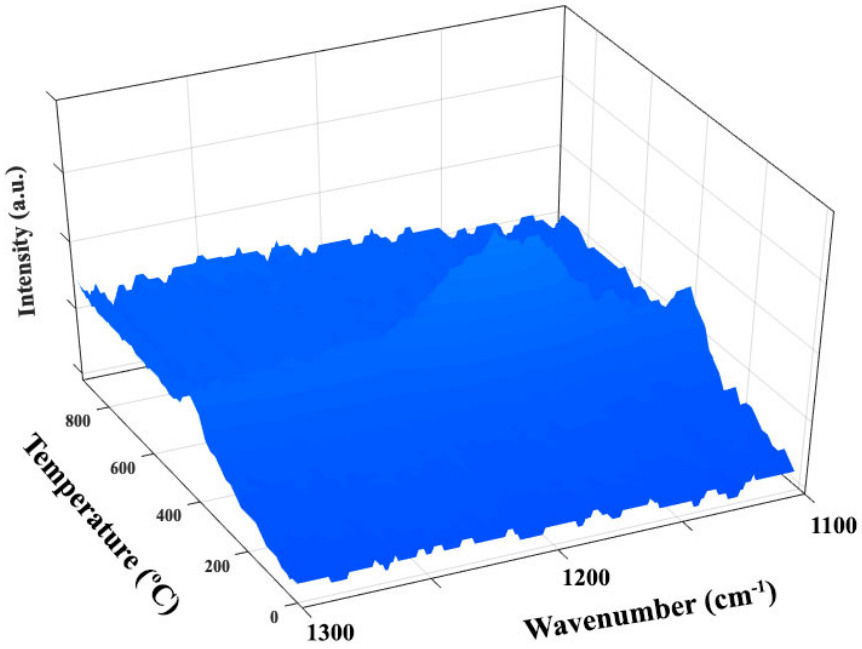


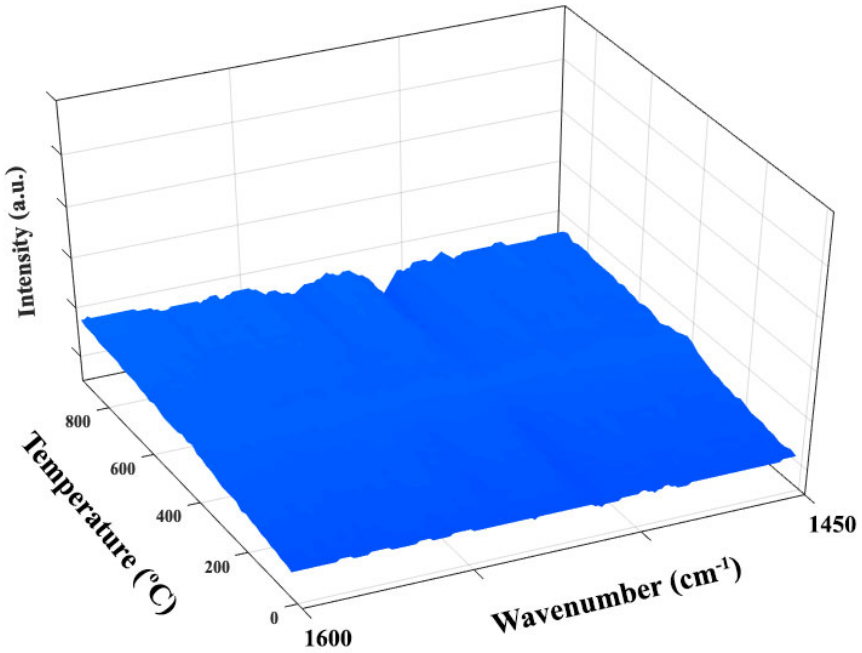
Figure S3: 3D FT-IR profiles of the evolved gases released from flax straw during pyrolysis (time based)



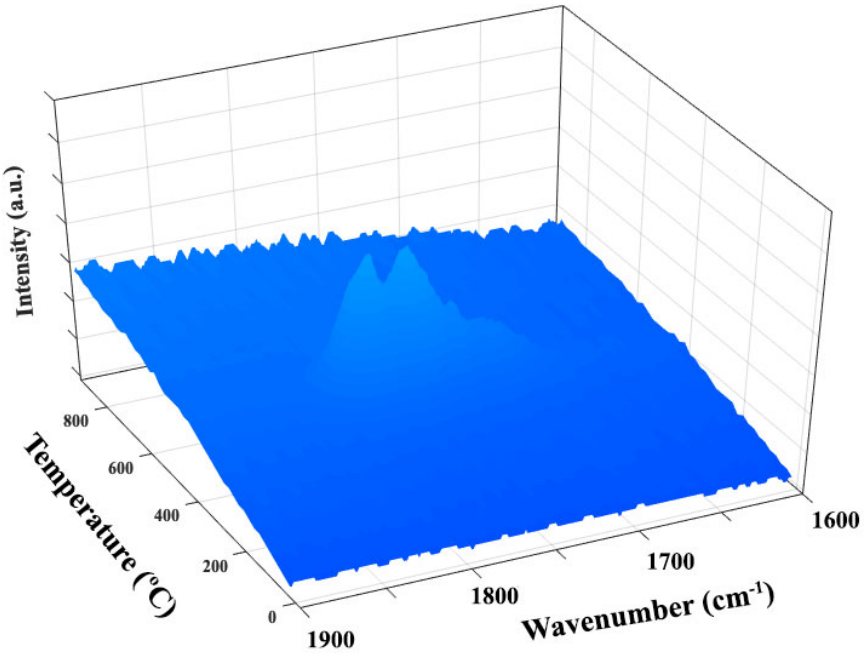
(a) 650-800 cm^{-1} Aromatic Region



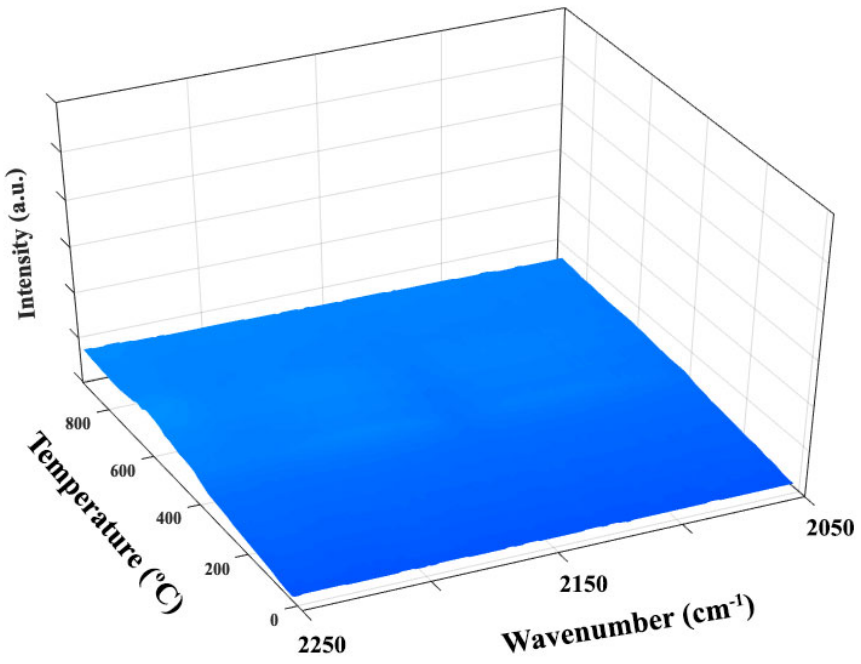
(b) 1100-1300 cm^{-1} Ethers and Alcohols



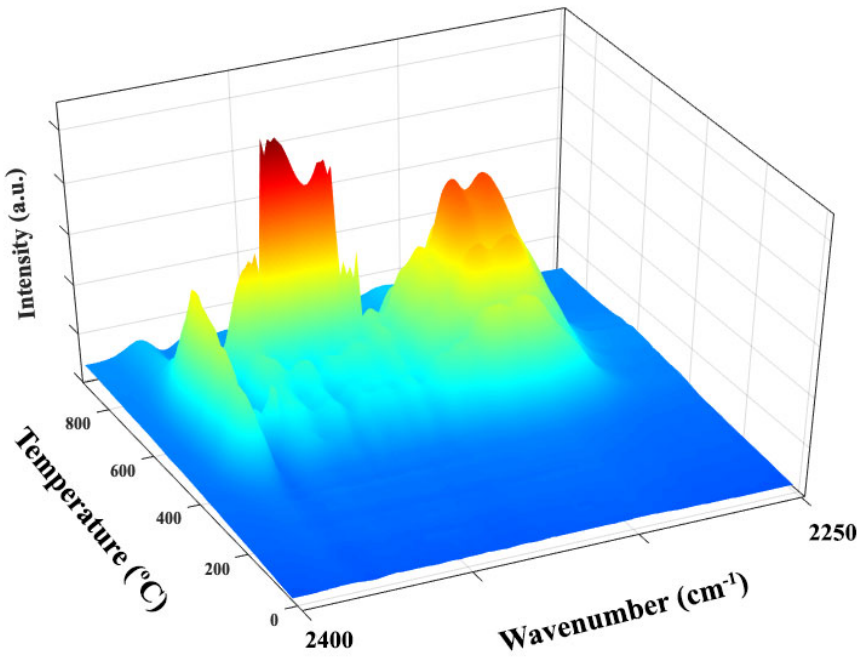
(c) 1450-1600 cm^{-1} Aromatics



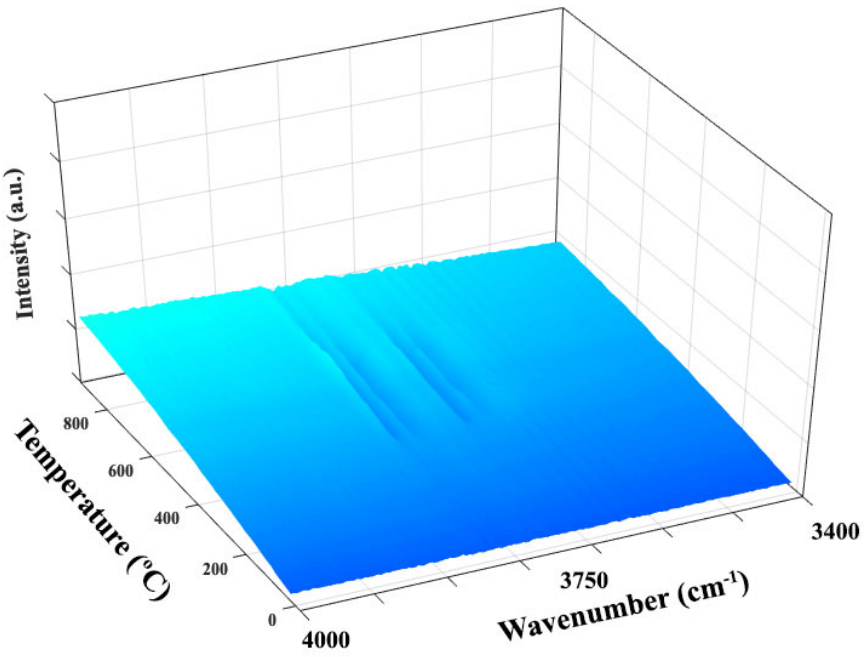
(d) 1600-1900 cm^{-1} Carboxylic acids



(e) 2050-2250 cm^{-1} CO



(f) 2250-2400 cm^{-1} CO_2



(g) 3400-4000 cm^{-1} Hydrogen bond

Figure S4: 3D FT-IR profiles of the evolved gases released from flax straw during combustion focused spectra in each region

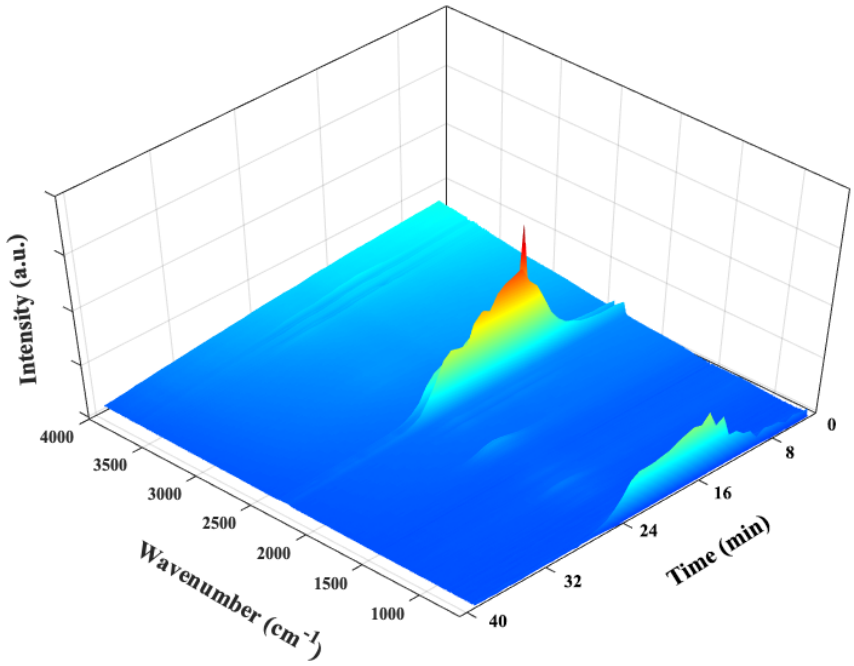


Figure S5: 3D FT-IR profiles of the evolved gases released from flax straw during combustion (time based)