

# Supplementary Materials

## Production and Characterization of Biodiesel Derived from a Novel Source *Koelreuteria Paniculata* Seed Oil

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**Description of *K. paniculata* (KP):****Scientific name:** *Koelreuteria paniculata***Common name(s):** Golden rain tree, varnish-tree**Family:** Sapindaceae**Uses:** shade; sidewalk cutout**S1. KP Plant Description**

KP grows 30 to 40 feet tall with an equal spread, in a broad, somewhat irregular globe-shape. Some trees appear vase-shaped. Although it has a character for being weakly wooded, it is rarely attacked by pests and grows in a wide range of soils, including high pH soils. KP tolerates dryness and casts little shade because of the open growth habit. It makes a good street or parking lot tree, particularly where overhead or soil space is limited due to its adaptive abilities. The tree grows moderately and bears large panicles of bright yellow flowers from May to July when few other trees bloom. It is not as showy as *Koelreuteria bipinnata* but is much more cold-tolerant. The seed pods look like brown Chinese lanterns and are held on the tree well into the fall. The inflorescences are very spectacular and contain ellipsoid capsules. The entire tree will be covered with inflorescences when in bloom. Capsules can be dried and the seeds can be separated using a harvester. Because of its aggressive growth habit, this is classed as a weed.

Cultivation: Once established, this species can thrive without irrigation. It can be grown on a wide range of soils either in monoculture or in mixed culture.

**S2. Mechanical Extraction of Seed**

The mechanical extraction of KP seeds was done by two different electric oil expeller machines, less power extractor (FANGTAI SHIBAYOUFANG FL-S2017 China) and a high power extractor (FANGTAI SHIBAYOUFANG J508, China). Pre-treatment of seed is very important for mechanical extraction which can increase the amount of oil recovery. After 2–3 revolutions, a large yield of crude KPSO was obtained. The oil removed from the seed by mechanical presses desires additional handling of extraction and filtration to produce a purer raw feedstock. The oil production of KPSO was calculated by the following Equation (1).

$$\text{Conversion \%} = \frac{\text{Obtained seed oil weight}}{\text{Total seed weight}} \times 100 \quad (1)$$

Further following steps were done to get the KPOB, filtration, rotary evaporation for access methanol, heating, trans-esterification, settling, separation and washing.

**S3. ICP-OES and EA Study of KP Biodiesel for Elemental Analysis**

For the presence of metals in the KPSO biodiesel, it was explored through Inductively Coupled Plasma Spectrometer (Spectro-blue, Germany) and Elemental Analyzer (Vario EL CUBE, Germany). For the ICP-OES test, We take 1 g of oil sample for incinerating. The ashing process is as follows: Increase the oven temperature to 200 °C in one hour, then increase the temperature to 500 °C and kept for 2 h, and finally increase to 800 °C and kept for 5 h. The ash was dissolved in 10 ml of 2% HNO<sub>3</sub>. The prepared sample of the KP biodiesel (KPBD) was used for elements finding and concentration tests.

Procedure for EA sample preparation: Element analyzer (Vario EL CUBE, Germany), the instrument was used for detecting the H, N, C and O concentration of KPBD. We take 0.5 ml KPBD, 3 ml concentrated HCl and 1 ml HNO<sub>3</sub> in a tube and was put them for 10–15 mins rest, to dissolve

the oil in the solution. Fresh reagents can be used for sample preparation. The aqua regia amount would be double than the sample. Then we take 1 ml prepared solution in a new tube and add deionized water up to 5 ml. We repeated the same technique 2–3 times until the sample becomes clean and clear to be used for C, H, N, and O concentration testing.

#### **S4. GC-MS Procedure**

The obtained KP biodiesel results were checked and tested by GCMS (QP2010SE, Shimadzu, Japan), furnished with a capillary column: PEG-20M (30 m × 0.32 mm × 1 μm film thickness). Helium gas flow rate 1.2 mL/min; split ratio 40:1; the injector temperature and injection volume were 220 °C and 1 uL; furnace heat up mode was 100 °C for 1 min, then from 100 °C rises to 210 °C at the increase rate of 10 °C/ min. Sensor heat mode was 210 °C for 20 mins; ion source temperature was 200 °C; for electron impact, 70 eV ionization mode used; the mass range was 35–500 m/z. The KP FAMES were identified with the mass spectrometry fragmentation design provided by the GCMS system software, as matched with those stored in the mass spectrometry library NIST14, and their fatty acid identity was further verifying by matching with known standards values.

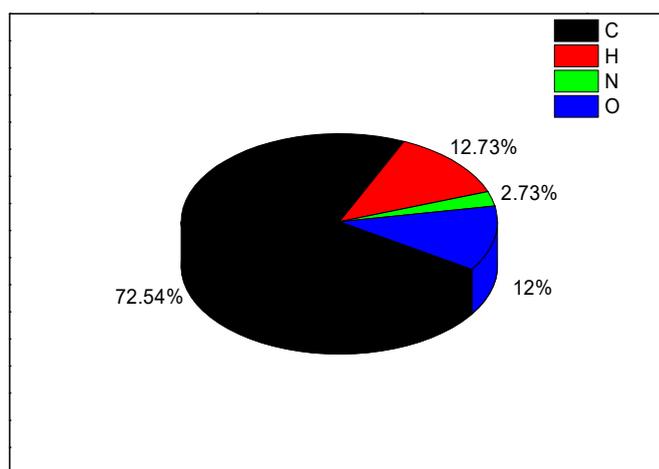


Figure S1. Shows KPBD EA (elemental analysis) for C, H, N, and O.

Table S1. Source collection, Oil extraction and transesterification of non-edible KP seed oil as biofuel.

Source Name	Solvent Extraction %	Mechanical Extraction %	Biodiesel Conversion %	Glycerin %	Soap %	Source Collected From
<i>Koelreuteria paniculata</i> (KP)	28–30	18.7	95.5	4.5	0	Binhai new area, Tianjin

Table S2. KP FAMEs process of optimization.

Amount of Oil Used (M/L)	The Molar Ratio of Oil to Alcohol	Temperature (°C)	Stirring Intensity (rpm)	Reaction Time (mins)	Amount of Catalyst Used		The Percentage Yield of Various Product		
					KOH (g)	CH <sub>3</sub> OH (ml)	Biodiesel (%)	Glycerol (%)	Soap (%)
50	4:1	65	700	60	0.45	12.5	79	15	6
50	5:1	65	700	60	0.40	10.0	88	10	2
50	6:1	65	700	60	0.32	8.3	94	6	0
50	7:1	65	700	60	0.26	7.14	86	8	6
50	6:1	65	700	60	0.22	8.3	71	20	9
50	6:1	65	700	60	0.26	8.3	87	8	5
50	6:1	65	700	60	0.32	8.3	93.6	6.4	0
50	6:1	65	700	60	0.42	8.3	89	8	3
50	6:1	60	700	60	0.32	8.3	76	20	4
50	6:1	65	700	60	0.32	8.3	95	4	1
50	6:1	70	700	60	0.32	8.3	91.8	6	2.2
50	6:1	65	500	60	0.32	8.3	78	20	2
50	6:1	65	600	60	0.32	8.3	92	8	0
50	6:1	65	700	60	0.32	8.3	95	5	0
50	6:1	65	700	40	0.32	8.3	76	18	6
50	6:1	65	700	60	0.32	8.3	92.4	5.6	2
50	6:1	65	700	80	0.32	8.3	95.2	3	1.8
50	6:1	65	700	100	0.32	8.3	89	8	3

**Table S3.** FTIR data presenting various functional groups in KP FAMES.

<b>Peak No.</b>	<b>Wavenumber (cm<sup>-1</sup>)</b>	<b>Group Attribution</b>	<b>Vibration Type</b>	<b>Absorption Intensity</b>
1	3465	-OH	Stretching	Weak
2	3007	=C-H	Stretching	Strong
3	2925	-CH <sub>2</sub>	Asymmetric stretching vibration	Strong
4	2854	-CH <sub>2</sub>	Asymmetric stretching vibration	Strong
5	1748	-C=O	Stretching	Strong
6	1641	-CH <sub>2</sub>	Shear type vibration	Middling
7	1435	Terminal Methyl	Stretching	Higher
8	1361	-CH <sub>3</sub>	Bending vibration	Middling
9	1170	C-O-C	Symmetric stretching vibration	Middling
10	1015	C-O-C	Vibration	Weak
11	724	-CH <sub>2</sub>	Plane rocking vibration	Weak

**Table S4.** <sup>1</sup>H NMR spectroscopic data showing the chemical composition of various methyl esters (Methoxy proton) in KP biodiesel (FAMES).

Peak No:	Peak Area/ Region/ ppm	Identified Compound	Chemical Structure
1	0.88	Terminal methyl protons	-CH <sub>3</sub>
2	0.99	Terminal methyl protons	-CH <sub>3</sub>
3	1.27	β-methyl protons	-CH <sub>2</sub>
4	1.65	β-methyl protons	-CH <sub>2</sub>
5	2.04	α –methylene protons	-CH <sub>2</sub>
6	2.61	α –methylene protons	-CH <sub>2</sub>
7	2.805	α –methylene protons	-CH <sub>2</sub>
8	3.59	Methoxy proton	-OCH <sub>3</sub>
9	3.853	Methoxy proton	-OCH <sub>3</sub>
10	5.32	Olefinic protons (unsaturated)	-HC=CH
11	5.44	Olefinic protons (unsaturated)	-HC=CH

**Table S5.**  $^{13}\text{C}$  NMR spectroscopic data showing the chemical shift values corresponding to various structural features in KP (Methoxy carbon) FAMES.

<b>Peak No:</b>	<b>Peak area/ region/ ppm</b>	<b>Identified compound</b>	<b>Chemical structure</b>
1	14.1	Terminal methyl carbon	$-\text{CH}_3$
2	22.6	Methylene carbon	$-\text{CH}_2$
3	34.1	Methylene carbon	$-\text{CH}_2$
4	51.38	Methoxy carbon	$-\text{OCH}_3$
5	127.84	Olefinic carbon	$\text{C}=\text{C}$
6	130.19	Olefinic carbon	$\text{C}=\text{C}$
7	174.20	Carbonyl carbon of ester	$-\text{COOCH}_3$

**Table S6.** Shows KPBD ICP-OES elements concentration (ug/g) in comparison with petro-diesel.

<b>Name of Elements</b>	<b>Ele. Conc in <math>\mu\text{g/L}</math></b>	<b>Ele. Conc in <math>\mu\text{g/g}</math> Experimental Result</b>	<b>Petro-Diesel <math>\mu\text{g/g}</math></b>	<b>The Density of KPBD in <math>\text{g/cm}^3</math></b>
Cr	1096	1246.8	–	0.879
Ni	578.7	658.36	–	0.879
Na	479	544.9	868.3	0.879
Sn	332.8	378.61	–	0.879
Al	304.9	346.87	–	0.879
Mn	80.92	92.05	–	0.879
Ti	56.61	64.40	–	0.879
Li	38.62	43.93	–	0.879
V	37.62	42.79	-	0.879
Cu	21.65	24.63	99.6	0.879
Ca	13.1	14.90	21.4	0.879
Mg	28.22	32.10	35.6	0.879
Bi	17.5	19.90	–	0.879
Zn	11.5	13.08	9.5	0.879
Co	9.398	10.69	21.2	0.879
K	5.40	6.14	213.3	0.879