Electronic Supplementary Information

Double bond isomerization of ethyl linoleate and vegetable oils to conjugated derivatives over an LDH supported ruthenium catalyst

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Structure of ethyl linoleate and conjugated ethyl linoleate along with the proton peak positions in ^{1}H NMR are given in Fig. S1 and S2 respectively. Protons considered for the calculation of conversion of ethyl linoleate and yield of products are also indicated.
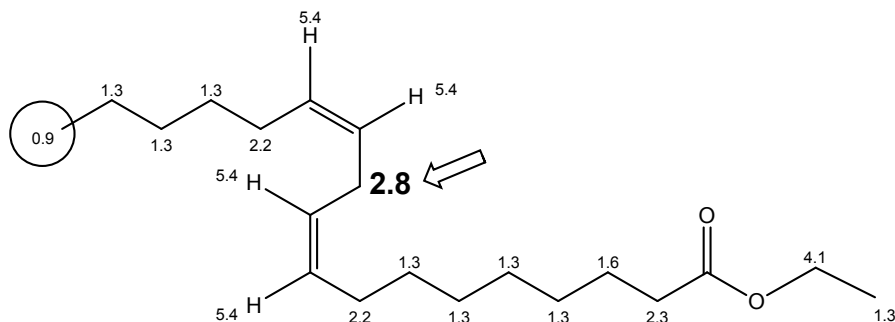

Fig. S1 Tentative proton peak positions in ethyl linoleate

Conversion of ethyl linoleate is calculated based on the decrease in the peak area of the bisallylic protons at 2.8 ppm in product relative to the reactant. The terminal methyl proton appears at 0.9 ppm was fixed as an internal standard.

$$\text{Conversion (\%)} = 100 * \left(\frac{\text{Area at 2.8 ppm before reaction - Area at 2.8 ppm after reaction}}{\text{Area at 2.8 ppm before reaction}} \right)$$
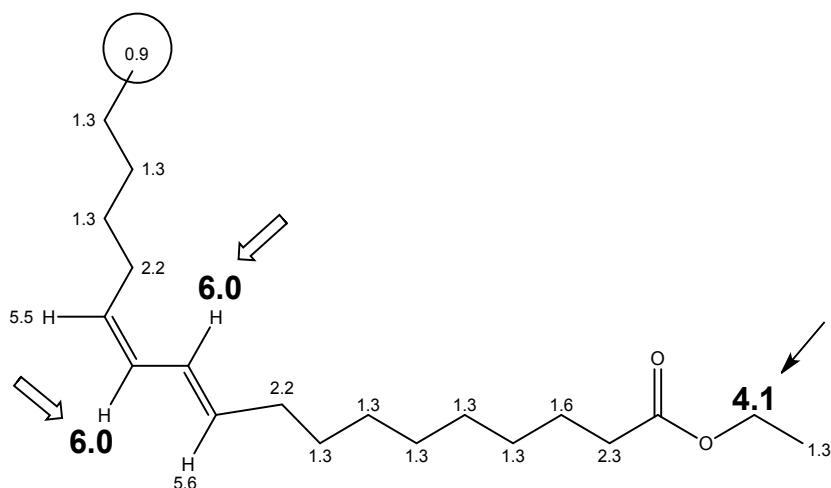

Fig. S2 Tentative proton peak positions in conjugated ethyl linoleate

Yield of the conjugated derivative is calculated based on the formation of new peaks in the region around 6 ppm in product. In this case also, the terminal methyl proton (0.9 ppm) was considered as internal standard. The isomerization product could be conjugated ethyl linoleate (CLA ester) (or) conjugated linoleic acid (CLA).

Yield of isomerized products (%) = 100 * Peak area around 6 ppm

Apart from double bond migration, there may be possibility of hydrolysis reaction owing to the presence of ionic liquid in the reaction medium. The hydrolysis product could be linoleic acid (LA) (or) conjugated linoleic acids (CLA). In this case, we are considering only the decrease in the peak area of -OCH$_2$ protons before and after the reaction.

$$\text{Yield of hydrolyzed products (\%)} = 100 * \left(\frac{\text{Area at 4.1 ppm before reaction - Area at 4.1 ppm after reaction}}{\text{Area at 4.1 ppm before reaction}} \right)$$

Preparation of reconstructed MgAl$_4$-LDH

1 M NaOH solution (20 ml) was prepared using decarbonated water and to this 250 mg of freshly prepared mixed oxides from MgAl$_4$-LDH (calcined at 500 °C for 5 h) was added under N$_2$ atmosphere. The solution was stirred at room temperature (27 °C) for 12 h and the obtained mixture was washed well till neutral pH. The material was dried under vacuum desiccator for 24 h (to prevent atmosphere contact) and stored in a tightly packed container in desiccator.
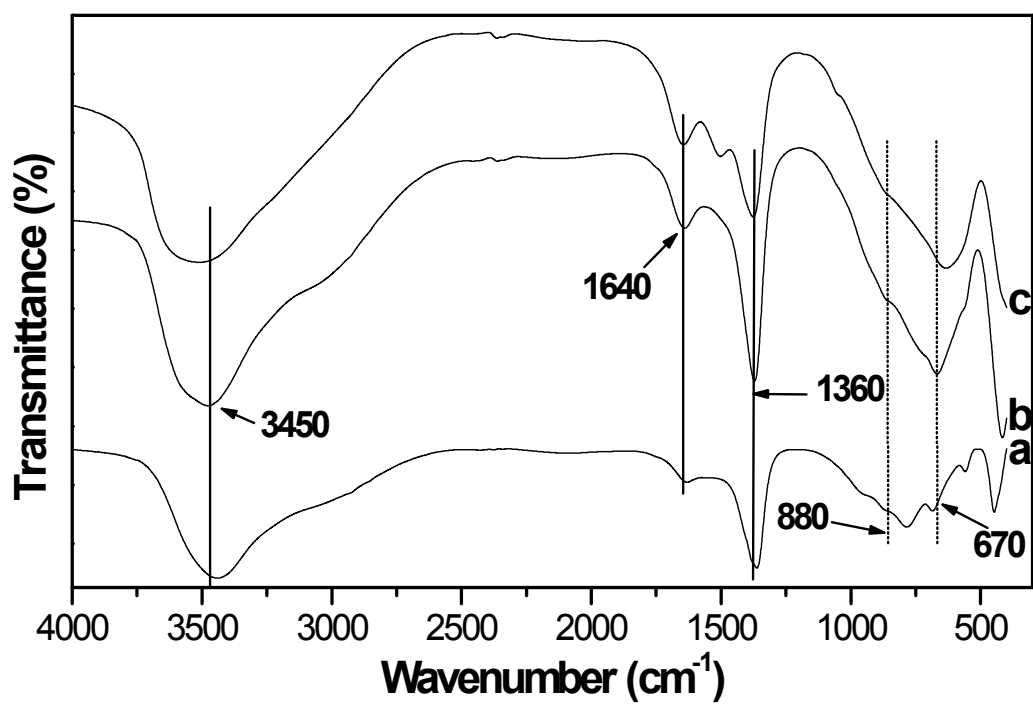
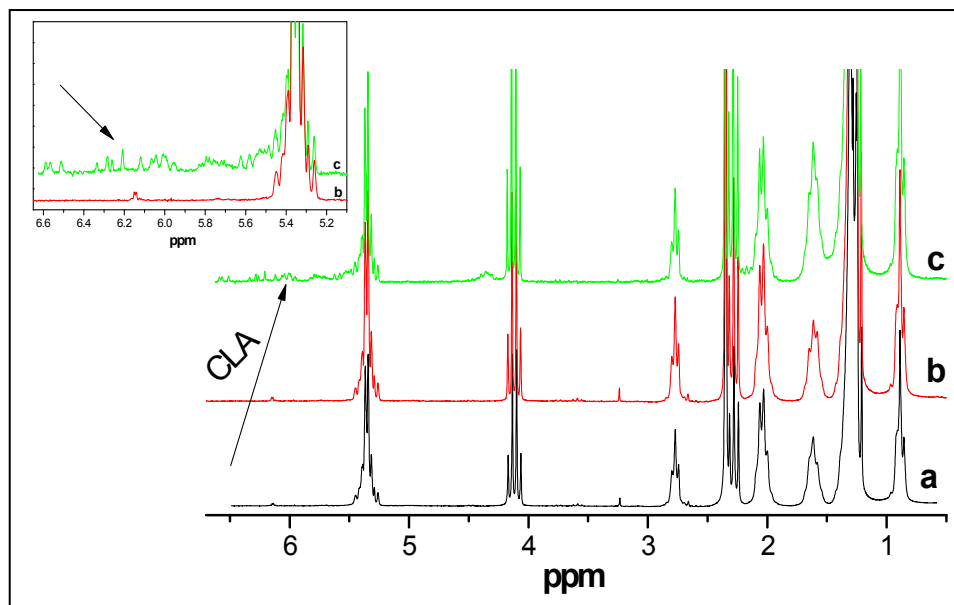**Fig. S3** FT-IR spectra of (a) MgAl$_2$-LDH, (b) MgAl$_3$-LDH, (c) MgAl$_4$-LDH

Fig. S4 ^{1}H NMR of spectra of (a) 0.5% Ru/MgAl$_4$-LDH, (b) 1% Ru/MgAl$_4$-LDH, (c) 5% Ru/MgAl$_4$-LDH catalysed product mixture; Inset: Expanded region of (b) and (c) from 6.6-5.2 ppm
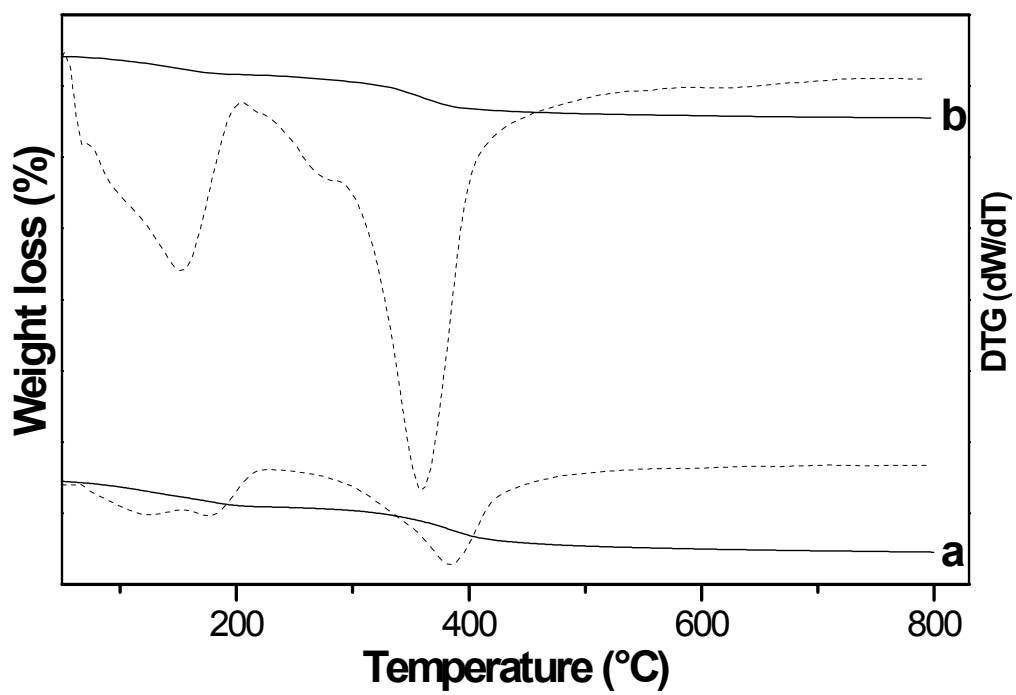
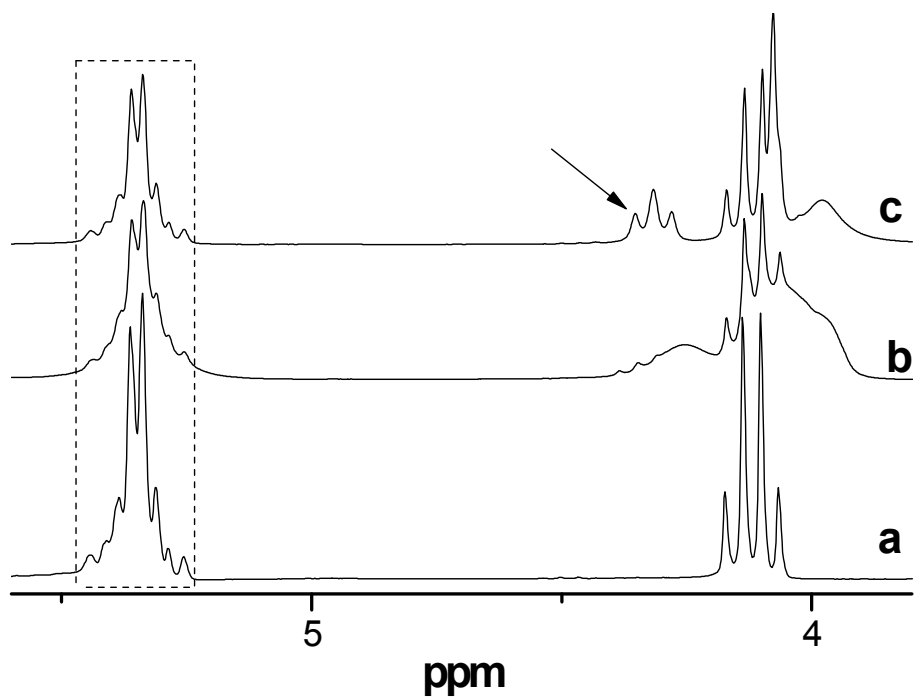**Fig. S5** TG-DTG profile of (a) MgAl$_4$-LDH, (b) 5% Ru/MgAl$_4$-LDH

Fig. S6 ^{1}H NMR spectra of (a) EL, (b) EL and BMImCl mixture, (c) EL and OMImCl mixture (arrow indicates methyl protons of ionic liquid)
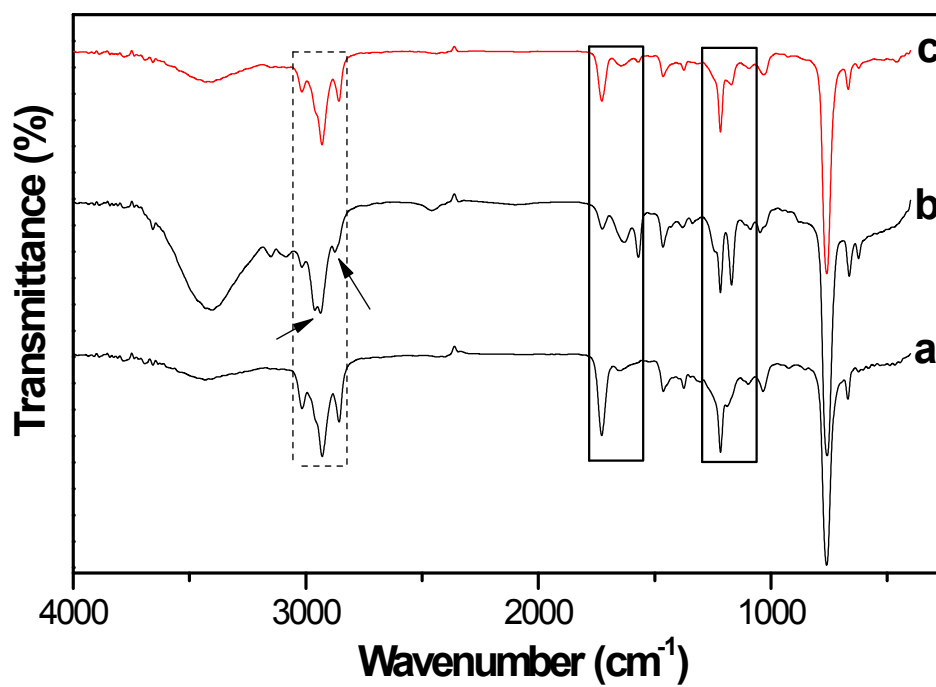
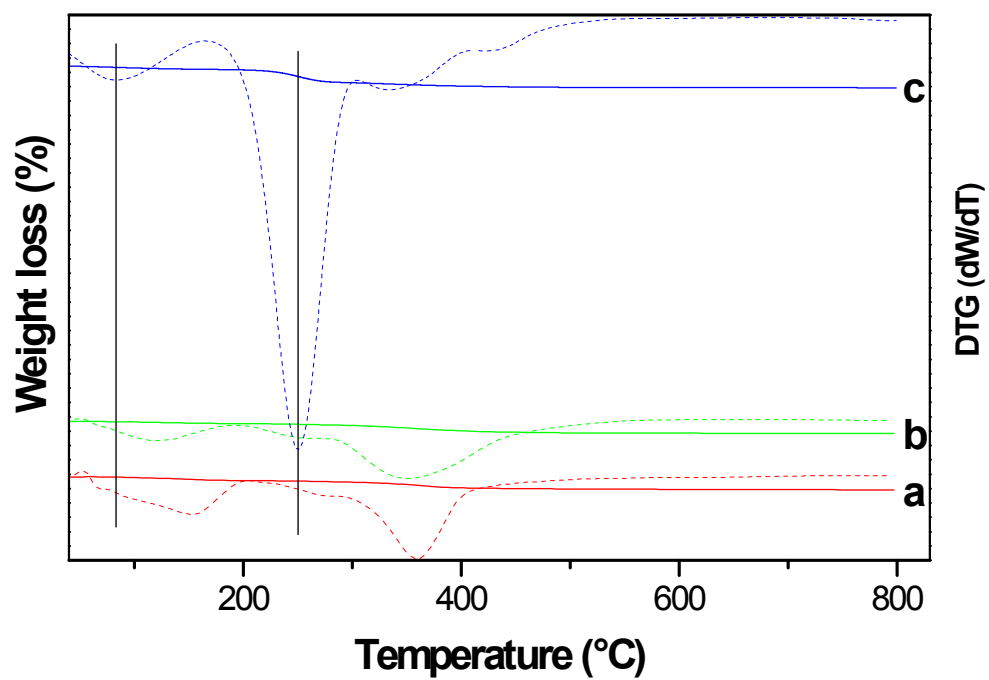**Fig. S7** FT-IR spectra of (a) EL, (b) EL and BMImCl mixture, (c) EL and OMImCl mixture

Fig. S8 TG-DTG profile for fresh and recovered catalysts (a) 5% Ru/MgAl$_4$-LDH, (b) 'a' after first cycle in BMImCl, (c) 'a' after first cycle in OMImCl
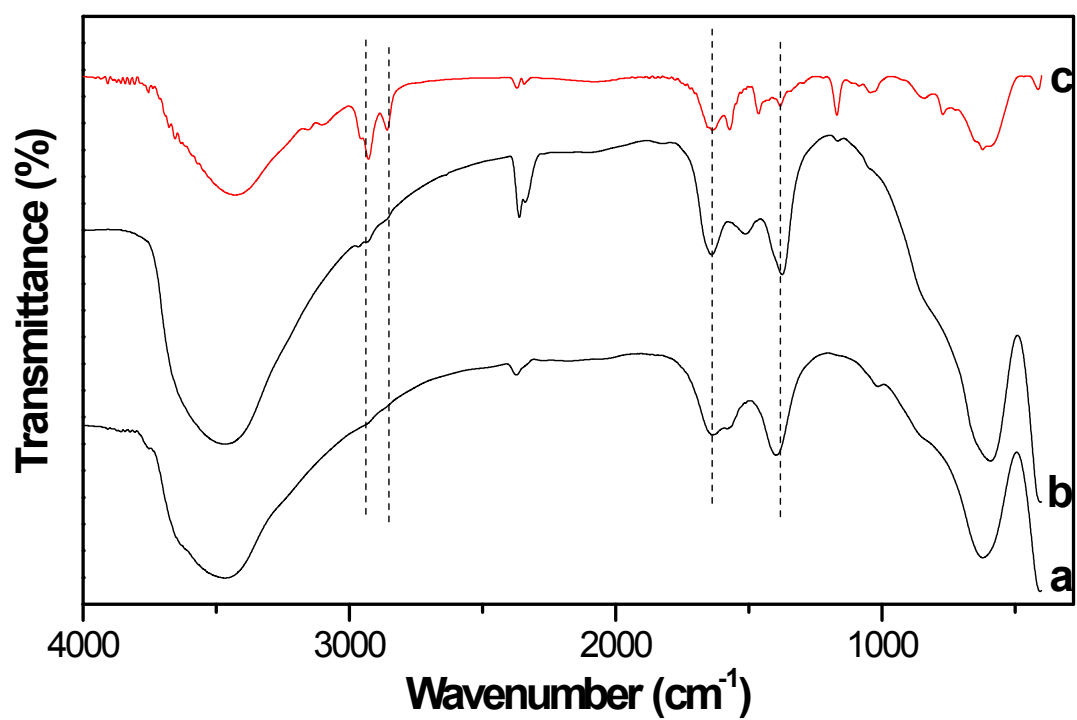
Fig. S9 FT-IR spectra of fresh and recovered catalysts (a) 5% Ru/MgAl$_4$-LDH, (b) 'a' after first cycle in BMImCl, (c) 'a' after first cycle in OMImCl

Table S1. Fatty acid compositions of vegetable oils

Name of the vegetable oil	Fatty acids (%)			
	Saturated		Unsaturated	
	Palmitic (16:0)[*]	Stearic (18:0)	Oleic (18:1)	Linoleic (18:2)
Sunflower oil	15	11	13	55
Once cooked (sunflower) oil	10	5	11	71
Doubly cooked (sunflower) oil	12	10	17	58
Corn oil	23	6	10	58
Soyabean oil	18	8	11	61
Gingelly oil	16	13	16	53

[*](x:y - No. of carbon atoms:unsaturated centers)

Table S2. Elemental chemical analysis and empirical formula of the MgAl-LDHs

Material	Mg/Al[a]		Empirical formula[b]
	Solution	Solid	
MgAl$_2$-LDH	2.0	2.0	[Mg$_{0.64}$Al$_{0.36}$(OH)$_2$](CO$_3$)$_{0.18}$ .0.74H$_2$O
MgAl$_3$-LDH	3.0	2.9	[Mg$_{0.73}$Al$_{0.27}$(OH)$_2$](CO$_3$)$_{0.14}$ .0.66H$_2$O
MgAl$_4$-LDH	4.0	3.7	[Mg$_{0.77}$Al$_{0.23}$(OH)$_2$](CO$_3$)$_{0.11}$ .0.80H$_2$O

[a]Atomic ratio; [b]Values rounded to significant figure

Table S3. Effect of amount of ionic liquid on the isomerization of ethyl linoleate[a]

Amount of ionic liquid (wt .%)	Conversion (%)	Yield (%)	
		Isomerized products	Hydrolyzed products
20	10	8	10
40	15	15	10
60	12	6	2
80	17	3	7
100	17	1	8
40[*]	63	1	63
40[$]	25	1	23

[a]EL = 250 mg, Toluene = 5 ml, Catalyst (MgAl$_4$-LDH) = 20 wt.% w.r.t. EL, Temp. = 90 °C, Time = 12 h; [*] Tetra butyl amine (TBA); [$] Tetra propyl ammonium hydroxide (TPAH)

Table S4. Time variation studies

Time	Conversion (%)	Yield (%) Isomerized products	Hydrolyzed products
1	2	1	0
4	6	4	0
8	15	10	0
12	42	29	0

[a]EL = 250 mg, Toluene = 5 ml, BMImCl = 40 wt.% w.r.t. EL, Catalyst (5% Ru/MgAl$_4$-LDH) = 20 wt.% w.r.t. EL, Temp. = 90 °C

Table S5. Recycle studies of 5% Ru/MgAl$_4$-LDH[a]

Cycle (Number)	Conversion (%)	Yield (%)	
		Isomerized products	Hydrolyzed products
1	42	29	0
2	38	18	23
3	17	4	7

[a]EL = 250 mg, Toluene = 5 ml, BMImCl = 40 wt.% w.r.t. EL, Catalyst = 20 wt.% w.r.t. EL, Temp. = 90 °C, Time = 12 h