

## Supplementary material

### Potassium Iodide-Polyethylene Glycol Catalyzed Cycloaddition Reaction of Epoxidized Soybean Oil Fatty Acid Methyl Esters and CO<sub>2</sub>

Wei Liu\*, Guanghui Lu, Bing Xiao, Chenfei Xie

E-mail address: [liuwei307@hotmail.com](mailto:liuwei307@hotmail.com) (Wei Liu)

#### 1. Materials and Methods

##### 1.1. Materials

CO<sub>2</sub> (99.995%) was supplied by Dumaoai Purge Gas Co., Ltd. (Shanghai, China). Epoxidized soybean oil (99%) and polyethylene glycol 1000 (99%) were purchased from Aladdin Industrial Co. (Shanghai, China). Potassium iodide (≥99.0%) was obtained from Kaitong Chemical Reagent Co., Ltd. (Tianjin, China). Calcium iodide (99%) was purchased from Xiya Reagent Co., Ltd. (Shandong, China). Potassium bromide (99%), sodium iodide (99%) and polyethylene glycol 400 (99%) were purchased from Kermel Chemical Reagent Co., Ltd. (Tianjin, China). Triethylene glycol (99.0%), tetraethylene glycol and zinc iodide (≥98%) were obtained from Macklin Biochemical Co., Ltd. (Shanghai, China). Polyethylene glycol 200 and polyethylene glycol 600 were purchased from Xiya Reagent Co., Ltd. (Shandong, China). Polyethylene glycol 800, polyethylene glycol 2000 and polyethylene glycol 4000 were obtained from TCI Development Co., Ltd. (Shanghai, China).

##### 1.2. Preparation of EMS

Epoxidized methyl soyates were prepared as described in the literature. Briefly, 200.0 g epoxidized soybean oil (ESO) was weighted into a 1000-ml three-necked

round-bottom flasks along with a mechanical stirrer. Sodium methoxide as a catalyst, 2.0 g (1 wt%), was dissolved in 60 ml methanol and then added to the epoxidized soybean oil in the reactor. The transesterification reaction was performed at 50 °C for 2 h with a violent agitation speed. After the reaction was completed, the epoxidized methyl soyates were obtained by static separation, water washing and drying treatment. Eventually, solvent and trace water were eliminated under negative pressure. Purity of the epoxidized methyl soyates was determined and analyzed by gas chromatography (Agilent 7890B) equipped with a DB-1HT capillary column (29.0 m×250 μm×0.1 μm) and a flame ionization detector (FID). Finally, the purity of the epoxidized methyl soyates (EMS) was above 99.0%.

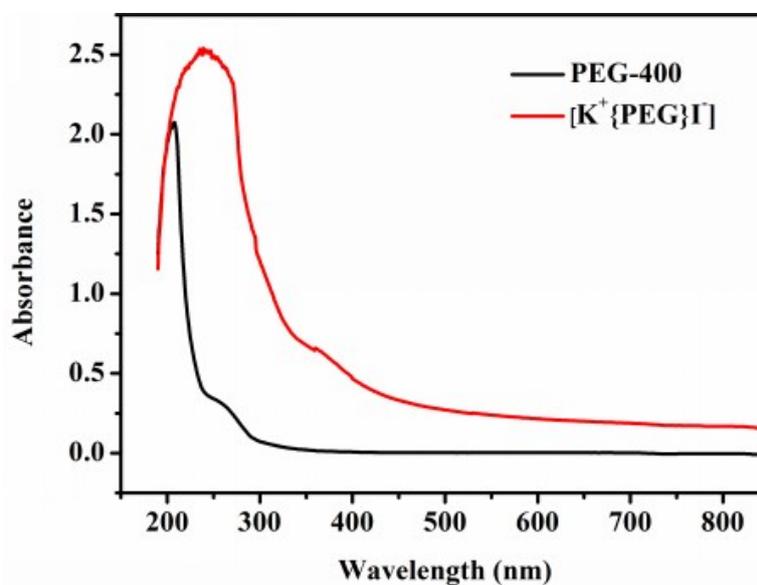
### **1.3. Synthesis of CMS**

5.0 g of EMS (epoxide number=6.16, i.e. 0.01925 mol epoxides) and catalyst were appended to the Parr stainless steel autoclave rigged with a gas inlet tube, through it, the autoclave was sealed. Before the reaction was started, the air in the autoclave was replaced by carbon dioxide (CO<sub>2</sub>) three times in order to clean out the air completely. Following this, the autoclave was maintained at the preset reaction temperature for 10 min. At the moment, the reaction mixture was pressured with CO<sub>2</sub> to a definite pressure at a definite stirring speed for different reaction time. After reaction finished, the autoclave was cooled to ambient temperature and the CO<sub>2</sub> was vented out. Subsequently, the metal halide and polyethylene glycol were completely removed by dissolving the reaction mixture in diethyl ether and then the reaction mixture was washed with saturated salt water for three times. After that, the organic layer was dehydrated with anhydrous sodium sulfate. Ultimately, the solvent was distilled under negative pressure and the final product was obtained.

### **1.4. Characterization of the CMS Product**

The addition of CO<sub>2</sub> to the epoxidized group to form the five-membered cyclic carbonate group was confirmed by FT-IR. Characteristic epoxide peaks of epoxidized methyl soyates were observed at 842-822 cm<sup>-1</sup>. As expected, the IR spectrum of

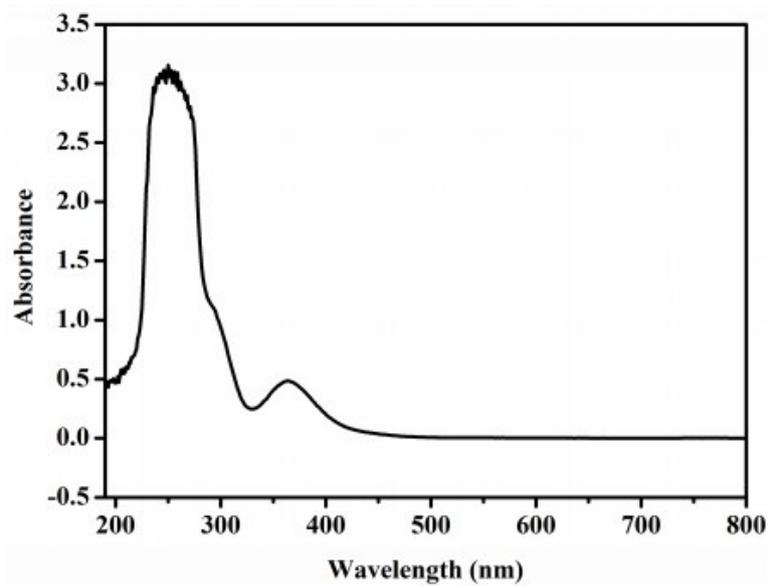
carbonated methyl soyates (CMS) lacked these epoxide peaks, while a strong absorption peak at 1,800-1,804  $\text{cm}^{-1}$  (C=O bond) bound up with carbonate was observed. Formation of the carbonate and the disappearance of the epoxide structures were further confirmed by  $^1\text{H-NMR}$  and  $^{13}\text{C-NMR}$  analysis. Both of  $^1\text{H-NMR}$  and  $^{13}\text{C-NMR}$  analysis were recorded using a Bruker Avance III HD 500 NMR spectrometer (Swiss) operating at a frequency of 500 MHz with tetramethylsilane (TMS) as the internal standard. In addition, it stated that the quantitative analysis of CMS was determined by GC.



**Fig. S1.** UV-vis spectra of PEG-400 and  $[\text{K}^+\{\text{PEG}\}\text{I}^-]$  complex



**Fig. S2.** The appearance of PEG-400/KI co-catalysts in reaction.



**Fig. S3.** UV-vis spectra of mixture of KI&PEG-400