Carbon dioxide as a sustainable resource for macrocyclic oligourea

Zhong Ying, Yanlei Dong, Jianwei Wang, Yancun Yu, Yihan Zhou, Yuequan Sun, Chao Zhang, Haiyang Cheng, Fengyu Zhao



Scheme S1 Synthesis of oligomer-4 from oligomer-1 and acetone



Figure S1 The MALDI-TOF mass spectrum of the oligomer-4.



Figure S2 The accurate molecular weight of the oligomer-3.



Figure S3 The fragment ion of the dimer for the oligomer-3.



Figure S4 The chemical structure for the trimer fragment ions of oligomer-3

GPC: The gel permeation chromatography (GPC) was used to determine the molecular weight of the oligomers and distribution with using a Waters instrument with a refractive index detector (waters 2414) and waters HPLC 2000 column. at a flow rate of 0.65 mL/min (eluent: 0.1mg/L sodium nitrate water solution; 30 °C). PAAS (sodium polyacrylate) standards (Waters) were used for calibration.



Figure S5 GPC curve of the oligomer-3



Figure S6 GPC curve of the oligomer-1

Molecular weight / Percentage of cyclic oligomer:

The molecular weight was determined according to the definition of the number average molecular weight and the weight average molecular weight.

$$M_n = \frac{\sum N_i M_i}{\sum N_i} \qquad M_w = \frac{\sum N_i M_i^2}{\sum N_i M_i}$$

 M_i is the ratio of mass and charge, and N_i stand for the number of the molecule with a molecular weight as M_i . The N_i increase linearly with the signal of the Mass Spectrum Instrument. Mn and Mw were calculated by means of accumulation for the each signal peak in the mass spectrum. In addition, the molecular weight and the percentage of cyclic oligomer were determined by PolyTools 1.0 software with the following formula:

$$Cyclic (\%) = \frac{\sum Intensity_{cyclic}}{\sum Intensity_{cyclic} + \sum Intensity_{others}}$$

