

Flexible Foams and Elastomers from Castor Oil

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Abstract

Self-transesterification of castor oil was employed to prepare higher molar mass polyols possessing interesting properties. Detailed structures of the polyols were studied using various standard techniques along with spectrometric analysis such as MALDI-TOF/MS. Polyurethane elastomers prepared from these polyols provided soft material with low Shore A hardness. These polyols were also tested in molded polyurethane foams and their polyurethane properties were compared with that of the commercial bio-polyols.

Background

- X-Polyol obtained from ring opening of epoxide soybean oil with methanol
- HF-Polyol prepared by hydroformylation/hydrogenation of soybean oil

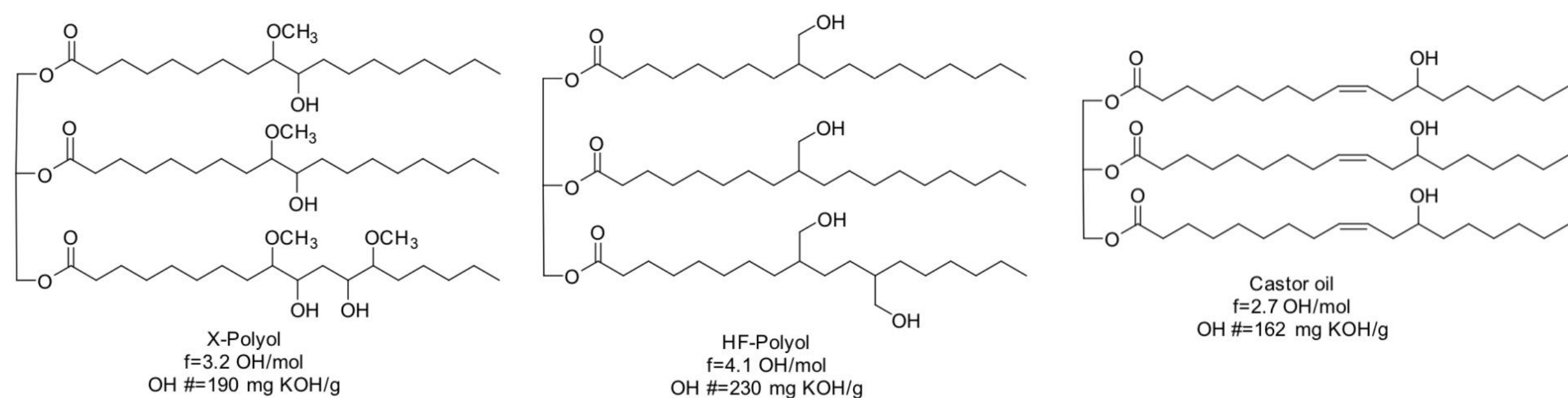
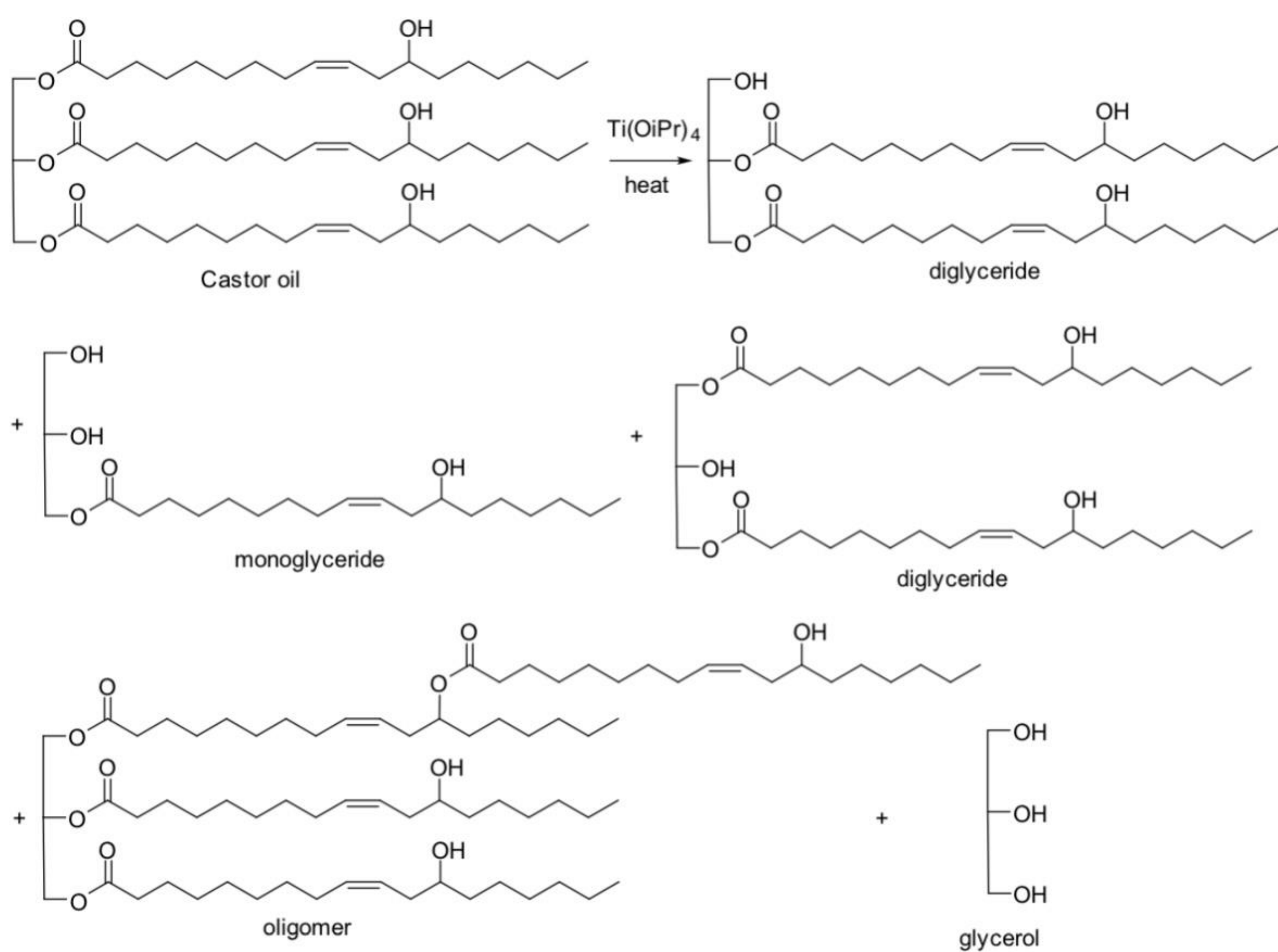


Fig. 1 Structures of starting materials for self condensation reaction

- Self condensation of castor oil produces a complex mixture of higher molecular weight oligomers, lower molecular weight diglycerides, monoglycerides, glycerol, etc.



Scheme 1 Proposed mechanism for self condensation of castor oil

Results & Discussion

- Viscosity of the polyols increases while the hydroxyl number of the polyols decreases with increase reaction time.

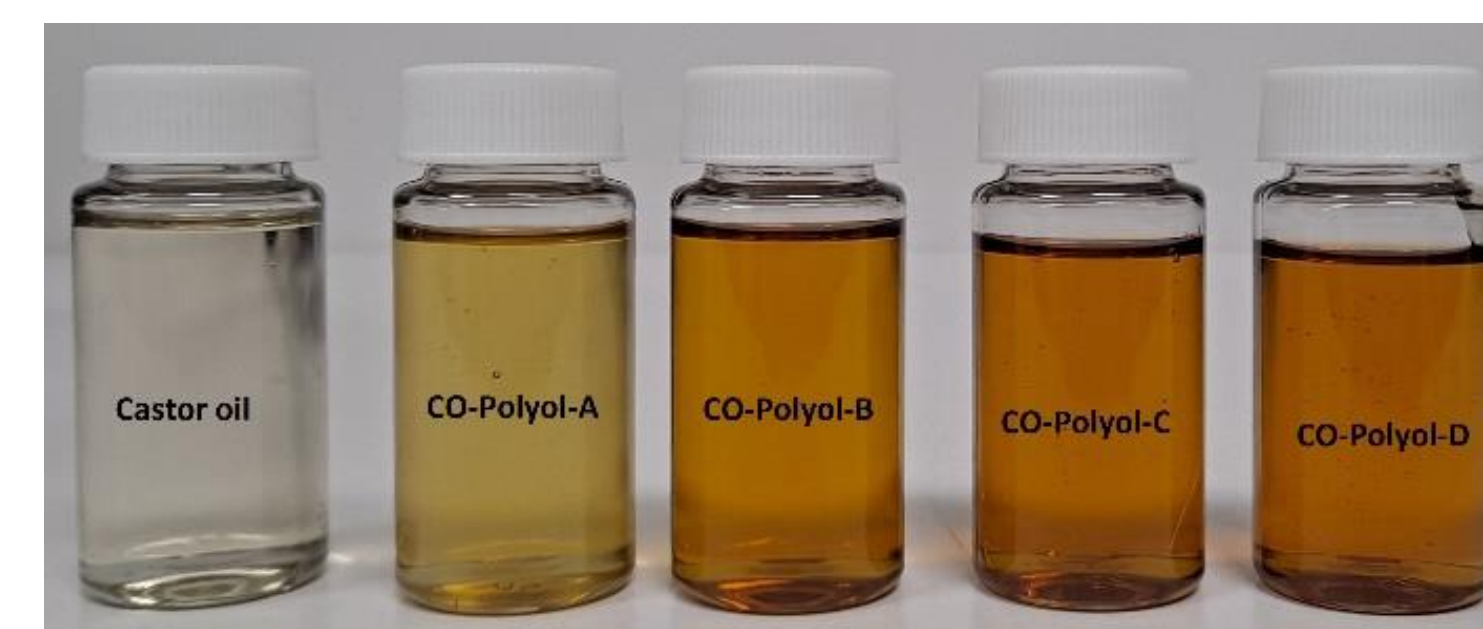


Fig. 2 Castor oil and self condensed polyols prepared from castor oil

| Polyols | Reaction time, h | Viscosity (Pa.s) @25 °C | Acid value Mg KOH/g | OH# (PAP), mg KOH/g | OH equiv. g/mol |
|-------------|------------------|-------------------------|---------------------|---------------------|-----------------|
| Castor Oil | 0 | ~ 0.6 | <1 | 158 | 355 |
| CO-Polyol-A | 5 | 1.4 | 0.8955 | 70 | 801 |
| CO-Polyol-B | 6 | 2.2 | 1.8003 | 60 | 935 |
| CO-Polyol-C | 8 | 2.1 | 0.9078 | 52 | 1078 |
| CO-Polyol-D | 10 | 2.4 | 1.8225 | 43 | 1305 |

Table 1: Properties of Castor oil and self condensed polyols synthesized from castor oil

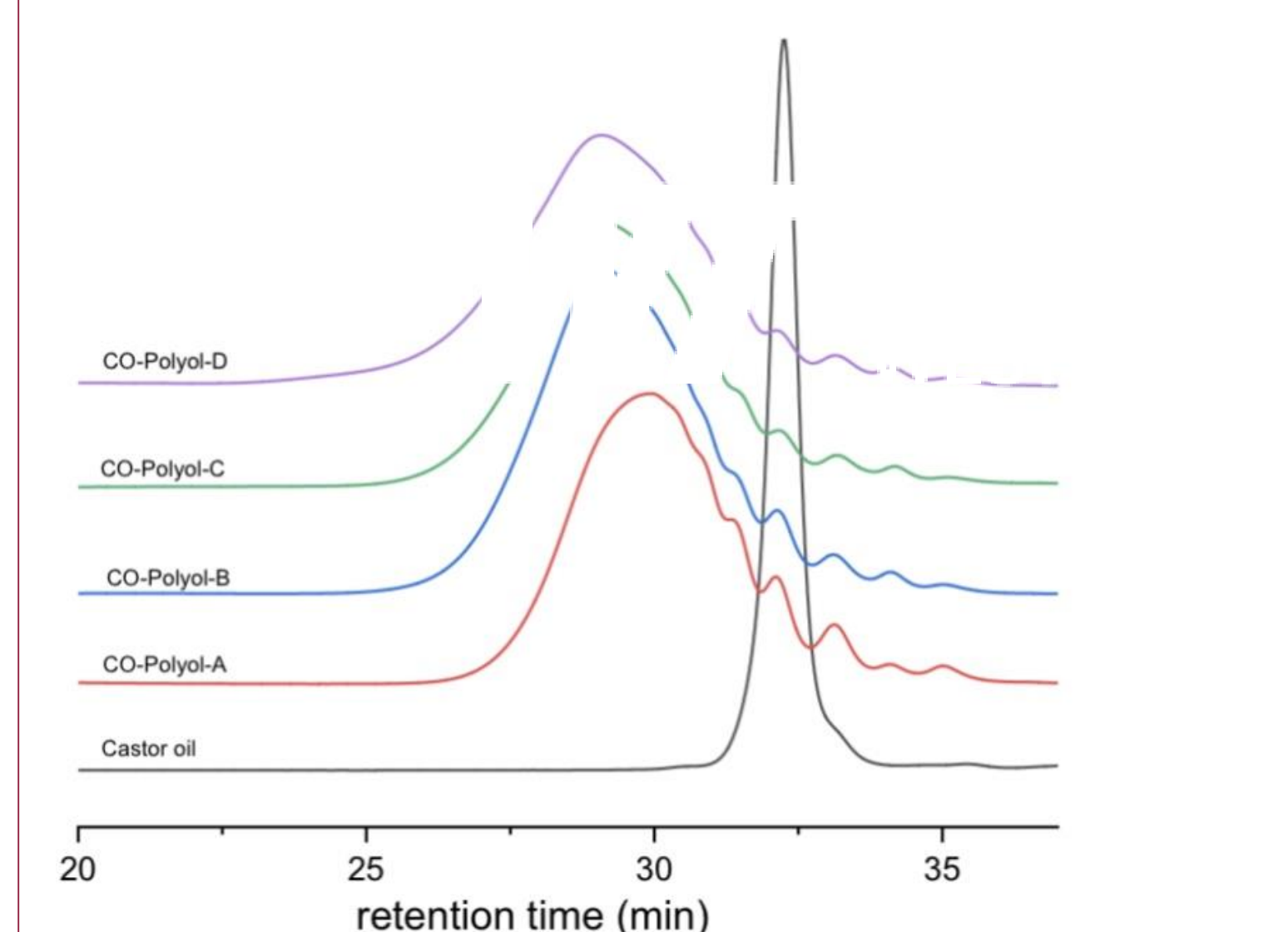


Fig. 3 SEC overlay of the polyols with castor oil

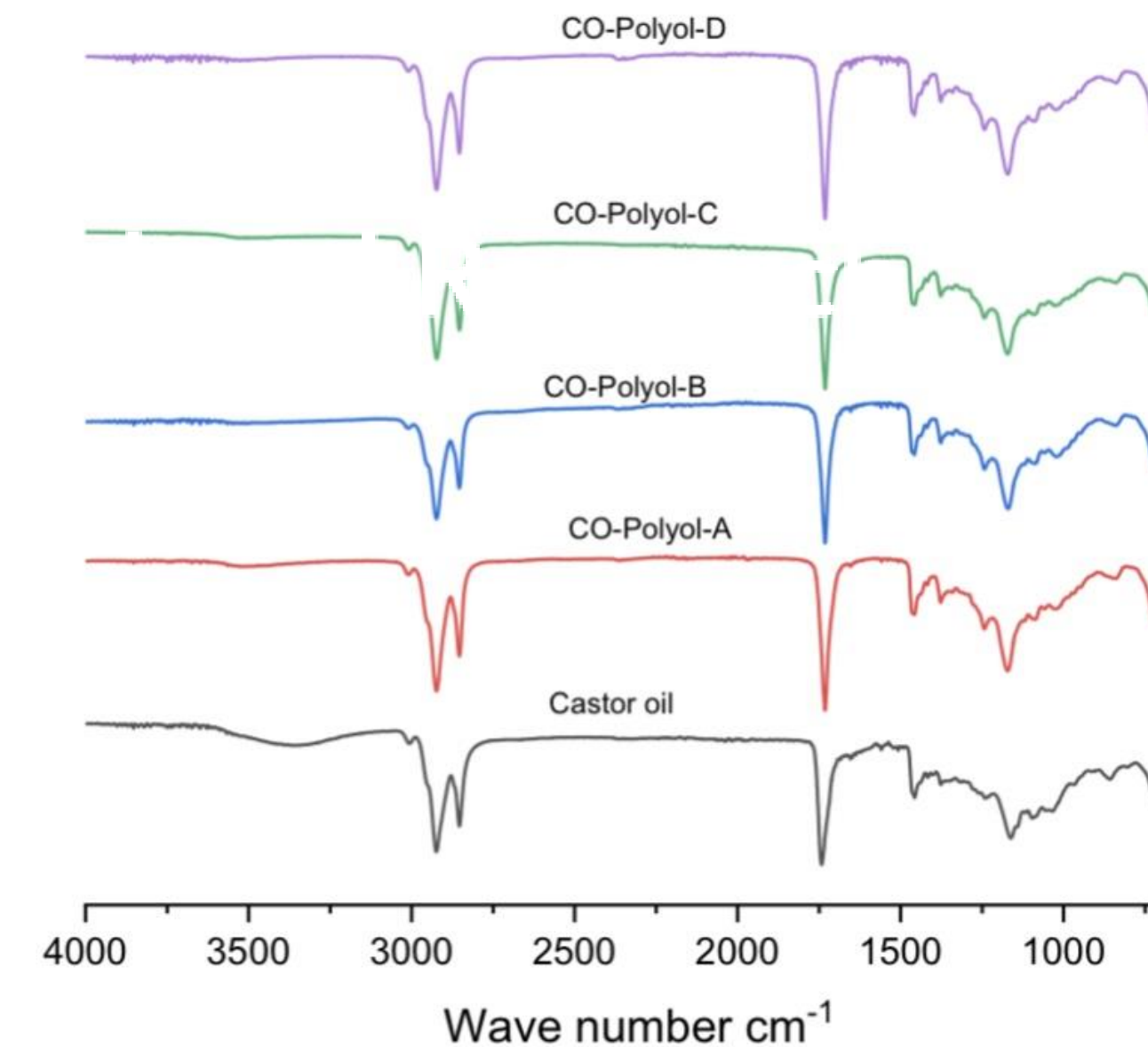


Fig. 4 FTIR overlay of the polyols with castor oil

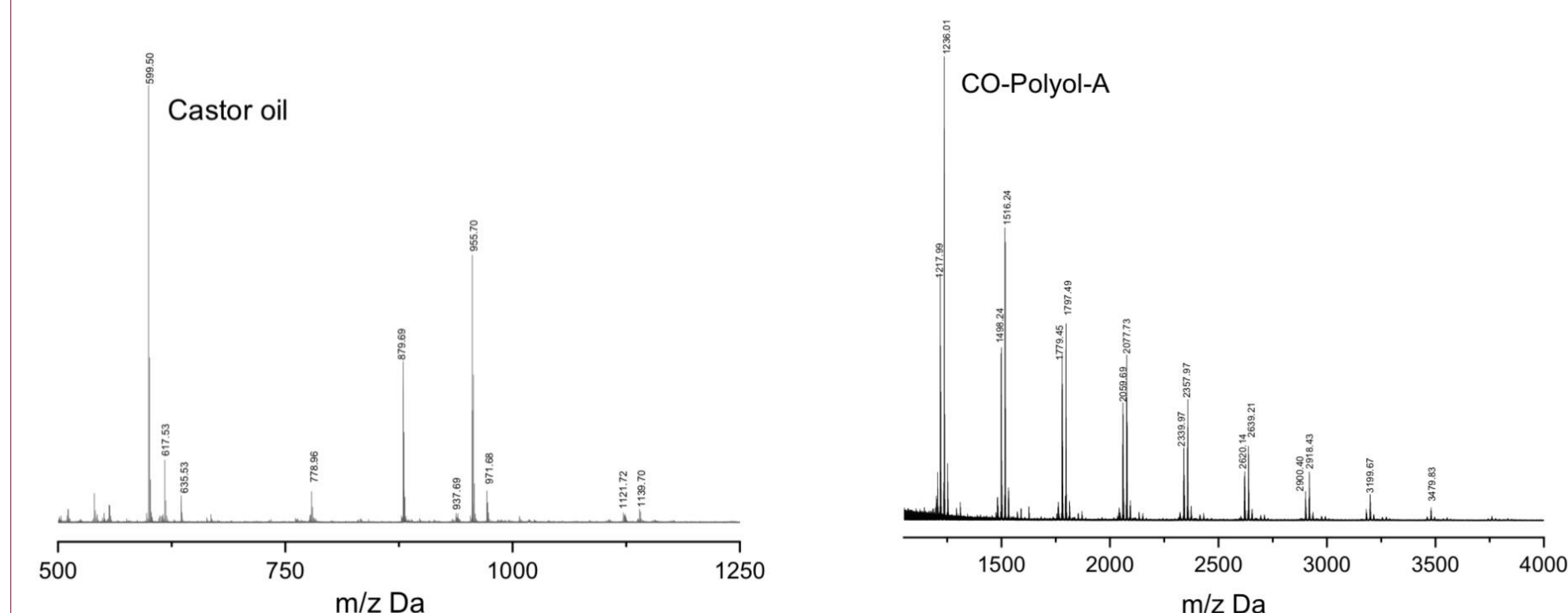


Fig. 5. MALDI-TOF/MS of castor oil and a polyol prepared from castor oil

Results & Discussion

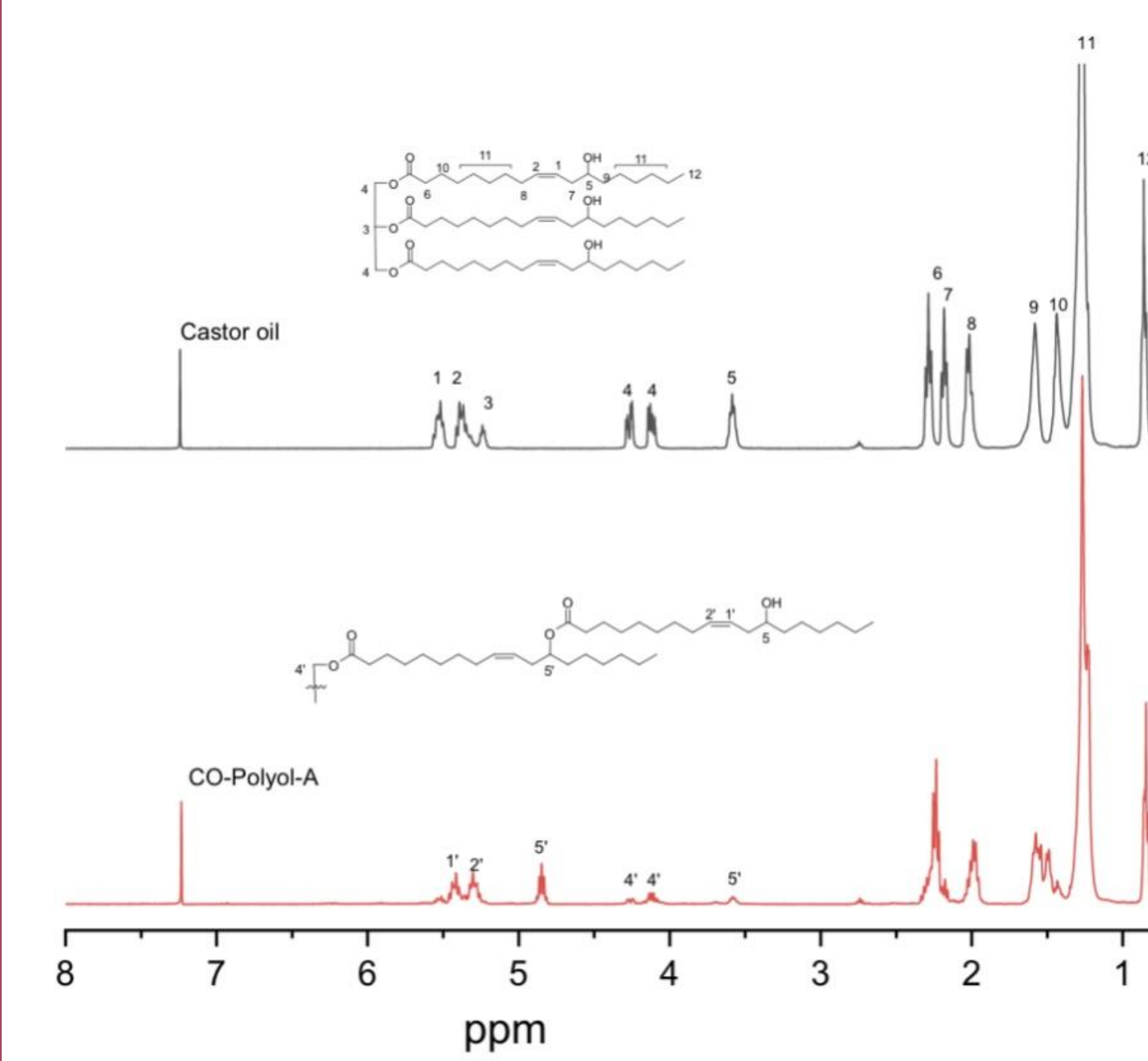


Fig. 6 ¹H NMR of castor oil and the polyol prepared from castor oil



Fig. 7 Elastomers prepared from castor oil and self condensed castor oil

- SEC overlay suggests the formation of higher molecular weight self-condensed polyols.

- NMR spectra of the polyols showed the formation of new ester bond.

- MALDI-TOF/MS confirms the structures of the polyols supporting the proposed mechanism.

- Degree of swelling $V_s/V_o = 3.1 - 3.8$
- Sol fraction = 4.7 – 17.3 %

| Elastomers | Tg, °C | Hardness, Shore A | Tensile Strength | Break Elongation, % |
|----------------|--------|-------------------|------------------|---------------------|
| Castor Oil-RM | 9.6 | 77±1 | 4.22±0.38 | 90.2±9.2 |
| CO-Polyol-A-RM | -48.7 | 48±3 | 0.51±0.05 | 36.2±6.3 |
| CO-Polyol-B-RM | -58.0 | 39±2 | 0.40±0.06 | 30.6±7.2 |
| CO-Polyol-C-RM | -58.6 | 30±3 | 0.29±0.01 | 30.7±4.4 |
| CO-Polyol-D-RM | -67.2 | 28±3 | 0.19±0.05 | 25.8±8.4 |

Table 2: Characteristics of elastomers obtained from castor oil and self condensed castor oil

- Split occurred in molded polyurethane foams prepared from 30 % self-condensed castor oil, therefore, not possible to analyze mechanical properties.
- Better results were obtained when the foams were formulated with a mixture of all 4 polyols.
- Optimization of the catalysts and TDI index may help achieve our goal to meet the current flexible foam requirement.

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References

- Z. S. Petrovic, *Polymer Reviews*, 2008, **48**, 109-155.
- M. Desroches, M. Escouvois, R. Auvergne, S. Caillol and B. Boutevin, *Polymer Reviews* 2012, **52**, 38- 79.
- Y. Li, X. Luo and S. Hu, *Journal*, (2015), DOI: https://doi.org/10.1007/978-3-319-21539-6_2.
- M. Ionescu, *Chemistry and Technology of Polyols for Polyurethanes*, Smithers-Rapra, Shawbury, Shropshire., 2016.
- M. Ionescu, D. Radojčić, X. Wan, M. L. Shrestha, Z. S. Petrović and T. A. Upshaw, *European Polymer Journal*, 2016, **84**, 736-749.