

Effects of Chemical Composition and Cross-Linking Degree on the Thermo-Mechanical Properties of Bio-Based Thermosetting Resins: A Molecular Dynamics Simulation Study

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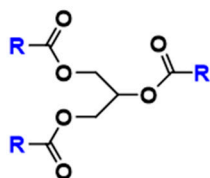
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The six molecular structures of EVO are named as a1, a2, a3, a4, a5, a6, as shown in Figure 1. The numbers of the six structures in ESO20, ESO40, ESO60, ESO80, ESO100 are shown in Table S1. The percentage of fatty acids in each system is shown in Figure S1.

Table S1. The composition of ESO in each system.

| | No. of a1 | No. of a2 | No. of a3 | No. of a4 | No. of a5 | No. of a6 | Total No. of EVO | Epoxy functionalities |
|-------|--------------|--------------|--------------|--------------|--------------|--------------|---------------------|--------------------------|
| ESO0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | - |
| ESO20 | 2 | 2 | 3 | 0 | 4 | 1 | 12 | 4.07 |
| ESO40 | 5 | 3 | 6 | 1 | 9 | 2 | 26 | 4.07 |
| ESO60 | 8 | 7 | 9 | 1 | 14 | 3 | 42 | 4.07 |

| | | | | | | | | |
|--------|----|---|----|---|----|---|----|------|
| ESO80 | 10 | 8 | 12 | 2 | 18 | 4 | 54 | 4.07 |
| ESO100 | 12 | 8 | 14 | 2 | 19 | 5 | 60 | 4.03 |



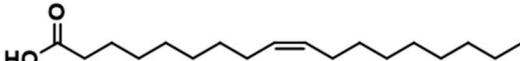
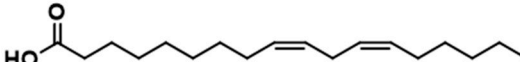
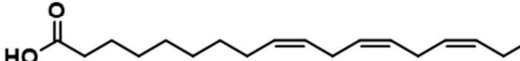
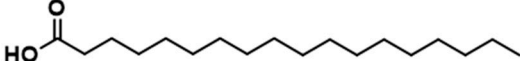
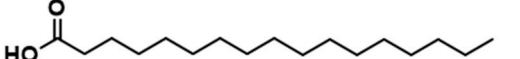
| | | ESO20 | ESO40 | ESO60 | ESO80 | ESO100 | |
|----|-----------|---|-------|-------|-------|--------|-------|
| R= | Oleic |  | 25% | 25.6% | 24.6% | 24.7% | 25% |
| | Linoleic |  | 50% | 51.3% | 50.8% | 50.6% | 50.6% |
| | Linolenic |  | 8.4% | 7.8% | 8.7% | 8.7% | 8.3% |
| | Stearic |  | 5.5% | 3.8% | 5.5% | 4.9% | 4.4% |
| | Palmitic |  | 11.1% | 11.5% | 10.3% | 11.1% | 11.7% |

Figure S1. The percentage of fatty acids in each system.