Supplementary material

Utilization of Phenolic Lignin Dimer Models for the Quantification of Monolignols in Biomass and in Its derived Organosolv Lignin via Thioacidolysis and GC-MS analysis.

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Table S1: Klason lignin (%, acid soluble and insoluble lignin) of three biomass types.

Biomass	**Aspen**	**Barley straw**	**Pine**
Klason lignin (%)	28.65	22.44	36.99

The lignin content was determined according to standard procedures.[1,2] For this purpose, 0.2 g of the sample was weighed to a glass beaker, 3 mL of sulfuric acid (72%) was added. The beaker was covered with aluminum foil and placed in a preheated water bath at 30 °C for one, while stirring occasionally. After removing the beaker from the water bath, 72 mL of ultrapure water was added to the solution and stirred thoroughly. The beaker was again covered with foil again and placed in the autoclave (121°C, 15 min). Then the samples were filtered, and the filtrate was collected. The volume of the filtrate was measured, and the filter with the lignin was washed with ultrapure water. The filter was dried at 105 °C and weighed until it reached a constant weight to obtain acid insoluble residue (AIR). The absorption of the filtrate was measured at 205 nm, and the absorption was kept between 0.2-0.8 AU with dilutions for measurement of the acid soluble lignin (ASL).[2] Total Klason lignin content (KL) was obtained as the sum of AIR and ASL percentages.

Table S2 Recovery test results of two LMCs (n = 8)

LMCs	**Spiked concentration (µmol/mL)**	**Mean recovery concentration (µmol/mL)**	**SD (µmol/mL)**	**RSD (%)**
GGE	0.7794	0.6929	0.012	8.65
SGE	1.1296	1.0973	0.022	10.07

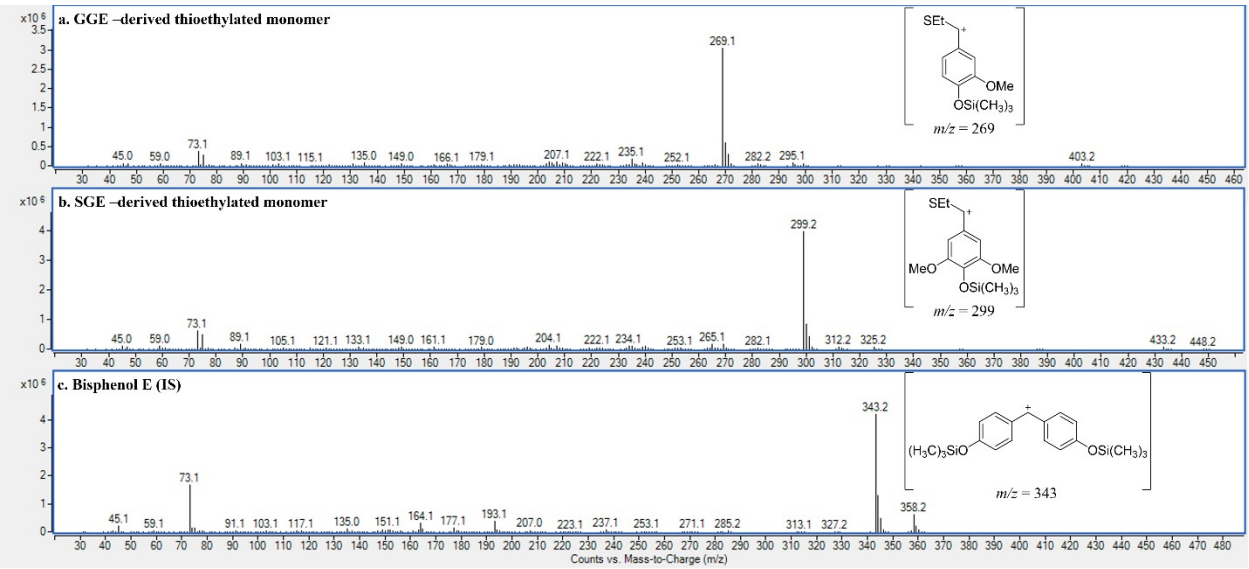

Fig. S1 Mass spectra of lignin model compound-derived thioethylated monomers and the internal standard. The structures are shown in each spectrum, illustrating the characteristic fragment ions with highest abundance.

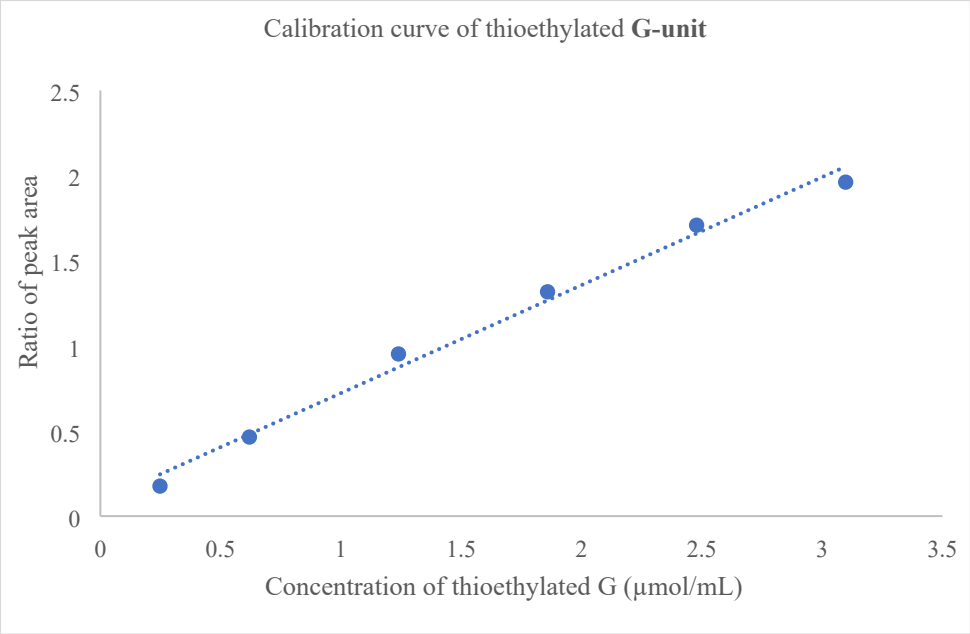

Fig. S2 Calibration curve built on peak area of thioethylated G-monomers released from GGE versus IS.

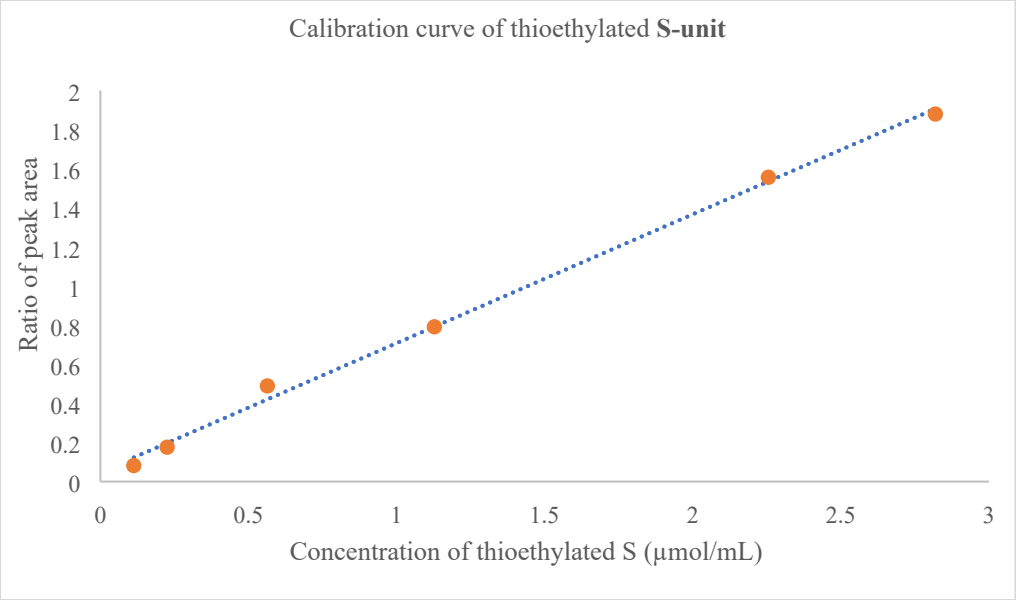

Fig. S3 Calibration curve built on peak area of thioethylated S-monomers released from SGE versus IS.

References

1 A. International and files indexed by mero, *Standard Test Method for Acid-Insoluble Lignin in Wood*, 2001.

2 A. Sluiter, B. Hames, R. Ruiz, C. Scarlata, J. Sluiter, D. Templeton and D. Crocker, *Determination of Structural Carbohydrates and Lignin in Biomass: Laboratory Analytical Procedure (LAP)*, 2008.