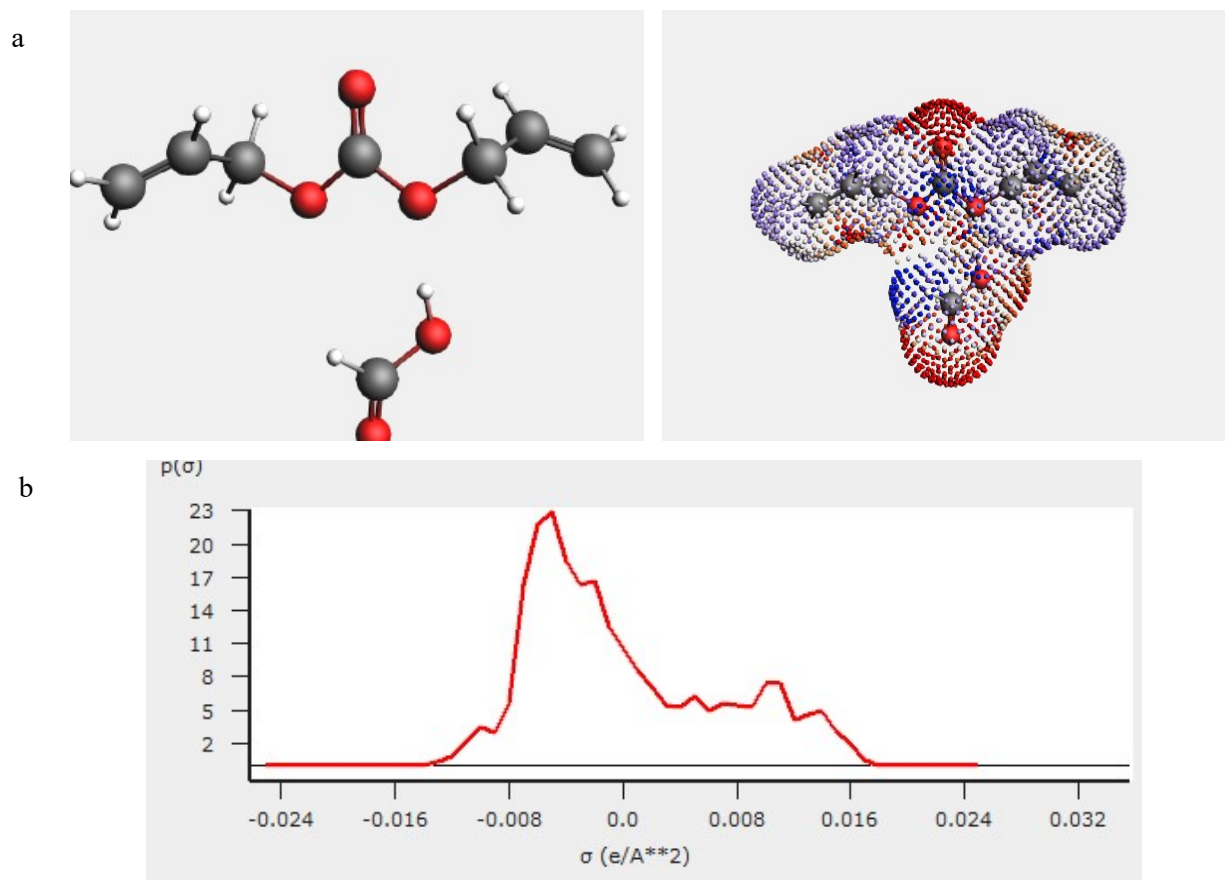
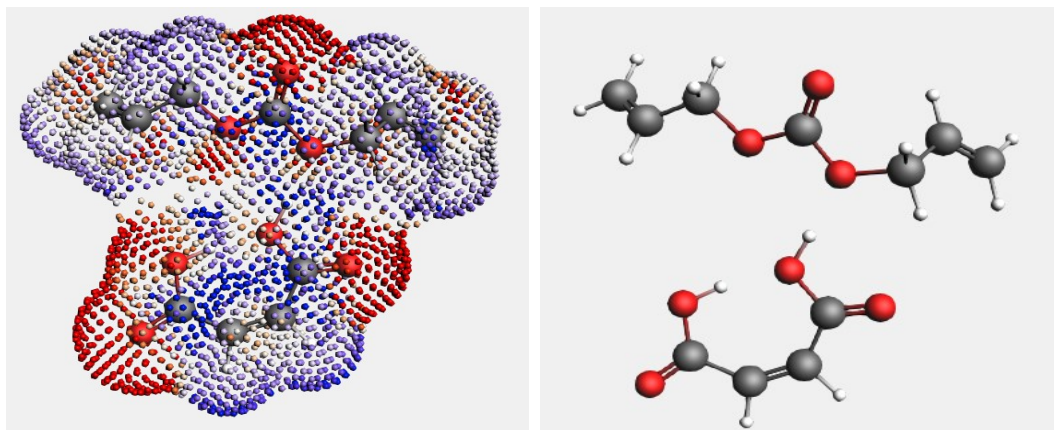


## Supporting Information

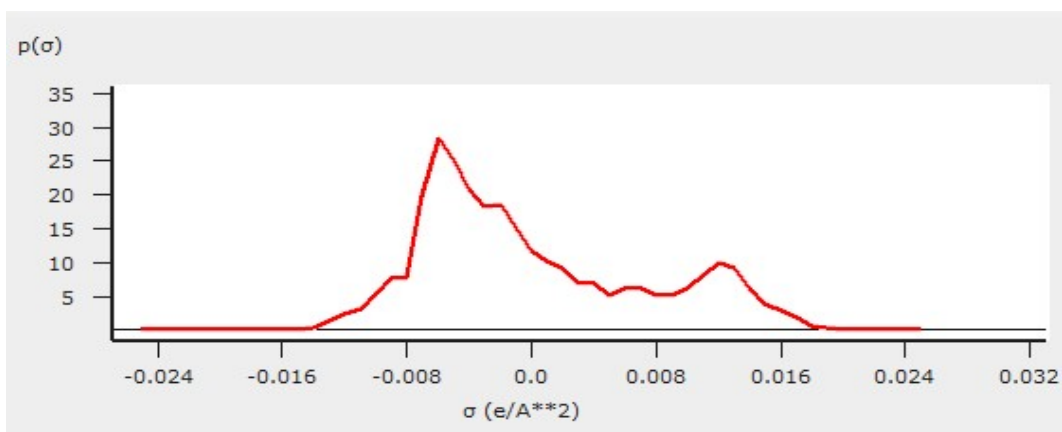


**Figure 1:** a) COSMO-RS model for geometrically optimized structure for DAC+FA solvent system b) Sigma profile for DAC+FA solvent system.

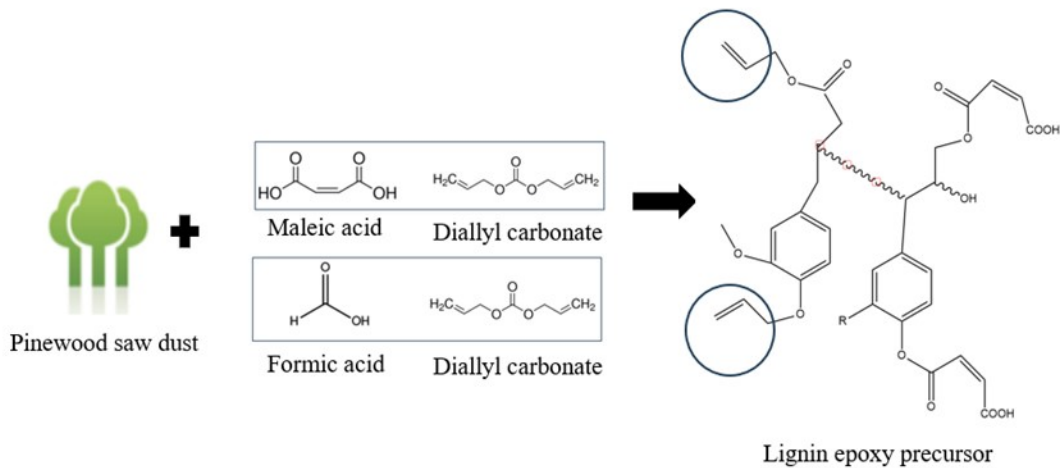
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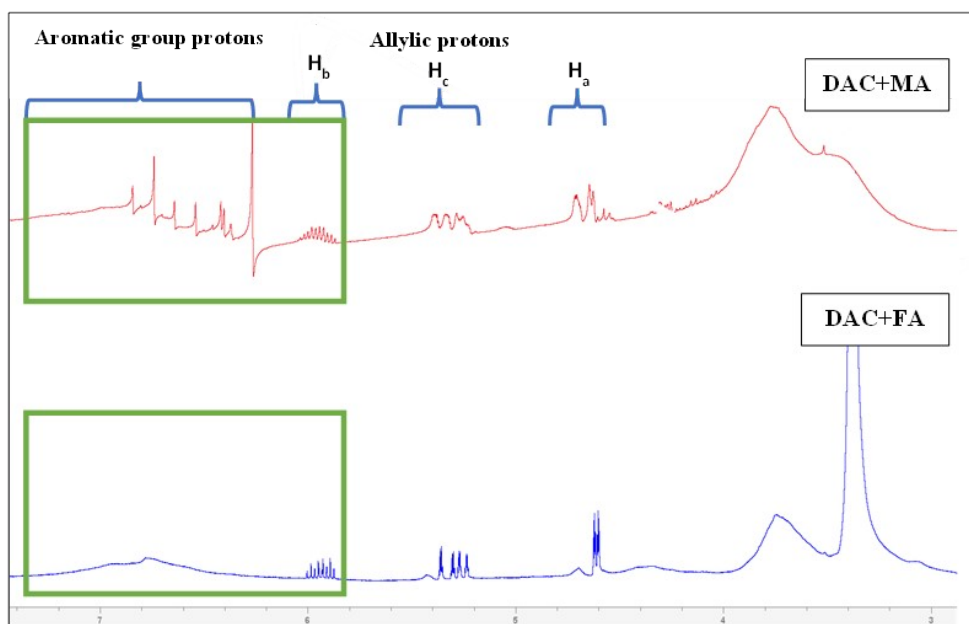
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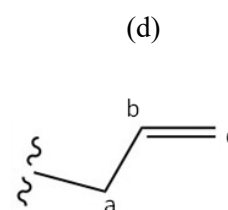
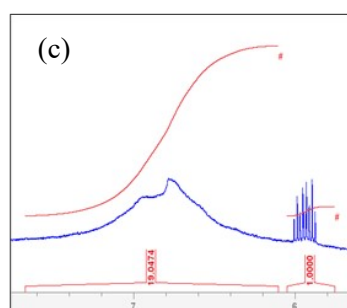
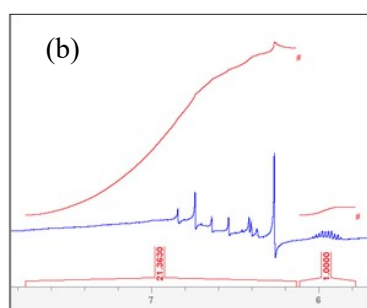
**Figure 2:** a) COSMO-RS model for geometrically optimized structure for DAC+MA solvent system b) Sigma profile for DAC+MA solvent system.



**Figure 3:** Reaction scheme for one-step extraction and functionalization of lignin. Pinewood saw dust was treated with solvent systems MA+DAC and MA+FA system, previously modeled in COSMO-RS software for experimental analysis.

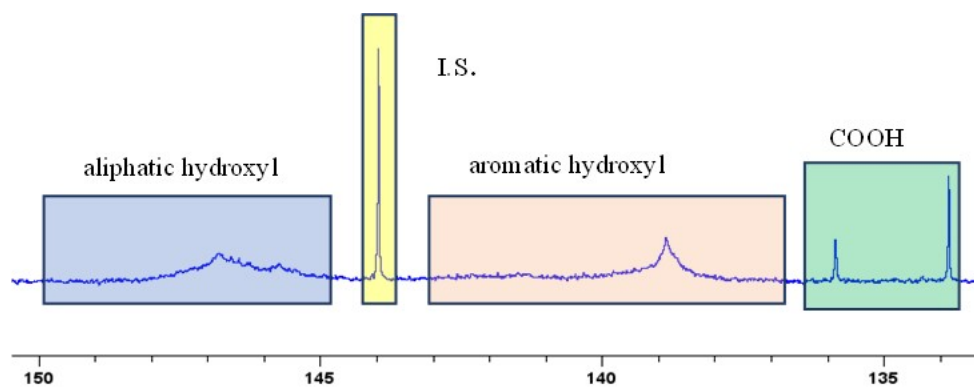


(a)

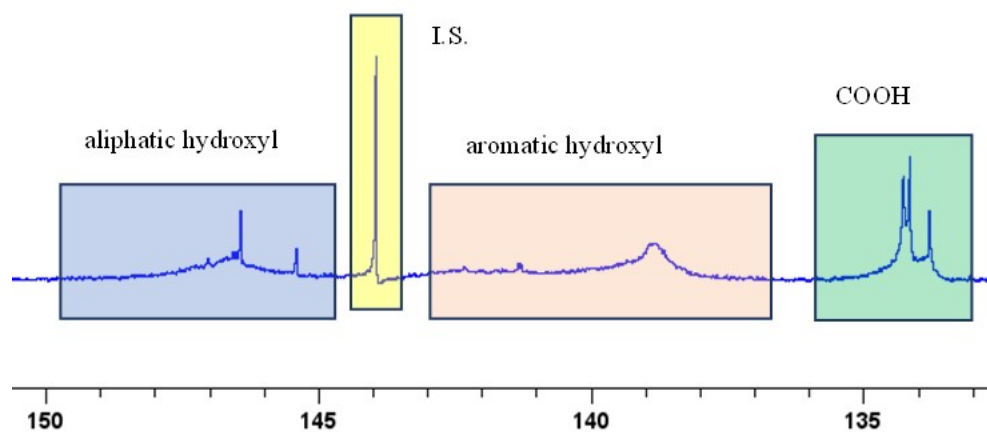


**Figure 4:** (a) H-NMR of lignin sample from DAC+MA and DAC+FA systems (b) Integration of DAC+MA system (c) Integration of DAC+FA system and (d) Different protons on allyl group. The allylation efficiency of both the solvent systems were compared by integrating the allyl proton in H-NMR.

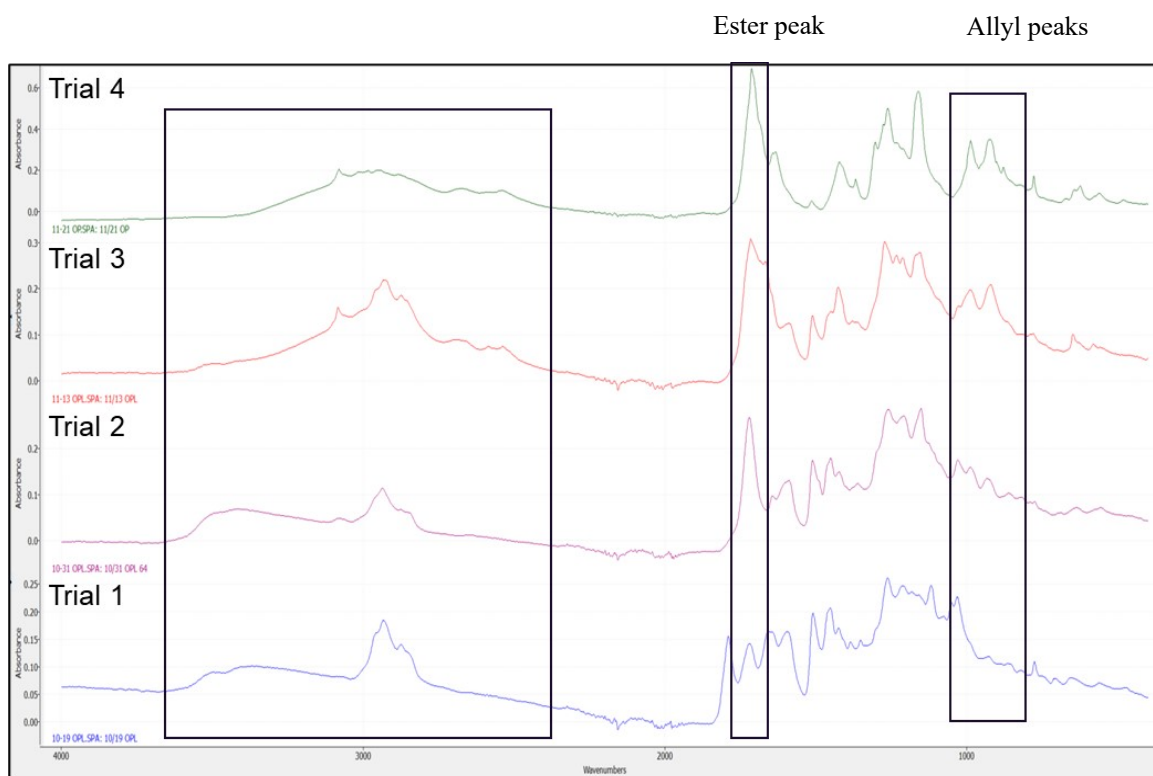
(a)



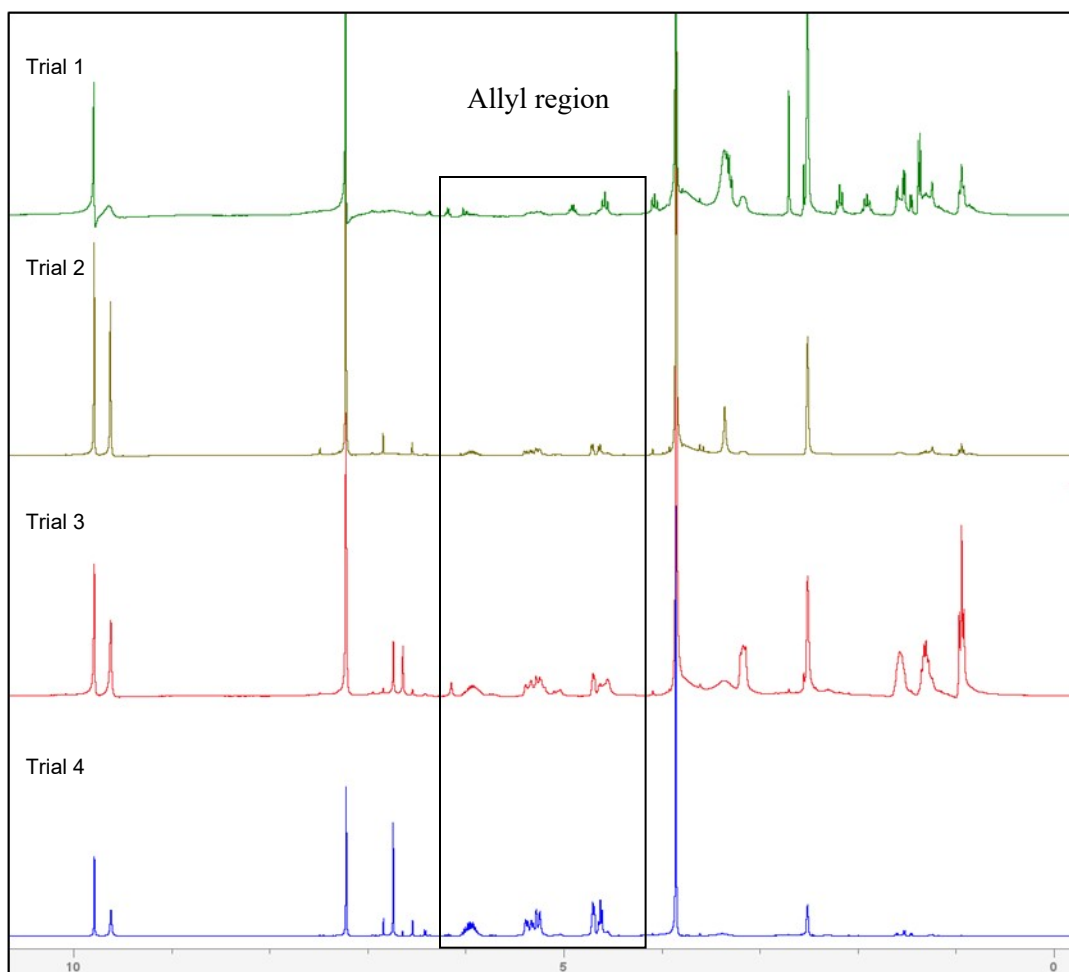
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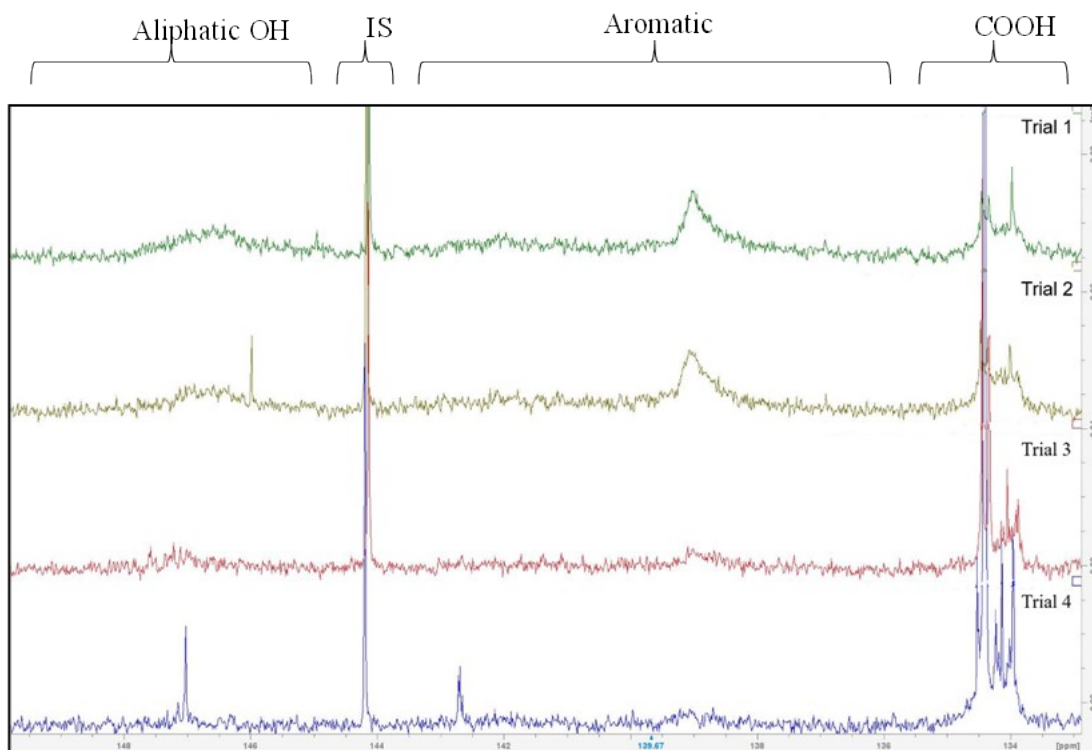
**Figure 5:** P-NMR of (a) DAC+FA system (b) DAC+MA system. Both the systems had similar aliphatic and aromatic hydroxyl groups with DAC+MA having higher amount of carboxylic acid groups due to a large peak in the region between 133-135 ppm.



**Figure 6:** FTIR spectra of samples from all four trials. FTIR revealed the presence of allyl peaks in the region between 900-1000 ppm. The peak intensity increases with increasing temperature from trial 1 to trial 4.



**Figure 7:** <sup>1</sup>H-NMR of lignin from various trials. Quantification of allyl peaks in the region 4-6 ppm was done using syringaldehyde as a standard whose peak appears at 9.8 ppm by integrating the area under the peaks.



**Figure 8:** P-NMR of lignin samples. Aliphatic hydroxyl group (145-150 ppm), aromatic hydroxyl group (137-143 ppm) and carboxylic acid groups (133-135 ppm) were quantified using cholesterol (144 ppm) as the standard in P-NMR.

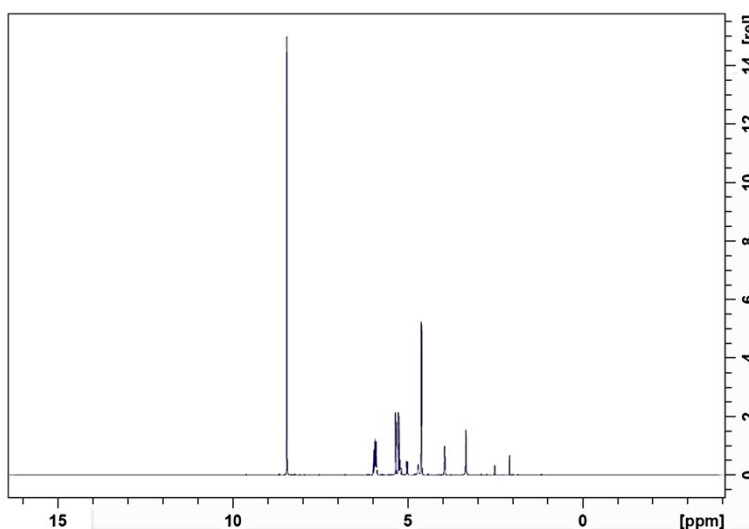


### Estimation of Purity of Recovered DAC from H-NMR using 1,4-Dinitrobenzene as Internal Standard:

To quantify the concentration of diallyl carbonate (DAC) in the recovered liquid, a quantitative  $^1\text{H}$  NMR analysis was conducted using 1,4-dinitrobenzene as an internal standard. A known amount of 1,4-dinitrobenzene (40 mg) was dissolved in 0.75 mL of d-DMSO, and a 50  $\mu\text{L}$  aliquot of the recovered DAC was taken for NMR analysis. The molar mass of 1,4-dinitrobenzene is 168.11 g/mol, corresponding to 0.000238 mol in the NMR tube. Each molecule of dinitrobenzene contributes four aromatic protons, giving a total of 0.000952 mmol of aromatic protons. In the spectrum, the aromatic region corresponding to these protons appeared at  $\sim 8.45$  ppm and was assigned an integral area of 1.00. The allylic protons (H<sub>b</sub>) of DAC, appearing between  $\delta = 5.8$ –6.3 ppm, exhibited an integral area of 0.60. Since the 1.00 integral represents 4 protons, the integral per proton is 0.25. This implies that the 0.60 integral corresponds to 2.4 protons. As each DAC molecule contributes 2 H<sub>b</sub> protons, the number of moles of DAC in the 50  $\mu\text{L}$  sample was calculated as below:

$$\begin{aligned}\text{Moles of DAC} &= \frac{2.4}{2} \times \text{moles of internal standard} \\ &= 1.2 \times 0.000238 \\ &= 0.0002856 \text{ moles.}\end{aligned}$$

Using the molecular weight of DAC (174.18 g/mol), the mass of DAC in the 50  $\mu\text{L}$  sample was determined to be  $0.0002856 \text{ mol} \times 174.18 \text{ g/mol} = 0.0497 \text{ g}$ . The mass of DAC in 6.8 ml of recovered DAC is 6.76g which is close to 100% purity since the density of DAC is 0.991g/ml at 25°C.



**Figure 9:** H-NMR of recovered DAC.

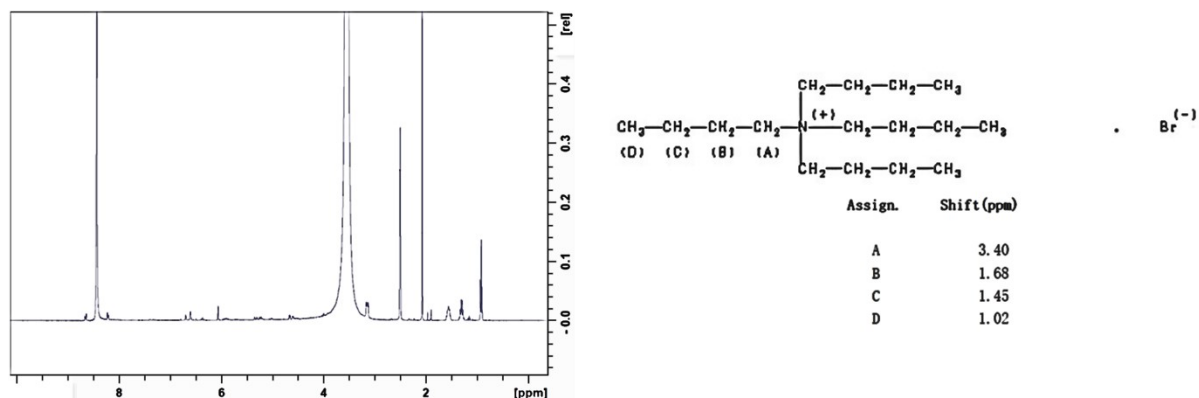
### Estimation of amounts of MA and TBAB in lignin filtrate from H-NMR using 1,4-Dinitrobenzene as Internal Standard:

To quantify the amount of TBAB in the lignin filtrate and to estimate the reusability of the solvent, a quantitative  $^1\text{H}$  NMR analysis was conducted using 1,4-dinitrobenzene as an internal standard. A known amount of 1,4-dinitrobenzene (39 mg) was dissolved in 0.75 mL of d-DMSO, and a 50  $\mu\text{L}$  aliquot of the recovered lignin filtrate was taken for NMR analysis. The molar mass of 1,4-dinitrobenzene is 168.11 g/mol, corresponding to 0.000232 mol in the NMR tube. Each molecule of dinitrobenzene contributes four aromatic protons, giving a total of 0.000928 mmol of aromatic protons. In the spectrum, the aromatic region corresponding to these protons appeared at  $\sim 8.45$  ppm and was assigned an integral area of 1.00. The terminal methyl protons (D) of TBAB, appearing at  $\delta = 1.02$  ppm, exhibited an integral area of 0.0457. Since the 1.00 integral represents 4 protons, the integral per proton is 0.25. This implies that the 0.0457 integral corresponds to 0.1828 protons. As each TBAB cation contributes 12 equivalent D protons, the number of moles of TBAB in the 50  $\mu\text{L}$  sample was calculated as below.

$$\begin{aligned} \text{Moles of TBAB in } 50 \mu\text{L aliquot} &= \frac{0.1828}{12} \times \text{moles of internal standard} \\ &= 0.0152 \times 0.000232 \\ &= 3.53 \times 10^{-6} \text{ moles.} \end{aligned}$$

Since 200 ml of lignin filtrate has been recovered, total amount of TBAB present is given below:

$$\begin{aligned} &= 3.53 \times 10^{-6} \times \frac{200}{0.05} \times \text{molecular weight of TBAB} \\ &= 3.53 \times 10^{-6} \times 4600 \times 322.368 \\ &= 4.5\text{g} \end{aligned}$$



**Figure 10:** H-NMR of TBAB in lignin filtrate.

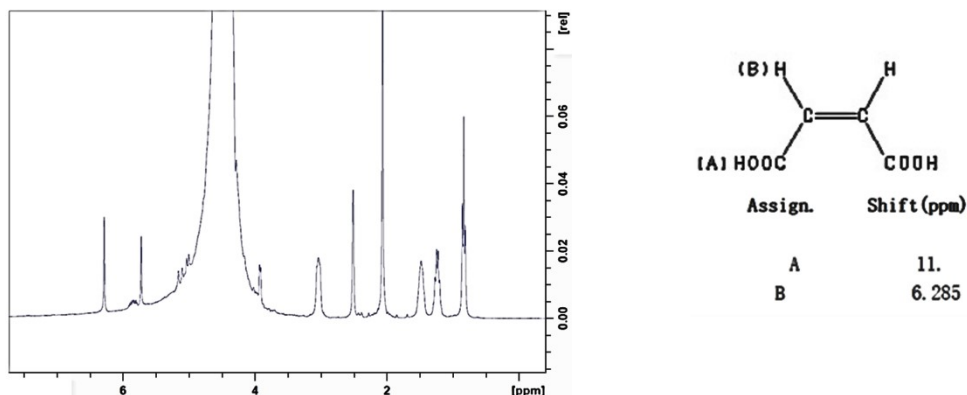
The amount of MA in 50  $\mu\text{L}$  aliquot was determined from weight of TBAB. From above calculations,  $3.53 \times 10^{-6}$  moles of TBAB is present in 50  $\mu\text{L}$  aliquot. In the spectrum, the region

corresponding to the terminal methyl protons (D) of TBAB, appearing at  $\delta = 1.02$  ppm, was assigned an integral area of 1.00. The vinylic protons (B) of MA, appearing at  $\delta = 6.29$  ppm, exhibited an integral area of 0.3372. Since the 1.00 integral represents 12 protons, the integral per proton is 0.0833. This implies that the 0.44 integral corresponds to 5.3 protons. As each MA molecule contributes two vinylic protons (B), the number of moles of MA in the 50  $\mu\text{L}$  sample was calculated as below.

$$\begin{aligned} \text{Moles of MA in } 50 \mu\text{L aliquot} &= \frac{5.3}{2} \times \text{moles of TBAB} \\ &= 2.65 \times 3.53 \times 10^{-6} \\ &= 9.4 \times 10^{-6} \text{ moles.} \end{aligned}$$

Since 200 ml of lignin filtrate has been recovered, total amount of MA present is given below:

$$\begin{aligned} &= 9.4 \times 10^{-6} \times \frac{200}{0.05} \times \text{molecular weight of MA} \\ &= 9.4 \times 10^{-6} \times 4600 \times 116.07 \\ &= 4.36\text{g} \end{aligned}$$



**Figure 11:** H-NMR of MA in lignin filtrate.

## E-factor calculation for different processes:

### 1. One-step extraction and functionalization of lignin directly from biomass

The input masses of different chemicals used in the one-step process are reported in table 1.

**Table 1:** Composition of different reactants used in the one-step process.

Inputs	Mass (g)
Pinewood sawdust	1
Diallyl carbonate	9.91
Maleic acid	5
TBAB	4.5
Total input mass	20.41

Recovered materials (approximate values):

Cellulose-rich residue – 0.51g

Acid insoluble lignin – 0.52g

Maleic acid – 4.36

TBAB – 4.5

DAC – 6.76

The output from the process includes 0.8 g of lignin as the primary product and 0.55 g of cellulose-rich residue as a co-product. A significant portion of the reagents has been recovered, including 90% of TBAB (4.05 g) and maleic acid (4.5 g), along with 60% of diallyl carbonate (6.0 g).

$$\text{Total Waste Mass} = \text{Total Input} - (\text{Recovered Materials} + \text{Product})$$

$$= 20.41 - (0.51 + 0.52 + 4.36 + 4.5 + 6.76)$$

$$= 3.76 \text{ g}$$

$$E = \frac{\text{Total waste mass}}{\text{Desired product mass(lignin)}}$$

$$= \frac{3.76}{0.52}$$

$$= 7.23$$

### 2. A Comparative Study of Lignin Recovery Conditions Using GVL-Organosolv and Lignin Characterization

Based on Tanis et al., 2025, to assess the efficiency of lignocellulosic fractionation under 80%  $\gamma$ -valerolactone (GVL) conditions, 1 g of dry Norway spruce was treated with a 10 mL solvent system (8.8 g GVL and 2.0 g DI water) at 140 °C in the presence of sulfuric acid (0.002 g, 0.01 M in the aqueous phase). Based on compositional analysis, the spruce contained 40.8% glucan (cellulose), 19.9% total hemicellulose, and 31.3% total lignin. Under these reaction conditions, which correspond to a delignification efficiency of 67% and a lignin recovery of 50%, approximately 0.210 g of lignin was solubilized, of which 0.157 g was recovered as precipitated lignin upon dilution with 100 mL of water. Simultaneously, 70% of the hemicellulose (0.139 g) was recovered as soluble sugars and oligosaccharides in the organosolv liquor. The cellulose-rich pulp retained about 95% of the original glucan content (0.388 g), along with 0.060 g of hemicellulose and 0.103 g of residual lignin, amounting to a total solid mass of approximately 0.551 g.<sup>47</sup> Although this paper doesn't explicitly mention on GVL recovery, based on Shuai et al. (2016), over 99.5% of  $\gamma$ -valerolactone (GVL) could be efficiently recovered from pretreated slurries using liquid CO<sub>2</sub> extraction, while removing less than 1% of solubilized sugars.<sup>46</sup>

**Table 2:** Composition of different reactants used in the GVL-Organosolv process.

Inputs	Mass (g)
Norway spruce chips	1
GVL	8.8
Sulfuric acid	0.002
Total input mass	9.802

Recovered materials (approximate values):

Cellulose-rich residue – 0.5g

Acid insoluble lignin – 0.16g

Hemicellulose – 0.14g

GVL recovered – 8.7g

Total Waste Mass = Total Input – (Recovered Materials)

$$= 9.802 - (0.5+0.16+0.14+8.7)$$

$$= 0.302\text{g}$$

$$E = \frac{\text{Total waste mass}}{\text{Desired product mass(lignin)}}$$

$$= \frac{0.302}{0.16}$$

$$= \mathbf{1.89}$$

### 3. Poplar lignin structural changes during extraction in $\gamma$ -valerolactone (GVL)

For the two-step GVL-assisted hydrolysis of 1 g of hybrid poplar line NM6 (*Populus nigra* × *Populus maximowiczii*), the input chemicals include 8.11 g of  $\gamma$ -valerolactone (GVL), 0.90 g of deionized water, and 0.075 g of sulfuric acid (85 mM), maintaining a 10 wt.% solids loading in a 9:1 GVL:H<sub>2</sub>O solvent system, as described by Cheng et al. (2022) in their study of tunable organosolv lignin extraction using GVL .<sup>48</sup> An additional 3.00 g of pure GVL was used to rinse residual GVL-soluble lignin from the cellulose-rich pulp. Based on Zamora et.al, the NM6 poplar contains approximately 39 wt.% cellulose, 21 wt.% hemicellulose, and 27 wt.% lignin.<sup>49</sup> From this, the recovered product masses were calculated as follows: 0.153 g of precipitated lignin (56.5% of initial lignin), 0.351 g of cellulose retained in the solid residue (assuming 90% of initial cellulose), and 0.105 g of hemicellulosic sugars released into the organosolv liquor (assuming 50% solubilization). Assuming the total cellulose-rich pulp to weigh approximately 0.573 g, composing of residual lignin, hemicellulose, and glucan.

**Table 3:** Composition of different reactants used in the GVL extraction process of poplar wood.

Inputs	Mass (g)
NM6	1
GVL	11.11
Sulfuric acid	0.075
Total input mass	12.185

Recovered materials (approximate values):

Cellulose-rich residue – 0.57g

GVL-soluble lignin – 0.15g

Hemicellulose – 0.105g

GVL recovered – 11g (assuming 99.5% recovery based on Shuai et al. (2016))

Total Waste Mass = Total Input – (Recovered Materials)

$$= 12.185 - (0.57+0.15+0.105+11)$$

$$= 0.307\text{g}$$

$$E = \frac{\text{Total waste mass}}{\text{Desired product mass(lignin)}}$$

$$= \frac{0.36}{0.15}$$

$$= 2.4$$

#### 4. Fractionation of lignocellulosic biomass to produce uncondensed aldehyde-stabilized lignin

Formaldehyde-assisted biomass fractionation of birch wood yields three major product streams: cellulose-rich solids, formaldehyde-stabilized lignin, and hemicellulose-derived diformylxylose. In this process, 1 g of dried biomass is treated with 1.16 mL of 37% formaldehyde, 2.1 mL of 1,4-dioxane, and 0.47 mL of 37% hydrochloric acid to extract lignin and stabilize reactive intermediates. The cellulose-rich residue accounts for approximately 43% of the initial biomass (0.430 g), while the isolated stabilized lignin represents 24% (0.240 g), and the diformylxylose fraction derived from hemicellulose accounts for 13.2% (0.132 g). This method enables selective fractionation while preserving lignin structure for downstream valorization.<sup>50</sup>

**Table 4:** Composition of different reactants used in the aldehyde-stabilized lignin extraction process.

Inputs	Mass (g)
Birchwood	1
Formaldehyde	0.465
Hydrochloric acid	0.207
1,4-Dioxane	10.31
Methanol	3.484
Sodium bicarbonate	0.75
Total input mass	16.22

Recovered materials (approximate values):

Cellulose-rich residue – 0.48g

Aldehyde-stabilized lignin – 0.27g

Hemicellulose – 0.20g

Total Waste Mass = Total Input – (Recovered Materials)

$$= 16.22 - (0.48 + 0.27 + 0.2)$$

$$= 15.27\text{g}$$

$$E = \frac{\text{Total waste mass}}{\text{Desired product mass(lignin)}}$$

$$= \frac{15.27}{0.27}$$

$$= 56.6$$

## 5. Simultaneous extraction and controlled chemical functionalization of hardwood lignin for improved phenolation

In this aldehyde-assisted fractionation process applied to 1 g of birchwood, terephthalic aldehyde (TALD) was used at a loading of 12.6 mmol/g, corresponding to 1.89 g of TALD. The reaction medium comprised 5 mL of 1,4-dioxane for solubilizing the biomass and aldehyde, and 0.16 mL

of 37% hydrochloric acid was added as the acid catalyst. Following the reaction, 0.23 g of sodium bicarbonate was introduced to neutralize the acidic mixture. During the post-reaction workup, an additional 4 mL of dioxane was used for washing the solid residue, 3 mL of dioxane was employed to redissolve the filtrate, and 80 mL of diethyl ether was used to precipitate the lignin. A further ~40 mL of diethyl ether was used for Soxhlet extraction to purify the lignin fraction. The recovered materials from this process included approximately 0.53 g of cellulose-rich solid, 0.21 g of aldehyde-stabilized lignin, and around 0.02 g of hemicellulose-derived products such as furfural, HMF, and TALDX.<sup>24,51</sup>

**Table 5:** Composition of different reactants used in the simultaneous extraction and functionalization process using TALD.

Inputs	Mass (g)
Birchwood	1
Terephthalic aldehyde	1.89
Hydrochloric acid	0.207
1,4-Dioxane	12.36
Sodium bicarbonate	0.23
Diethyl ether	57
Total input mass	72.7

Recovered materials (approximate values):

Cellulose-rich residue – 0.53g

Aldehyde-stabilized lignin – 0.21g

Hemicellulose (furfural, HMF, TALDX) – 0.02g

Total Waste Mass = Total Input – (Recovered Materials)

$$= 72.7 - (0.53 + 0.21 + 0.02)$$

$$= 71.94\text{g}$$

$$E = \frac{\text{Total waste mass}}{\text{Desired product mass(lignin)}}$$

$$= \frac{71.94}{0.21}$$

$$= 342.57$$

## 6. Deep Eutectic solvents

The E-factor for the deep eutectic solvent (DES) process of extracting lignin, based on Yujin et al., was calculated to evaluate its sustainability.<sup>52</sup>



**Table 6:** Composition of different reactants used in the process based on Yujin et.al.

Inputs	Mass (g)
Pinewood	1
Choline Chloride	5
Lactic Acid	3.3
Formic acid	1.7
Ethanol	18
Total Input Mass	29

The final products include 0.27g of lignin and 0.07g of glucan based on the yield values of lignin and glucan which were around 72% and 18% approximately based on the paper.<sup>52</sup> Based on paper, DES is recovered and based on the assumption that 80% ethanol is recovered, the total waste mass is calculated (the paper doesn't discuss about the recovery of ethanol that is added post DES treatment to reduce viscosity). The total product mass, focusing on lignin, is 0.27g. The original composition of pinewood powder (*Pinus rigida*) was determined based on Kwon et.al.<sup>96</sup>

Recovered materials (approximate values):

Cellulose-rich residue – 0.5g

Lignin – 0.27g

Hemicellulose– 0.14g

Ethanol (assuming 80% recovery)– 14.4g

DES (complete recovery/) – 10g

$$\text{Total waste mass} = \text{Total input mass} - \text{Total recovered mass} - \text{Total product mass}$$

$$= 29 - (0.5 + 0.27 + 0.14 + 14.4 + 10)$$

$$= 3.69\text{g}$$

$$\begin{aligned} E &= \frac{\text{Total waste mass}}{\text{Desired product mass(lignin)}} \\ &= \frac{3.69}{0.27} \\ &= 13.7 \end{aligned}$$

## Hazard score and GHS weight calculations for different processes

### 1. One-step process for extraction and functionalization

**Table 7:** Different chemicals and their hazard scores.

Chemical	Hazard Classification	Hazard Type	Category	Hazard Score	Total Hazard Score
Maleic acid	Health	Skin sensitizer	1	5	21
		Eye damage	1	5	
		Skin corrosion	1b	4	
		Acute oral toxicity	4	2	
		Acute dermal toxicity	4	2	
		Specific organ toxicity	3	3	
		None	—	1	
Diallyl carbonate	Physical Environmental	Aquatic toxicity	3	3	13
		Skin irritation	2	5	
		Eye irritation	2a	5	
		Specific organ toxicity	3	3	
		Flammable	3	3	
		None	—	1	
		None	—	1	
TBAB	Health	Skin irritation	2	5	14
		Eye irritation	2b	4	
		Acute oral toxicity	4	2	
		Reproductive toxicity	2	3	
		None	—	1	
		Aquatic toxicity	3	3	
		Aquatic toxicity	3	3	

**Table 8:** Total hazard scores in health, physical and environmental categories.

Chemical	E-Score (Human Health Hazard)	Z-Score (Physical Hazard)	B-Score (Aquatic toxicity)
Maleic acid	21	1	3
Diallyl carbonate	13	3	1
TBAB	14	1	3

## 2. A Comparative Study of Lignin Recovery Conditions Using GVL-Organosolv and Lignin Characterization

**Table 9:** Different chemicals and their hazard scores.

Chemical	Hazard Classification	Hazard Type	Category	Hazard Score	Total Hazard Score
$\gamma$ -Valerolactone (GVL)	Health	Skin irritation	2	5	10
		Eye irritation	2a	5	
	Physical	None	—	1	1
	Environmental	Aquatic toxicity	—	1	1
Sulfuric acid	Health	Skin corrosion	1a	5	13
		Eye damage	1	5	
		Specific organ toxicity	3	3	
	Physical	Corrosive to metals	1	5	5
	Environmental	Aquatic toxicity	3	3	3

**Table 10:** Total hazard scores in health, physical and environmental categories.

Chemical	E-Score (Human Health Hazard)	Z-Score (Physical Hazard)	B-Score (Aquatic toxicity)
$\gamma$ -Valerolactone (GVL)	10	1	1
Sulfuric acid	13	5	3

### 3. Poplar lignin structural changes during extraction in $\gamma$ -valerolactone (GVL)

**Table 11:** Different chemicals and their hazard scores.

Chemical	Hazard Classification	Hazard Type	Category	Hazard Score	Total Hazard Score
$\gamma$ -Valerolactone (GVL)	Health	Skin irritation	2	5	10
		Eye irritation	2a	5	
	Physical Environmental	None	—	1	1
		Aquatic toxicity	—	1	1
Sulfuric acid	Health	Skin corrosion	1a	5	13
		Eye damage	1	5	
		Specific organ toxicity	3	3	
	Physical	Corrosive to metals	1	5	5
	Environmental	Aquatic toxicity	3	3	3

**Table 12:** Total hazard scores in health, physical and environmental categories.

Chemical	E-Score (Human Health Hazard)	Z-Score (Physical Hazard)	B-Score (Aquatic toxicity)
$\gamma$ -Valerolactone (GVL)	10	1	1
Sulfuric acid	13	5	3

#### 4. Fractionation of lignocellulosic biomass to produce uncondensed aldehyde-stabilized lignin

**Table 13:** Different chemicals and their hazard scores.

Chemical	Hazard Classification	Hazard Type	Category	Hazard Score	Total Hazard Score
Methanol	Health	Specific organ toxicity	1	5	14
		Acute oral toxicity	3	3	
		Acute dermal toxicity	3	3	
		Acute inhalation toxicity	3	3	
		Flammable liquid	2	4	
Formaldehyde	Health	None	1	1	36
		Acute oral toxicity	3	3	
		Acute inhalation toxicity	3	3	
		Acute dermal toxicity	3	3	
		Skin corrosion	1b	4	
		Eye damage	1	5	
		Skin sensitization	1	5	
		Germ cell mutagenicity	2	3	
		Carcinogenicity	1a	5	
		Specific organ toxicity	1	5	
		Flammable	3	3	
	Physical				3

	Environmental	liquid Aquatic toxicity	3	3	3
Hydrochloric acid	Health	Skin corrosion	1b	4	12
		Eye damage	1	5	
		Specific target organ toxicity	3	3	
	Physical	Corrosive to metals	1	5	5
	Environmental	Aquatic toxicity	3	3	3
1,4 - Dioxane	Health	Eye damage	2a	5	12
		Specific target organ toxicity	3	3	
		Carcinogenicity	1b	4	
	Physical	Flammable	2	4	4
	Environmental	liquid Aquatic toxicity	4	2	2
Sodium bicarbonate	Health	Skin irritation	3	4	9
		Eye irritation	2b	4	
		Acute oral toxicity	5	1	
	Physical	None	—	—	—
	Environmental	Aquatic toxicity	—	1	1

**Table 14:** Total hazard scores in health, physical and environmental categories.

Chemical	E-Score (Human Health Hazard)	Z-Score (Physical Hazard)	B-Score (Aquatic toxicity)
Formaldehyde	36	3	3
Hydrochloric acid	12	5	3
Methanol	14	4	1
1,4 - Dioxane	12	4	2
Sodium bicarbonate	9	—	1

## 5. Simultaneous extraction and controlled chemical functionalization of hardwood lignin for improved phenolation

**Table 15:** Different chemicals and their hazard scores.

Chemical	Hazard	Hazard Type	Category	Hazard	Total
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	Classification				Score	Hazard Score
Diethyl ether	Health	Acute oral toxicity	4	2	5	
		Specific target organ toxicity	3	3		
		Flammable liquid	1	5	5	
	Environmental	Aquatic toxicity	4	2	2	
Terephthalic aldehyde	Health	Eye irritation	2a	5	8	
		Specific target organ toxicity	3	3		
		None				
	Physical					
	Environmental	Aquatic toxicity	2	4	4	
Hydrochloric acid	Health	Skin corrosion	1b	4	12	
		Eye damage	1	5		
		Specific target organ toxicity	3	3		
	Physical	Corrosive to metals	1	5	5	
	Environmental	Aquatic toxicity	3	3	3	
1,4 - Dioxane	Health	Eye damage	2a	5	12	
		Specific target organ toxicity	3	3		
		Carcinogenicity	1b	4		
	Physical	Flammable liquid	2	4	4	
	Environmental	Aquatic toxicity	4	2	2	
Sodium bicarbonate	Health	Skin irritation	3	4	9	
		Eye irritation	2b	4		
		Acute oral toxicity	5	1		
	Physical	None				
	Environmental	Aquatic toxicity	1	1	1	

**Table 16:** Total hazard scores in health, physical and environmental categories.

Chemical	E-Score (Human Health Hazard)	Z-Score (Physical Hazard)	B-Score (Aquatic toxicity)
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Diethyl ether	5	5	2
Terephthalic aldehyde	8	—	4
Hydrochloric acid	12	5	3
1,4 - Dioxane	12	4	2
Sodium bicarbonate	9	—	1

## 6. Deep Eutectic solvents

**Table 17:** Different chemicals and their hazard scores.

Chemical	Hazard Classification	Hazard Type	Category	Hazard Score	Total Hazard Score
Choline chloride	Health	Skin irritation	2	5	14
		Eye irritation	2a	5	
		Specific organ toxicity	3	3	
		Acute oral toxicity	5	1	
	Physical	None	—	1	1
Lactic acid	Environmental	Aquatic toxicity	—	1	1
		Skin corrosion	1c	3	8
	Health	Eye damage	1	5	
		None	—	1	1
		Aquatic toxicity	—	1	1
Formic acid	Health	Skin corrosion	1a	5	15
		Eye damage	1	5	
		Acute inhalation toxicity	3	3	
		Acute oral toxicity	4	2	
	Physical	Flammable liquid	3	3	3
	Environmental	Aquatic toxicity	3	3	3
		Eye irritation	2a	5	5
Ethanol	Health	Flammable liquid	2	4	4
	Physical	Aquatic toxicity	—	1	1
		Acute oral toxicity	4	2	2



**Table 18:** Total hazard scores in health, physical and environmental categories.

Chemical	E-Score (Human Health Hazard)	Z-Score (Physical Hazard)	B-Score (Aquatic toxicity)
Choline chloride	14	1	1
Lactic acid	8	1	1
Formic acid	15	3	3
Ethanol	5	4	1