Supplementary Information

A predictive toolset for the identification of effective lignocellulosic pretreatment solvents: A case study of solvents tailored for lignin extraction

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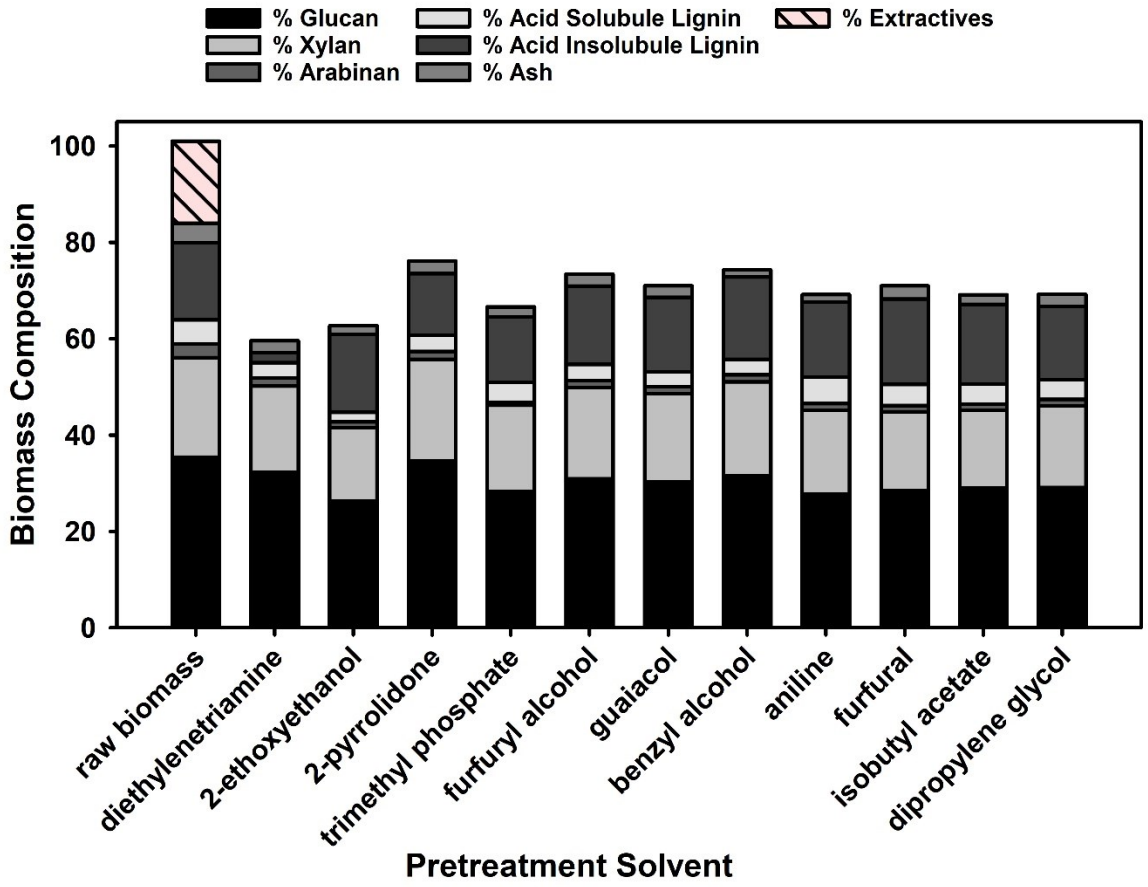


Fig. S1 Biomass yield and composition after pretreatment of sorghum with the organic solvents. The composition of the untreated "raw biomass" is also displayed.

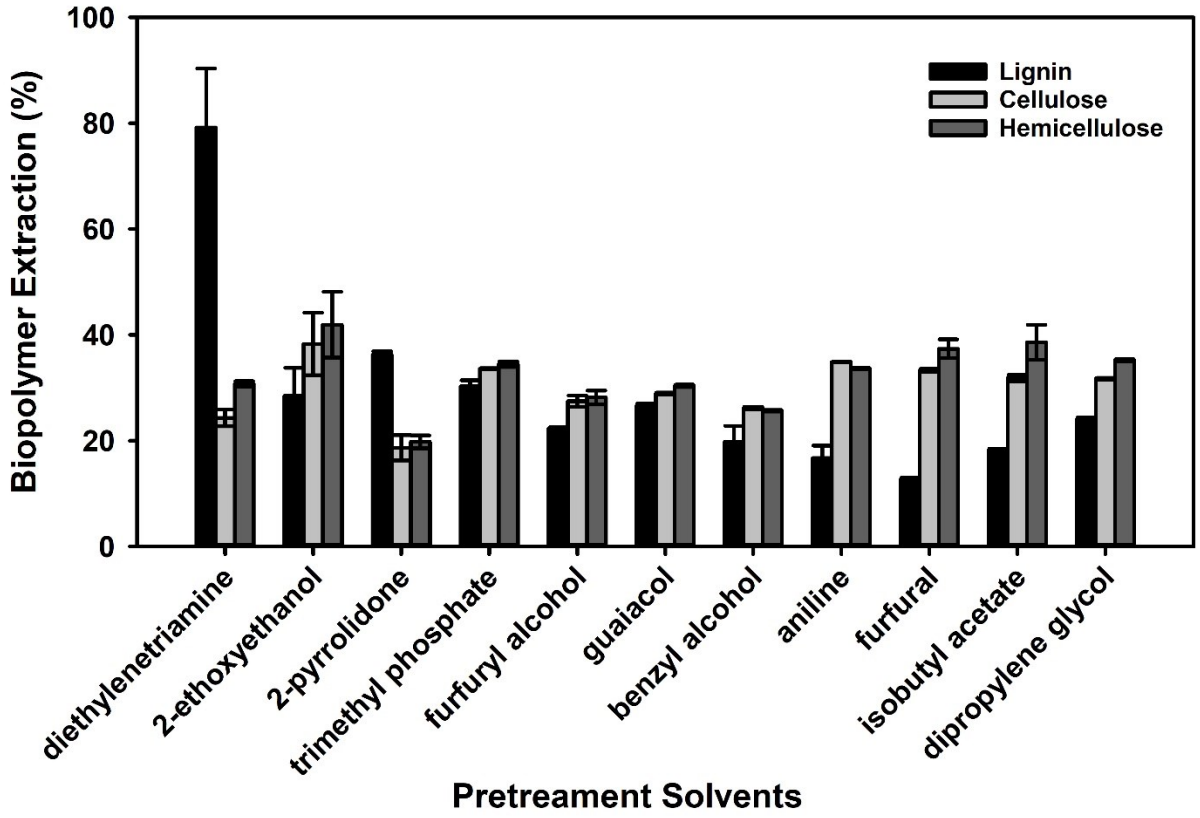
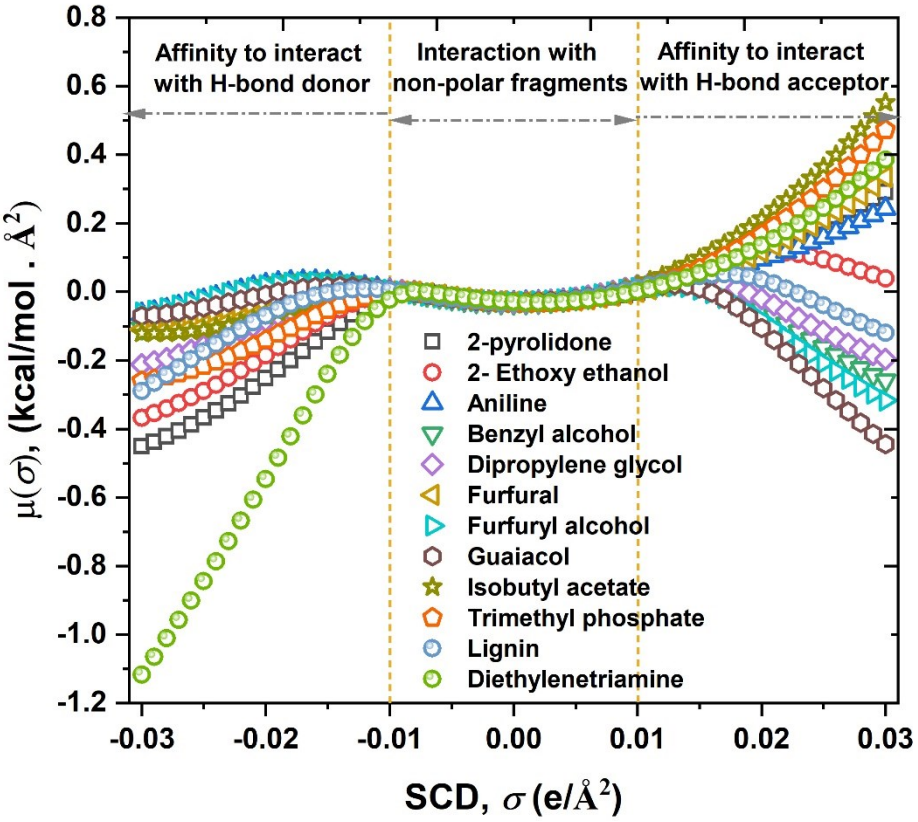
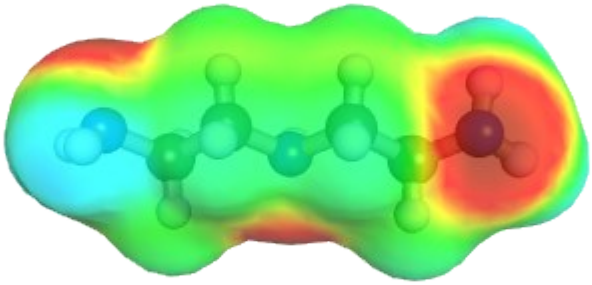


Fig. S2 Amount of each biopolymer (lignin, cellulose, and hemicellulose) that was removed during pretreatment and solvent recovery.



(a)



(b)

Fig. S3 (a) Sigma potentials of lignin and molecular solvents predicted by COSMO-RS. (b) COSMO cavity (surface polarity) diagram of diethylenetriamine (here the extent of screening charge varies from -0.03 e.Å^{-2} (red) to +0.03 e.Å^{-2} (blue)). The intermediate (non-polar) region is represented by green and yellow colors.

Table S1: Predicted excess enthalpy, activity coefficient, and viscosity of amines for cellulose by COSMO-RS

Solvent	H^E (kcal/mol)	ln(Υ)	Viscosity, cP
1,3-diaminopropane	-1.57	-5.01	0.63
1,4-diaminobutane (Putrescine)	-1.55	-4.79	0.76
1,5-diaminopentane (Cadaverine)	-1.56	-4.63	0.89
1,2-diaminopropane	-1.48	-4.58	0.57
Spermine	-1.57	-4.64	6.82
Spermidine	-1.55	-4.60	2.26
2,2-dimethyl-1,3-propanediamine	-0.88	-2.13	0.50
Ethylenediamine	-1.46	-4.84	0.54
Diethylenetriamine	-1.42	-4.50	1.42
Pentylamine	0.07	-0.04	0.65
Aniline	-1.43	-3.04	0.37
2-ethoxy Ethanol	-0.07	-0.32	1.47
2-pyrolidone	-0.54	-2.25	0.78
Trimethyl phosphate	-0.29	-0.92	0.63
Furfuryl alcohol	0.01	-0.12	1.51
Guaiacol	0.01	-0.08	3.77
Benzyl alcohol	0.03	0.01	1.60
Furfural	0.01	-0.21	0.64
Isobutyl acetate	-0.11	-0.05	0.36
Dipropylene glycol	0.00	-0.06	8.27

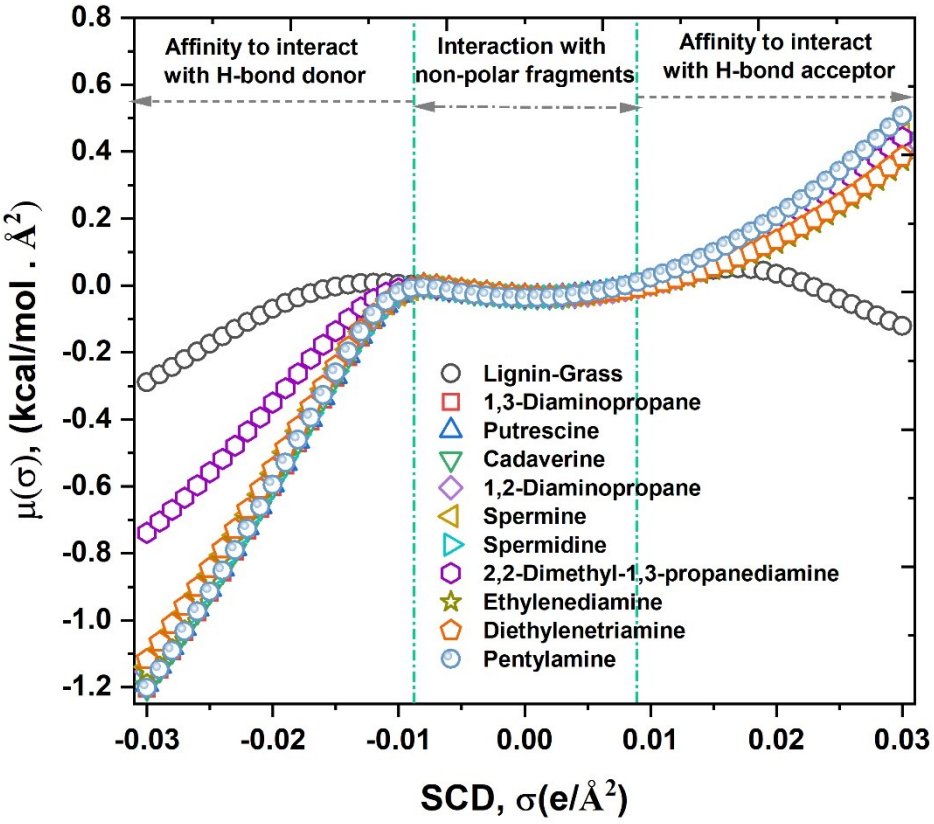


Fig. S4 COSMO-RS-based predicted sigma potentials of lignin and amines.

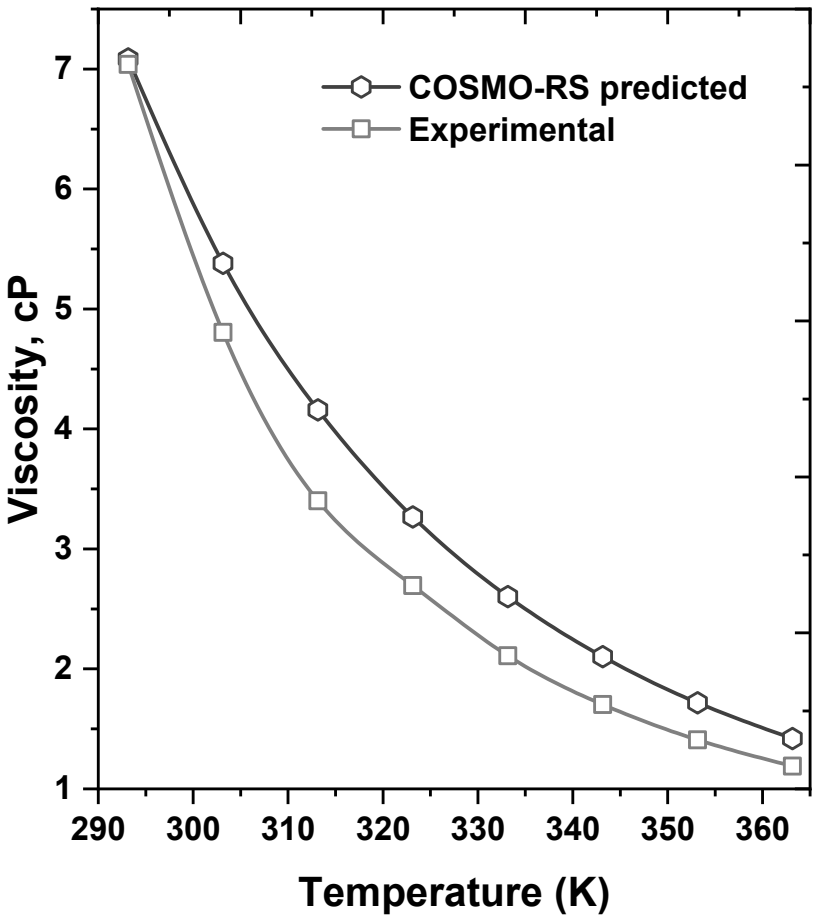


Fig. S5 Experimental and COSMO-RS predicted viscosities of diethylenetriamine at different temperatures.

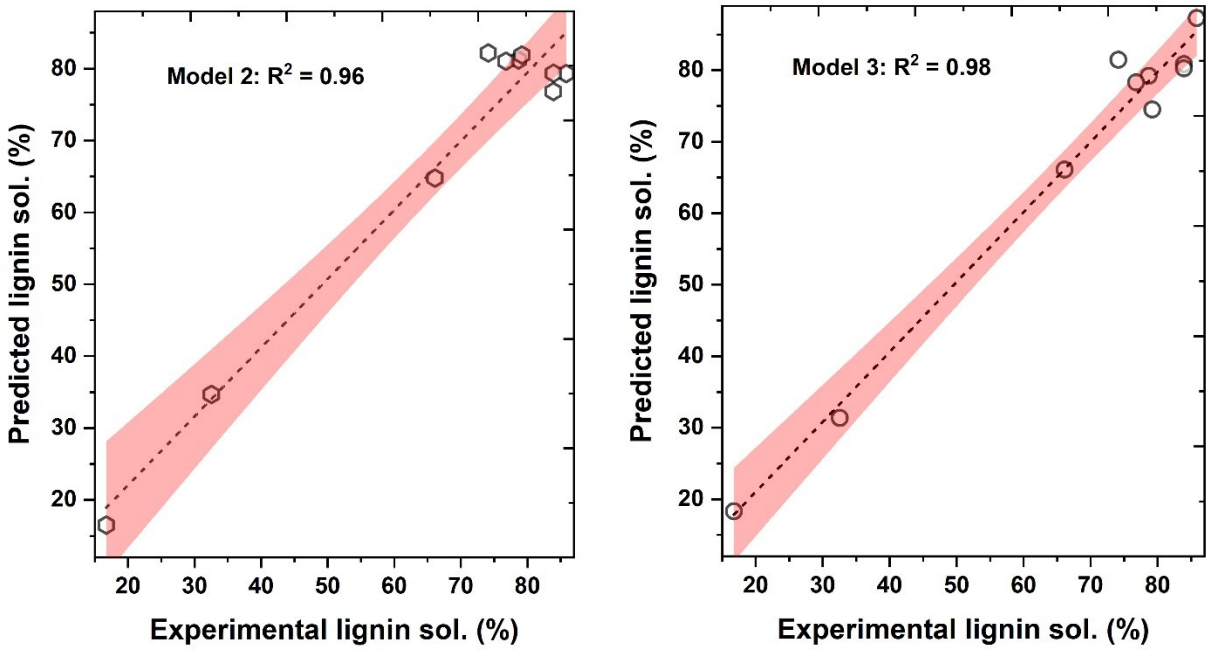


Fig. S6 Experimental and COSMO-RS-based developed models 2 & 3 predicted lignin solubility for amines with 95% confidence error band.

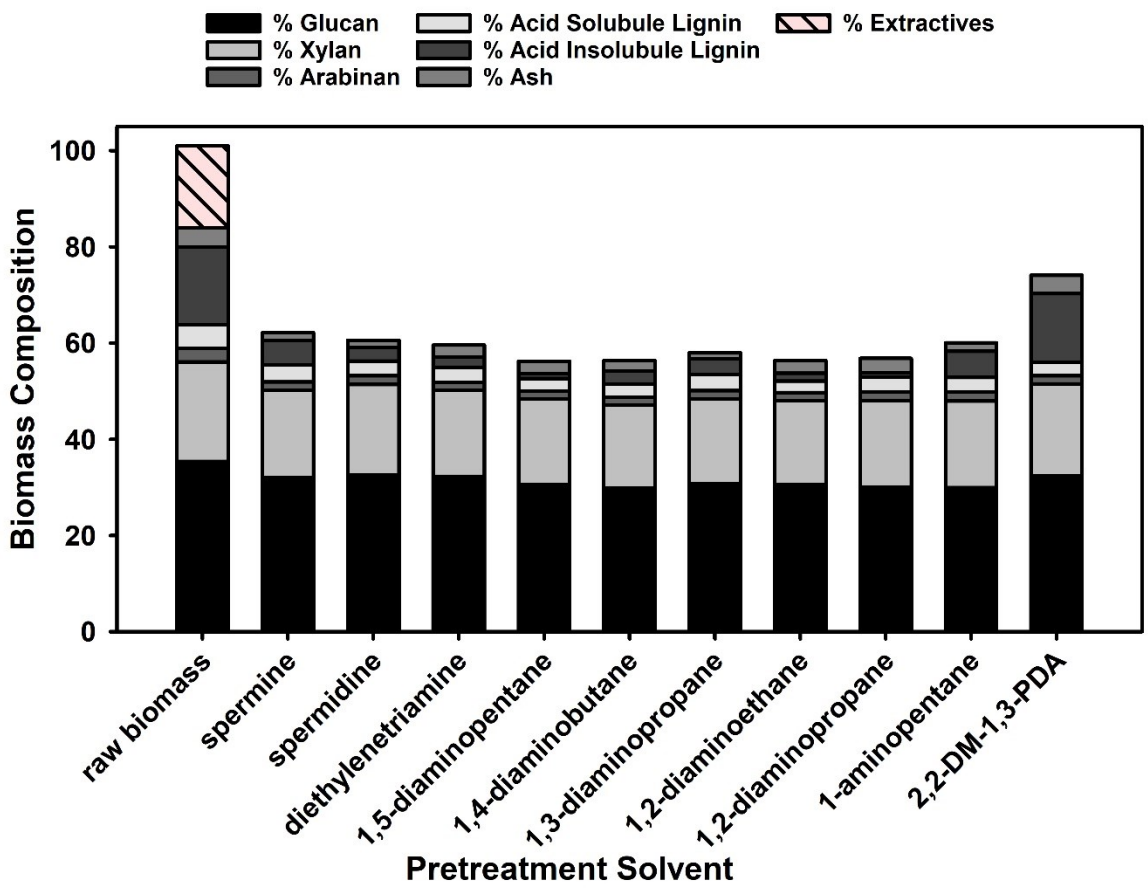


Fig. S7 Biomass yield and composition after pretreatment of sorghum with the amies. The composition of the untreated "raw biomass" is also displayed.

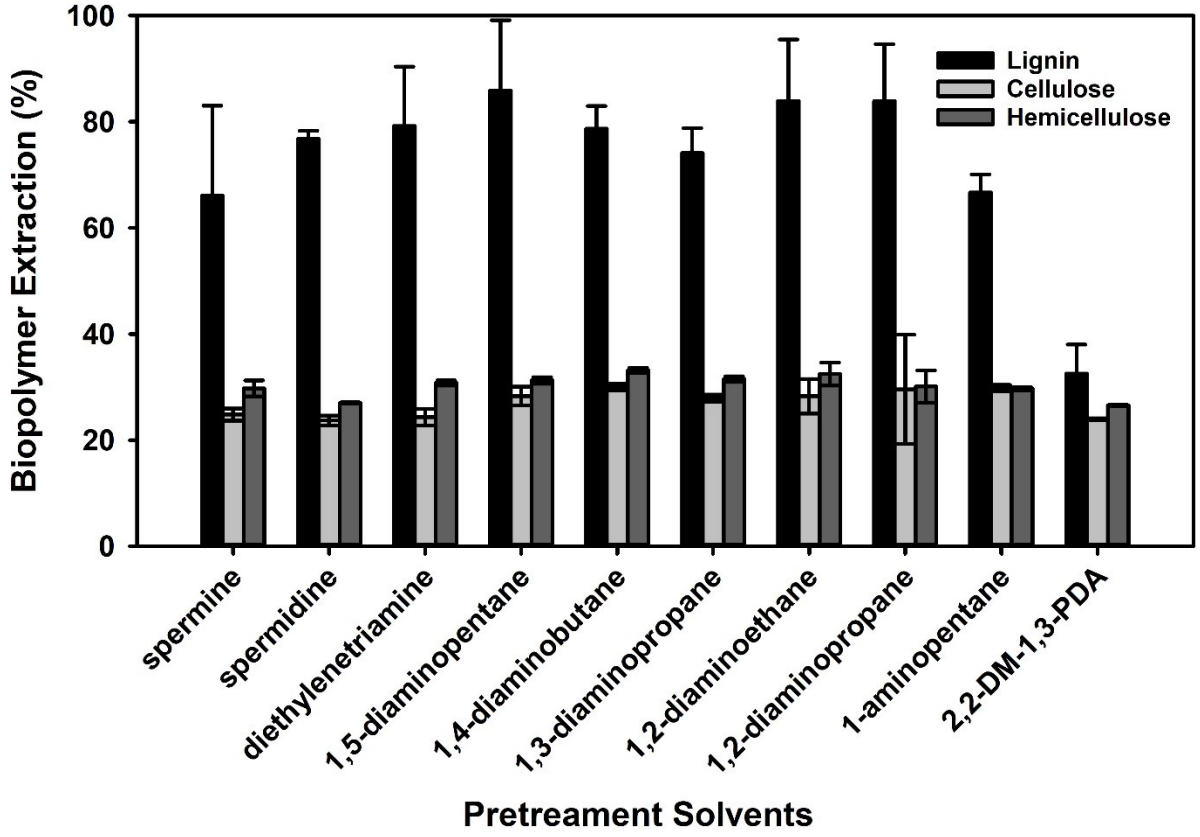


Fig. S8 Amount of each biopolymer (lignin, cellulose, and hemicellulose) that was removed during pretreatment and solvent recovery.

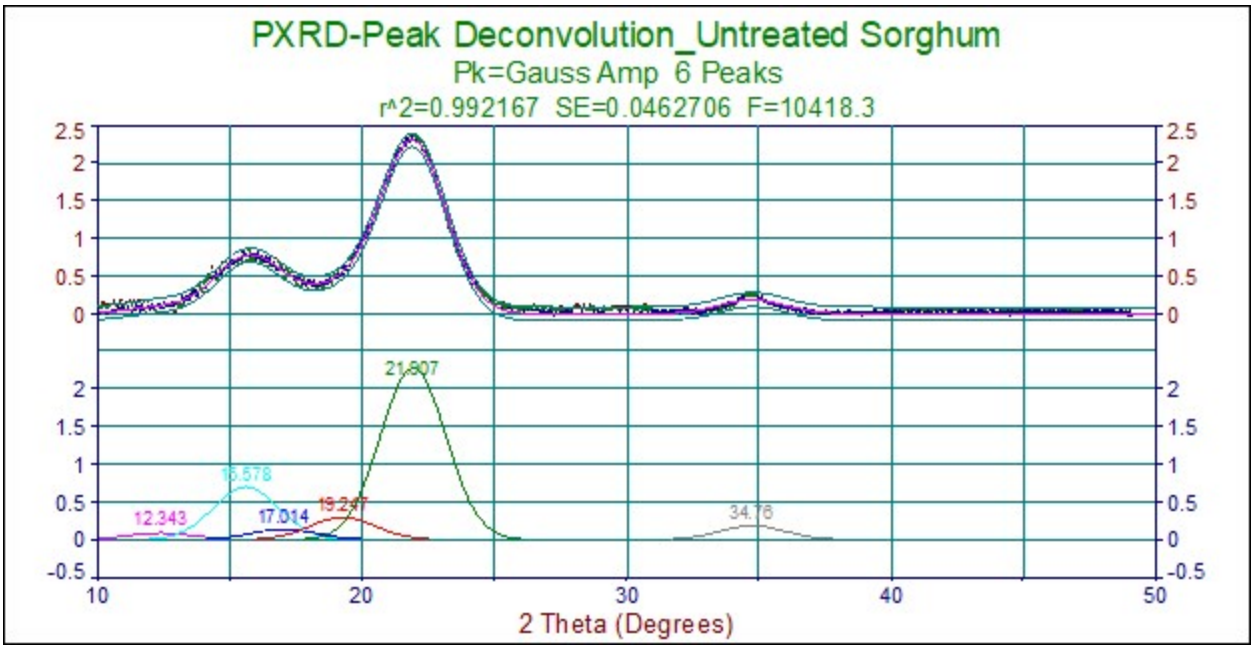


Fig. S9 X-ray diffraction profiles for untreated sorghum along with results from peak deconvolution.

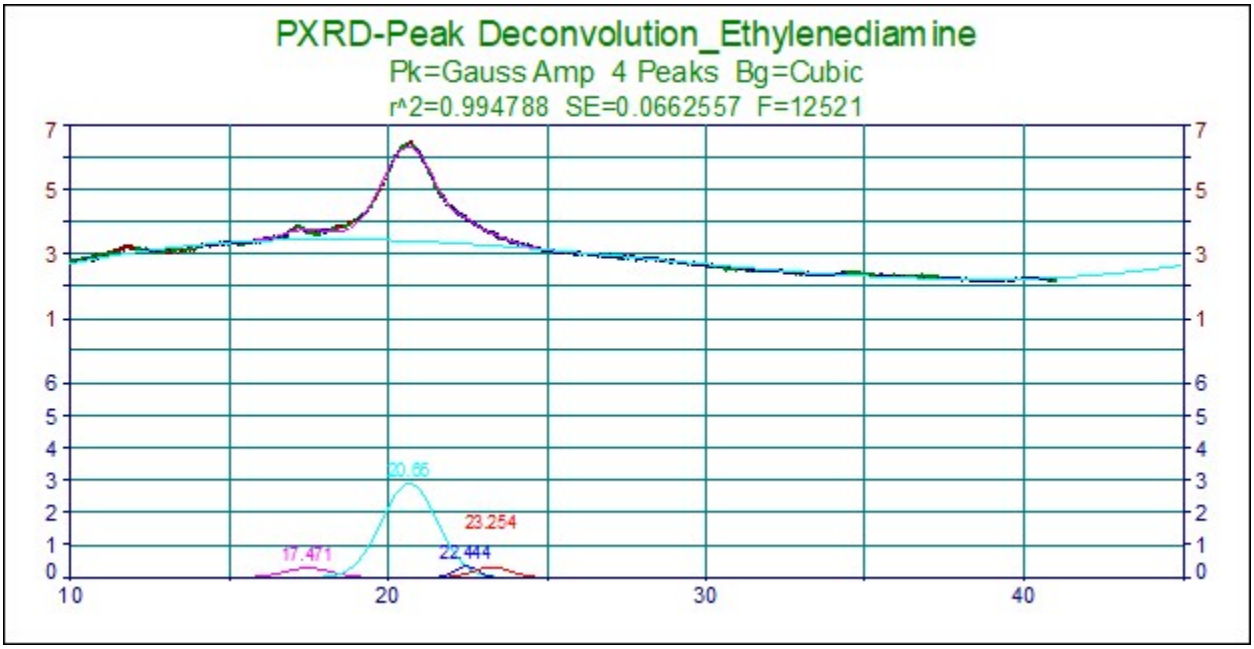


Fig. S10 X-ray diffraction profiles for ethylenediamine-treated sorghum along with results from peak deconvolution.

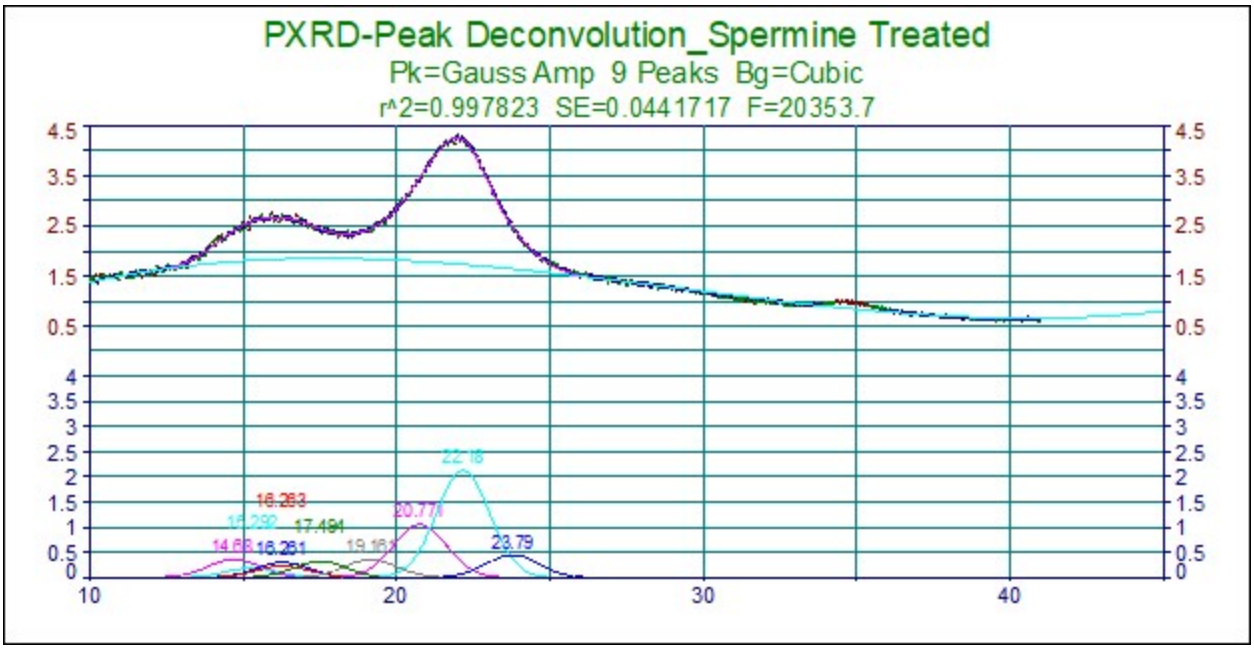
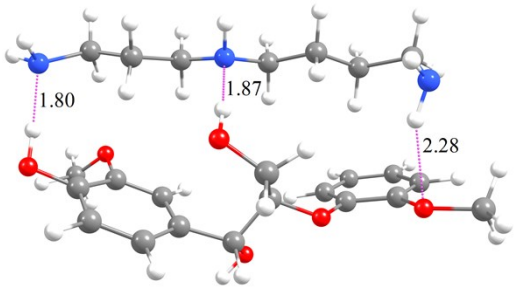


Fig. S11 X-ray diffraction profiles for spermine-treated sorghum along with results from peak deconvolution.



(a) Lignin-spermidine-1
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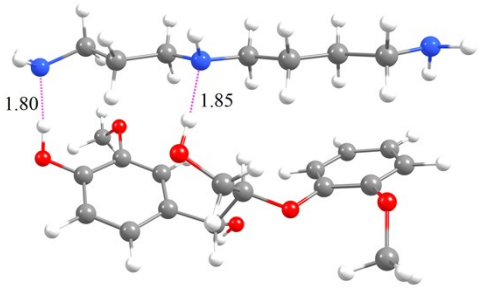

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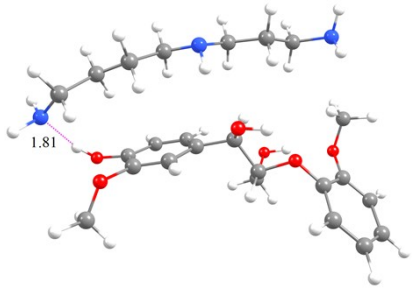

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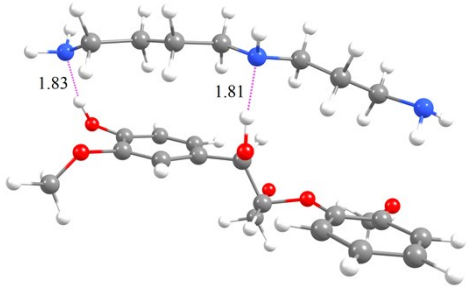

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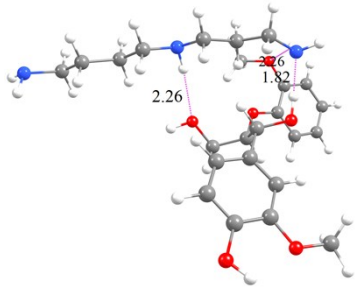

(e) Lignin-spermidine-5
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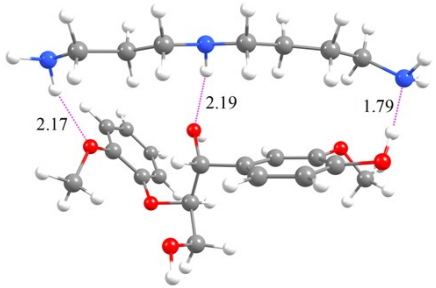

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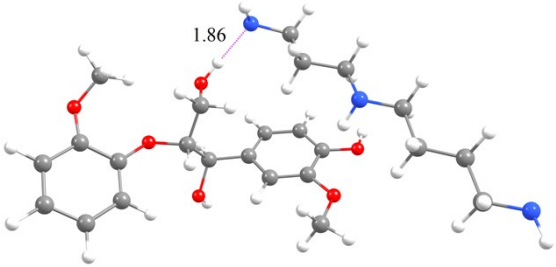

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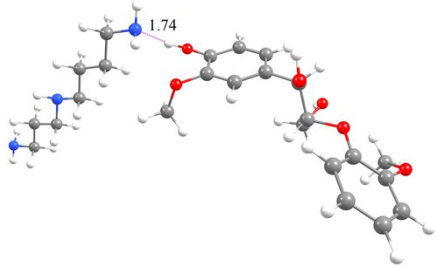

(h) Lignin-spermidine-8
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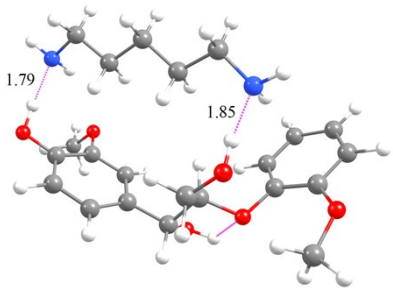
Fig. S12: The optimized configurations of lignin-spermidine-n (n=1-8) at B3LYP-GD3BJ/6-311+g(d,p) level. The hydrogen bonds are indicated by dashed lines and bond distances are given in Å.

Table S2: Hydrogen bonds, relative optimized complex energy ($\Delta E_{relative}$), and Fi-SAFT predicted interaction energy (I.E.) between the different conformers of lignin and spermidine

Lignin–spermidine	H-bonding	Distance (Å)	$\Delta E_{relative}$[a], (kJ/mol)	I. E., (kJ/mol)
Conformer 1	O23-H42…N43	1.80	0.00	-133.37
	O13-H32…N47	1.87		
	N52-H64…O8	2.28		
Conformer 2	O23-H42…N43	1.80	2.93	-131.61
	O13-H32…N47	1.85		
Conformer 3	O23-H43…N53	1.81	24.16	-95.29
Conformer 4	O23-H42…N52	1.83	30.41	-138.36
	O11-H31…N47	1.81		
Conformer 5	O11-H31…N43	1.82	33.07	-81.00
	N47-H71…O13	2.26		
	N43-H53…O8	2.26		
Conformer 6	O23-H42…N52	1.79	45.10	-107.82
	N47-H71…O11	2.19		
	N43-H53…O8	2.17		
Conformer 7	O13-H32…N42	1.86	57.12	-70.95
Conformer 8	O23-H42…N52	1.74	77.17	-59.88

[a] $\Delta E_{relative}$ (kJ/mol) = ($E_{conformer1} - E_{conformer\ (1\ to\ n)}$) × 2625.5



(a) Lignin-1,5-diaminopentane-1
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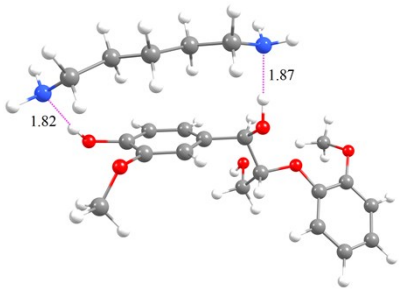

(b) Lignin-1,5-diaminopentane-2
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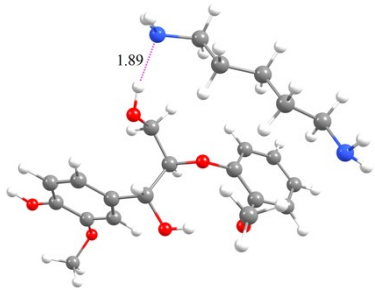

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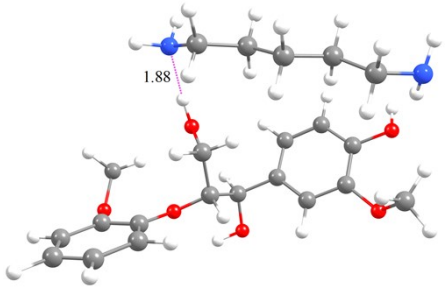

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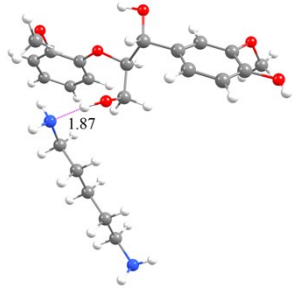

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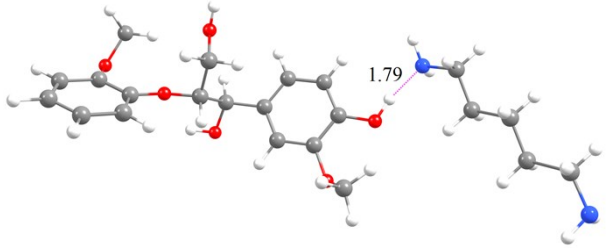

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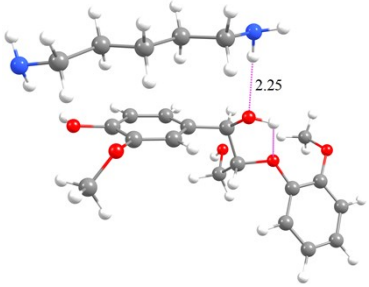

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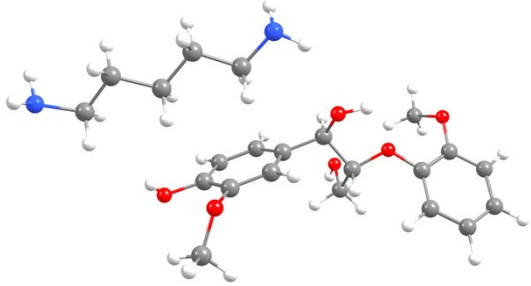

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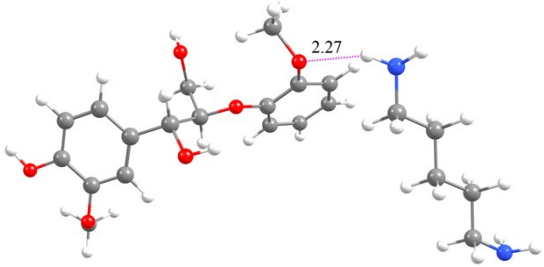


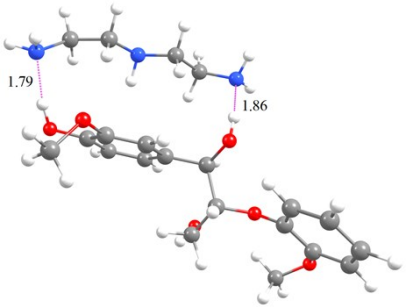
(i) Lignin-1,5-diaminopentane-9
E = -1420.08029283

Fig. S13: The optimized configurations of lignin-1,5-diaminopentane-n (n=1-9) at B3LYP-GD3BJ/6-311+g(d,p) level. The hydrogen bonds are indicated by dashed lines and bond distances are given in Å.

Table S3: Hydrogen bonds, relative optimized complex energy ($\Delta E_{relative}$), and Fi-SAFT predicted interaction energy (I.E.) between the different conformers of lignin and 1,5-diaminopentane

Lignin–1,5-diaminopentane	H-bonding	Distance (Å)	$\Delta E_{relative}$[a], (kJ/mol)	I. E., (kJ/mol)
Conformer 1	O23-H43…N44	1.79	0.00	-122.45
	O13-H32…N50	1.85		
Conformer 2	O11-H31…N44	1.87	26.89	-106.28
	O23-H43…N50	1.82		
Conformer 3	O13-H32…N50	1.89	40.87	-70.77
Conformer 4	O13-H32…N44	1.88	50.04	-62.30
Conformer 5	O13-H32…N44	1.87	56.00	-58.87
Conformer 6	O23-H43…N44	1.79	65.91	-52.77
Conformer 7	N44-H52…O11	2.25	75.29	-38.68
Conformer 8	-	-	88.35	-27.12
Conformer 9	N44-H51…O8	2.27	95.71	-22.16

[a] $\Delta E_{relative}$ (kJ/mol) = $(E_{conformer1} - E_{conformer\ (1\ to\ n)}) \times 2625.5$



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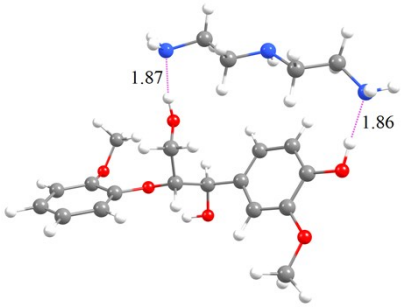

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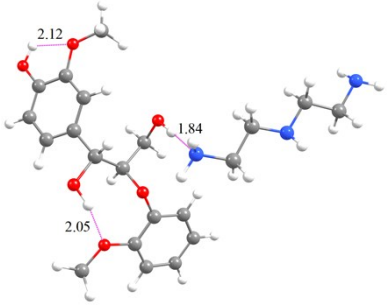

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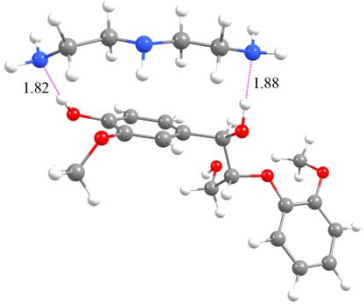

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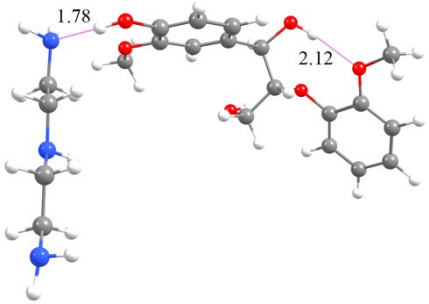

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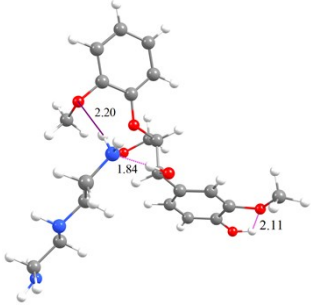

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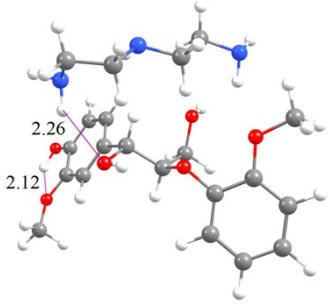

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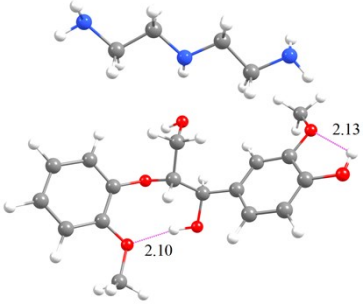

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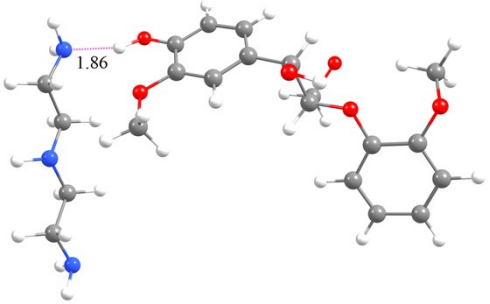

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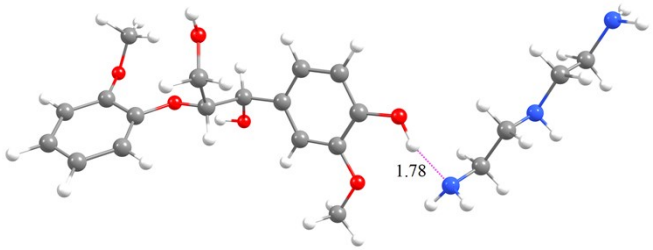
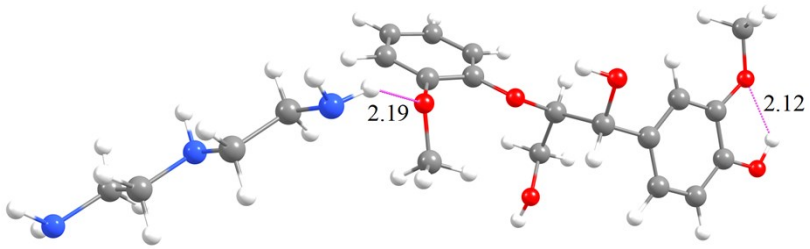


(j) Lignin-diethylenetriamine-10
E = -1436.12848412



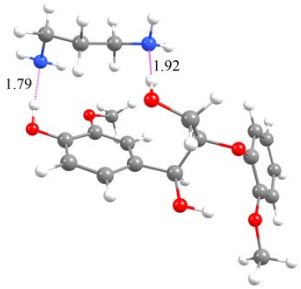
(k) Lignin-diethylenetriamine-11
E = -1436.12100633

Fig. S14: The optimized configurations of lignin-diethylenetriamine-n (n=1-11) at B3LYP-GD3BJ/6-311+g(d,p) level. The hydrogen bonds are indicated by dashed lines and bond distances are given in Å.

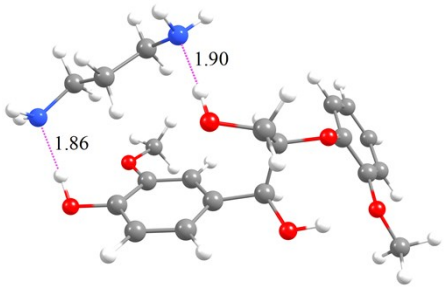
Table S4: Hydrogen bonds, relative optimized complex energy ($\Delta E_{relative}$), and Fi-SAFT predicted interaction energy (I.E.) between the different conformers of lignin and diethylenetriamine

Lignin–diethylenetriamine	H-bonding	Distance (Å)	$\Delta E_{relative}$[a], (kJ/mol)	I. E., (kJ/mol)
Conformer 1	O11-H31…N50	1.86	0.00	-114.94
	O23-H43…N44	1.79		
Conformer 2	O23-H43…N44	1.86	0.33	-92.71
	O13-H32…N50	1.87		
Conformer 3	O13-H32…N44	1.84	0.73	-49.82
Conformer 4	O23-H43…N50	1.82	0.80	
	O11-H31…N44	1.88		
Conformer 5	O23-H43…N50	1.78	5.75	-45.78
Conformer 6	O11-H31…N50	1.84	6.70	-60.67
	N50-H63…O8	2.20		
Conformer 7	N44-H52…O11	2.26	9.13	-48.87
Conformer 8	-	-	14.02	-29.47
Conformer 9	O23-H43…N50	1.86	18.96	-50.62
Conformer 10	O23-H43…N44	1.78	27.77	-43.33
Conformer 11	N44-H51…O8	2.19	47.39	-18.45

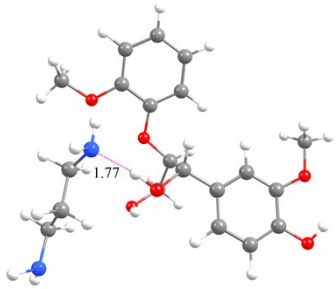
[a] $\Delta E_{relative}$ (kJ/mol) = ($E_{conformer1} - E_{conformer\ (1\ to\ n)}$) × 2625.5



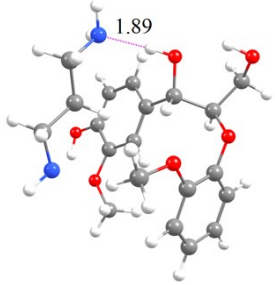
(a) Lignin-1,3-diaminopropane -1
E = -1341.45575324



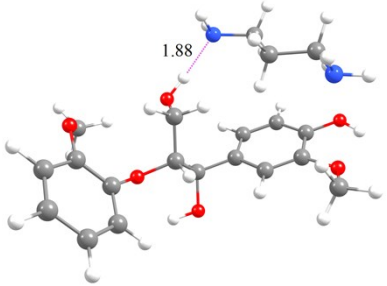
(b) Lignin-1,3-diaminopropane -2
E = -1341.45419475



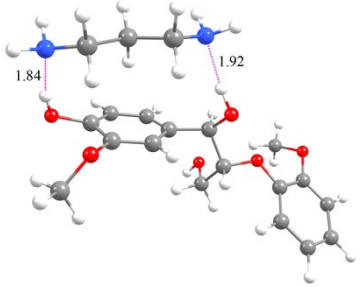
(c) Lignin-1,3-diaminopropane -3
E = -1341.45350033



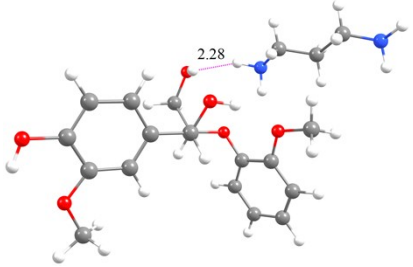
(d) Lignin GGE-1,3-diaminopropane -4
E = -1341.45198078



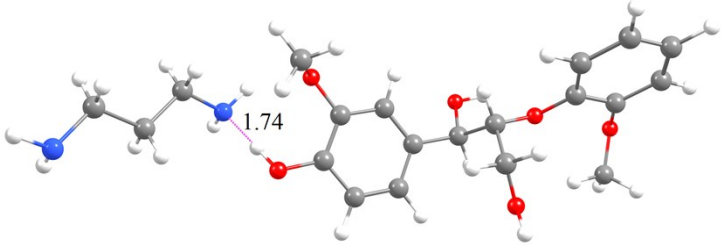
(e) Lignin-1,3-diaminopropane -5
E = -1341.45048815



(f) Lignin-1,3-diaminopropane -6
E = -1341.4459659



(g) Lignin-1,3-diaminopropane -7
E = -1341.44466136



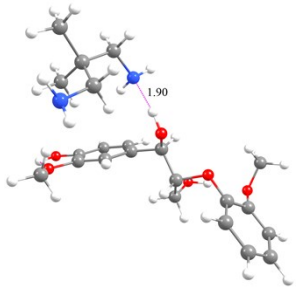
(h) Lignin-1,3-diaminopropane -8
E = -1341.44070271

Figure S15: The optimized configurations of lignin-1,3-diaminopropane-n (n=1-8) at B3LYP-GD3BJ/6-311+g(d,p) level. The hydrogen bonds are indicated by dashed lines and bond distances are given in Å.

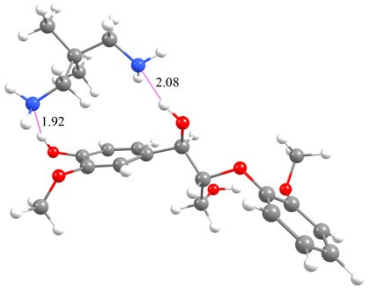
Table S5: Hydrogen bonds, relative optimized complex energy ($\Delta E_{relative}$), and Fi-SAFT predicted interaction energy (I.E.) between the different conformers of lignin and 1,3-diaminopropane

Lignin–1,3-diaminopropane	H-bonding	Distance (Å)	$\Delta E_{relative}$[a], (kJ/mol)	I. E., (kJ/mol)
Conformer 1	O23-H43…N48	1.79	0.00	-90.26
	O13-H32…N44	1.92		
Conformer 2	O23-H43…N48	1.86	4.09	-83.02
	O13-H32…N44	1.90		
Conformer 3	O11-H31…N44	1.77	5.91	-74.70
Conformer 4	O11-H31…N48	1.89	9.90	
Conformer 5	O13-H32…N48	1.88	13.82	-65.86
Conformer 6	O23-H43…N44	1.84	25.68	-98.69
	O11-H31…N48	1.92		
Conformer 7	N48-H55…O13	2.28	29.11	-26.17
Conformer 8	O23-H43…N48	1.74	39.50	-57.90

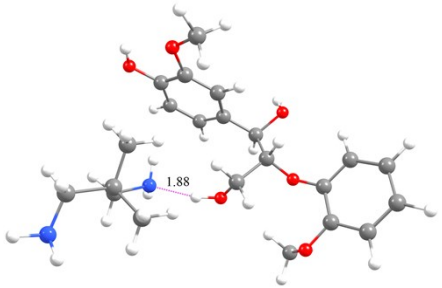
[a] $\Delta E_{relative}$ (kJ/mol) = $(E_{conformer1} - E_{conformer\ (1\ to\ n)}) \times 2625.5$



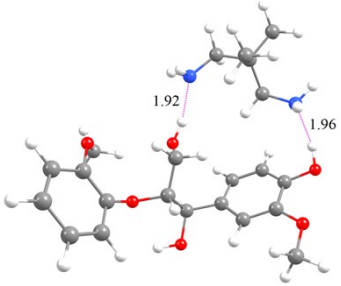
(a) Lignin-22DM13PDA-1
E = -1420.11242186



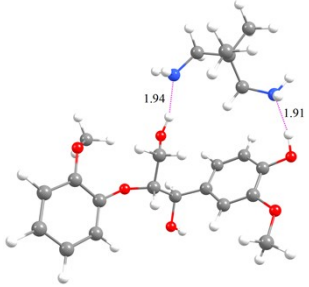
(b) Lignin-22DM13PDA-2
E = -1420.10768821



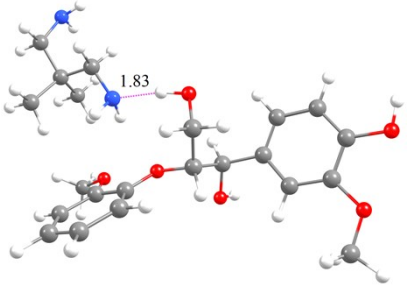
(c) Lignin-22DM13PDA-3
E = -1420.10321594



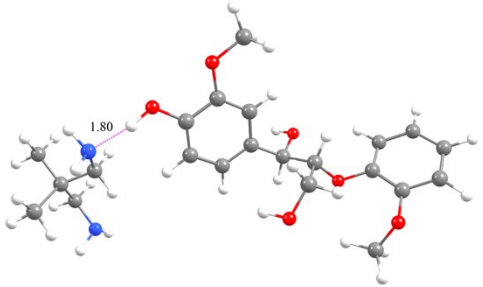
(d) Lignin-22DM13PDA-4
E = -1420.10300804



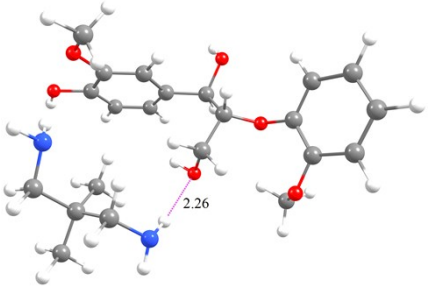
(e) Lignin-22DM13PDA-5
E = -1420.10083435



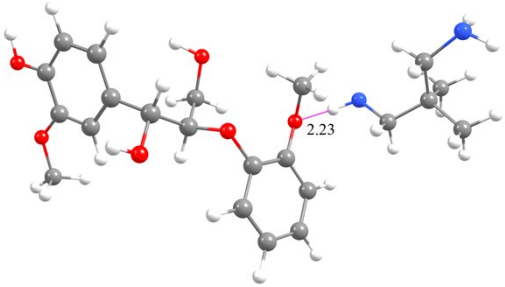
(f) Lignin-22DM13PDA-6
E = -1420.09981939



(g) Lignin-22DM13PDA-7
E = -1420.09523625



(h) Lignin-22DM13PDA-8
E = -1420.09065721



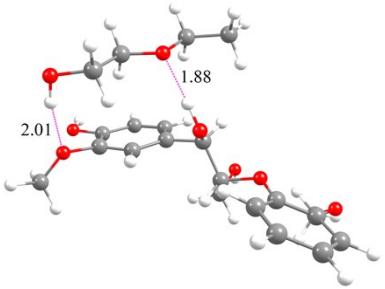
(i) Lignin-22DM13PDA-9
E = -1420.08301598

Figure S16: The optimized configurations of lignin-2,2-dimethyl-1,3-propanediamine (22DM13PDA)-n (n=1-8) at B3LYP-GD3BJ/6-311+g(d,p) level. The hydrogen bonds are indicated by dashed lines and bond distances are given in Å.

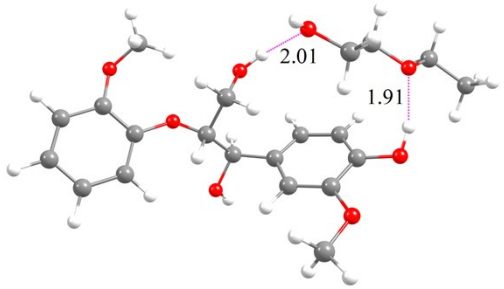
Table S6: Hydrogen bonds, relative optimized complex energy ($\Delta E_{relative}$), and Fi-SAFT predicted interaction energy (I.E.) between the different conformers of lignin and 2,2-dimethyl-1,3-propanediamine (2,2-DM-1,3-PDA)

Lignin–(2,2-dimethyl-1,3-propanediamine)	H-bonding	Distance (Å)	$\Delta E_{relative}$[a], (kJ/mol)	I. E., (kJ/mol)
Conformer 1	O11-H31…N44	1.90	0.00	-60.58
Conformer 2	O23-H43…N48	1.92	12.42	-90.16
	N48-H55…O20	2.28		
	O11-H31…N44	2.08		
Conformer 3	O13-H32…N48	1.88	24.16	-56.03
Conformer 4	O13-H32…N44	1.92	24.70	-80.24
	O23-H43…N48	1.96		
Conformer 5	O13-H32…N44	1.94	30.41	-80.93
	O23-H43…N48	1.91		
Conformer 6	O13-H32…N48	1.83	33.07	-64.82
Conformer 7	O23-H43…N48	1.80	45.10	-56.20
Conformer 8	N48-H55…O13	2.26	57.12	-37.61
Conformer 9	N44-H61…O8	2.23	77.17	-20.48

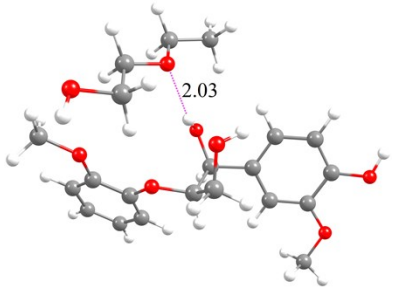
[a] $\Delta E_{relative}$ (kJ/mol) = ($E_{conformer1} - E_{conformer\ (1\ to\ n)}$) × 2625.5



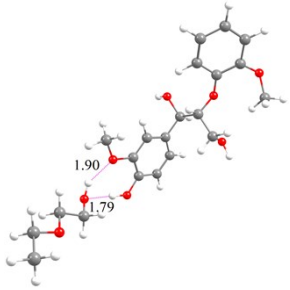
(a) Lignin-2-ethoxy ethanol-1
E = -1420.50316587



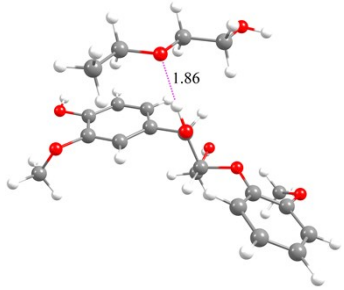
(b) Lignin-2-ethoxy ethanol-2
E = -1420.5006484



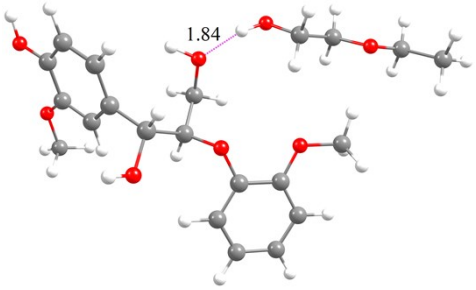
(c) Lignin-2-ethoxy ethanol-3
E = -1420.49843929



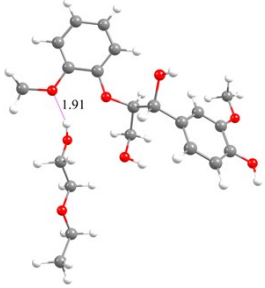
(d) Lignin-2-ethoxy ethanol-4
E = -1420.49841527



(e) Lignin-2-ethoxy ethanol-5
E = -1420.49726424



(f) Lignin-2-ethoxy ethanol-6
E = -1420.4965459



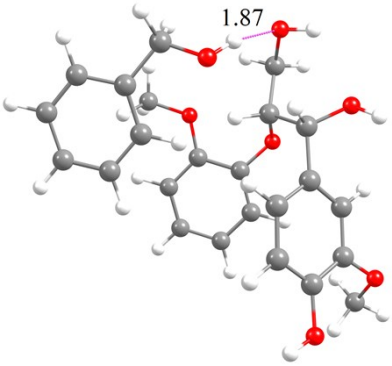
(g) Lignin-2-ethoxyethanol-7
E = -1420.49530012

Figure S17. The optimized configurations of lignin-2-ethoxy ethanol-n (n=1-7) at B3LYP-GD3BJ/6-311+g(d,p) level. The hydrogen bonds are indicated by dashed lines and bond distances are given in Å.

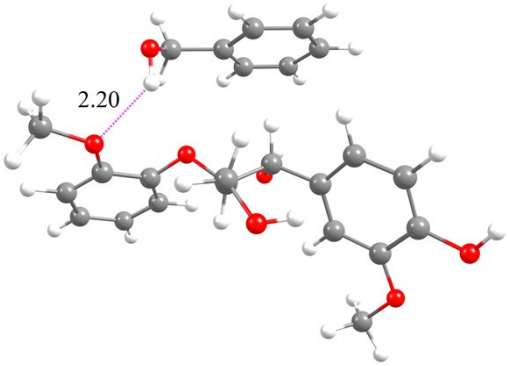
Table S7: Hydrogen bonds, relative optimized complex energy ($\Delta E_{relative}$), and Fi-SAFT predicted interaction energy (I.E.) between the different conformers of lignin and 2-ethoxy ethanol

Lignin–2-ethoxy ethanol	H-bonding	Distance (Å)	$\Delta E_{relative}$[a], (kJ/mol)	I. E., (kJ/mol)
Conformer 1	O11-H31…O46	1.88	0.00	-69.48
	O50-H59…O20	2.01		
Conformer 2	O23-H43…O46	1.91	6.61	-66.11
	O13-H32…O57	2.01		
Conformer 3	O11-H31…O46	2.03	12.40	-45.90
Conformer 4	O23-H43…O57	1.79	12.47	-38.10
	O57-H59…O20	1.90		
Conformer 5	O11-H31…O46	1.86	15.49	-51.66
Conformer 6	O57-H59…O13	1.84	17.37	-43.75
Conformer 7	O57-H59…O8	1.91	20.64	-42.46

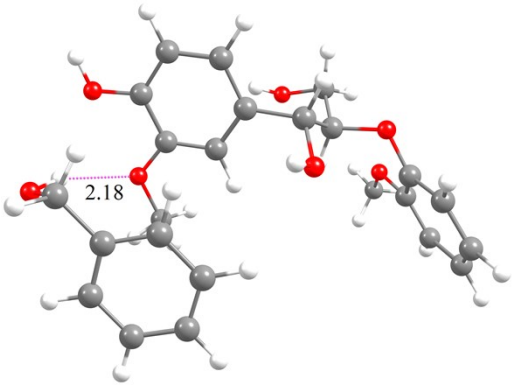
[a] $\Delta E_{relative}$ (kJ/mol) = ($E_{conformer1} - E_{conformer\ (1\ to\ n)}$) × 2625.5



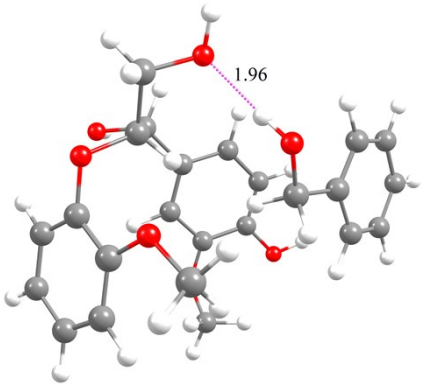
(a) Lignin-benzyl alcohol-1
E = -1458.41067599



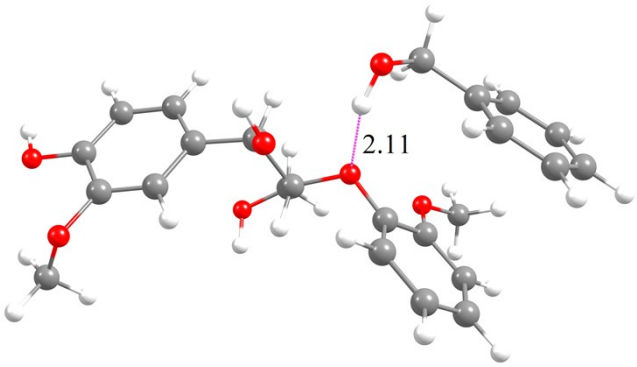
(b) Lignin-benzyl alcohol-2
E = -1458.41057868



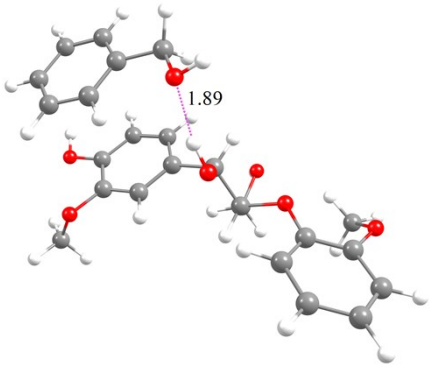
(c) Lignin-benzyl alcohol-3
E = -1458.40667195



(d) Lignin-benzyl alcohol-4
E = -1458.40262718



(e) Lignin-benzyl alcohol-5
E = -1458.40145676



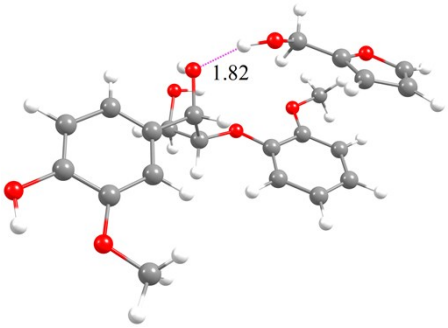
(f) Lignin-benzyl alcohol-6
E = -1458.39798136

Figure S18: The optimized configurations of lignin-benzyl alcohol-n (n=1-6) at B3LYP-GD3BJ/6-311+g(d,p) level. The hydrogen bonds are indicated by dashed lines and bond distances are given in Å.

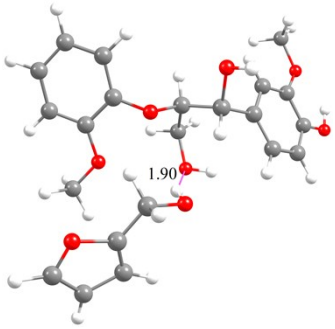
Table S8: Hydrogen bonds, relative optimized complex energy ($\Delta E_{relative}$), and Fi-SAFT predicted interaction energy (I.E.) between the different conformers of lignin and benzyl alcohol

Lignin–benzyl alcohol	H-bonding	Distance (Å)	$\Delta E_{relative}$[a], (kJ/mol)	I. E., (kJ/mol)
Conformer 1	O51-H59…O13	1.87	0.00	-65.90
Conformer 2	O51-H59…O8	2.20	0.26	-67.40
Conformer 3	O51-H59…O20	2.18	10.51	-50.42
Conformer 4	O51-H59…O13	1.96	21.12	-65.16
Conformer 5	O51-H59…O1	2.11	24.19	-59.60
Conformer 6	O11-H31…O51	1.89	33.31	-55.21

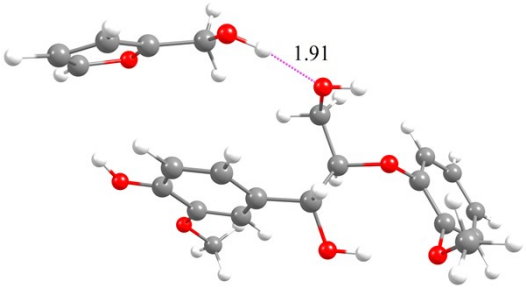
[a] $\Delta E_{relative}$ (kJ/mol) = $(E_{conformer1} - E_{conformer\ (1\ to\ n)}) \times 2625.5$



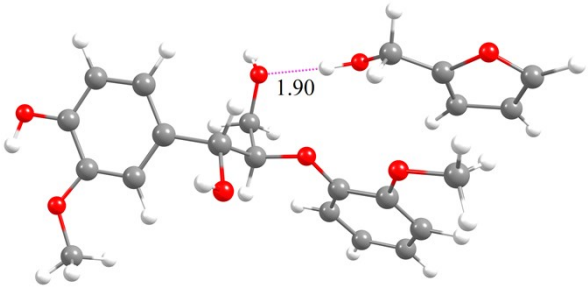
(a) Lignin-furfuryl alcohol-1
E = -1456.19460258



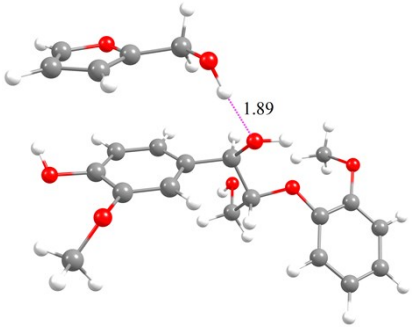
(b) Lignin-furfuryl alcohol-2
E = -1456.19115991



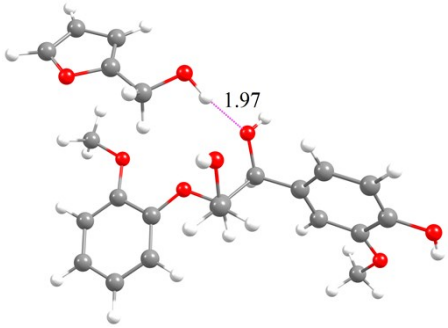
(c) Lignin-furfuryl alcohol-3
E = -1456.18603716



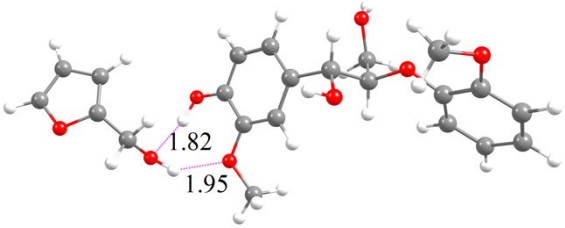
(d) Lignin-furfuryl alcohol-4
E = -1456.18559915



(e) Lignin-furfuryl alcohol-5
E = -1456.18031223



(f) Lignin-furfuryl alcohol-6
E = -1456.17917738



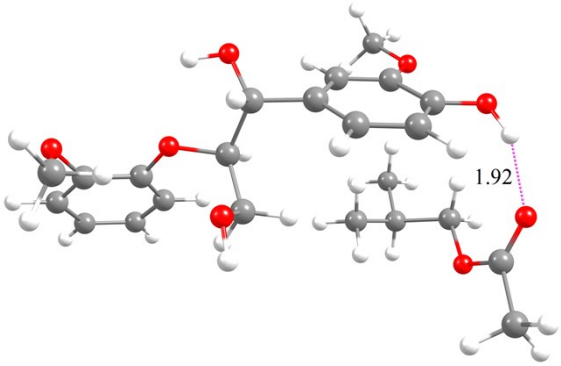
(g) Lignin-furfuryl alcohol-7
E = -1456.17756777

Figure S19: The optimized configurations of lignin-furfuryl alcohol-n (n=1-7) at B3LYP-GD3BJ/6-311+g(d,p) level. The hydrogen bonds are indicated by dashed lines and bond distances are given in Å.

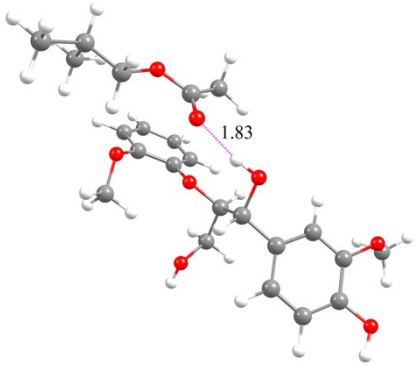
Table S9: Hydrogen bonds, relative optimized complex energy ($\Delta E_{relative}$), and Fi-SAFT predicted interaction energy (I.E.) between the different conformers of lignin and furfuryl alcohol

Lignin–furfuryl alcohol	H-bonding	Distance (Å)	$\Delta E_{relative}$[a], (kJ/mol)	I. E., (kJ/mol)
Conformer 1	O50-H56…O11	1.82	0.00	-63.51
Conformer 2	O50-H56…O13	1.90	9.03	-64.35
Conformer 3	O50-H56…O13	1.91	22.48	-53.37
Conformer 4	O50-H56…O13	1.90	23.63	-59.64
Conformer 5	O50-H56…O11	1.89	37.50	-60.56
Conformer 6	O50-H56…O11	1.97	40.48	-66.95
Conformer 7	O23-H43…O50	1.82	44.70	-44.01
	O50-H56…O20	1.95		

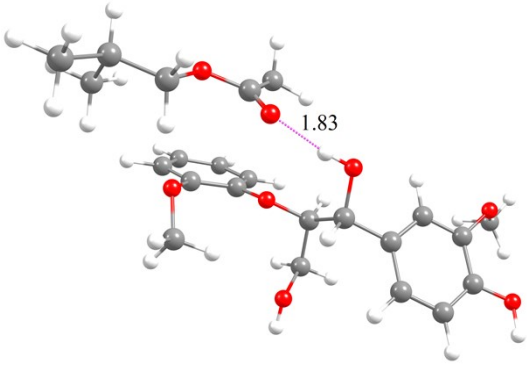
[a] $\Delta E_{relative}$ (kJ/mol) = ($E_{conformer1} - E_{conformer\ (1\ to\ n)}$) × 2625.5



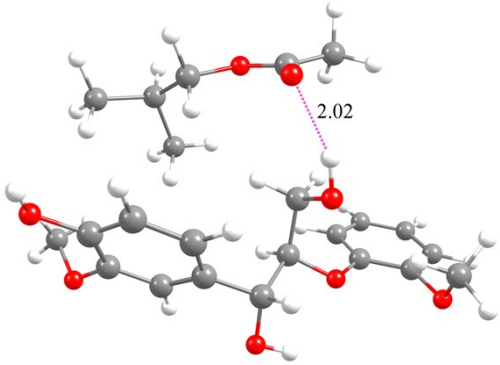
(a) Lignin-isobutyl acetate -1
E = -1497.98931539



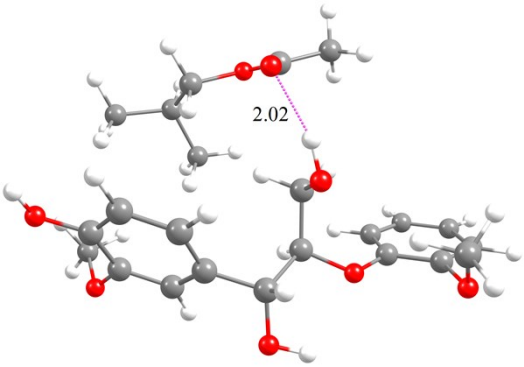
(b) Lignin-isobutyl acetate -2
E = -1497.98696768



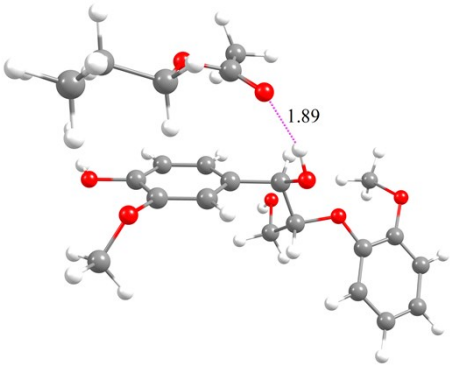
(c) Lignin-isobutyl acetate -3
E = -1497.98696767



(d) Lignin-isobutyl acetate -4
E = -1497.98661456



(e) Lignin-isobutyl acetate -5
E = -1497.98661456



(f) Lignin-isobutyl acetate -6
E = -1497.98247558

Figure S20: The optimized configurations of lignin-isobutyl acetate -n (n=1-6) at B3LYP-GD3BJ/6-311+g(d,p) level. The hydrogen bonds are indicated by dashed lines and bond distances are given in Å.

Table S10: Hydrogen bonds, relative optimized complex energy ($\Delta E_{relative}$), and Fi-SAFT predicted interaction energy (I.E.) between the different conformers of lignin and isobutyl acetate

Lignin–isobutyl acetate	H-bonding	Distance (Å)	$\Delta E_{relative}$[a], (kJ/mol)	I. E., (kJ/mol)
Conformer 1	O23-H43…O46	1.92	0.00	-56.61
Conformer 2	O11-H31…O46	1.83	6.16	-53.87
Conformer 3	O11-H31…O46	1.83	6.16	-53.87
Conformer 4	O13-H32…O46	2.02	7.09	-49.05
Conformer 5	O13-H32…O46	2.02	7.09	-49.05
Conformer 6	O11-H31…O46	1.89	17.95	-52.81

[a] $\Delta E_{relative}$ (kJ/mol) = ($E_{conformer1} - E_{conformer\ (1\ to\ n)}$) × 2625.5

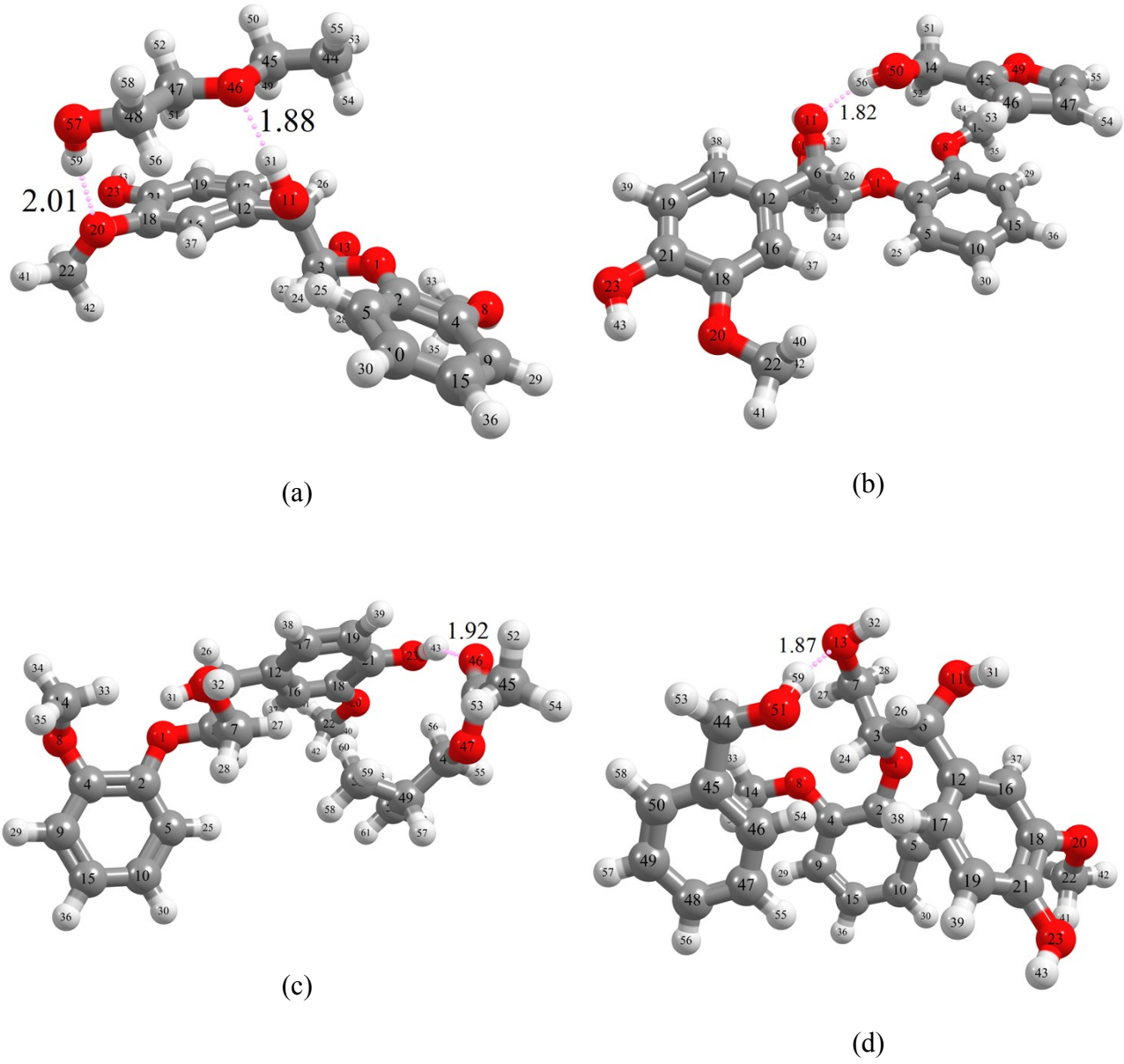


Fig. S21 Optimized geometries for lignin GGE–organic solvents (a) 2-ethoxyethanol, (b) furfuryl alcohol, (c) isobutyl acetate, and (d) benzyl alcohol. The H-bonds are indicated by dotted lines, the bond lengths are in Angstrom (Å) and given with corresponding atom numbers. The color scheme used for different atoms is C (gray), O (red), and H (white), respectively.

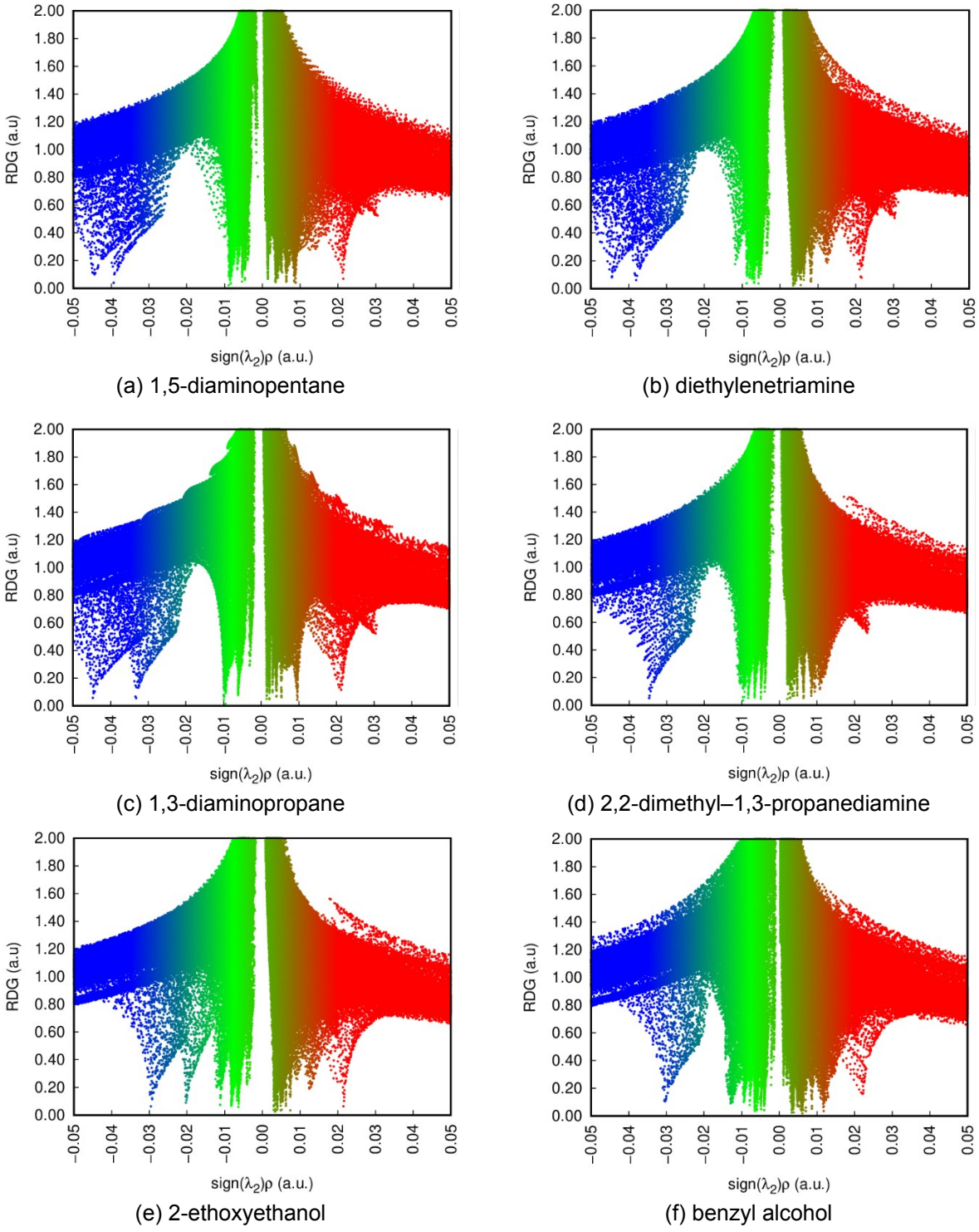


Fig. S22 RDG scatter plots (isovalue 0.5 a.u.) of lignin-amine/organic solvents. The RDG scatters are colored on a blue-green-red scale according to values of sign(λ_2)$\rho(r)$, ranging from -0.045 to 0.025. Blue indicates strong attractive interactions, green indicates the vdW interaction, and red indicated steric repulsions

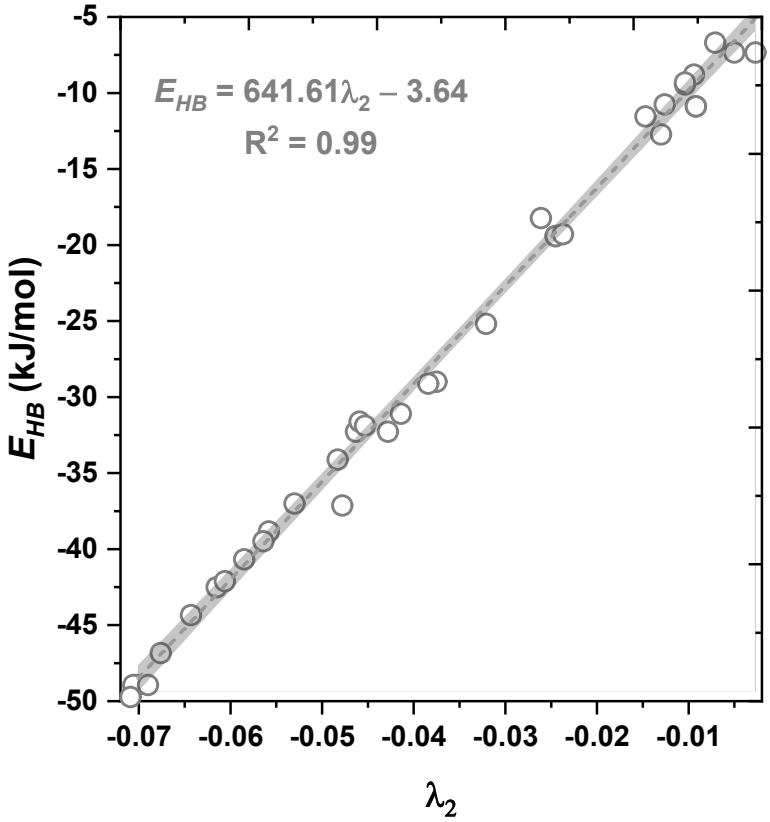


Fig. S23 Correlation between QTAIM–based Hessian second eigenvalue (λ_2) and H-bonding energies (E_{HB}) of lignin-amine/organic solvent systems.

Cartesian coordinates (in Å) and calculated lowest energy conformers of lignin-amine/organic solvent complexes (most stable energy conformer) optimized at B3LYP-GD3BJ/6-311+g(d,p) level of theory and basis set.

Lignin–Spermidine-1

72

Energy: -1554.13158473

O	-2.09189	-1.61079	-0.54387
C	-2.90623	-1.24205	0.48611
C	-0.71601	-1.19588	-0.56057
C	-4.26208	-1.00617	0.15950
C	-2.48940	-1.11268	1.80819
C	0.17840	-2.42957	-0.37878
C	-0.51576	-0.46095	-1.90145
O	-4.59275	-1.15091	-1.15741
C	-5.15237	-0.61618	1.15836
C	-3.38773	-0.71157	2.80027
O	-0.16042	-2.98376	0.90117
C	1.64754	-2.08528	-0.46622
O	0.67327	0.29068	-1.98014
C	-5.96672	-1.05242	-1.52556
C	-4.71410	-0.46076	2.47658
C	2.26973	-1.43569	0.60299
C	2.39032	-2.34360	-1.61723
C	3.58777	-1.01384	0.50679
C	3.70379	-1.89865	-1.72989
O	4.15680	-0.34721	1.57657
C	4.30926	-1.19513	-0.68920
C	5.19297	-1.07956	2.24613
O	5.57519	-0.71937	-0.83893
H	-0.51914	-0.49665	0.25766
H	-1.46802	-1.36200	2.05851
H	-0.08707	-3.13949	-1.17348
H	-0.49672	-1.19157	-2.71561
H	-1.41057	0.15801	-2.05072
H	-6.18646	-0.41462	0.91408
H	-3.04368	-0.61215	3.82314
H	0.43275	-3.72308	1.07059
H	0.64711	1.03376	-1.33516
H	-6.35182	-0.04046	-1.36326
H	-6.00007	-1.27763	-2.59029
H	-6.57489	-1.78028	-0.97767
H	-5.41838	-0.14911	3.23896
H	1.92561	-2.85307	-2.45448

Lignin–1,5-diaminopentane-1

64

Energy: -1420.11676348

O	-2.58256	-1.48202	0.12276
C	-3.20120	-0.44034	0.78952
C	-1.24958	-1.21718	-0.38427
C	-4.44611	0.05746	0.35583
C	-2.58818	0.11899	1.91617
C	-0.35472	-2.40415	0.04505
C	-1.30826	-1.01142	-1.89966
O	-5.19060	-0.37576	-0.68875
C	-4.99896	1.14726	1.04756
C	-3.14819	1.19996	2.58863
O	-0.57970	-2.69989	1.42074
C	1.10845	-2.07791	-0.15552
O	-2.25812	-0.05027	-2.30182
C	-4.93942	-1.62397	-1.35172
C	-4.36198	1.72228	2.13847
C	1.83099	-1.43641	0.85316
C	1.74971	-2.34828	-1.36615
C	3.14556	-1.04236	0.64365
C	3.05480	-1.92086	-1.59402
O	3.82495	-0.39540	1.66420
C	3.76185	-1.23004	-0.60827
C	4.84194	-1.20346	2.27739
O	5.01117	-0.77108	-0.87584
H	-0.87020	-0.31181	0.09497
H	-1.64847	-0.30915	2.24618
H	-0.62216	-3.27562	-0.56987
H	-0.29799	-0.76012	-2.24981
H	-1.59394	-1.95514	-2.37693
H	-5.94859	1.52635	0.68873
H	-2.64953	1.61827	3.45471
H	-1.53783	-2.73671	1.53540
H	-2.14350	0.79343	-1.80294
H	-4.81614	-2.43379	-0.62998
H	-5.82954	-1.79844	-1.95618
H	-4.05943	-1.54395	-1.98577
H	-4.81904	2.56530	2.64371
H	1.37888	-1.25072	1.81898

H	4.27323	-2.05243	-2.63873
H	4.78461	-1.99048	2.69744
H	5.57381	-0.42568	3.03149
H	6.00005	-1.33984	1.55602
H	5.61418	0.23099	-0.54256
N	5.65143	2.01799	-0.30105
C	4.49572	2.54124	0.46025
C	3.19227	2.35099	-0.31766
C	1.97249	2.47062	0.59615
N	0.72539	2.49866	-0.17663
C	-0.48964	2.55539	0.64821
C	-1.72602	2.78885	-0.21727
C	-3.03943	2.55786	0.53077
C	-4.28986	2.80210	-0.33255
N	-4.37757	2.05091	-1.58942
H	5.70082	2.45352	-1.21915
H	6.52062	2.24665	0.17347
H	4.61731	3.60275	0.71759
H	4.44536	1.97186	1.38936
H	-1.69949	3.81035	-0.62211
H	-1.67588	2.11435	-1.07704
H	-3.06322	1.52978	0.90555
H	-3.08997	3.20981	1.41230
H	-4.36599	3.86689	-0.58092
H	-5.17310	2.56169	0.26812
H	-3.72618	2.41099	-2.27772
H	-4.15225	1.06978	-1.45554
H	3.17877	1.36971	-0.79808
H	3.12944	3.09796	-1.12039
H	2.06452	3.35965	1.24375
H	1.94051	1.59885	1.25728
H	-0.58205	1.59940	1.17548
H	-0.42071	3.33537	1.42440
H	0.73910	3.30238	-0.80072
H	1.73184	-1.25064	1.52549
H	1.21894	-2.87393	-2.15309
H	3.54269	-2.08980	-2.54663
H	4.39522	-2.08266	2.75300
H	5.31591	-0.58162	3.03795
H	5.58575	-1.52068	1.54052
H	5.12634	0.14860	-0.50437
N	5.19844	1.82395	0.11791
C	4.17136	2.76848	-0.37580
C	2.78751	2.12925	-0.29638
C	1.63584	3.05269	-0.69821
C	0.28932	2.32976	-0.59325
C	-0.91108	3.18084	-0.99968
N	-2.15307	2.39626	-0.88109
H	6.12323	2.24164	0.07595
H	5.00794	1.58801	1.08909
H	4.41192	3.01332	-1.41513
H	4.17662	3.71180	0.18935
H	2.62249	1.77326	0.72670
H	2.77262	1.23903	-0.93083
H	1.78258	3.40715	-1.72648
H	1.62936	3.94527	-0.05977
H	0.14732	1.98143	0.43788
H	0.31198	1.43248	-1.22059
H	-0.80588	3.48435	-2.04617
H	-0.93309	4.10143	-0.39764
H	-2.36027	2.18997	0.09370
H	-2.95085	2.91352	-1.23767

Lignin–diethylenetriamine-1

63

Energy: -1436.13906674

O	3.11245	-0.08582	-0.53046
C	4.01847	0.19851	0.45660
C	1.86721	-0.72272	-0.20858
C	5.38523	0.07454	0.13421
C	3.64919	0.66993	1.71887

Lignin–1,3-diaminopropane-1

58

Energy: -1341.45575324

O	-2.68377	0.33035	-1.44402
C	-3.44234	0.88154	-0.44463
C	-1.28838	0.06423	-1.14650
C	-4.43184	0.09110	0.17421
C	-3.29072	2.21164	-0.07046

C	0.72555	0.24948	-0.55217	C	-1.20285	-1.10064	-0.13078
C	1.81018	-2.05254	-0.94634	C	-0.64023	-0.20069	-2.51067
O	5.85076	-0.29361	-1.10099	O	-4.50946	-1.20675	-0.24822
C	6.34336	0.41890	1.08836	C	-5.24690	0.65494	1.15647
C	4.61866	0.99709	2.66428	C	-4.10122	2.77243	0.91766
O	0.83470	1.32956	0.36067	O	-1.80979	-2.26786	-0.66136
C	-0.64265	-0.41355	-0.47983	C	0.22460	-1.38113	0.27398
O	1.79525	-1.80966	-2.35534	O	0.76983	-0.23795	-2.46633
C	5.30733	-1.46233	-1.72739	C	-5.42762	-2.08342	0.40020
C	5.97033	0.87469	2.34964	C	-5.07690	1.99135	1.52629
C	-1.30842	-0.51091	0.74407	C	0.88702	-0.45269	1.08417
C	-1.25933	-0.93987	-1.61741	C	0.92042	-2.48897	-0.19385
C	-2.56160	-1.10462	0.83197	C	2.23706	-0.60250	1.38421
C	-2.52248	-1.52456	-1.53975	C	2.27308	-2.63668	0.09993
O	-3.21352	-1.13183	2.05055	O	2.94923	0.28859	2.16690
C	-3.20174	-1.59726	-0.32135	C	2.96027	-1.69482	0.86108
C	-3.29774	-2.43418	2.64614	C	2.21315	1.16339	3.00944
O	-4.44848	-2.13459	-0.27535	O	4.28596	-1.87089	1.10081
H	1.81655	-0.94080	0.86360	H	-0.83833	0.95804	-0.69556
H	2.59932	0.83349	1.92186	H	-2.53556	2.80279	-0.57598
H	0.90433	0.58719	-1.57959	H	-1.75605	-0.77383	0.76378
H	0.91010	-2.59381	-0.63267	H	-0.98050	-1.16982	-2.87970
H	2.69148	-2.63959	-0.66117	H	-1.01237	0.57172	-3.19905
H	7.38562	0.31619	0.80998	H	-6.01117	0.06292	1.64142
H	4.31258	1.36794	3.63587	H	-3.97587	3.81169	1.19743
H	0.47217	2.13725	-0.06792	H	-2.73483	-2.03949	-0.83009
H	1.71426	-2.65187	-2.81193	H	1.11309	0.61350	-2.12765
H	4.33538	-1.26354	-2.17832	H	-5.28420	-3.05747	-0.06417
H	6.02968	-1.74580	-2.49395	H	-5.21506	-2.15651	1.47191
H	5.21662	-2.28002	-1.00219	H	-6.46119	-1.75597	0.24809
H	6.73099	1.13330	3.07720	H	-5.71728	2.41418	2.29158
H	-0.86559	-0.09258	1.63976	H	0.33594	0.39505	1.47430
H	-0.74631	-0.88797	-2.57121	H	0.41147	-3.21223	-0.81593
H	-3.02094	-1.90551	-2.42370	H	2.83806	-3.48007	-0.27937
H	-3.81430	-3.13756	1.98665	H	1.68101	1.93291	2.43566
H	-3.86223	-2.31389	3.57092	H	2.94448	1.64703	3.65715
H	-2.29625	-2.81385	2.87718	H	1.49129	0.61200	3.62139
H	-5.03720	-1.58087	0.30921	H	4.75836	-1.00205	1.01640
N	-6.18676	-0.29537	0.79823	N	1.95271	2.26398	-1.63513
C	-5.84617	0.81153	-0.12740	C	3.17835	2.08414	-0.83175
C	-4.61980	1.59597	0.37183	C	4.05759	0.97816	-1.42357
N	-3.72310	1.91933	-0.73718	C	5.47205	0.94678	-0.83921
C	-2.54741	2.68009	-0.32102	N	5.48890	0.57329	0.58886
C	-1.63782	2.94055	-1.52008	H	3.76227	3.01507	-0.75501
N	-0.33871	3.47944	-1.07016	H	2.86791	1.80794	0.17764
H	-7.13397	-0.62276	0.63275	H	3.56386	0.01116	-1.29565

H	-6.13902	0.00810	1.76650
H	-6.68870	1.49378	-0.28759
H	-5.61259	0.36182	-1.09614
H	-4.11430	1.01278	1.15637
H	-4.93985	2.53563	0.83508
H	-3.40503	1.04476	-1.14954
H	-2.88449	3.63661	0.09888
H	-1.96650	2.16794	0.46142
H	-1.43948	1.98978	-2.02434
H	-2.15445	3.59171	-2.23568
H	0.25756	3.69400	-1.86379
H	-0.46684	4.34948	-0.56030
H	4.15168	1.14430	-2.50354
H	6.06026	0.19825	-1.37674
H	5.95179	1.92208	-1.01471
H	4.89743	1.17954	1.14928
H	6.43022	0.63534	0.96435
H	1.32514	2.92473	-1.18699
H	2.18326	2.65352	-2.54579

Lignin–22DM13PDA-1

64

Energy: -1420.11242186

O	2.71136	0.66074	-0.24024
C	3.87140	0.71117	0.48410
C	1.72612	-0.32026	0.16246
C	5.06184	0.30953	-0.14134
C	3.90933	1.18339	1.79544
C	0.48009	-0.02110	-0.67478
C	2.28795	-1.73126	-0.03505
O	5.02909	-0.21011	-1.42277
C	6.26990	0.37469	0.54559
C	5.12022	1.24275	2.48291
O	0.02351	1.27302	-0.30376
C	-0.59816	-1.07525	-0.47762
O	2.66342	-1.98815	-1.37980
C	4.82819	0.77011	-2.45917
C	6.30047	0.83654	1.86081
C	-1.39435	-1.04124	0.67617
C	-0.81239	-2.07407	-1.42330
C	-2.39012	-1.98963	0.86820
C	-1.81135	-3.03271	-1.23275
O	-3.25012	-2.04823	1.93317
C	-2.60299	-2.99535	-0.09500
C	-3.20166	-1.00362	2.90787
O	-3.59262	-3.91715	0.08048
H	1.47431	-0.17484	1.22148
H	2.98402	1.50508	2.25896
H	0.79648	-0.03609	-1.72518
H	1.52572	-2.46300	0.23667
H	3.13950	-1.87049	0.64349

Lignin–2-ethoxy ethanol-1

59

Energy: -1420.50316587

O	2.67427	-0.32913	-0.41507
C	3.52709	0.20113	0.51943
C	1.42798	-0.90705	-0.00718
C	4.90909	0.04743	0.29123
C	3.08826	0.93630	1.62304
C	0.28577	-0.07190	-0.60510
C	1.41473	-2.36788	-0.43528
O	5.43985	-0.58120	-0.80474
C	5.81379	0.63090	1.17886
C	4.00502	1.50141	2.50670
O	0.33791	1.19025	0.04622
C	-1.07561	-0.72495	-0.43864
O	1.42140	-2.44013	-1.86279
C	4.94968	-1.87739	-1.16603
C	5.37209	1.35243	2.28412
C	-1.78090	-0.56456	0.75458
C	-1.67358	-1.44238	-1.47411
C	-3.07168	-1.05350	0.90524
C	-2.95393	-1.97155	-1.32169
O	-3.77614	-0.68419	2.03052
C	-3.67272	-1.76697	-0.14444
C	-4.21306	-1.73415	2.91033
O	-4.95958	-2.19966	0.03039
H	1.33537	-0.88312	1.08384
H	2.02730	1.11012	1.74271
H	0.50006	0.03128	-1.67537
H	0.51972	-2.85023	-0.02397
H	2.30155	-2.85425	-0.01307

H	7.17010	0.04596	0.03965	H	6.86989	0.49976	0.97469
H	5.14156	1.61104	3.50217	H	3.64574	2.07635	3.35242
H	-0.73435	1.48036	-0.89310	H	-0.37476	1.75093	-0.31202
H	3.46861	-1.47722	-1.55339	H	1.46113	-3.36411	-2.12553
H	5.64406	1.49975	-2.44894	H	4.00244	-1.81422	-1.70182
H	4.83821	0.22217	-3.40109	H	5.71760	-2.31362	-1.80610
H	3.86813	1.27467	-2.32898	H	4.82844	-2.50485	-0.27470
H	7.24232	0.87980	2.39501	H	6.09201	1.79574	2.96224
H	-1.24345	-0.24247	1.38930	H	-1.35569	0.01445	1.56443
H	-0.18332	-2.12009	-2.30498	H	-1.13446	-1.58917	-2.40254
H	-1.99096	-3.81253	-1.96310	H	-3.41871	-2.51655	-2.13850
H	-2.22387	-0.97881	3.40127	H	-4.91874	-2.39779	2.40846
H	-3.96732	-1.25065	3.64184	H	-4.69971	-1.23773	3.74871
H	-3.42494	-0.03045	2.46014	H	-3.34992	-2.30295	3.27106
H	-4.03867	-3.71461	0.91400	H	-5.28134	-2.60354	-0.78220
N	-2.21719	1.39800	-2.08980	C	-0.33379	2.83718	-3.00360
C	-3.43196	2.22530	-1.95194	C	-1.70310	2.33989	-2.57739
C	-4.12450	2.08742	-0.57689	O	-1.84984	2.54697	-1.16949
C	-3.12826	2.50052	0.52994	C	-3.14444	2.20025	-0.67290
N	-3.70656	2.41749	1.88148	C	-3.21273	2.57944	0.80451
H	-3.13196	3.26881	-2.09566	H	-1.82513	1.26978	-2.79957
H	-4.17601	1.99460	-2.72844	H	-2.49723	2.88440	-3.10618
C	-5.33552	3.03938	-0.57762	H	-3.32131	1.12462	-0.79580
C	-4.61405	0.64367	-0.37046	H	-3.91950	2.74054	-1.23156
H	-2.26950	1.83094	0.50877	H	-0.19720	2.68336	-4.07728
H	-2.74984	3.50721	0.28986	H	0.46147	2.30640	-2.47602
H	-2.98551	2.59841	2.57231	H	-0.23184	3.90330	-2.78948
H	-4.41881	3.12687	2.02087	H	-2.33854	2.17318	1.32558
H	-6.01068	2.81197	-1.40800	O	-4.42947	2.13771	1.38872
H	-5.02126	4.08409	-0.67482	H	-3.17841	3.66689	0.90388
H	-5.91659	2.93950	0.34283	H	-4.33517	1.21158	1.65350
H	-2.44256	0.40808	-2.02762				
H	-1.80898	1.53881	-3.00926				
H	-5.31696	0.35752	-1.15940				
H	-5.12057	0.54723	0.59110				
H	-3.78897	-0.07087	-0.37159				

Lignin–benzyl alcohol-1

59

Energy: -1458.41067599

O	-0.55354	0.82959	1.77957
C	-0.36769	-0.53211	1.69391
C	0.11915	1.64943	0.80921
C	0.91492	-1.11563	1.77915

Lignin–furfuryl alcohol-1

56

Energy: -1456.19460258

O	0.56593	-1.13900	1.25839
C	1.29970	0.00731	1.40289
C	-0.85089	-1.09594	1.07714
C	2.69743	-0.18783	1.48669

C	-1.48657	-1.34863	1.59807	C	0.77718	1.29195	1.48549
C	-0.85516	2.27190	-0.21189	C	-1.22565	-0.72236	-0.37905
C	0.87914	2.71516	1.60316	C	-1.32208	-2.48807	1.50138
O	1.96526	-0.25455	1.91589	O	3.11522	-1.48144	1.38322
C	1.03723	-2.50489	1.72331	C	3.53131	0.91201	1.65313
C	-1.36169	-2.73667	1.55971	C	1.62664	2.39141	1.65079
O	-1.47873	3.40737	0.41079	O	-0.77350	-1.70478	-1.31228
C	-1.84675	1.27060	-0.75767	C	-2.71763	-0.46113	-0.49147
O	1.42136	3.73977	0.75214	O	-0.63844	-3.51472	0.76973
C	3.27749	-0.79701	2.04399	C	4.51444	-1.74670	1.46296
C	-0.09711	-3.31130	1.61347	C	2.99619	2.20052	1.73270
C	-3.10600	1.10914	-0.17836	C	-3.22982	0.75754	-0.02140
C	-1.48777	0.44941	-1.82652	C	-3.59213	-1.41089	-1.00791
C	-4.00160	0.15317	-0.64700	C	-4.59570	1.00643	-0.06090
C	-2.36835	-0.52037	-2.29591	C	-4.96584	-1.16371	-1.04924
O	-5.25014	0.08448	-0.08134	O	-5.21561	2.15686	0.35849
C	-3.62852	-0.67346	-1.72043	C	-5.47570	0.03529	-0.57542
C	-5.55363	-1.12177	0.63303	C	-4.41275	3.22033	0.85830
O	-4.54010	-1.59396	-2.16707	O	-6.81699	0.27105	-0.62150
H	0.82200	1.04654	0.23868	H	-1.30849	-0.36527	1.75259
H	-2.45320	-0.86885	1.54252	H	-0.29010	1.45204	1.41871
H	-0.22691	2.61798	-1.04158	H	-0.68576	0.19494	-0.63212
H	1.71531	2.24275	2.11473	H	-1.15759	-2.61219	2.57641
H	0.20530	3.14868	2.34460	H	-2.38499	-2.60635	1.29043
H	2.01491	-2.96408	1.76695	H	4.60302	0.77973	1.69216
H	-2.24722	-3.35619	1.47957	H	1.20476	3.38793	1.70458
H	-2.16855	3.73484	-0.17631	H	-0.70675	-2.56448	-0.86385
H	0.69192	4.33101	0.52740	H	0.30009	-3.43817	0.98833
H	3.94287	0.06069	2.13083	H	5.05237	-1.26120	0.64453
H	3.36047	-1.41386	2.94557	H	4.61317	-2.82743	1.37238
H	3.55696	-1.37920	1.16309	H	4.92314	-1.42517	2.42741
H	0.01960	-4.38828	1.57462	H	3.66395	3.04622	1.84211
H	-3.40597	1.71632	0.66662	H	-2.55104	1.51282	0.35592
H	-0.51989	0.56732	-2.30116	H	-3.19993	-2.33937	-1.40239
H	-2.08499	-1.15354	-3.13195	H	-5.65570	-1.89291	-1.45648
H	-4.87262	-1.24630	1.48272	H	-3.70812	3.57316	0.09768
H	-5.49839	-1.99613	-0.01875	H	-5.10211	4.02274	1.11503
H	-6.57151	-1.00340	1.00291	H	-3.86305	2.91212	1.75443
H	-4.16682	-2.08355	-2.90712	H	-6.97917	1.15614	-0.26924
C	3.64686	1.69477	-1.09477	C	2.48365	-0.85005	-1.99985
C	3.68304	0.19067	-1.27286	C	3.40066	0.31108	-1.80844
C	2.51671	-0.56023	-1.41504	C	3.23417	1.65337	-1.92290
C	2.57128	-1.95131	-1.49832	C	4.50607	2.24676	-1.61784
C	3.79858	-2.60928	-1.45343	C	5.35130	1.22269	-1.34040
C	4.97323	-1.86411	-1.33062	O	4.69232	0.02525	-1.45435
C	4.91331	-0.47552	-1.24279	O	1.29041	-0.38922	-2.60628

O	2.38179	2.24266	-1.42878	H	2.98968	-1.60055	-2.62668
H	3.89398	1.92527	-0.04879	H	2.28100	-1.32322	-1.02988
H	4.43259	2.14889	-1.71415	H	2.31480	2.14332	-2.19428
H	1.56555	-0.04927	-1.45416	H	4.75350	3.29663	-1.60898
H	1.65097	-2.51782	-1.58298	H	6.39222	1.16444	-1.07072
H	3.84272	-3.69077	-1.51689	H	0.56322	-0.95787	-2.30142
H	5.93450	-2.36556	-1.30407				
H	5.83120	0.09711	-1.14504				
H	2.14721	2.90476	-0.75603				

Lignin–isobutyl acetate-1

63

Energy: -1497.98931539

O	-3.20375	0.46385	0.38795
C	-4.02043	-0.21512	-0.47350
C	-1.77885	0.28050	0.35542
C	-5.38132	-0.26682	-0.10817
C	-3.60795	-0.80234	-1.67025
C	-1.21754	1.45268	1.19190
C	-1.40097	-1.10012	0.87464
O	-5.82946	0.33297	1.04021
C	-6.29850	-0.87258	-0.95973
C	-4.53947	-1.41683	-2.50954
O	-1.74915	2.67710	0.69231
C	0.29178	1.49843	1.11160
O	-1.81215	-1.20196	2.24107
C	-5.41080	-0.28854	2.26757
C	-5.88570	-1.44740	-2.16227
C	0.91275	2.21335	0.08000
C	1.07619	0.78601	2.01270
C	2.29797	2.21045	-0.05941
C	2.46566	0.77526	1.87763
O	2.97687	2.85382	-1.05240
C	3.08982	1.47675	0.85020
C	2.23516	3.65694	-1.96107
O	4.43925	1.49053	0.67242
H	-1.40404	0.39843	-0.66722
H	-2.56663	-0.77261	-1.96248
H	-1.52751	1.30017	2.23094
H	-0.31867	-1.22513	0.77619
H	-1.89908	-1.85988	0.26180
H	-7.33913	-0.88035	-0.65741
H	-4.20287	-1.86402	-3.43774
H	-2.70501	2.55983	0.62599

H	-1.66835	-2.10411	2.54010
H	-4.32279	-0.33312	2.34597
H	-5.81634	0.32852	3.06892
H	-5.83130	-1.29870	2.33807
H	-6.61112	-1.91788	-2.81523
H	0.28982	2.77584	-0.60013
H	0.60603	0.23398	2.81903
H	3.08337	0.22108	2.57518
H	2.97007	4.09711	-2.63345
H	1.69216	4.45358	-1.44112
H	1.52564	3.05629	-2.54281
H	4.82094	0.69367	1.07658
C	4.62977	-2.25489	0.82514
C	4.60027	-3.55044	1.59337
O	5.04421	-1.20626	1.27611
O	4.14909	-2.42073	-0.41215
C	4.11863	-1.29068	-1.33168
C	2.85070	-1.36720	-2.17462
C	1.59458	-1.34740	-1.29649
C	2.85657	-0.19690	-3.16941
H	4.84326	-3.36246	2.63697
H	3.61929	-4.02047	1.50497
H	5.33409	-4.23809	1.16505
H	5.01526	-1.36407	-1.95253
H	4.15933	-0.35968	-0.77193
H	2.87319	-2.30984	-2.73486
H	0.69424	-1.41222	-1.91478
H	1.58827	-2.19028	-0.60169
H	1.54240	-0.42366	-0.71496
H	1.96308	-0.22402	-3.79867
H	3.72994	-0.23125	-3.82757
H	2.87327	0.76028	-2.63950