Supporting information

Integration of acetic acid catalysis with one-pot protic ionic liquid configuration to achieve high-efficient biorefinery of poplar biomass

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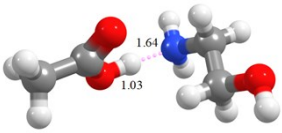
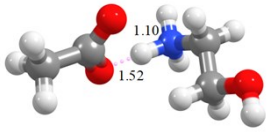
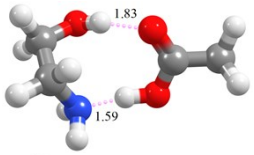
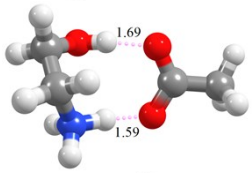
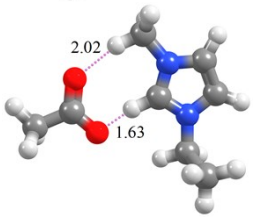
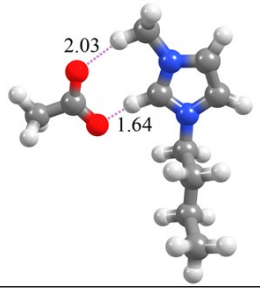
Table S1: Favorability of proton transfer between acetic acid and ethanolamine and interaction energies between molecular species of acid and base and ionic species of anion and cation of IL computed by quantum chemical calculations at B3LYP-GD3BJ/6-311+G(d,p) level of theory.

Type	Chemical structure	$\Delta E_{reaction}$ (kcal/mol)	Interaction energies (kcal/mol)
Neutral species (HAc + EOA) Conformer 1		0.98	-14.98
Ionic Species ([EOA][OAc]) Conformer 1			-132.84
Neutral species (HAc + EOA) Conformer 2		-1.68	-22.73
Ionic Species ([EOA][OAc]) Conformer 2			-139.39
$[C_2C_1Im][OAc]$		-	-101.65
$[C_4C_1Im][OAc]$		-	-100.67

Proton Affinity of acetic acid is 342.33 kcal/mol and ethanolamine is 220.87 kcal/mol; Favorability of proton transfer calculated as: $\Delta E_{reaction} = E_{ionic} - E_{neutral}$

Fig. S1 Synthesis and characterization of ethanolamine acetate ([EOA][OAc]). (A)[EOA][OAc] formation from ethanolamine and acetic acid. (B)NMR spectrum of [EOA][OAc]. (C) DSC and TGA spectrum of [EOA][OAc].

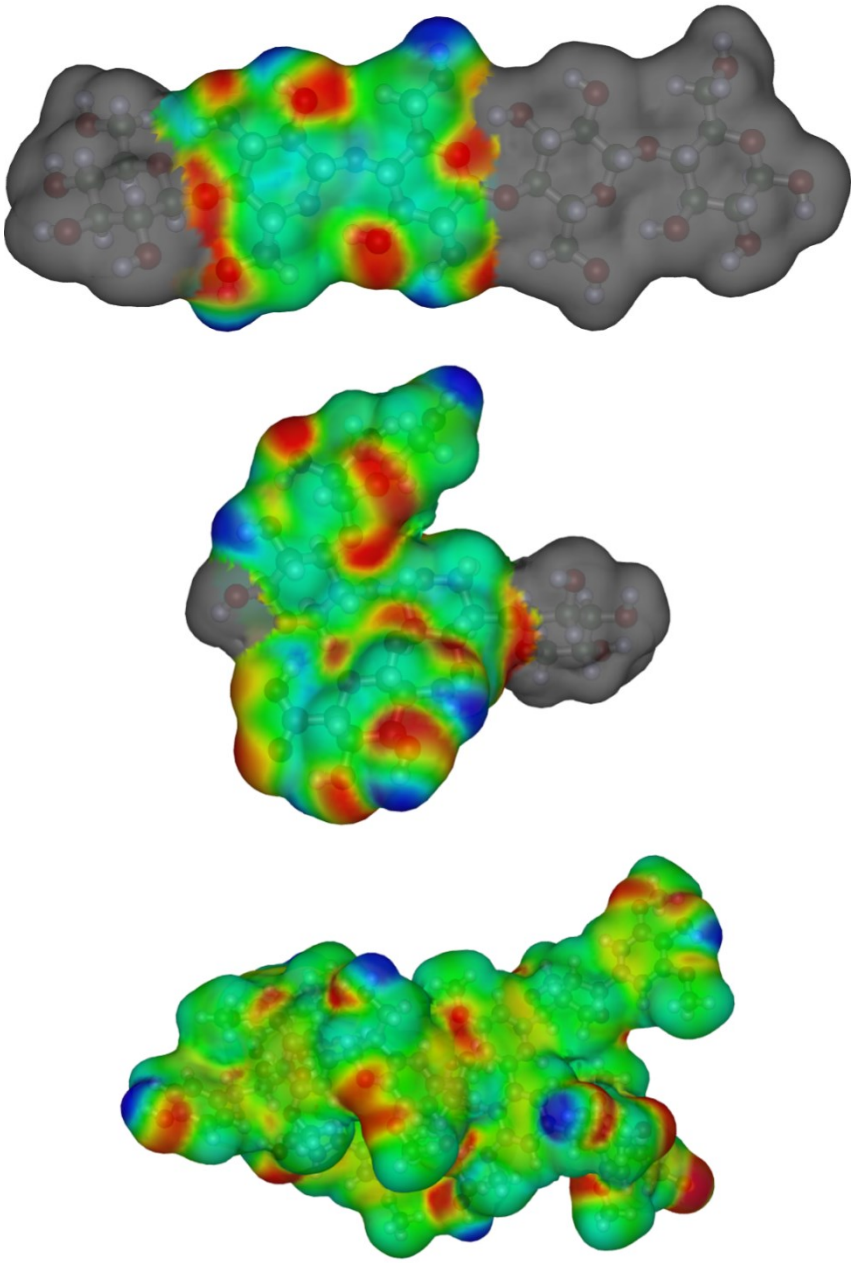


Fig. S2 COSMO-RS charge surface of cellulose (mid-dimer of cellopentoase), hemicellulose, and lignin. Here the extent of screening charge varies from -0.03 e/Å^2 (red: polar region) to +0.03 e/Å^2 (blue: polar region). Red color indicates positive surface screening charges resulting from negative

partial charges within molecule, blue color indicates negative surface charges resulting from positive partial charges, and green color represents neutral charges (non-polar region)

Cartesian coordinates (in Å) of isolated molecules of neutral and ionic species optimized at B3LYP-GD3BJ/6-311+g(d,p) level of theory and basis set.

Acetic acid ([HAc])
Energy: -229.104667

C	-0.51636	0.28023	0.00000
O	-1.05453	1.35820	0.00000
O	-1.21930	-0.88248	0.00000
H	-2.15937	-0.64710	0.00000
C	0.96638	0.02788	0.00000
H	1.49763	0.97677	-0.00001
H	1.24277	-0.55675	-0.88043
H	1.24277	-0.55674	0.88043

Acetate [[OAc]$^-$)
Energy: -228.555355

C	-0.90160	0.00001	-0.01738
C	0.66320	-0.00002	-0.01162
O	-1.44294	-1.13300	-0.00481
O	-1.44290	1.13304	-0.00481
H	1.05862	-0.89809	-0.49569
H	1.05863	0.89790	-0.49598
H	1.00699	0.00017	1.03026

Ethanolamine ([EOA])
Energy: -210.365070

N	-1.65818	0.16355	-0.08231
C	0.77176	0.44119	-0.09415
C	-0.37942	-0.55135	-0.00736
O	1.98995	-0.29308	0.03859
H	-2.42357	-0.47410	-0.26687
H	-1.86621	0.63926	0.78958
H	0.72328	0.96922	-1.05363
H	0.67839	1.18684	0.70901
H	-0.25233	-1.15461	0.90301
H	-0.31468	-1.23474	-0.85806
H	2.73099	0.30781	-0.07783

Ethanolammonium ([EOA]$^+$)
Energy: -210.706082

N	1.21601	0.96131	0.00000
C	-0.44090	-0.92762	0.00000
C	-0.25883	0.58868	0.00000
O	-1.83663	-1.09409	0.00000
H	1.34035	1.97838	0.00000
H	1.69744	0.59279	0.82679
H	1.69744	0.59279	-0.82679
H	0.02972	-1.36656	-0.89213
H	0.02972	-1.36656	0.89213
H	-0.70271	1.03514	0.88929
H	-0.70271	1.03514	-0.88929
H	-2.06889	-2.02940	0.00000

Water
Energy: -76.433974

O	0.00000	-0.00000	0.39017
H	0.00000	0.76357	-0.19509
H	0.00000	-0.76357	-0.19509

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

EthA-Ace_Ethanol-React-Conf1
-439.650221969
-439.477162
Neutral species (HAc + EOA)
Conformer 1
19
Energy: -439.477162
I.E. (kcal/mol) = -14.98

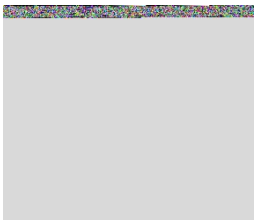
N	-0.93758	1.70667	-0.05322
C	-1.96898	-0.43355	0.55686
C	-1.83834	0.63284	-0.51634
O	-2.87406	-1.42471	0.06422
H	-0.81753	2.39485	-0.79059
H	-1.35393	2.20494	0.72942
H	0.55239	1.14766	0.33383
H	-0.98930	-0.87479	0.76689
H	-2.35329	0.00775	1.48561
H	-2.83264	1.01265	-0.77582
H	-1.39779	0.18965	-1.41062
H	-2.94391	-2.13669	0.71097
C	1.93046	-0.16816	-0.13259
C	3.29881	-0.64996	0.27641
H	4.01562	0.17292	0.22703
H	3.27675	-0.99797	1.31186
H	3.62696	-1.45940	-0.37252
O	1.49172	0.83139	0.62304
O	1.28834	-0.64359	-1.05596

EOA-Ace_React-New-Conf2
-439.656192288
-439.483297
Neutral species (HAc + EOA)
Conformer 2
19
Energy: -439.483297
I.E. (kcal/mol) = -132.84

N	1.28262	1.47664	-0.17978
C	2.44149	-0.71962	-0.02728
C	2.02183	0.54802	0.70360
O	1.37613	-1.37975	-0.69982
H	1.27321	2.40534	0.23287
H	1.75807	1.56955	-1.07395
H	-0.25401	1.11250	-0.36064
H	2.92018	-1.38876	0.69971
H	3.18641	-0.48207	-0.79270
H	2.92273	1.01389	1.11817
H	1.36669	0.29845	1.54284
H	0.56320	-1.32551	-0.16250
C	-1.78464	-0.08296	0.07597
C	-3.28795	-0.14487	0.04149
H	-3.70727	0.69419	0.60136
H	-3.63897	-0.05389	-0.98894
H	-3.64128	-1.08170	0.46681
O	-1.29549	1.02493	-0.44111
O	-1.08960	-0.98292	0.54251

EthA-Ace_Ethanol-Prod-Conf1
-439.649768543
-439.475600
Ionic Species ([EOA][OAc])
Conformer 1
19
Energy: -439.475600
I.E. (kcal/mol) = -22.73

N	0.87741	1.69518	-0.02866
C	1.94571	-0.46675	-0.55182
C	1.73102	0.59730	0.51053
O	2.78864	-1.45184	0.04043
H	0.70322	2.39804	0.68685
H	1.32042	2.17113	-0.81347
H	-0.09582	1.30342	-0.35492
H	0.98430	-0.89694	-0.84900
H	2.42107	-0.03285	-1.44032
H	2.68215	1.01555	0.83912
H	1.19733	0.17672	1.36003
H	2.90292	-2.18297	-0.57814
C	-1.87227	-0.08488	0.10007
C	-3.17068	-0.80705	-0.24166
H	-3.93632	-0.08579	-0.53871
H	-3.00895	-1.47149	-1.09524
H	-3.53565	-1.39426	0.60080
O	-1.40805	0.68595	-0.81335
O	-1.32799	-0.27143	1.20804

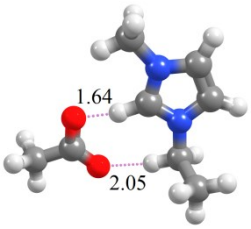


EMIM-Ace-4
Energy: -573.397700765
-573.165549

[C_2C_1Im][OAc]-Conformer 1
26
Energy: -573.165549

EOA-Ace_Prod-New-Conf2
-439.660907913
-439.485982
Ionic Species ([EOA][OAc])
Conformer 2
19
Energy: -439.485982
I.E. (kcal/mol) = -139.39

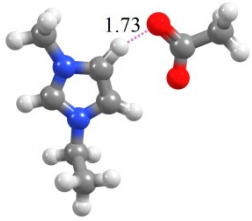
N	1.38494	1.46881	-0.23792
C	2.31757	-0.80324	0.13595
C	1.93528	0.52281	0.78661
O	1.33348	-1.28291	-0.75793
H	1.42181	2.43121	0.09243
H	1.90335	1.42307	-1.11399
H	0.35262	1.23507	-0.42662
H	2.53105	-1.51957	0.93955
H	3.23524	-0.67998	-0.44511
H	2.80210	0.98016	1.26309
H	1.15104	0.39357	1.53196
H	0.44183	-1.27686	-0.32360
C	-1.75123	-0.05674	-0.00223
C	-3.26016	-0.02641	0.19578
H	-3.50464	0.66791	1.00504
H	-3.75272	0.34514	-0.70553
H	-3.65243	-1.01127	0.44738
O	-1.21761	1.00343	-0.45589
O	-1.12494	-1.10660	0.30184



EMIM-Ace-3
Energy: -573.397537013
-573.165323
[C_2C_1Im][OAc]-Conformer 2
26
Energy: -573.165323
I.E. (kcal/mol) = -104.95

I.E. (kcal/mol) =

C	-0.56754	0.30374	0.12323
N	-0.89538	1.59044	-0.04142
C	-2.27234	1.72226	0.02813
C	-2.78215	0.47893	0.23850
N	-1.70319	-0.38744	0.29657
C	0.08055	2.67080	-0.25387
C	-1.74050	-1.84952	0.48431
C	-2.24972	-2.58295	-0.75325
H	-2.76353	2.67490	-0.07180
H	-3.79968	0.14790	0.35467
H	1.07847	2.21608	-0.25504
H	-0.12240	3.15382	-1.21075
H	-0.00828	3.39833	0.55419
H	-2.36762	-2.05438	1.35513
H	-0.71825	-2.14766	0.72005
H	-2.24809	-3.65860	-0.56274
H	-1.60171	-2.38941	-1.61035
H	-3.27012	-2.28760	-1.01104
H	0.46293	-0.17215	0.13032
H	4.92963	-0.14678	-0.16989
O	2.64559	0.93703	-0.17292
C	2.76796	-0.29626	0.01411
C	4.17174	-0.90301	0.03492
O	1.80126	-1.10714	0.19616
H	4.35841	-1.35346	1.01407
H	4.23739	-1.70506	-0.70532
C	-0.67942	-0.43910	-0.02970
N	-1.58044	-1.42900	0.04625
C	-2.85065	-0.91144	-0.14498
C	-2.69928	0.42642	-0.33876
N	-1.34303	0.69815	-0.26559
C	-1.22096	-2.82857	0.28773
C	-0.69501	2.02255	-0.40347
C	-0.95544	2.91370	0.80658
H	-3.73444	-1.52583	-0.13195
H	-3.43092	1.19337	-0.52561
H	-1.56228	-3.44713	-0.54329
H	-0.13584	-2.88548	0.36601
H	-1.67653	-3.17403	1.21673
H	-1.07891	2.47240	-1.32223
H	0.37542	1.81673	-0.51720
H	-0.45253	3.87167	0.65676
H	-0.54700	2.46083	1.71262
H	-2.02043	3.11091	0.96114
H	0.43803	-0.60508	0.07176
H	4.73874	0.58460	-0.22215
O	1.97394	-1.15159	0.20934
C	2.69228	-0.13197	-0.05473
C	4.20653	-0.34395	-0.01533
O	2.24815	1.00489	-0.33976
H	4.49848	-0.72862	0.96568
H	4.48752	-1.10053	-0.75359



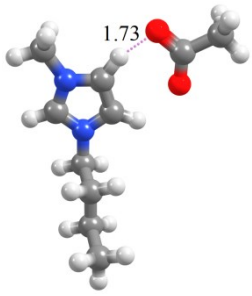
EMIM-Ace-2
Energy: -573.377019020
-573.144813
[C_2C_1Im][OAc]-Conformer 3
26
Energy: -573.144813
I.E. (kcal/mol) = `-90.95`

C	-2.22225	0.98490	-0.14701
N	-1.06913	1.64772	0.01859
C	-0.01319	0.75635	-0.04150

BMIM-Ace
Energy: -652.046858844
-651.755225
[C_4C_1Im][OAc]-Conformer 1
32
Energy: -651.755225
I.E. (kcal/mol) = `-104.08`

C	-0.54677	0.91820	-0.20081
N	-1.14163	2.05352	0.18308

C	-0.56261	-0.47328	-0.24839	C	-0.22239	3.08824	0.13431
N	-1.93649	-0.31356	-0.31379	C	0.95588	2.55544	-0.28788
C	-0.92939	3.09037	0.21758	N	0.72986	1.20487	-0.49332
C	-2.91939	-1.39399	-0.49082	C	-2.55486	2.15248	0.57978
C	-3.03705	-2.28169	0.74563	C	1.71055	0.18773	-0.91148
H	1.07413	0.99388	0.06041	C	2.65710	-0.21725	0.22034
H	-0.02711	-1.40527	-0.34725	H	-0.48240	4.09953	0.39587
H	-0.36501	3.51901	-0.61040	H	1.91319	3.01585	-0.46103
H	-1.91703	3.54747	0.26450	H	-3.08065	2.80317	-0.12059
H	-0.39469	3.27552	1.14869	H	-2.97419	1.13953	0.55580
H	-2.60668	-1.97417	-1.36103	H	-2.61467	2.56758	1.58674
H	-3.87521	-0.92573	-0.73298	H	2.26254	0.58927	-1.76534
H	-3.76724	-3.07242	0.55830	H	1.12952	-0.67129	-1.25084
H	-3.36747	-1.70680	1.61374	C	3.64380	-1.30354	-0.22299
H	-2.08157	-2.75129	0.98583	H	2.05902	-0.58212	1.06186
H	-3.20819	1.41769	-0.15032	H	3.20898	0.66103	0.57652
H	4.99337	-0.48436	-0.88022	H	-0.98600	-0.12411	-0.27294
O	2.79131	0.81401	0.16039	H	-2.55002	-3.89578	0.54266
C	3.03364	-0.42389	0.01464	O	-3.24669	-0.85932	0.37305
C	4.51402	-0.82842	0.04202	C	-2.54558	-1.81573	-0.03352
O	2.17734	-1.32729	-0.16362	C	-3.15768	-3.21735	-0.06267
H	5.02471	-0.33752	0.87413	O	-1.33975	-1.71916	-0.43462
H	4.62537	-1.91107	0.11590	H	-4.18167	-3.20679	0.31087
				H	-3.14322	-3.60065	-1.08692
				H	4.22859	-0.94033	-1.07701
				H	3.08107	-2.17257	-0.58107
				C	4.59225	-1.73510	0.89890
				H	5.19469	-0.89426	1.25673
				H	5.27880	-2.51344	0.55662
				H	4.03658	-2.13431	1.75241



BMIM-Ace-2
Energy: -652.026212225
-651.734571
[C_4C_1Im][OAc]-Conformer 1
32
Energy: -651.734571
I.E. (kcal/mol) = -90.05

C	-0.76361	2.10503	-0.18268
N	0.53371	2.20151	0.14078
C	1.13635	0.96464	-0.00082
C	0.16108	0.11047	-0.42024
N	-1.01338	0.83554	-0.53087
C	1.22426	3.41971	0.56387
C	-2.32495	0.29107	-0.91105
C	-2.97325	-0.52290	0.21160
H	2.20781	0.71349	0.19055
H	0.27842	-0.94112	-0.63339
H	2.00367	3.66559	-0.15714
H	0.50922	4.23916	0.62537
H	1.67916	3.25544	1.54025
H	-2.17197	-0.32542	-1.79949
H	-2.95859	1.13276	-1.20005
C	-4.32482	-1.10986	-0.21195
H	-3.10323	0.11814	1.09103
H	-2.29446	-1.32895	0.50806
H	-1.48191	2.90710	-0.17034
H	5.38723	-2.03239	-0.58015
O	3.68375	-0.18205	0.34487
C	3.41603	-1.38114	0.02423
C	4.58885	-2.36971	0.08729
O	2.29206	-1.81606	-0.33413
H	5.00233	-2.38351	1.09989
H	4.27462	-3.37519	-0.19548
H	-4.18231	-1.74706	-1.09247
H	-4.99414	-0.29892	-0.52465
C	-4.99197	-1.92105	0.90215
H	-4.36232	-2.76010	1.21159
H	-5.95046	-2.32850	0.57169
H	-5.17964	-1.30255	1.78499

Cartesian coordinates (in Å) of cellulose, hemicellulose, and lignin optimized at B3LYP-GD3BJ/6-311+g(d,p) level of theory and basis set.

Cellulose
Energy:

O	-3.97005	-0.78334	-0.38733
C	-3.45387	0.42223	0.20636
C	-6.31021	-0.17228	-0.00392
C	-5.22365	-1.25842	0.13154
O	-6.67309	2.25136	0.13739
O	-3.94836	2.73719	0.53099
C	-5.49482	-2.52089	-0.69081
O	-2.24280	0.71044	-0.39844
C	-4.43229	1.55367	-0.07879
C	-5.80185	1.18948	0.48500
O	-6.78000	-3.01717	-0.37297
O	1.30602	0.68012	0.41922
C	1.75025	-0.47701	-0.30127
C	-1.04432	0.17430	0.17742
C	0.06347	1.21699	-0.03754
O	-1.53561	-2.20862	-0.19705
O	1.13829	-2.73048	-0.83878
C	-0.16717	2.50971	0.72388
O	2.97423	-0.85889	0.21795
C	0.74242	-1.60237	-0.08026
C	-0.65391	-1.14181	-0.50361
O	0.87672	3.40035	0.34376
O	6.53377	-0.80660	-0.49354
C	6.94010	0.41264	0.14493
C	4.15971	-0.31359	-0.37446
C	5.27922	-1.31421	-0.04310
O	3.67176	2.11332	-0.29210
O	6.27362	2.69683	0.45365
C	5.08583	-2.66428	-0.71066

O	8.17815	0.76621	-0.35917
C	5.92935	1.49669	-0.21284
C	4.50972	1.07363	0.18409
O	6.10420	-3.52414	-0.20797
O	11.72663	0.81078	0.46104
C	12.11943	-0.41792	-0.11227
C	9.34772	0.27661	0.31019
C	10.47568	1.27493	-0.03838
O	8.88469	-2.16207	0.39551
O	11.55421	-2.74297	-0.18350
C	10.21654	2.65126	0.55274
O	13.40870	-0.68539	0.35547
C	11.12803	-1.48914	0.33119
C	9.71824	-1.14621	-0.13924
O	11.07428	3.58217	-0.09590
O	-12.70242	0.16385	-0.48097
O	-9.07237	0.71096	-0.13371
C	-8.66221	-0.62661	0.23453
C	-11.43998	0.27730	0.15525
C	-10.34106	0.79962	-0.78607
O	-11.97312	-1.60891	1.60811
O	-9.33615	-2.52203	1.55793
C	-10.50712	2.27233	-1.15246
O	-7.42257	-0.51431	0.83855
C	-9.67007	-1.18754	1.23921
C	-11.06891	-1.12452	0.62511
O	-11.78366	2.42582	-1.77621
H	-3.33477	0.27470	1.29282
H	-6.62723	-0.08508	-1.05057
H	-5.12984	-1.51456	1.19688
H	-7.58467	1.94741	0.28971
H	-4.68416	3.36675	0.50296
H	-5.40648	-2.24986	-1.75517
H	-4.70351	-3.25146	-0.46721
H	-4.50183	1.66504	-1.17149
H	-5.70269	1.11556	1.58150
H	-6.88043	-3.89046	-0.77035
H	1.82827	-0.23481	-1.37475
H	-1.18928	-0.00015	1.25287
H	0.12514	1.45311	-1.11184
H	-2.43329	-1.92758	-0.45201
H	0.38376	-3.33771	-0.81156
H	-1.16083	2.89971	0.47125
H	-0.13797	2.29220	1.80269
H	0.73365	-1.82757	0.99728
H	-0.63532	-0.95468	-1.59064

H	0.79192	4.21055	0.86073
H	6.97953	0.25976	1.23704
H	4.03288	-0.23961	-1.46419
H	5.30149	-1.46586	1.04807
H	2.79438	2.04916	0.12504
H	5.50841	3.27817	0.32347
H	4.07863	-3.03431	-0.48362
H	5.17365	-2.53047	-1.79960
H	5.96618	1.62297	-1.30604
H	4.46740	1.00641	1.28320
H	6.07338	-4.35379	-0.69939
H	12.11046	-0.33117	-1.21687
H	9.17860	0.27094	1.39699
H	10.51613	1.37467	-1.13511
H	8.01278	-2.13244	-0.03669
H	10.82280	-3.35323	-0.00425
H	9.15779	2.90015	0.40395
H	10.41738	2.59910	1.63451
H	13.51244	-1.64736	0.30479
H	11.13890	-1.49683	1.43258
H	9.70093	-1.16178	-1.24062
H	10.92197	4.44671	0.30469
H	-12.86625	1.00809	-0.93266
H	-8.61380	-1.25481	-0.66703
H	-11.49184	0.94289	1.03356
H	-10.34712	0.19207	-1.70468
H	-12.85857	-1.54276	1.22249
H	-10.10792	-2.87468	2.02581
H	-10.43587	2.87163	-0.23322
H	-9.69219	2.57438	-1.82353
H	-9.63725	-0.53944	2.12951
H	-11.08261	-1.78384	-0.25917
H	-11.94268	3.36520	-1.92967

Hemicellulose
Energy:

C	2.75287	-0.05346	-0.49459
H	2.97542	-0.41632	-1.50345
C	2.10152	1.33311	-0.55179
H	2.72693	2.04501	-1.09537
H	1.96366	1.71298	0.47359
O	0.86659	1.27844	-1.24996
C	-0.11194	0.50515	-0.59551
H	-0.35924	0.93055	0.39087
C	0.39200	-0.94624	-0.43501
H	0.41148	-1.40702	-1.43044
C	1.79966	-1.03065	0.18905
H	1.71255	-0.73047	1.24414
O	-1.21820	0.59550	-1.46073
O	-0.54847	-1.63248	0.41791
C	-0.67584	-3.01037	0.31393
O	2.30272	-2.34688	0.08159
H	2.02669	-2.82463	0.88376
O	3.95883	0.00344	0.27804
C	-2.47786	0.20270	-0.93242
H	-2.35570	-0.36102	-0.00576
C	-3.11444	-0.71508	-1.97107
H	-2.49368	-1.59840	-2.11796
H	-3.22761	-0.19517	-2.93352
O	-4.38022	-1.17675	-1.49363
C	-5.29526	-0.10021	-1.32214
H	-5.42859	0.39794	-2.29929
C	-4.78685	0.92330	-0.29807
H	-4.76358	0.42816	0.68296
C	-3.37088	1.41558	-0.63960
H	-3.42789	2.04306	-1.54198
O	-6.49751	-0.59667	-0.82645
O	-5.68245	2.03530	-0.28353
O	-2.73335	2.10598	0.42235
H	-6.56301	1.68741	-0.08036
C	5.13040	0.23273	-0.44665
H	5.02859	1.12234	-1.09745
C	6.24947	0.46394	0.57141
H	6.29895	-0.42970	1.21075
O	5.42060	-0.90196	-1.24466
C	7.57323	0.63625	-0.16307
H	7.50991	1.55092	-0.77652
C	6.60998	-0.73127	-2.01429
H	6.52770	0.13643	-2.68795

H	6.72077	-1.62957	-2.62425
C	7.82262	-0.54506	-1.09766
H	7.94205	-1.44983	-0.48076
O	6.03557	1.63891	1.34254
H	5.19216	1.51835	1.80068
O	8.67529	0.72050	0.73046
H	8.47163	1.43140	1.35461
O	8.96315	-0.32772	-1.90946
H	9.67281	-0.05886	-1.30830
H	-6.88702	-1.18561	-1.48791
O	-2.03025	-3.28378	-0.11965
C	-0.48393	-3.66348	1.68917
H	0.03330	-3.42285	-0.41691
C	-0.70920	-5.16362	1.57020
C	-2.31349	-4.67062	-0.28445
C	-2.09952	-5.46580	1.03237
H	-1.66490	-5.11485	-1.05604
C	-3.75932	-4.88746	-0.73525
O	-2.16848	-6.85896	0.83142
H	-2.84443	-5.12365	1.76956
H	-2.97760	-7.02239	0.31083
O	-4.17452	-6.02836	-0.85076
O	-4.54907	-3.84809	-0.95747
H	-4.12981	-2.97304	-0.82496
O	-0.49609	-5.71944	2.85920
H	0.02261	-5.57366	0.85405
H	-1.22668	-3.22435	2.36962
O	0.83163	-3.40727	2.17120
H	-0.66673	-6.66975	2.78721
H	0.99352	-4.06192	2.86846
C	-3.26811	3.35624	0.87623
C	-1.56744	4.87713	1.14682
C	-2.58312	5.58904	0.24134
O	-2.33571	3.86267	1.80014
C	-0.94178	5.77330	2.20154
H	-0.78011	4.43462	0.51820
C	-3.44118	4.42043	-0.24749
H	-4.21143	3.18422	1.40376
O	-1.99536	6.29668	-0.82739
H	-3.22527	6.23741	0.86002
O	-4.78432	4.81503	-0.42791
H	-2.98826	4.05660	-1.18156
H	-5.29251	4.00418	-0.59112
H	-1.35198	6.89573	-0.41818
H	-1.73657	6.15058	2.86090
O	-0.29818	6.83414	1.48962

H	-0.22624	5.20791	2.81499
H	0.00422	7.49329	2.12558

Lignin
Energy:

C	-12.98341	-6.54505	1.94275
C	-12.05938	-6.01483	0.89111
C	-11.46119	-4.81724	0.95605
C	-10.51204	-4.23175	-0.00163
C	-10.05280	-2.92713	0.23404
C	-9.14861	-2.31105	-0.63812
O	-8.64783	-1.05588	-0.46043
C	-9.17097	-0.27535	0.61017
C	-8.70439	-2.99617	-1.78680
C	-9.16579	-4.31100	-2.02050
O	-8.68026	-4.89903	-3.15332
C	-9.12001	-6.21181	-3.46485
C	-10.05542	-4.92244	-1.13577
O	-14.18941	-6.97432	1.31090
O	-7.75900	-2.48801	-2.63609
C	0.30844	1.26665	-3.50983
C	1.10097	2.29477	-2.98886
C	2.27950	2.62462	-3.65462
C	2.67638	1.94260	-4.79538
C	1.89794	0.90859	-5.33514
C	0.69970	0.59920	-4.68390
O	3.86616	2.36351	-5.31763
O	2.37976	0.28339	-6.44736
C	-0.96827	0.83515	-2.79795
C	-0.72881	-0.32778	-1.80863
O	-1.42143	2.01840	-2.11697
C	0.12692	-1.47524	-2.35557
O	-0.38382	-2.04445	-3.54937
O	-1.96761	-0.87825	-1.26114
C	-5.50878	-1.04571	-3.48818
C	-4.70203	-2.18126	-3.36510
C	-3.51094	-2.12605	-2.64085
C	-3.10298	-0.91856	-2.03638
C	-3.93469	0.20761	-2.11694
C	-5.12070	0.13684	-2.86296
C	-4.57936	2.84641	0.48271
C	-4.69518	1.76582	-0.37913
C	-3.66878	1.40377	-1.27528
C	-2.48142	2.14535	-1.27357

C	-2.34946	3.24086	-0.37193
C	-3.39024	3.58986	0.48303
O	-2.67761	-3.20473	-2.46816
C	-3.17174	-4.50187	-2.81433
C	-6.79852	-1.10111	-4.28899
C	-8.05431	-1.31365	-3.41939
C	-9.30271	-1.49127	-4.29087
O	-10.52351	-1.35968	-3.57656
C	-5.74343	3.22383	1.35900
C	-6.69616	4.30009	0.77598
C	-7.86823	3.73304	-0.01655
O	-8.80180	3.30831	0.98278
O	-1.15385	3.89853	-0.42888
C	-0.95306	4.98837	0.45709
C	5.67489	2.74686	-3.70788
C	6.44279	3.58751	-2.90482
C	7.49969	3.07094	-2.16370
C	7.86467	1.71712	-2.24512
C	7.11367	0.88787	-3.11342
C	6.01642	1.39827	-3.81140
O	8.99110	1.33191	-1.56918
O	7.53298	-0.40695	-3.24676
C	4.44552	3.32069	-4.38585
C	3.31038	3.69198	-3.37030
C	2.76218	5.10282	-3.58037
O	3.79649	6.02620	-3.23533
C	1.63333	-0.81374	-6.95509
C	6.60534	-1.39442	-3.69805
C	9.54350	0.93898	4.46630
C	8.13388	1.51268	4.62350
C	8.03631	3.01344	4.26420
C	8.11354	3.34686	2.78103
C	6.94918	3.64629	2.07148
C	7.00970	3.89406	0.70501
O	5.84183	4.19707	0.03512
C	5.67434	5.59926	-0.20373
C	8.21969	3.79367	-0.00651
C	9.40899	3.57681	0.71818
O	10.66601	3.48653	0.20425
C	10.99201	4.00934	-1.08822
C	9.33523	3.37794	2.10702
O	9.70510	-0.30156	5.12623
O	8.23798	3.96704	-1.38198
C	1.91632	-3.64154	6.58777
C	2.04502	-2.89657	5.25185
C	2.18717	-1.34190	5.42676

C	3.52863	-0.76819	5.00884
C	4.64761	-1.02110	5.80971
C	5.89876	-0.53669	5.42263
O	7.06194	-0.79908	6.09842
C	7.00137	-1.50818	7.32822
C	6.04423	0.25487	4.26791
C	4.91160	0.47724	3.46523
O	5.13412	1.18695	2.32078
C	4.04192	1.43689	1.43692
C	3.65980	-0.02741	3.83614
O	3.08228	-3.53373	7.40068
O	7.27182	0.67647	3.80948
O	6.82607	3.46865	4.86341
C	-1.97321	-6.56987	0.35845
C	-1.11881	-5.49044	1.01511
C	-1.67233	-5.10965	2.41289
C	-0.96075	-3.92712	3.04625
C	-1.40036	-2.62161	2.75482
C	-0.74689	-1.49723	3.27325
O	-1.09386	-0.20268	3.05407
C	-2.24059	0.04854	2.24298
C	0.37156	-1.72758	4.09125
O	1.11686	-0.73270	4.65180
C	0.81266	-3.00973	4.38178
C	0.14865	-4.12515	3.87326
O	-1.46596	-6.79872	-0.95934
O	-7.03706	0.11537	-4.99613
C	7.59950	-3.31712	-0.19707
C	6.32382	-4.09936	-0.23005
C	5.14537	-3.54206	0.08855
C	3.84865	-4.20529	0.27075
C	3.70514	-5.60083	0.38354
C	2.47354	-6.18632	0.64160
O	2.40432	-7.55083	0.81771
C	1.79750	-8.25655	-0.26800
C	1.32350	-5.38152	0.81052
O	0.18656	-6.04920	1.18154
C	1.44458	-3.99776	0.67079
C	2.69024	-3.42740	0.40668
O	8.29987	-3.41409	-1.44040
O	-3.06786	-4.86200	2.23093
C	-6.46099	4.35893	3.19991
C	-7.36128	4.88660	2.05072
C	-8.81104	4.31567	2.00988
C	-9.89484	5.36212	1.76596
C	-9.95407	6.51813	2.54554

C	-10.97042	7.46331	2.36839
O	-10.92619	8.60637	3.12641
C	-12.08241	8.89559	3.91883
C	-11.94492	7.25290	1.38486
C	-11.89645	6.07388	0.61949
C	-10.88802	5.13230	0.80467
O	-5.30427	3.78910	2.59270
O	-12.92360	8.17802	1.15838
O	-12.91522	5.98655	-0.30102
C	-12.94222	4.85966	-1.16673
C	8.46854	0.13525	0.50229
C	9.06972	0.05722	-0.89476
C	10.55861	-0.33130	-0.83410
C	11.36130	-0.08721	-2.09274
C	10.93269	-0.55386	-3.34699
C	11.71814	-0.38602	-4.47981
C	12.96109	0.25328	-4.38119
C	13.40323	0.72479	-3.14324
C	12.60254	0.55015	-2.01284
O	7.05604	0.19285	0.38581
O	13.69210	0.38720	-5.52862
O	10.53745	-1.74249	-0.50350
H	-12.49894	-7.39260	2.45907
H	-13.17372	-5.76980	2.70204
H	-11.89138	-6.68680	0.05179
H	-11.69086	-4.18200	1.81186
H	-10.40354	-2.40063	1.11296
H	-8.71415	0.71109	0.53491
H	-10.25922	-0.16842	0.53040
H	-8.92146	-0.71554	1.58354
H	-8.62556	-6.47795	-4.40025
H	-8.83279	-6.93144	-2.68766
H	-10.20732	-6.25416	-3.60734
H	-10.39900	-5.93035	-1.32493
H	-14.70530	-7.46356	1.96471
H	0.78155	2.82698	-2.10068
H	0.08330	-0.21377	-5.04556
H	-1.70566	0.52589	-3.54471
H	-0.21524	0.08966	-0.93457
H	0.21696	-2.22865	-1.56234
H	1.12965	-1.09916	-2.57281
H	-1.11243	-2.63020	-3.28257
H	-5.01903	-3.10637	-3.83103
H	-5.75033	1.01609	-2.94548
H	-5.58947	1.15019	-0.35865
H	-3.29146	4.41502	1.17617

H	-2.44466	-5.21313	-2.42002
H	-4.14843	-4.67592	-2.34996
H	-3.26288	-4.61692	-3.90139
H	-6.73659	-1.94991	-4.98955
H	-8.19051	-0.44965	-2.76140
H	-9.30154	-0.70087	-5.04498
H	-9.23259	-2.46174	-4.80607
H	-10.60196	-2.12204	-2.98818
H	-6.34327	2.31961	1.56036
H	-6.12238	5.04209	0.21478
H	-7.61294	2.86091	-0.62547
H	-8.31542	4.49633	-0.66882
H	0.05431	5.35557	0.25574
H	-1.67447	5.79569	0.27696
H	-1.02096	4.67657	1.50696
H	6.20048	4.63956	-2.81061
H	5.44239	0.75716	-4.46750
H	4.72797	4.19750	-4.97719
H	3.69568	3.63242	-2.34706
H	1.87292	5.24857	-2.94939
H	2.45147	5.22679	-4.62862
H	3.51078	6.91278	-3.48872
H	2.21558	-1.21198	-7.78733
H	1.49241	-1.59337	-6.19639
H	0.64908	-0.49543	-7.32322
H	7.04303	-2.35152	-3.41168
H	5.63653	-1.27729	-3.20092
H	6.46498	-1.34168	-4.78463
H	9.76939	0.85519	3.39273
H	10.27079	1.63102	4.90687
H	7.83442	1.43120	5.67140
H	8.89794	3.48465	4.76796
H	5.98472	3.64972	2.56095
H	5.50683	6.13551	0.74000
H	6.55407	6.02073	-0.70279
H	4.80909	5.71293	-0.85882
H	12.08351	4.05693	-1.10457
H	10.63760	3.35214	-1.88217
H	10.58121	5.01322	-1.22846
H	10.27287	3.20736	2.62675
H	8.86656	-0.77794	5.03306
H	1.66505	-4.69537	6.39912
H	1.09945	-3.21143	7.17602
H	2.92158	-3.29250	4.72069
H	2.00082	-1.07810	6.47500
H	4.53174	-1.61219	6.71041

H	8.02934	-1.55320	7.68933
H	6.37466	-0.98565	8.05987
H	6.61781	-2.52630	7.18769
H	4.45398	2.04329	0.63105
H	3.63698	0.50136	1.03413
H	3.24349	1.99021	1.94409
H	2.78219	0.16000	3.23386
H	3.79706	-3.99588	6.94191
H	6.71027	4.39635	4.61724
H	-1.90947	-7.48268	0.96722
H	-3.01549	-6.23554	0.33281
H	-1.09533	-4.61165	0.36194
H	-1.51949	-5.99415	3.05172
H	-2.25773	-2.49806	2.10409
H	-2.35357	1.13202	2.20886
H	-2.11108	-0.33636	1.22537
H	-3.14227	-0.39252	2.68648
H	0.49775	-5.13140	4.08484
H	-1.87050	-7.60846	-1.29476
H	-6.23087	0.32970	-5.48388
H	7.36358	-2.27518	0.05040
H	8.23334	-3.71331	0.61592
H	6.40557	-5.15965	-0.46598
H	5.13846	-2.46662	0.26999
H	4.56366	-6.25987	0.30714
H	2.41199	-8.17829	-1.17516
H	1.74612	-9.30425	0.03840
H	0.79122	-7.88177	-0.48036
H	0.58815	-3.35345	0.82712
H	2.76694	-2.34585	0.33339
H	9.14484	-2.95171	-1.29915
H	-3.39926	-4.48057	3.05493
H	-6.12472	5.14280	3.88393
H	-6.99383	3.59449	3.78757
H	-7.37763	5.97721	2.03395
H	-9.04266	3.78143	2.94017
H	-9.21776	6.72422	3.31625
H	-11.82893	9.78132	4.50469
H	-12.95774	9.10169	3.29806
H	-12.30526	8.06474	4.60070
H	-10.85204	4.22071	0.22281
H	-13.47440	7.82390	0.44228
H	-13.80462	4.99887	-1.81973
H	-12.03065	4.80157	-1.77318
H	-13.05955	3.92644	-0.60325
H	8.79299	-0.75499	1.06180

H	8.86486	1.01736	1.01417
H	8.54139	-0.69966	-1.46999
H	11.03573	0.22177	-0.01156
H	9.96206	-1.02912	-3.44005
H	11.38637	-0.73692	-5.45132
H	14.36658	1.22418	-3.06077
H	12.95182	0.92326	-1.05308
H	6.68898	0.53641	1.21693
H	14.51403	0.85266	-5.32537
H	11.45051	-2.05820	-0.53075