Techno-economic and environmental evaluation of producing chemicals and drop-in aviation biofuels via aqueous phase processing

Supplementary material

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Supplementary Information*

* Refer to the manuscript for details and references.

Table S1. Net aggregated resource requirements to produce 1 MJ of hydrogen in the 12 hydrogen pathways described in the text, and the lifecycle emissions from its production. Negative values are due to co-product displacement. Simulation year: 2015.

Resources		Hydrogen pathways											
		1	2	3	4	5	6	7	8	9	10	11	12
Crude oil	J	4.66E+03	1.57E+04	6.53E+04	2.11E+04	UOP LLC Confidential	2.02E+04	1.21E+06	4.13E+04	7.26E+03	9.00E+02	2.16E+02	4.41E+04
Natural gas	J	1.49E+06	7.20E+04	6.59E+05	2.02E+06		1.03E+04	1.52E+05	1.48E+05	1.40E+05	1.78E+04	4.57E+03	9.32E+05
Coal	J	3.13E+04	1.35E+06	1.51E+05	1.33E+05		1.97E+06	3.72E+04	5.04E+04	2.23E+05	2.96E+04	8.82E+03	1.80E+06
Pet coke	J	8.11E+00	2.73E+01	1.14E+02	3.67E+01		3.51E+01	2.11E+03	7.19E+01	1.26E+01	1.57E+00	3.77E-01	7.68E+01
Bitumen	J	7.03E+02	2.37E+03	9.85E+03	3.19E+03		3.04E+03	1.83E+05	6.23E+03	1.10E+03	1.36E+02	3.26E+01	6.66E+03
Shale oil	J	1.07E+03	3.60E+03	1.50E+04	4.84E+03		4.62E+03	2.78E+05	9.46E+03	1.66E+03	2.06E+02	4.96E+01	1.01E+04
Nuclear energy	J	5.53E+03	2.38E+04	1.67E+04	2.35E+04		2.42E+03	6.68E+03	8.90E+03	1.04E+06	1.20E+06	1.56E+03	3.17E+05
Renewable energy													
Hydroelectric	J	1.93E+03	8.31E+03	5.82E+03	8.18E+03		8.44E+02	2.28E+03	3.10E+03	1.37E+04	1.82E+03	5.42E+02	1.11E+05
Geothermal	J	1.21E+02	5.20E+02	3.64E+02	5.12E+02		5.28E+01	1.46E+02	1.94E+02	8.58E+02	1.14E+02	3.39E+01	6.92E+03
Solar	J	1.61E+02	6.94E+02	4.87E+02	6.84E+02		7.06E+01	1.95E+02	2.59E+02	1.15E+03	1.52E+02	1.39E+06	9.25E+03
Wind	J	1.37E+03	5.92E+03	4.15E+03	5.83E+03		6.02E+02	1.66E+03	2.21E+03	9.77E+03	1.30E+03	3.86E+02	7.88E+04
Unspecified	J	1.41E+02	6.09E+02	4.27E+02	6.00E+02		6.19E+01	1.71E+02	2.27E+02	1.01E+03	1.33E+02	3.98E+01	8.11E+03
Biomass													
Forest residues	J	3.75E+02	1.62E+03	9.24E+02	1.59E+03		1.64E+02	4.53E+02	6.04E+02	2.67E+03	3.54E+02	1.06E+02	2.15E+04
	g	1.87E-02	8.04E-02	4.59E-02	7.92E-02		8.17E-03	2.25E-02	3.00E-02	1.33E-01	1.76E-02	5.25E-03	1.07E+00
Switchgrass	J	-	-	-	-		-	-	2.38E+06	-	-	-	-
	g								1.42E+02				
Corn	J	-	-	1.99E+06	-		-	-	-	-	-	-	-
	g			1.25E+02									
Soybean	J	-	-	-2.44E+05	-		-	-	-	-	-	-	-
	g			-1.32E+01									
Sugarcane	J	-	-	4.01E+01	-		-	-	-	-	-	-	-
	g			1.10E-02									
Water	cm^3	1.50E+02	1.42E+02	2.44E+03	1.66E+02		2.55E+02	4.21E+02	2.10E+02	3.46E+02	3.53E+02	9.18E+00	2.09E+03
Lifecycle emissions	gCO_2e	92.4	41.7	18.2	135.2	0.11	178.0	182.5	29.8	31.4	4.1	1.2	239.0

Table S2. Chemical Engineering Plant Cost Index (CEPCI)

	2010	2011	2012	2013	2014	2015
Jan	532.9	564.8	593.6	571.2	572.8	573.1
Feb	539.1	574.6	596.3	569.9	574.9	570.5
Mar	541.8	575.9	596.1	568.3	571.5	568.6
Apr	555.3	582.3	595.9	569.4	573.6	562.9
May	558.2	581.9	593.8	566.5	574.3	560.5
Jun	556.4	588.9	585.6	564.8	576.2	558.3
Jul	550.7	593.2	582.2	564	576.9	556.3
Aug	549.5	596.1	576.6	564.8	578.7	553.9
Sep	552.5	596	577.4	567.3	580.1	550.3
Oct	556.3	594	575.4	567.5	579.7	547.2
Nov	556.7	590.8	570.6	566.6	578.4	542.8
Dec	560.3	590.1	571.9	567.5	575.7	537.1
Ave	550.8	585.7	584.6	567.3	576.1	556.8

Table S3. Acetone prices that this study relies on, $/t.

	2010	2011	2012	2013	2014	2015
Jan	1257	1411	1780	1618	1786	1389
Feb	1301	1543	1548	1755	1830	1213
Mar	1301	1587	1748	1667	1720	1146
Apr	1345	1830	1691	1459	1676	1036
May	1213	1764	1519	1457	1609	970
Jun	1146	1609	1433	1565	1504	970
Jul	1124	1499	1204	1565	1552	992
Aug	1014	1477	1232	1653	1609	926
Sep	1014	1411	1261	1653	1609	794
Oct	1080	1279	1290	1587	1786	750
Nov	1036	1124	1407	1521	1653	794
Dec	1080	1124	1506	1631	1587	794
Ave	1159	1472	1468	1594	1660	981

Table S4. Electricity prices that this study relies on, ¢/kWh.

	2010	2011	2012	2013	2014	2015
Jan	6.5	6.53	6.44	6.5	6.98	6.63
Feb	6.55	6.63	6.45	6.66	7.12	6.9
Mar	6.53	6.53	6.46	6.64	6.99	6.81
Apr	6.55	6.53	6.38	6.58	6.77	6.6
May	6.64	6.68	6.53	6.75	6.83	6.71
Jun	6.96	7.14	6.89	7.25	7.39	7.1
Jul	7.23	7.31	7.13	7.45	7.62	7.44
Aug	7.22	7.4	7.08	7.37	7.51	7.32
Sep	7	7.15	6.97	7.22	7.37	7.18
Oct	6.8	6.77	6.62	6.87	7.07	6.88
Nov	6.56	6.53	6.5	6.65	6.75	6.62
Dec	6.6	6.51	6.52	6.66	6.7	6.42
Ave	6.76	6.81	6.66	6.88	7.09	6.88

Table S5. Hydrochloric acid prices that this study relies on, $/t.

	2010	2011	2012	2013	2014	2015
Jan	151	130	265	232	215	224
Feb	142	130	265	212	207	214
Mar	140	127	265	211	171	153
Apr	140	113	265	208	160	107
May	140	113	264	208	135	98
Jun	140	113	264	208	150	94
Jul	140	113	263	206	176	91
Aug	140	143	254	226	187	80
Sep	137	153	255	226	220	80
Oct	136	170	264	226	242	77
Nov	131	265	264	226	251	61
Dec	130	265	256	215	245	61
Ave	139	153	262	217	197	112

Table S6. Ruthenium prices, $/kg

	2010	2011	2012	2013	2014	2015
Jan	5433	5787	3567	2755	1866	1810
Feb	5892	5787	4088	2733	2045	1800
Mar	6109	5787	4070	2733	2185	1774
Apr	6720	5787	3714	2733	2315	1608
May	7831	5787	3697	2733	2315	1608
Jun	7745	5787	3697	2733	2254	1571
Jul	6766	5787	3697	2699	2189	1426
Aug	6350	5647	3613	2479	2180	1350
Sep	6079	5393	3537	2013	2046	1350
Oct	5718	4731	3537	1833	1894	1350
Nov	5626	4114	3171	1833	1865	1350
Dec	5773	3601	2894	1833	1865	1350
Ave	6337	5333	3607	2426	2085	1529

Table S7. Platinum prices, $/kg

	2010	2011	2012	2013	2014	2015
Jan	50467	57521	48529	52944	45900	40201
Feb	49041	58903	53398	53983	45448	38811
Mar	51498	56912	53518	51023	46870	36893
Apr	55315	57827	51197	47980	46241	37305
May	52606	57610	47438	47727	46988	36965
Jun	50148	57124	46603	46154	46908	35234
Jul	49113	56644	45961	45169	48125	32833
Aug	49639	58201	46857	48191	46786	31882
Sep	51263	56458	52116	47131	44036	31385
Oct	54460	49474	52737	45580	40740	31559
Nov	54587	51428	50759	45821	39127	28815
Dec	55247	47210	51192	43727	39391	27824
Ave	51949	55443	50026	47952	44713	34142

Table S8. Acetic acid prices that this study relies on, $/t.

	2010	2011	2012	2013	2014	2015
Jan	513	650	562	607	725	713
Feb	513	650	590	627	726	700
Mar	537	650	597	682	726	700
Apr	537	651	572	695	739	700
May	537	676	572	659	723	700
Jun	537	625	572	685	733	700
Jul	537	635	572	648	733	700
Aug	537	650	645	667	722	700
Sep	537	650	665	667	703	687
Oct	537	630	608	667	713	687
Nov	537	625	607	708	713	687
Dec	563	625	607	725	713	687
Ave	535	643	597	670	722	697

Table S9. Furfural and hydroxymethylfurfural prices that this study relies on, $/t.

	2010	2011	2012	2013	2014	2015
Jan	1237	2655	1982	1380	1627	1639
Feb	1377	2778	1737	1314	1774	1550
Mar	1411	2610	1783	1354	1634	1571
Apr	1432	2698	1869	1564	1583	1637
May	1739	2558	1793	1404	1481	1488
Jun	1446	2539	1587	1484	1399	1485
Jul	1791	2817	1494	1402	1438	1538
Aug	1551	2366	1462	1300	1568	1734
Sep	1615	2188	1398	1466	1343	1487
Oct	1633	2151	1657	1492	1269	1528
Nov	2195	2006	1874	1600	1621	1404
Dec	2532	1975	2101	1572	1670	1828
Ave	1663	2445	1728	1444	1534	1574

Table S10. Natural gas prices that this study relies on, $/mmBtu.

	2010	2011	2012	2013	2014	2015
Jan	5.84	4.49	2.67	3.33	4.7	2.97
Feb	5.32	4.09	2.53	3.33	5.98	2.85
Mar	4.29	3.97	2.16	3.8	4.88	2.80
Apr	4.04	4.24	1.95	4.17	4.63	2.58
May	4.15	4.31	2.43	4.04	4.56	2.84
Jun	4.8	4.54	2.45	3.83	4.57	2.77
Jul	4.63	4.42	2.96	3.62	4.01	2.83
Aug	4.31	4.05	2.84	3.43	3.89	2.76
Sep	3.89	3.89	2.85	3.62	3.92	2.65
Oct	3.43	3.56	3.32	3.67	3.77	2.32
Nov	3.71	3.26	3.54	3.62	4.1	2.08
Dec	4.25	3.16	3.34	4.24	3.43	1.92
Ave	4.39	4	2.75	3.73	4.37	2.61

Table S11. Propane prices that this study relies on, $/gal.

	2010	2011	2012	2013	2014	2015
Jan	1.31	1.35	1.29	0.84	1.4	0.48
Feb	1.28	1.38	1.22	0.86	1.44	0.57
Mar	1.14	1.4	1.26	0.89	1.06	0.54
Apr	1.14	1.45	1.2	0.94	1.1	0.55
May	1.08	1.52	0.95	0.93	1.04	0.47
Jun	1.04	1.52	0.79	0.86	1.05	0.39
Jul	1.01	1.53	0.88	0.92	1.04	0.41
Aug	1.07	1.53	0.9	1.06	1.02	0.37
Sep	1.13	1.56	0.91	1.11	1.06	0.45
Oct	1.23	1.47	0.96	1.14	0.94	0.45
Nov	1.25	1.46	0.89	1.18	0.8	0.43
Dec	1.3	1.4	0.8	1.28	0.56	0.39
Ave	1.17	1.46	1	1	1.04	0.46

Table S12. Naphtha prices that this study relies on, $/gal.

	2010	2011	2012	2013	2014	2015
Jan	1.88	2.36	2.75	2.86	2.68	1.32
Feb	1.93	2.52	2.93	3.16	2.61	1.58
Mar	2.05	2.83	3.01	2.97	2.63	1.56
Apr	2.13	3.03	2.88	2.43	2.66	1.59
May	1.95	2.88	2.66	2.35	2.68	1.74
Jun	1.96	2.69	2.38	2.24	2.76	1.73
Jul	1.91	2.83	2.45	2.61	2.64	1.37
Aug	1.86	2.7	2.86	2.6	2.5	1.2
Sep	1.93	2.61	2.97	2.57	2.41	1.24
Oct	2.06	2.62	2.78	2.54	2.02	1.25
Nov	2.12	2.5	2.78	2.51	1.83	1.26
Dec	2.29	2.56	2.83	2.74	1.32	1.12
Ave	2.01	2.68	2.77	2.63	2.4	1.41

Table S13. Jet fuel prices that this study relies on, $/gal.

	2010	2011	2012	2013	2014	2015
Jan	2.05	2.62	3.09	3.09	2.92	1.5
Feb	1.99	2.84	3.21	3.22	2.97	1.76
Mar	2.11	3.13	3.26	2.97	2.89	1.63
Apr	2.24	3.27	3.23	2.81	2.89	1.7
May	2.06	3.09	2.97	2.73	2.87	1.85
Jun	2.06	3.05	2.68	2.77	2.88	1.73
Jul	2.02	3.13	2.89	2.89	2.82	1.54
Aug	2.08	3.01	3.16	3	2.84	1.39
Sep	2.11	2.95	3.19	2.93	2.73	1.39
Oct	2.25	2.97	3.11	2.89	2.46	1.39
Nov	2.32	3.05	2.96	2.83	2.3	1.33
Dec	2.45	2.87	2.94	2.96	1.8	1.08
Ave	2.15	3	3.06	2.92	2.7	1.52

Table S14. Diesel fuel prices that this study relies on, $/gal.

	2010	**2011**	**2012**	**2013**	**2014**	**2015**
Jan	2.07	2.64	3.08	3.1	3.12	1.68
Feb	2.04	2.84	3.22	3.24	3.23	1.99
Mar	2.16	3.13	3.3	3.04	2.99	1.86
Apr	2.28	3.27	3.24	2.9	2.96	1.84
May	2.14	3.04	2.99	2.89	2.94	1.97
Jun	2.11	3.05	2.71	2.89	2.96	1.89
Jul	2.07	3.17	2.92	3.02	2.88	1.68
Aug	2.12	3.01	3.18	3.07	2.85	1.52
Sep	2.18	2.98	3.23	3.05	2.74	1.51
Oct	2.3	3.01	3.24	3	2.53	1.47
Nov	2.38	3.1	3.18	2.94	2.43	1.41
Dec	2.5	2.94	3.07	3.05	2.03	1.14
Ave	2.2	3.02	3.11	3.02	2.81	1.66

Table S15. Details of major streams in Biorefinery 1. The streams are shown on a process flow diagram in Figure S2.

	P01	P05	P06	H04	H06	H17	H22A	H27	H34	H40	H55	C01	C03	C07	C12	C14	C21	C27	C31	C36	C50	B01
Temperature, K	298.1	473.1	473.1	384.2	473.1	434.5	309.2	383.1	383.1	523.1	310.4	298.1	473.1	453.0	453.2	493.0	371.9	648.1	443.0	423.1	300.3	374.4
Pressure, atm	1.0	16.1	16.0	54.4	54.0	1.1	1.1	54.3	54.0	61.1	1.0	1.0	15.8	16.1	15.7	35.5	1.1	36.4	35.5	34.6	0.9	1.0
Mass flow, kg/h	24,395.2	52,575.7	52,575.7	76,512.8	76,512.8	2,280.7	9,966.7	8,084.8	7,832.2	2,827.8	1,920.2	12,731.9	32,462.7	8,579.4	13,279.9	18,156.4	17,996.1	4,818.8	4,110.9	2,311.9	2,293.7	25,972.9
Water[1]	1,788.2	29,968.8	29,975.5	30,965.0	31,900.2	-	1,003.2	-	-	-	-	12,727.3	15,787.4	3,060.1	-	Trace	597.9	597.9	41.6	41.5	8.9	14,889.5
Cellulose	9,971.2	9,971.2	9,350.0	-	-	-	-	-	-	-	-	-	9,350.0	-	-	-	-	-	-	-	-	-
Xylan	4,218.8	4,218.8	544.2	-	-	-	-	-	-	-	-	-	544.2	-	-	-	-	-	-	-	-	544.2
Lignin	5,606.8	5,606.8	5,606.8	-	-	-	-	-	-	-	-	-	5,606.8	-	-	-	-	-	-	-	-	5,606.8
Acetate	1,175.6	1,175.6	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Ash	526.8	526.8	526.8	-	-	-	-	-	-	-	-	-	526.8	-	-	-	-	-	-	-	-	526.8
Soluble lignin	474.8	474.8	474.8	474.8	474.8	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	474.8
Uronic acids	633.0	633.0	633.0	633.0	633.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	633.0
Oxalic acid	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Sulfuric acid	-	-	-	-	-	-	-	-	-	-	-	4.6	240.4	235.8	Trace	Trace	Trace	-	-	-	-	4.4
HCl[1]	-	-	-	600.1	600.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Acetic acid	-	-	1,175.6	1,175.6	1,175.6	0.9	0.9	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5 sugar olig.	-	-	2,869.8	2,869.8	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6 sugar mono.	-	-	402.4	402.4	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5 sugar mono.	-	-	639.2	639.2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
HMF	-	-	201.5	201.5	446.5	0.4	0.4	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Furfural	-	-	176.2	176.2	2,347.9	2,279.4	2,279.4	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
THF	-	-	-	36,547.9	36,547.9	-	5,640.5	5,640.5	5,226.8	223.8	-	-	-	-	-	-	-	-	-	-	-	-
Sodium chloride	-	-	-	1,827.4	1,827.4	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6 humins	-	-	-	-	52.3	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2,649.5
C5 humins	-	-	-	-	507.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	507.0
Acetone	-	-	-	-	-	-	689.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
NaOH	-	-	-	-	-	-	353.4	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
FAF	-	-	-	-	-	-	-	2,444.3	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H-FAF	-	-	-	-	-	-	-	-	2,605.3	2,604.1	-	-	-	-	-	-	-	-	-	-	-	-
C1 alkane	-	-	-	-	-	-	-	-	-	-	34.6	-	-	-	-	-	-	-	-	-	-	-
C2 alkane	-	-	-	-	-	-	-	-	-	-	0.4	-	-	-	-	-	-	-	-	-	-	-
C3 alkane	-	-	-	-	-	-	-	-	-	-	11.5	-	-	-	-	-	-	-	-	-	-	-
C4 alkanes	-	-	-	-	-	-	-	-	-	-	59.1	-	-	-	-	-	-	-	-	-	Trace	-
C5 alkanes	-	-	-	-	-	-	-	-	-	-	2.2	-	-	-	-	-	-	-	-	-	-	-
C6 alkanes	-	-	-	-	-	-	-	-	-	-	18.6	-	-	-	-	-	-	-	-	-	-	-
C7 alkanes	-	-	-	-	-	-	-	-	-	-	15.3	-	-	-	-	-	-	-	-	-	-	-
C8 alkanes	-	-	-	-	-	-	-	-	-	-	6.8	-	-	-	-	-	-	-	-	-	684.5	-
C9 alkanes	-	-	-	-	-	-	-	-	-	-	14.9	-	-	-	-	-	-	-	-	-	-	-
C10 alkanes	-	-	-	-	-	-	-	-	-	-	14.7	-	-	-	-	-	-	-	-	-	-	-
C11 alkanes	-	-	-	-	-	-	-	-	-	-	23.2	-	-	-	-	-	-	-	-	-	-	-
C12 alkanes	-	-	-	-	-	-	-	-	-	-	304.2	-	-	-	-	-	-	-	-	-	593.9	-
C13 alkanes	-	-	-	-	-	-	-	-	-	-	1,414.6	-	-	-	-	-	-	-	-	-	-	-
C16 alkanes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	569.4	-
C20 alkanes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	432.0	-
Formic acid	-	-	-	-	-	-	-	-	-	-	-	-	288.3	306.2	-	18.1	-	-	-	-	-	42.0
Levulinic acid	-	-	-	-	-	-	-	-	-	-	-	-	108.7	4,968.8	-	4,860.1	-	-	-	-	-	94.6
GVL	-	-	-	-	-	-	-	-	-	-	-	-	7.5	6.0	83.9	82.4	4,194.0	4,110.1	0.3	0.3	0.3	0.1
SBP	-	-	-	-	-	-	-	-	-	-	-	-	2.6	2.5	13,196.0	13,195.9	13,177.2	83.9	0.1	0.1	0.1	-
CO2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.2	0.2	1,784.1	12.9	0.4	-
MBA	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	26.8	26.8	4.5	4.4	4.1	-
C4 alkene	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2,280.3	Trace	-	-
C8 alkenes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	672.5	-	-
C12 alkenes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	586.9	-	-
C16 alkenes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	564.4	-	-

[1]Note that hydrochloric acid is not available at 100% purity. This analysis considers the use of 36% HCl solutions, the HCl and water contents of which are included in their respective rows.

Table S16. Details of major streams in Biorefinery 2. The streams are shown on a process flow diagram in Figure S2.

	P01	P05	P06	H04	H06	H17	H22A	H27	H34	H40	H55	C01	C03	C07	C12	C14	C21	C27	C31	C36	C50	B01
Temperature, K	298.1	473.1	473.1	384.2	473.1	434.5	309.2	383.1	383.1	523.1	310.4	298.1	473.1	453.0	453.2	493.0	371.9	648.1	443.0	423.1	300.3	374.3
Pressure, atm	1.0	16.1	16.0	54.4	54.0	1.1	1.1	54.3	54.0	61.1	1.0	1.0	15.8	16.1	15.7	35.5	1.1	36.4	35.5	34.6	0.9	1.0
Mass flow, kg/h	24,395.2	52,575.7	52,575.7	76,512.8	76,512.8	2,474.7	10,813.9	8,821.6	8,543.8	3,125.7	2,215.7	12,731.9	32,462.7	8,579.4	13,279.9	18,156.4	17,996.1	4,818.8	4,110.9	2,311.9	2,293.7	25,628.7
Water[1]	1,788.2	29,968.8	29,975.5	30,965.0	32,022.2	-	1,088.4	-	-	-	-	12,727.3	15,787.4	3,060.1	-	Trace	597.9	597.9	41.6	41.5	8.9	14,889.5
Cellulose	9,971.2	9,971.2	9,350.0	-	-	-	-	-	-	-	-	-	9,350.0	-	-	-	-	-	-	-	-	-
Xylan	4,218.8	4,218.8	544.2	-	-	-	-	-	-	-	-	-	544.2	-	-	-	-	-	-	-	-	544.2
Lignin	5,606.8	5,606.8	5,606.8	-	-	-	-	-	-	-	-	-	5,606.8	-	-	-	-	-	-	-	-	5,606.8
Acetate	1,175.6	1,175.6	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Ash	526.8	526.8	526.8	-	-	-	-	-	-	-	-	-	526.8	-	-	-	-	-	-	-	-	526.8
Soluble lignin	474.8	474.8	474.8	474.8	474.8	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	474.8
Uronic acids	633.0	633.0	633.0	633.0	633.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	633.0
Oxalic acid	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Sulfuric acid	-	-	-	-	-	-	-	-	-	-	-	4.6	240.4	235.8	Trace	Trace	Trace	-	-	-	-	4.4
HCl[1]	-	-	-	600.1	600.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Acetic acid	-	-	1,175.6	1,175.6	1,175.6	1.1	1.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5 sugar olig.	-	-	2,869.8	2,869.8	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6 sugar mono.	-	-	402.4	402.4	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5 sugar mono.	-	-	639.2	639.2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
HMF	-	-	201.5	201.5	469.1	0.4	0.4	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Furfural	-	-	176.2	176.2	2,547.6	2,473.1	2,473.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
THF	-	-	-	36,547.9	36,547.9	-	6,119.8	6,119.8	5,664.2	247.4	-	-	-	-	-	-	-	-	-	-	-	-
Sodium chloride	-	-	-	1,827.4	1,827.4	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6 humins	-	-	-	-	20.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2,617.3
C5 humins	-	-	-	-	195.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	195.0
Acetone	-	-	-	-	-	-	747.6	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
NaOH	-	-	-	-	-	-	383.5	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
FAF	-	-	-	-	-	-	-	2,701.7	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H-FAF	-	-	-	-	-	-	-	-	2,879.7	2,878.3	-	-	-	-	-	-	-	-	-	-	-	-
C1 alkane	-	-	-	-	-	-	-	-	-	-	39.9	-	-	-	-	-	-	-	-	-	-	-
C2 alkane	-	-	-	-	-	-	-	-	-	-	0.5	-	-	-	-	-	-	-	-	-	-	-
C3 alkane	-	-	-	-	-	-	-	-	-	-	13.3	-	-	-	-	-	-	-	-	-	-	-
C4 alkanes	-	-	-	-	-	-	-	-	-	-	68.2	-	-	-	-	-	-	-	-	-	Trace	-
C5 alkanes	-	-	-	-	-	-	-	-	-	-	2.5	-	-	-	-	-	-	-	-	-	-	-
C6 alkanes	-	-	-	-	-	-	-	-	-	-	21.5	-	-	-	-	-	-	-	-	-	-	-
C7 alkanes	-	-	-	-	-	-	-	-	-	-	17.6	-	-	-	-	-	-	-	-	-	-	-
C8 alkanes	-	-	-	-	-	-	-	-	-	-	7.9	-	-	-	-	-	-	-	-	-	684.5	-
C9 alkanes	-	-	-	-	-	-	-	-	-	-	17.2	-	-	-	-	-	-	-	-	-	-	-
C10 alkanes	-	-	-	-	-	-	-	-	-	-	16.9	-	-	-	-	-	-	-	-	-	-	-
C11 alkanes	-	-	-	-	-	-	-	-	-	-	26.8	-	-	-	-	-	-	-	-	-	-	-
C12 alkanes	-	-	-	-	-	-	-	-	-	-	351.1	-	-	-	-	-	-	-	-	-	593.9	-
C13 alkanes	-	-	-	-	-	-	-	-	-	-	1,632.3	-	-	-	-	-	-	-	-	-	-	-
C16 alkanes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	569.4	-
C20 alkanes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	432.0	-
Formic acid	-	-	-	-	-	-	-	-	-	-	-	-	288.3	306.2	-	18.1	-	-	-	-	-	42.0
Levulinic acid	-	-	-	-	-	-	-	-	-	-	-	-	108.7	4,968.8	-	4,860.1	-	-	-	-	-	94.6
GVL	-	-	-	-	-	-	-	-	-	-	-	-	7.5	6.0	83.9	82.4	4,194.0	4,110.1	0.3	0.3	0.3	0.1
SBP	-	-	-	-	-	-	-	-	-	-	-	-	2.6	2.5	13,196.0	13,195.9	13,177.2	83.9	0.1	0.1	0.1	-
CO2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.2	0.2	1,784.1	12.9	0.4	-
MBA	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	26.8	26.8	4.5	4.4	4.1	-
C4 alkene	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2,280.3	Trace	-	-
C8 alkenes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	672.5	-	-
C12 alkenes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	586.9	-	-
C16 alkenes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	564.4	-	-

[1]Note that hydrochloric acid is not available at 100% purity. This analysis considers the use of 36% HCl solutions, the HCl and water contents of which are included in their respective rows.

Table S17. Details of major streams in Biorefinery 3. The streams are shown on a process flow diagram in Figure S2.

	P01	P05	P06	H04	H06	H17	H22A	H27	H34	H40	H55	C01	C03	C07	C12	C14	C21	C27	C31	C36	C50	B01
Temperature, K	298.1	473.1	473.1	384.2	473.1	434.5	309.2	383.1	383.1	523.1	310.4	298.1	473.1	453.0	453.1	493.0	374.3	648.1	443.0	423.1	300.3	374.8
Pressure, atm	1.0	16.1	16.0	54.4	54.0	1.1	1.1	54.3	54.0	61.1	1.0	1.0	15.8	16.1	15.7	35.5	1.1	36.4	35.5	34.6	0.9	1.0
Mass flow, kg/h	24,395.2	52,575.7	52,575.7	76,512.8	76,512.8	2,280.7	9,966.7	8,084.8	7,832.2	2,827.8	1,920.2	13,542.7	32,207.5	6,193.0	13,258.0	16,814.1	16,707.8	3,528.7	3,001.1	1,687.8	1,674.5	28,548.7
Water[1]	1,788.2	29,968.8	29,975.5	30,965.0	31,900.2	-	1,003.2	-	-	-	-	13,538.0	15,787.4	2,249.4	-	Trace	446.5	446.5	30.3	30.2	6.4	15,426.7
Cellulose	9,971.2	9,971.2	9,350.0	-	-	-	-	-	-	-	-	-	9,350.0	-	-	-	-	-	-	-	-	-
Xylan	4,218.8	4,218.8	544.2	-	-	-	-	-	-	-	-	-	544.2	-	-	-	-	-	-	-	-	544.2
Lignin	5,606.8	5,606.8	5,606.8	-	-	-	-	-	-	-	-	-	5,606.8	-	-	-	-	-	-	-	-	5,606.8
Acetate	1,175.6	1,175.6	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Ash	526.8	526.8	526.8	-	-	-	-	-	-	-	-	-	526.8	-	-	-	-	-	-	-	-	526.8
Soluble lignin	474.8	474.8	474.8	474.8	474.8	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	474.8
Uronic acids	633.0	633.0	633.0	633.0	633.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	633.0
Oxalic acid	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Sulfuric acid	-	-	-	-	-	-	-	-	-	-	-	4.7	240.4	235.7	Trace	Trace	Trace	-	-	-	-	4.4
HCl[1]	-	-	-	600.1	600.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Acetic acid	-	-	1,175.6	1,175.6	1,175.6	0.9	0.9	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5 sugar olig.	-	-	2,869.8	2,869.8	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6 sugar mono.	-	-	402.4	402.4	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5 sugar mono.	-	-	639.2	639.2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
HMF	-	-	201.5	201.5	446.5	0.4	0.4	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Furfural	-	-	176.2	176.2	2,347.9	2,279.4	2,279.4	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
THF	-	-	-	36,547.9	36,547.9	-	5,640.5	5,640.5	5,226.8	223.8	-	-	-	-	-	-	-	-	-	-	-	-
Sodium chloride	-	-	-	1,827.4	1,827.4	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6 humins	-	-	-	-	52.3	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	4,727.3
C5 humins	-	-	-	-	507.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	507.0
Acetone	-	-	-	-	-	-	689.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
NaOH	-	-	-	-	-	-	353.4	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
FAF	-	-	-	-	-	-	-	2,444.3	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H-FAF	-	-	-	-	-	-	-	-	2,605.3	2,604.1	-	-	-	-	-	-	-	-	-	-	-	-
C1 alkane	-	-	-	-	-	-	-	-	-	-	34.6	-	-	-	-	-	-	-	-	-	-	-
C2 alkane	-	-	-	-	-	-	-	-	-	-	0.4	-	-	-	-	-	-	-	-	-	-	-
C3 alkane	-	-	-	-	-	-	-	-	-	-	11.5	-	-	-	-	-	-	-	-	-	-	-
C4 alkanes	-	-	-	-	-	-	-	-	-	-	59.1	-	-	-	-	-	-	-	-	-	Trace	-
C5 alkanes	-	-	-	-	-	-	-	-	-	-	2.2	-	-	-	-	-	-	-	-	-	-	-
C6 alkanes	-	-	-	-	-	-	-	-	-	-	18.6	-	-	-	-	-	-	-	-	-	-	-
C7 alkanes	-	-	-	-	-	-	-	-	-	-	15.3	-	-	-	-	-	-	-	-	-	-	-
C8 alkanes	-	-	-	-	-	-	-	-	-	-	6.8	-	-	-	-	-	-	-	-	-	499.8	-
C9 alkanes	-	-	-	-	-	-	-	-	-	-	14.9	-	-	-	-	-	-	-	-	-	-	-
C10 alkanes	-	-	-	-	-	-	-	-	-	-	14.7	-	-	-	-	-	-	-	-	-	-	-
C11 alkanes	-	-	-	-	-	-	-	-	-	-	23.2	-	-	-	-	-	-	-	-	-	-	-
C12 alkanes	-	-	-	-	-	-	-	-	-	-	304.2	-	-	-	-	-	-	-	-	-	433.6	-
C13 alkanes	-	-	-	-	-	-	-	-	-	-	1,414.6	-	-	-	-	-	-	-	-	-	-	-
C16 alkanes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	415.7	-
C20 alkanes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	315.4	-
Formic acid	-	-	-	-	-	-	-	-	-	-	-	-	144.4	156.0	-	11.6	-	-	-	-	-	29.6
Levulinic acid	-	-	-	-	-	-	-	-	-	-	-	-	1.6	3,547.2	-	3,545.6	-	-	-	-	-	67.9
GVL	-	-	-	-	-	-	-	-	-	-	-	-	4.0	3.0	61.2	60.2	3,061.9	3,000.6	0.2	0.2	0.2	0.1
SBP	-	-	-	-	-	-	-	-	-	-	-	-	1.9	1.8	13,196.8	13,196.6	13,179.1	61.2	0.1	0.1	0.1	-
CO2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.1	0.1	1,302.4	9.4	0.3	-
MBA	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	20.2	20.2	3.3	3.2	3.0	-
C4 alkene	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1,664.7	Trace	-	-
C8 alkenes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	490.9	-	-
C12 alkenes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	428.5	-	-
C16 alkenes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	412.0	-	-

[1]Note that hydrochloric acid is not available at 100% purity. This analysis considers the use of 36% HCl solutions, the HCl and water contents of which are included in their respective rows.

Table S18. Details of major streams in Biorefinery 4. The streams are shown on a process flow diagram in Figure S2.

	P01	P05	P06	H04	H06	H17	H22A	H27	H34	H40	H55	C01	C03	C07	C12	C14	C21	C27	C31	C36	C50	B01
Temperature, K	298.1	473.1	473.1	384.2	473.1	434.5	-	-	-	-	-	298.1	473.1	453.0	453.2	493.0	371.9	648.1	443.0	423.1	300.3	374.4
Pressure, atm	1.0	16.1	16.0	54.4	54.0	1.0	-	-	-	-	-	1.0	15.8	16.1	15.7	35.5	1.1	36.4	35.5	34.6	0.9	1.0
Mass flow, kg/h	24,395.2	52,575.7	52,575.7	76,512.8	76,512.8	2,280.7	-	-	-	-	-	12,731.9	32,462.7	8,579.4	13,279.9	18,156.4	17,996.1	4,818.8	4,110.9	2,311.9	2,293.7	25,972.9
Water[1]	1,788.2	29,968.8	29,975.5	30,965.0	31,900.2	-	-	-	-	-	-	12,727.3	15,787.4	3,060.1	-	Trace	597.9	597.9	41.6	41.5	8.9	14,889.5
Cellulose	9,971.2	9,971.2	9,350.0	-	-	-	-	-	-	-	-	-	9,350.0	-	-	-	-	-	-	-	-	-
Xylan	4,218.8	4,218.8	544.2	-	-	-	-	-	-	-	-	-	544.2	-	-	-	-	-	-	-	-	544.2
Lignin	5,606.8	5,606.8	5,606.8	-	-	-	-	-	-	-	-	-	5,606.8	-	-	-	-	-	-	-	-	5,606.8
Acetate	1,175.6	1,175.6	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Ash	526.8	526.8	526.8	-	-	-	-	-	-	-	-	-	526.8	-	-	-	-	-	-	-	-	526.8
Soluble lignin	474.8	474.8	474.8	474.8	474.8	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	474.8
Uronic acids	633.0	633.0	633.0	633.0	633.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	633.0
Oxalic acid	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Sulfuric acid	-	-	-	-	-	-	-	-	-	-	-	4.6	240.4	235.8	Trace	Trace	Trace	-	-	-	-	4.4
HCl[1]	-	-	-	600.1	600.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Acetic acid	-	-	1,175.6	1,175.6	1,175.6	0.9	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5 sugar olig.	-	-	2,869.8	2,869.8	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6 sugar mono.	-	-	402.4	402.4	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5 sugar mono.	-	-	639.2	639.2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
HMF	-	-	201.5	201.5	446.5	0.4	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Furfural	-	-	176.2	176.2	2,347.9	2,279.4	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
THF	-	-	-	36,547.9	36,547.9	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Sodium chloride	-	-	-	1,827.4	1,827.4	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6 humins	-	-	-	-	52.3	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2,649.5
C5 humins	-	-	-	-	507.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	507.0
Acetone	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
NaOH	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
FAF	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H-FAF	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C1 alkane	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C2 alkane	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C3 alkane	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C4 alkanes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	Trace	-
C5 alkanes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6 alkanes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C7 alkanes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C8 alkanes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	684.5	-
C9 alkanes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C10 alkanes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C11 alkanes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C12 alkanes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	593.9	-
C13 alkanes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C16 alkanes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	569.4	-
C20 alkanes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	432.0	-
Formic acid	-	-	-	-	-	-	-	-	-	-	-	-	288.3	306.2	-	18.1	-	-	-	-	-	42.0
Levulinic acid	-	-	-	-	-	-	-	-	-	-	-	-	108.7	4,968.8	-	4,860.1	-	-	-	-	-	94.6
GVL	-	-	-	-	-	-	-	-	-	-	-	-	7.5	6.0	83.9	82.4	4,194.0	4,110.1	0.3	0.3	0.3	0.1
SBP	-	-	-	-	-	-	-	-	-	-	-	-	2.6	2.5	13,196.0	13,195.9	13,177.2	83.9	0.1	0.1	0.1	-
CO2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.2	0.2	1,784.1	12.9	0.4	-
MBA	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	26.8	26.8	4.5	4.4	4.1	-
C4 alkene	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2,280.3	Trace	-	-
C8 alkenes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	672.5	-	-
C12 alkenes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	586.9	-	-
C16 alkenes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	564.4	-	-

[1]Note that hydrochloric acid is not available at 100% purity. This analysis considers the use of 36% HCl solutions, the HCl and water contents of which are included in their respective rows.

Table S19. Details of major streams in Biorefinery 5. The streams are shown on a process flow diagram in Figure S2.

	P01	P05	P06	H04	H06	H17	H22A	H27	H34	H40	H55	C01	C03	C07	C12	C14	C21	C27	C31	C36	C50	B01
Temperature, K	298.1	433.1	433.1	384.2	473.1	434.5	309.2	383.1	383.1	523.1	310.4	298.1	467.8	453.0	453.2	493.0	371.6	648.1	443.0	423.1	300.3	374.4
Pressure, atm	1.0	16.1	16.0	54.4	54.0	1.1	1.1	54.3	54.0	61.1	1.0	1.0	15.8	16.1	15.7	35.5	1.1	36.4	35.5	34.6	0.9	1.0
Mass flow, kg/h	24,395.2	52,575.7	52,575.7	76,324.2	76,324.2	2,423.0	10,588.5	8,589.4	8,321.0	3,004.5	2,040.2	12,687.6	32,736.6	8,974.2	13,282.3	18,326.6	18,158.7	4,982.0	4,251.2	2,390.8	2,372.0	25,895.2
Water[1]	1,788.2	29,818.9	29,469.4	30,458.9	31,737.3	-	1,065.7	-	-	-	-	12,683.0	15,877.3	3,194.3	-	Trace	617.1	617.1	43.1	42.9	9.2	14,936.5
Cellulose	9,971.2	9,971.2	9,669.1	-	-	-	-	-	-	-	-	-	9,669.1	-	-	-	-	-	-	-	-	-
Xylan	4,218.8	4,218.8	316.4	-	-	-	-	-	-	-	-	-	316.4	-	-	-	-	-	-	-	-	316.4
Lignin	5,606.8	5,606.8	5,606.8	-	-	-	-	-	-	-	-	-	5,606.8	-	-	-	-	-	-	-	-	5,606.8
Acetate	1,175.6	1,175.6	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Ash	526.8	526.8	526.8	-	-	-	-	-	-	-	-	-	526.8	-	-	-	-	-	-	-	-	526.8
Soluble lignin	474.8	474.8	474.8	474.8	474.8	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	474.8
Uronic acids	633.0	633.0	633.0	633.0	633.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	633.0
Oxalic acid	-	149.8	149.8	149.8	149.8	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Sulfuric acid	-	-	-	-	-	-	-	-	-	-	-	4.7	241.8	237.1	Trace	Trace	Trace	-	-	-	-	4.5
HCl[1]	-	-	-	598.6	598.6	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Acetic acid	-	-	1,175.6	1,175.6	1,175.6	1.0	1.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5 sugar olig.	-	-	565.8	565.8	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6 sugar mono.	-	-	236.3	236.3	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5 sugar mono.	-	-	3,488.1	3,488.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
HMF	-	-	69.6	69.6	213.5	0.2	0.2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Furfural	-	-	194.1	194.1	2,494.4	2,421.8	2,421.8	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
THF	-	-	-	36,456.7	36,456.7	-	5,992.3	5,992.3	5,552.9	237.7	-	-	-	-	-	-	-	-	-	-	-	-
Sodium chloride	-	-	-	1,822.8	1,822.8	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6 humins	-	-	-	-	30.7	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2,716.6
C5 humins	-	-	-	-	537.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	537.0
Acetone	-	-	-	-	-	-	732.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
NaOH	-	-	-	-	-	-	375.5	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
FAF	-	-	-	-	-	-	-	2,597.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H-FAF	-	-	-	-	-	-	-	-	2,768.1	2,766.8	-	-	-	-	-	-	-	-	-	-	-	-
C1 alkane	-	-	-	-	-	-	-	-	-	-	36.8	-	-	-	-	-	-	-	-	-	-	-
C2 alkane	-	-	-	-	-	-	-	-	-	-	0.4	-	-	-	-	-	-	-	-	-	-	-
C3 alkane	-	-	-	-	-	-	-	-	-	-	12.2	-	-	-	-	-	-	-	-	-	-	-
C4 alkanes	-	-	-	-	-	-	-	-	-	-	62.8	-	-	-	-	-	-	-	-	-	Trace	-
C5 alkanes	-	-	-	-	-	-	-	-	-	-	2.3	-	-	-	-	-	-	-	-	-	-	-
C6 alkanes	-	-	-	-	-	-	-	-	-	-	19.8	-	-	-	-	-	-	-	-	-	-	-
C7 alkanes	-	-	-	-	-	-	-	-	-	-	16.2	-	-	-	-	-	-	-	-	-	-	-
C8 alkanes	-	-	-	-	-	-	-	-	-	-	7.3	-	-	-	-	-	-	-	-	-	707.9	-
C9 alkanes	-	-	-	-	-	-	-	-	-	-	15.9	-	-	-	-	-	-	-	-	-	-	-
C10 alkanes	-	-	-	-	-	-	-	-	-	-	15.6	-	-	-	-	-	-	-	-	-	-	-
C11 alkanes	-	-	-	-	-	-	-	-	-	-	24.7	-	-	-	-	-	-	-	-	-	-	-
C12 alkanes	-	-	-	-	-	-	-	-	-	-	323.2	-	-	-	-	-	-	-	-	-	614.2	-
C13 alkanes	-	-	-	-	-	-	-	-	-	-	1,503.0	-	-	-	-	-	-	-	-	-	-	-
C16 alkanes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	588.9	-
C20 alkanes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	446.7	-
Formic acid	-	-	-	-	-	-	-	-	-	-	-	-	312.1	331.1	-	19.0	-	-	-	-	-	43.7
Levulinic acid	-	-	-	-	-	-	-	-	-	-	-	-	175.5	5,202.5	-	5,027.0	-	-	-	-	-	99.0
GVL	-	-	-	-	-	-	-	-	-	-	-	-	8.1	6.5	86.7	85.1	4,337.2	4,250.4	0.3	0.3	0.3	0.1
SBP	-	-	-	-	-	-	-	-	-	-	-	-	2.7	2.6	13,195.5	13,195.4	13,176.7	86.7	0.1	0.1	0.1	-
CO2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.2	0.2	1,845.0	13.3	0.4	-
MBA	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	27.6	27.6	4.6	4.5	4.2	-
C4 alkene	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2,358.1	Trace	-	-
C8 alkenes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	695.4	-	-
C12 alkenes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	606.9	-	-
C16 alkenes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	583.6	-	-

[1]Note that hydrochloric acid is not available at 100% purity. This analysis considers the use of 36% HCl solutions, the HCl and water contents of which are included in their respective rows.

Table S20. Details of major streams in Biorefinery 6. The streams are shown on a process flow diagram in Figure S2.

	P01	P05	P06	H04	H06	H17	H22A	H27	H34	H40	H55	C01	C03	C07	C12	C14	C21	C27	C31	C36	C50	B01
Temperature, K	298.1	413.1	413.1	384.2	473.1	434.5	309.2	383.1	383.1	523.1	310.4	298.1	464.9	453.0	453.1	493.0	372.7	648.1	443.0	423.1	300.3	374.4
Pressure, atm	1.0	16.1	16.0	54.4	54.0	1.1	1.1	54.3	54.0	61.1	1.0	1.0	15.8	16.1	15.7	35.5	1.1	36.4	35.5	34.6	0.9	1.0
Mass flow, kg/h	24,395.2	52,575.7	52,575.7	78,722.8	78,722.8	2,490.8	10,883.0	8,826.3	8,550.5	3,086.1	2,095.6	11,865.5	29,898.9	7,626.7	13,272.3	17,674.0	17,531.3	4,353.2	3,710.4	2,086.7	2,070.2	24,414.3
Water[1]	1,788.2	29,818.9	29,515.1	30,504.6	31,997.3	-	1,095.3	-	-	-	-	11,861.2	14,586.3	2,725.1	-	Trace	543.2	543.2	37.6	37.4	8.0	13,778.0
Cellulose	9,971.2	9,971.2	8,438.6	-	-	-	-	-	-	-	-	-	8,438.6	-	-	-	-	-	-	-	-	-
Xylan	4,218.8	4,218.8	236.3	-	-	-	-	-	-	-	-	-	236.3	-	-	-	-	-	-	-	-	236.3
Lignin	5,606.8	5,606.8	5,606.8	-	-	-	-	-	-	-	-	-	5,606.8	-	-	-	-	-	-	-	-	5,606.8
Acetate	1,175.6	1,175.6	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Ash	526.8	526.8	526.8	-	-	-	-	-	-	-	-	-	526.8	-	-	-	-	-	-	-	-	526.8
Soluble lignin	474.8	474.8	474.8	474.8	474.8	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	474.8
Uronic acids	633.0	633.0	633.0	633.0	633.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	633.0
Oxalic acid	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Sulfuric acid	-	-	-	-	-	-	-	-	-	-	-	4.3	222.1	217.8	Trace	Trace	Trace	-	-	-	-	4.1
HCl[1]	-	149.8	149.8	617.6	617.6	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Acetic acid	-	-	1,175.6	1,175.6	1,175.6	1.2	1.2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5 sugar olig.	-	-	720.8	720.8	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6 sugar mono.	-	-	1,306.1	1,306.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5 sugar mono.	-	-	3,172.7	3,172.7	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
HMF	-	-	277.7	277.7	1,073.1	2.1	2.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Furfural	-	-	341.6	341.6	2,564.3	2,487.6	2,487.6	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
THF	-	-	-	37,617.4	37,617.4	-	6,158.7	6,158.7	5,707.2	244.2	-	-	-	-	-	-	-	-	-	-	-	-
Sodium chloride	-	-	-	1,880.9	1,880.9	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6 humins	-	-	-	-	169.8	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2,513.9
C5 humins	-	-	-	-	518.9	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	518.9
Acetone	-	-	-	-	-	-	752.3	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
NaOH	-	-	-	-	-	-	385.9	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
FAF	-	-	-	-	-	-	-	2,667.6	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H-FAF	-	-	-	-	-	-	-	-	2,843.3	2,841.9	-	-	-	-	-	-	-	-	-	-	-	-
C1 alkane	-	-	-	-	-	-	-	-	-	-	37.8	-	-	-	-	-	-	-	-	-	-	-
C2 alkane	-	-	-	-	-	-	-	-	-	-	0.5	-	-	-	-	-	-	-	-	-	-	-
C3 alkane	-	-	-	-	-	-	-	-	-	-	12.6	-	-	-	-	-	-	-	-	-	-	-
C4 alkanes	-	-	-	-	-	-	-	-	-	-	64.5	-	-	-	-	-	-	-	-	-	Trace	-
C5 alkanes	-	-	-	-	-	-	-	-	-	-	2.4	-	-	-	-	-	-	-	-	-	-	-
C6 alkanes	-	-	-	-	-	-	-	-	-	-	20.4	-	-	-	-	-	-	-	-	-	-	-
C7 alkanes	-	-	-	-	-	-	-	-	-	-	16.7	-	-	-	-	-	-	-	-	-	-	-
C8 alkanes	-	-	-	-	-	-	-	-	-	-	7.5	-	-	-	-	-	-	-	-	-	617.9	-
C9 alkanes	-	-	-	-	-	-	-	-	-	-	16.3	-	-	-	-	-	-	-	-	-	-	-
C10 alkanes	-	-	-	-	-	-	-	-	-	-	16.0	-	-	-	-	-	-	-	-	-	-	-
C11 alkanes	-	-	-	-	-	-	-	-	-	-	25.4	-	-	-	-	-	-	-	-	-	-	-
C12 alkanes	-	-	-	-	-	-	-	-	-	-	332.0	-	-	-	-	-	-	-	-	-	536.1	-
C13 alkanes	-	-	-	-	-	-	-	-	-	-	1,543.8	-	-	-	-	-	-	-	-	-	-	-
C16 alkanes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	514.0	-
C20 alkanes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	389.9	-
Formic acid	-	-	-	-	-	-	-	-	-	-	-	-	247.4	264.5	-	17.1	-	-	-	-	-	37.7
Levulinic acid	-	-	-	-	-	-	-	-	-	-	-	-	26.2	4,412.2	-	4,386.0	-	-	-	-	-	84.1
GVL	-	-	-	-	-	-	-	-	-	-	-	-	6.0	4.7	75.7	74.4	3,785.4	3,709.7	0.3	0.3	0.3	0.1
SBP	-	-	-	-	-	-	-	-	-	-	-	-	2.3	2.2	13,196.6	13,196.5	13,178.1	75.7	0.1	0.1	0.1	-
CO2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.2	0.2	1,610.3	11.6	0.3	-
MBA	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	24.4	24.4	4.0	4.0	3.7	-
C4 alkene	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2,058.1	Trace	-	-
C8 alkenes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	607.0	-	-
C12 alkenes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	529.7	-	-
C16 alkenes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	509.4	-	-

[1]Note that hydrochloric acid is not available at 100% purity. This analysis considers the use of 36% HCl solutions, the HCl and water contents of which are included in their respective rows.

Table S21. Details of major streams in Biorefinery 7. The streams are shown on a process flow diagram in Figure S2.

	P01	P05	P06	H04	H06	H17	H22A	H27	H34	H40	H55	C01	C03	C07	C12	C14	C21	C27	C31	C36	C50	B01
Temperature, K	298.1	433.1	433.1	384.2	473.1	434.5	309.2	383.1	383.1	523.1	310.4	298.1	467.7	453.0	453.2	493.0	372.1	648.1	443.0	423.1	300.3	374.4
Pressure, atm	1.0	16.1	16.0	54.4	54.0	1.1	1.1	54.3	54.0	61.1	1.0	1.0	15.8	16.1	15.7	35.5	1.1	36.4	35.5	34.6	0.9	1.0
Mass flow, kg/h	24,395.2	52,575.7	52,575.7	77,087.1	77,087.1	2,390.0	10,444.0	8,471.6	8,206.9	2,963.0	2,011.9	12,415.2	31,559.2	8,284.1	13,277.4	18,017.6	17,861.7	4,684.5	3,995.4	2,246.9	2,229.3	25,374.2
Water[1]	1,788.2	29,818.9	29,454.4	30,443.9	31,838.8	-	1,051.2	-	-	-	-	12,410.7	15,366.0	2,955.3	-	Trace	582.1	582.1	40.5	40.3	8.6	14,485.4
Cellulose	9,971.2	9,971.2	9,086.8	-	-	-	-	-	-	-	-	-	9,086.8	-	-	-	-	-	-	-	-	-
Xylan	4,218.8	4,218.8	379.7	-	-	-	-	-	-	-	-	-	379.7	-	-	-	-	-	-	-	-	379.7
Lignin	5,606.8	5,606.8	5,606.8	-	-	-	-	-	-	-	-	-	5,606.8	-	-	-	-	-	-	-	-	5,606.8
Acetate	1,175.6	1,175.6	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Ash	526.8	526.8	526.8	-	-	-	-	-	-	-	-	-	526.8	-	-	-	-	-	-	-	-	526.8
Soluble lignin	474.8	474.8	474.8	474.8	474.8	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	474.8
Uronic acids	633.0	633.0	633.0	633.0	633.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	633.0
Oxalic acid	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Sulfuric acid	-	149.8	149.8	149.8	149.8	-	-	-	-	-	-	4.5	234.0	229.5	Trace	Trace	Trace	-	-	-	-	4.3
HCl[1]	-	-	-	454.8	454.8	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Acetic acid	-	-	1,175.6	1,175.6	1,175.6	1.0	1.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5 sugar olig.	-	-	234.2	234.2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6 sugar mono.	-	-	684.0	684.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C5 sugar mono.	-	-	3,719.6	3,719.6	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
HMF	-	-	209.1	209.1	625.7	0.7	0.7	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Furfural	-	-	241.2	241.2	2,460.5	2,388.3	2,388.3	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
THF	-	-	-	36,825.8	36,825.8	-	5,910.5	5,910.5	5,477.1	234.4	-	-	-	-	-	-	-	-	-	-	-	-
Sodium chloride	-	-	-	1,841.3	1,841.3	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
C6 humins	-	-	-	-	88.9	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2,613.0
C5 humins	-	-	-	-	518.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	518.1
Acetone	-	-	-	-	-	-	722.0	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
NaOH	-	-	-	-	-	-	370.3	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
FAF	-	-	-	-	-	-	-	2,561.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-
H-FAF	-	-	-	-	-	-	-	-	2,729.8	2,728.5	-	-	-	-	-	-	-	-	-	-	-	-
C1 alkane	-	-	-	-	-	-	-	-	-	-	36.3	-	-	-	-	-	-	-	-	-	-	-
C2 alkane	-	-	-	-	-	-	-	-	-	-	0.4	-	-	-	-	-	-	-	-	-	-	-
C3 alkane	-	-	-	-	-	-	-	-	-	-	12.1	-	-	-	-	-	-	-	-	-	-	-
C4 alkanes	-	-	-	-	-	-	-	-	-	-	61.9	-	-	-	-	-	-	-	-	-	Trace	-
C5 alkanes	-	-	-	-	-	-	-	-	-	-	2.3	-	-	-	-	-	-	-	-	-	-	-
C6 alkanes	-	-	-	-	-	-	-	-	-	-	19.5	-	-	-	-	-	-	-	-	-	-	-
C7 alkanes	-	-	-	-	-	-	-	-	-	-	16.0	-	-	-	-	-	-	-	-	-	-	-
C8 alkanes	-	-	-	-	-	-	-	-	-	-	7.2	-	-	-	-	-	-	-	-	-	665.3	-
C9 alkanes	-	-	-	-	-	-	-	-	-	-	15.6	-	-	-	-	-	-	-	-	-	-	-
C10 alkanes	-	-	-	-	-	-	-	-	-	-	15.4	-	-	-	-	-	-	-	-	-	-	-
C11 alkanes	-	-	-	-	-	-	-	-	-	-	24.3	-	-	-	-	-	-	-	-	-	-	-
C12 alkanes	-	-	-	-	-	-	-	-	-	-	318.8	-	-	-	-	-	-	-	-	-	577.2	-
C13 alkanes	-	-	-	-	-	-	-	-	-	-	1,482.2	-	-	-	-	-	-	-	-	-	-	-
C16 alkanes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	553.4	-
C20 alkanes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	419.9	-
Formic acid	-	-	-	-	-	-	-	-	-	-	-	-	277.0	295.0	-	17.9	-	-	-	-	-	40.8
Levulinic acid	-	-	-	-	-	-	-	-	-	-	-	-	72.6	4,796.4	-	4,723.8	-	-	-	-	-	91.3
GVL	-	-	-	-	-	-	-	-	-	-	-	-	7.0	5.6	81.5	80.1	4,076.1	3,994.6	0.3	0.3	0.3	0.1
SBP	-	-	-	-	-	-	-	-	-	-	-	-	2.5	2.4	13,195.9	13,195.8	13,177.2	81.5	0.1	0.1	0.1	-
CO2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.2	0.2	1,734.0	12.5	0.4	-
MBA	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	26.1	26.1	4.3	4.3	4.0	-
C4 alkene	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	2,216.2	Trace	-	-
C8 alkenes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	653.6	-	-
C12 alkenes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	570.4	-	-
C16 alkenes	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	548.5	-	-

[1]Note that hydrochloric acid is not available at 100% purity. This analysis considers the use of 36% HCl solutions, the HCl and water contents of which are included in their respective rows.

Table S22. Representative red maple wood composition adjusted based on Zhang et al. 2013. Uronic acids are assumed to be the only extractives (Jara 2010). Moisture content is assumed to be 7.3%.

Dry composition	**%**
Cellulose (glucan)	44.1
Hemicellulose (xylan)	18.7
Lignin	24.8
Soluble lignin	2.1
Acetate	5.2
Uronic acids	2.8
Ash	2.3
Total	100.0

Table S23. Pretreatment reactor material inputs based on 100 a.u. of dry red maple wood, reactions, reactor conditions and yields for different pretreatment techniques.

		Pretreatment techniques			
		Hot water	Oxalic acid	Hydro-chloric acid	Sulfuric acid
		Biorefinery model			
		1-4	5	6	7
Material inputs, a.u.	Dry biomass	100	100	100	100
	Moisture in biomass	7.9	7.9	7.9	7.9
	Additional water	124.6	124.0	124.0	124.0
	Acid	-	0.7	0.7	0.7
Reactor conditions	Temperature, °C	200	160	140	160
	Pressure, psi (kPa)	235 (1620)	235 (1620)	235 (1620)	235 (1620)
	Residence time, min	11.2	27.5	51	27.5
Reactions and % yields	Cellulose → Glucooligomers	6.2	3	15.4	8.9
	Glucooligomers + H_2O → Glucose	100.0	100.0	100.0	100.0
	Glucose → HMF + 3 H_2O	41.7	29.6	23.3	30.4
	Xylan → Xylooligomers	87.1	92.5	94.4	91.0
	Xylooligomers + H_2O → Xylose	21.9	85.5	81.9	93.9
	Xylose → Furfural + 3 H_2O	30.1	8.0	14.4	9.2
	Acetate → Acetic acid	100.0	100.0	100.0	100.0

Table S24. Cellulose deconstruction reactions and percent reaction yields for low and high yield cases. All reactions take place under 200°C and 230 psi (1586 kPa) at a residence time of 1 hour.

	Low yield	High yield
Biorefinery model	3	Others
Cellulose → Glucooligomers	100.0	100.0
Glucooligomers + H_2O → Glucose	100.0	100.0
Glucose → Levulinic acid + Formic acid + H_2O	55.0	75.0
Glucose → C_6 Humins	45.0	25.0

Table S25. Percent conversion and molar selectivities derived from experimental data (Xing et al. 2010) to be applied in the hydrodeoxygenation reactor for the low and high yield cases.

% Molar selectivity of alkanes based on carbon number												
C_1	C_2	C_3	C_4	C_5	C_6	C_7	C_8	C_9	C_{10}	C_{11}	C_{12}	C_{13}
15.7	0.10	1.90	7.40	0.22	1.58	1.11	0.44	0.85	0.75	1.08	13.0	55.9

% Conversion	
Low yield	High yield
91	95

Table S26. Lifecycle production emissions of biorefinery products in gCO_2e/kg for chemicals and gCO_2e/MJ for fuels compared with their conventional counterparts.

		Biorefineries						
Products	**Conv.**	**1**	**2**	**3**	**4**	**5**	**6**	**7**
Acetic acid	620[a,d]	267	272	281	92.4	276	262	267
HMF		416	425	439	144	430	410	416
Furfural		N/A	N/A	N/A	160	N/A	N/A	N/A
Natural gas	17.5[b,d]	49.3	48.4	53.5	N/A	51.4	47.9	47.1
Propane		49.2	48.3	53.5	N/A	51.4	47.8	47.1
Naphtha	16.9[c,d]	50.3	49.4	54.4	37.2	52.5	48.8	48.1
Jet fuel	13.5[c,e]	53.6	52.8	58.0	38.2	55.9	52.1	51.5
Diesel	18.0[c,d]	49.8	48.9	54.0	36.7	52.0	48.3	47.7

[a]Acetic acid production from methanol carboxylation.
[b]Natural gas from shale and crude oil.
[c]Product from crude oil refining.
[d]Data from GREET.net.
[e]Data from Stratton et al. 2010.

Table S27. Cost of hydrogen in 2010 USD based on the Hydrogen Analysis (H2A) carried out by the U.S. Department of Energy. A large-scale central plant is assumed unless noted otherwise. Start of production is assumed to take place in 2010. Plant sizes (kg/day) have been rounded. CCS: Carbon capture and storage.

Feedstock/Utility	Technology	Plant size	Notes	H_2 cost
Natural gas	Steam reforming	380,000	-	1.78
		380,000	With CCS	2.19
		380,000	Improved efficiency	1.69
		380,000	With CCS, improved efficiency	2.11
		1,500	Small-scale distributed plant	4.46
Biomass, hybrid poplar	Gasification	150,000	-	2.39
		150,000	Improved efficiency	2.16
Coal	Gasification	300,000	-	1.41
		300,000	With CCS	2.05
		250,000	Improved efficiency	1.43
		250,000	With CCS, improved efficiency	1.97
Water/Grid electricity	PEM electrolysis	50,000	-	5.37
		50,000	With future efficiency	4.04
	Solid oxide electrolysis	50,000	-	5.04
		50,000	With improved efficiency	3.72
	Photoelectrochemical	50,000	Technology option 1	4.82
		50,000	Technology option 2	5.99
Water/Solar energy	Thermolysis	100,000	-	4.03

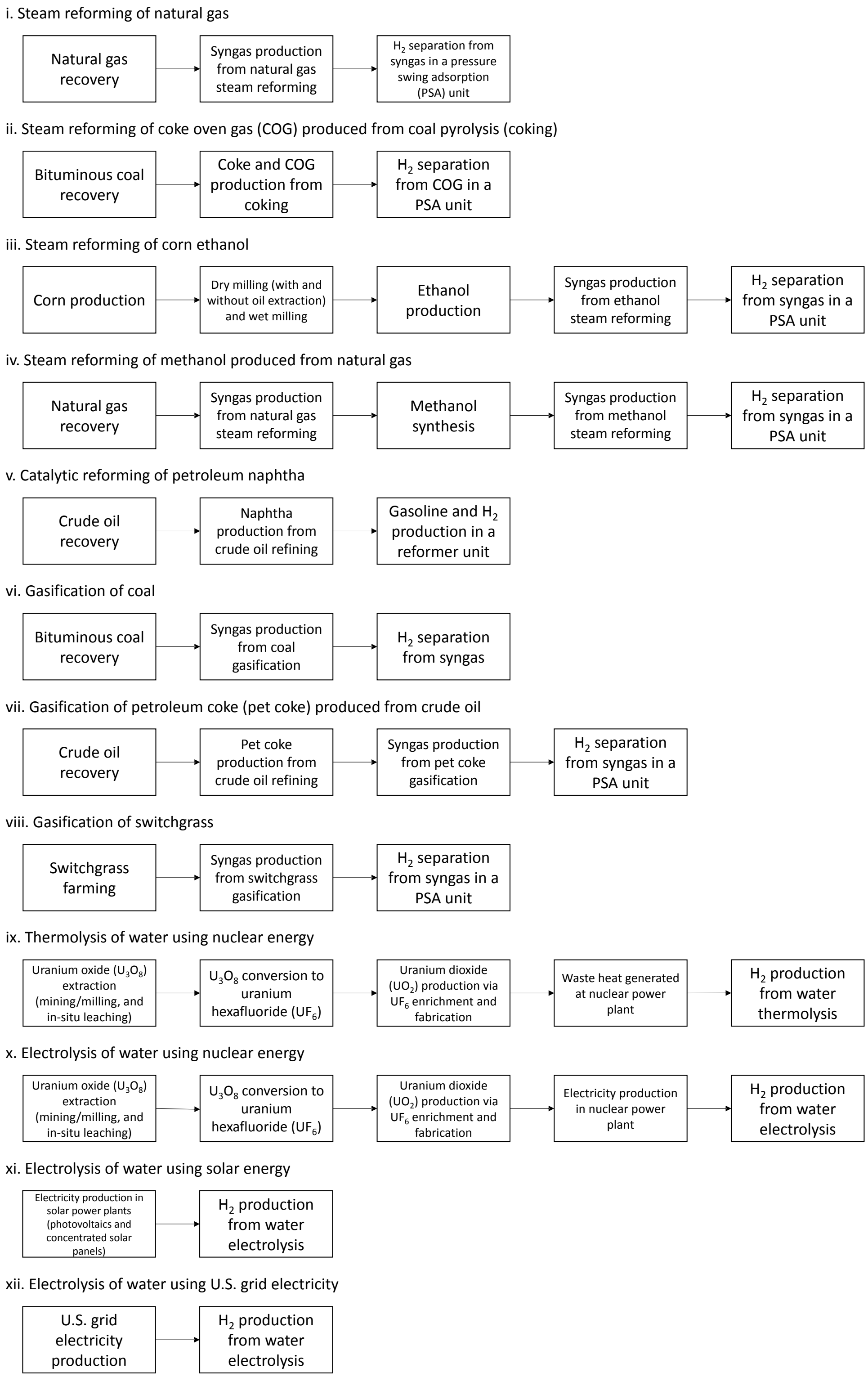

Figure S1. Process overview of the 12 hydrogen pathways employed in the lifecycle analysis calculations. Note that many lifecycle steps have been omitted for simplicity (e.g. transportation steps, water gas shift reaction, etc.).

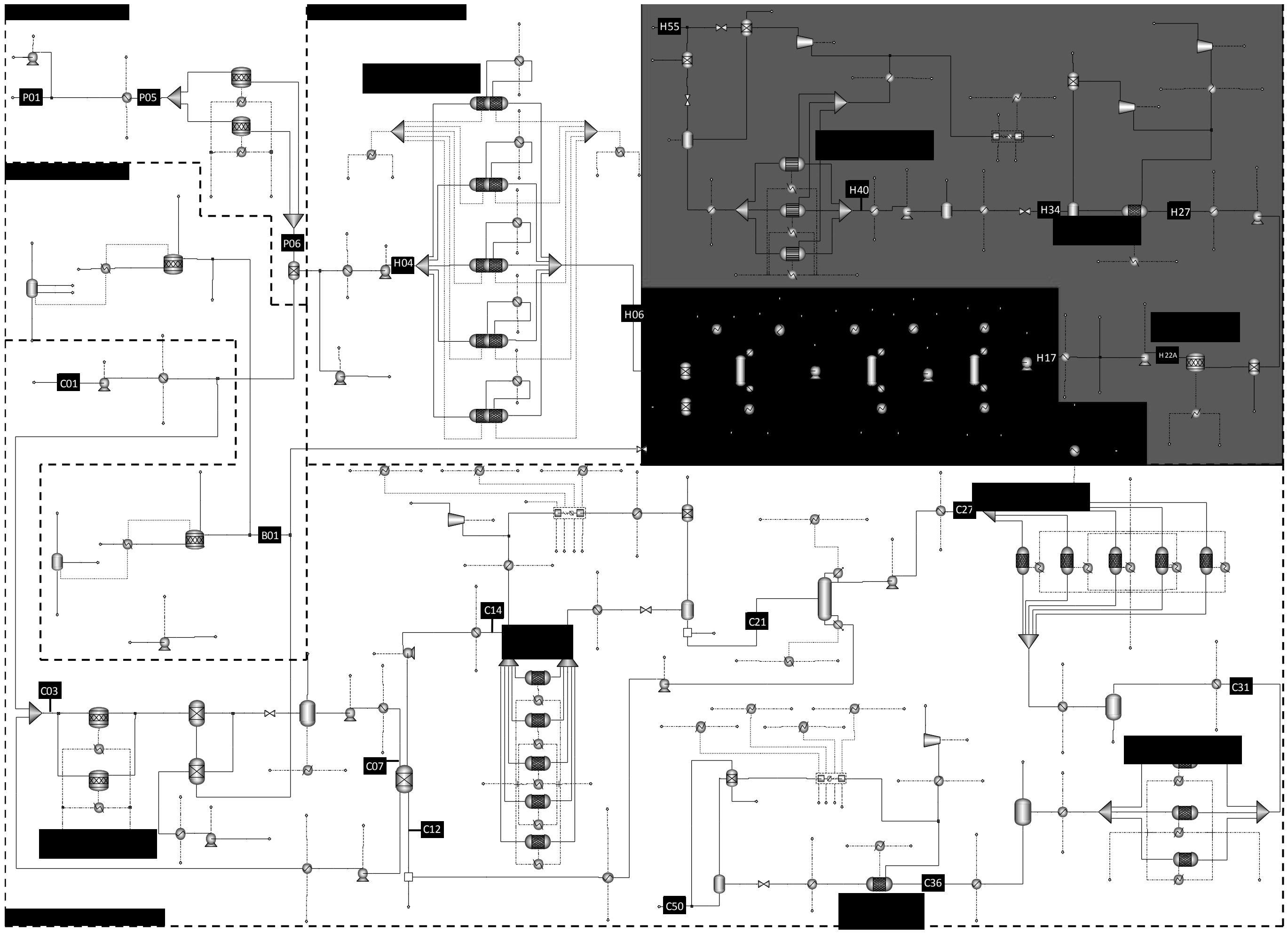

Figure S2. Aspen Plus® process flow diagram (PFD) of a single train outlining the four processing sections (pretreatment, cellulose processing, hemicellulose processing, utility) and the reactors. Unit operations in the shaded area do not exist in Biorefinery 4. Details of the streams shown are given for each Biorefinery model from Table S15 to Table S21. Recycle of streams utilized via calculator blocks are not visible in this PFD.

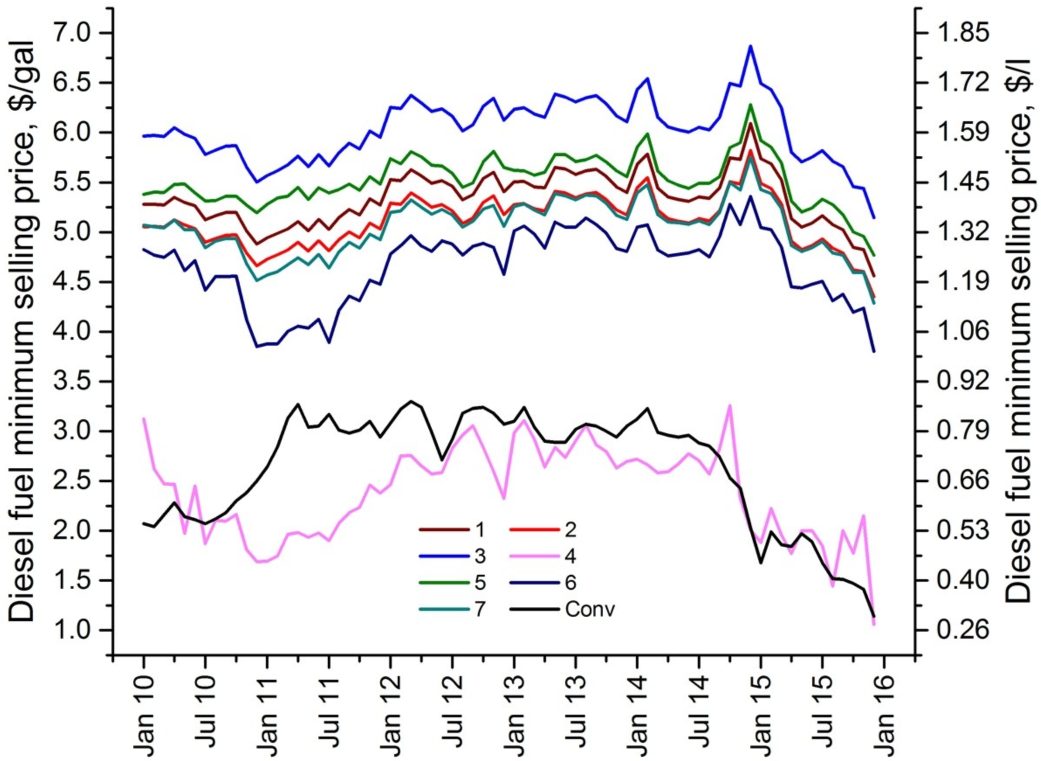

Figure S3. Minimum selling prices (MSP) of diesel fuels from the biorefinery models under consideration for the time period from January 2010-December 2015. Also shown are the conventional diesel fuel prices for comparison purposes.