Supporting Information

Meta-Analysis of Life Cycle Energy and Greenhouse Gas Emissions for Priority Bio-based Chemicals

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Part I: Method

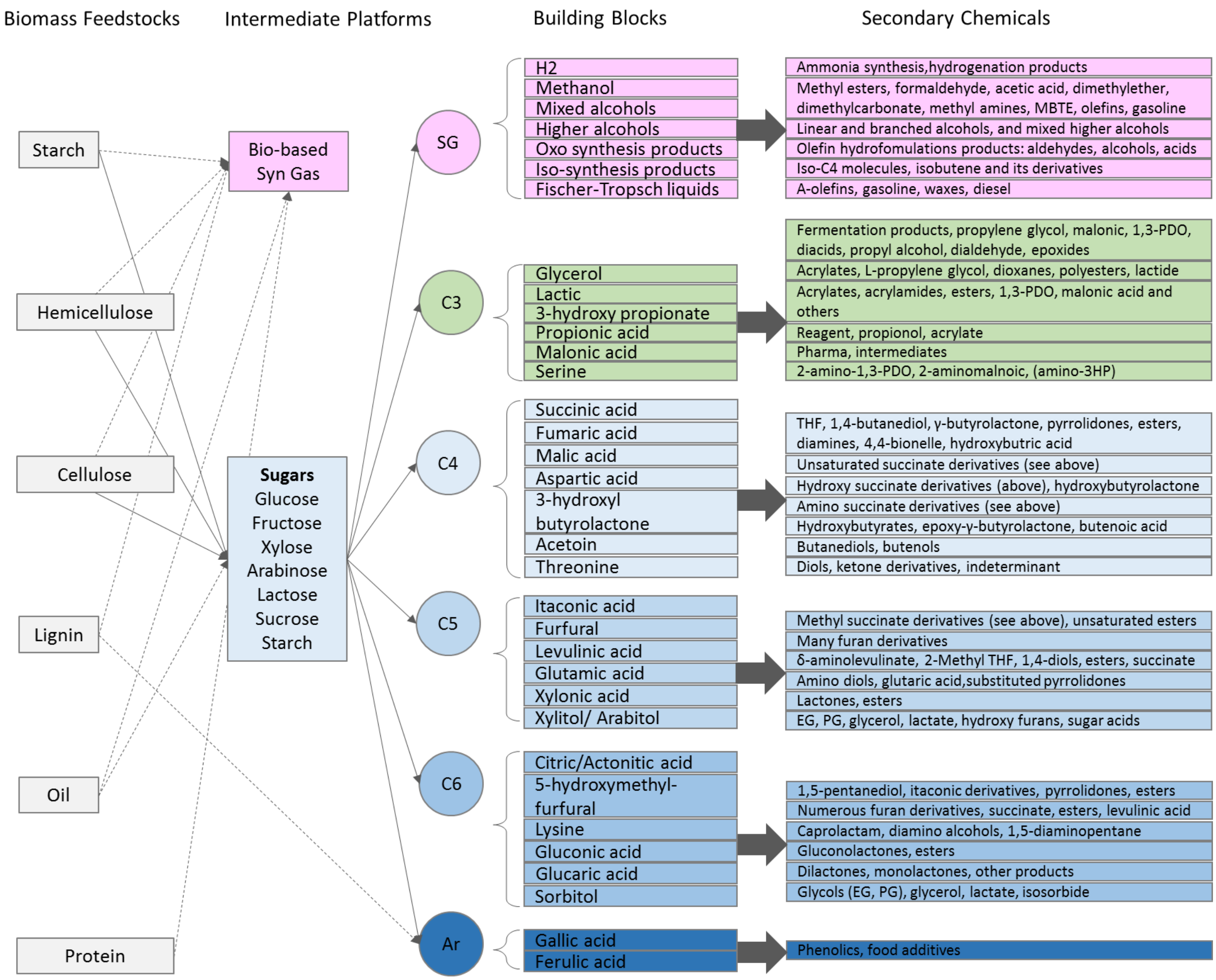

Figure S1. Primary building blocks and secondary chemicals (partially adopted and modified from figure 3 of the U.S. DOE repoert[1])

[1] Werpy, T.; Petersen, G.; Aden, A.; Bozell, J.; Holladay, J.; White, J.; Manheim, A.; Eliot, D.; Lasure, L.; Jones, S. *Top value added chemicals from biomass. Volume 1-Results of screening for potential candidates from sugars and synthesis gas*; DTIC Document: 2004.

Table S1. Life cycle GHG emission and energy use values for studied cases (including carbon sequestration)

Chemical	Feedstock	GHG (kg CO_2 eq./kg)	Energy Use (MJ/kg)	Note
Succinic acid	Corn Corn stover Lignocellulose sugarcane	-0.18 0.88 0.83-3.13 0.8-3.1 0.43 (-0.16)-2.13 (-0.2)-2.1 0.2-2.5	CED: 34.7 NREU: 32.7 NREU: 27-67 NREU: 28-66.5 Fossil fuel input: 28 NREU: 5-45 NREU: 5.4-44.9 NREU: 15-54.5	4 cases for corn grain, 1 case for corn stover, 2 cases for sugarcane and 1 for lignocellulosic source
Polyethylene furan dicarboxylate (PEF)	Corn starch	2.05	NREU: 33.8	Another case was also found for PEF from corn starch with just relative GHG reduction values
Propionic acid	Rapeseed meal Potato juice Sugarbeet Potato molasses artichoke	1.35 3.2 3.6 3.1 3.8	CED: 39 - - - -	Life cycle energy use was found for the first case from rapeseed meal
Itaconic acid	Softwood Corn	-0.36 0.75	CED: 15 CED: 24.8	
Polyjydroxy butyric acid (PHB)	Eucalyptus Poplar Sugarcane Corn	2.44 2.08 2.6 (-4)-(-1.6)	- - CED: 44.7 Fossil fuel input: (-6)-8	Life cycle energy use were reported for the last two cases
Xylitol	Corn stover Corn cobs Pulp and paper stream	-0.93 37.16 2.15	Fossil fuel input: 3 - -	Another case was found for pulp and paper stream which had the relative GHG reduction
Phenol	Poplar Eucalyptus	3.38 4.19	- -	Relative energy reductions were

				reported
Methanol	Waste wood	0.08	-	Relative energy reduction was reported
Vanillin	Wood Timber and wood chips	1.6 -0.09	NREU: 44.1 CED: 36.5	
Styrene	Forest residue	-0.002	Fossil fuel input: 0.14	
Adipic acid	Corn Lignin-based phenol Lignocellulosics sugarcane	0.20 9.2 9.2 -1.29 6 5.6 3.8	- NREU: 195 NREU: 44.5-195.4 CED: 35.5 NREU: 21.5-134.4 NREU: 86 NREU: 3.2-85.7	3 cases for corn grain, 1 case for lignin-based phenol, 1 case for lignocellulosics and 2 cases for sugarcane
Polylactic acid (PLA)	Corn Poplar Eucalyptus Sugarcane lignocellulosics	1.8 0.4-2.4 1.16-2.36 3.16 3.77 (-0.9)-1 (-0.13)-0.96 0.5 (-0.4)-1.5	Fossil fuel input:54 NREU: 40.1-60.8 NREU: 49-61 - - NREU: 13.2-32.9 NREU: 21-33 NREU: 30.45 NREU: 25.1-45.3	3 cases for corn, 1 case for poplar, 1 case for eucalyptus, 3 cases for sugarcane and 1 case for lignocellulosics
Polyhydroxy alkanoate (PHA)	Corn Corn stover Sugarcane lignocellulosics	0.48-4.48 (-0.22)-4.27 (-0.7)-6.9 0.25-0.5 (-3.7)-6.9 (-2.5)-6.9	NREU: 59.17-88 NREU: 38-112 NREU: 33.3- 111.6 NREU: 44-60 NREU: (-23.5)-109 NREU: 3.4-111.5	3 cases for corn, 1 case for corn stover, 1 case for sugarcane and 1 case for lignocellulosics
1,3-butadiene	Corn Wheat/rye/sugar beet sugarcane	2.3-4 1.04-2.18 2.04-3.62	NREU: 30-40 NREU: 90-115 NREU: 60-85	
Ethyl lactate	Corn	0.11-0.75	-	Energy use was not reported
p-xylene	Corn Red oak	5.5-9.86 1.13-2.49	- -	Energy use was not reported

Low density polyethylene (LDPE)	Corn Switchgrass Sugarcane	2.6 -2.9 -1.3 0.3-2.6	- - - CED: 102	1 case for corn grain, 1 case for switchgrass and two cases for sugarcane
Polyethylene (PE)	Corn stover	-0.75	Fossil fuel input: 32	
High density polyethylene (HDPE)	Sugarcane	(1.5)-(-0.3)	NREU: 18	
1,3-propanediol (PDO)	Corn Algae Sugarcane lignocellulosics	2.7 0.57-1.17 0.5-1.8 6.67 (-1.5)-(-0.5) (-1.7)-1.8 (-0.8)-1.8	Fossil fuel input: 43 NREU: 38-52 NREU: 19.8-91.5 Fossil fuel input: 120 NREU: (-9)-7 NREU: (-16.5)-63.5 NREU: (-16.5)-63.5	3 cases for corn grain, 1 case for algae (hydroxypropioni c acid) , 2 cases for sugarcane an d1 case for lignocellulosics
1,4-butanediol	Corn stover	1.05	Fossil fuel input: 45	
Acrylic acid	Algae	2.26	Fossil fuel input: 49	From hydroxypropionic acid derived from algae
Iso-butanol	Corn stover	0.31	Fossil fuel input: 38	
n-butanol	Corn Sugarcane Lignocellulosics	0.7-1.1 0.61-1.11 (-2.1)-(-1.7) (-2.18)-(-1.68) (-0.5)-(-1)	NREU: 6.6-63.9 NREU: 27-67 NREU: (-40.9)- 7.4 NREU: 27-67 NREU: (-19.8)- 32.5	2 cases from corn, 2 cases from sugarcane and 1 case from lignocellulosics
Acetic acid	Corn Sugarcane Lignocellulosics	4.23-6.63 4.2-6 2.33-4.72 2.3-4.7 3.1-5	NREU: 109-145 NREU: 38.9-144.9 NREU: 71-106 NREU: 17.6-106.3 NREU:27-123.4	2 cases for corn grain, 2 cases for sugarcane and 1 case for lignocellulosics

Table S2. Bio-based chemicals and their fossil-based counterpart- sourced from ecoinvent unit processes

Bio-based chemical	Fossil-based equivalent
Polyethylene furandicarboxylate (PEF)	Polyethylene terephthalate resin, at plant/kg NREL/RNA
Polyhydroxy alkanoate (PHA)	High density polyethylene resin, at plant/NREL/RNA
p-xylene	p-xylene, production, at plant/RER
Styrene	Styrene, at plant/ RER

Table S3. Bio-based chemicals and their fossil-based counterparts- sourced from literature

Bio-based chemical	Fossil-based equivalents
Succinic acid	Maleic anhydride, succinic acid
Polyethylene furandicarboxylate (PEF)	PET resin
Propionic acid	Propionic acid
Itaconic acid	Polyacrylic acid
Polyhydroxy butyric acid (PHB)	Polyethylene terephthalate (PET), low density polyethylene (LDPE)
Xylitol*	-
Phenol	Phenol (from cumene)
Methanol	Methanol
Vanillin	Formaldehyde resin
Styrene	Styrene
Adipic acid	Adipic acid
Polylactic acid (PLA)	Propylene resin (PP), polyethylene terephthalate (PET), polystyrene (PS)
Polyhydroxy alkanoate (PHA)	High density polyethylene (HDPE), polystyrene (PS)
1,3-butadiene	1,3-butadiene
Ethyl lactate	Polytrimethylene terephthalate (PTT)
p-Xylene	p-Xylene
Low density polyethylene (LDPE)	Low density polyethylene (LDPE)
Polyethylene	Polyethylene
High density polyethylene (HDPE)	High density polyethylene (HDPE)
1,3-propanediol (1,3-PDO)	1,3-propanediol (1,3-PDO)
1,4-butanediol	1,4-butanediol
Acrylic acid	Acrylic acid
Iso-butanol	Iso-butanol
n-Butanol	n-Butanol, maleic anhydride
Acetic acid	Acetic acid

* No data were found for the fossil-based equivalent of xylitol

Note: For each building block, several counterparts are considered sourcing from the case studies, second column in this table list all the counterparts considered for various cases

Table S4. Molecular complexity for select bio-based compounds

CAS #	Biochemical	Molecular Complexity	Note
106-99-0	1,3- butadiene	21	
504-63-2	1,3- propandiol	12.4	
110-63-4	1,4- butanediol	17.5	
503-66-2	3-hydroxypropionic acid	50	
64-19-7	Acetic Acid	31	
79-10-7	Acrylic acid	55.9	
124-04-9	Adipic acid	114	
7643-75-6	Arabinitol	76.1	*L-arabinitol
617-45-8	Aspartic acid	133	*L-aspartic acid
92-52-4	Biphenyl	100	
71-36-3	Butanol	13.1	
N/A	Cresol/Resorcinol	N/A	
110-82-7	Cyclohexane	15.5	
97-64-3	Ethyl Lactate	79.7	
56-81-5	Glycerol	25.2	
78-83-1	Isobutanol	17.6	
97-65-4	Itaconic acid	158	
N/A	Low-density polyethylene (LDPE)	N/A	
67-56-1	Methanol	2	
872-50-4	N-methylpyrrolidone	90.1	
106-42-3	P-Xylene	48.8	
108-95-2	Phenol	46.1	
N/A	Polyethylene	N/A	
N/A	Polyethylene (HDPE)	N/A	
N/A	Polyethylene furandicarboxylate (PEF)	N/A	
N/A	Polyhydroxyalkanoate (PHA)	N/A	
N/A	Polyhydroxybutyric acid (PHB)	N/A	
N/A	Polylactic acid (PLA)	N/A	
504-63-2	Propandiol (PDO)	12.4	*1,3-Propanediol
504-63-2	Propanediol	12.4	*1,3-Propanediol
79-09-4	Propionic acid	40.2	
57-55-6	Propylene glycol	20.9	
50-70-4	Sorbitol	105	*D-Sorbitol
100-42-5	Styrene	68.1	
110-15-6	Succinic acid	92.6	
121-34-6	Vanilic acid	168	
121-33-5	Vanillin	135	
87-99-0	Xylitol	76.1	

*Proxy Compound

Values for molecular complexity were obtained from PubChem.

Part II: Results

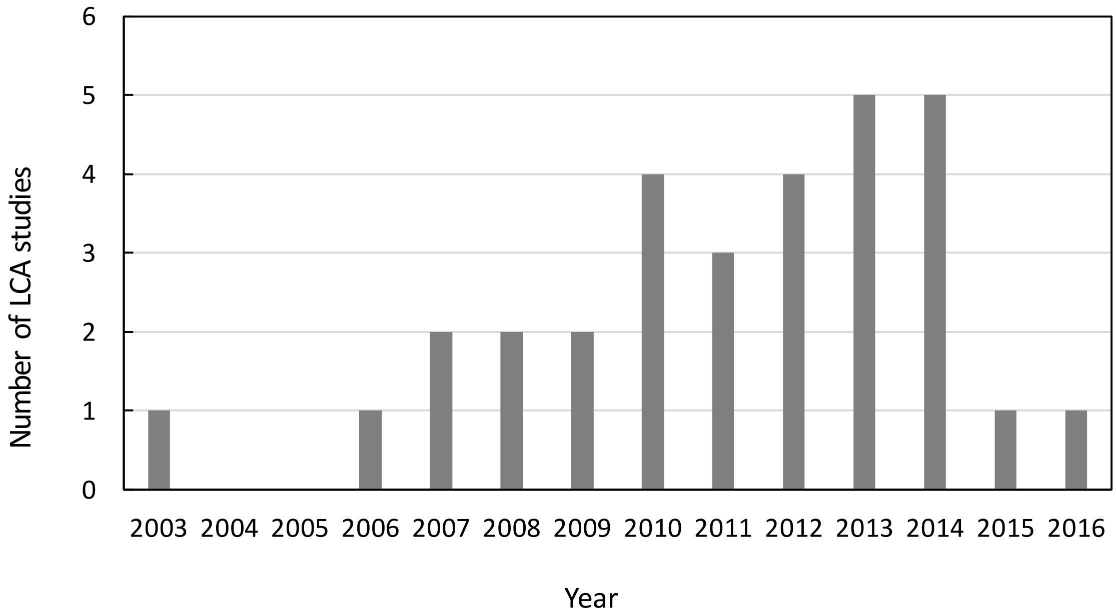

Figure S2. Trend of LCA publications under review

Table S5. Grouping information using the Tukey method and 90% confidence for factor, *Conversion Platform* for *response factor* absolute greenhouse gas emissions

Factor Level	N	Mean	Grouping
Thermochemical	7	6.68	A
Biochemical	57	2.024	B
Chemical	10	1.907	A B
Hybrid	9	0.903	B
Catalytic	1	0.2032	A B

Means that do not share a letter are significantly different

Table S6. Tukey simultaneous tests for differences of means, 90% confidence for factor, *Conversion Platform* for *response factor* absolute greenhouse gas emissions

Difference of Levels	Difference of Means	SE of Difference	90% CI	T-Value	Adjusted P-Value
Catalytic - Biochemical	-1.82	4.42	(-12.88, 9.24)	-0.41	0.994
Chemical - Biochemical	-0.12	1.5	(-3.88, 3.64)	-0.08	1
Hybrid - Biochemical	-1.12	1.57	(-5.05, 2.81)	-0.71	0.953
Thermochemical - Biochemical	**4.66**	**1.75**	**(0.27, 9.05)**	**2.66**	**0.07**
Chemical - Catalytic	1.7	4.59	(-9.80, 13.20)	0.37	0.996
Hybrid - Catalytic	0.7	4.62	(-10.86, 12.26)	0.15	1
Thermochemical - Catalytic	6.48	4.68	(-5.24, 18.20)	1.38	0.64
Hybrid - Chemical	-1	2.01	(-6.04, 4.03)	-0.5	0.987
Thermochemical - Chemical	4.78	2.16	(-0.63, 10.18)	2.21	0.186
Thermochemical - Hybrid	**5.78**	**2.21**	**(0.25, 11.31)**	**2.62**	**0.077**

Table S7. Analysis of Covariance (ANCOVA) for the response variable of *absolute greenhouse gas emissions* and covariate of *complexity*

Source	DF	Adj. SS	Adj. MS	F-Value	P-Value
Complexity	1	11.01	11.01	0.41	0.525
Error	58	1557.92	26.86		
Lack-of-Fit	18	481.48	26.75	0.99	0.486
Pure Error	40	1076.44	26.91		
Total	59	1568.93			

Table S8. Analysis of Covariance (ANCOVA) for the response variable of *relative greenhouse gas emissions* and covariate of *complexity*

Source	DF	Adj. SS	Adj. MS	F-Value	P-Value
Complexity	1	0.05	0.04996	0.07	0.788
Error	55	37.7326	0.68605		
Lack-of-Fit	17	23.0343	1.35496	3.5	0.001
Pure Error	38	14.6982	0.3868		
Total	56	37.7825			

Table S9. Analysis of Covariance (ANCOVA) for response variable of *absolute greenhouse gas emissions* and covariate of *molecular weight*

Source	**DF**	**Adj. SS**	**Adj. MS**	**F-Value**	**P-Value**
Molecular Weight	1	69.88	69.88	2.7	0.106
Error	58	1499.05	25.85		
Lack-of-Fit	16	247.95	15.5	0.52	0.921
Pure Error	42	1251.1	29.79		
Total	59	1568.93			

Table S10. Analysis of Covariance (ANCOVA) for response variable of *relative greenhouse gas emissions* and covariate of *molecular weight*

Source	**DF**	**Adj. SS**	**Adj. MS**	**F-Value**	**P-Value**
Molecular Weight	1	0.0089	0.00885	0.01	0.91
Error	55	37.7737	0.68679		
Lack-of-Fit	15	23.0469	1.53646	4.17	0
Pure Error	40	14.7268	0.36817		
Total	56	37.7825			

Table S11. 1-way Analysis of Variance (ANOVA) for response variable of *absolute greenhouse gas emissions*- 1st set of parameters

Source	**DF**	**Adj. SS**	**Adj. MS**	**F-Value**	**P-Value**
Feedstock	12	117.9	9.822	0.46	0.933
Error	73	1570.3	21.511		
Total	85	1688.2			

Factor**:** Feedstock; ***Levels*****:** 13; ***Values*****:** Algae, Artichoke, Corn, Lignocellulose, Mixed, Potato, Rapeseed, Residue, Sugarbeet, Sugarcane, Switchgrass, Waste, and Woody Biomass

Table S12. 1-way Analysis of Variance (ANOVA) for response variable of *relative greenhouse gas emissions*- 1st set of parameters

Source	**DF**	**Adj. SS**	**Adj. MS**	**F-Value**	**P-Value**
Feedstock	12	10.09	0.8406	1.4	0.184
Error	71	42.5	0.5986		
Total	83	52.59			

Factor: Feedstock; ***Levels***: 13; ***Values***: Algae, Artichoke, Corn, Lignocellulose, Mixed, Phenol, Potato, Rapeseed, Residue, Sugarbeet, Sugarcane, Switchgrass, Waste, and Woody Biomass

Table S13. 1-way Analysis of Variance (ANOVA) for the response variable of *absolute greenhouse gas emissions*- 2nd set of parameters

Source	DF	Adj. SS	Adj. MS	F-Value	P-Value
Composition	1	9.2	9.204	0.46	0.499
Error	84	1678.99	19.988		
Total	85	1688.2			

Factor: Building Blocks; ***Levels***: 2; ***Values***: Sugar, Lignin

Table S14. 1-way Analysis of Variance (ANOVA) for the response variable of *relative greenhouse gas emissions*- 2nd set of parameters

Source	DF	Adj. SS	Adj. MS	F-Value	P-Value
Composition	1	0.4264	0.4264	0.67	0.415
Error	82	52.1613	0.6361		
Total	83	52.5877			

Factor: Building Blocks; ***Levels***: 2; ***Values***: Sugar, Lignin

Table S15. 1-way Analysis of Variance (ANOVA) for the response variable of *absolute greenhouse gas emissions*- 3rd set of parameters

Source	DF	Adj. SS	Adj. MS	F-Value	P-Value
Conversion Platform	4	162.1	40.54	2.11	0.087
Error	79	1516	19.19		
Total	83	1678.1			

Factor: Conversion; ***Levels***: 5; ***Values***: Biochemical, Catalytic, Chemical, Hybrid, Thermochemical

Table S16. 1-way Analysis of Variance (ANOVA) for the response variable of *relative greenhouse gas emissions*- 3rd set of parameters

Source	DF	Adj. SS	Adj. MS	F-Value	P-Value
Conversion Platform	4	1.17	0.2925	0.45	0.77
Error	78	50.34	0.6454		
Total	82	51.51			

Factor: Conversion; ***Levels***: 5; ***Values***: Biochemical, Catalytic, Chemical, Hybrid, Thermochemical

Table S17. 1-way Analysis of Variance (ANOVA) for the response variable of *absolute greenhouse gas emissions*- 4th set of parameters

Source	DF	Adj. SS	Adj. MS	F-Value	P-Value
Geography	4	28.4	7.1	1.41	0.242
Error	54	271.2	5.022		
Total	58	299.6			

Factor: Geography; ***Levels***: 5; ***Values***: Thailand, Europe, USA, Canada, and Brazil

Table S18. 1-way Analysis of Variance (ANOVA) for the response variable of *relative greenhouse gas emissions*- 4th set of parameters

Source	DF	Adj. SS	Adj. MS	F-Value	P-Value
Geography	4	0.5438	0.1359	0.17	0.954
Error	55	44.6105	0.8111		
Total	59	45.1543			

Factor: Geography; ***Levels***: 5; ***Values***: Thailand, Europe, USA, Canada, and Brazil

Table S19. 1-way Analysis of Variance (ANOVA) for the response variable of *absolute greenhouse gas emissions*- 5th set of parameters

Source	DF	Adj. SS	Adj. MS	F-Value	P-Value
LCA Coproduct Handling Method	3	16	5.333	0.91	0.439
Error	65	378.91	5.829		
Total	68	394.9			

Factor: LCA Coproduct Handling Method; ***Levels***: 4; ***Values***: Economic, Hybrid, Mass, System Boundary Expansion

Table S20. 1-way Analysis of Variance (ANOVA) for the response variable of *relative greenhouse gas emissions*- 5th set of parameters

Source	DF	Adj. SS	Adj. MS	F-Value	P-Value
LCA Coproduct Handling Method	3	0.9539	0.318	0.42	0.742
Error	63	48.1231	0.7639		
Total	66	49.077			

Factor: LCA Coproduct Handling Method; ***Levels***: 4; ***Values***: Economic, Hybrid, Mass, System Boundary Expansion

Table S21. 1-way Analysis of Variance (ANOVA) for the response variable of *absolute greenhouse gas emissions*- 6th set of parameters

Source	DF	Adj. SS	Adj. MS	F-Value	P-Value
Land Use Change	2	27.07	13.53	0.68	0.511
Error	83	1661.13	20.01		
Total	85	1688.2			

Factor: Land Use Change; ***Levels***: 3; ***Values***: No LUC, dLUC, and dLUC & ILUC
Land Use Change (LUC); Direct Land Use Change (dLUC); Indirect Land Use Change (ILUC)

Table S22. 1-way Analysis of Variance (ANOVA) for the response variable of *relative greenhouse gas emissions*- 6th set of parameters

Source	DF	Adj. SS	Adj. MS	F-Value	P-Value
Land Use Change	2	1.656	0.8282	1.32	0.274
Error	81	50.931	0.6288		
Total	83	52.588			

Factor: Land Use Change; ***Levels***: 3; ***Values***: No LUC, dLUC, and dLUC & ILUC
Land Use Change (LUC); Direct Land Use Change (dLUC); Indirect Land Use Change (ILUC)

Table S23. ANCOVA and ANOVA summary results for bio-based chemicals greenhouse gas emissions meta-data

Parameter	Covariate or Factor	Factor Levels	Response Factor	P-value	Statistically Significant (α = 10%)
Complexity	Covariate	-	GHG Absolute	0.525	No
Complexity	Covariate	-	GHG Relative	0.788	No
Molecular Weight	Covariate	-	GHG Absolute	0.106	No
Molecular Weight	Covariate	-	GHG Relative	0.91	No
Feedstock	Factor	13	GHG Absolute	0.933	No
Feedstock	Factor	13	GHG Relative	0.184	No
Composition	Factor	2	GHG Absolute	0.499	No
Composition	Factor	2	GHG Relative	0.415	No
Conversion Platform	**Factor**	**5**	GHG Absolute	0.087	Yes
Conversion Platform	Factor	5	GHG Relative	0.77	No
Geography	Factor	5	GHG Absolute	0.242	No
Geography	Factor	5	GHG Relative	0.954	No
LCA Coproduct Handling Method	Factor	4	GHG Absolute	0.439	No
LCA Coproduct Handling Method	Factor	4	GHG Relative	0.742	No
Land Use Change	Factor	3	GHG Absolute	0.511	No
Land Use Change	Factor	3	GHG Relative	0.274	No

Table S24. Grouping information using the Tukey method and 90% confidence for factor, *Conversion Platform* for *response factor* absolute nonrenewable energy use

Factor Level	N	Mean	Grouping
Thermochemical	1	2.600	A
Hybrid	4	-0.131	B
Biochemical	38	-0.2976	B
Chemical	1	-0.5000	B

Means that do not share a letter are significantly different

Table S25. Tukey simultaneous tests for differences of means, 90% confidence for factor, *Conversion Platform* for *response factor* absolute nonrenewable energy use

Difference of Levels	Difference of Means	SE of Difference	90% CI	T-Value	Adjusted P-Value
Chemical - Biochemical	-0.202	0.555	(-1.517, 1.112)	-0.36	0.983
Hybrid - Biochemical	0.166	0.288	(-0.516, 0.848)	0.58	0.938
Thermochemical - Biochemical	**2.898**	**0.555**	**(1.583, 4.212)**	**5.22**	**0**
Hybrid - Chemical	0.369	0.612	(-1.082, 1.819)	0.6	0.931
Thermochemical - Chemical	**3.1**	**0.774**	**(1.266, 4.934)**	**4**	**0.001**
Thermochemical - Hybrid	**2.731**	**0.612**	**(1.281, 4.182)**	**4.46**	**0**

Table S26. Grouping information using the Tukey method and 90% confidence for factor, *LCA Coproduct Handling Method* for *response factor* absolute nonrenewable energy use

Factor Level	N	Mean	Grouping
Mass	5	0.493	A
Hybrid	36	-0.2833	B
Economic	1	-0.7300	AB
System Expansion	1	-0.7700	AB

Means that do not share a letter are significantly different

Table S27. Tukey simultaneous tests for differences of means, 90% confidence for factor, *LCA Coproduct Handling Method* for *response factor* absolute nonrenewable energy use

Difference of Levels	Difference of Means	SE of Difference	90% CI	T-Value	Adjusted P-Value
Hybrid - Economic	0.447	0.669	(-1.137, 2.030)	0.67	0.908
Mass – Economic	1.223	0.722	(-0.488, 2.934)	1.69	0.341
System Expansion - Economic	-0.04	0.933	(-2.249, 2.169)	-0.04	1
Mass - Hybrid	**0.776**	**0.315**	**(0.031, 1.522)**	**2.47**	**0.081**
System Expansion - Hybrid	-0.487	0.669	(-2.070, 1.097)	-0.73	0.885
System Expansion - Mass	-1.263	0.722	(-2.974, 0.448)	-1.75	0.313

Table S28. Grouping information using the Tukey method and 90% confidence for factor, *Land Use Change* for *response factor* absolute nonrenewable energy use

Factor Level	N	Mean	Grouping
dLUC & ILUC	2	0.92	A
No LUC	39	-0.2366	B
dLUC	4	-0.6112	B

Means that do not share a letter are significantly different

Table S29. Tukey simultaneous tests for differences of means, 90% confidence for factor, *Land Use Change* for *response factor* absolute nonrenewable energy use

Difference of Levels	Difference of Means	SE of Difference	90% CI	T-Value	Adjusted P-Value
dLUC – No LUC	-0.375	0.335	(-1.081, 0.331)	-1.12	0.508
dLUC & ILUC – No LUC	**1.152**	**0.463**	**(0.177, 2.126)**	**2.49**	**0.044**
dLUC & ILUC – dLUC	**1.526**	**0.553**	**(0.362, 2.691)**	**2.76**	**0.023**

Table S30. Analysis of Covariance (ANCOVA) for the response variable of *absolute nonrenewable energy use* and covariate of *complexity*

Source	DF	Adj. SS	Adj. MS	F-Value	P-Value
Complexity	1	4426	4426	2.57	0.12
Error	28	48175	1721		
Lack-of-Fit	5	24825	4965	4.89	0.003
Pure Error	23	23350	1015		
Total	29	52601			

Table S31. Analysis of Covariance (ANCOVA) for the response variable of *relative absolute nonrenewable energy use* and covariate of *complexity*

Source	DF	Adj. SS	Adj. MS	F-Value	P-Value
Complexity	1	0.0096	0.00963	0.03	0.874
Error	28	10.4454	0.37305		
Lack-of-Fit	5	6.3124	1.26248	7.03	0
Pure Error	23	4.133	0.1797		
Total	29	10.455			

Table S32. Analysis of Covariance (ANCOVA) for response variable of *absolute nonrenewable energy use* and covariate of *molecular weight*

Source	DF	Adj. SS	Adj. MS	F-Value	P-Value
Molecular Weight	1	1557	1557	0.85	0.363
Error	28	51043	1823		
Lack-of-Fit	5	27693	5539	5.46	0.002
Pure Error	23	23350	1015		
Total	29	52601			

Table S33. Analysis of Covariance (ANCOVA) for response variable of *relative nonrenewable energy use* and covariate of *molecular weight*

Source	DF	Adj. SS	Adj. MS	F-Value	P-Value
Molecular Weight	1	0.4714	0.4714	1.32	0.26
Error	28	9.9836	0.3566		
Lack-of-Fit	5	5.8506	1.1701	6.51	0.001
Pure Error	23	4.133	0.1797		
Total	29	10.455			

Table S34. 1-way Analysis of Variance (ANOVA) for response variable of *absolute nonrenewable energy use* - 1st set of parameters

Source	DF	Adj. SS	Adj. MS	F-Value	P-Value
Feedstock	5	9823	1965	1.49	0.214
Error	39	51268	1315		
Total	44	61091			

Factor**:** Feedstock; ***Levels*****:** 13; ***Values*****:** Algae, Artichoke, Corn, Lignocellulose, Mixed, Potato, Rapeseed, Residue, Sugarbeet, Sugarcane, Switchgrass, Waste, and Woody Biomass

Table S35. 1-way Analysis of Variance (ANOVA) for response variable of *relative nonrenewable energy use* - 1st set of parameters

Source	DF	Adj. SS	Adj. MS	F-Value	P-Value
Feedstock	5	2.543	0.5087	1.12	0.367
Error	39	17.755	0.4553		
Total	44	20.299			

Factor: Feedstock; ***Levels***: 13; ***Values***: Algae, Artichoke, Corn, Lignocellulose, Mixed, Phenol, Potato, Rapeseed, Residue, Sugarbeet, Sugarcane, Switchgrass, Waste, and Woody Biomass

Table S36. 1-way Analysis of Variance (ANOVA) for the response variable of *absolute nonrenewable energy use* - 2nd set of parameters

Source	**DF**	**Adj. SS**	**Adj. MS**	**F-Value**	**P-Value**
Composition	1	66.2	66.22	0.05	0.83
Error	43	61024.3	1419.17		
Total	44	61090.6			

Factor: Building Blocks; ***Levels***: 2; ***Values***: Sugar, Lignin

Table S37. 1-way Analysis of Variance (ANOVA) for the response variable of *relative nonrenewable energy use* - 2nd set of parameters

Source	**DF**	**Adj. SS**	**Adj. MS**	**F-Value**	**P-Value**
Composition	1	0.0809	0.08094	0.17	0.68
Error	43	20.2178	0.47018		
Total	44	20.2988			

Factor: Building Blocks; ***Levels***: 2; ***Values***: Sugar, Lignin

Table S38. 1-way Analysis of Variance (ANOVA) for the response variable of *absolute nonrenewable energy use* - 3rd set of parameters

Source	**DF**	**Adj. SS**	**Adj. MS**	**F-Value**	**P-Value**
Conversion Platform	3	490.6	163.5	0.11	0.954
Error	40	60129.9	1503.2		
Total	43	60620.5			

Factor: Conversion; ***Levels***: 5; ***Values***: Biochemical, Catalytic, Chemical, Hybrid, Thermochemical

Table S39. 1-way Analysis of Variance (ANOVA) for the response variable of *relative nonrenewable energy use* - 3rd set of parameters

Source	**DF**	**Adj. SS**	**Adj. MS**	**F-Value**	**P-Value**
Conversion Platform	3	8.291	2.7637	9.22	0
Error	40	11.995	0.2999		
Total	43	20.286			

Factor: Conversion; ***Levels***: 5; ***Values***: Biochemical, Catalytic, Chemical, Hybrid, Thermochemical

Table S40. 1-way Analysis of Variance (ANOVA) for the response variable of *absolute nonrenewable energy use* - 4th set of parameters

Source	DF	Adj. SS	Adj. MS	F-Value	P-Value
Geography	4	2079	519.6	0.57	0.689
Error	26	23837	916.8		
Total	30	25916			

Factor: Geography; ***Levels***: 5; ***Values***: Thailand, Europe, USA, Canada, and Brazil

Table S41. 1-way Analysis of Variance (ANOVA) for the response variable of *relative nonrenewable energy use* - 4th set of parameters

Source	DF	Adj. SS	Adj. MS	F-Value	P-Value
Geography	4	0.8092	0.2023	0.4	0.809
Error	26	13.241	0.5093		
Total	30	14.0502			

Factor: Geography; ***Levels***: 5; ***Values***: Thailand, Europe, USA, Canada, and Brazil

Table S42. 1-way Analysis of Variance (ANOVA) for the response variable of *absolute nonrenewable energy use* - 5th set of parameters

Source	DF	Adj. SS	Adj. MS	F-Value	P-Value
LCA Coproduct Handling Method	3	1787	595.6	0.4	0.757
Error	39	58775	1507.1		
Total	42	60562			

Factor: LCA Coproduct Handling Method; ***Levels***: 4; ***Values***: Economic, Hybrid, Mass, System Boundary Expansion

Table S43. 1-way Analysis of Variance (ANOVA) for the response variable of *relative nonrenewable energy use* - 5th set of parameters

Source	DF	Adj. SS	Adj. MS	F-Value	P-Value
LCA Coproduct Handling Method	3	3.247	1.0825	2.49	0.075
Error	39	16.959	0.4348		
Total	42	20.206			

Factor: LCA Coproduct Handling Method; ***Levels***: 4; ***Values***: Economic, Hybrid, Mass, System Boundary Expansion

Table S44. 1-way Analysis of Variance (ANOVA) for the response variable of *absolute greenhouse gas emissions*- 6th set of parameters

Source	DF	Adj. SS	Adj. MS	F-Value	P-Value
Land Use Change	2	1539	769.5	0.54	0.585
Error	42	59552	1417.9		
Total	44	61091			

Factor: Land Use Change; ***Levels***: 3; ***Values***: No LUC, dLUC, and dLUC & ILUC
Land Use Change (LUC); Direct Land Use Change (dLUC); Indirect Land Use Change (ILUC)

Table S45. 1-way Analysis of Variance (ANOVA) for the response variable of *relative nonrenewable energy use* - 6th set of parameters

Source	DF	Adj. SS	Adj. MS	F-Value	P-Value
Land Use Change	2	3.199	1.5997	3.93	0.027
Error	42	17.099	0.4071		
Total	44	20.299			

Factor: Land Use Change; ***Levels***: 3; ***Values***: No LUC, dLUC, and dLUC & ILUC
Land Use Change (LUC); Direct Land Use Change (dLUC); Indirect Land Use Change (ILUC)

Table S46. ANCOVA and ANOVA summary results for bio-based chemicals nonrenewable energy use meta-data

Parameter	Covariate or Factor	Factor Levels	Response Factor	P-value	Statistically Significant (α = 10%)
Complexity	Covariate	-	NREU Absolute	0.12	No
Complexity	Covariate	-	NREU Relative	0.874	No
Molecular Weight	Covariate	-	NREU Absolute	0.363	No
Molecular Weight	Covariate	-	NREU Relative	0.26	No
Feedstock	Factor	13	NREU Absolute	0.214	No
Feedstock	Factor	13	NREU Relative	0.367	No
Composition	Factor	2	NREU Absolute	0.83	No
Composition	Factor	2	NREU Relative	0.68	No
Conversion Platform	Factor	4	NREU Absolute	0.954	No
Conversion Platform	**Factor**	**4**	**NREU Relative**	**0**	**Yes**
Geography	Factor	5	NREU Absolute	0.689	No
Geography	Factor	5	NREU Relative	0.809	No
LCA Coproduct Handling Method	Factor	4	NREU Absolute	0.757	No
LCA Coproduct Handling Method	**Factor**	**4**	**NREU Relative**	**0.075**	**Yes**
Land Use Change	Factor	3	NREU Absolute	0.585	No
Land Use Change	**Factor**	**3**	**NREU Relative**	**0.027**	**Yes**

Table S47. 1-way Analysis of Variance (ANOVA) for the *response variable* of Greenhouse Gas Emissions (Absolute)

Source	DF	Adj. SS	Adj. MS	F-Value	P-Value
Plant Capacity	**2**	**157.5**	**78.77**	**3.99**	**0.022**
Error	77	1520.6	19.75		
Total	79	1678.1			

Factor: Plant Capacity; ***Levels***: 3; ***Values***: Commercial Scale, Pilot Scale, Lab Scale

Table S48. Grouping Information Using the Tukey Method and 90% Confidence for Factor *Plant Capacity* with response factor *GHG Absolute*

Factor Level	N	Mean	Grouping
Pilot Scale	5	7.44	A
Lab Scale	11	2.862	A B
Commercial Scale	64	1.705	B

Means that do not share a letter are significantly different

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Table S49. Tukey Simultaneous Tests for Differences of Means, 90% Confidence for Factor *Plant Capacity* with response factor *GHG Absolute*

Difference of Levels	Difference of Means	SE of Difference	90% CI	T-Value	Adjusted P-Value
Lab Scale - Commercial Scale	1.16	1.45	(-1.87, 4.18)	0.80	0.706
Pilot Scale - Commercial Scale	**5.73**	**2.06**	**(1.43, 10.04)**	**2.78**	**0.019**
Pilot Scale - Lab Scale	4.57	2.40	(-0.42, 9.57)	1.91	0.143

Table S50. 1 Way Analysis of Variance (ANOVA) for the *Response Variable*: Greenhouse Gas Emissions (Relative)

Source	DF	Adj. SS	Adj. MS	F-Value	P-Value
Plant Capacity	**2**	**3.139**	**1.5695**	**2.43**	**0.095**
Error	74	47.821	0.6462		
Total	76	50.960			

Factor: Plant Capacity; ***Levels***: 3; ***Values***: Commercial Scale, Pilot Scale, Lab Scale

Table S51. Grouping Information Using the Tukey Method and 90% Confidence for Factor *Plant Capacity* with response factor *GHG Relative*

Factor Level	N	Mean	Grouping
Lab Scale	11	-0.084	A
Commercial Scale	64	-0.5992	A
Pilot Scale	2	-1.098	A

Means that do not share a letter are significantly different

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Table S52. Tukey Simultaneous Tests for Differences of Means, 90% Confidence for Factor *Plant Capacity* with response factor *GHG Relative*

Difference of Levels	Difference of Means	SE of Difference	90% CI	T-Value	Adjusted P-Value
Lab Scale - Commercial Scale	0.516	0.262	(-0.032, 1.063)	1.96	0.128
Pilot Scale - Commercial Scale	-0.499	0.577	(-1.703, 0.705)	-0.87	0.664
Pilot Scale - Lab Scale	-1.015	0.618	(-2.304, 0.274)	-1.64	0.235

Table S53. CO_2 emissions from EOL phase of bio-based and fossil-based chemicals

Bio-based chemical/ fossil-based counterpart	EOL CO_2 emissions (kg CO_2/ kg)	Comparative EOL results (bio-based relative to fossil-based chemicals)
Succinic acid	1.49	-17%
Adipic acid	1.80	
Succinic acid	1.49	-17%
Maleic anhydride	1.79	
PEF	1.92	-39%
PET	3.14	
Itaconic acid	1.69	-7%
Polyacrylic acid	1.83	
PHB	1.69	-32%
PET	2.50	
PHB	1.69	-46%
LDPE	3.13	
PLA	1.46	-53%
PET	3.14	
PLA	1.46	-56%
PS	3.37	
PLA	1.46	-53%
PP	3.13	
PHA	2.04	-35%
HDPE	3.15	
PHA	2.04	-38%
PS	3.37	
Ethyl lactate	1.86	-20%
PTT	2.34	

Table S54. Cradle-to-grave GHG emissions for bio-based chemicals relative to petrochemical counterparts

Bio-based chemical	Cradle-to-grave GHG emissions, % change from petrochemical counterpart		
	Low value	Average	High value
Succinic acid	-92%	-70%	-46%
PEF	-	-47%	-
Propionic acid	-40%	-22%	-11%
Itaconic acid	-71%	-59%	-46%
PHB	-138%	-61%	-31%
Phenol	-28%	-23%	-19%
Methanol	-	-15%	-
Vanillin	-54%	-37%	-19%
Adipic acid	-89%	12%	90%
PLA	-91%	-57%	-35%
PHA	-135%	-26%	89%
1,3-butadiene	-20%	7%	35%
Ethyl lactate	-65%	-59%	-54%
LDPE	-95%	-44%	16%
PE	-	-114%	-
HDPE	-68%	-56%	-45%
Propanediol	-99%	-62%	-42%
1,4-Butanediol	-	-64%	-
i-Butanol	-	-63%	-
n-Butanol	-97%	-64%	-19%
Acetic acid	-36%	9%	70%
p-Xylene	34%	143%	298%
Acrylic acid	-83%	-61%	-61%

[*] Note: For some of the bio-based chemicals mentioned in this table, cradle to grave GHG results are available from the reference studies and may be different from what reported here. For the values mentioned in this table, the main assumption is that, the carbon content in the composition of each building block is going to be released as CO_2 during EOL scenarios.