Platform Chemicals from Biomass Fermentation

a Report Prepared for Chemistry Innovation KTN

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Platform Chemicals from Biomass Fermentation

The following table shows the main platform chemicals and derivatives that could be derived from processing of plant biomass in a biorefinery, and includes glycerol generated as a by-product from bio-diesel.

The material name, structure, applications and current production volumes are given if available.

The principal sources of information used were:

- "Medium and Long-term Opportunities and Risks of the Biotechnological Production of Bulk Chemicals from Renewable Resources - The Potential of White Biotechnology", final report of the BREW project, University of Utrecht, 2006
- "Top Value Added Chemicals from Biomass: Volume I—Results of Screening for Potential Candidates from Sugars and Synthesis Gas" National Renewable Energy Laboratory, Pacific NorthWest National Laboratory, US Department of Energy Biomass Programme, 2004
- "Handbook of Industrial Chemistry - Organic Chemicals" Ali, Mohammad Farhat; El Ali, Bassam M.; Speight, James G. © 2005 McGraw-Hill
- www.wikipedia.org

The table covers a selection of the potential platform chemicals and derivatives that are reported in these and other publications. The criteria for selection were:

- Could be produced from a feedstock suitable for biofuel production
- Known biotechnological or chemical route to material
- Known or predicted industrial application

Direct extracts from plant biomass (eg plant sterols, artemisinin, plant waxes etc) have been excluded from this table.

General Points

The chemicals produced from a fermentation biorefinery have two important characteristics:

- They are typically oxygenates

  Starting from sugars and starches which are highly oxygenated, the vast majority of potential platform chemicals that have been described also carry at least one oxygen atom – sometimes several. This is important for downstream processing. The petrochemical based chemical industry traditionally manipulates the main structure of a molecule as a hydrocarbon; adding hetero-atoms at a later stage in the process. In contrast, when starting from bio-based platform chemicals oxygen is almost always already present. This dramatically changes the synthetic strategies for reaching target molecules. As a result bio-based platform chemicals cannot easily be introduced into the material flows for the current mainstream chemical industry.

- They are typically multifunctional

  The majority of the platform chemicals and their derivatives have more than one functional group available for further reaction. This multifunctional nature makes them extremely flexible when devising synthetic strategies, and makes them particularly appropriate for polymerisation reactions; e.g. the production of polyesters, polyethers and polyurethanes.

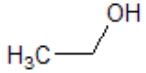
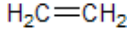
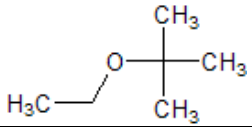
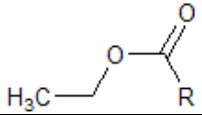
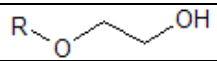
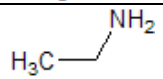
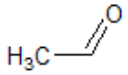
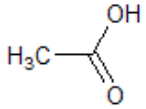
Given these characteristics, the platform chemicals and their derivatives listed currently find application in:

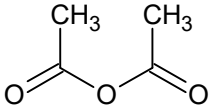
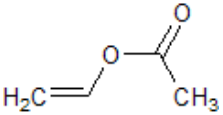
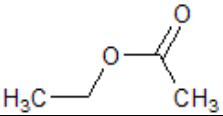
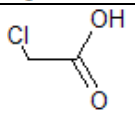
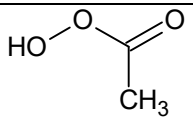
- Fuel and fuel additives
- Solvents
- Polymers
- Coatings adhesives sealants and elastomers
- Lubricants and hydraulic fluids
- Surfactants
- Cosmetic ingredients

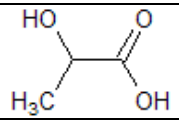
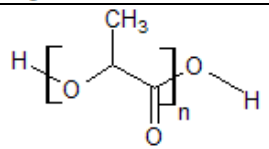
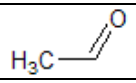
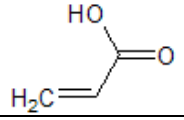
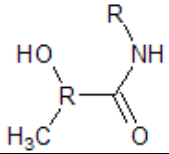
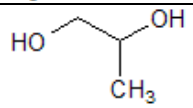
Notes on the Tables

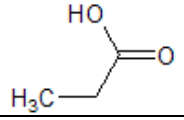
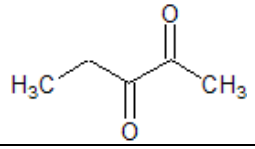
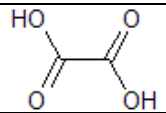
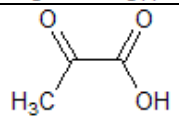
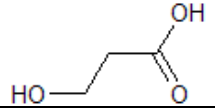
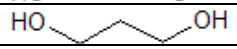
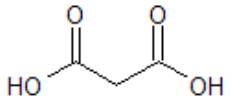
The tables in this appendix show information about the platform chemicals and their derivatives. The column headings are:

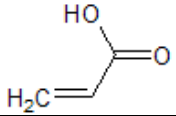
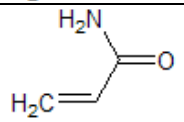
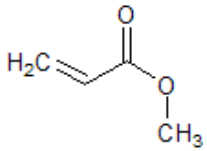
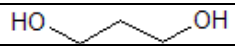
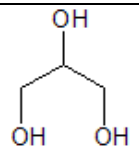
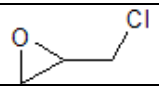
- Carbon number — Number of carbon atoms in the backbone of the platform chemical. Ranges from 2 to 6.
- Platform chemical — The name of the platform chemical with a specific carbon number.
- Derivative — The name of a derivative of a specific platform chemical.
- Structure — The molecular structure of the platform chemical or derivative. In cases where the structure is variable, either no structure or a ‘typical’ structure is given.
- Applications — Known or predicted applications of the platform chemical or derivative. Almost all of these are current commercial applications.
- Production — Information on the global production of the chemical where known.

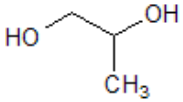
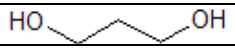
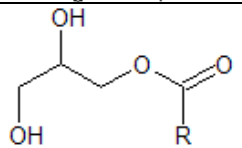
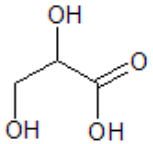
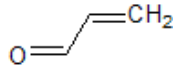
Carbon Number	Platform Chemical	Derivatives	Structure	Applications	Production
2	Ethanol			▪ 70% fuel, ▪ 20% industrial, ▪ 10% beverages	40bn litres in 2003. >90% by fermentation.
		Ethylene		Key chemical building block : ▪ Polyethylene ▪ PVC ▪ Ethylene oxide ▪ Ethylene glycols	94 Mt (2002)
		Ethyl *tert*-butyl ether		Fuel additive. Competes with MTBE and Ethanol	5 bn litres p.a.
		Ethyl esters		Greener solvents	1 Mt p.a. of ethyl acetate
		Ethylethers		Solvents and medical applications	
		Glycolethers		Solvents – cellosolve and carbitols	
		Ethylamine		▪ Solvent ▪ Synthetic intermediate	80 kt p.a.
		Acetaldehyde		Production of: ▪ Acetic acid and anhydride ▪ Pyridine	1.35 Mt (1993)
2	Acetic acid			Production of: ▪ Vinyl acetate ▪ Acetic anhydride Used as a solvent	>7 Mt p.a. 190 kt by fermentation

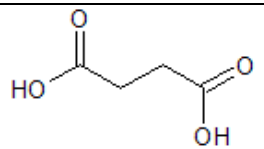
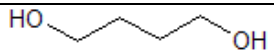
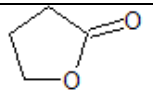
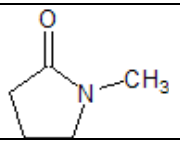
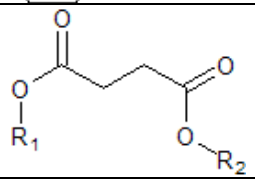
		Acetic anhydride		Acetylating agent for alcohols and amines Dehydrating agent	1-2 Mt p.a.
		Vinyl acetate		Monomer for polymer and copolymer production: ▪ Polyvinylacetate ▪ Polyvinylalcohol ▪ Ethylene – vinyl acetate	4 Mt p.a.(2002)
		Ethyl acetate		Green solvent	1 Mt p.a.
		Chloroacetic acid		Production of: ▪ Carboxymethylcellulose ▪ Phenoxy herbicides As a difunctional reactive intermediate	370 kt p.a.
		Peracetic acid		▪ Antimicrobial ▪ Bleaching agent ▪ Oxidising agent to produce epoxides and alcohols	18 kt p.a.

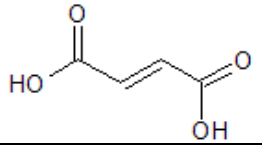
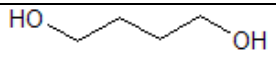
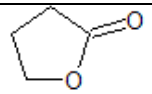
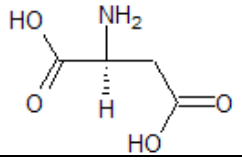
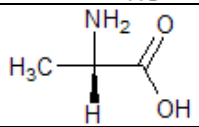
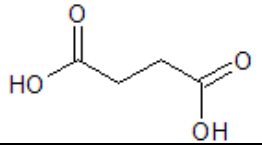
Carbon Number	Platform Chemical	Derivatives	Structure	Applications	Production
3	Lactic acid			▪ Food and beverages ▪ Green solvents ▪ Bio-polymers	150 kt in 2002 – almost entirely by fermentation
		Polylactic acid		▪ Compostable polymer from renewable source ▪ Packaging ▪ Fibres and Textiles	140 kt p.a. production capacity
		Lactic acid salts		▪ Food and beverages ▪ Permeation enhancer (medical)	
		Esters		▪ Green solvents (eg ethyl lactate)	5 kt p.a.
		Chiral esters		▪ Chiral synthons for pharmaceuticals and agrochemicals	
		Acetaldehyde		▪ Common 2 carbon building block in synthesis	
		Acrylic acid		▪ Acrylates ▪ Polymers and copolymers for coatings, adhesives, sealants and elastomers	>2 Mt p.a.
		Lactamides		▪ Plasticisers	
		1,2-Propanediol		▪ moisturizer in medicines, cosmetics, food, and tobacco products ▪ medical and sexual lubricant ▪ emulsification agent ▪ solvent for food colors and flavourings	0.9 Mt p.a. €1000-€1200/t

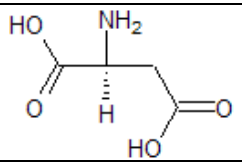
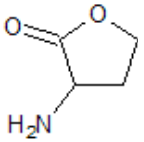
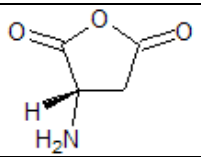
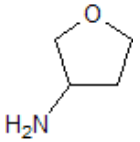
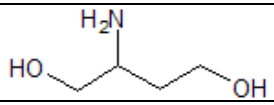
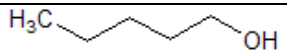
				▪ humectant ▪ carrier in fragrance oils ▪ non-toxic antifreeze ▪ main ingredient in cosmetic products, including baby wipes, bubble baths, deodorants, shampoos, and hair dyes ▪ working fluid in hydraulic presses	
		Propionic acid		▪ Preservative ▪ Esters used as solvents ▪ Chemical intermediate	130 kt (1989)
		2,3-Pentadione		▪ Solvent ▪ Flavour synthesis ▪ Chemical intermediate	
		Oxalic acid		▪ Mordant for dyeing ▪ Household chemicals ▪ Rust remover and rust proofer	
		Pyruvic acid		▪ Medical applications ▪ Production of plant growth regulators	
3	3-Hydroxypropionic acid			▪ Acrylic polymers ▪ Speciality polyesters	
		1,3-Propanediol		▪ Polymer building block (PTT)	80 kt p.a.
		Malonic acid		▪ Synthetic intermediate for pharmaceuticals, agrochemicals and flavors & fragrances compounds.	

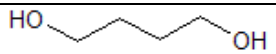
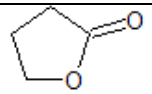
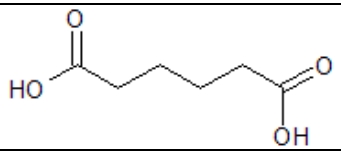
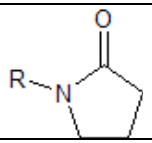
		Acrylic acid		▪ Acrylates ▪ Polymers and copolymers for coatings, adhesives, sealants and elastomers	>2 Mt p.a.
		Acrylamide		Production of polymers and modified copolymers for: ▪ waste and sewage treatment, ▪ paper and pulp manufacturing ▪ oil recovery and ore processes ▪ soil stabilizer ▪ adhesive coating ▪ food processing.	
		Methyl acrylate		Production of: ▪ coatings, elastomers, adhesives, thickeners, ▪ amphoteric surfactants, ▪ fibers, plastics, textiles and inks.. Chemical synthesis.	
3	1, 3-Propanediol			▪ Polymer building block (PTT)	80 kt p.a.
		Polytrimethylene terephthalate		▪ Fibres and textiles ▪ Engineering plastics Brand names Sorona and Corterra	>100 kt p.a. installed capacity
		Polyurethanes		▪ Chain extender for thermoplastic polyurethanes – replacement for 1,4-butanediol	
		Copolyester ethers		▪ High performance elastomers	
3	Glycerol			▪ Triacetin ▪ Food additive ▪ Pharmaceuticals ▪ Personal Care ▪ Polyols ▪ Alkyd resins ▪ Tobacco ▪ Explosives ▪ Detergents ▪ Cellophane	600 kt p.a. in Europe (2006). Increased from ~200 kt in 2000. Expected to continue to rise due to increased production of biodiesel 2006 price ~500€/t – a historically low level.
		Epichlorohydrin		▪ Epoxy resins ▪ Paper chemicals	1.2 Mt p.a. $2300/t

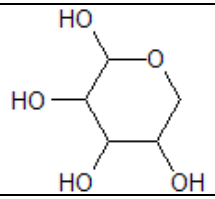
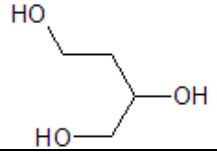
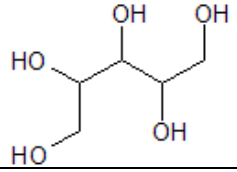
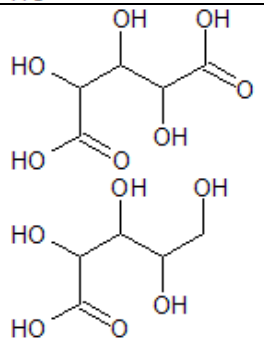
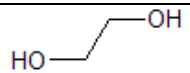
				▪ Water treatment ▪ Polyglycerols	
		1,2-propanediol		▪ moisturizer in medicines, cosmetics, food, and tobacco products ▪ medical and sexual lubricant ▪ emulsification agent ▪ solvent for food colors and flavourings ▪ humectant ▪ carrier in fragrance oils ▪ non-toxic antifreeze ▪ main ingredient in cosmetic products, including baby wipes, bubble baths, deodorants, shampoos, and hair dyes ▪ working fluid in hydraulic presses	0.9 Mt p.a. €1000-€1200/t
		1,3-Propanediol		▪ Polymer building block (PTT)	80 kt p.a.
		Mono-, di- and tri-esters		▪ Food additives ▪ Emulsifiers	
		Polyglycerols		▪ Non-ionic surfactants. ▪ Emulsifiers in food, cosmetics etc ▪ Antifogging agents in polyolefin films	
		Glyceric acid		▪ Potential for PLA analogues with different properties	
		Acrolein		▪ Acrylic acid esters, ▪ Polymers, ▪ Detergents	

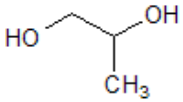
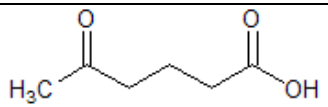
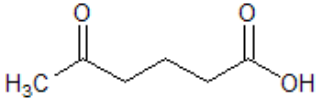
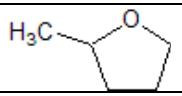
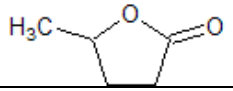
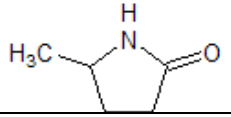
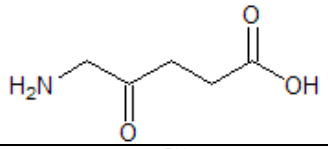
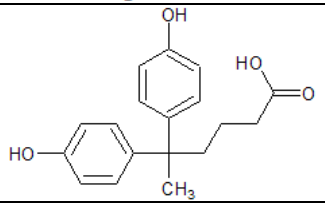
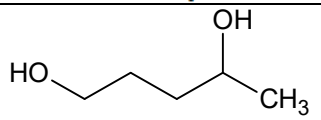
Carbon Number	Platform Chemical	Derivatives	Structure	Applications	Production
4	Succinic acid			▪ Sweetener in food and beverages	16 kt p.a.
		1,4-Butanediol		▪ Polybutylene terephthalate (PBT) ▪ Polybutylene succinate (PBS)	512 kt p.a. (1995)
		γ-Butyrolactone		▪ Solvent for polymers and agrochemicals. ▪ Intermediate in the manufacture of pyrrolidone derivatives	
		Tetrahydrofuran		▪ Solvent ▪ Thermoplastic polyurethanes, ▪ Elastic fibres, ▪ Moulded elastomers, ▪ Copolyesters and copolyamides.	140 kt p.a. (1992)
		N-Methyl-2-pyrrolidone (NMP)		▪ Solvent ▪ Reaction medium	30 kt p.a.
		Di-esters		▪ Green solvents ▪ Fuel oxygenates	
		Polyamides			
		Polyesters		▪ e.g. polybutylene succinate	

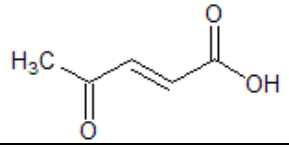
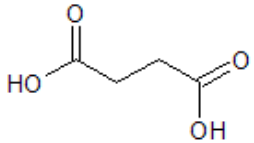
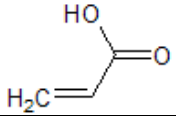
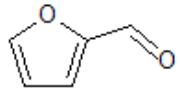
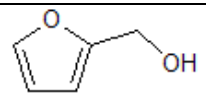
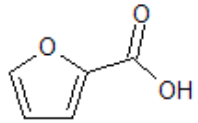
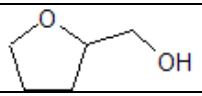
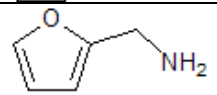
4	Fumaric Acid			▪ Unsaturated polyester resins ▪ Food additive ▪ Animal feed ▪ Dye mordant ▪ Polyhydric alcohols	12 kt p.a.
		1,4-Butanediol		▪ Polybutylene terephthalate (PBT) ▪ Polybutylene succinate (PBS)	512 kt p.a. (1995)
		γ-Butyrolactone		▪ Solvent for polymers and agrochemicals. ▪ Intermediate in the manufacture of pyrrolidone derivatives	
		Tetrahydrofuran		▪ Solvent ▪ Thermoplastic polyurethanes, ▪ Elastic fibres, ▪ Moulded elastomers, ▪ Copolyesters and copolyamides.	140 kt p.a. (1992)
		Unsaturated polyesters		Replaces maleic acid and maleic anhydride for polyesters with: ▪ Improved thermal stability ▪ Greater hardness	
		L-Aspartic acid		Production of sweetener aspartame	13 kt p.a.
		L-Alanine			
		Succinic acid		▪ Sweetener in food and beverages	16 kt p.a.

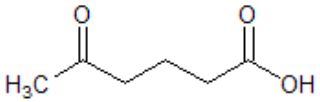
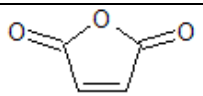
4	Aspartic Acid			Production of sweetener aspartame	13 kt p.a.
		Amino-γ-butyrolactone		Potential polymer and solvent applications	
		Aspartic anhydride		Potential polymer and solvent applications	
		3-Aminotetrahydrofuran		Potential polymer and solvent applications	
		2-Amino-1,4,-butanediol		Potential polymer and solvent applications	
		Polyaspartic acid		Potential substitute for polyacrylates and polycarboxylates. Potential applications in: ▪ Detergents, ▪ Water treatment, ▪ Corrosion inhibition ▪ Super-absorbers.	
4	1-Butanol			▪ Solvent ▪ Thinner for varnishes and lacquers ▪ Plasticizers ▪ Butylamines ▪ Butyl acetate, ▪ Acrylic esters, ▪ Glycol esters.	2 Mt p.a.

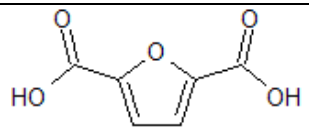
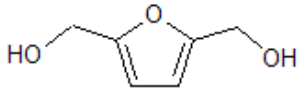
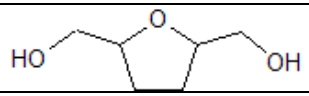
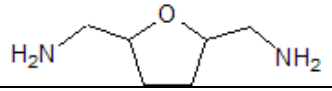
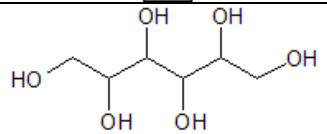
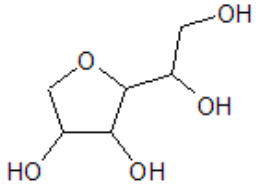
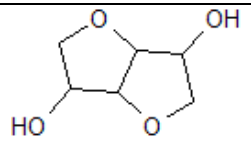
4	1,4-Butanediol			▪ Polybutylene terephthalate (PBT) ▪ Polybutylene succinate (PBS)	512 kt p.a. (1995)
		Polybutylene terephthalate (PBT)			340 kt p.a. (1997)
		Polybutylene succinate (PBS)			33 kt p.a. installed capacity 2006
		Polyurethanes			
		γ-Butyrolactone		▪ Solvent for polymers and agrochemicals. ▪ Intermediate in the manufacture of pyrrolidone derivatives	
		Tetrahydrofuran		▪ Solvent ▪ Thermoplastic polyurethanes, ▪ Elastic fibres, ▪ Moulded elastomers, ▪ Copolyesters and copolyamides.	140 kt p.a. (1992)
		Adipic acid		▪ Nylon 66 ▪ Lubricant esters ▪ Plasticizers ▪ Polyurethanes	2.5 Mt p.a.
		Pyrrolidones		▪ Chemical intermediate	

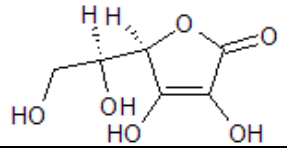
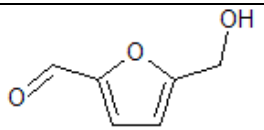
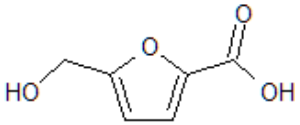
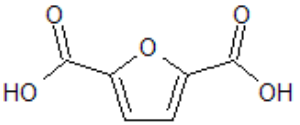
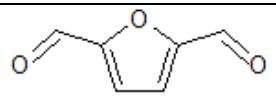
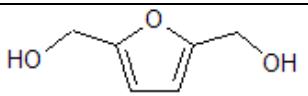
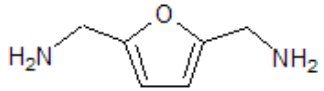
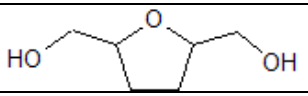
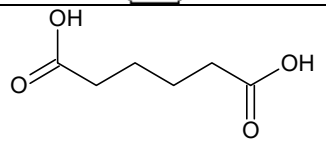
Carbon Number	Platform Chemical	Derivatives	Structure	Applications	Production
5	Xylose / Arabinose			▪ Source of C5 sugars for chemical synthesis	
		1,2,4-Butanetriol		▪ Explosive ▪ Propellant ▪ Chiral synthon	
		Xylitol / Arabinitol		▪ Sweetener	
		Xylaric, Xylonic, Arabonic, Arabinoic acid		▪ Potential uses in new polymers	
		Polyesters		▪ Xylitol/arabinitol with other glycols for unsaturated polyesters	
		Ethylene and propylene glycol		▪ Deicer ▪ Automotive antifreeze	

				▪ Building block unsaturated polyesters	
		Levulinic acid		See below	See below
5	Levulinic acid			▪ Chemical intermediate	450 t p.a.
		Methyltetrahydrofuran		▪ Solvent ▪ Fuel oxygenate ▪ Chemical intermediate	
		Esters		▪ Fuel oxygenates	
		γ-Valerolactone		▪ Solvent ▪ Chemical intermediate	
		5-Methyl-2-pyrrolidone		▪ Solvent ▪ Chemical intermediate	
		δ-Amino-levulinic acid		▪ Herbicide	
		Diphenolic acid		▪ Potential replacement for Bisphenol-A	
		1,4-Pentanediol		▪ Diol for polyesters	

		β-Acetyl-acrylic acid		▪ Co-polymers	
		Succinic acid		▪ Sweetener in food and beverages	16 kt p.a.
		Acrylic acid		▪ Acrylates ▪ Polymers and copolymers for coatings, adhesives, sealants and elastomers	>2 Mt p.a.
5	Furfural			▪ Extraction solvent ▪ Nematicide ▪ Fungicide ▪ Resins	200 kt – 300 kt
		Furfuryl alcohol		▪ Resins	120 kt – 180 kt p.a.
		Furoic acid			
		Tetrahydrofurfuryl alcohol		▪ Solvent ▪ Industrial cleaning	
		Furfuryl amine		▪ Pharmaceuticals	
		Tetrahydrofuran		▪ Solvent ▪ Thermoplastic polyurethanes, ▪ Elastic fibres, ▪ Moulded elastomers, ▪ Copolyesters and copolyamides.	140 kt p.a. (1992)

		Levulinic acid		▪ Chemical intermediate	450 t p.a.
		Maleic anhydride		▪ Important chemical intermediate	
		Thermoset resins		▪ Foundry binder	

Carbon Number	Platform Chemical	Derivatives	Structure	Applications	Production
6	2,5-Furandicarboxylic acid			▪ Potential as monomer to replace terephthalic acid	
		2,5-Dihydroxymethylfuran		▪ Potential use in new polyesters	
		2,5-Dihydroxymethyl-tetrahydrofuran		▪ Potential use in new polyesters	
		2,5-Bis(aminomethyl)-tetrahydrofuran		▪ Potential use in new polyamides	
6	Sorbitol			▪ Sweetener ▪ Humectant ▪ Thickener ▪ Cryo-stabiliser ▪ Amateur rocket fuel	1.1 Mt p.a.
		1,4-Sorbitan		▪ Esters used as non-ionic surfactants ▪ Solubiliser ▪ Emulsifier	50 kt p.s.
		Isosorbide		▪ Pharmaceutical (vasodilator) ▪ Esters used as solvent in cosmetics ▪ Potential for use as diol in polyesters ▪ Potential for plasticizers	800 t p.a.
		Polyetherpolyols		▪ Polyurethane synthesis	

		Ascorbic acid		▪ Salts – antioxidants for aqueous systems ▪ Esters – antioxidants for non-aqueous systems	
6	5-Hydroxymethylfufural			▪ Phenolic resins	
		5-Hydroxymethyl-furoic acid			
		2,5-Furan dicarboxylic acid		▪ Green alternative to terephthalic acid	
		Furandialdehyde		▪ Potential for new polyesters	
		2,5-Dihydroxymethylfuran		▪ Potential for new polyesters	
		2,5-Diaminomethylfuran		▪ Potential for new polyamides	
		2,5-Dihydroxymethyl-tetrahydrofuran		▪ Potential for new polyesters	
6	Adipic acid			▪ Nylon 66 ▪ Lubricant esters ▪ Plasticizers ▪ Polyurethanes	2.5 Mt p.a.

		Polyamides		▪ Engineering plastics ▪ Fibres	
		Polyurethanes			
		Esters		▪ Lubricants ▪ Solvents	