Supplementary information

Appendix 1: Survey of available Green Chemistry metrics

Abiotic Depletion Potential[1]	$Index_{ADP} = ADP \cdot mass\ of\ product$ ADP values from reference tables
Acidification Potential[1,2]	$AP =$ where a: number of dissociable H^+ in the formed acid $Index_{AP} = AP \cdot mass\ of\ product$
Atmospheric Acidification Potential[3]	$AP = \frac{Total\ mass\ of\ SO2\ equivalents}{Mass\ of\ Product}$
Atom Economy[4,5,6]	$\frac{MW\ of\ product(s)}{MW\ of\ all\ reagents} \cdot 100\%$
Actual Atom Economy[3]	$AAE = AE \times \varepsilon$
Atom Utilisation[7]	$\frac{mass\ of\ product}{total\ mass\ of\ all\ substances\ produced}$
Bioaccumulation[1] Octanol-water partition Coefficient (K_{ow}) Bioconcentration factor	logP or $\log K_{ow}$ $K_{ow} = \frac{concentration\ in\ octanol\ phase}{concentration\ in\ water}$ $BCF = \frac{concentration\ in\ tissue\ of\ aquatic\ org.}{concentration\ in\ water}$
Carbon Efficiency[3,4]	$\frac{mass\ of\ carbon\ in\ product}{total\ mass\ of\ carbon\ in\ key\ reagents}$
E-factor[5,8,9,10]	$\frac{m_A}{m_p} + \frac{m_B}{m_p} + \frac{m_{aux}}{m_p} + \frac{m_s}{m_p} - 1$ where A,B: reactants, p: product, aux: auxiliaries, s: solvents
E-factor based on mass	$E_m = \frac{1}{RME} - 1$
E-factor based on Molecular Weight	$E_{MW} = \frac{[(MW) \times (Stoichiometric\ coefficient)]_{waste}}{[(MW) \times (Stoichiometric\ coefficient)]_{product}}$
Effective Mass Yield[7,11]	$\frac{mass\ of\ product}{mass\ of\ non-benign\ reagent}$
Elemental Efficiency[7]	$\frac{mass\ of\ element\ in\ product}{total\ mass\ of\ element\ in\ stoichiometric\ reagents}$
Emissions of specific compound released[12]	$E_i = \frac{mass\ of\ compound\ \ i\ released\ as\ CO_2}{basis\ of\ mass\ balance\ calculations}$ [g CO_2 / kg of intermediate crystallised]
Energy Efficiency[6]	From a complete life cycle $\frac{theoretical\ energy\ demand}{actual\ energy\ spent}$ For individual process $\frac{energy\ spent\ on\ step}{overall\ energy\ spent}$
Energy Intensity[4]	$EI = \frac{total\ process\ energy}{mass\ product}$

Environmental Quotient[3]	$EQ = E \cdot Q$ Where E: E-factor, Q: Environmentally hazardous quotient
Eutrophication Potential[2]	$EP = \frac{Total\ Mass\ of\ phosphate\ equivalents}{Mass\ of\ Product}$ $Index_{EP} = EP \cdot m_{\text{ass of product}}$
Global Warming[1]	$\frac{kg\ CO2\ eq}{kg\ of\ product}$
Global Warming Potential[1,3,13]	$GWP = \frac{Total\ mass\ of\ CO2\ equivalents}{Mass\ of\ Product}$ $GWP = \frac{\left[\frac{NC}{MW}\right] of\ a\ compound}{\left[\frac{NC_{CO2}}{MW_{CO2}}\right]}$ where NC: number of carbon
Green House Gases emissions[6]	$\sum (GHG_i \cdot P_i)$ Where P_i: Global warming potential factor
Human Toxicity by Ingestion Potential[1]	$INGTP = \frac{\left[\frac{C_W}{LD_{50}}\right]}{\left[\frac{C_{W,tot}}{LD_{50,\ tot}}\right]}$ where C_w: concentration in water $I_{INGTP} = INGTP \cdot m$
Human Toxicity by Inhalation Potential[4]	$INHTP = \frac{\left[\frac{C_a}{LD_{50}}\right]}{\left[\frac{C_{a,tot}}{LD_{50,\ tot}}\right]}$ where C_a: airborne concentration of the emitted chemical $I_{INHTP} = INHTP \cdot m$
Mass Intensity[4,8,12,13]	$\frac{total\ mass\ input\ excluding\ water}{mass\ of\ product}$
Material Inputs Per Unit Service (MIPS)[6]	$\frac{weighted\ material\ input\ over\ life\ cycle}{units\ of\ service\ obtainable}$
Material Recovery Parameter[3]	$MRP = \frac{Total\ mass\ of\ reaction\ and\ postreaction\ solvents + mass\ o}{Total\ mass\ of\ reaction\ and\ postreaction\ solvents + mas}$
Ozone depleting gas emissions[1,6]	$\sum (ODG_i \cdot P_i)$ Where P_i: Potency factor
Persistence – Aerobic Biodegradation Rate[1]	$I = 3.199 + a_1 f_1 + a_2 f_2 + \ldots + a_m MW$
Persistence and Bioaccumulative[4]	$\frac{total[mass\ persistent + bioaccumulative]}{mass\ of\ product}$ $\frac{total[mass\ persistent + bioaccumulative]}{\frac{EC_{50a\ material}}{EC_{50\ DDT\ control}}}$
Photochemical oxidation (smog) potential[3]	$PCOP = \frac{Total\ mass\ of\ ethylene\ eq.}{Mass\ of\ product}$

PMI Complexity Model[14]	$PMI = 131 + 26C + 40H - 515A + 57(C - 1.5)(H - 8)$ Where C: total number of chiral centres, H: total number of heteroatoms, A: fraction aromatic $A = \frac{aromatic\ heavy\ atoms + heteroaromatic\ heavy\ atoms}{heavy\ atoms}$
Primary Energy Usage	$\frac{kg\ fuel}{kg\ product}$
Process Mass Intensity (Overall)[15,16]	$\frac{total\ mass\ in\ a\ process\ or\ process\ step}{mass\ of\ product}$
Process Solvent Mass Intensity[4]	$\frac{total\ solvent\ input\ excluding\ water}{mass\ of\ product}$
Process Water Mass Intensity	$\frac{fresh\ water - recycled\ water}{mass\ of\ product}$
Process Water Use	$\frac{amount\ of\ water\ used}{unit\ of\ product}$
Raw Material Use	$\frac{mass\ raw\ material}{mass\ product}$
Reaction Mass Efficiency (RME) (Tot.)[4,8,6,11,9]	$\frac{mass\ of\ products}{mass\ of\ all\ reactants}$
RME: Excess reagent used, reaction catalyst and solvent disposed, workup and purification materials disposed	$(\varepsilon)(AE)\left(\frac{1}{SF}\right)\left(\frac{1}{1 + \left(\frac{\varepsilon(\mathrm{AE})[c + s + \omega]}{(SF)(m_p)}\right)}\right)$ Where ε: yield, AE: atom economy, SF: stoichiometric factor, c: catalyst, s: solvent, ω: waste, m_p: mass of product
RME: No excess reagent used, reaction catalyst and solvent disposed, workup and purification materials disposed	$(\varepsilon)(AE)\left(\frac{1}{1 + \left(\frac{\varepsilon(\mathrm{AE})[c + s + \omega]}{(m_p)}\right)}\right)$
RME: No excess reagent used, reaction catalyst disposed, solvent recovered, workup and purification materials disposed	$(\varepsilon)(AE)\left(\frac{1}{1 + \left(\frac{\varepsilon(\mathrm{AE})[c + \omega]}{(m_p)}\right)}\right)$
RME: No excess reagent used, reaction catalyst disposed, solvent recovered, workup and purification materials recovered	$(\varepsilon)(AE)\left(\frac{1}{1 + \left(\frac{\varepsilon(\mathrm{AE})[c]}{(m_p)}\right)}\right)$
RME: Excess reagent used, reaction catalyst recovered, solvent recovered, workup and purification materials recovered	$(\varepsilon)(AE)\left(\frac{1}{SF}\right)$
RME: No excess reagent used, reaction catalyst recovered, solvent recovered, workup and purification materials recovered	$(\varepsilon)(AE)$
Reaction Yield[3]	$\varepsilon = \frac{Mass\ of\ product}{Theoretical\ mass\ of\ product}$
Recyclability	$\frac{number\ of\ different\ materials}{unit\ of\ product}$
Renewability[6]	$\frac{rate\ of\ consumption\ of\ renewable\ energy}{overall\ rate\ of\ energy\ consumption}$

Renewability Index[3]	$RI = \frac{Total\ energy\ supplied\ from\ renewable\ resources}{Total\ energy\ supplied\ to\ the\ process}$
Renewable Intensity[13]	$\frac{mass\ of\ all\ renewably\ derived\ materials\ used}{mass\ of\ product}$
Risk Index	$I = P \cdot m$ where P: risk potential, m: mass of chemical risk
Smog Formation[1]	$SFP = \frac{MIR}{MIR_{ROG}}$ where MIR: maximum Incremental Reactivity ROG: Reactive organic gases $I_{SFP} = SFP \cdot m$
Solvent recovery Energy[3]	$\frac{total\ solvent\ recover\ energy\ requirements}{mass\ of\ final\ product}$
Solvent Intensity[12,13]	$\frac{mass\ of\ solvent}{mass\ of\ product}$
Stoichiometric Factor[3,9,11]	$SF = 1 + \frac{\sum mass_{excess\ reagent}}{\sum mass_{stoichiometric\ reagent}}$ $SF = 1 + \frac{(AE)\sum mass_{excess\ reagent}}{theoretical\ mass\ of\ product}$
VOCs emissions	$\frac{solvent\ recycled}{total\ solvent\ use}$
Waste Intensity[12,13]	$\frac{total\ waste\ produced}{total\ mass\ input}$
Waste treatment energy[3]	$\frac{waste\ treatment\ energy\ requirements}{kg\ of\ final\ product}$
Water Consumption	Volume of water consumed in the process ore process unit

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