

Index

a

- abiotic resource depletion 79
- acetone 81
- acid gas scrubbing 13
- acidification 79, 109
 - potential 108
- active pharmaceutical ingredient (API) 105, 196
 - artemether (ARM) 171
 - batch manufacturing process 175
 - environmental life cycle impacts 106
 - production process at Sanofi 174
- N*-acyl pyrazine 57
- adipic acid (ADA) 107, 187
 - direct microflow synthesis 188
 - life cycle assessment (LCA)
 - for continuous flow 190
 - for two-step conventional synthesis 191
 - production routes 188
 - quantitative results for 192
 - two-step conventional synthesis 189, 191
- Aggregated Computational Toxicology Resource (ACToR) 35, 37
- alkyl boronic acid 59
- Alzheimer's disease 113
- American Apparel & Footwear Association (AAFA) 238
- American Chemical Society (ACS) 157
 - Green Chemistry Pharmaceutical Roundtable 106, 201
- Ames mutagenicity assay 38
- amidation 181
- 7-aminocephalosporic acid (7-ACA) 109
- analytic hierarchy process (AHP) 130
- Andraos algorithm 76
- anthraquinone oxidation (AO) process 190, 194
- antioxidant 167
- Apple® products 115

aqueous phase biocatalytic process 222

- artemether 171
- Artemisia annua* 171
- artemisinin-based drugs 171, 172
- artesunate 171
- aspirin 50, 56, 75
 - synthesis, reaction network for 75
- Association of the British Pharmaceutical Industry (ABPI) and Carbon Trust's tool 115
- atom economy (AE) 12, 16, 158, 192, 214
- atorvastatin 218
 - biocatalytic synthesis 219
- auxiliary material 73
- azidation 180
 - β -azidation reactions 81, 82

b

- balanced chemical equations 64
- BASF methodology 114
- BASF's Eco-efficiency analysis 114
- basification 79
- batch processing 175, 178. *See also* sustainable batch design
 - chemical manufacturing 192
 - and continuous micromixer parameters 165
 - and continuous operation, cost analysis of 178
 - procedures 199
 - reaction conditions of 167
 - reactor process 170, 171, 187
 - vs. continuous operation 160
- BatchRetroLC 131, 141
- benzene chlorination 5, 77, 88
- benzene/toluene/xylene (BTX) 288
- benzoic acid 75, 88
- benzoyl chloride 168
 - phase transfer catalysis of 167

- toxicity potentials, biphasic reaction 169
- bioaccumulation 43, 79
- bio-based chemicals 6, 109
- biocatalytic processes 207, 285
 - atom economy 214
 - biocatalyst/reaction development 217
 - biocatalytic route to atorvastatin 218
 - Carbon Mass Efficiency 214
 - claimed environmental benefits 211
 - design/development 210
 - E-factor 216
 - efficiency 209
 - environmental benefits 211
 - methodology 223
 - potential staged approach to benchmark 214
 - process development 221
 - process mass intensity 215
 - reaction development, evaluation of 215
 - route feasibility, evaluation 214
 - route selection 216
 - sitagliptin 219
 - solvent intensity 215
 - structure 208
 - sustainability 207, 210
 - early stage assessment 213
 - quantitative measuring 212
 - synthetic processes 286
 - two-stage development paradigm 211
 - water intensity 216
- biocide-coated medical textiles 106
- bioconcentration factor (BCF) 38
- biofuels 112
- biomass utilization 5
- biomaterials 116
- bisphenol A (BPA) 233, 241, 269
- blister pack carbon footprint 115
- Boc protection
 - group 61
 - phenylalanine 59
- bond economy 12
- boronic acid 57
- boronic ester 73
 - cleavage 67
- bortezomib 50, 56, 57, 59, 63, 73, 74
- Brundtland Report 131
- butadiene 187, 289
- 1-butyl-3-methylimidazolium chloride 167
- 1-butylsulfonate-3-methylimidazolium 167

- c**
- CA Green Chemistry Act 16
- calcination 88
- California Act 16
- California Office of Environmental Health Hazard Assessment 234
- California Safer Consumer Products Act 263
- CAPEX cost analysis 188
- caprolactam routes 109
- carbon efficiency 12, 158, 162
- carbon footprint analysis 116
- carbon mass efficiency (CME) 214, 218
- carbon monoxide 6
- carbonyldiimidazole (CDI) 73
- carboxylic acid 89
- carcinogenicity 81
- carcinogenic, mutagenic, or toxic to reproduction (CMR) 258
- cascading reactions, into a microreactor flow network 179
- case study
 - aspirin 74
 - Case I 84
 - Case II 85
 - Case III 85
 - Case IV 85
 - Case V 86
 - Case VI 86
 - environmental and safety–hazard impact 78
 - input energy 84
 - material efficiency 76
 - reaction network 74
- bortezomib 56
 - material efficiency 64
- millennium pharmaceuticals' process 59
- pharma-sintez process 62
- synthesis strategy, for future optimization 72
- catalytic transformation 2
- catechol 88
- C-efficiency 192
- cell death 56
- cereal crop preservation 114
- chain optimization 103
- chemical additives 114
- chemical alternatives assessment 18
- chemical efficiency 11
- chemical engineers 11
- Chemical Footprint Project 256, 259
 - chemical inventory 256
 - disclosure and verification 256
 - footprint measurement 256
 - management strategy 256
- chemical hazard assessment (CHA) 6, 9, 231–233, 244, 271
 - case studies 264

- Levi Strauss & Co. (LS&Co.) 267
 - challenges 271
 - filling data gaps 272
 - into green product design 272
 - transparency 271
 - characteristics 232
 - chemical alternatives assessment 263
 - chemical footprint project 255
 - comprehensive/abbreviated forms 247
 - consumer product
 - companies 232
 - design/development considerations 235
 - sector 242, 256
 - Cradle to Cradle Certified™ Product Program 262
 - declare label 261
 - defined 243
 - endocrine disrupting chemical used in lining 269
 - estimated cost and time 257
 - GC3 joint statement on green chemistry/safer alternatives 238
 - GHS hazard classifications 245
 - globally harmonized system of classification and labelling 244
 - GreenScreen for safer chemicals 248, 250
 - GreenScreen list translator (GS LT) 253
 - hazard endpoints 248
 - health product declaration 260
 - Health Product Declaration Version 2.0 (HPD) 259
 - Living Product Challenge™ (LPC) 262
 - nonprofit organization (NPO) 235
 - quick chemical assessment tool (QCAT) 252
 - red list declare label 259
 - retailer initiatives 237, 239
 - state initiatives 240
 - substitution and regrettable 233
 - United States Environmental Protection Agency 260, 264
 - uses 255
 - worldwide GHS implementation 246
 - chemical intensification 180
 - Chemical of High Concern (CoHC) 258
 - chemical reactions 10, 12, 81
 - chemical risk assessment 45
 - chemical selectivity 10
 - chemicals legislation 6
 - Chemicals Management Software 238
 - chemical transformations 2, 12
 - chemists, integrating sustainable/green chemistry 281
 - chemoenzymatic conversions 208
 - chemoselectivity 10
 - Children's Safe Products Act (CSPA) 240
 - chiral compounds 10
 - chloridehydroxylation 180
 - chlorine 89
 - CleanGredients database 266
 - Clean Production Action (CPA) 255
 - closed-paths (CP) 144
 - CML impact scores 173
 - Coca-Cola Company 96
 - contamination 159
 - continuous end-to-end pharmaceutical manufacturing 201
 - continuous flow 187
 - microflow process 167, 195
 - millireactor-based process 174
 - processing 187, 200
 - reactors 73, 190
 - continuous process 175
 - advantages of 160
 - production 162
 - at small scale 159
 - synthesis process 170
 - continuous tablet production 201
 - conventional batch API manufacturing process (AP) 177
 - convergent approaches 57
 - convergent plans 54
 - convergent strategy 64
 - costing metrics 209
 - Cradle to Cradle Products Innovation Institute (C2CPII) 237, 262
 - cradle-to-gate life cycle 109
 - crude batch/continuous operation, ecological profile comparison of 175
 - cryogenic system 167
 - crystallization 177
 - cumene hydroperoxide 75
 - cumene oxidation 88
 - cumulative energy demand (CED) 108, 166, 168, 172
 - demand 166
 - impact 166
 - for microreactor processing 167
 - current continuous processing (CP1) 175
 - 4-cyanophenylboronic acid 197
 - cyclohexane 187
 - cyclohexene 187
 - production 191
- d**
- database algorithms 49
 - data gap (DG) 7, 248
 - data transparency 101
 - DEAM 98

- Declare Assessment 259
- Department of Energy (DOE) 288
- Department of Toxic Substances Control (DTSC) 267
- Design for the Environment (DfE) Program 246
- Design Institute for Physical Property Data (DIPPR) database 84
- DfE AA method 251
- dichloromethane 181
- di(2-ethylhexyl)phthalate (DEHP) 234
- 2,6-difluorobenzyl alcohol 186
- 2,6-difluorobenzyl azide 180, 181, 183
- dihydroartemisinin (DHA) 171
- DINP's Prop 65 234
- 1,3-dipolar Huisgen cycloaddition 181
- dipolarophile 185
- drug discovery 157

- e**
- eco-efficiency 178, 179
 - alternative 115
 - assessment 114
- EcoIndicator 99 method 95
- Eco-Invent method 98
- ecological niche 3
- economic analysis 195
- economic benefits 200
- economic competitiveness 162
- economic evaluation 170
- economic improvements 162
- Eco-Profiles Web site 109
- ecorepel® 269
- ecosystem 3
- ecotoxicity 7
 - hazard data 8
- E-factors 12, 56, 77, 162, 223
- effective mass yield 13
- EI99 scores 107
- electricity demand 167
- Ellen MacArthur Foundation 236
- (E)-methyl-3-methoxyacrylate (EMMA)
 - 181, 182
- enantiomers 10
- endocrine disruption 81
- energy consumption 87, 158, 167, 168, 175
- energy demand 169
- energy efficiency 3, 157
- energy input consumption 56
- engineering metrics 6
- enterprise resource planning (ERP) 138
- enthalpic contribution 86
- enthalpy 84
- environmental burdens 178

- environmental chemistry 1
- environmental efficiency 178
- environmental factor (E-factor) 162
- environmental, health, and safety (EHS) 35
- Environmental Health Perspectives (EHP) 270
- environmental indicator 149
- Environmental Product Declarations (EPD) 97
- environmental protection 179
 - technology 31
- Environment, Safer Choice program 16
- enzymatic pathways 44
- enzyme modification 209
- EPISuite™ 37
 - toolbox 35
- Escherichia coli* 142, 221
- ethanol 171
- etherification 172
- European Union's Classification and Labelling (CLP) 268
- eutrophication potential 3
- explosivity 7
 - strength 79
 - vapor 79

- f**
- fermentation 142
 - operation 144
 - processes 207, 211
- final products profiles 152
- flammability 7
- FLASC™ tool 105, 109
- flash point 7, 81
- flowsheet decomposition 144
- fossil-based plastics 109
- fossil fuels 96
- Frank Lautenberg Chemical Safety Act of 2016 6, 16
- fresh water
 - aquatic ecotoxicity potential 169
 - sediment ecotoxicity potential 169
- furfural 6

- g**
- GABI 98
- gaseous hydrochloric acid 88
- gastrointestinal tract (GI) 41
- Gauging Reaction Effectiveness for the Environmental Sustainability of Chemistries with a multi-Objective Process Evaluator (GREENSCOPE) 34
 - sustainability indicators 35
- generic convergent process, consisting steps 55
- generic linear process steps 54

- GlaxoSmithKline (GSK) 105, 110, 116
 – methodology 106
 – Solvent Selection Guide 110
 Globally Harmonized System (GHS) of
 Classification and Labeling of
 Chemicals 244
 global warming 7, 79, 96, 109, 115, 140, 198
 global warming potential (GWP) 107, 108, 168,
 185, 199
 glucose dehydrogenase (GDH) 218
 – recycle reaction 218
 green chemistry 1, 2, 4, 6, 9, 11, 14, 17, 29, 32,
 49, 90, 157–159, 174, 194, 200, 231
 – ACS-GCI Roundtable 160
 – to assess microflow processing metrics 163
 – chemicals 194
 – manufacturing processes 209
 – metrics 162, 214, 217, 285, 289
 – evolution of 11
 – safer chemical design, life cycle thinking 30
 Green Chemistry and Commerce Council
 (GC3) 236
 Green Chemistry Institute (GCI) 157
 green engineering 29, 157–159, 174, 194, 200
 – safer chemical design
 – life cycle thinking 30
 greener chemistry 12
 greenhouse gas (GHG) 109
 – emissions 199
 green metrics 158, 200
 – analysis 49
 – for direct microflow route and two-step
 conventional routes 193
 greenness 44, 53
 – measuring with LCI/A applications 103
 – chemical route comparison 106
 – footprinting 115
 – material assessment 109
 – probing case studies 103
 – product LCAs 112
 Greenpeace's Detox Campaign 235
 GreenScreen 7, 246, 248
 – assessments 248, 251
 – list translator 255, 263
 – scores 254
 – for safer chemicals 249
- h***
 halohydrin dehalogenase (HHDH) 218
 hazard 9
 – assessment 7, 246
 – data 7
 – reduction 46
- solvents 42
 – substances 157
 – waste 3
 Hazard Identification and Ranking System
 (HIRA) 134
 2-(H-benzotriazole-1-yl)-1,1,3,3-
 tetramethyluronium tetrafluoroborate
 (TBTU) 61, 73
 Health Product Declaration® (HPD) 259
 Healthy Building Network's Pharos Assessment
 Tool 254
 high-performance liquid chromatography
 (HPLC) 287
 high-temperature flow chemistry protocol 187
 high-throughput screening (HTS) 37
 Hock oxidation-rearrangement 77
 H₂O₂ production 190, 191
 H₂O₂ synthesis 194
 hotspots identification 32, 96
 Huisgen cycloaddition 181, 182
 – dipolarophile 185
 human toxicity potential (HTP) 108, 168,
 169, 185
 hydrogenation catalyst 177
 hydrogen gas generation (HG) 79
 hydrogen peroxide 88, 187, 190
 hydroquinone 88
- i***
 ideal material efficiency conditions 53
 impact sensitivity 79
 incineration 112
 Indicator Sensitivity Analysis (ISA) 142
 – ISA 95 132
 indigo production 114
 ingestion toxicity 79
 inhalation toxicity 79
 Inherently Safer Design (ISD) 135
 Inherent Safety Index (ISI) 134
 in-situ product removal (ISPR) 218
 Integrated Inherent Safety Index (IISI) 135
 Integrated Risk Information System (IRIS) 35
 intensification, process alternatives for 174
 intensified chemistry 187
 International Agency for Research on Cancer
 (IARC) 253
 International Conference on Chemicals
 Management (ICCM) 282
 International Living Future Institute
 (ILFI) 237, 259, 262
 International Standards Organization
 (ISO) 32, 132
 – 14000 series (14040, 14044) 97

- standards 101
- International Sustainable Chemistry Collaborative Centers (ISC3) 283
- Interstate Chemicals Clearinghouse (IC2) 241
- ionic liquids 168, 169
- iridium 2, 3
- isobutyl boronic acid 62, 63
- isoprene 289
- isosteres 42

- k**
- kernel 74
- ketoreductase (KRED) 218
- key input material (KIM) 179, 196
- key output material (KOM) 175
 - recovery 178
- Kolbe–Schmitt synthesis 108

- l**
- LCIA categories, reduction 183
- Leadership in Energy and Environmental Design (LEED) 249
- Lennox-Gastaut syndrome 180
- Lewis acid 60
- life cycle approach 95
- life cycle assessment (LCA) 32, 107, 132, 158, 162, 163, 171, 209, 232
 - assessments of formulated products 113
 - assess microflow processing 163
 - complete picture 191
 - components of 33
 - for continuous flow 190
 - data 115
 - evolution of 96
 - goal/scope definition 33
 - methodology
 - goal and scope 98
 - impact assessment 99
 - interpretation 99
 - inventory analysis 98
 - pharmaceutical product, cradle-to-gate 113
 - simplified LCA (SLCA) 163, 168
 - streamlined 102
 - study for two-reactor network process designs 184
 - treatment options 112
 - for two-step conventional synthesis 191
 - life cycle costing (LCC) 195
 - analysis 159
 - applications with continuous microflow processing, snapshot on 196
 - chemical production processes 198
 - composition of 195
- life cycle evaluation 95
- life cycle inventory and assessment (LCI/A) 3, 33, 34, 95, 101, 103, 184, 187
 - application 104
 - batch/continuous multistep processing 185
 - cradle-to-gate 106
 - data 95
 - databases 99
 - impact categories 9
 - limitations 100
 - as measure of greenness 103
 - methodologies 101
 - score 110
- life cycle practice, historical evolution 97
- lipophilic compounds 43
- liquid-liquid extraction 190
- List Translator-1 chemicals (LT-1's) 258
- lithium diisopropylamide (LDA) 60
- lithium hexamethyldisilazane (LiHMDS) 61

- m**
- macro-economic factors 100
- macroscale reactors 161
- manufacturing restricted substances list (MRSL) 267
- marine aquatic ecotoxicity potential 169
- marine sediment ecotoxicity potential 169
- market competitiveness 127
- mass efficiency 16, 194
- mass intensity (MI) 15, 16, 158, 162
- mass productivity 16, 158, 162
- material efficiency 53, 115
 - analysis for synthesis plans 50
 - metrics 52
- Material Health Certificate (MHC) 262
- material performances 72
- material recovery parameter (MRP) 52
- material selection 110
- material value-added (MVA) 144
- maximal State-Task Network (mSTN) 128
- metal oxides 88
- methane 191
- methanol 171
- methyl 1-(2,6-difluorobenzyl)-1H-1,2,3-triazole-4-carboxylate 184, 186, 187
- microchemical process 197
- micro-economic factors 100
- microflow
 - processing 199
 - production 200
 - reactors 161
 - synthesis in interdigital mixer 168
 - technology 200

- micromixer 168
 microprocess engineering 197
 microreaction technology-based
 processes 167, 199
 microreactors 107, 166, 167, 171
 – flow networks 186
 microstructured reactors 197
 Millennium Pharmaceuticals' process 64, 65,
 67, 68
 – bortezomib process 59–61, 62
 – – global efficiency metrics for 69
 – – intrinsic efficiency metrics 67
 – global metrics analysis for 71
 – linear process 69
 miniaturization 161
 miniflow technology 161
 Minnesota Department of Health (MDH) 240
 Minnesota Pollution Control Agency
 (MPCA) 240
 mixed-integer linear programming (MILP) 128
 mixed-integer nonlinear programming
 (MINLP) 128
 Mixed-Logic Dynamic Optimization 129
 molecular initiating events (MIE) 37
 multifaceted process optimization *versus*
 process intensification 174
 multiobjective genetic algorithm (MOGA)
 – fuzzy logic concepts 130
 multiparameter variations 179
 multistage synthetic route 12
 multistep microreactor flow network 181
 multivariate approach to assessment 18
- n**
 naphthalene 75
 National Fire Protection Association
 (NFPA) 163
 – rating 181
 National Retail Federation 238
 N-Boc-L-phenylalanine 61
 net present value (NPV) 130, 196
 nitrobenzene 180
 nitrogen gas 88
 nitrous oxide 88
 N,N'-carbonyldiimidazole (CDI) 63
 N,O-bis(trimethylsilyl)-acetamide (BSA) 63
 nondominating sorting genetic algorithm
 (NSGA-II) 130
 nonenzymatic process 44
 nonrenewable resource 4
 – conservation 282
 – depletion 126
 normal-boundary intersection (NBI) 130
 nosocomial infections 106
 Novozymes 112
 NO_x emissions 108
 N scaling factors 51
- o**
 occupational exposure limit 79
 1-octadecyl-3-methylimidazolium
 bromide 167
 Office of Environmental Health Hazard
 Assessment (OEHHA) 234
 Office of Research and Development (ORD) 38
 operation time factor (OTF) 144
 optimal batch plant topology 149
 optimal plant scheduling 150
 optimization
 – process alternatives for 174
 – strategies 49
 OptimRetHeat 131
 Oregon Toxic-Free Kids Act 241
 organic solvents 16, 178
 Organization for Economic Cooperation and
 Development (OECD) 35, 282, 283
 ortho-phthalate plasticizers 233
 – diisononyl phthalate (DINP) 234
 oxidant 88
 oxidative process 89
 1-oxybenzotriazole unit 73
 oxygen balance 79
 o-xylene 75
 ozone-depleting 4, 7, 79
 – potential 3, 108
- p**
 Pareto nondominant solution 130
 – ϵ -constraint method 131
 path flow decomposition approach 129
 peptide coupling reagents 73
 peptide-like coupling reactions 73
 perfluorooctanesulfonic acid (PFOS) 268
 perfluorooctanoic acid (PFOA) 268
 persistent, bioaccumulative, and toxic
 (PBT) 232, 258
 petrochemical process 12, 107
 PFC-free replacement technology 269
 pH adjustment 13
 pharmacodynamics 44
 Pharma-Sintez bortezomib process 63, 64, 66,
 69, 72
 – convergent bortezomib route 65
 – global efficiency metrics for 69
 – global metrics analysis for 71
 – – individual steps 70

- intrinsic efficiency metrics for 67
 - Pharma-Sintez route 72
 - Pharos Project Chemical Screen Library (Pharos) 259
 - phase transfer catalysis 168-170
 - phase transition 84, 86
 - phenol 56, 75, 88, 89, 168
 - from glucose, biotechnological route 89
 - plans, synthesis tree representation 80
 - production 88
 - syntheses
 - BI(waste) results 81
 - energy consumption data for 86
 - global E-factor breakdown for 80
 - global material efficiency metrics for 80
 - plans 76
 - toxicity potentials, biphasic reaction of 169
 - phenylalanine 57
 - L-phenylalanine 73
 - phenyl benzoate synthesis 167, 168
 - cost evaluation 167
 - phosphates reduce water hardness 244
 - photochemical ozone creation potential (POCP) 109
 - photo oxidant creation potential 108
 - phthalate plasticizers 244
 - pinanediol boronic ester 62
 - plasmodium falciparum 171
 - pollution prevention 96
 - polyvinyl chloride (PVC) 234
 - plastics 232
 - pot economy 13
 - pregablin 105
 - preliminary cost analysis 197
 - Prezista 201
 - Pr₂NET 73
 - process characteristics
 - of considered batch scenarios 176
 - of continuous process 177
 - process-design intensification 161
 - process intensification tools 194
 - process mass intensity (PMI) 15, 158, 162
 - process optimization opportunities 50
 - process safety 160
 - process sensitivity analysis 146
 - process simulation 188
 - and CAPEX cost study 188
 - Product Category Rules (PCR) 97, 110
 - product diversity 159
 - production cost breakdown 196
 - product quality 159, 160
 - Program for Assisting the Replacement of Industrial Solvents (PARIS)
 - user-friendly graphical user interface 42
 - Prop 65-listed substances
 - into drinking water sources 240
 - proteasome 56
 - purification 142
 - protocols 73
 - 2-pyrazine carboxylic acid 62
- q**
- quantitative and other structure activity relationship (Q/SAR) models 251
 - quantitative structure-activity relationship (QSAR) 18, 35
 - methodologies 38
 - modeling 38, 249
- Quick Chemical Assessment Tool (QCAT) 252
- r**
- raw material (RM) 148
 - raw materials consumption 194
 - reaction mass efficiency (RME) 14, 49, 50, 158
 - RME_{kernel} values 72
 - reaction network strategies
 - to synthesize bortezomib 59
 - to synthesize pyrazine 58
 - variety of 58
 - REACTION spreadsheets 51, 56
 - reaction yield 51
 - ReCiPe 132
 - recycling, role of 171
 - Redlich-Kwong equation 86
 - Registration, Evaluation, Authorization and Restriction of Chemicals (REACH) 16
 - legislation 7
 - regrettable substitution 234, 268
 - renewable bio-based feedstocks 207
 - renewable catalyst 212
 - renewable energy 194
 - restricted substances list (RSL) 267
 - Retailer Regulation 237-239
 - reverse Lipinski 41
 - risk reduction strategy 41
 - rufinamide process 180, 181
 - routes, comparison of 182
- s**
- safer chemical design 29
 - alternatives assessment (AA) 45
 - attributes and measurement metrics 39
 - chemicals attributes
 - good character 36
 - potency/efficacy, maximize uses 40

- tools for characterizing 37
- economic efficiency 40
- hazardous functional groups, minimize the incorporation 42
- life cycle assessment (LCA) 31, 32
- life cycle, stages 33
- life cycle thinking 30, 31
- limited bioavailability 41
- limited environmental mobility 41
- limited persistence/bioaccumulation 43
- pH 44
- protocol for approaching 45
- quick transformation to innocuous products 44
- risk assessment 45
- seven virtues and four turpitutes of 36
- strive to reduce/eliminate the use 40
- toxicity 41, 42
- training 46
- Safer Chemical Ingredients List (SCIL) 261, 265
- safer chemicals, challenge 29
- Safer Choice
 - on CleanGredients 265
 - criteria 261, 266
 - logo 267
 - program 264-266
- safety-hazard constraints 89
- safety-hazard impact 56
- safety-hazard index (SHI) 74, 79
- Sanofi Company 174
- scaling factors 51, 53, 56
- SciVeraLENS 246
- SEEBalance® 113
- selectivity 187, 199
- sertraline 105
- shikimic acid 89
- SimaPro 98
- simulated annealing (SA) 130
- single innovation drivers 171
- single-step analyses in batch and flow 181
- sitagliptin
 - antidiabetic compound 219
 - biocatalytic synthesis 220
- skin dose 79
- skin sensitization 232
- small scale reactors 161
- smog formation 79
- social indicators 134
- societal values 100
- sodium borohydride 171
- sodium hydroxide 75
- sodium tripolyphosphate (STPP) 244
- solvent free methodologies 90
- solvent load 200
 - improvements 187
- solvent rate 162
- solvent selection 110
- solvent swap
 - to recover product 222
- space-time yield 208
- state-of-the-art batch process 136
- State-Task Network (STN) 147
 - representation, product recipe 148
- Strategic Approach to International Chemicals Management (SAICM) 282, 283
- streamlined life cycle assessment 102
- sulfonic acid 89
- sulfur dioxide 181
- SuperPro Design
 - insulin process, flowsheet of 143
- sustainability 17, 30, 162
 - assessment 287
 - batch design (*see* sustainable batch design (SBD))
 - of biocatalytic processes 207
 - chemical process evaluation-metrics 34
 - chemistry 282, 283
 - development 281, 282
 - metrics 31
 - molecular design 31
 - procurement 241
 - safer chemical design, life cycle thinking 30
 - toolbox 274
- sustainable batch design (SBD) 7, 125
 - batch design 125
 - – assessment 131
 - – challenges 126
 - – characteristics 125
 - – design and retrofit 127
 - – process sustainability 126
 - – State of the Art 126
 - – framework (SBD-FRAME) 126
 - – assessment 147
 - – batch indicators for insulin production 145
 - – business planning 138
 - – case studies 142
 - – compound specification 137
 - – design of batch process 147
 - – economic assessment 136, 138
 - – environmental assessment 135, 139
 - – fermentation 144
 - – flow diagram 137
 - – integration task characterization 148
 - – ISA 95 framework 132, 133
 - – mass indicators for insulin production 145
 - – methodologies 141

- – primary recovery 145
- – process recipe 138
- – purification 146
- – retrofit 142
- – retrofitting 136
- – scheduling 138
- – series of reactions 145
- – social assessment 140
- – waste recovery/disposal 138
- SustainPro tool 131, 142
- symmetric fuzzy linear programming (SFLP) 130

- t**
- Tait equation 86
- tegretol 113
- terrestrial ecotoxicity potential 108, 169
- tetrahymena pyriformis IGC₅₀ 38
- tetralone 105
- tetramethyl bisphenol F (TMBPF) 270
- The Society of Environmental Toxicology and Chemistry 97
- thionyl chloride 181
- three-reaction network process designs 184
- TidalVision USA 242
- titanium silicates 88
- toluene 5, 75
- toluene oxidation 76, 88
- Tool for the Reduction and Assessment of Chemical and other environmental Impacts (TRACI) 35
- total cradle-to-gate energy consumption 106
- toxicity 29, 41
 - hazard profile 37
- Toxicity Estimation Software Tool (TEST) 35, 38
- toxicity pathways 44
- toxicity potentials 168
- toxicological sciences 30
- toxicology tests 35
- toxicophores 42, 45
- Toxic Substances Control Act (TSCA) 6
- ToxServices' Full Materials DisclosureTM (ToxFMDTM) Program 262
- trade-offs 96, 100
- transformation 179
 - equipment flowsheet 144
- trifluoroacetic acid (TFA) 61
- Trp-LE'-MET-proinsulin 142
- true greenness of a process 95
- two-liquid phase biocatalysis 223

- u**
- UMBERTO 98
- United Kingdom's National Health System's "Green House Gas" 115
- α,β-unsaturated ketones 81, 82
- US EPA Safer Choice Program 260
- US National Academy of Science 18

- v**
- Valspar's Safety 271
- vanadium pentoxide 82
- vancomycin hydrochloride 106
- vector magnitude ratio (VMR) 83
- scores 83
- Ventolin 116
- very persistent or very bioaccumulative in the environment (vPvB) 232

- w**
- Washington Department of Ecology (WA DOE) 252
- waste disposal 199
- waste materials 81
- Waste Reduction Algorithm (WAR) 35, 132
- wastewater treatment plants 13
- water intensity (WI) 217
- water reuse optimization 128
- World Summit on Sustainable Development 283

- x**
- xylene 5
 - p-xylene 289

- z**
- zeolites 88
- zero discharge of toxic chemicals (ZDHC) program 236
- zinc chloride 60
- Z-isomeric compound 175
- Zoloft® 105