Sustainability Decision Making for Renewable Biomass Energy Production: Integrated Algal
Bio-energy and Environmental Remediation Systems

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Abstract

In this dissertation, a combination of life cycle modeling and laboratory experiments is used to evaluate the feasibility and sustainability of simultaneous biomass energy production and environmental remediation via the synergies of algal bioenergy generation and wastewater treatment polishing. Life cycle approaches include both life cycle assessment (LCA) and life cycle costing (LCC), for assessing environmental and economic performances, respectively, of integrated algae cultivation and dairy manure wastewater treatment on small dairy farms in the Southeastern US. Laboratory experiments are designed to evaluate algae-mediated removal of both environmental estrogens and the estrogenic toxicity they induce. The results indicate that the integrated systems will deliver not only algae-derived energy (as bio-electricity) but also water quality improvement, the latter via removal of aqueous nutrients (nitrogen and phosphorus) comprising eutrophication potential and also anthropogenic estrogenic compounds from wastewater. Additional work comprises expansion of the current LCA framework to include estrogenicity as an environmental impact category, and improvement of two LCA and LCC metrics; i.e., energy return on investment (EROI) and economic meta-model for algae bio-energy based on published LCCs. Results from this work will not only improve sustainability decision-making related to the proposed algae-to-energy systems, but also constitute methodological advancements to increase LCA's usefulness during design of sustainable water-energy systems.

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Definition of Acronyms and Symbols

17 α	17 α -estradiol
AD	anaerobic digestion scenario
AOM	algal organic matter
ATS	algae turf scrubber
E1	estrone
E2	17 β -estradiol
E3	estriol
EN	net energy use
EROI	energy return on investment
EsP	estrogenicity potential impact factor
EUT	net eutrophication potential
GHG	greenhouse gas
GWP	net global warming potential
HPLC	high-performance liquid chromatography
LCA	life cycle assessment
LCC	life cycle cost analysis
MACRS	modified accelerated cost recovery system
NPV	net present value
OPS	algae cultivation in open ponds
REF	conventional reference scenario
TN	total nitrogen
TP	total phosphorus
WWTP	waste water treatment plants

Related Publications and Presentations

Colosi, L. M.; **Zhang, Y. L.**; Clarens, A. F.; White, M. A., 2012. Will algae produce green? Using published life cycle assessments as a starting point for economic evaluation for future algae-to-energy systems. *Biofuels* 3 (2), 129-142.

Zhang, Y. L.; Colosi, L.M., 2013. Practical ambiguities during calculation of energy ratios and their impacts on life cycle assessment calculations. *Energy Policy* 57, 630-633.

Zhang, Y. L.; White, M.A.; Colosi, L.M., 2013. Environmental and economic assessment of integrated systems for dairy manure treatment coupled with algae bioenergy production. *Bioresource Technology* 130, 486-494.

Zhang, Y. L.; White, M. A.; Clarens, A. F.; Colosi, L. M., 2011. Comparative LCA and economic analysis of integrated algae-dairy manure treatment systems for small farms. Oral presentation at *LCA-XI International Conference*, Chicago, Illinois, USA, Oct 4-6.

Zhang, Y. L.; Clarens, A. F.; White, M. A.; Colosi, L. M., 2013. Algal biofuels are financially promising. Poster presentation at *Advanced Energy*, New York, USA, April 30 – May 1.

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1. Introduction

1.1. Algae-to-energy systems: A green answer for increasing energy demand?

As energy consumption has increased over the last several decades, so too has interest in sustainable, non-fossil energy sources. Biofuels are considered to be one particularly attractive source of alternative energy for use in the US, because they can be produced domestically and are theoretically carbon-neutral. Algae biofuels are one class of biofuels with unique characteristics compared to conventional feedstocks (e.g., corn and soybeans) which may make them especially suitable for widespread deployment in the US. First, unlike terrestrial plants, algae can be grown on non-arable land using fresh, brackish, or even saline water (Chisti, 2007), still achieving much higher productivity per unit area. A second appealing feature is that algae do not directly compete with production of food crops (Benemann & Oswald, 1996; Sheehan et al., 1998). Third, algae's fast growth rate and aquatic habitat make them ideal for uptake of anthropogenic carbon dioxide (CO₂) and removal of certain water pollutants (Benemann and Oswald, 1996). These characteristics make algae not only appealing for biofuel production but also attractive on the basis of environmental considerations.

There have been numerous studies addressing algae-to-bioenergy systems over the past several decades. These have focused on a variety of bench-scale research topics, such as: identifying algae strains exhibiting high lipid content, enhancing algae lipid production by genetic modification, etc. More recently, considerable studies have focused on the environmental impacts associated with hypothetical large-scale algae-to-bioenergy systems. This has been done using what's called life cycle assessment (LCA). LCA is a widely accepted quantitative accounting tool for evaluating the environmental effects of

products, process, or services by computing the energy/material inputs and wastes released to the environment, and also assessing the potential environmental impacts of those energy, materials, and wastes (Nordic Council, 1995). LCA has become an actively researched area and has been increasingly applied in academic and industrial fields for evaluation of anticipated environmental impacts. Several analyses have also used a related tool, life cycle costing (LCC), which focuses on assessing the likely economic feasibility of algae-derived bioenergy platforms.

The algae LCA and LCC studies published to date reveal that algae-derived bioenergy is not likely to be truly sustainable at large scales without significant improvement in several areas (Clarens et al., 2010; Lundquist et al., 2010; Mata et al., 2010). Clarens et al. (2010) reported that energy production from algae cultivated in first-generation open pond systems tends to be more environmentally burdensome than energy production from canola, corn, or switch grass under some conditions. LCC analyses from Davis et al. (2011) and Gallagher et al. (2011) also show that the economics of micro-algal biofuel production are unlikely to be competitive with traditional fossil fuel in the near term. In all of these studies, the authors pointed to the need for improved access to low cost, low energy-intensity nutrient (nitrogen and phosphorus) sources to improve the overall environmental and economic bottom lines. This is because commercial fertilizers are among the most burdensome inputs for an algae-to-energy system, comprising up to 50% of overall system energy consumption during algae cultivation and conversion into biofuels (Clarens et al, 2010; Davis et al., 2011; Stephens et al., 2010; Stephenson et al., 2010).

1.2. Integration of algae cultivation and wastewater treatment

To improve the performance of algae cultivation, previous LCA studies have proposed the integration of algae cultivation and wastewater treatment (Clarens et al., 2010; Stephenson et al., 2010). In fact, it has become widely accepted in LCA studies to assume that large-scale algae cultivation systems will use recycled wastes from other sectors as “burden-free” inputs; e.g., flue gas for CO₂ supply, or municipal wastewater effluent for N and P supply (Clarens et al., 2011; Pittman et al., 2011; Sander & Murphy, 2010; Stephenson et al., 2010). This approach significantly improves the environmental performance of algae-derived energy sources in at least two ways: on the one hand, use of nutrients from wastewater effluent reduces the very high energy consumption associated with commercial fertilizer production; on the other hand, algae-mediated nutrient removal reduces energy consumption during wastewater treatment, because N and P removal are very energy intensive processes. Another appealing feature of integrated algae cultivation and wastewater treatment is that algae may be able to “polish” the treated effluent; i.e., remove “emerging contaminants” such as personal care products, estrogens, pharmaceuticals, etc. Traditional municipal wastewater treatment plants (WWTPs) are not typically designed for the effective removal of these chemicals, and as a result, many can be found in detectable concentration in water body worldwide (Wilson et al., 2003). Previous studies have demonstrated that algae may be capable of removing certain emerging contaminants to some extent via combination of biotransformation, bioconcentration, and biosorption interactions that are not well understood at present (Lai et al., 2002; Faramarze et al., 2008).

Although the synergies of algae cultivation and wastewater treatment seem promising, several practical limitations currently prevent this approach from being implemented at large-scale. First, the nutrient concentrations in municipal wastewater effluents are quite low: 3-8 mg/L N and 1-2 mg/L P in secondary effluent from an activated sludge treatment plant with biological nutrient removal (Carey & Migliaccio, 2009). This limits the amounts of energy savings which can be achieved via fertilizer avoidance and wastewater treatment offsets (Clarens et al., 2010). Second, municipal WWTPs are usually located in urban areas where vacant land is quite scarce and expensive. This makes it difficult to co-locate large algae farms nearby to WWTPs.

1.3. Integration of algae cultivation and dairy manure wastewater treatment

Besides municipal wastewater, an alternative nutrient source for algae cultivation is nutrient-rich animal waste, e.g., dairy manure. Historically, nutrient-rich dairy manure waste has been an environmental liability for the farms that generate it. Water quality impairment in Chesapeake Bay (the largest estuary in the United States) has been largely attributed to runoff and discharge of nutrients from agriculture, of which 18% of N and 25% of P arises from animal wastes (Chesapeake Bay Foundation, 2004). Animal waste is also an increasing source of greenhouse gas (GHG) emissions, including methane (CH₄) and nitrous oxide (N₂O). The US Environmental Protection Agency (EPA) estimates that GHG emissions from animal wastes increased by almost 60% during the period between 1990 and 2009 (EPA, 2010). Finally, dairy manure contributes to impairment of the water supply via introduction of emerging contaminants, including the steroid hormones and other so-called “environmental estrogens”. Feces and urine from livestock are known to be the principal source of these contaminants into the water supply (Khanal et al., 2006),

based on field studies which have shown that estrogens within manure are sufficiently mobile to impact surface and groundwater quality (Hanselman et al., 2003). Groundwater and runoff collected from research plots receiving dairy manure effluent had estrogen concentrations ranging from 2.1 to 41 ng/L (Dyer et al., 2001; Khanal et al., 2006). Livestock excrete a total estrogenic activity of 48.5 tonnes EEQ (17 beta-estradiol equivalents) per year in the USA, 93% of which is from dairy manure (Khanal et al., 2006; Lange et al., 2002). These chemicals are of increasing environmental concern because they are known to adversely affect the reproductive biology of aquatic wildlife (fish, turtles, frogs, etc) even at very low concentrations (10-100 ng/L) (Hanselman et al., 2003; Oberdorster & Cheek, 2001; Tyler et al., 1998).

Despite the challenges noted above, the relatively high N and P contents in dairy manure could make it a valuable nutrient source for algae farming. N and P excretion from dairy cow is about 108 and 20 kg/yr-cow respectively, such that cattle waste slurries can be expected to contain ~4300 mg/L N and ~800 mg/L P (Van Horn et al., 1994). These concentrations are many times higher than in municipal wastewater effluent. Thus, the possible synergies associated with integration of algae cultivation and wastewater treatment are even more pronounced for the case of dairy manure wastewaters. The dairy manure waste could provide a concentrated source of “free” nutrients, and algae production could mitigate eutrophication potential, global warming potential (GWP), and possible water quality impairment from estrogenic compounds. It’s also possible that integration of dairy waste management and algae cultivation could make the combined system more financially attractive than either individual system, since wastes from dairy farming would be used as inputs for production of algae-derived bioelectricity.

2. Research Objectives

The overall goal of this research is to develop the knowledge required by farmers, wastewater treatment plants, and the energy generation sector to choose which waste-to-energy system is optimally sustainable with respect to its environmental and financial feasibility. This knowledge could also help formulate local, regional, and national policies (economic incentives, etc) that motivate individual stakeholders to make environmentally sound choices. The first step towards this goal is understanding how traditional manure waste management strategies compare with novel, algae-integrated management on the basis of environmental and economic performance. This is done via life cycle assessment and life cycle costing modeling. The second step is assessing algae mediated removal of emerging contaminants (as pertaining to estrogens in this research) via bench scale experiments. Finally, related additional work will focus on improving LCA and LCC methodologies to better understand ecosystem services delivered by integrated algal energy production and wastewater management systems.

Specifically, this dissertation consists of the four following objectives.

Objective 1. Evaluate the environmental and economic impacts of integrating algal bioenergy production with dairy manure waste treatment by using life cycle assessment (LCA) and life cycle cost (LCC) analysis. This objective is discussed in Chapter 3.

Objective 2. Characterize algae-mediated removal of selected estrogenic compounds , and their associated estrogenic toxicity, from simulated dairy manure wastewater effluent; apportioning apparent removal among

biotransformation, sorption, and direct photolysis; establishing an estrogenicity potential impact factor (EsP) as a novel LCA endpoint, so that water quality impairment (or mitigation thereof) can be fully accounted for during LCA using data similar to that arising from the bench scale experiments. This objective is discussed in Chapter 4.

Objective 3. Evaluate practical difficulties with the widely-used LCA metric known as EROI (energy return on investment) and establish a consistent methodology for use in LCA to better address sustainability decision-making as it pertains to waste-to-energy systems. This objective is discussed in Chapter 5.

Objective 4. Establish an economic meta-model for algal bio-energy production based on previously published LCCs, to better understand the financial feasibility of algal bioenergy at present and in the near future. This objective is discussed in Chapter 6.

Each objective is the topic of one dissertation chapter, as noted above. Figure 1 shows how the individual chapters fit within the overall framework of the dissertation research, contributing to a comprehensive assessment of ecosystem services delivered by integrated algae cultivation and waste treatment systems.

Figure 1. The overall framework of the dissertation, with interactions among four key research objectives.

3. LCA & LCC of Integrated Algae Cultivation and Dairy Manure Management

This chapter summarizes dissertation content pertaining to Objective 1. In this chapter, life cycle assessment (LCA) and life cycle costing (LCC) are used to assess the environmental and economic performance of integrated algae bioenergy production and dairy manure waste management on small dairy farms. This will provide first-sight information of what economic and environmental benefits could arise from the synergies between algae energy production and dairy manure waste management. The material in this chapter was adapted from Zhang et al. (2013), which had been published in *Bioresource Technology* (Zhang et al., 2013).

3.1. Background

3.1.1. Limitations of conventional dairy manure waste management

The most widely used manure management strategy at present is on-farm land application. There are, however, some limitations of this application, such as the short season of the year when wastes can be land-applied, low nutrient utilization by crops, nutrient leaching/runoff, and the large land area required for complete consumption of the waste. These factors pose both technical and economic challenges for dairy farmers (Adey et al., 1993; Kaiser, 2001; Van Horn et al., 1994). For many years, the conventional manure waste management, on-farm land application, has been a considerable expenditure for dairy farmers, roughly 30-100 \$/head (Fulhage & Pfost, 2003). Significant technical challenges include runoff and discharge of environmental contaminants such as nutrients, estrogens, etc. As a result, water quality in water bodies adjacent to dairy farms has been impaired and eutrophication has become an increasing concern in these regions.

3.1.2. Emerging approaches for dairy manure management

Although there has been significant efforts towards mitigation of eutrophication in impacted watersheds (e.g., the Chesapeake Bay), progress has been slow (Jones et al., 2010). Several new technical and economic approaches have been proposed, including nutrient credit trading (Commonwealth of Virginia 2005; Jones et al., 2010; Selman et al., 2009). Nutrient trading markets allow agents that reduce their nutrient runoff or discharges below target levels to sell their surplus reductions as “credits” to other agents. Preliminary analyses of this approach indicate that several environmental and economic benefits could be achieved following establishment of a robust nutrient trading market, including: 1) creation of new revenues for the agricultural sector and other credit generators; 2) accelerated nutrient load reductions; and 3) more rapid development of low-cost and high-effectiveness nutrient reduction practices (Jones et al., 2010).

The establishment of nutrient credit trading would be one additional, financial, incentive for farmers to consider integrated algae farming and dairy manure waste management. A number of bench-scale and pilot-scale studies performed over the past decade have evaluated algae growth on animal waste effluents as nutrient source, including: An et al. (2003); González et al. (1997); Kebede-Westhead et al. (2003); and Mulbry et al. (2008a, 2008b). Taken together, these studies demonstrate algae’s ability to utilize nutrients from a variety of waste effluents. However, there have been no-full scale LCA and LCC studies to assess how utilization of these new approaches could affect the overall sustainability of dairy manure management.

3.1.3. Algae cultivation systems: OPS and ATS

The best-studied configuration for large-scale algae cultivation is the open pond system (OPS). This configuration is widely considered to be the most feasible cultivation configuration for algae-to-energy systems, primarily because it has been widely used in algae LCA and LCC studies to date (Clarens et al., 2010; Clarens et al., 2011; Park et al., 2011; Davis et al., 2011). One alternative to OPS for algae cultivation at large scale is the so-called “algae turf scrubber” system (ATS). This system has been evaluated in a small number of previous studies, which have documented its ability to produce sustained algae yields of up to 40 g dry solids (DS)/m²-day with concomitant N and P removals up to 90% and 100%, respectively, from animal manure effluents, wastewater, or river water (Adey et al., 1993; Craggs et al., 1996; Kebede-Westhead et al., 2003; Mulbry et al., 2008a, 2008b). There has been no formal LCA study conducted of the ATS system to date, so its environmental impacts remain unknown. Pizarro et al. (2006) evaluated the likely economic performance of using ATSS to treat dairy manure effluents on large dairy farms (1000 cows); however, this study omitted several possible revenue streams that could accrue from integration of dairy manure waste management and algae cultivation for energy production.

3.2. Methodology

The following paragraphs briefly summarize the methodology. Please see Appendix A for detailed information.

Complementary life cycle assessment (LCA) and life cycle costing (LCC) analysis were performed to evaluate the environmental impacts and economic feasibility, respectively, of four on-farm dairy waste management approaches. Figure 2 depicts the four selected nutrient management scenarios, as modeled for a typical small dairy farm (100 cows) in Virginia. These scenarios include: a conventional reference (REF) scenario, whereby manure is stored at the farm where it is generated and then directly applied to

Figure 2. Schematic graphic of four evaluated manure waste management scenarios. A is algae biomass, B is biogas (CH_4), L is liquid digestate, M is manure, and S is solid digestate. Adapted from Zhang et al. (2013).

on-farm agricultural lands; an anaerobic digestion scenario (AD), corresponding to the reference system plus addition of an anaerobic digester where manure is converted into biogas for production of bioelectricity, liquid digestate for on-farm application, and solid digestate for use as soil amendment; and two algae scenarios, in which nutrient-rich

digester liquid is used to cultivate algae in either an open pond system (OPS) or an algae turf scrubber (ATS), and resulting biomass is co-digested with manure to increase bioelectricity production. In all cases, nutrient and other characteristics of dairy manure were based on Van Horn et al. (1994). On-farm land application (for scenarios REF and AD) was assumed to occur during the crop growing season, which is March through September in the southeast USA. Algae cultivation was assumed to occur from March through November (Mulbry et al., 2008; Pizarro et al., 2006). Wastes generated and collected outside of the biomass growing seasons were stored on-farm in lagoons for next growing season.

The functional unit was defined as management of as much manure is produced per year on a 100-cow dairy farm. Systems boundaries of all four scenarios were “cradle to gate” for dairy manure management, encompassing all processes associated with dairy manure waste treatment. These processes included collection and storage of manure waste, extraction of raw resources required for the production of energy/material inputs, bioelectricity generation for on-farm use or sale to local grid, and disposition/export of residual materials. Cow breeding and manure collection were excluded from system boundary, because these activities are already be in place at all farms and, therefore, held in common for all evaluated scenarios. Environmental impacts associated with infrastructure and equipment were calculated by multiplying material inputs and their corresponding environmental impact factors obtained from the ecoinvent database (Weidema, 2007), and they were further divided by an assumed 20-years of system life time for direct comparison with annual impacts in each scenario.

All LCA and LCC models were built in Microsoft Excel, and the Crystal Ball commercial suite was used to automate Monte Carlo analyses for characterization of input and output uncertainty. LCA models evaluated direct land use and three categories of environmental impacts for each of the four evaluate systems. The three environmental impacts were: net energy use (EN), net eutrophication potential (EUT), and net global warming potential (GWP). LCC models were constructed based on LCA mass-flow models. The outcome of LCC analysis was net present value (NPV) over the entire system lifetime (20 years) for each scenario, based on three types of cash flows: initial outlay, annual operating cost, and annual revenue. Initial outlay was the total capital investment required for purchase of materials and equipment, construction costs, and miscellaneous costs. Annual operating costs included energy, labor, capital depreciation, and other operating costs. Annual revenues consisted of five possible sources: 1) sale of corn (for REF and AD); 2) sale of biogas-derived bioelectricity (for AD, OPS, and ATS); 3) sale of N and P treatment credits, using the 80% of REF nutrient loadings as “baseline” and assuming that the nutrient loading reductions achieved by each “best management practice” (AD, OPS, and ATS) are eligible to be sold (Branosky et al., 2011; Maryland Department of Agriculture, 2008); 4) sale of carbon dioxide (CO₂) credits within the national carbon market (for AD, OPS, and ATS) (Cap-and-Trade Program, 2012; Chicago Climate Change, 2011), which is the reduction of CO₂ emission compared to scenario REF; and, 5) sale of post-digestion residuals for use as soil amendment (i.e., fertilizer) (AD, OPS, ATS) (Tambone et al, 2009).

3.3. Results & Discussion

3.3.1. Nutrient Flows

Figure 3 summarizes the total nitrogen (TN) and total phosphorus (TP) flows in each of the four evaluated scenarios.

Figure 3. Nitrogen (N) and phosphorus (P) flows for each modeled nutrient management scenario. Adapted from **Zhang et al. (2013)**.

It is assumed that each cow excretes 2,578 kg of waste per year as feces and urine, roughly 80% of which is volatile (Van Horn et al., 1994). Total nitrogen (TN) and total phosphorus (TP) excretion is 108 kg per cow per year and 20 kg per cow per year, respectively.

For REF, the manure slurry is either used directly for on-farm land application or stored for use in the next growing season, depending on the time of year. The biologically available TN mass for on-farm land application is 2,710 kg per year per 100 cows after N losses during storage and spreading (see Section 3.4 of Appendix A).

In the AD scenario, the manure slurry first undergoes anaerobic digestion, wherein 30% of TN and 60% of TP are retained in the solid digestate. Post-digestion effluent is then transferred to a storage tank for separation into solid and liquid streams. The solids are shipped off-farm for use as land amendment at a sale price of roughly \$12/Mg. The liquid is either used directly for on-farm land application or stored for the next growing season, depending on the time of year. The biologically available TN mass in the post-digestion effluent for on-farm land application is 1,141 kg/year per 100 cows after N losses during storage and spreading (see section 3.4 of Appendix A).

Regarding the OPS and ATS scenarios, the manure slurry first undergoes anaerobic digestion, just the same as in AD. The post-digestion slurry is then transferred to a storage tank for solid/liquid separation. Solids are shipped off-farm, and storage N losses in the liquid stream are the same as in AD scenario. Assuming 275 operational days per year (March through November) for algae cultivation, the post-digestion TN and TP masses give rise to 118 or 153 Mg of algae biomass per year in the OPS or ATS scenario, respectively. The difference between these yields is attributed to the difference of algae yield (ash free dry mass): 12.6 g/m²-day in OPS versus 18.5 g/m²-day in ATS.

3.3.2. Direct Land Use

Direct land use is the land area required for manure management in each scenario; i.e., corn cultivation on undigested or digested manure waste for REF and AD, or the footprint required for algae cultivation in an OPS and ATS system. Corn's nitrogen demand ("agronomic N rate) was assumed to be 157kg/ha TN on typical dairy farms in Virginia (Evanylo 2009). The total quantity of N available to plants was 2,710 and 1,141 kg N/yr for REF and AD, respectively. Average land use requirements for on-farm dairy manure management were therefore 17.7 ha for REF and 7.4 ha for AD, which are roughly 12% and 5% of the average farm size in this region (155 ha) (Groover, 1998), respectively.

Regarding the OPS and ATS scenarios, total quantities of N and P available from dairy manure after digestion are 6,722 kg N/yr and 788 kg P/yr, respectively. The algal uptake rate of P from dairy manure is up to 100%, greater than that of N (Mulbry et al., 2008). Therefore, the OPS and ATS systems were sized to completely consume all of the available P. The OPS and ATS land area requirements were roughly 3.4 ha for OPS and 2.6 ha for ATS. Thus, both algae systems require less direct land use than REF and AD, and each will require no more than 3% of the average farm size in this region (155 ha) (Groover, 1998). This suggests that farms will not need to purchase additional land to implement an algae-mediated nutrient management system.

3.3.3. Environmental Impacts

Figure 4 summarizes environmental impacts of all four evaluated nutrient management scenarios. The three evaluated environmental impacts include net eutrophication potential (EUT), net energy use, and net global warming potential (GWP)

(based on GHG emissions). From these results, AD, OPS, and ATS are environmentally preferable to REF. These impacts are discussed in the following paragraphs.

Figure 4. LCA results for delivery of one functional unit in each manure management scenario. EN is energy use (in GJ/yr), GWP is global warming potential (in Mg CO₂-eq/yr), and EUT is eutrophication potential in (kg PO₄-eq/yr). For EUT and GWP, values greater than zero indicate net output from the system boundaries, values less than zero indicate net input across the system boundaries. For EN, values greater than zero indicate net energy consumption, values less than zero indicate net energy generation. Error bars are 25-75% percentile ranges for Monte Carlo output. Adapted from **Zhang et al. (2013)**.

3.3.3.1. Net Eutrophication Potential (EUT)

On-farm land application (REF) constitutes the most widely-used manure management practice at present. But this methodology is problematic with respect to nutrient control for several reasons, most notably: 1) considerable release of N and P during storage and land spreading, 2) significant runoff of N and P following waste application, and 3) large land areas required for manure management due to the relatively short duration of the growing season when waste can be applied (Van Horn et al., 1994). It was hypothesized that the improved nutrient control afforded by an AD, OPS, or ATS

system could be an incentive for farms to improve their manure management strategy, especially in the face of increasingly stringent environmental regulations, but it was necessary to evaluate what EUT performance enhancement each system would deliver.

From Figure 4, AD offers considerable EUT improvement over REF, and both algae systems offer dramatic EUT reductions compared to AD and REF. The EUT values for both OPS and ATS are roughly 325 kg PO₄-eq/yr per functional unit, which is nearly seven times smaller than for AD (2162 kg PO₄-eq/yr) and roughly nine times smaller than for REF (3024 kg PO₄-eq/yr). For both algae cases (OPS and ATS), the nutrient-rich liquid digestate is recycled into the algae cultivation system instead of spread onto farmland. This essentially eliminates the N and P fluxes which would otherwise occur following land application of raw or digested manure waste, as in the REF and AD cases, respectively. The difference in EUT between REF and AD reflects partial nutrient removal during digestion: roughly 30% of pre-digestion N and 60% of pre-digestion P are separated from the post-digestion liquid effluent via various processes.

3.3.3.2. Net Energy Use (EN)

As shown in Figure 4, the three scenarios incorporating anaerobic digestion (AD, OPS, and ATS) exhibit net energy production per FU. Only REF exhibits net energy consumption. Table 1 lists detailed information about energy generation and energy consumption for each scenario. Energy generation calculations accounted for both direct energy production (i.e., bioelectricity derived from biogas via anaerobic digestion) and indirect energy offsets (i.e., use of solid digestate to offset commercial fertilizer production, and production of corn as co-product). Energy consumption calculations also accounted for both direct energy consumption and upstream energy inputs associated

with production of system infrastructure and input materials.

Regarding direct energy generation, only the manure slurry is digested to produce biogas in the AD scenario. For the OPS and ATS scenarios, the manure slurry is co-digested with algae biomass, increasing the quantity of digestible biomass by roughly 60%. This gives rise to increased bioelectricity generation. The amounts of CH₄-derived bioelectricity produced per FU are 1,662 GJ/year for OPS and 1,802 GJ/year for ATS, compared to only 1,044 GJ/year for AD (Table 1). It should be emphasized that the bioelectricity figures for the algae cases may be underestimates, based on limited data from bench-scale experiments which show increased methane production during digestion of algae with a carbon-rich co-substrate (e.g., manure) (Yen and Brune, 2007); however, this possible impact was not accounted for in this study due to data scarcity.

Table 1. Overview of annual energy use for each scenario (GJ/yr)¹.

Process	REF	AD	OPS	ATS
<i>Energy Inputs</i>				
Manure land application (fuel)	195	183		
Algae cultivation			272	846
<i>Electricity</i>			55	846
<i>Nutrients supply</i>			217	0
Anaerobic digestion		100	341	386
<i>Electricity</i>		86	308	347
<i>Heat</i>		14	33	39
Infrastructure ²	4	19	627	143
<i>Energy Outputs</i>				
Bioelectricity generation		-1,044	-1,662	-1,817
Soil amendment offset ³		-101	-189	-199
Corn silage offset ⁴	-19	-8		
Total Energy Input	199	302	1,240	1,375
Total Energy Output	-19	-1,153	-1,851	-2,016
Net Energy Balance	180	-851	-611	-641

¹ Adapted from Zhang et al. (2013). For more detailed information, please see Table S10 of the SI in Appendix A.

² Accounts for “annualized” infrastructure energy burdens assuming a 20-years useful lifetime.

³ Accounts for digestate solids used as soil amendment.

⁴ Accounts for corn grown on manure-applied lands.

Regarding indirect energy generation, the masses of solid digestate produced per FU are 156, 232, and 256 Mg/year in the AD, OPS, and ATS scenarios, respectively. These quantities account for energy offsets of 101 GJ/year, 189 GJ/year, and 199 GJ/year, respectively. REF produces only a small amount of energy production, 1.1 GJ/ha per FU, which is an offset associated with production of corn silage.

Energy consumption was also evaluated for in each scenario. Not surprisingly, REF requires the lowest energy consumption (199 GJ/yr per FU), because it involves the least number of steps. Energy consumption in this scenario is mostly associated with operation of manure spreading, including upstream impacts associated with production of the necessary diesel fuel.

Energy consumption for AD (301 GJ/year per FU) was roughly 1.5 times that of REF. This is because energy consumed by land application of liquid digestate is held in common between the AD and REF scenarios, whereas anaerobic digestion requires additional energy input.

Energy requirements for OPS (1,240 GJ/yr) and ATS (1,375 GJ/yr) were understandably greater than for either AD or REF. This is because additional energy is required for algae cultivation beyond what is consumed for operation of the anaerobic digester and application of the liquid digestate. Direct energy use will be a key factor in decision making about on-farm waste nutrient management, because farms have to pay for it. From Table 1, heat consumption is roughly the same in both algae systems (~30 GJ/FU), but electricity consumption varies dramatically: 363 GJ/FU for OPS versus 1,193 GJ/FU for ATS. The difference arises mostly from cultivation usage (55 GJ/FU in OPS versus 846 GJ/FU in ATS), since both systems use about the same amount for

anaerobic digestion. Cultivation-phase electricity usage of ATS is primarily attributed for water pumping, accounting for 47% of overall energy usage. From Table 1, direct energy use for algae cultivation and digestion processes constitutes 50% of total energy consumption per FU in OPS and 90% in ATS. This may make OPS seemingly more desirable than ATS for an algae farming entity, together with the fact that the total amount of energy consumed per FU is also smaller in OPS than in ATS.

From Table 1, there is a dramatic difference in energy consumption for *nutrients* (mainly CO₂ because N and P come from manure waste) between the OPS and ATS systems. In the OPS, pure CO₂ or air is generally bubbled into the growth medium to provide a carbon source for algae photosynthesis (Benemann and Oswald, 1996). The upstream burdens associated with the production of CO₂ account for nearly one-quarter (17%) of total energy usage in the OPS system. This is consistent with previous OPS studies (Clarens 2010, Lundquist et al., 2010). In contrast, ATS requires neither commercial fertilizer nor CO₂ because the shallow, continuously pumped configuration enables algae taking CO₂ from the atmosphere, which is one of the principal benefits of the ATS for on-farm dairy waste nutrient management (Mulbry et al., 2008a).

Finally, regarding upstream infrastructure burdens, Table 1 indicates that there is a significant difference in the extent to which upstream energy use for production of infrastructure contributes to overall energy consumption in each algae system. Annualized infrastructure energy burdens account for 50% of total energy use per FU in the OPS system but only 10% in the ATS. This difference makes re-design of the OPS infrastructure a potentially useful strategy for improving overall energy efficiency of algae-to-energy systems. In contrast, it would seem not worthwhile to try to optimize

ATS infrastructure burdens because they account for such a small fraction of overall energy consumption in that system.

In summary, referring again to Figure 4 and Table 1, the AD scenario is most energetically favorable because it mediates the largest difference between energy outputs (both direct and indirect) and energy inputs (direct, upstream, and infrastructure). In comparison, the OPS and ATS scenarios exhibit increased energy production, but the increases in energy output do not counterbalance the increased energy consumption required for construction and operation of either algae scenario. The REF scenario is least energetically desirable, even though it consumes the least amount of energy per FU, because it produces such a small amount of energy offset.

3.3.3.3. Net Global Warming Potential (GWP)

There is frequently a link between energy consumption and greenhouse gas (GHG) emissions per FU, thus it is not surprising that the EN and GWP performances exhibit qualitatively similar trends in Figure 4. The REF scenario exhibits the worst performance (437 Mg CO₂-eq/FU). This is attributed to the significant emissions of gaseous CH₄ and N₂O, both of which have very strong GWP impacts.

The GWP performances of AD (337 Mg CO₂-eq/FU), OPS (309 Mg CO₂-eq/FU), and ATS (242 Mg CO₂-eq/FU) are all better than REF, for at least two reasons. First, all three improved systems dramatically reduce emissions of strongly global-warming CH₄ and N₂O. Second, all three include one or more CO₂-sequestering processes; e.g., anaerobic digestion and/or CO₂ recycling. During digestion, not all organic material is converted into biogas. Carbon comprises 30% of the digestate material, of which 80% of is accounted for as GWP sequestration, because it is not directly returned to the

atmosphere when the biogas is combusted (Hue and Sobieszczyk, 1999; Moorhead et al., 1987; Tambone et al, 2009;), With respect to CO₂ recycling, only the ATS system exhibits true CO₂ reuse, whereby the flux of CO₂ out of the atmosphere into algae biomass (via photosynthesis) is roughly equivalent to the flux of CO₂ into the atmosphere during biogas combustion. Thus, ATS is nearly net CO₂-neutral for *direct* GHG flows. In contrast, the OPS requires large quantities of compressed virgin CO₂ as input for algae cultivation, such that the combustion GHG flux cannot be directly offset by photosynthesis. Moreover, the manufacture of the virgin CO₂ engenders significant *upstream* GWP emissions. Thus, the combined direct and upstream GWP impacts associated with commercial CO₂ render OPS worse than AD for GWP performance.

3.3.4. Economic Feasibility

A life cycle costing (LCC) analysis was undertaken in parallel with the LCA to assess the economic viability of each scenario. The key metric was net present value (NPV) for an assumed system lifetime equal to 20 years. Positive NPV indicates that the system is economically profitable. The results of LCC analysis are summarized in Figure 5 and Table 2.

Figure 5. LCC results for delivery of one functional unit in each manure management scenario. 3a (left): Net present value (NPV) for each system. Error bars are 25-75% percentile ranges for Monte Carlo output. 3b (right): Probability density function for Monte Carlo NPV output, where $P(NPV)$ is the probability of achieving a particular NPV value. Adapted from **Zhang et al. (2013)**.

Table 2. Capital costs, annual operational costs, and annual revenues for each manure management scenario¹.

Cash Flow	REF	AD	OPS	ATS
Capital Costs	\$ 102,000	\$ 334,349	\$ 574,987	\$ 595,832
Manure land application	\$ 102,000	\$ 95,696		
Anaerobic digestion		\$ 238,653	\$ 283,430	\$ 288,530
Algae cultivation			\$ 291,557	\$ 307,302
Annual Operational Costs	\$ 9,200	\$ 40,741	\$ 94,835	\$ 106,391
Manure on-farm land application	\$ 9,200	\$ 8,631		
Anaerobic digestion		\$ 32,109	\$ 43,851	\$ 45,507
Algae cultivation			\$ 50,984	\$ 60,684
Annual Revenues	\$ 12,637	\$ 51,980	\$ 303,127	\$306,539
Corn	\$ 12,637	\$ 5,321		
Bio-electricity		\$ 16,827	\$ 26,781	\$ 29,266
N credit sale		\$ 26,662	\$ 271,742	\$ 271,742
P credit sale		\$ 61	\$ 123	\$ 123
Carbon credit sale		\$ 1,264	\$ 1,733	\$ 2,374
Digestate		\$ 1,844	\$ 2,748	\$ 3,034

¹ Adapted from **Zhang et al. (2013)**. For more detailed information, please see Sections 7.1, 7.2, and 7.3 of the SI in Appendix A.

Figure 5a summarizes net present value (NPV) for all four nutrient management strategies (in Panel a). From this figure, OPS and ATS exhibit economically favorable performances, as indicated by $NPV > 0$. Values were \$853,250 for OPS, and \$790,280 for ATS. In contrast, REF and AD exhibit NPVs of -\$62,279 and -\$211,126 respectively. This is consistent with previous observations that dairy manure management via land application is quite costly, approaching \$50-120/cow-yr (Ribaud et al., 2003; Van Horn et al., 1994). Thus, both algae systems (OPS and ATS) are economically favorable compared to the non-algae systems (REF and AD).

From Table 2, nutrients credits constitute the main revenue source in the algae scenarios, accounting for 88% of overall income for both OPS and ATS. Sensitivity analysis also shows that the price of nutrient credits, (especially nitrogen), is the most important factor affecting the magnitude of NPV (see Table S23 of SI). In the absence of any nitrogen credits, the two algae scenarios (OPS and ATS) exhibit negative NPV. The break-even price for nitrogen credits, at which $NPV = 0$, is roughly \$14/lb N (see Figure S9 of SI in appendix A). This is substantially higher than the value estimated by Pizarro et al. (2006) for economically advantageous ATS operation (\$4/lb N). The difference between these two estimates likely reflects Pizzaro's omission of downstream processing costs (e.g., digestion and electricity generation equipment, etc.). Other relevant economic benchmarks include the market price at which farmers are expected to sell nutrient credits (\$20/lb N) and expected costs for various proposed nutrients management strategies (from \$30-\$600/lb) according to Jones et al. (2010) and Van Houtven et al. (2012). From these data, both OPS and ATS could be very cost-competitive in the geographic regions where sustainable nutrient credit markets are likely to exist, e.g., Chesapeake Bay area

(Jones et al., 2012; Stephenson & Shabman, 2011; Van Houstven et al., 2012).

Two other considerations affecting the relative economic appeal of possible dairy waste management strategies include *risk* and *scale*. Regarding risk, comparison of NPV distributions (as opposed to mean or median values) reveals that two algae scenarios (OPS, ATS) exhibit small risk. This is evident in the NPV distributions for OPS and ATS (Figure 5b), whereby each system has small likelihood of delivering NPV < 0: roughly 10%. Regarding scale, farm size significantly affects expected economic performance. This is because capital costs for digestion systems do not scale linearly with increasing farm size (see 7.1 of SI in Appendix A), and this may also be true for algae cultivation systems. If so, OPS, and ATS systems could become even more economically attractive for herd sizes larger than the 100-cow farm selected for this study.

3.3.5. Assessment of Overall Favorability

In evaluating the overall sustainability of possible manure waste nutrient management systems, environmental and economic performances are important considerations. For the four management strategies evaluated in this study, all three “improved” scenarios (AD, OPS, and ATS) were found to be far environmentally superior to the reference scenario (scenario REF: storage and land application). The direct land use requirement for REF was more than twice as large as for AD, OPS, or ATS. For energy production, REF was the only scenario that resulted in net energy consumption. With respect to economic feasibility, both algae systems (OPS and ATS) exhibit similar performance and are preferable to REF and AD. Thus, either algae system offers more favorable land, environmental, and economic performance.

Still, OPS, and ATS systems are unlikely to be profitable on the basis of energy

production alone, since their economic performances are highly dependent on the price of nutrient credits. This means that farmers may be unwilling to invest in ATS (or even OPS) systems, despite their environmental preferability, since they may be unable to achieve their full potential in the absence of a robust nutrient credit market. This observation highlights the need for environmental policies which offer financial incentive for environmentally responsible technologies, such that economic favorability is better aligned with environmental favorability during on-farm decision-making.

3.4. Conclusions

This section provides conclusive evidence that adoption of “improved” nutrient management strategies will dramatically improve the sustainability of manure management on small dairy farms. Addition of digestion with or without algae cultivation makes farm operations net positive in energy production. Use of an algae system, for beneficial recycling of nutrient-rich liquid digestate, further improves environmental and economic performances. However, energy production itself is unlikely to be profitable. The environmental and economic benefits of these integrated systems could only be achieved if economic incentives (e.g., nutrient credits) are in place to motivate environmentally-responsible decision-making. In this section, only one economic incentive, nutrient credits arising from nutrient removal, was accounted for. Considering the various types of environmental pollutants that are present in dairy manure, it is also necessary to explore other possible ecosystem services that could be delivered by integrated algae cultivation and dairy manure management systems. This topic is addressed in Chapter 4.

4. Characterizing Algae-mediated Removal of Estrogenic Compounds and Establishing of Estrogenicity Potential Impact Factor (EsP)

This chapter discusses work related to Objective 2 of the overall dissertation. In particular, bench-scale laboratory experiments are designed to characterizing algae-mediated removal of four estrogens (i.e., 17 α -estradiol, 17 β -estradiol, estrone, and estriol) and the corresponding estrogenicity induced. Specific interests included: 1) apportioning apparent removal among biotransformation, sorption, and direct photolysis; 2) quantifying estrogenicity removal mediated by algae *Scenedesmus dimorphus*; 3) assessing the effect of estrogen concentrations on algae growth. At the same time, an estrogenicity potential impact factor (EsP) as a novel LCA endpoint would be established by using data similar to that arising from the bench scale experiments.

4.1. Background

4.1.1. Estrogenic Pollution from Dairy Manure Wastewater

Current management and regulations for manure wastewater are primarily focused on nutrients removal (Bradford et al., 2008). Nevertheless, there are other environmental considerations associated with dairy manure waste, one of which is the presence of estrogens and other hormones. The natural steroidal estrogens, also known as the C18 steroidal group, include estrone (E1), 17 β -estradiol (E2), estriol (E3), and 17 α -estradiol (17 α). Table 3 summarizes the structure and key properties of several especially relevant environmental estrogens. Dairy cows excrete 17 α , E2, E1, and E3, with 17 α being the dominant estrogen (Khanal et al., 2006; Hanselman et al., 2003).

Table 3. Chemical structures of selected steroidal hormones¹.

Steroid Hormone	Symbol	Chemical Structure	MW ² , g/mol	E2-Eq ³
Estrone	E1		270.4	0.1-0.2
17 β -estradiol	E2		272.4	1
Estriol	E3		288.4	0.02
17 α -estradiol	17 α		272.4	1-2

¹ Modified from **Khanal et al. (2006)**.

² MW is molecular weight

³ E2-Eq is “E2 equivalent” where E2 is 17 β -estradiol; larger values indicate stronger estrogenic toxicity.

The behavior of estrogenic compounds has been previously studied in the natural environment and engineered systems. There are three possible mechanisms of estrogen removal: volatilization, sorption, and degradation. Regarding volatilization, it has been demonstrated that natural estrogens are not easily volatilized under normal temperature and pressure conditions (Khanal et al., 2006). In contrast, estrogens are known to readily sorb onto organic solids such as WWTP sludge or various sediments. Finally, biodegradation is a well-known mechanism of estrogen removal from municipal wastewaters, even though the exact mechanisms of removal for each specific compound are not completely understood (Colucci et al., 2001; Raman et al., 2001; Ternes et al., 1999). In activated sludge wastewater treatment systems, removal efficiencies for E2 and E1 are 70-95% and 20-70%, respectively (Johnson and Sumpter 2001). Thus, even well-operated systems cannot achieve complete removal of estrogenic compounds. For the

specific case of dairy manure management, a typical treatment strategy may comprise covered or uncovered lagoons, in which estrogen removal may be as low as 15%-23% over several months (Zheng et al, 2012). Therefore, it is desirable to identify new farm-appropriate manure wastewater treatment strategies, to mitigate runoff of steroid estrogens and reduce water quality impairment.

4.1.2. Algae-mediated Estrogen Removal

Compared to the large number of studies about WWTP estrogen removal via activated sludge treatment, there has been less studies on estrogen removal mediated by algae culture. Historically, bacteria and fungi have been considered the microorganisms of choice for biotransformation of organic compounds, thus algae-mediated processes have traditionally been overlooked in the literature (Faramarzi et al., 2008). Abul-Hajj and Qian (1986) first studied steroid transformation reactions mediated by various algae strains, and a small number of subsequent studies have demonstrated that algae may possess several attributes which make them uniquely well-suited for removal of estrogens (and other emerging contaminants) from water and wastewater effluents (Lai et al., 2002; Mason et al., 1996; Pflugmacher et al., 1999). First, algae's genetic and biochemical diversity enable the rapid production of organic, high surface area carbonaceous material ("algal organic matter" – AOM), with diverse chemical structures and properties, in a short time of period. This facilitates the bio-sorption of various organic contaminants (Lai, et al., 2002; Faramarzi et al., 2008). Second, there is limited evidence to suggest that microalgae possess several enzymes in common with mammalian livers, which enable them to mediate various steroid estrogen reactions, including: hydroxylation, reduction, hydroxyl oxidation, and side-chain degradations (Faramarzi et al. 2008; Lai et al. 2002).

From this limited information, it seems algae can reduce estrogen concentrations by bio-sorption and biotransformation, but possibly with increased specificity and efficiency compared to activated sludge treatment (Lai et al., 2002). Additional information is required to better understand the mechanisms by which algae mediate estrogen removal and to assess what effect these reactions have on overall estrogenic toxicity, not just the concentrations of the parent compounds themselves.

4.1.3. Estrogenicity Removal

It has been previously demonstrated that biological estrogen degradation (in activated sludge, etc) frequently proceeds stepwise with production of multiple metabolic intermediates. In many cases, the intermediate products may exhibit appreciable estrogenic toxicity. For example, in the most common degradation route, E2 is initially oxidized to E1 which exhibits 10-20% of E2's starting estrogenic toxicity (Khanal et al., 2006). In some cases, the metabolites may be more strongly estrogenic than the parent compounds such that "treatment" increases, instead of decreases, the estrogenic potency. Therefore, it is necessary to evaluate estrogenic toxicity (estrogenicity) over time during reactions designed to remove estrogenic parent compounds. This can be done using several popular assays, including: receptor binding assays, reporter gene expression assays using cultured cells and yeast cells (YES), and a MCF-7 cell proliferation assay (E-Screen) (Nishihara et al., 2000). Among all of these, the MCF-7 (E-Screen) method is generally accepted to be the most sensitive, accurate, and predictive of actual outcomes in mammals (Isidori et al., 2010; Soto et al., 1991, 1995).

The E-Screen assay measures proliferation (increase in number) of estrogen-sensitive human breast cancer MCF-7 cells following exposure to the prototypical female

sex hormone (17 β -estradiol – “E2”) or other chemicals bearing structural similarity to E2. More strongly estrogenic substances engender greater proliferation, which is quantified via DNA quantification. Results are in units of “M E2 equivalents”, to articulate what molar concentration of 17 β -estradiol would elicit the same (“equivalent”) MCF-7 proliferation response.

4.1.4. Estrogenicity Potential Impact Factor (EsP)

Energy use, eutrophication potential, global warming potential, land use, and water use are examples of the many “impact categories” that have been established for use in comprehensive LCA analyses. However, there is currently no estrogenicity potential impact factor, despite the fact that exposure to estrogens causes serious adverse ecological effects and many chemicals exhibit estrogenic activity (Nishihara et al., 2000). This makes it such that current LCA practice cannot adequately capture estrogenicity removal as a possible benefit of a proposed product or service. This serious shortcoming must be addressed before the benefits of the proposed on-farm algae dairy waste management system can be fully articulated.

4.2. Methodology

Laboratory experiments were designed to characterize the interaction of algae and selected estrogens during simulated cultivation conditions. Parameters of interest include rate of estrogen removal, rate of estrogenic toxicity reduction, the correlation between algae growth rate and estrogen concentration, identification of mechanisms of estrogen removal (e.g. biotransformation, direct photolysis, and sorption), and possible pathways of estrogens biotransformation mediated by algae culture. The experimental results, together with previously published estrogenicity data obtained from different assays,

were used to establish estrogenicity potential impact factor (EsP) as a novel LCA impact factor category. The following paragraphs summarize the methodology applied in this section. Please see Appendix B & C for detailed information.

4.2.1. Chemicals and Culture Media

Analytical standards for estrone, estriol, 17 β -estradiol, and 17 α -estradiol were purchased from Sigma-Aldrich (St.Louis). Individual stock solutions of each estrogen were prepared in HPLC grade methanol (Fisher Scientific Inc) at 100 mg/L. The stock solutions were stored at -20 °C for up to one month.

Algae were cultivated in protease-peptone medium (PPM) and modified Bold 3N medium (MB3N). All culture chemicals were purchased from Fisher Scientific Inc. Please see Appendix B for detailed information for medium preparation.

4.2.2. Algae-mediated Estrogen Removal

The algae used in this research was a freshwater species, *Scenedesmus dimorphus*. A three-step process was used to grow the algae in monoculture at high density without introducing bacterial contamination. This was done to help ensure that all results are accurate and reproducible. First,

Figure 6. Experimental algae cultivation set up.

algae were transferred from a solid slant tube stock provided by the UTEX culture

collection and inoculated into 15 mL screw-capped test tubes filled with 10 mL protease-peptone medium. These tubes were then incubated for 5 days in a rotator subjected to 12 hours of illumination (cool white fluorescent growth lamp with 125-W 6500-K) and 12 hours of darkness per day. Cultures were then transferred to 250-mL flasks containing 50 mL protease-peptone medium and incubated for another 5 days in a shaker subjected to the same light-dark sequencing. Finally, these cultures were transferred to 1000-mL flasks and adjusted to a final volume of 500 mL in MB3N. The flasks were incubated until cultures reached stationary phase (8-10 days), again using the same light-dark sequencing as in previous culture steps. During this step, the flasks were stirred by magnet (200-300 rpm) and continuously aerated using filtered air flowing at 7 scfm. Figure 6 depicts the experimental set-up for algae cultivation.

Four sets of duplicate reactors were used to characterize possible mechanisms of estrogen removal (e.g. biotransformation, direct photolysis, and bio-sorption). These included: 1) algae (A), which was algae cultivated as described above, in media containing 5 ug/L of each individual estrogen; 2) dark control (DC), which was media without algae containing 5 ug/L of each individual estrogen, in foil-wrapped tubes to prevent illumination ; 3) light control (LC), which was media containing 5 ug/L of each individual estrogen, subject to the light-dark sequencing noted above, but without any algae; and, 4) algae sorption control (AAC), which was autoclaved algae, in foil-wrapped tubes to prevent illumination, in media containing 5 ug/L of each individual estrogen.

50-mL samples were collected from each reactor at 0, 6, 24, 48, 96, 144, and 192 hours over a period of 8 days. For the A reactors, optical density (at 662 nm), direct

counting of algae cell, and dry mass were measured to determine their correlation. For the A & AAC reactors, collected samples were filtered through 0.7- μ m pore size glass microfiber filters (Millipore) to separate algae cells from growth medium. For the DC & LC reactors, collected samples were subject to the extraction and quantification procedures summarized in Figure 7 and described below.

Estrogens in the filtrate were extracted and concentrated using a previously validated solid phase extraction (SPE) method. Oasis[®] HLB SPE 3cc (160 mg) cartridges were conditioned with 3 mL methanol and then equilibrated with 3 mL LC-MS grade water. Filtrate was then loaded onto each cartridge, drop-wise at a rate of 5-6ml/min until roughly 50 mL had been passed through. The cartridge was then washed with 3 mL of a 5% methanol-water solution (v/v) and eluted two times with 1 mL methanol. The eluate was vacuum-dried to dryness overnight and then reconstituted in 400 μ L HPLC grade methanol. The reconstituted solution was syringe-filtered using 0.22- μ m pore size syringe filters (Fisher Scientific Inc). Extracted samples were stored at -20 °C for up to three months before HPLC analysis. Further kinetic experiments (A reactors) were undertaken using different estrogen concentrations (17 β -Estradiol: 50 μ g/L, 100 μ g/L) to determine the effect of substrate level on the interaction of estrogen and algae growth.

Figure 7. Procedures for estrogens extraction. A is “algae”, AAC is “autoclaved algae control”, LC is “light control”, and DC is “dark control”.

A high-performance liquid chromatography (HPLC) method was developed to measure the concentrations of estrogens in extracted samples. The instrument was a Shimadzu 2010-AB HPLC with both UV and fluorescence detectors. Estriol, 17 β -estradiol, and 17 α -estradiol were measured by the fluorescence detector with excitation at 280 nm and emission at 310 nm. Estrone was quantified using the UV detector at 280 nm. Chromatographic separation was achieved using a 250 $\times$ 2.1 mm C18 column (Thermo Scientific) and the following gradient program for HPLC grade water (A) and acetonitrile (B) pumped at 0.5 ml/min: 0-8 min, 20% B; 8-18 min: 20% $\rightarrow$ 35% of B; 18-30 min: 35% $\rightarrow$ 50% of B; 30-32 min: 50% $\rightarrow$ 20% of B; 32-35 min: 20% of B. Injection volume was 20 μ l. The retention times were 11.9 min for estriol, 23.4 min for 17 β -estradiol, 24.5 min for 17 α -estradiol, and 25.9 min for estrone. Table 4 summarizes main HPLC parameters for these four estrogens. Figure 8 summarizes chromatograms for these four estrogens using the described method. Figures 9 and 10 are standards calibration curves.

Table 4. HPLC method parameters for four estrogenic compounds.

Compound	Formula	Molecular Weight	Retention time, min	IDL ¹ , ug/L
Estriol	C ₁₈ H ₂₄ O ₃	288.4	11.9	20
17 β -Estradiol	C ₁₈ H ₂₄ O ₂	272.4	23.4	20
17 α -Estradiol	C ₁₈ H ₂₄ O ₂	272.4	24.5	20
Estrone	C ₁₈ H ₂₂ O ₂	270.4	25.9	50

¹ IDL, instrument detection limit;

Figure 8. Representative chromatograms for the HPLC method use to analyze estrogen concentrations. The top panel shows the resolution of the four estrogens in pure, virgin medium. The middle panel shows the background peaks arising from organic materials in the post-cultivation algae medium, in the absence of estrogens. The bottom panel shows the four estrogens spiked into the algae background. In all cases, the four estrogens of interest show distinct, clearly-resolved peaks that are suitable for analyzing concentrations.

Figure 9. Standard calibration curves for estriol, 17β-estradiol, and 17α-estradiol by fluorescence detector.

Figure 10. Standard calibration curves for estrone by UV detector.

4.2.3. Estrogenicity Analysis (E-Screen)

The so-called E-Screen assay was used to assess changes in estrogenic toxicity occurring during algae-mediated estrogen removal. This work was performed in cooperation with Dr. Mussie Habteselassie, an assistant professor in the Department of Crop and Soil Sciences at the University of Georgia (Griffin). His group has published extensively using this assay (e.g., Mao et al., 2010). We used a modified version of an MCF-7 protocol described by Mao et al. (2010), with different sample pretreatment, to analyze algae (A) samples at time intervals of 0 hours, 24 hours, and 192 hours and light control (LC) samples at time intervals of 0 hours and 192 hours. These samples were collected from one-half of the same vials described in 4.2.2. 1 mL aliquots of the SPE eluates were vacuum-dried to dryness overnight and then reconstituted in 200 μ L HPLC grade methanol, which served as the stock solution, and were stored at -20 °C for up to one month for analysis. 10 μ L of the stock solution was diluted 10,000 $\times$ via serial dilution of 10 μ L of sample into 990 μ L of Dulbecco's Modification of Eagle's Medium (DMEM) (MP Biomedicals LLC, Solon, Ohio). 100 μ L of each diluted sample was then added to the wells of a 96-well plate containing cells and 900 μ L of DMEM for E-screen test.

4.2.4. Establishment of Estrogenicity Potential Impact Factor (EsP)

The growing body of *in vitro* estrogenicity assay data was used to standardize previously published estrogenicity measurements for a diverse array of environmental estrogens. Although there are many different methods used for empirical estrogenicity measurement, all assays utilize 17 β -estradiol as positive control and report their results in

units of E2 equivalents. Therefore, the estrogenicity potential impact factor (EsP) is reported using these same units.

Among all the assays, the yeast estrogenicity screen (YES) has been most conclusively cross-validated with other assays. It has also been widely

used to test various chemicals, and, as such, large quantities of YES estrogenicity data are available (Fang et al., 2000). Therefore, YES estrogenicity data will be used to establish an estrogenicity potential impact factor in this research. Figure 8 depicts the proposed methodology for use of an estrogenicity potential impact factor (EsP), using the established LCA impact category eutrophication potential as analogy. The critical part of creating EsP values will be assigning equivalency factors (Y) to each known estrogenic chemical. First, we cross-referenced all published YES estrogenicity data against other data sources. Second, data from all sources was normalized to E2-equivalents in a manner consistent with the output from YES and other assays.

Figure 11. Computation of the existing eutrophication potential impact (left) and a proposed estrogenicity potential impact (right).

4.3. Results and Discussion

4.3.1. Algae Cultivation

Figure 12A shows a typical algae growth curve produced in our lab. From this figure, the algae enter exponential growth at around 1 day post-incubation. Stationary stage is achieved in about 4 days post-incubation. Information from the growth curve was used to establish sampling times for the experiments evaluating algae-mediated estrogen removal. In particular, more samples were collected before 4 days, because Figure 12A indicates that the algae reach stationary phase at around 4 days. Figure 12B shows the significant linear correlation between optical density at 662 nm, which corresponds to the maximum absorbance for *chlorophyll a*, and algae dry mass. Therefore, optical density at 662 nm was used for quantifying algae dry mass in further experiments.

Figure 12. Algae cultivation results. *A (left):* Algae growth curve. *B (right):* A linear correlation between optical density and algae dry mass.

4.3.2. The Effect of Estrogen Concentration on Algae Growth

Dairy cows excrete considerable amount of estrogens, ranging from below detection limit (BDL) up to 370, 239, and 543 ug/kg (dry weight) for 17 α -estradiol, 17 β -

estradiol, and estrone, respectively (Hanselman et al., 2003). Given the total solids content in dairy manure, roughly 10% (Van Horn et al., 1994), the concentration of individual estrogens in dairy manure slurry is up to 54 ug/L. It was originally supposed that high concentrations of estrogens might suppress algae growth, which could be problematic for algae-mediated dairy manure waste scrubbing systems. To investigate the effect of estrogens on algae growth rate, algae cultures were incubated with three different concentration of 17 β -estradiol: 5 ug/L, 50 ug/L, and 100 ug/L. Algae without estrogen was used as the control. Surprisingly, higher 17 β -estradiol concentrations, up to 100 ug/L, were found to stimulate instead of suppress algae growth (Figure 13). Compared to the control (no 17 β -estradiol added), algae dry masses in the samples with 50 ug/L and 100 ug/L 17 β -estradiol were 19% and 34% higher, respectively, after 10 days of incubation. One possible explanation for this observation is that estrogens can be utilized by algae as nutrients to facilitate algal growth. Although most algae are phototrophic organisms, and thus use radiant energy to produce energy and cellular biomass, there are reports that some microalgal species are able to grow heterotrophically or mixotrophically and attain higher biomass yield than those achievable in photoautotrophic systems (Apt and Behrens, 1999; Della Greca et al., 1997; Faramarzi et al., 2008). For example, the yield of algae *Scenedesmus quadricauda* increased about 60% when using organic substrates at 0.001% of concentration (Della Greca et al., 1997).

Figure 13. Algae growth rates at three different concentrations of 17 β -estradiol. Error bars are standard deviations from duplicate samples.

4.3.3. Algae-mediated Estrogen Removal

4.3.3.1. Evaluating the Mechanisms of Estrogen Removal

Figure 14 summarizes the fates of four estrogens (estriol, 17 β -estradiol, 17 α -estradiol, and estrone) under different experimental conditions: 1) a dark control (DC) without algae, as the baseline; 2) a light control (LC) without algae, to quantify estrogen removal via direct photolysis (i.e., the reduction of estrogen in LC minus the reduction of estrogen in DC); 3) an autoclaved algae control (AAC) to test estrogen removal via sorption by the algae cells (i.e., the reduction of estrogen in AAC minus the reduction of estrogen in DC); and, 4) a live algae (A) culture to analyze the estrogen removal via biotransformation by algae (i.e., the reduction of estrogen in A minus the total removal of estrogen in AAC and LC).

Figure 14. Fates of four tested estrogens in four different conditions. X axis presents incubation time (hours); Y axis presents estrogen removal rate (C/C_0 , %). Error bars are standard deviation for 2 replicates.

Estrogen Removal by Direct Photolysis. Compared to the dark control (DC), the concentration of all four estrogens in the light control (LC) batches remained relatively constant, and no significant reductions were observed. This indicates that there was little to no direct photolysis removal for these four estrogens. This is not surprising, as previous studies have demonstrated that the degradation of free estrogens is achieved mainly through biotic routes (Khanal et al., 2006; DEPA, 2004). In particular, Jürgens et al. (2001) compared estradiol direct photolysis and biodegradation half-lives. They reported that the half-life of estradiol, assuming first-order decay via biotic routes, was as low as 0.2 days; whereas the half-life of direct photolysis under ideal conditions was at least 10 days. The results from this study confirmed that direct photolysis is not effective for estrogen removal.

Estrogen Removal by Sorption. For the algae sorption controls (AAC), no significant sorption was observed for all the four estrogens, although slightly decreases occurred for the concentrations of estrone and estriol: roughly 9% reductions after 8 days. Because they are non-volatile and slightly hydrophobic compounds, theoretically, estrogens should be easily adsorbed from the liquid phase to the solid phase. The sorption capacity coefficient (K_f) values of estradiol and estrone vary from 4-667 ng/g in different types of soil and sediment (Khanal et al., 2006). However, the results of this study indicated that the sorption of estrogen onto autoclaved algae biomass was not significant. Similar results were also observed by Lai et al. (2002), who reported only a small amount of estrogens (<9%) partitioned to the alive algae cell when investigating the fates of estrogens in *Chlorella vulgaris*. The reason for the contradiction of sorption between

algae cell and soil / sediment may be that the algae cells have lesser sorption capacity than soil or sediment.

Estrogen Removal by Algae-Mediated Biotransformation. In the active algae culture (A), the apparent concentrations of all four estrogens decreased by more than 90% over 8 days. At the end of this period, only 10% of the initial 17α -estradiol concentration remained, and the residual concentrations of 17β -estradiol, estrone, and estriol were all below the detection limit. The concentrations of 17β -estradiol and estriol fell rapidly, exhibiting >90% removal during the first 6 hours of incubation. The reduction of 17α -estradiol and estrone occurred more slowly, after roughly 24 hours. These results indicate that live algae cells are extremely effective at reducing estrogen concentrations. Also, the removal processes exhibit different effects on each individual estrogen.

These observations are consistent with limited data from a previous study of estrogen removal by the alga *Chlorella vulgaris*, as reported by Lai et al. (2001). In the previous study, Lai et al. (2001) observed that the oxidation half-time of estradiol decreased from 48 hours to only 3 hours in the presence a live algae culture. The removal rates 17β -estradiol and estriol in Figure 14 (90% in the first 6 hours), are slightly faster than what was reported by Lai et al. (2001). Lai et al. also observed a slower rate of initial degradation for estrone. From Figure 14, the removal of estrogen was 25% over 48 hours, which is faster than the 10% removal over 48 hours reported by Lai et al.

The residual estrone concentration in Figure 14 is less than the HPLC detection limit (50 ppb in HPLC vial). For the extraction procedure used in this study ($125\times$ after accounting for recovery efficiency), this detection limit corresponds to a concentration of

about 0.4 ug/L in sample. Thus, Figure 14 exhibits roughly 90% removal of estrone, compare to the initial concentration of 5 ug/L. This removal is somewhat better than has been previously reported for conventional wastewater treatment plants (Khanal et al., 2006), 25-80%. This suggests that algae-mediated estrone removal may be more efficient than traditional wastewater treatment plant processes.

4.3.4. Biotransformation Pathways of Estrogens by *Scenedesmus dimorphus*

From previous investigations of estrogen biodegradation, the four estrogens evaluated in this study can be interconverted to one another as the apparent concentrations are reduced (Lai et al., 2001; Zheng et al., 2012). Our results suggest that these inter-conversions may also occur during removal mediated by *Scenedesmus dimorphus*.

Biotransformation Pathway for Estriol. During 8 days of incubation time, there was no observation of estradiol or estrone in the algal culture spiking with estriol. The concentration of estriol decreased 96% in the first 6 hours as shown in Figure 14C, and no other estrogens analyzed in this study were observed. In particular, there was no observation of estradiol or estrone in the algal culture spiked with estriol. The results indicate that estriol was converted to some unknown products very rapidly by algae *Scenedesmus dimorphus*. This is in contrast to previously published studies in which there was no conclusive evidence showing the removal or biotransformation of estriol by algae *Chlorella vulgaris* (Lai et al., 2001) within 48 hours.

Biotransformation Pathway for Estrone. In the algal culture spiked with estrone, there was no change in estrone concentration during the first 24 hours of incubation

(Figure 15). After 24 hours, the estrone concentration begins to decline slowly, and there 17 β -estradiol becomes present at slowly increasing concentrations (0.19-0.30 ug/L). This suggests that estrone may be bio-transformed into 17 β -estradiol during these reactions. This conversion involves reduction requiring the addition of two hydrogen atoms to each estrone molecule to produce one molecule of 17 β -estradiol. Estriol and 17 α -estradiol were also observed in the reaction mixture towards the end of the incubation (around 192 hours), but their concentrations were below the quantification level. The low abundances of these compounds may reflect the low initial concentration of the parent compound (estrone at 5ug/L), or they may be intermediate metabolites with short half-lives in this particular reaction mixture. Thus, the conversion of estrone to estriol and 17 α -estradiol will require further confirmation.

Figure 15. Changes with time after spiking algae culture with estrone (5ug/L). Error bars are standard deviation for 2 replicates.

Biotransformation Pathway for 17 α -Estradiol. A significant decrease of 17 α -estradiol was observed within 48 hours (Figure 16). There was an increase in estrone concentration (up to ~1.0 ug/L) during the same interval. This suggests that estrone is a key biotransformation product of 17 α -estradiol in the presence of active *Scenedesmus dimorphus*. The same observation, although in slower rate, has been reported by Zheng et al. (2012) in anaerobic dairy lagoon water under anaerobic conditions. This conclusion is also supported by considering the total mass balance of 17 α -estradiol and estrone, whereby the amount of 17 α -estradiol removed from solution (0.0029 uM) was roughly equal to the amount of estrone that was introduced (0.0031 uM). The conversion of 17 α -estradiol into estrone involves oxidation requiring the removal of two hydrogen atoms per molecule of 17 α -estradiol.

Figure 16. Changes with time after spiking algae culture with 17 α -estradiol (5ug/L). Error bars are standard deviation for 2 replicates.

During the period from 96-192 hours, 17 β -estradiol appeared in the reaction mixture and was detected at concentrations on the range of 0.35- 0.19 ug/L. Interestingly, the appearance of 17 β -estradiol occurred during the same period as estrone concentration was decreasing. Given that 17 β -estradiol appeared after the estrone had already been produced, and estrone was converted into 17 β -estradiol from Figure 15, it seems likely that the 17 β -estradiol observed in this experiment corresponds to a reaction product of the estrone intermediate. At later periods, a small quantity of estriol was observed in the reaction mixture, but the concentration could not be quantified because it was less than the detection limit.

Biotransformation Pathway for 17 β -Estradiol. The concentration of 17 β -estradiol dropped more than 90% in the first 6 hours when this compound was evaluated at an initial concentration of 5 ug/L. Estrone and 17 α -estradiol were observed as reaction products around 96 hours, and estriol was observed towards the end of incubation time (192 hours), but its concentration was below the quantification limit for the method used in this study. 17 β -estradiol is of particular concern because it is strongly estrogenic and has been used as the representative estrogen for many studies (Bisagno et al., 2003; Mao et al., 2010). To better understand the transformation mechanisms of 17 β -estradiol, further experiments were undertaken by spiking the algae culture with two much higher starting concentrations of 17 β -estradiol: 50ug/L and 100ug/L. The results from these experiments are summarized in Figure 17.

Figure 17. Changes with time after spiking algae culture with 17β-estradiol (50 ug/L, 100 ug/L). X axis is incubation time (hours); Y axis is estrogen concentration in the algae medium (ug/L). A: (upper) initial condition is 100 ug/L 17β-estradiol; B: (lower) initial condition is 50 ug/L 17β-estradiol. Error bars are standard deviation for duplicate samples.

Comparison of Panels A and B in Figure 17 indicates that the changes of the individual parent compound (17β -estradiol) and biotransformed products (17α -estradiol, estrone, and estriol) were very similar for both high-range initial concentrations. For both reactions, all four target estrogens were present in the algal culture during some portion of the incubation period. The concentration of 17β -estradiol rapidly declined during the first 24 hours, whereas the concentration of estrone quickly increased during the same period. More than 80% of the initial 17β -estradiol appears to be converted into estrone, which was much more significant than the 6% of estrone that was converted into estradiol for the reverse reaction (Figure 15). The conversion of 17β -estradiol into estrone was also more significant and occurred more rapidly than the transformation of 17α -estradiol into estrone (42% from Figure 16), which might contribute to the fact that 17α -estradiol exhibited a longer half-life than 17β -estradiol during these experiments. After 24-48 hours, the estrone concentration decreased rapidly, ultimately dropping below the quantification limit by the end of the incubation time. As the estrone concentration was decreasing, small quantities of estriol and 17α -estradiol appeared in the reaction mixture, though there is a substantial difference between the amount of estrone removed (~ 0.2 μ M and 0.1 μ M for the experiments with 100 μ g/L and 50 μ g/L 17β -estradiol, respectively) and the combined amounts of estriol and 17α -estradiol observed (0.018 μ M and 0.006 μ M for the experiments with 100 μ g/L and 50 μ g/L 17β -estradiol, respectively). One possible explanation for this observation may be that the estrone was converted primarily into estriol, which was then rapidly converted to unknown metabolites, consistent with Figure 14C.

Summary of Estrogen Biotransformation Reactions. In summary, the results presented in Figures 15-17 demonstrate that the four target estrogens selected for this study are interconverted among one another by reactions occurring in the presence of *Scenedesmus dimorphus*. Figure 18 presents a possible transformation pathway for these four estrogens based on these observations, whereby both 17 β -estradiol and 17 α -estradiol were first bio-transformed into estrone, which was then further transformed into estriol or converted back to 17 β -estradiol or 17 α -estradiol. Estriol was further degraded to unknown products and was likely not converted back into estrone or estradiol. Thus, all of the estrogens with two oxygen molecules (17 β -estradiol, 17 α -estradiol, and estrone) are inter-convertible during interactions with *Scenedesmus dimorphus*, and the sole three-oxygen form (estrone) is an important intermediate for further biotransformation and degradation. Lai et al. (2002) also reported 17 β -estradiol and estrone to be inter-convertible during reactions mediated by *Chlorella vulgaris*, and, similar to Figure 18, the estrone was then converted into estriol (Figure 19). They did not observe subsequent removal of the estriol into other products; however, this could be because their incubation time was only 48 hours, compared to nearly 200 hours duration used in this study.

There has been no previously published study regarding the biotransformation pathway of 17 α -estradiol in the presence of active algae biomass. Our results indicate this estrogen could share the same transformation pathway as 17 β -estradiol under algal culture conditions (although at a much longer half-life), and that both estradiol isomers may be inter-convertible via estrone as the intermediate. Considering the large amount of 17 α -estradiol that is excreted in dairy manure, the information about this estrogen arising

from this study is important for understanding the benefits of algae-mediated livestock manure waste treatment.

Figure 18. Possible biotransformation pathways of 17 β -estradiol, 17 α -estradiol, estrone, and estriol by the algae *Scenedesmus dimorphus*.

Figure 19. Proposed biotransformation pathway of steroid estrogens by *C. vulgaris*. Adapted from Lai et al. (2002).

In terms of the total amount of steroid estrogen removed by *Scenedesmus dimorphus*, roughly 95% of the total estrogens were removed during individual (single-chemical) reactions with 17β -estradiol, estrone, and estriol. Roughly 85% of total estrogens were removed during individual (single-chemical) reactions with 17α -estradiol. This is surprisingly high, given that many of the removal reactions are initiated by conversion of one estrogen into another. Thus, algae-mediated treatment is much more effective for estrogens removal compared to other engineered systems (Khanal et al., 2006; Zheng et al., 2012). In a study investigating the fates of estrogens in dairy lagoon waters under anaerobic condition, the removals of 17α -estradiol, 17β -estradiol and estrone were only 15-23% after 52 days of incubation (Zheng et al., 2012). In conventional wastewater treatment plants, the removal of 17β -estradiol, estrone, and estriol are roughly 85%-99%, 25% -80%, and 0%-89%, respectively (Khanal et al., 2006). Our results indicate that algae cultivation could be a promising approach for controlling estrogen pollution.

4.3.5. Estrogenicity Removal Mediated by *Scenedesmus dimorphus*

Figures 14-17 show that roughly 85-95% of the total estrogen concentrations were removed in the presence of the *Scenedesmus dimorphus* during a period of 8 days. However, many of the removal reactions comprised inter-conversions among the target estrogens, and it was not possible to fully account for all by-products. Thus, the estrogen concentrations alone were not adequate to assess whether or not algae-mediated reactions reduce the estrogenic toxicity of digested dairy manure waste. For this reason, we used a standard *in vitro* assay to measure estrogenic toxicity over time during algae culture.

The estrogenicity assay produces data that are in units of “relative estrogenic effect (REE)”, which is defined as the ratio between the cell yield for MCF-7 tumor cells exposed to a water sample of interest and the cell yield for identical MCF-7 cells exposed to a solution comprising 10^{-9} M 17β -estradiol. The control cell count (denominator) is multiplied by 100 such that REE can be reported as a percentage, using the 10^{-9} M 17β -estradiol solution as reference for 100% “relative estrogenicity”. Our results from the estrogenicity assay are summarized in Figure 20. Here we see that there is very little change in REE over 8 days. Only the 17β -estradiol experiment exhibits a statistically significant difference (at $\alpha = 0.05$) in estrogenicity; whereby, the initial estrogenic toxicity is reduced by roughly 30% over the cultivation period. This decrease occurred during the first 24 hours, prior to collection of the first sample at 24 hours of Figures 14A. In the light control experiments, there was no significant change of estrogenicity for all the target estrogens, which is consistent with the results of estrogen concentration in light control as shown in Figure 14.

Comparison of Figure 14 and Figure 20 indicates that there is a significant mismatch between removal of the individual parent compounds ($\geq 85\%$) and removal of their combined toxicity effects ($\leq 30\%$). This suggests that the unknown transformation products existing at the end of the cultivation period are still exhibiting considerable estrogenic activity. For the specific case of 17β -estradiol, the decrease in estrogenic toxicity during the first 24 h is consistent with conversion of the parent compound into estrone during that interval, because estrone is only 10-20% as estrogenic as 17β -estradiol (Table 3). Conversion of estrone into estriol (Figure 17) would manifest a

further drop in estrogenic toxicity, but transformation back to either 17β -estradiol or 17α -estradiol would increase the estrogenicity back to its initial level.

There have been very few studies assessing the removal of estrogenic toxicity as mediated by algae, especially in comparison to the large volume of work that has been done to evaluate estrogenicity removal during municipal wastewater treatment (WWTPs). The total estrogenicity reduction in WWTPs varies dramatically, from almost complete removal to almost zero removal (0-99%) (Coors et al., 2004; Murk et al., 2002; Sun et al., 2008; Svenson et al., 2003). Much of the removal, when it does occur, is generally achieved biologically, e.g., aerobically activated sludge. For example, the average removal efficiency in plants without biological treatment is only 18%, compared to an average efficiency of 81% in plants with activated sludge treatment. Svenson et al. (2003) reported that activated sludge treatment was more effective than trickling filters, whereas chemical precipitation without biological treatment showed little estrogenicity removal. However, it should be noted that the composition of municipal wastewater is very different from that of dairy manure waste, whereby dairy manure waste has much higher concentrations of estrogenic compounds.

Another engineering system often studied for estrogen removal is anaerobic digestion. Although it is a biological process, anaerobic digestion does not favor estrogen or estrogenicity removal as activated sludge does. For example, Zhao et al. (2007) reported that all the removal of estrogens E2 and E3 were achieved by the aeration process, and anaerobic digestion showed little or no capability of estrogens removal. Some studies even found that the total estrogenic activity actually increased during anaerobic sludge digestion (Teske et al., 2007).

Our study is the first to analyze algae-mediated removal of estrogenic toxicity in mixtures containing steroid estrogens that are present at high concentrations in livestock (specifically dairy) manure wastes. Preliminary results suggest that rapid removal of the parent compounds is not well correlated with removal of estrogenic effects. Further research, specifically analysis of the bio-transformation products and assessment of their ecological or human health impacts, is warranted, so that we can better evaluate the ecological services afforded by the proposed algae cultivation system.

Figure 20. Measurements of total estrogenic toxicity over time, during reaction with *Scenedesmus dimorphus*. Starting concentration of each estrogen was 5 ug/L: X axis is the incubation time (hours), and Y axis is the ratio of relative estrogenic effect (REE) at sampling time to that at initial point (REE / REE₀). There was no estrogenicity test for light control samples at 24 hours. Error bars are equal to 95% confidence interval with 6 replicates (two experimental replicates at each sampling time × three replicate wells per sample during E-screen = 6).

4.3.6. Establishment of an Estrogenicity Potential (EsP)

To reiterate from Section 4.1.4, it was previously impossible to account for changes in estrogenic toxicity within an LCA framework, because there were no standardized impact factors or units. To remedy this, we created an estrogenicity potential (EsP) that can be used to account for estrogenicity reduction as part of a full life-cycle accounting of a product or service. The first step was collecting estrogenicity measurements for 635 chemicals from previous publications. Although these data were obtained by a variety of assays, most of them (425 chemicals) were from a YES study conducted by Nishihara et al. (2000). From Table 5, it is apparent that the data derived from the various studies are not immediately comparable because different authors present different value and different units. But, linear regression reveals that there are significant linear relationship between data from Nishihara et al. (2000) and other studies. Thus, it is possible to report EsP values for more than 635 chemicals.

Table 5. Summary of published estrogenicity data for formulation of an estrogenicity potential (EsP) impact factor during LCA.

No. of chemicals	Test assay	Linear correlation (R^2 value) ^a	Result Unit	Unit Meaning	Reference
425	Yeast two hybrid assay	1	REC ₁₀ (M)	Concentration of test chemical showing 10% of the highest activity level of 10 ⁻⁷ M E2	Nishihara et al., 2000
146	Yeast two hybrid assay	0.94	REC ₁₀ (M)	Concentration of test chemical showing 10% of the highest activity of E2	Ogawa et al., 2005
46	Recombinant yeast cell bioassay	0.86	RP	Relative potency compared to E2 (100) by molar mass	Coldham et al., 1997
35	Yeast two hybrid assay	NA ^b	REP _E	The ratio of tested chemicals to E2	Hayakawa et al., 2007
31	Yeast two hybrid assay	0.94	REC ₁₀ (M)	Concentration of test chemical showing 10% of the highest activity level of 10 ⁻⁶ M E2	Kawamura et al., 2003
27	Yeast two hybrid assay	0.98	RA _{E2}	Ratio toward estrogenic activity of E2	Kawagoshi et al., 2002
24	Yeast based reporter gene assay	0.69	RIE	The ratio between maximum beta-galactosidase activity achieved with the test compound and that of E2 (multiplied by 100)	Fang et al., 2000
22	Yeast two hybrid assay	NA ^b	REP _E	The ratio of tested chemical to E2	Hayakawa et al., 2011
16	Yeast based reporter gene assay	0.86	PR	The potency ratio of tested chemical over E2	Gaido et al., 1997
11	Yeast two hybrid assay	NA ^b	REC ₁₀ (M)	Concentration of test chemical showing 10% of the highest activity level of 0.01 mg/L E2	Eguchi et al., 2002
2	Yeast two hybrid assay	NA ^c	REC ₁₀ (M)	Concentration of test chemical showing 10% of the highest activity of E2	Shioji et al., 2006

^a Linear correlation based on the data from Nishihara et al. (2000); ^b No linear correlation available due to no specific data; ^c No linear correlation available due to few data.

As described in 4.3.4, all available YES data were standardized against the estrogenicity equivalence of 17 β -estradiol (E2). EsP impact factors for all compounds were then assigned values to indicate their estrogenic toxicity relative to that of 17 β -estradiol (E2). In this way, the EsP values for all chemicals can be expressed using the same units. Table 6 is an example of how EsP values were formulated from different resources. These results show that 17 β -estradiol has strongest estrogenic potency, which supports the results in section 4.4.5, whereby most significant estrogenicity removal was observed only for the sample that had been originally spiked with 17 β -estradiol. EsP for other chemicals please see Appendix C.

Table 6. Established estrogenicity potential factors (EsP) for estrogen 17 β -estradiol, 17 α -estradiol, estrone, and estriol based on previous published data.

Source				17 β -estradiol	17 α -estradiol	Estrone	Estriol
Coldham et al 1997							
Original Value, RP ¹				100	5.25	9.6	0.63
Estrogenicity	impact	factor	1		0.0525	0.096	0.0063
Gaido et al 1996							
Original Value, PR ²				1			273
Estrogenicity	impact	factor	1				0.004
Kawagoshi et al 2002							
Original Value, RA ³				1	0.01		
Estrogenicity	impact	factor	1		0.01		
Nishihara et al 2000							
Original Value, REC10 (M) ⁴				3.00E-10	4.00E-09	3.00E-10	3.00E-07
Estrogenicity	impact	factor	1		0.075	1	0.001
Average EsP				1	0.0458	0.55	0.003

¹ RP is the relative potency compared to E2; ² PR is the ratio of EC50 (chemical) over EC50 (17 β -estradiol); ³ RA is the ratio towards estrogenic activity of 17 β -estradiol; ⁴ REC10 (M) is the concentration of tested compound showing 10% of the activity of 10⁻⁷ M 17 β -estradiol.

EsP data could be used to evaluate changes in estrogenicity potential associated with a specific process or product of interest, as part of a larger LCA analysis. One example application would be assessing the efficiency of estrogenicity reduction among various tertiary treatments (e.g., sonolysis, UV direct photolysis, etc).

4.4. Conclusion

This section provides clear evidence from bench-scale experiments that algae (specifically *Scenedesmus dimorphus*) effectively bio-transform 17 α -estradiol, 17 β -estradiol, estrone, and estriol, achieving up to 95% removal. This level of removal makes algae-mediated estrogen removal more effective than other engineered systems (e.g., conventional wastewater treatment plants or anaerobic digesters), especially for estrone. Both estradiol isomers (17 α -estradiol and 17 β -estradiol) are inter-convertible via estrone as the intermediate. Estrone can also be degraded to estriol which is further degraded to unknown products. However, the removal of estrogenic toxicity is not as significant as the biodegradation of estrogens. To better evaluate and compare the ecological services that algae cultivation systems could offer, further research should focus on: 1) investigating estrogenicity removal in other engineering systems such as conventional wastewater treatment plants; 2) analyzing the currently unknown biotransformation products; and 3) assessing their ecological or human health impacts.

5. Energy Return on Investment (EROI)

This section discussed the Objective 3 of the overall dissertation. It will be demonstrated how different EROI formulations give rise to a wide range of output values and how this ambiguity then makes it difficult to properly assess the energetic favorability of a particular energy system or to make accurate comparisons among multiple systems. The material in this chapter was adapted from Zhang & Colosi (2013), which had been published in *Energy Policy* (Zhang & Colosi, 2013).

5.1. Background

The search for environmentally sustainable and economically viable alternatives to fossil-based energy sources has made life cycle assessment (LCA) and other systems-level energy analyses increasingly important research topics. This has stimulated concurrent development of appropriate metrics for comparison among possible energy-producing systems. One particularly relevant class of LCA metrics comprises the various “energy ratios.” These account for both energy generation (E_{OUT}) and energy consumption (E_{IN}) associated with a given system, as means to assess the production *efficiency* of a particular energy system. Two popular names for such ratios include the “net energy ratio” (NER) and “energy return on investment” (EROI). NER can be computed using either combination of E_{IN} and E_{OUT} as numerator and denominator (i.e., $NER = E_{IN}/E_{OUT}$ or $NER = E_{OUT}/E_{IN}$); however, EROI is only computed using E_{OUT} as numerator and E_{IN} as denominator, such that larger values are indicative of more efficient energy production (Cleveland et al, 1984).

The rapidly evolving field of algal biofuels LCA has developed in parallel with the various energy ratios over the past 3-5 years. Accordingly, several recently published

algae LCA studies have made reference to self-normalized energy metrics, including: NER in Batan et al (2010), Jorquera et al (2010), and Khoo et al (2011); and EROI in Clarens et al (2011), and Colosi et al (2012). In each of these studies, the energy ratio metric is used to assess overall sustainability of a particular system (using $EROI = 1$ as cutoff) and/or to facilitate comparison among multiple candidate systems. Simultaneously, energy ratios (most notably EROI) have also been the subject of several *theoretical* studies. These studies have focused on: assessing the impact of hypothetical systems boundaries on EROI calculations, accounting for differences in energy quality, treatment of non-energy inputs and outputs (i.e., “co-products”), relating EROI to economic performance at a societal level, and estimating a minimum EROI (3:1) an energy-producing system must achieve to maintain the current quality of life in the absence of readily-available fossil fuels (Hall et al, 2009; Mulder and Hagens, 2008; Murphy and Hall, 2010; Murphy et al, 2011).

This research seeks to illustrate previously undocumented *practical* difficulties associated with computation and interpretation of a meaningful energy ratio metric. This is done using previously published life cycle inventory data for algal biofuels and also corn and switchgrass ethanol. The use of actual LCA data makes it possible to achieve three goals: 1) demonstrate the susceptibility of EROI to inadvertent or purposeful manipulation; 2) identify unique practical issues associated with EROI computation for algae and other biofuels crops that will likely be used to create appreciable bioelectricity or other non-fuel co-products; and 3) highlight the need for increased transparency in EROI calculations. In this way, the algae LCA data are used to build upon and

contextualize much of the ongoing theoretical debate about improvement of the energy ratio as a useful LCA metric.

5.2. Methodology

Several types of EROI calculations were computed using available algae biofuel and corn ethanol data from: the fully configurable EBAMM meta-model inventories (Farrell et al., 2006), the MABEL algae LCA meta-model (Liu et al., 2012), and a number of recently published corn ethanol EROI calculations (Murphy et al., 2011 a, 2011 b; Murphy & Hall, 2010). It was expected that these calculations would show dramatic variability in EROI for individual crops, possibly skewing comparisons between multiple crops or multiple ways to produce a single crop (e.g., OPS versus ATS algae systems).

The array of various calculation strategies was then analyzed for its compatibility with GREET v. 1.8 (Wang, 2007) and EBAMM (Farrell et al., 2006), since these two models have considerable influence among biofuels LCA practitioners. Finally, a framework was used to resolve current EROI ambiguity by: 1) categorizing (naming) the various EROI calculations so that authors can clearly referenced what type of computation is used in a particular study; 2) proposing a standardized calculation for future use, to communicate the ratio of energy outputs and inputs in a more direct and easily understood way.

5.3. Results and Discussion

5.3.1 Demonstrating the Ambiguity of EROI Calculations

EROI or NER metrics are used to communicate information about the favorability of an energy-producing system, either relative to some threshold value or for comparison

with one or more possible alternatives. This information is essential for rapid commercialization of alternative energy technologies and formulation of meaningful energy policies. Despite this, there is no standardized protocol for how to compute EROI or NER. As a result, there may be several seemingly valid approaches to calculate either metric for the same dataset, each of which gives rise to a different result. Figure 21 demonstrates this ambiguity for the specific case of bio-energy production from microalgae. These data correspond to algae cultivation in open ponds, with subsequent conversion of algal lipids into biodiesel via transesterification and anaerobic digestion of residual biomass into methane-derived bio-electricity. From Figure 21, the same six life cycle quantities (A-F) can be assembled into at several different EROI ratios, all of which are mathematically valid. It should be emphasized that other additional EROI formulations also exist, but that the formulas in Figure 21 were selected for demonstration purposes.

<p>Energy Quantities from Previously Published Algal Biofuels LCAs</p> <p>A. Biodiesel energy (from algae lipids) B. Bioelectricity (from digestion of non-lipids) C. Fertilizer offsets (from digestate residuals) D. Electricity for cultivation, conversion E. Heat for cultivation, conversion F. Upstream burdens for input materials</p>	$EROI_1 = \frac{A + B \times IF_E + C}{D \times IF_E + E + F}$ $EROI_{2A} = \frac{A + \parallel B - D \parallel \times IF_E + C}{E + F}$ $EROI_{2B} = \frac{A + C}{\parallel D - B \parallel \times IF_E + E + F}$	$EROI_{3A} = \frac{A + \parallel C - F \parallel + \parallel B - D \parallel \times IF_E}{E}$ $EROI_{3B} = \frac{A + \parallel C - F \parallel}{\parallel D - B \parallel \times IF_E + E}$ $EROI_{3C} = \frac{A + \parallel B - D \parallel \times IF_E}{\parallel F - C \parallel + E}$ $EROI_{3D} = \frac{A}{\parallel D - B \parallel \times IF_E + \parallel F - C \parallel + E}$
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Figure 21. Possible formulations for EROI based on life cycle quantities from previously published life cycle assessment (LCA) studies of bio-energy production from microalgae. Quantities A-C and D-F are energy inputs and outputs, respectively, from a meta-analysis by Liu et al (2012). IF_E refers to the impact factor for displaced/consumed electricity from the US grid; whereby 3.47 MJ of primary energy is required to produce 1 MJ of electricity, such that the total multiplier is $IF_E = 1 \text{ MJ} + 3.47 \text{ MJ/MJ} = 4.47 \text{ MJ}$ total energy per MJ electricity displaced/consumed (Weidema, 2007). Adapted from **Zhang & Colosi (2013)**.

The EROI formulations in Figure 21 differ primarily in their treatment of surpluses (or deficits), more specifically, in the assignment of systems boundaries for quantifying net energy creation or consumption. For algae LCAs, two types of surpluses are particularly relevant: the difference in the amount of *electricity* brought in from the grid to power cultivation and conversion processes versus the amount produced on-site via methane combustion; and, the difference in the amount of *upstream energy* required to produce cultivation and conversion inputs versus the amount of energy *offset* via avoidance of fertilizer production when solid residuals from anaerobic digestion are used as nutrient-rich soil amendments. In $EROI_1$, there is no attempt to quantify either surplus; all outputs are added together linearly as the numerator, and all inputs are added together linearly as the denominator. In $EROI_2$, it is assumed that the bio-electricity produced on site (B) is first used for system operation on-site and then the surplus is then exported. The difference between quantities B and D (electricity output and input, respectively) is computed first, and the magnitude is then moved to either the numerator if positive (to connote net generation – i.e., surplus, as in $EROI_{2A}$) or the denominator if negative (to connote net consumption – i.e., deficit, as in $EROI_{2B}$). In both formulations, the net difference is multiplied by an empirical impact factor (IF_E) to account for upstream energy consumption during electricity production. The $EROI_3$ formulations demonstrate similar treatment of the energy surplus/deficit arising from comparison of upstream burdens for materials versus energy offsets for material co-products. As with $EROI_2$, the magnitude of this quantity is taken to the numerator if positive ($EROI_{3A}$ or $EROI_{3B}$) or denominator if negative ($EROI_{3C}$ or $EROI_{3D}$). The four formulations for $EROI_3$ account for all possible combinations of electricity quantities (D vs. B) and materials quantities (C

vs. F). It is expected that only one of the two formulations for $EROI_2$ and one of the four formulations for $EROI_3$ should be computed for a given dataset, based on the magnitudes of the electricity and materials energy surpluses/deficits.

Table 7 summarizes the EROI values computed using the multiple formulations from Figure 21 and previously published algae LCA data. It should be emphasized that the EROI values in each row of a single column are computed using the same exact values of quantities A-F. Despite this, there is significant variation in the EROI values that can be computed from a single dataset. In most cases, the largest EROI value for a given dataset is up to 2-3 times greater than the smallest value. This dramatically affects the interpretation of these metrics. For example, use of $EROI_1$ makes the performance of the algae system described by Stephenson et al (2011) (A_{ST}) seem marginal to fair; whereas, use of $EROI_3$ makes this system seemingly capable of supporting what Hall et al (2009) have categorized as a “sustainable society”. The obvious disparity among these values makes it hard to accurately assess this system’s commercial and environmental appeal.

Table 7. Example EROI calculations using previously published algae LCA data and multiple seemingly valid EROI formulations ¹.

Item	Dataset ^a					
	A_{CL}	A_L	A_{CA}	A_{SA}	A_{ST}	A_G
A	33,264	33,264	33,264	35,844	32,736	1,055
B	11,097	11,770	8,899	13,483	13,904	363
C	2,000	1,605	2,553	2,430	740	50
D	8,887	8,919	9,508	8,129	10,668	483
E	3,403	22,583	3,398	4,025	7,953	1,056
F	13,982	3,662	13,973	15,899	3,083	198
$EROI_1$	1.5	1.3	1.3	1.8	1.6	0.6
$EROI_2^b$	2.6 (A)	1.8 (A)	1.8 (B)	3.1 (A)	4.3 (A)	0.4 (B)
$EROI_3^b$	2.6 (C)	1.9 (C)	1.9 (D)	3.4 (C)	4.6 (C)	0.4 (D)
<i>Reported EROI</i> ^c	2.8	1.9	1.9	3.4	4.6	NA

Items A-F correspond to Figure 18.

¹ Adapted from **Zhang & Colosi (2013)**.

^a First five columns are from a meta-analysis of algae LCAs by Liu et al (2012): A_{CL} – Clarens et al (2010), A_L – Lardon et al (2010), A_{CA} – Campbell et al (2010), A_{SA} – Sander and Murthy (2010), and A_{ST} – Stephenson et al (2010). A_G corresponds to the harmonized model from GREET 1 (2012).

^b Letters in parentheses indicate which of multiple $EROI_2$ or $EROI_3$ formulations was used, based on lettering from Figure 1.

^c Denotes the EROI value reported by the authors of the original publication.

Table 8 contains LCA data for production of bio-ethanol, as taken from the widely-cited EBAMM meta-model (Farell et al, 2006). Two of the EBAMM scenarios, “Ethanol Today” and “CO₂ Intensive”, are based on existing technologies for current production of corn ethanol. In contrast, the “Cellulosic” EBAMM scenario refers to anticipated technologies for production of switchgrass-derived ethanol. The interpretations of items A-F for the EBAMM scenarios are analogous to what was presented in Figure 21, with some minor adaptation: A corresponds to production of 100% neat bio-ethanol instead of biodiesel; C corresponds to energy offsets for material co-products including oils, animal feed, and others. Items D, E, and F are unchanged compared to their definitions in Figure 21. Item B is zero for both corn ethanol scenarios because EBAMM does not account for electricity as an energy co-product during corn ethanol production. From Table 8, the EROI values computed using the EBAMM

“Cellulosic” scenario demonstrate considerable variability, ranging from 1.2 (marginal) to 8.1 (excellent). This suggests that EROI ambiguity is not only restricted to algae, but rather that this phenomenon may occur for biofuels calculations in general. Interestingly, there is almost zero variability among EROI values for either corn ethanol scenario.

Table 8. Example EROI calculations using previously published ethanol LCA data and multiple seemingly valid EROI formulations ¹.

Item	Ethanol Dataset from EBAMM		
	<i>Corn – Today</i>	<i>Corn – CO₂ Intensive</i>	<i>Switchgrass – Cellulosic</i>
A	21.2	21.2	21.2
B	0	0	26.3
C	4.1	4.1	4.8
D	0.2	1.1	26.4
E	17.2	19.9	2.5
F	3.2	3.0	0.5
<i>EROI₁</i>	1.2	0.9	1.2
<i>EROI₂^a</i>	1.2 (B)	0.9 (B)	7.1 (B)
<i>EROI₃^a</i>	1.2 (B)	0.9 (B)	8.1 (B)
<i>Reported EROI^b</i>	1.2	1.1	8.2

Items A-F are slightly modified from Figure 18.

¹ Adapted from **Zhang & Colosi (2013)**.

^a Letters in parentheses indicate which of multiple EROI₂ or EROI₃ formulations was used, based on lettering from Figure 1.

^b Denotes the EROI value reported by the authors of the original publication.

The LCA data from Tables 7 and 8 can be used to show that selection of EROI formula impacts selection among alternative biofuel platforms, since the different EROI formulations give rise to different favorability rankings among the evaluated energy-producing systems. This is demonstrated in Table 9 using averages from each type of dataset: all algae scenarios together versus the two EBAMM corn ethanol scenarios together versus the EBAMM cellulosic scenario. From this data, policy decisions could be impacted by choice of EROI formulation. If the most straightforward approach (*EROI₁*) is used, all three biofuels platforms appear equally marginal, with algae exhibiting slight preferability. In contrast, use of *EROI₂* or *EROI₃* suggests that

switchgrass-derived cellulosic ethanol is far superior to algae, which is appreciably better than corn ethanol, which is itself marginal. Likewise, use of $EROI_3$ instead of $EROI_2$ further dramatizes the disparities in cellulosic ethanol versus algae and algae versus corn ethanol.

Table 9. Average values for the EROI formulations in Tables 7 and 8, with preferability rankings for algae (A), EBAMM corn scenarios (EC), and the EBAMM switchgrass-derived cellulosic ethanol scenario (ESC)¹.

Form	Average EROI Value			Preferability Ranking ^a
	<i>Algae (A)</i>	<i>EBAMM – Corn (EC)</i>	<i>EBAMM Cellulosic (ESC)</i>	
$EROI_1$	1.4	1.1	1.1	$EC \approx ESC < A$
$EROI_2$	2.3	1.1	7.1	$EC < A < ESC$
$EROI_3$	2.5	1.1	8.1	$EC < A < ESC$

¹ Adapted from **Zhang & Colosi (2013)**.

^a Unity (1) is included in rankings as indication of the energy breakeven point, whereby energy production is equal to energy consumption for a particular system.

5.3.2. Observations and Implications

Comparison between Tables 7 and 8 indicates that corn ethanol LCA data is apparently less susceptible to mathematical variability in EROI compared to the algae LCA data or the switchgrass ethanol data from EBAMM. This may be because the corn ethanol system does not produce an appreciable amount of bio-electricity as co-product. From Table 7, the difference between electricity production and consumption ($\|D-B\|$) is correlated with extent of variability among multiple computed EROI values. For example, the A_{SA} and A_{ST} datasets exhibit the largest values of $\|D-B\|$ and the largest differences between minimum and maximum EROI: 3.4 versus 1.8 for A_{SA} , and 4.6 versus 1.6 for A_{ST} .

EROI may be especially sensitive to the magnitude of $\|D-B\|$ because this term is multiplied by a factor of ~ 4.5 (IF_E) in either the numerator (for electricity surpluses) or

the denominator (for electricity deficits). Previously published work has shown that the magnitude of the electricity surplus/deficit term (i.e., $\|D-B\| \times IF_E$) can sometimes dominate the entire EROI ratio (Farrell et al., 2006; Liu et al., 2012). Applying the EROI formulations from Figure 21 to the algae life cycle data in Clarens et al (2011) (specifically Table S10 of their Supporting Information), there is much greater variability in EROI for systems producing only bioelectricity compared to systems producing both biodiesel and bioelectricity: EROI = 1.5-3.2 for anaerobic digestion of the bulk algae biomass to produce methane-derived bioelectricity, and EROI = 3.6-5.5 for direct combustion of the bulk algae biomass to produce bioelectricity; versus EROI = 1.2-1.5 and EROI = 1.8-2.7 for systems producing roughly equal amounts of energy as biodiesel and electricity, whereby electricity arises from either anaerobic digestion or direct combustion, respectively. EROI is thus very sensitive to accumulation of an electricity deficit or surplus, in part because grid electricity is so burdensome to produce and its upstream energy impact is so high. It should be emphasized the selection of IF_E value can have dramatic impacts on EROI computation and that not all EROI formulations are equally sensitive to changes in IF_E . Thus, it is problematic that the energy-intensiveness of electricity production varies by geographic location and also changes over time (Gagnon et al, 2002).

From a historical perspective, the mathematical ambiguity of the energy ratio metrics may have been overlooked primarily because early work was so focused on corn ethanol, and this system apparently exhibits less EROI variability than other biofuels. But, as the search for robust biofuels alternatives accelerates, it will be necessary to improve the usefulness of these metrics by standardizing their formulation for improved

interpretation. In a recent review of twelve algal biofuels LCA studies, it was demonstrated that co-products are critical for achieving favorable energy performance (Colosi et al, 2012). To the extent that this is true for other biofuels platforms, the ambiguity of the EROI ratio must be resolved.

5.4. Conclusions and Recommendations

In general, EROI is supposed to characterize the ratio of energy benefits (i.e., amount generated) to energy costs (i.e., amount consumed) for any hypothetical energy process, with the understanding that, as EROI approaches the cutoff ratio (1.0), the thermodynamic and economic favorability of the process decreases. Although all of the EROI formulations are mathematically meaningful, each of them represents different physical significance and system boundaries. $EROI_2$ and $EROI_3$ can only be applied to certain systems that allow internal recirculation of bioelectricity and other co-products. This method has at least two drawbacks: 1) very restricted applicability due to the fact that industrial specialization make it impossible to generate all products and co-products (biofuels, bio-electricity, fertilizer, etc) in one industrial sector; and 2) masking the internal circulation of high quality energy (electricity), thereby understating the energetic costs and overstating the energy benefits. In light of this, $EROI_1$ appears to be the most straightforward and conservative method, and it is applicable to any system regardless of its LCA system boundaries. $EROI_1$ is also seemingly most consistent with the work of Murphy & Hall (2010) and Murphy et al. (2011), who have indicated, for theoretical systems, that co-products should be categorized as energy output during EROI computation. Therefore, we conclude that $EROI_1$ is the most preferred method for calculation of the energy ratio metric, and we suggest that it is the form of EROI that

should be used in all future studies. Additionally, all EROI calculations should be thoroughly documented, with explicit denotation of how numerators and denominators are calculated, for maximal transparency and ease of interpretation by other researchers.

6. Economic Meta-Analysis for Algae Derived Biofuels

In this section, a meta-analysis of five previously published economic evaluations of algae-to-fuel systems was developed to better understand the near-term economic viability of deploying this technology at large scale. The meta-model uses data from other analyses, as standardized to a generic framework for financial assumptions. These data correspond to algae cultivation in open ponds followed by algae oil extraction, biodiesel conversion, and anaerobic digestion of the residual algae cake for bioelectricity generation.

6.1. Background

Life Cycle Costing (LCC) is a framework for evaluating economic feasibility, based on computation of all costs and revenues associated with energy flows, materials inputs, and processes through all stages of a process or product's life cycle. Many LCC studies use an existing LCA framework as a starting point (Colosi et al., 2012); however, there have been many fewer algae LCCs than algae LCAs published to date. What's more, the algae LCCs that have been published do not appear to give consistent results. This makes it difficult to understand what the likely economic performance of large-scale algae-to-energy systems could be. The estimated costs for algal oil or biodiesel span nearly two orders of magnitude, from 0.9 \$/gal to \$42.6/gal (Sun et al., 2011). This is surprising given that most studies have assessed essentially the same system, whereby algae are cultivated in open ponds, the oil fraction is extracted with solvent and then converted to fuels, and residual algae biomass is used to produce co-products.

We hypothesized that the disparate results from differently studies could be attributed to methodological differences, considering that different authors used different

functional units, system boundaries, allocation schemes, and economic parameters (tax rate, cost depreciation, internal return rate, etc). We further hypothesized that harmonization of these different methodological approaches, into an economic meta-analysis for algae derived biofuels, would offer better understanding of the likely economic performance of deploying this technology at large scale. This premise was based on a previous work, in which a similar meta-analysis approach was successfully applied to harmonize data from six published algae LCA studies (Liu et al, 2012). The current study is the logical extension of the previous meta-modeling work; with a focus on the economic viability, rather than environmental preferability, of algae-derived fuels.

6.2. Methodology

Five previously published economic analyses of systems producing algae biofuel in open ponds were incorporated into an LCC meta-model. These studies include: a systems and economic analysis of algae grown in ponds for conversion of CO₂ to biomass by Benneman & Oswald (1996); a cost-effectiveness analysis of algae-derived energy production in the EU by Kovacevic and Wesseler (2010); an economic and technical evaluation of microalgae biofuels by Stephens et al. (2010); a techno-economic analysis of autotrophic microalgae cultivation for fuel production by Davis et al. (2011); and an economic analysis of biodiesel production from algae by Gallagher (2011).

To build the normalized models, data from these studies were extracted and then standardized to ensure uniform system boundaries, functional units, by-product allocation schemes, and model input assumptions. The functional unit was defined as 10 million gal/yr of biodiesel. Standardized system boundaries and by-product allocation schemes are depicted in Figure 22, which reflects emerging trends in the algae biofuel industry

(Clarens et al., 2011; Davis et al., 2011; Gallagher, 2011). Two scenarios were modeled based on the information from the original studies: a *base case*, which assumes moderate algal oil yield achievable using current technology; and a *projected case*, which assumes that higher algal oil yields will be made possible by technological improvements and/or process optimization in the near future. The base case results correspond to the “probable algae yield” case (30 g/m²-day) in Benemann & Oswald (1996), the “open ponds” case in Davis et al. (2011), the “medium algae yield” scenario in Gallagher (2011), the “base case” in Kovacevic & Wesseler (2010), and the “base case” in Stephenson et al. (2010). The projected case correspond to the “high algae yield” case (60 g/m²-day) in Benemann & Oswald (1996), the “high algae yield” scenario in Gallagher (2011), the “high-yield case” in Kovacevic & Wesseler (2010), and the “projected case” in Stephenson et al. (2010). Thus, there was one dataset for both the base case and the projected case from each of the five original papers except Davis et al. (2011), which did not include a “projected” case.

Figure 22. Sytem configuration of algae-to-biofuel system. Most economic studies for algal biofuel have focused on algae cultivation in open ponds, algal oil extraction with solvent, and biodiesel producing via conversion. Upstream input (e.g., fertilizer, flue gas or commercial CO₂ as carbon source, etc.) are needed for algae cultivation; algal oil are extracted from algae and then converted to biodiesel; and residual non-lipid algae cake are used for anaerobic digestion for nutrient recycling and bio-electricity generation.

The net present value (NPV) was computed for each modeled dataset, based on three types of cash flows: total capital cost, annual operating cost, and annual revenue. Total capital cost was the capital investment required for purchase of materials and equipment, construction costs, and miscellaneous costs. Annual operating costs included energy, labor, capital depreciation, and other operating costs. Annual revenues consisted of all revenues gained from the sale of biodiesel and by-products. The results are presented using break-even costs of biodiesel, which was defined as the sale price of algal biodiesel required to achieve $NPV = 0$. It was expected that incorporation of data from five different authors, from different countries around the world, into a single unified framework would yield robust information about the relative economic favorability of the proposed algae systems, and this data could be easily compared with external benchmarks for meaningful interpretation of algae's favorability compared to other biofuels candidates. The original and normalized assumptions were summarized in Appendix D.

6.3. Results and Discussion

6.3.1. Normalized Results Arising from Meta-Model

Figure 23 depicts intermediate and final results arising from normalization of the original data from five separate algae LCC studies. In general, the cost estimates across all five studies become increasingly consistent with increased standardization. This makes the data easier to interpret in a meaningful way.

Figure 23. Normalized results of algal biodiesel cost: intermediate and final results from standardization of algae LCC data from five studies. The 1st normalization corrected differences in functional unit and financial assumptions. The 2nd normalization accounted for differences in systems boundaries and co-product allocations. The 3rd normalization adjusted for differences in key technical assumptions. The “base case” corresponds to prove algae oil yields. The “projected case” accounts for expected improvements in technology and/or process operations. Coefficients of variation (CVs) are presented above each data grouping. This parameter is defined as the ratio of the standard deviation to the mean, whereby smaller values indicate greater consistency among the five studies.

The “original results” data for both the base case and the projected case in Figure 23 correspond to each study’s original data following unit conversions so that all results can be presented in dollars per gallon (\$/gal) and are directly comparable to one another. The original data had been presented in various units, including dollars per gallon, dollars per barrel, dollars per gigajoule, etc. Following conversion to a consistent set of units, the estimated cost of algae biofuels varied between \$1.33-26.68/gal for the base case and \$0.93-10.52/gal for the projected case. The dramatic variability for both cases makes it difficult to assess the likely economic feasibility of algae-derived biofuels with any level of confidence.

The next step of the harmonization process corresponds to the “1st normalization” in Figure 23. This step constituted standardization of the functional unit across all studies, using 10 million gal/yr biodiesel as the common functional unit. Several financial assumptions were also standardized, including project life time, discount rate, tax rate, capital depreciation method, etc (see Appendix D). The original studies used a variety of relevant, but different, functional units: biodiesel production in 400 ha open ponds, 10 MM gal/yr biodiesel, algal oil production in 500 ha open ponds, etc. After standardization of the functional unit, it was necessary to account for costs associated with conversion of the algal oil into biodiesel for two of the papers: Benemann and Oswald, 1996; and, Stephenson et al., 2011. This is because these papers only accounted for the costs to produce algal oil instead of algal biodiesel. The financial assumptions used by each set of authors were also very different from each other; input values ranged from 15-30 years for projected useful lifetime, 5-10% for discount rate, 7-30 years for depreciation timeframe, etc. The standardized financial assumptions used in the meta-model included

20 years of project lifetime, 10% discount rate, 7 years of depreciation according to the modified accelerated cost recovery system (MACRS), and the use of 2012 US currency.

The adjustments comprising the first normalization step made the results of four studies much more consistent with one another. The revised estimated costs for algal biodiesel were \$2.18-10.98/gal for the base case and from \$1.21-4.51/gal for the projected case for all data except the base case from Stephenson et al. (2010). This data was unique because the original study had assumed that revenue from biodiesel was much smaller than revenue from β -carotene, a high value co-product comprising 0.1% of algae biomass and selling for roughly \$600/kg. For this reason, the biodiesel sale price required to achieve NPV = 0 was much less than in any other the studies.

A second normalization step was then performed to standardize systems boundaries and assumptions about co-products. The results from this step correspond to the “2nd Normalization” data in Figure 23. The system boundaries definitions within the original studies varied significantly, whereby some authors accounted for all processes generating algal oil (“farm to gate”) and others accounted for all processes through delivery of algal biodiesel at a retail fueling station (i.e., “farm to pump”). All system boundaries were changed to be “farm to pump”, for consistency across all studies and to capture the total cost to individual biodiesel consumers. This change made it necessary to add on distribution costs, for transport of the biodiesel from the biodiesel factory to fueling stations, for four of the five original studies: Benemann & Oswald, 1996; Davis et al., 2011; Gallagher, 2011; and Stephenson et al., 2010. It was assumed that distribution costs are roughly \$0.27/gal, based on Kovacevic & Wesseler (2010). Regarding co-products, it was assumed that non-lipid algae residuals would be subject to anaerobic

digestion to produce biogas (methane) that could then be combusted to produce bio-electricity. This approach had been previously modeled in several of the original studies (Benemann & Oswald, 1996; Davist et al., 2011; Kovacevic & Wessler, 2010). Following standardization of system boundaries and co-product processing, the breakeven costs for biodiesel were revised to \$2.47-33.36/gal for the base case and \$1.81-4.74/gal for the projected case.

The third and final step of the standardization process accounted for technical assumptions pertaining to algae oil yield, algae biomass yield, oil content, and lipid extraction efficiency. Although all five of the original studies had essentially modeled the same system (Figure 22) and most of them cited data from Benemann and Oswald (1996), there was still significant variability in the assumed values of these parameters. To eliminate this superficial variability of these parameters, uniform assumptions were applied to all five studies (Table 10). The results from this normalization step, corresponding to the “3rd Normalization” data in Figure 23, are more uniform than for any other step in the normalization process. Breakeven biodiesel prices are \$5.0-9.62/gal for the base case and \$2.76-4.39/gal for the projected case. The increased uniformity of these estimates demonstrates that the results of the five original LCCs are fundamentally consistent, despite the seeming disparity of original data. More importantly, the narrower range of breakeven cost estimates enables direct comparison between algae biodiesel and selected benchmarks.

Table 10. Assumptions of technical parameters defined in the meta-model.

Case	Algae biomass yield (g/m ² -day)	Algae oil content (fraction)	Oil extraction loss factor (fraction)
Base case	25	0.3	0.1
Projected	45	0.4	0.05

6.3.2. Comparison of Normalized Cost of Algal Biodiesel with the Selected Benchmarks

We chose the current retail price of petroleum diesel and commercially-available (e.g., soy) biodiesel (B100) as two relevant benchmarks for the meta-analyzed algae LCC data. This price is roughly \$3.99/gal for petroleum diesel and \$4.29/gal for biodiesel (B100) according to the DOE's Alternative Fuels Data Center (US DOE, 2013). This comparison is summarized in Table 11. From this data, the average cost of algal biodiesel corresponding to the base case is roughly 81% and 70% higher than retail price for petroleum diesel and B100. In contrast, the average cost of algal biodiesel corresponding to the projected case is quite competitive; 10% and 17% lower than the retail price of diesel and B100, respectively. It should be noted that the projected break-even price for algal biodiesel assumes that there will be a federal subsidy at \$1/gal, consistent with current practice (26 US § 40, 2013; Callagher, 2011). This subsidy is of course subjected to policy change.

Table 11. The comparison of the prices for algal biodiesel and selected benchmarks

Fuels	Algal biodiesel (base case)	Algal biodiesel (projected case)	Gasoline	Biodiesel (B100)
Price, \$/gal	7.24±2.20	3.58±0.89	3.99	4.29

The base case results presented in Table 11 suggest that algal biodiesel produced by first-generation algae-to-fuel systems cannot compete on a cost basis with petroleum diesel or biodiesel from conventional terrestrial sources. This could explain why this concept, for production of algal biodiesel, has not yet been put into place at successful commercial venture, and why tremendous research and development (R&D) are still underway for more applicable algae-to-fuel technologies. However, the results for the projected case offer a much more optimistic outlook for the economic viability of algae-derived biodiesel. The average cost of the four projected case data points is \$2.76/gal, which is 10% and 17% less than the current retail price for petroleum diesel and commercially available B100 from terrestrial sources, respectively. Even the highest anticipated cost for the projected case, \$4.39/gal, is only 2% and 10% greater than the current diesel price and B100 price, respectively. From a long-term perspective, algal biodiesel will be more financially competitive, because the price of petroleum fuels is expected to keep increasing into the future. The forecasted price of diesel will be around 4.28\$/gal in 2025 (US EIA, 2013), roughly equal to the highest anticipated cost of algae biodiesel under the projected case. Based on these results, algae-derived biodiesel could become financially appealing if the technological advancements or process optimization changes anticipated by the original LCC authors are brought to bear in the future.

Noting that the system configuration modeled in this analysis (Figure 22) represents the most studied algae cultivation configuration to date; however, this is only the first generation conceptualization of algae-to-fuels systems. There are many other technologies currently under R&D, which have been less discussed in the LCC or LCC literature because they are still unproven, that could revolutionize the production of algae

derived energy; e.g., wet oil recovery, oil secretion, hydrothermal liquefaction, genetic modification, ethanol production, pyrolytic conversion, etc (Liu et al., 2013; Luo et al., 2010, Miao et al., 2004; Vasudevan et al., 2012). For example, Vasudevan et al. (2012) assessed the environmental performance of three algal biofuels technology options, e.g., dry oil extraction, wet oil recovery, and oil secretion. The results showed that the net energy ration (NER, energy output / energy input) of under-development wet oil recovery could achieve 2.5, whereas the NER of well-established dry oil extraction was only 0.3. Another study reported that the energy return on investment (EROI) of algae biofuels produced by hydrothermal liquefaction could achieve up to 3, which is two times higher than that of algal biofuels produced by first-generation technologies (Liu et al., 2012; Liu et al., 2013). It could be expected that the economic viability of these new technologies would also be more optimistic along with the improved energy balance, because economic performance of energy systems is generally associated with their energy balance. Interestingly, most of the new technologies involve algal oil recovery, which indicates that the optimization of algal oil yield could make significant progress for the overall system performance. Still, there is much less LCA or LCC information regarding these under-development technologies, since most of them are still at the early stage of R&D, As these technologies mature, the LCA and LCC analyses will need to be updated accordingly.

6.3.3. Sensitivity Analysis

Given the inherent uncertainty associated with current economic assessment for algae-to-fuels systems that have yet to be deployed at large scale, sensitivity analysis is an important tool for identifying current bottlenecks and prioritizing areas that need to be

improved before better financial performance can be achieved. To conduct a sensitivity analysis, two scenarios corresponding to the base case and the projected case were modeled using the same system boundaries and functional unit, but selected input technical and financial parameters were made stochastic instead of deterministic. The input distributions for these parameters were mostly based on the ranges of values collected from all five original LCC studies, with external references used to fill some data gaps. Monte Carlo analysis was then performed using the Crystal Ball add-in for Microsoft Excel, and tornado plots were generated for each modeled scenario. These plots are a visual representation of which parameters most strongly impact the overall economic performance of the system (i.e., net present value). To generate these plots, each input parameter is increased and decreased by $\pm 10\%$, and the recording percent change in output parameter is recorded for each change in input parameter. This process is repeated systematically, one at a time, for all stochastic input parameters. The model is most sensitive to those inputs that mediate the largest changes in output response. Figure 24 is the tornado plot showing the top five inputs to which the NPV modeling is most sensitive, for both the base case and the projected case.

A (Base case)

B (Projected case)

Figure 24. Tornado plots reveal the extent to which the net present value of algae-to-fuel systems are sensitive to a 10% change in input parameters for base case (upper) and projected case (lower). The centerline represents the baseline case. The dark- and light-shaded values indicate direct and inverse relationships, respectively. For example, A 10% increase in algae oil content increases the net present value from 0.31 to 0.42 million dollars in base case, or ~30%.

In both scenarios, *algae oil content* most strongly affects the economic performance of algal biodiesel. This is not surprising, considering that the increased algae oil content contributes to improved overall economic performance in two ways: 1) increasing the amount of revenue arising from the desired final product (algal biodiesel); and 2) reducing the capital and operating costs associated with oil extraction and anaerobic digestion of the residual algae cake, because a smaller quantity of algae is produced when the algae oil content increases. This conclusion, that algae oil content is a critical parameter for the performance of algae-to-energy systems, is consistent with previous work in this area (Colosi et al., 2012; Vasudevan et al., 2012).

Most of the five most impactful parameters for both scenarios pertain to algal oil yield, rather than diesel conversion: algae oil content, open pond cost, and algae biomass yield for base case; and algae oil content, cultivation operational cost, open pond cost, and algae biomass yield for projected case. This indicates that improved performance in algae cultivation & algal oil recovery (e.g., increasing algae biomass yield and/or algae oil yield and reducing algae cultivation cost), could significantly improve the financial viability of algal biodiesel. It should be noted that these factors only account for top five parameters for first-generation algae technology (open pond cultivation plus conversion into biodiesel with production of biogas from residuals); therefore, different factors may affect the performance of other configurations for algae-to-energy systems.

6.4. Conclusions

The results of an economic meta-analysis indicate that first-generation algae-to-fuels systems are likely to be less financially viable compared to commercially available biodiesel so long as the base case conditions remain true. But there is significant

potential for improvement in financial performance as new technologies and/or optimized operations come online (as in the projected case). This conclusion, arising from the synthesis of five existing algae CC studies, suggests that algal biofuels have real potential but that the technology still needs to be improved. A sensitivity analysis highlights several particularly important areas for progress, mostly pertaining to improving algae cultivation and the quality of the algae biomass.

7. Conclusion and Future Work

In this dissertation, both modeling and experimental approaches were utilized to create knowledge that improves sustainability decision making of water-energy systems. In particular, it has been demonstrated that there are significant benefits to combining bio-energy production and water quality treatment into integrated systems. LCA and LCC modeling results demonstrate the synergies between algal energy production and dairy manure waste management will deliver improved economic and environmental performance for both systems. This conclusion is also supported by the bench-scale experiments, which have demonstrated the high efficiency of estrogen removal compared to conventional wastewater treatment processes. Furthermore, the results of economic meta-analysis for algal biodiesel reinforce the necessity of this integration, because the current algae-to-fuels system is not economic viable on its own and, as such, other economic incentives (e.g., ecosystem services) will be necessary to improve the overall financial feasibility of algae-to-energy systems.

To fully understand the benefits of the synergies between algal energy production and wastewater treatment, future work should focus on the following three areas.

1) Comparing the removal efficiency of estrogenicity mediated by algae growth and conventional tertiary treatments. The estrogenicity potential (EsP) data, established in this study, will be used to compare algae-mediated estrogenicity reduction against conventional tertiary treatments on the basis of cost, energy use, and GHG emissions per fixed quantity of EsP removal. This information will then be used to determine which treatment is most environmental favorable and cost effective per unit EsP reduction, which enables LCA or LCC better capturing estrogenicity removal as a valuable environmental service during algae –to-energy systems or in other engineering systems.

2) Analyzing the currently unknown biotransformation products of estrogens mediated by algae culture and assessing their estrogenic toxicity. As described in Chapter 4, both estradiol and estrone can be biotransformed into estriol, which is then further biodegraded to unknown products still exhibiting considerable estrogenicity. There is no study to date explaining the whole pathway for estriol in algae culture. Thus it is warranted to investigate the possible pathway for estriol biodegradation in algae culture and assess their estrogenic activity, which will enable better understanding the mechanisms of estrogens biodegradation mediated by algae culture and evaluating the benefits of estrogen removal arising from algae cultivation. For this purpose, LC-MS or GC-MS can be used to character the chemical structure of possible biodegraded products from estriol.

3) Exploring other water quality improvements arising from algae cultivation. Except for estrogens studied in this dissertation, there present other emerging contaminants, such as antibiotics and personal care products, which conventional wastewater treatment plants are not designed for. A great number of previous studies

have indicated that conventional wastewater treatment plants are not effective to remove these contaminants and are largely responsible for their spreading from municipal sewage to surface water (Schluter et al., 2007; Zhang et al., 2009). The results of this dissertation suggest that algae culture exhibit high efficiency of removing estrogens via biotransformation such as oxidation and hydroxylation. This could be also true for the removal of other emerging contaminants with similar structure via similar mechanisms. One or two antibiotics and personal care products, that are widely present in wastewater, should be chosen as the target compounds to investigate their removal or biodegradation mediated by algae culture.

The proposed future work, together with the results of this dissertation, will provide valuable information about what benefits could arise from the integration of algal bioenergy production and wastewater treatment, which can be further used for optimizing algae-to-energy systems to achieve environmental and economic sustainability.

8. References

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Appendix A: Supporting Information for Objective 1

This section is the detailed model documentation for objective 1 -- LCA & LCC of integrated algae cultivation and dairy manure management. This material has been published as the support information for Zhang et al. (2013).

1 Model Overview

Life cycle assessment (LCA) and life cycle costing (LCC) were performed to evaluate the environmental impacts and economic feasibility, respectively, of four dairy manure waste management systems. The reference scenario (REF) corresponds to conventional management practices, whereby manure is stored and then directly applied to on-farm agricultural lands. The anaerobic digestion (AD) corresponds to the reference system plus addition of an anaerobic digester for improved manure management. In this scenario, manure is converted into biogas, liquid digestate, and solid digestate. These products are then used for bioelectricity generation, on-farm land application, and soil amendment, respectively. The third scenario corresponds to integrated anaerobic digestion and algae cultivation in an open pond system (OPS). Similarly, the fourth scenario corresponds to integrated anaerobic digestion and algae cultivation in an algae turf scrubbing system (ATS). In both OPS and ATS, algae biomass is co-digested with manure to increase bioelectricity and soil amendment production. In addition, the OPS or ATS algae systems serve as means to effectively recycle nutrients from the liquid digestate. More detailed information for each scenario is described in Section 2.

1.1 System Boundaries

System boundaries corresponded to “cradle to farm gate” analyses, including all energy and material inputs corresponding to extraction of raw materials, manufacturing, use, and delivery of product (bioelectricity) and co-product (solid digestate residuals for use as soil amendment). All processes and facilities associated with cow breeding and manure collection were excluded from this analysis, since it was assumed that they would already exist on farms considering implementation of any one of the four modeled systems.

1.2 Functional Unit and LCA/LCC Outputs

The functional unit (FU) for the LCA and LCC analyses was treatment of as much waste is produced by 100 cows per year; i.e., approximately 6.9 kg/cow-day of dry mass (Van Horn et al., 1994). This is because we wished to model operations on a “typical” dairy farm in a Southeastern US state (e.g., Virginia). According to Groover (1998), average dairy herd size in Virginia is 115 cows per farm, and average land area is 382 acres (155 ha).

LCA outputs from modeled scenario included: energy use (GJ/yr), global warming potential (GWP) (kg CO₂-eq/yr), and eutrophication potential (kg PO₄-eq/yr). The principal LCC output for each modeled scenario was net present value (NPV). All models were built in Microsoft Excel, with the Crystal Ball add-in to facilitate Monte Carlo analysis.

2 Overview of Modeled Scenarios

2.1 Reference Scenario (REF)

Figure S1 shows system boundaries for the reference scenario (REF). Key processes in the REF scenario include manure storage and land application. It is assumed that dairy manure is collected and then stored on-farm as a slurry; either as excreted or with some minimal addition of water, in either tanks or earthen ponds located outside of the animal housing facilities (IPCC 2006). During the summer growing season (March to September), stored slurry is applied to on-farm agricultural fields for crop growth.

Figure S1. A schematic overview of Scenario 1 – REF. Double lines denote system boundaries, single lines denote modeled unit processes, and dashed lines denote material flows.

2.2 Manure Anaerobic Digestion (AD)

Figure S2 shows system boundaries for the AD scenario, the improved manure management system in which anaerobic digestion is used to convert dairy manure into bioelectricity and soil amendment. It is assumed that dairy manure is collected daily and sent to an anaerobic digester. After digestion, liquid digestate and solid digestate are separated via gravity-induced sedimentation and subsequent belt filter pressing. The liquid stream is stored for on-farm land application during the summer growing season (March-September) to support crop growth. The solid stream is further dewatered and then sold as soil amendment. Biogas is collected from the digester and sent to a micro-turbine for electricity generation. This electricity is used to power on-farm operations. Any surplus electricity is sold back to the local grid.

Figure S2. A schematic overview of AD. Double lines denote system boundaries, single lines denote modeled unit processes, and dashed lines denote material flows.

2.3 Algae Cultivation and Co-Digestion with Manure (OPS and ATS)

Figure S3 shows system boundaries for the OPS and ATS scenarios. Both scenarios include three main components: algae cultivation in either an OPS or ATS system; anaerobic digestion of dairy waste and algae biomass in the same digester; and bioelectricity generation. It is assumed that algae cultivation proceeds from March through November (Pizarro et al., 2006). During this period, liquid digestate is routed through the algae cultivation system to recycle nutrients (nitrogen – N, and phosphorus – P) into algae biomass. The harvested algae is then co-digested with the manure. During December-February, when the algae cultivation systems are not in operation, dairy manure effluent is stored on-farm for later use. As in AD, digester biogas is used to produce bioelectricity, and all surpluses are sold back to the grid. Also, digester solids are dewatered via belt filter press (BFP) and then sold for use as soil amendment.

Figure S3. A schematic of the OPS and ATS scenarios. Double lines denote system boundaries, single lines denote modeled unit processes, and dashed lines denote material flows.

3 Manure Storage and On-Farm Land Application

In the REF and AD scenarios, semi-liquid materials (i.e., stored manure slurry or post-digestion liquid effluent, respectively) are spread over on-farm agricultural lands to support crop growth. According to Groover (1998), a typical dairy farm in Virginia will comprise 130 acres of corn, 69 acres of hay, and 44 acres of “other” crops. For simplicity, it was assumed in this analysis that all nutrient-rich land-applied liquid wastes are used for corn cultivation.

3.1 Manure Characterization

The characteristics of dairy manure vary widely with location and feed method. For simplicity, it was assumed that manure has the characteristics summarized in Table S1. These are based on a report from Van Horn et al. (1994).

Table S1. Dairy manure characteristics based on Van Horn et al (1994).

Total Excretion (kg/cow-day)	Total Dry Matter (kg/cow-day)	Volatile Solids (g/cow-day)	Total Nitrogen ^a (g/cow-day)	NH ₃ -N ^a (g/cow-day)	Total Phosphorus ^a (g/cow-day)
56.7	6.9	5,730	296	112	54

^a Total N, ammonia as N (NH₃-N), and total P concentrations are for total manure (i.e., solids plus liquids).

3.2 Land Area Requirements and Crop Productivity

For on-farm application, manure must be applied at a rate that meets but does not exceed the nutrient requirements of the crop being grown in a particular soil. This rate is generally computed based on the crop's nitrogen demand ("agronomic N rate"), because nitrogen is the nutrient in highest demand for most crops; and because nitrogen is the growth-limiting nutrient most likely to run off (leach out of) an agricultural field if it is applied in excess of crop needs (Evanylo, 2009). Table S2 summarizes distributions for typical corn yields and the corresponding agronomic N rate in Virginia (Evanylo, 2009).

Table S2. Input distribution data for corn yield and agronomic N rate on typical dairy farms in Virginia. Data are from (Evanylo, 2009), as converted to SI units.

Model Parameter	Distribution Type	Minimum	Maximum	Likeliest
Nitrogen use, kg/ha	Triangular	123	179	157
Corn yield, Mg/ha ^a	Uniform	6.9	8.8	NA

^a In-field corn yield with 35-42% of dry matter at harvest (Brann et al., 2009).

Nitrogen in manure comprises both inorganic N (primarily NH₃) and organic N. When manure is stored and applied on land, some NH₃ is transported into the air via volatilization. The remaining inorganic N is assumed to be completely and directly available for uptake by plants (See Section 3.4 for detailed information and calculations). In contrast, organic N must be mineralized into inorganic N by soil microorganisms to become biologically available for plants. In light of this, it was assumed that 25% of the organic N in dairy manure is usable by crops during the year that it is land-applied (Wiens et al., 2008).

The total quantity of N available to plants in land-applied dairy manure comprises inorganic N remaining after volatilization plus 25% of total organic N. For the REF and AD cases, this corresponds to roughly 2,710 and 1,141 kg N/yr (average values), respectively. Based on these values, and the agronomic N rates in Table S2, average land use requirements for on-farm dairy manure management are 17.7 ha for the REF case and 7.4 ha for the AD case.

3.3 Energy Use

Energy consumption during on-farm application of dairy manure was accounted for as the diesel fuel for the manure loading and spreading equipment. Based on the average farm size of 155 ha (1.55 km²) noted in Section 1.2, it was assumed that the average on-farm travel distance is 1 km. Diesel consumption rates then were taken from the literature (Dalgaard et al., 2001; Mcfate, 1983; Pick & Netik, 1989) and incorporated into the following triangular distribution: minimum = 0.4, maximum = 1.8, and likeliest = 0.6. Units were L diesel per Mg manure transported per km (L/Mg-km). The energy content for diesel fuel was 35.9 MJ/L (Dalgaard et al., 2001).

3.4 Nutrient Losses and Manure Emissions

Nutrient losses and methane (CH₄) emissions during manure storage and application are a significant source of eutrophication potential and global warming potential, respectively. It was thus necessary to incorporate these fluxes into the LCA models to fully understand how dairy manure management choices could affect the surrounding environment. Nutrient losses were modeled using a protocol based on published reports from the US Environmental Protection Agency (EPA 2003, 2005) and others. Methane emissions were modeled based on published reports from the Intergovernmental Panel on Climate Change (IPCC 2006, Ar4 2007).

Nitrogen Losses for the REF and AD Cases. It was assumed that there are five major types of nitrogen losses from liquid dairy wastes: direct nitrous oxide (N₂O) emissions, nitric oxide (NO) emissions, N volatilization, N leaching/runoff, and indirect N₂O emissions. These five quantities are summed together to compute total nitrogen losses. Table S3 provides data for undigested manure slurry, as used to compute nitrogen losses for the REF case. Table S4 provides data for digested dairy manure, as used to compute nitrogen losses for the AD case. In both tables, emission factors are provided for storage and application.

Table S3. N emission factors for storage and land application of undigested manure slurry.

Factor	Storage or Application	Model Distribution	Minimum Value	Maximum Value	Likeliest Value	References
EF ₁	Storage	Triangular	0.0025	0.01	0.005	IPCC 2006
	Application	Triangular	0.005	0.02	0.01	IPCC 2006
EF ₂	Storage	Triangular	0.0005	0.002	0.001	IPCC 2006
	Application	NA	NA	NA	0.0055	Vries et al., 2010
EF ₃	Storage	Triangular	0.15	0.45	0.40	IPCC 2006
	Application	Triangular	0.05	0.5	0.2	IPCC 2006
EF ₄	Application	Triangular	0.18	0.21	0.20	Ortenblad, 2000
						Vries et al., 2010;
EF ₅		Uniform			0.01	IPCC 2006
EF ₆		Uniform			0.0075	IPCC 2006

Table S4. N emission factors for storage and land application of digested manure.

Factor	Storage or Application	Model Distribution	Minimum Value	Maximum Value	Likeliest Value	References
EF ₁	Storage	NA	NA	NA	0	IPCC 2006
	Application	Triangular	0.005	0.02	0.01	IPCC 2006
EF ₂	Storage	Triangular	0.0005	0.002	0.001	IPCC 2006
	Application	NA	NA	NA	0.0055	Vries et al., 2010
EF ₃	Storage	Triangular	0.20	0.80	0.35	IPCC 2006
	Application	Triangular	0.05	0.5	0.2	IPCC 2006
EF ₄	Application	Triangular	0.10	0.19	0.15	Vries et al., 2010; Ortenblad, 2000
EF ₅		Uniform			0.01	IPCC 2006
EF ₆		Uniform			0.0075	IPCC 2006

Nitrogen loss calculations are summarized using Equations S1-S5 below and the factors in tables above.

$$Y_1 = X_{TN} \times EF_1 \times 44/28 \quad \text{Eq. S1}$$

Where: Y_1 is direct N₂O emissions, in kg N₂O;
 X_{TN} is total nitrogen (TN) concentration, in kg N;
 EF_1 is an empirical emission factor, in kg N₂O-N/kg TN;
44/28 is a conversion factor for the ratio of N mass in N₂O.

$$Y_2 = X_{TN} \times EF_2 \times 30/14 \quad \text{Eq. S2}$$

Where: Y_2 is NO emissions, in kg NO;
 X_{TN} is total nitrogen (TN) concentration, in kg N;
 EF_2 is an empirical emission factor, in kg NO-N/kg TN;
30/14 is a conversion factor for the ratio of N mass in NO.

$$Y_3 = X_{TN} \times EF_3 \quad \text{Eq. S3}$$

Where: Y_3 is N volatilization losses, in kg N;
 X_{TN} is total nitrogen (TN) concentration, in kg N;
 EF_3 is an empirical estimate for the fraction of manure nitrogen that volatilizes as NH₃.

$$Y_4 = X_{TN} \times EF_4 \quad \text{Eq. S4}$$

Where: Y_4 is N runoff (leaching) losses, in kg N;
 X_{TN} is total nitrogen (TN) concentration, in kg N;
 EF_4 is an empirical estimate for the fraction of manure nitrogen that leaches out of solution into runoff water.

$$Y_5 = (Y_3 \times EF_5 + Y_4 \times EF_6) \times 44/28 \quad \text{Eq. S5}$$

Where: Y_5 is indirect N₂O emissions resulting from volatilization of NH₃ and leaching of nitrate (IPCC, 2006), in kg N₂O;
 Y_3 is N volatilization losses, in kg N;

EF_5 is an empirical factor for N_2O emission from volatilized N, on the order of 0.01 kg N_2O -N/kg volatilized N.

Y_4 is N runoff (leaching) losses, in kg N;

EF_6 is an empirical factor for N_2O emission from runoff N, on the order or 0.0075 kg N_2O -N/kg runoff N;

44/28 is a conversion factor for the ratio of N mass in N_2O .

Nitrogen Losses for the OPS and ATS Cases. A different approach was used to compute nitrogen losses for the OPS and ATS cases compared to the REF and AD cases. This is because post-digestion liquid is diluted and applied to the algae cultivation systems daily, with no need for prolonged storage during March-November. It was thus assumed that there is no N leaching or runoff from the OPS or ATS during this part of the year, because both are closed systems. Also, because the liquid digestate must be diluted roughly 40 times and N emissions are dramatically reduced for dilution ratios greater than 2:1 (Amon et al., 2006), it was assumed that N losses due to N volatilization are negligible during the algae cultivation season. Thus, it was assumed that there are no N losses from the OPS or ATS systems during March-November. For December-February, nitrogen losses from the OPS and ATS systems were computed using the same method as for AD system.

Phosphorus Losses. As noted in Section 3.2, nitrogen is much more likely run off than phosphorus following land application of liquid dairy wastes. Also, phosphorus losses are more difficult to estimate than nitrogen losses, because its immobility varies strongly as a function of soil type (Vries et al., 2010). In light of these factors, an empirical loss factor ($0.6\% \times$ total phosphorus) was used to estimate phosphorus losses from land-applied dairy solids (EPA, 2003).

Nutrient Losses from Post-Digestion Solids. It was assumed that the solid residuals arising from manure/algae digestion in the AD, OPS, and ATS cases would be sold for use as soil amendment at off-farm locations. Nutrient losses of these solids were purposefully excluded from the LCA, because it was presumed that mobilization of nitrogen and phosphorus from the solids is desirable to support plant growth. Also, the off-site locations were considered to be outside the system boundaries for the AD, OPS, and ATS systems.

Methane Emissions. Equation S6 was used to compute fugitive methane emissions arising during manure storage and application. These were accounted for as one contributor to global warming potential (GWP). Table S5 contains empirical emissions factors referenced in Equation 6. See Section 6.2 for additional GWP calculations.

$$Y = X_{VS} \times VS_{B_0} \times MCF \times D_{CH_4} \quad \text{Eq. S6}$$

Where: Y is CH₄ emissions during manure management, in kg CH₄;
 X_{VS} is manure volatile solids, in kg;
 VS_{B0} is maximum CH₄ productivity, in m³ CH₄/kg VS.
 MCF is an empirical methane conversion factor;
 D_{CH4} is the density of methane gas at STP, 1.0 kg/m³.

Table S5. Methane (CH₄) emission factors for manure management.

Factor	Model Distribution	Minimum Value	Maximum Value	Likeliest Value	References
VS_{B0}	Triangular	0.20	0.28	0.24	Safley et al., 1992 IPCC 2006
MCF – Storage	Triangular	0.17	0.39	0.25	^a IPCC 2006
MCF – Digestion	NA	NA	NA	0.1	IPCC 2006

^a Values based on average annual temperature in Virginia, min = 7 °C; max = 19 °C; likeliest = 14 °C (Virginia Climate Description, 2011).

4 Algae Cultivation

4.1 Algae Cultivation in Open Ponds (OPS)

LCA impacts for algae cultivation in open ponds (OPS) was modeled based on existing frameworks from Clarens et al. (2010, 2011); specifically, LCA models correspond to “Scenario A” from Clarens et al. (2011). Three significant modifications to this model are described below.

Climate inputs, including photosynthetically active radiation (PAR), temperature, wind speed, relative humidity, and precipitation corresponds to the southeastern USA (i.e., Virginia) instead of the southwestern USA. These inputs were based on information from Clarens et al (2010).

Algae yield data correspond to freshwater instead of brackish-to-saline yields, based on information from Clarens et al (2010).

N and P concentrations in the irrigating medium have been changed to 3 g/L N and 0.3 g/L total P to reflect nutrient concentrations in liquid digestate. These are considerably higher than the corresponding nutrient concentrations in municipal wastewater effluent. Finally, CO₂ for algae photosynthesis was obtained from methane combustion and commercial virgin CO₂, roughly 222 and 52 Mg/yr respectively.

Algae stoichiometry was based on the Redfield ratio, $C_{106}H_{181}O_{45}N_{15}P$ (Redfield 1958). This formulation was used to characterize the ash-free algae biomass. Ash content for OPS algae was taken from Clarens et al (2011) and set to the following triangular distribution: minimum = 9.8%, maximum = 18.6%, and likeliest = 11.2%. OPS algae yield was also taken from Clarens et al (2010). Monthly yields and overall annual yield are summarized in Table S6.

Table S6. Monthly yields of freshwater OPS algae for PAR conditions similar to Virginia, USA.

Month	Algae Yield, Mg AFDW/ha ^a
March	2.9
April	3.5
May	4.1
June	4.2
July	4.2
August	3.8
September	3.1
October	2.5
November	1.7
Annual ^b	30.1

^a AFDW is ash free dry weight.

^b Average annual yield corresponds roughly to 12.6 g AFDW/m²-day.

4.2 Algae Cultivation in Algae Turf Scrubber (ATS) Systems

4.2.1 ATS Configuration

ATS infrastructure was modeled using data from previously published reports of pilot-scale dairy effluent treatment and an economic assessment of ATS-mediated dairy manure treatment, with some modification (Mulbry et al., 2008b; Pizarro et al., 2006). Each ATS module was assumed to be 10 m wide by 100 m long (Figure S4), for a total footprint of 1,000 m². There is a 2% slope along length. Each module comprises a 0.75-mm thick HDPE landfill liner covered with 6-mm mesh nylon netting, plus an underground sump with dimensions 10 m long by 5 m wide by 2 m deep. Total sump volume is 100 m³. The sump is located near the top (upstream) end of each ATS module. A submerged water pump is located within the sump to deliver water at a flow rate of 1200 L/min onto the ATS module. From the bottom end of the ATS model, the spent algae medium flows through a 100-m long, 6-in diameter PVC pipe back to the sump. Liquid digestate is added to the sump for nutrients delivery to the ATS biomass. No CO₂ supply is required beyond what enters the ATS via gas transfer from the atmosphere (Mulbry et al., 2008b).

It was assumed that multiple ATS modules comprise a single system. It was also assumed that all modules comprising a single ATS system share algae processing equipment and facilities, such as the algae harvester, belt filter press, etc.

Figure S4. A schematic depiction of one 1000-m² ATS algae cultivation module.

4.2.2 Electricity Consumption for ATS Operations

Electricity is consumed for pumping, mixing, harvesting, and algae dewatering. Electricity calculations for these processes are summarized in the following paragraphs.

Pumping. Electricity demand for pumping algae medium out of the sump to the top of the ATS module and then back from the collection tank into the sump was calculated using the standard pump power equation (Equation S7).

$$W = h g q / \eta \quad \text{Eq. S7}$$

Where: W is energy required for water pumping within each individual ATS module, in J/s);

h is dynamic differential pump head, in m, from Equation S8;

g is the acceleration of gravity, 9.81 N/kg;

q is flow rate for one floway unit, 1200 L/s;

η is pumping efficiency (85%).

$$h = h_1 + h_2 + h_3 \quad \text{Eq. S8}$$

Where: dynamic differential pump head, in m;

h_1 is static pump head, in 4.5 m;

h_2 is friction head loss, as computed using the Hazen-Williams Equation (Equation S9) and converted into m from ft;

h_3 is fittings head loss, in m, as computed using Equation S10.

$$h_2 = \left[0.2083 \times \left(\frac{100}{c} \right)^{1.852} \times q^{1.852} \right] \div d_h^{4.8655} \quad \text{Eq. S9}$$

Where: h_2 is pipe friction head loss (in ft) per 100 feet of pipe;
 c is the Hazen-Williams roughness constant (130 for PVC pipe);
 q is flow rate, as converted from 1200 L/min to 316 gal/min;
 d_h is inside hydraulic diameter (6 in, PVC).

$$h_3 = k \times v^2 / 2g \quad \text{Eq. S10}$$

Where: h_3 is pipe fitting head loss per elbow or “T”, in m;
 k is pipe fitting resistance co-efficient, 0.45 for elbow and 0.3 for “T”;
 g is the acceleration of gravity, 9.81 N/kg;
 v is flow velocity, as computed using quotient of flow rate over pipe cross-sectional area, in L/s.

From Equations S8-S10, the dynamic differential pump head in each ATS module was roughly 5 m. Using this value in conjunction with Equation S7, the amount of electricity consumed for pumping in each ATS module is 25 GJ/yr.

Mixing. The electricity requirement for mixing recycle water and liquid digestate within the underground sump was calculated according to the method of Clarens et al (2010) in their Supporting Information document (Section 3.3.1). Mixing consumes 0.800 GJ per ATS module.

Harvesting and Dewatering. Electricity demand for algae harvesting and dewatering was computed based on parameters from Pizarro et al (2006). In their study, power costs for harvesting and dewatering were \$1,200/ha-yr, assuming \$0.06/kWh. Therefore, it was assumed that each 1000-m² ATS module requires 7.2 GJ for harvesting and dewatering.

4.2.3 ATS Yield and Biomass Characterization

Algae yield and biomass characteristics for the ATS system were based on previous pilot-scale experiments (Kebede-Westhead et al, 2003, 2004; Mulbry et al, 2001, 2008a, 2008b; Pizarro et al, 2006). Dry biomass yield and ash content were set to triangular distributions. The distribution for dry biomass yield (in g/m²-d) was: minimum = 18, maximum = 25, and likeliest value = 22. The distribution for ash content was: minimum = 12%, maximum = 18%, and likeliest value = 16%. Carbon, nitrogen, and phosphorus contents were set to uniform distributions over the following ranges: C = 44.5% ± 2.5%, N = 7.0% ± 0.7%, P = 0.86% ± 0.05%.

4.3 Algae Cultivation Area Requirement

The estimated quantities of total nitrogen (TN) and total phosphorus (TP) excreted from a 100-cow farm are 10,804 kg/yr and 1,971 kg/yr, respectively. For OPS and ATS case, the manure is digested and the liquid digestate, containing 70% and 40% of total N and P input (Fuchs et al, 2001), is then used to supply N and P requirements. During non-cultivation season (December-February), the digestate effluent is stored for later use, and 841 kg N loses via volatilization during storage period. Therefore, total N and P available for OPS and ATS algae cultivation are 6,722 kg N/yr (24.5 kg N/day) and 788 kg P/yr (2.88 kg P/day) respectively. The OPS and ATS cultivation area is sized to completely consume the amounts of N and P.

Because phosphorus is the limiting nutrient when the liquid digestate is applied for algae cultivation. The OPS and ATS module were thus sized to consume all of the available phosphorus. It was also necessary to account for the TP arising from co-digestion of the algae biomass with the dairy manure, since it had been previously demonstrated that only 60% of post-digestion algae P makes its way into the solid digestate (Fuchs et al., 2000). Equation S11 was used to calculate the amount of area required to completely consume the amount of P in the liquid digestate arising from co-digestion of both dairy manure and algae biomass on a 100-cow farm in Virginia.

$$Y = m / (f \times a \times n) \quad \text{Eq. S11}$$

Where: Y is total area required to consume P in the liquid digestate, in m^2 ;

m is manure TP input for algae cultivation, in 2867 g/day;

f is mass fraction of P in algae biomass, 0.013 for OPS algae and 0.009 for ATS algae (Mulbry et al., 2008);

a is mass fraction of algae P entering solid digestate, 0.60 (Table S8);

n is algae productivity, 12.6 g/day-m (ash free dry weight, Table S6) for OPS algae and 22 g/day- m^2 for ATS algae.

From Equation S11, the OPS and ATS land area required to completely consume liquid digestate N is roughly 34,029 m^2 (3.4 ha) and 25,643 m^2 (2.6 ha), respectively.

5 Anaerobic Digestion

Anaerobic digestion was modeled as part of the AD, OPS, and ATS scenarios. Calculations pertaining to several digestion sub-processes are summarized in the following paragraphs.

5.1 Digester Capacity

A report of manure digestion on mid-sized dairy farms by Goodrich (2005) was the principal source of information about digestion and digesters. All calculations for the present study were based on Goodrich's System #2 (an upright mixed digester). Retention time was 14 days.

It was assumed that all dairy manure, comprising 10% dry solids (DS) by mass, is collected from dairy barns and sent to an anaerobic digester for digestion. For Scenario AD, the average effluent flow rate on a 100-cow farm is 6.9 m³/day. One single digester, sized to accommodate 100 cows will be sufficient for this scenario. For the OPS and ATS scenarios, in which algae biomass is co-digested with the dairy manure, additional capacity is required. For the OPS scenario, the additional load is 3.23 m³/day. For the ATS scenario, the additional load is 4.11 m³/day. For these cases, the digesters are sized to accommodate 150 and 160 “cow-equivalents”, respectively.

5.2 Algal Homogenization

Previous studies have reported that homogenization significantly improves algae digestibility (Stephenson et al. 2010; Sialve et al, 2009; Samson & Leduy, 1983). Electricity consumption was 67 MJ/m³ algae slurry per pass (Stephenson et al, 2010). It was assumed that two passes would be required to achieve nearly complete (96%) cell disruption (Stephenson et al, 2010).

5.3 Digestion Products and Energy Consumption

Tables S7 and S8 summarize anaerobic digestion parameters for digestion of dairy manure and algae biomass. These are based on previous bench-scale digestion studies, as noted in each table.

Table S7. Parameters used to model anaerobic digestion of dairy manure.

Parameter	Model Distribution	MIN	MAX	Likeliest Value	References
VSS removal (fraction)	NA	NA	NA	0.46	Van Horn et al., 1994
Methane production efficiency (L CH ₄ /g VSS)	Triangular	0.32	0.47	0.42	Van Horn et al., 1994 Ward et al., 2008
Biogas methane fraction (vol/vol)	Triangular	0.60	0.64	0.61	Hills & Roberts, 1981 Van Horn et al., 1994
Biogas CO ₂ fraction (vol/vol)	Triangular	0.30	0.35	0.31	Hills & Roberts, 1981 Van Horn et al., 1994
N in liquid digestate (fraction)	Triangular	0.65	0.75	0.70	Fuchs et al., 2010 Pizarro et al., 2006
N in solid digestate (fraction)	Triangular	0.25	0.35	0.30	Fuchs et al., 2010
N mineralized (fraction)	Triangular	0.57	0.67	0.62	Amon et al., 2006 Vries et al., 2010
NH ₃ -N in liquid digestate (fraction)	Triangular	0.70	0.80	0.75	Fuchs et al., 2000
NH ₃ -N in solid digestate (fraction)	Triangular	0.20	0.30	0.25	Fuchs et al., 2000
P in liquid digestate (fraction)	Triangular	0.35	0.45	0.40	Fuchs et al., 2000
P in solid digestate (fraction)	Triangular	0.55	0.65	0.60	Fuchs et al., 2000

Table S8. Parameters used to model anaerobic digestion of algae biomass.

Parameter	Model Distribution	MIN	MAX	Likeliest Value	References
VSS removal (fraction)	Triangular	0.21	0.60	0.41	Samson & Leduy, 1983 Golueke et al, 1975 Yen & Brune, 2007
Methane production efficiency (L CH ₄ /g VSS)	Triangular	0.18	0.99	0.49	Sialve et al, 2009
Biogas methane fraction (vol/vol)	Triangular	0.46	0.76	0.72	Sialve et al, 2009
Biogas CO ₂ fraction (vol/vol)	Triangular	0.08	0.31	0.22	Sanchez et al, 1993
N in liquid digestate (fraction)	Triangular	0.40	0.57	0.43	Anasruron et al, 2010 Sialve et al, 2010 Starman 2009
N in solid digestate (fraction)	Triangular	0.43	0.60	0.57	Anasruron et al, 2010 Sialve et al, 2010 Starman 2009
N mineralized (fraction)	Triangular	0.57	0.67	0.62	Amon et al, 2006 Vries et al, 2010
NH ₃ -N in liquid digestate (fraction)	Triangular	0.70	0.80	0.75	Fuchs et al, 2000
NH ₃ -N in solid digestate (fraction)	Triangular	0.20	0.30	0.25	Fuchs et al, 2000
P in liquid digestate (fraction)	Triangular	0.35	0.45	0.40	Fuchs et al, 2000
P in solid digestate (fraction)	Triangular	0.55	0.65	0.60	Fuchs et al, 2000

Empirical regression equations from Soda et al (2010) were used to estimate electricity and heat consumption during anaerobic digestion. These are Equations S 12 and S13, respectively.

$$Y = 2587 \times X^{0.944} \quad \text{Eq. S12}$$

Where: Y is electricity consumption for digestion, in kWh/t-DS;

X is manure or manure + algae loading rate, in t-DS/d.

$$Z = 42540 \times X^{-1.011} \quad \text{Eq. S13}$$

Where: Z is heat consumption, in MJ/t-DS;

X is manure or manure + algae loading rate, in t-DS/d.

5.4 Dewatering of the Digestate Solids

It was assumed that a screw press is used to dewater digestate solids, based on common practice in farms. Equation S14 was used to compute electricity consumption during digestate dewatering (Moller et al., 2000).

$$Y = 0.5 \times X \quad \text{Eq. S14}$$

Where: Y is BFP electricity consumption, in kWh/yr;

X is manure or manure + algae slurry, in t / yr.

5.5 Methane Combustion

Methane in the biogas produced during anaerobic digestion is combusted in a micro-turbine to generate bioelectricity. Methane energy content and turbine efficiency were both taken from Masters (2008). Energy content was 50 MJ/kg. Turbine efficiency was set to the following triangular distribution: minimum = 0.50, maximum = 0.60, likeliest value = 0.53.

5.6 Soil Amendment Yield

It was assumed that BFP-separated solids are used as soil amendment (i.e., fertilizer), to offset use of commercial fertilizer. Nutrient content and bioavailability were used to determine what mass of digestate solids could be used in place of 1 kg of commercial fertilizer. Pertinent parameters for these calculations are summarized in Table S9. Nitrogen and phosphorus offsets were first converted into an equivalent amount of ammonium phosphate ($\text{H}_{12}\text{N}_3\text{O}_4\text{P}$) offset. Excess nitrogen was converted into urea offset. Overall, 1 kg of solid digestate accounts for roughly 0.0025 kg of $\text{H}_{12}\text{N}_3\text{O}_4\text{P}$ offset and 0.027 kg of urea offset.

Table S9. Parameters used to compute soil amendment offsets for solid digestate.

Parameter	Distribution	MIN	MAX	Likeliest	References
N use efficiency, fraction	NA	NA	NA	0.36	N mass balance ^a
P use efficiency, fraction	Uniform	0.05	0.10	NA	Warman & Termeer, 2005

^a N use efficiency is ratio of inorganic N to total N in the solid digestate (see Table S7 and S8)

5.7 CO₂ Sequestration into Solid Digestate

Since no external CO₂ is supplied to the ATS system, all carbon that ultimately makes its way into the solid digestate (for use as soil amendment) can be considered effectively “sequestered.” The GWP offset associated with sequestration of this carbon is given by Equation S15.

$$Y = (1 - m) \times f \times X \times \frac{44}{12} \quad \text{Eq. S15}$$

Where: m is carbon mineralization fraction, minimum 0.16, maximum 0.42, most likely 0.20 (Moorhead et al., 1987);

Y is mass of CO₂-eq sequestered as solid digestate, in kg/yr;

X is mass of solid algal digestate mass, in kg/yr;

f is carbon fraction in algae digestate.

A distribution of values for f (the carbon fraction in solid algae digestate) was based on published literature reports. The triangular distribution was as follows: min = 0.32, max = 0.42, likeliest value = 0.37 (Hue and Sobieszczyk, 1999; Tambone et al, 2009).

6 Environmental Impact Factors Calculations

Model inputs and outputs were used to evaluate three kinds of environmental impacts associated with production of one functional unit in each of the four modeled scenarios. Evaluated LCA impacts included: total energy use, total greenhouse gas emissions (i.e., global warming potential, GWP), and total eutrophication potential (EUT). Impact factors for input materials (including energy) were taken from the ecoinvent database via Simapro v 2 (Weidema, 2007).

All capital equipment (most notably the ATS system and the anaerobic digester) were assumed to have a useful lifetime of twenty years. For computation of “annualized” life cycle impacts, all environmental impacts associated with a particular piece of capital infrastructure or equipment were divided by twenty.

6.1 Energy Use

Energy use accounts for total energy consumption for production of one functional unit. This includes all direct energy (electricity, heat, diesel), upstream energy use for

production of input materials. Energy use is reported in GJ per year. Table S10 provides an overview of energy consumption, by process, for each modeled scenario. This is an expanded version of Table 1 from the main paper.

Table S10. Energy use (GJ/yr), by process, for each of the four modeled scenarios. Positive values indicate energy consumption, negative numbers indicate energy production.

Process	REF	AD	OPS	ATS
<i>Energy Inputs</i>				
Manure land application	195	183		
Fuel (transportation)	195	183		
Algae cultivation			272	846
Electricity			55	846
Water pumping			5843	641
Mixing			4	21
CO ₂ recycle pumping			9	
Harvesting and dewatering				185
Nutrients supply			216	
Phosphorus & Nitrogen			0	
Virgin CO ₂			216	
Anaerobic digestion		100	341	382
Electricity		86	308	343
Algae thickening			9	
Algae homogenization			158	201
Anaerobic digestion		83	137	137
Screw press		3	4	5
Fuel (heating)		14	33	38
Infrastructure burden ¹	4	14	418	102
<i>Energy Outputs</i>				
Bioelectricity generation		-1,044	-1,662	-1,803
Soil amendment offset		-101	-189	-199
Crops (corn silage) offset ²	-19	-8		
Total Energy Input	199	297	1,031	1,320
Total Energy Output	-19	-1,153	-1,851	-2,002
Net Energy Balance	180	-856	-820	-672

¹ Accounts for “annualized” infrastructure energy burdens (i.e., energy consumption associated with production of anaerobic digester, whereby overall burdens have been divided by the assumed 30-years useful lifetime to estimate annual impact.

² Accounts for corn grown on manure-applied lands.

6.2 Global Warming Potential (GWP)

GWP accounts for total GHG emissions associated with production of one functional unit, including upstream emissions for production of material and energy inputs. GWP is reported in kg CO₂-equivalents per year (kg CO₂-eq/yr), based on a 100-year GWP time horizon (Table S11).

Table S11. Impact factors for computation of global warming potential (GWP).

Emission Species	Chemical Formula	Global Warming Potential (100 years), kg CO ₂ -eq/kg
Carbon dioxide	CO ₂	1
Methane	CH ₄	21
Nitrous oxide	N ₂ O	310

6.3 Eutrophication Potential (EUT)

EUT accounts for all waterborne emissions of nutrients and other chemicals associated with production of one functional unit, including production of upstream material and energy inputs and volatilization/leaching of nutrients from land-applied manure. EUT is reported in units of kg of PO₄-equivalents per year (kg PO₄-eq/yr). Impact factors are summarized in Table S12.

Table S12. Impact factors for computation of eutrophication potential (EUT).

Emission Species	Chemical Formula	Eutrophication Potential, kg PO ₄ -eq/kg
Nitrogen monoxide	NO	0.20
Nitrogen oxides	NO _x	0.13
Ammonium	NH ₄ ⁺	0.33
Nitrogen	N	0.42
Phosphorus	P	3.06

7 Life Cycle Cost (LCC) Analysis

An LCC analysis was computed based on the results of LCA inventories for all four evaluated scenarios. Three principal cash flows were accounted for, including: initial outlays, annual operational costs, and annual revenues.

7.1 Initial Outlay

The initial outlay accounts for infrastructure costs, major facilities costs, working capital, engineering, and contingencies.

Capital costs for the REF scenarios include purchase of manure loading, spreading, and application equipment. In the AD scenario, capital costs include purchase of manure loading, spreading, and application equipment, purchase and construction of the anaerobic digester, and bioelectricity generation systems. For both the OPS scenario and the ATS scenario, capital costs include purchase of the same equipment from the AD scenario plus the algae cultivation system (as sized to produce one functional unit). In all

scenarios, costs associated with farm construction, livestock breeding, and manure collection was excluded.

Tables S13, S14, S15, and S16 summarize initial outlays for the REF, AD, OPS, and ATS scenarios, respectively. Tabulated values are mean values from empirical output distributions. Table S13. Initial outlays for the REF scenario.

Item	Unit Price (\$/cow)	Total Price (\$/FU)	References
Manure on-farm application system (equipment, construction, miscellanea)	1020 ¹	102,000	Fulhage & Psoft, 2003

¹ Based on use of a regression model (Figure S5 below) for farm-sizes between 150 and 600 cows (Fulhage & Psoft, 2003), assuming 100 “cow-equivalents” for the REF scenario.

Figure S5: Regression model of costs for manure land application systems. Original data was from Fulhage & Psoft (2003).

Table S14. Initial outlays for the AD scenario.

Item	Unit Price (\$/100 cow)	Total Price (\$/FU)	References
Anaerobic digestion system		238,652	
<i>Liquid storage facility</i>	NA ¹	NA	
<i>Digester tank</i>	68,200	68,200	<i>Goodrich, 2005</i>
<i>Building</i>	20,667	20,667	<i>Goodrich, 2005</i>
<i>Boilers and heat exchangers</i>	8,267	8,267	<i>Goodrich, 2005</i>
<i>Gas recirculation pump</i>	4,133	4,133	<i>Goodrich, 2005</i>
<i>Screw press</i>	22,400 (100 kg/hr) ²	22,400	<i>Moller et al., 2000</i>
<i>Micro-turbine</i>	75,000 (200 cows) ³	75,000	<i>Goodrich, 2005</i>
<i>Miscellanea (engineering, etc).</i>		39,985 ⁵	<i>Benemann and Oswald, 1996; Pizarro et al., 2006</i>
<i>Manure application system</i>	102,000 ⁴	95,696 ⁶	<i>Fulhage & Psoft, 2003</i>
Total Initial Outlay – AD	352,943	334,349	

¹ Assumes that a liquid storage facility already exists on farm.

² Price was changed to 2012 US dollar.

³ For capacity equivalent to the amount of biogas arising from 200 cows.

⁴ Same price as REF system; see Table S13.

⁵ This cost includes engineering and contingencies, 15% of total direct capital, and working capital, 25% of net operating cost (Table S17).

⁶ This cost is different from the cost for 100 cows because there is less dairy manure for land application after anaerobic digestion (equivalent to 94 cows after anaerobic digestion)..

Table S15. Initial outlays for the OPS scenario.

Item	Unit Price (\$)	Total Price (\$/FU)	References
Algae Cultivation System		291,557 ¹	
<i>Infrastructure and equipment</i>	56,604/ha	194,371	<i>Resurreccion et al.</i>
<i>Miscellanea (start-up, engineering, etc.)</i>	28,302/ha	97,186	<i>Resurreccion et al.</i>
Energy Generation System		283,430	
<i>Algae homogenizer</i>	24,500 ²	24,500	
<i>Digester tank</i>	68,200 per 100 cows	77,468 ⁶	<i>Goodrich, 2005</i>
<i>Screw press</i>	22,400 ³	22,400	<i>Moller et al., 2000</i>
<i>Boilers and heat exchangers</i>	8,267 per 100 cows	9,390 ⁶	<i>Goodrich, 2005</i>
<i>Gas recirculation pump</i>	4,133 per 100 cows	4,695 ⁶	<i>Goodrich, 2005</i>
<i>Liquid storage facilities</i>	NA ⁴	NA	
<i>Micro-turbine</i>	75,000 ⁵	75,000	<i>Goodrich, 2005</i>
<i>Building cost</i>	20,667 per 100 cows	23,475 ⁶	<i>Goodrich, 2005</i>
<i>Miscellanea (engineering, etc.)</i>	40,417 per 100 cows	46,502 ⁷	<i>Goodrich, 2005;</i> <i>Benemann and Oswald,</i> <i>1996; Pizarro et al., 2006</i>
Total Initial Outlay – OPS		574,987	

¹Direct land use for OPS system sized to produce one FU per year is 4.7 ha. For OPS systems, FU corresponds to 165 cow-equivalents worth of digestion capacity to accommodate digestion of both manure and algae.

²Price corresponds to ultra-high pressure homogenizer (12,000 psi, 400 L/h) See Dairy Engineering (Nov 2011).

³ Price was changed to 2012 US dollar.

⁴ Assumes that on-farm liquid storage facilities already exist.

⁵For capacity equivalent to the amount of biogas arising from 200 cows.

⁶Based on use of linear regression models (Figure S6 below) for farm-sizes between 100 and 300 cows (Goodrich, 2005), assuming 165 “cow-equivalents” for the OPS scenario.

⁷ This cost includes engineering and contingencies, 15% of total direct capital, and working capital, 25% of net operating cost (Table S17).

Figure S6: Regression models for energy generation system based on Goodrich (2005).

Table S16. Initial outlays for the ATS scenario.

Item	Unit Price (\$)	Total Price (\$/FU)	References
Algae cultivation system		307,302 ¹	
<i>ATS screen</i>	6,090/ha	15,617	<i>Pizarro et al, 2006</i>
<i>Algae harvesting equipment</i>	7,000/ha	17,950	<i>Pizarro et al, 2006</i>
<i>Electrical supply and distribution</i>	3,000/ha	7,693	<i>Pizarro et al, 2006</i>
<i>HDPE liner and installation</i>	33,000/ha	84,623	<i>Pizarro et al, 2006</i>
<i>Instrumentation and machinery</i>	500/ha	1,282	<i>Pizarro et al, 2006</i>
<i>Pump</i>	8,455/ha	21,681	<i>Pizarro et al, 2006</i>
<i>Roads, drainage</i>	7,000/ha	17,950	<i>Pizarro et al, 2006</i>
<i>Site preparation, grading, and compaction</i>	34,000/ha	87,187	<i>Pizarro et al, 2006</i>
<i>Miscellanea</i>		53,319 ⁶	<i>Pizarro et al, 2006</i> <i>Benemann & Oswald 1996</i>
Energy generation system		288,120	
<i>Algae homogenizer</i>	24,500 ²	24,500	
<i>Digester tank</i>	68,200 per 100 cows	79,994 ⁷	<i>Goodrich, 2005</i>
<i>Screw press</i>	22,400 ³	22,400	<i>Moller et al., 2000</i>
<i>Boilers and heat exchangers</i>	8,267 per 100 cows	9,696 ⁷	<i>Goodrich, 2005</i>
<i>Gas recirculation pump</i>	4,133 per 100 cows	4,848 ⁷	<i>Goodrich, 2005</i>
<i>Liquid storage facilities</i>	NA ⁴	NA	
<i>Micro-turbine</i>	75,000 ⁵	75,000	<i>Goodrich, 2005</i>
<i>Building cost</i>	20,667 per 100 cows	24,241 ⁷	<i>Goodrich, 2005</i>
<i>Miscellanea (engineering, etc).</i>	40,417 per100 cows	47,441 ⁸	<i>Goodrich, 2005;</i> <i>Pizarro et al., 2006</i>
Total Initial Outlay – ATS		595,421	

¹ Direct land use for ATS system sized to produce one FU per year is 3 ha. For ATS systems, FU corresponds to 170 cow-equivalents worth of digestion capacity to accommodate digestion of both manure and algae.

² Price for ultra-high pressure homogenizer (12,000 psi, 400 L/h) See Dairy Engineering Company (2011).

³ Price was changed to 2012 US dollar.

⁴ Assumes that on-farm liquid storage facilities already exist.

⁵ For capacity equivalent to the amount of biogas arising from 200 cows.

⁶ Includes engineering and contingencies, 15% of total direct capital, and working capital, 25% of net operating cost (Table S17).

⁷ Based on use of linear regression models (Figure S6) for farm-sizes between 100 and 300 cows (Goodrich, 2005), assuming 170 “cow-equivalents” for the ATS scenario.

⁸ Includes engineering and contingencies, 15% of total direct capital, and working capital, 25% of net operating cost (Table S17).

7.2 Annual Operational Cost

Annual operational costs include: power (electricity and fuel), labor, capital, insurance, systems maintenance, etc. Electricity cost (\$0.097/kWh) was based on an EIA report (2011). Labor and overhead were 10% of total capital cost, based on Benemann & Oswald (1996). Insurance, maintenance, reports, and other costs were taken as 5% of total capital cost (Benemann & Oswald, 1996). Table S17 summarizes these quantities.

Table S17. Net annual operational costs (per FU) for the four evaluated scenarios.

Cost Item	REF, \$	AD, \$	OPS, \$	ATS, \$
Manure land application system	9,200	8,631		
<i>Direct supply (electricity, fuel, fertilizer)</i>	4,100	3,846		
<i>Labor and overhead</i> ¹	NA ³	NA ³		
<i>Insurance, maintenance, reports, etc</i> ²	5100	4,785		
Algae cultivation system			50,984	60,884
<i>Direct supply (electricity, fuel, fertilizer)</i>			7,251	22,787
<i>Labor and overhead</i> ¹			29,156	25,398
<i>Insurance, maintenance, reports, etc</i> ²			14,578	12,699
Anaerobic digestion system		32,109	43,851	45,355
<i>Direct supply (electricity, fuel, fertilizer)</i>		2,309	8,312	9,253
<i>Labor and overhead</i> ¹		19,867	23,693	24,068
<i>Insurance, maintenance, reports, etc</i> ²		9,933	11,846	12,034
Total Net Operating Cost (\$/FU)	9,200	40,741	94,835	106,239

¹ This value is 10% of total direct capital cost (Benemann & Oswald, 1996).

² This value is 5% of total capital cost (Benemann & Oswald, 1996).

³ "Direct supply" includes labor and overhead cost, based on Feinerman (2004).

7.3 Annual Revenues

Two approaches were required to compute annual revenues for REF versus AD, OPS, and ATS. This is because the two systems produced different sets of sellable products. Table S18 summarizes annual revenues for each of the four evaluated scenarios.

For the REF scenario, annual revenues were derived only from the sale of corn produced on manure-applied lands. The value of this corn was assigned to the following triangular distribution: minimum = \$198/Mg, maximum = \$278/Mg, likeliest = \$234/Mg (MSU, 2011). For the AD, OPS, and ATS systems, it was assumed that revenues are derived from: the sale of corn (REF and AD), sale of methane-derived bioelectricity back to the grid, sale of nutrient credits, sale of carbon (CO₂) credits, and sale of solid digestate as soil amendment. It was assumed that bioelectricity is sold back to the US grid for less than the retail price (\$0.058/kWh sale price vs. \$0.097/kWh purchase price) (EIA, 2011). Nutrient credit were accounted for N and P loading reduction compared to 80% of nutrient loading in scenario REF. Figure S7 illustrates the computation of nutrient credit (nitrogen) for scenario AD, OPS, and ATS. Nitrogen credits were assigned to a triangular distribution: minimum = \$8/lb N, maximum = \$50/lb N, likeliest = \$20/lb N (Jones et al., 2010). Phosphorus credits were assigned to a uniform distribution over the range \$11-15/kg P (Greenhalgh and Sauer, 2003:). Carbon credits were assigned a value of

minimum, \$0.001\$/kg CO₂, maximum, \$0.03/kg CO₂, most likeliest \$0.005/ kg CO₂ (Chicago Climate Change 2011; Nordhaus 2008). Finally, the value of soil amendment was assumed to be \$7.9-15.8/Mg (uniform distribution) (Waste and Resources Action Program, Feb 2009).

Figure S7: Nitrogen credit illustration for improved scenarios (AD, OPS, ATS).

Table S18. Annual revenues (per FU) for the four evaluated scenarios.

Item	Scenario REF	Scenario AD	Scenario OPS	Scenario ATS
Sale of corn	12,637	5,321		
Sale of bioelectricity (surplus)		16,827	26,780	29,037
Sale of nutrients credits (N)		26,662	271,742	271,742
Sale of nutrient credits (P)		61	123	123
Sale of carbon credits (CO ₂)		1,269	1,849	2,389
Sale of digestate		1,844	2,748	3,012
Total Revenue (\$/FU)	12,637	51,985	303,242	306,303

7.4 Assessing Financial Feasibility

Net present value (NPV) was used to as metric to assess the financial feasibility of each system. Based on standard practice, NPV values greater than zero are indicative of a profitable project. Discount rate was assumed to be a triangular distribution: minimum = 5%, maximum = 15%, likeliest = 10% (Adey et al., 2011; Amer et al., 2011; Campbell et al., 2011; Davis et al., 2011; Fischer et al., 2011; Gallagher, 2011; Garafolo, 2011; Zamalloa et al., 2011). Tax rate was 23.6%. Project lifetime was 20 years. Investment depreciation was computed by using seven years depreciation schedule under the Modified Accelerated Cost Recovery System (MACRS) (Department of The Treasury). Table S19-22 summarizes 20 yrs cash flows for each scenario.

Table S19: 20 years cash flows for scenario REF

Cash flows	Years								
	1	2	3	4	5	6	7	8	9-20
Initial outlay	10,200								
Depreciation base ¹	10,200								
Revenue	12,637	12,637	12,637	12,637	12,637	12,637	12,637	12,637	12,637
- Operating cost	9,200	9,200	9,200	9,200	9,200	9,200	9,200	9,200	9,200
- Depreciation	14,576	24,980	17,840	12,740	9,109	9,098	9,109	4,549	-
7 yrs MACRS depreciation	14.29%	24.49%	17.49%	12.49%	8.93%	8.92%	8.93%	4.46%	-
Taxable income	-11,139	-21,543	-14,403	-9,303	-5,672	-5,662	-5,672	-1,112	3,437
- Taxes	-2,629	-5,084	-3,399	-2,196	-1,339	-1,336	-1,339	-263	811
Aftertax income	-8,510	16,459	11,004	-7,108	-4,333	-4,325	-4,333	-850	2,626
+ Depreciation	14,576	24,980	17,840	12,740	9,109	9,098	9,109	4,549	-
Cash flow	6,066	8,521	6,836	5,632	4,775	4,773	4,775	3,699	2,626
NPV	-62,279								

¹ Depreciation base is the initial outlay excluding miscellaneous cost (working and engineering capital).

Table S20: 20 years cash flows for scenario AD

Cash flows	Years								
	1	2	3	4	5	6	7	8	9-20
Initial outlay	334,349								
Depreciation base ¹	294,363								
Revenue	51,985	51,985	51,985	51,985	51,985	51,985	51,985	51,985	51,985
- Operating cost	40,741	40,741	40,741	40,741	40,741	40,741	40,741	40,741	40,741
- Depreciation	42,065	72,090	51,484	36,766	26,287	26,257	26,287	13,129	-
7 yrs MACRS depreciation	14.29%	24.49%	17.49%	12.49%	8.93%	8.92%	8.93%	4.46%	0.00%
Taxable income	-30,820	-60,845	-40,240	-25,522	-15,042	-15,013	-15,042	-1,884	11,244
- Taxes	-7274	-14360	-9497	-6023	-3550	-3543	-3550	-445	2654
Aftertax income	-23,547	-46,486	-30,743	-19,499	-11,492	-11,470	-11,492	-1,440	8,591
+ Depreciation	42,065	72,090	51,484	36,766	26,287	26,257	26,287	13,129	-
Cash flow	18,518	25,604	20,741	17,267	14,794	14,787	14,794	11,689	8,591
NPV	-211,093								

¹ Depreciation base is the initial outlay excluding miscellaneous cost (working and engineering capital).

Table S21: 20 years cash flows for scenario OPS

Cash flows	Years								
	1	2	3	4	5	6	7	8	9-20
Initial outlay	574,987								
Depreciation base ¹	431,300								
Revenue	303,242	303,242	303,242	303,242	303,242	303,242	303,242	303,242	303,242
- Operating cost	94,835	94,835	94,835	94,835	94,835	94,835	94,835	94,835	94,835
- Depreciation	61,633	105,625	75,434	53,869	38,515	38,472	38,515	19,236	-
7 yrs MACRS depreciation	14.29%	24.49%	17.49%	12.49%	8.93%	8.92%	8.93%	4.46%	0.00%
Taxable income	85,141	-2,844	57,538	100,668	131,377	131,463	131,377	169,935	208,407
- Taxes	20,093	-671	13,579	23,758	31,005	31,025	31,005	40,105	49,184
Aftertax income	65,048	-2,173	43,959	76,910	100,372	100,438	100,372	129,830	159,223
+ Depreciation	61,633	105,625	75,434	53,869	38,515	38,472	38,515	19,236	-
Cash flow	126,681	103,453	119,393	130,780	138,887	138,910	138,887	149,066	159,223
NPV	853,999								

¹ Depreciation base is the initial outlay excluding miscellaneous cost (working and engineering capital).

Table S22: 20 years cash flows for scenario ATS

Cash flows	Years								
	1	2	3	4	5	6	7	8	9-20
Initial outlay	595,421								
Depreciation base ¹	494,662								
Revenue	306,303	306,303	306,303	306,303	306,303	306,303	306,303	306,303	306,303
- Operating cost	106,239	106,239	106,239	106,239	106,239	106,239	106,239	106,239	106,239
- Depreciation	70,687	121,143	86,516	61,783	44,173	44,124	44,173	22,062	-
7 yrs MACRS depreciation	14.29%	24.49%	17.49%	12.49%	8.93%	8.92%	8.93%	4.46%	0.00%
Taxable income	129,376	78,921	113,547	138,280	155,890	155,940	155,890	178,002	200,064
- Taxes	30,533	18,625	26,797	32,634	36,790	36,802	36,790	42,008	47,215
Aftertax income	98,844	60,296	86,750	105,646	119,100	119,138	119,100	135,993	152,849
+ Depreciation	70,687	121,143	86,516	61,783	44,173	44,124	44,173	22,062	-
Cash flow	169,531	181,438	173,266	167,429	163,274	163,262	163,274	158,055	152,849
NPV	790,087								

¹ Depreciation base is the initial outlay excluding miscellaneous cost (working and engineering capital).

The overall NPV is \$-62,279, \$-211,093, \$853,999, and \$790,087 for scenario REF, AD, OPS, and ATS respectively. Figure S8 depicts the relationship between NPV and nutrient credit price for scenario AD, OPS, and ATS.

Figure S8: Net present value versus nutrient credit price.

7.5 Sensitivity Analysis of NPV

Sensitivity analysis was performed to understand what input parameters most directly impact NPV. Table S23 summarizes the top three most impactful factors affecting NPV result for each modeled manure waste management strategy, when all inputs were subjected to a standard perturbation ($\pm 10\%$).

Table S23: Sensitivity analysis of NPV for each scenario – top three most impactful inputs.

Rank	Scenario REF	Scenario AD	Scenario OPS	Scenario ATS
1	NH ₃ -N loss factor	N credit price	N credit price	N credit price
2	Manure land application cost	Discount Rate	Discount Rate	Discount Rate
3	Discount rate	N fraction in solid digestate	N fraction in solid digestate	Algae N content

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Appendix B: Medium Used for *Scenedesmus dimorphus* Cultivation

B.1 Proteose-Peptide Medium

1). Add proteose-peptone to Bristol Medium.

*For 1.5% agar medium, add 15 g of agar into the flask; do not mix.

2). Cover and autoclave medium.

B.2 Bristol Medium

H.C. Bold's modification of Bristol's recipe (Bold 1949). General purpose freshwater medium and as Bristol's solution, an essential component of other media.

1). To approximately 900 mL of dH₂O add each of the components in the order specified while stirring continuously.

2). Bring total volume to 1 L with dH₂O.

*For 1.5% agar medium, add 15 g of agar into the flask; do not mix.

3). Cover and autoclave medium.

4). Store at refrigerator temperature.

#	Component	Amount	Stock Solution Concentration	Final Concentration
1	NaNO ₃ (Fisher BP360-500)	10 mL/L	10 g/400mL dH ₂ O	2.94 mM
2	CaCl ₂ ·2H ₂ O (Sigma C-3881)	10 mL/L	1 g/400mL dH ₂ O	0.17 mM
3	MgSO ₄ ·7H ₂ O (Sigma 230391)	10 mL/L	3 g/400mL dH ₂ O	0.3 mM
4	K ₂ HPO ₄ (Sigma P 3786)	10 mL/L	3 g/400mL dH ₂ O	0.43 mM
5	KH ₂ PO ₄ (Sigma P 0662)	10 mL/L	7 g/400mL dH ₂ O	1.29 mM
6	NaCl (Fisher S271-500)	10 mL/L	1 g/400mL dH ₂ O	0.43 mM

B. 3 Modified Bold 3N Medium

Modification of Bold's recipe. General purpose freshwater medium used for axenic cultures, especially blue-greens and reds.

1). To approximately 850 mL of dH₂O, add each of the components in the order specified

(except vitamins) while stirring continuously.

2). Bring the total volume to 1 L with dH₂O.

*For 1.5% agar medium, add 15 g of agar into the flask; do not mix.

3). Cover and autoclave medium.

4). When cooled add vitamins.

*For agar medium, add vitamins, mix, and dispense before agar solidifies.

5). Store at refrigerator temperature.

#	Component	Amount	Stock Solution Concentration	Final Concentration
1	NaNO ₃ (Fisher BP360-500)	30 mL/L	10 g/400mL dH ₂ O	8.82 mM
2	CaCl ₂ ·2H ₂ O (Sigma C-3881)	10 mL/L	1 g/400mL dH ₂ O	0.17 mM
3	MgSO ₄ ·7H ₂ O (Sigma 230391)	10 mL/L	3 g/400mL dH ₂ O	0.3 mM
4	K ₂ HPO ₄ (Sigma P 3786)	10 mL/L	3 g/400mL dH ₂ O	0.43 mM
5	KH ₂ PO ₄ (Sigma P 0662)	10 mL/L	7 g/400mL dH ₂ O	1.29 mM
6	NaCl (Fisher S271-500)	10 mL/L	1 g/400mL dH ₂ O	0.43 mM
7	<u>P-IV Metal Solution</u>	6 mL/L		
8	<u>Soilwater: GR+ Medium</u>	40 mL/L		
9	<u>Vitamin B₁₂</u>	1 mL/L		
10	<u>Biotin Vitamin Solution</u>	1 mL/L		
11	<u>Thiamine Vitamin Solution</u>	1 mL/L		

B.4 P-IV Metal Solution

1). To approximately 950 mL of dH₂O, add the nutrients in the order listed while stirring continuously.

Note: The Na₂EDTA should be fully dissolved before adding other components.

2). Bring total volume to 1 L with dH₂O.

3). Store at refrigerator temperature.

#	Component	Amount	Stock Solution Concentration	Final Concentration
1	Na ₂ EDTA·2H ₂ O (Sigma ED255)	0.75 g/L		2 mM
2	FeCl ₃ ·6H ₂ O (Sigma 1513)	0.097 g/L		0.36 mM
3	MnCl ₂ ·4H ₂ O (Baker 2540)	0.041 g/L		0.21 mM
4	ZnCl ₂ (Sigma Z-0152)	0.005 g/L		0.037 mM
5	CoCl ₂ ·6H ₂ O (Sigma C-3169)	0.002 g/L		0.0084 mM
6	Na ₂ MoO ₄ ·2H ₂ O (J.T. Baker 3764)	0.004 g/L		0.017 mM

Note: Final concentration listed is for the stock solution.

B.5 Soil Water: GR+ Medium

The basic garden-type soilwater; includes a pinch of CaCO₃, which is added to the soil and water prior to steaming; suitable for most phototrophic freshwater algae.

1). Combine all components listed.

2). Cover the medium container and steam for 2 consecutive days, 3 hours on each day. Pasteurization is a gradual rising of temperature to approximately 95°C in 15 minutes. Then increased just over 98°C for the 3 hour duration. Cooling occurs gradually at room temperature.

3). Refrigerate 24 hours or more and bring to room temperature before using.

#	Component	Amount	Stock Solution Concentration	Final Concentration
1	Green House Soil	1 tsp/200 mL dH ₂ O		
2	CaCO ₃ (optional) (Fisher C 64)	1 mg/200 mL dH ₂ O		0.05 mM

Appendix C: Estrogenicity Potential Impact Factor (EsP)

Note: For chemicals that had several reported estrogenicity values from difference references, **bolded text** indicates the normalized average EsP, and *italicized text* indicates the original data.

Chemical	CAS No.		Original Estrogenicity & Unit		Reference	Normalized EsP	
1-(2-Tolyl)biguanide	93-69-6	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
1,1,1,2-Tetrachloroethane	630-20-6	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
1,1,3-Tris(2-methyl-4-hydroxy-5- <i>tert</i> -butylphenyl)butane	1843-03-4	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
1,2,3-Trichlorobenzene	87-61-6	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
1,2,3-Trichloropropane	96-18-4	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
1,2,3-Trimethylbenzene	526-73-8	>	4.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	7.50E-08
1,2,4,5-Tetramethylbenzene	95-93-2	>	4.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	7.50E-08
1,2,4-Trichlorobenzene	120-82-1	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
1,2,4-Trimethylbenzene	95-63-6	>	4.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	7.50E-08
1,2-benzanthraquinone	2498-66-0	<	1.00E-06	REP ²	Hayakawa et al 2011	<	1.00E-06
1,2-chrysenequinone			5.00E-05	REP ²	Hayakawa et al 2011		5.00E-05
1,2-Dibromo-3-chloropropane	96-12-8	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
1,2-Dibromoethane	106-93-4	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
1,2-Dichlorobenzene	95-50-1	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
1,2-Diethylbenzene	135-01-3	>	4.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	7.50E-08
1,2-Dimethylnaphthalene	573-98-8	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
1,2-Dinitrobenzene	528-29-0	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
1,2-Epoxyethylbenzene	96-09-3					<	3.20E-07

		>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
		>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
1,2-naphthoquinone	524-42-5	<	1.00E-06	REP ²	Hayakawa et al 2011	<	1.00E-06
1,3,5-Triethyltoluene		>	4.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	7.50E-08
1,3,5-Trimethyl-2,4,6-tris(3,5-di- <i>tert</i> -butyl-4-hydroxybenzyl) benzene	1709-70-2	>	1.00E-04	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-06
1,3,5-Trimethylbenzene	108-67-8	>	4.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	7.50E-08
1,3,5-Triphenylcyclohexane	28336-57-4	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
1,3,5-Tris(3,5-di- <i>tert</i> -butyl-4-hydroxybenzyl)-s-triazine-2,4,6-(1 <i>H</i> ,3 <i>H</i> ,5 <i>H</i>) trione	27676-62-6	>	1.00E-04	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-06
1,3,5-Tris(4- <i>tert</i> -butyl-3-hydroxy-2,6-dimethylbenzyl)-1,3,5-triazine-2,4,6-(1 <i>H</i> ,3 <i>H</i> ,5 <i>H</i>) trione	40601-76-1	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
1,3,5-tri- <i>tert</i> -butylbenzene	1460-02-2	>	1.00E-04	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-06
1,3-Dichloro-2-propanol	96-23-1	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
1,3-Dichloropropene, mixture	542-75-6	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
1,3-Dimethylbenzene < <i>m</i> -Xylene>	108-38-3	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
1,3-Diphenylguanidine	102-06-7	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
1,3-Diphenylpropane	1081-75-0					<	3.20E-07
		>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
		>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
1,4-anthraquinone	635-12-1	<	1.00E-06	REP ²	Hayakawa et al 2011	<	1.00E-06
1,4-Benzoquinone dioxime	105-11-3	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07

1,4-chrysenequinone	100900-16-1	<	1.00E-06	REP ²	Hayakawa et al 2011	<	1.00E-06
1,4-Dichlorobenzene	106-46-7	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
1,4-Dichlorobenzene	106-46-7	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
1,4-Diethylbenzene	105-05-5					<	2.08E-07
		>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
		>	4.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	7.50E-08
1,4-Dioxane	123-91-1	>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-05
1,4-phenanthrenequinone	569-15-3	<	1.00E-06	REP ²	Hayakawa et al 2011	<	3.00E-04
1,6-Dinitropyrene	42397-64-8	>	1.00E-06	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-04
1,8-Dimethylnaphthalene	569-41-5	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
1,8-Dinitropyrene	42397-65-9	>	1.00E-06	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-04
10-hydroxybenz[a]anthracene	69884-53-3		3.20E-03	REP	Hayakawa et al 2007		3.20E-03
10-hydroxybenzo[a]pyrene	56892-31-0					<	5.15E-05
		<	1.00E-04	REP	Hayakawa et al 2007	<	1.00E-04
		>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
10-hydroxybenzo[b]fluoranthene		<	1.00E-04	REP	Hayakawa et al 2007	<	1.00E-04
10-hydroxybenzo[e]pyrene		<	1.00E-04	REP	Hayakawa et al 2007	<	1.00E-04
11H-benzo[a]fluoren-11-one	479-79-8	<	1.00E-06	REP ²	Hayakawa et al 2011	<	1.00E-06
11H-benzo[b]fluoren-11-one	3074031	<	1.00E-06	REP ²	Hayakawa et al 2011	<	1.00E-06
11-hydroxybenz[a]anthracene		<	1.00E-04	REP	Hayakawa et al 2007	<	1.00E-04
11-hydroxybenzo[a]pyrene	56892-32-1					<	5.15E-05
		<	1.00E-04	REP	Hayakawa et al 2007	<	1.00E-04
		>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06

11-hydroxybenzo[b]fluoranthene	<	1.00E-04	REP	Hayakawa et al 2007	<	1.00E-04
11-hydroxybenzo[g]chrysene	<	1.00E-04	REP	Hayakawa et al 2007	<	1.00E-04
12-hydroxybenzo[a]pyrene	56892-33-2				<	5.15E-05
	<	1.00E-04	REP	Hayakawa et al 2007	<	1.00E-04
	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
12-hydroxybenzo[b]fluoranthene		1.00E-04	REP	Hayakawa et al 2007		1.00E-04
13-hydroxybenzo[g]chrysene	<	1.00E-04	REP	Hayakawa et al 2007	<	1.00E-04
17α-Estradiol	57-91-0					4.58E-02
		4.00E-09	REC ₁₀ (M) ¹	Nishihara et al 2000		7.50E-02
		1.00E-02	RA _{E2}	Kawagoshi et al 2002		1.00E-02
		5.25	RP ¹	Coldham et al 1997		5.25E-02
17α-Ethynylestradiol	57-63-6					1.02E+00
		2.00E-10	REC ₁₀ (M) ¹	Nishihara et al 2000		1.50E+00
		7.00E-01	RA _{E2}	Kawagoshi et al 2002		7.00E-01
		88.8	RP ¹	Coldham et al 1997		8.88E-01
		100	RIE	Fang et al 2000		1.00E+00
17β-Estradiol	50-28-2					1.00E+00
		3.00E-10	REC ₁₀ (M) ¹	Nishihara et al 2000		1.00E+00
		3.40E-10	REC ₁₀ (M) ⁴	Kawamura et al 2003		1.00E+00
		3.40E-10	REC ₁₀ (M) ³	Ogawa et al 2005		1.00E+00
		1.00	PR	Gaido et al 1996		1.00E+00
		1	RA _{E2}	Kawagoshi et al 2002		1.00E+00
		100	RP ¹	Coldham et al 1997		1.00E+00
		100	RIE	Fang et al 2000		1.00E+00

17β-Estradiol-3(β-D-glucuronide)			0.32	RP ¹	Coldham et al 1997	3.20E-03
17β-Estradiol-3-glucuronide-17-sulfate			0	RP ¹	Coldham et al 1997	0.00E+00
17β-Estradiol-3-sulfate	481-96-9		0.01	RP ¹	Coldham et al 1997	1.00E-04
1a-Phenyl-4a-(1'-phenylethyl)tetralin		>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
1a-Phenyl-4e-(1'-phenylethyl)tetralin		>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
1-Butanol	71-36-3	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
1-Chloro-2,4-dinitrobenzene	97-00-7	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
1-Chloro-2-nitrobenzene	88-73-3	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
1e-Phenyl-4a-(1'-phenylethyl)tetralin		>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
1e-Phenyl-4e-(1'-phenylethyl)tetralin		>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
1-hydroxy-9-fluorenone	6344-60-1	<	1.00E-06	REP ²	Hayakawa et al 2011	< 1.00E-06
1-hydroxybenz[a]anthracene	69847-26-3	<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
1-hydroxybenzo[a]pyrene	13345-23-8	<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
1-hydroxybenzo[b]fluoranthene		<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
1-hydroxybenzo[c]phenanthrene		<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
1-hydroxychrysene	63019-38-5		4.20E-04	REP	Hayakawa et al 2007	4.20E-04
1-hydroxypyrene	5315-79-7					1.20E-04
			2.40E-04	REP	Hayakawa et al 2007	2.40E-04
		>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
1-Methylnaphthalene	90-12-0	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
1-Naphthol	90-15-3					1.00E-06
			1.00E-06	RA _{E2}	Kawagoshi et al 2002	1.00E-06
		<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04

1-Nitropyrene	5522-43-0	>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-05
1-Nonanol	143-08-8	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
1-Tridecanol	112-70-9	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
2-(2'-Hydroxy-3',5'-di- <i>tert</i> -amylphenyl) benzotriazole	25973-55-1	>	1.00E-04	REC ₁₀ (M) ⁴	Kawamura et al 2003	<	3.40E-06
2-(2'-Hydroxy-3',5'-di- <i>tert</i> -butylphenyl)-5-chlorobenzotriazole	3864-99-1	>	1.00E-04	REC ₁₀ (M) ⁴	Kawamura et al 2003	<	3.40E-06
2-(2'-Hydroxy-3'-<i>tert</i>-butyl-5'-methylphenyl)-5-chlorobenzotriazole	3896115					<	3.40E-06
		>	1.00E-04	REC ₁₀ (M) ⁴	Kawamura et al 2003	<	3.40E-06
		>	1.00E-04	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-06
2-(2'-Hydroxy-5'-methylphenyl) benzotriazole	2440-22-4					<	3.40E-07
		>	1.00E-03	REC ₁₀ (M) ⁴	Kawamura et al 2003	<	3.40E-07
		>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
2-(4-Morpholinodithio)benzothiazole	95-32-9	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
2-(Morpholinothio)benzothiazole	102-77-2	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
2-(Phenylmethyl)phenol < <i>o</i> -Benzylphenol> [phenolic resin]	28994-41-4	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
2,2',2''-Nitrilotriethanol	102-71-6	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000		3.00E-07
2,2',4,4'-Tetrahydroxybenzophenone	131-55-5		1.40E-05	REC ₁₀ (M) ⁴	Kawamura et al 2003		2.14E-05
2,2,4-Trimethyl-1,3-pentanediol diisobutyrate	6846-50-0	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
2,2-Bis(4-hydroxy-3-methylphenyl)propane	79-97-0		3.00E-06	REC ₁₀ (M) ¹	Nishihara et al 2000		1.00E-04
2,2-Bis(4-hydroxy-phenyl)butane	77-40-7		3.00E-06	REC ₁₀ (M) ¹	Nishihara et al 2000		1.00E-04

2,2-bis[4-(2-hydroxy-3-methacryloxypropoxy)phenyl]propane (BisGMA)	1565-94-2	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
2,2-bis[4(methacryloxy)]phenyl propane (BisMEPP)	24448-20-2	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
2,2-bis[4(methacryloxypolyethoxy)phenyl]propane (MPEPP)		>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
2,2'-Dibenzothiazolyl disulfide	120-78-5	>	1.00E-04	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-06
2,2'-Dihydroxy-4,4'-dimethoxybenzophenone	131-54-4	>	1.00E-03	REC ₁₀ (M) ⁴	Kawamura et al 2003	<	3.40E-07
2,2'-Dihydroxy-4-methoxybenzophenone	131-53-3						3.40E-07
<i>2,2'-Dihydroxy-4-methoxybenzophenone</i>	<i>131-53-3</i>		<i>1.00E-03</i>	<i>REC₁₀ (M)⁴</i>	<i>Kawamura et al 2003</i>		<i>3.40E-07</i>
<i>2,2'-Dihydroxy-4-methoxybenzophenone</i>	<i>131-53-3</i>		<i>1.00E-03</i>	<i>REC₁₀ (M)³</i>	<i>Ogawa et al 2005</i>		<i>3.40E-07</i>
2,2'-Dihydroxybenzophenone	835-11-0	>	1.00E-03	REC ₁₀ (M) ⁴	Kawamura et al 2003	<	3.40E-07
2,2'-Dihydroxybiphenyl	1806-29-7	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
2,2'-Ethylidenebis(4,6-di- <i>tert</i> -butylphenol)	35958-30-6	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
2,2'-Methylenebis (4-ethyl-6- <i>tert</i> -butylphenol)	88-24-4	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
2,2'-Methylenebis (6- <i>tert</i> -butyl-4-methylphenol)	119-47-1	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
2,2'-Methylenebis(4-methyl-6-methylcyclohexylphenol)	77-62-3	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
2,2'-Oxamidobis[ethyl-3-(3,5-di- <i>tert</i> -butyl-4-hydroxyphenyl) propionate]	70331-94-1	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
2,3,4,4'-Tetrahydroxybenzophenone	31127-54-5		3.60E-05	REC ₁₀ (M) ⁴	Kawamura et al 2003		9.44E-06

2,3',4,4'-Tetrahydroxybenzophenone	61445-50-9		2.40E-04	REC ₁₀ (M) ⁴	Kawamura et al 2003	1.42E-06
2,3,4,5-TCB-4'-ol			77	RIE	Fang et al 2000	7.70E-01
2',3',4',5'-Tetrachloro-4-biphenylol	67651-34-7		0.82	RP ¹	Coldham et al 1997	8.20E-01
2,3,4-Trihydroxybenzophenone	1143-72-2		9.00E-06	REC ₁₀ (M) ⁴	Kawamura et al 2003	3.78E-05
2,3,6-Trimethylphenol	2416-94-6		3.00E-07	RA _{E2}	Kawagoshi et al 2002	3.00E-07
2,3,7,8-Tetrachlorodibenzo- <i>p</i> -dioxin	1746-01-6		0.26	RP ¹	Coldham et al 1997	2.60E-01
2,3-Xylenol	526-75-0		9.00E-07	RA _{E2}	Kawagoshi et al 2002	9.00E-07
2,4,4'-Trihydroxybenzophenone	1470-79-7		1.80E-05	REC ₁₀ (M) ⁴	Kawamura et al 2003	1.89E-05
2,4,5-Trichlorophenol	95-95-4	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
2,4,5-Trichlorophenoxyacetic acid	93-76-5	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
2,4,6-TCB-4'-ol			67.6	RIE	Fang et al 2000	6.76E-01
2,4,6-Tribromophenol	118-79-6	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
2',4',6'-Trichloro-4-biphenylol	14962-28-8					4.63E-03
2',4',6'-Trichloro-4-biphenylol	14962-28-8		4.00E-07	REC ₁₀ (M) ¹	Nishihara et al 2000	7.50E-04
2',4',6'-Trichloro-4-biphenylol	14962-28-8		1	RP ¹	Coldham et al 1997	1.00E-02
2,4,6-Trichlorophenol	88-06-2	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
2,4,6-Triphenyl-1-hexene	18964-53-9	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
2,4-Bis-(<i>n</i> -octylthio)-6-(4-hydroxy-3,5-di- <i>tert</i> -butylanilino)-1,3,5-triazine	991-84-4	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
2,4-Diaminotoluene	95-80-7	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
2,4-Dibromophenol	615-58-7	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
2,4-Dichloroaniline	554-00-7	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
2,4-Dichlorophenol	120-83-2		4.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	7.50E-06

2,4-Dichlorophenoxyacetic acid (2,4-D)	94-75-7	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
2,4-Dihydroxybenzophenone	131-56-6		1.80E-06	REC ₁₀ (M) ⁴	Kawamura et al 2003		1.89E-04
2,4-Dimethylphenol	105-67-9						1.00E-07
2,4-Dimethylphenol	105-67-9		1.00E-07	RA _{E2}	Kawagoshi et al 2002		1.00E-07
2,4-Dimethylphenol	105-67-9	>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-05
2,4-Dinitroaniline	97-02-9	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
2,4-Dinitrophenol	51-28-5	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
2,4-Diphenyl-1-butene		>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
2,4-Diphenyl-4-methyl-1-pentene	6362-80-7		6.60E-05	REC ₁₀ (M) ³	Ogawa et al 2005		5.15E-06
2,4-Di- <i>tert</i> -butylphenol	96-76-4	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
2,4-Di-<i>tert</i>-butylphenyl-3,5-di-<i>tert</i>-butyl-4-hydroxybenzoate	4221-80-1					<	3.40E-07
2,4-Di- <i>tert</i> -butylphenyl-3,5-di- <i>tert</i> -butyl-4-hydroxybenzoate	4221-80-1	>	1.00E-03	REC ₁₀ (M) ⁴	Kawamura et al 2003	<	3.40E-07
2,4-Di- <i>tert</i> -butylphenyl-3,5-di- <i>tert</i> -butyl-4-hydroxybenzoate	4221-80-1	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
2,5-Bis(5'-<i>tert</i>-butyl-2'-benzoxazolyl)thiophene	7128-64-5					<	3.40E-06
2,5-Bis(5'- <i>tert</i> -butyl-2'-benzoxazolyl)thiophene	7128-64-5	>	1.00E-04	REC ₁₀ (M) ⁴	Kawamura et al 2003	<	3.40E-06
2,5-Bis(5'- <i>tert</i> -butyl-2'-benzoxazolyl)thiophene	7128-64-5	>	1.00E-04	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-06
2,5-Bis(<i>tert</i> -butylperoxy)-2,5-dimethylhexane	78-63-7	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07

2,5-DCB-4'-ol			65	RIE	Fang et al 2000		6.50E-01
2',5'-dichloro-4-biphenylol			0.62	RP ¹	Coldham et al 1997		6.20E-01
2,5-Dichloroaniline	95-82-9	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
2,5-Dichlorophenol	583-78-8	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
2,5-Di- <i>tert</i> -amylhydroquinone	79-74-3	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
2,5-Di- <i>tert</i> -butylhydroquinone	88-58-4	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
2,6-Dimethylnapthalene		>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
2,6-Di- <i>tert</i> -butyl-4-ethylphenol	4130-42-1	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
2,6-Di-<i>tert</i>-butyl-4-methylphenol	128-37-0					<	1.67E-06
<i>2,6-Di-tert-butyl-4-methylphenol</i>	<i>128-37-0</i>		0	RP ¹	<i>Coldham et al 1997</i>		<i>0.00E+00</i>
<i>2,6-Di-tert-butyl-4-methylphenol</i>	<i>128-37-0</i>	>	1.00E-04	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	<	3.00E-06
<i>2,6-Di-tert-butyl-4-methylphenol</i>	<i>128-37-0</i>	>	1.00E-03	REC ₁₀ (M) ³	<i>Ogawa et al 2005</i>	<	3.40E-07
2,6-Xylenol	576-26-1		1.00E-07	RA _{E2}	Kawagoshi et al 2002		3.00E-03
2-[2'-Hydroxy-3',5'-bis(α,α-dimethylbenzyl)phenyl]-2H-benzotriazole	70321-86-7					<	3.40E-06
<i>2-[2'-Hydroxy-3',5'-bis(α,α-dimethylbenzyl)phenyl]-2H-benzotriazole</i>	<i>70321-86-7</i>	>	1.00E-04	REC ₁₀ (M) ⁴	<i>Kawamura et al 2003</i>	<	3.40E-06
<i>2-[2'-Hydroxy-3',5'-bis(α,α-dimethylbenzyl)phenyl]-2H-benzotriazole</i>	<i>70321-86-7</i>	>	1.00E-04	REC ₁₀ (M) ³	<i>Ogawa et al 2005</i>	<	3.40E-06
2-Aminoanthracene	613-13-8	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
2-Aminoanthraquinone	117-79-3	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
2-Aminotoluene (<i>o</i> -toluidine)	95-53-4	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
2-Butoxyethyl phthalate		>	4.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	7.50E-08
2-Chloro-1,1,2-trifluoroethyl ethyl ether	310-71-4	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06

2'-Chloro-4-biphenylol			0.0037	RP ¹	Coldham et al 1997	3.70E-03
2-Ethoxyethanol	110-80-5					< 1.65E-06
2-Ethoxyethanol	110-80-5	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
2-Ethoxyethanol	110-80-5	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
2-Ethyltoluene	611-14-3	>	4.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 7.50E-08
2-Hydroxy benzo[a]pyrene	56892-30-9					6.00E-06
2-Hydroxy benzo[a]pyrene	56892-30-9		5.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	6.00E-06
2-Hydroxy benzo[a]pyrene	56892-30-9	<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
2-Hydroxy fluorene			1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	3.00E-06
2-Hydroxy-4-methoxybenzophenone	131-57-7					5.15E-07
2-Hydroxy-4-methoxybenzophenone	131-57-7		6.60E-04	REC ₁₀ (M) ⁴	Kawamura et al 2003	5.15E-07
2-Hydroxy-4-methoxybenzophenone	131-57-7		6.60E-04	REC ₁₀ (M) ³	Ogawa et al 2005	5.15E-07
2-Hydroxy-4-methoxybenzophenone-5-sulfonic acid	4065-45-6	>	1.00E-03	REC ₁₀ (M) ⁴	Kawamura et al 2003	< 3.40E-07
2-Hydroxy-4-n-octyloxybenzophenone	1843-05-6					< 3.40E-07
2-Hydroxy-4-n-octyloxybenzophenone	1843-05-6	>	1.00E-03	REC ₁₀ (M) ⁴	Kawamura et al 2003	< 3.40E-07
2-Hydroxy-4-n-octyloxybenzophenone	1843-05-6	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
2-Hydroxy-5-methylbenzophenone	1470-57-1		1.30E-04	REC ₁₀ (M) ⁴	Kawamura et al 2003	2.62E-06
2-hydroxybenz[a]anthracene		<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
2-hydroxybenzo[b]fluoranthene		<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
2-hydroxybenzo[c]phenanthrene		<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
2-Hydroxybenzophenone	117-99-7		6.20E-04	REC ₁₀ (M) ⁴	Kawamura et al 2003	5.48E-07
2-Hydroxybiphenyl (OPP)	90-43-7	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
2-hydroxychrysene	65945-06-4		4.20E-03	REP	Hayakawa et al 2007	4.20E-03

2-Hydroxydibenzofuran	86-77-1	>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-05
2-Hydroxyethyl methacrylate (HEMA)	868-77-9	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
2-hydroxyfluorene	2443-58-5		5.60E-04	REP	Hayakawa et al 2007	5.60E-04
2-hydroxynaphthalene	135-19-3	<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
2-hydroxyphenanthrene	605-55-0		7.50E-04	REP	Hayakawa et al 2007	7.50E-04
2-Mercaptobenzothiazole	149-30-4					< 1.67E-06
2-Mercaptobenzothiazole	149-30-4	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
2-Mercaptobenzothiazole	149-30-4	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
2-Mercaptoimidazoline	96-45-7	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
2-Methacryloyloxyethyl phenyl phosphate (Phenyl-P)	64716-34-3	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
2-Methyl-1-propanol	78-83-1	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
2-Methyl-6-tert-butylphenol	2219-82-1	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
2-Methylphenol (o-cresol)	95-48-7	>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-05
2-Methylpyridine	109-06-8	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
2-Naphthol	135-19-3		4.00E-06	RA _{E2}	Kawagoshi et al 2002	4.00E-06
2-Nitrofluorene	607-57-8	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
2-Nitrophenol	88-75-5	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
2-Phenylene diamine	95-54-5	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
2-sec-Butylphenol	89-72-5	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
2-tert-Butyl-4-methylphenol	2409-55-4	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
2-tert-Butylphenol	88-18-6	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
3,3',4,4',5-Pentachlorobiphenyl (PCB 126)	57465-28-8	>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-05

3,3',5,5'-TCB-4,4'-diol			83.5	RIE	Fang et al 2000	8.35E-01
3,3',5,5'-Tetrachloro-4,4'-biphenyldiol	13049-13-3		0.016	RP ¹	Coldham et al 1997	1.60E-04
3,3'-Thiodipropionic acid di- <i>n</i> -dodecyl ester <Dilauryl thiodipropionate>	123-28-4	>	1.00E-04	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-06
3,3'-Thiodipropionic acid di- <i>n</i> -octadecyl ester <Distearyl thiodipropionate>	693-36-7	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
3,3'-Thiodipropionic acid di- <i>n</i> -tetradecyl ester <Dimyristyl thiodipropionate>	16545-54-3	>	1.00E-04	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-06
3,4-Dichlorophenol	95-77-2		2.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	1.50E-05
3,4-dihydrobenz[<i>a</i>]anthracen-1[2H]-one	57652-74-1	<	1.00E-06	REP ²	Hayakawa et al 2011	< 1.00E-06
3,4-Xylenol	95-65-8		3.00E-07	RA _{E2}	Kawagoshi et al 2002	3.00E-07
3,5-Dimethylphenol <3-xyleneol>	108-68-9	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
3,8-Dihydroxy-2-chlorodibenzofuran			8.00E-07	REC ₁₀ (M) ¹	Nishihara et al 2000	3.75E-04
3-Aminophenol	591-27-5	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
3-Ethyltoluene	620-14-4	>	4.00E-03	REC₁₀ (M)¹	Nishihara et al 2000	3.00E-05
3-Hydroxy benzo[<i>a</i>]pyrene	13345-21-6					3.00E-05
3-Hydroxy benzo[<i>a</i>]pyrene	13345-21-6		1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	3.00E-05
3-Hydroxy benzo[<i>a</i>]pyrene	13345-21-6	<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
3-Hydroxy-2,8-dichlorodibenzofuran		>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-05
3-hydroxybenz[<i>a</i>]anthracene	4834-35-9		4.20E-03	REP	Hayakawa et al 2007	4.20E-03
3-hydroxybenzo[<i>b</i>]fluoranthene		<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
3-hydroxybenzo[<i>c</i>]phenanthrene		<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
3-hydroxybenzo[<i>j</i>]fluoranthene		<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
3-hydroxybenzo[<i>k</i>]fluoranthene			1.30E-04	REP	Hayakawa et al 2007	1.30E-04

3-Hydroxybenzophenone	13020-57-0		1.00E-05	REC ₁₀ (M) ⁴	Kawamura et al 2003	3.40E-05
3-hydroxychrysene	63019-39-6	<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
3-hydroxydibenz[<i>a,h</i>]anthracene	1421-80-3	<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
3-hydroxyfluoranthene			4.20E-04	REP	Hayakawa et al 2007	4.20E-04
3-hydroxyphenanthrene	605-87-8	<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
3-Methylcholanthrene (MC)	56-49-5	>	2.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.50E-05
3-Nitrofluoranthene	892-21-7	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
3-Nitrophenol	554-84-7	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
3- <i>tert</i> -Butylphenol	585-34-2	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
4-(1-cyclohexyl-2-methylpropan-2-yl)phenol			1.97E-07	REC ₁₀ (M) ²	Shioji et al 2006	1.97E-07
4-(1-cyclohexylpropyl)phenol			3.02E-09	REC ₁₀ (M) ²	Shioji et al 2006	3.02E-09
4-(2,2,4,4-tetramethylpentan-3-yl)phenol			2.36E-08	REC ₁₀ (M) ²	Shioji et al 2006	2.36E-08
4-(2,2-dimethylheptan-3-yl)phenol			3.91E-07	REC ₁₀ (M) ²	Shioji et al 2006	3.91E-07
4-(2,2-dimethylheptan-4-yl)phenol			1.29E-07	REC ₁₀ (M) ²	Shioji et al 2006	1.29E-07
4-(2,3-dimethylheptan-2-yl)phenol			9.29E-07	REC ₁₀ (M) ²	Shioji et al 2006	9.29E-07
4-(2,4,4-trimethylhexan-2-yl)phenol			3.90E-08	REC ₁₀ (M) ²	Shioji et al 2006	3.90E-08
4-(2,4-dimethylheptan-2-yl)phenol			6.69E-07	REC ₁₀ (M) ²	Shioji et al 2006	6.69E-07
4-(2,5,5-trimethylhexan-2-yl)phenol			1.96E-07	REC ₁₀ (M) ²	Shioji et al 2006	1.96E-07
4-(2,5-dimethylheptan-2-yl)phenol			7.44E-07	REC ₁₀ (M) ²	Shioji et al 2006	7.44E-07
4-(2,6-dimethylheptan-2-yl)phenol			2.60E-06	REC ₁₀ (M) ²	Shioji et al 2006	2.60E-06
4-(2,6-dimethylheptan-4-yl)phenol			3.03E-07	REC ₁₀ (M) ²	Shioji et al 2006	3.03E-07
4-(2-cyclohexylpropan-2-yl)phenol			8.06E-09	REC ₁₀ (M) ²	Shioji et al 2006	8.06E-09
4-(2-methylheptan-2-yl)phenol			1.39E-06	REC ₁₀ (M) ²	Shioji et al 2006	1.39E-06
4-(2-methyl-hexan-2-yl)phenol			8.26E-07	REC ₁₀ (M) ²	Shioji et al 2006	8.26E-07

4-(2-methyloctan-2-yl)phenol	30790-78-4		1.61E-06	REC ₁₀ (M) ²	Shioji et al 2006	1.61E-06
4-(3,3,4,4-tetramethylpentan-2-yl)phenol			7.37E-10	REC ₁₀ (M) ²	Shioji et al 2006	7.37E-10
4-(3,3-dimethylpentan-2-yl)phenol			1.41E-08	REC ₁₀ (M) ²	Shioji et al 2006	1.41E-08
4-(3,5,5-trimethylhexan-3-yl)phenol			1.49E-07	REC ₁₀ (M) ²	Shioji et al 2006	1.49E-07
4-(3-ethylheptyl)phenol			5.86E-07	REC ₁₀ (M) ²	Shioji et al 2006	5.86E-07
4-(3-ethylpentyl)phenol			8.86E-08	REC ₁₀ (M) ²	Shioji et al 2006	8.86E-08
4-(3-methyloctan-3-yl)phenol			1.00E-06	REC ₁₀ (M) ²	Shioji et al 2006	1.00E-06
4-(4,4-dimethylpentan-2-yl)phenol			6.18E-08	REC ₁₀ (M) ²	Shioji et al 2006	6.18E-08
4-(4-ethyl-2-methylhexan-2-yl)phenol			1.25E-07	REC ₁₀ (M) ²	Shioji et al 2006	1.25E-07
4-(4-methyloctan-4-yl)phenol			1.41E-06	REC ₁₀ (M) ²	Shioji et al 2006	1.41E-06
4-(5-ethylheptan-3-yl)phenol			1.21E-07	REC ₁₀ (M) ²	Shioji et al 2006	1.21E-07
4-(branched)-Nonylphenol	84852-15-3		2.00E-07	REC ₁₀ (M) ¹	Nishihara et al 2000	1.50E-03
4-(nonan-2-yl)phenol			1.36E-06	REC ₁₀ (M) ²	Shioji et al 2006	1.36E-06
4-(nonan-3-yl)phenol			1.12E-06	REC ₁₀ (M) ²	Shioji et al 2006	1.12E-06
4-(nonan-4-yl)phenol			7.81E-07	REC ₁₀ (M) ²	Shioji et al 2006	7.81E-07
4-(nonan-5-yl)phenol			1.02E-06	REC ₁₀ (M) ²	Shioji et al 2006	1.02E-06
4-(pentan-2-yl)phenol			1.13E-06	REC ₁₀ (M) ²	Shioji et al 2006	1.13E-06
4,4'-Butylidenebis(3-methyl-6- <i>tert</i> -butylphenol)	85-60-9	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
4,4'-Butylidenebis(3-methyl-6- <i>tert</i> -butylphenyl ditridecyl)phosphite	13003-12-8	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
4,4'-Dibenzoylquinone dioxime	120-52-5	>	1.00E-04	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-06
4,4'-Dihydroxybenzophenone	611-99-4					4.97E-06
4,4'-Dihydroxybenzophenone	611-99-4		3.80E-05	REC ₁₀ (M) ⁴	Kawamura et al 2003	8.95E-06

4,4'-Dihydroxybenzophenone	611-99-4		3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	1.00E-06
4,4'-Dihydroxybiphenyl	92-88-6		5.00E-06	REC ₁₀ (M) ¹	Nishihara et al 2000	6.00E-05
4,4'-Dithiodimorpholine	103-34-4	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
4,4'-Isopropylidenediphenol alkyl(C ₁₂ -C ₁₅)phosphite	3315-29-5		4.40E-05	REC ₁₀ (M) ³	Ogawa et al 2005	7.73E-06
4,4'-Methylenebis (2,6-di- <i>tert</i> -butylphenol)	118-82-1	>	1.00E-04	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-06
4,4'-Thiobiphenyl	6954-27-4		3.00E-06	REC ₁₀ (M) ¹	Nishihara et al 2000	1.00E-04
4,4'-Thiobis(3-methyl-6- <i>tert</i> -butylphenol)	96-69-5	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
4-Acryloyloxyethyl trimetric acid (4-AETA)		>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
4-Acryloyloxyethyl trimetric acid anhydrate (4-AET)		>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
4-Amino butylbenzoate	94-25-7	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
4-Aminobenzoic acid	150-13-0	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
4-Aminobenzoic acid diglucoside		>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
4-Bromophenol	106-41-2		8.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	3.75E-06
4-CB-4'-ol			73.3	RIE	Fang et al 2000	7.33E-01
4-Chloro-3,5-xyleneol	88-04-0		1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	3.00E-06
4-Chloro-3-methylphenol	59-50-7		5.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	6.00E-02
4'-Chloro-4-biphenylol	28034-99-3		0.06	RP ¹	Coldham et al 1997	5.00E-09
4-Chloroaniline	106-47-8	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
4-Chloronitrobenzene	100-00-5	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
4-Chlorophenol	106-48-9		2.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	1.50E-06
4-Chlorotoluene	106-43-4	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06

4-Cyclohexylphenol [phenolic resin]	1131-60-8		6.20E-07	REC ₁₀ (M) ³	Ogawa et al 2005	5.48E-04
4-Ethylphenol	123-07-9					5.15E-06
4-Ethylphenol	123-07-9		3.00E-07	RA _{E2}	Kawagoshi et al 2002	3.00E-07
4-Ethylphenol	123-07-9		3.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	1.00E-05
4-Hydroxy-2',3,5,5'-tetrachlorobiphenyl		>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-05
4-Hydroxy-2',4'-dimethoxybenzophenone	41351-30-8		4.00E-05	REC ₁₀ (M) ⁴	Kawamura et al 2003	8.50E-06
4-Hydroxy-4'-chlorobenzophenone	42019-78-3		2.20E-06	REC ₁₀ (M) ⁴	Kawamura et al 2003	1.55E-04
4-Hydroxy-4'-monochlorobiphenyl		>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-05
4-Hydroxyacetophenone	99-93-4		2.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	1.50E-06
4-hydroxybenz[a]anthracene			7.50E-03	REP	Hayakawa et al 2007	7.50E-03
4-Hydroxybenzaldehyde	123-08-0	>	3.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.00E-07
4-hydroxybenzo[a]pyrene	37574-48-4					< 5.15E-05
4-hydroxybenzo[a]pyrene	37574-48-4	<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
4-hydroxybenzo[a]pyrene	37574-48-4	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
4-hydroxybenzo[c]phenanthrene		<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
4-hydroxybenzo[e]pyrene			4.20E-04	REP	Hayakawa et al 2007	4.20E-04
4-Hydroxybenzoic acid	99-96-7	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
4-Hydroxybenzophenone	1137-42-4		4.50E-06	REC ₁₀ (M) ⁴	Kawamura et al 2003	7.56E-05
4-hydroxychrysene	63019-40-9	<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
4-Hydroxymethyl-2,6-di-tert-butylphenol	88-26-6	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
4-hydroxyphenanthrene	7651-86-7	<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
4-Hydroxytamoxifen	68392-35-8		0.0073	RP ¹	Coldham et al 1997	7.30E-03
4-Hydroxy-tamoxifen	68392-35-8	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06

4-iso-Propyl-3-methylphenol	3328022	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
4-Methacryloyloxyethyl trimetric acid anhydrate (4-MET)		>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
4-Methacryloyloxyethyl trimetric acid (4-META)		>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
4-Methylphenol (p-cresol)	106-44-5						5.50E-07
4-Methylphenol (p-cresol)	106-44-5		1.00E-07	RA _{E2}	Kawagoshi et al 2002		1.00E-07
4-Methylphenol (p-cresol)	106-44-5		3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000		1.00E-06
4-n-Butylphenol	1638-22-8						2.00E-05
4-n-Butylphenol	1638-22-8		1.00E-05	RA _{E2}	Kawagoshi et al 2002		1.00E-05
4-n-Butylphenol	1638-22-8		1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000		3.00E-05
4-n-Heptylphenol	1987-50-4						1.02E-05
4-n-Heptylphenol	1987-50-4		2.00E-05	RA _{E2}	Kawagoshi et al 2002		2.00E-05
4-n-Heptylphenol	1987-50-4	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
4-n-Hexylphenol	2446-69-7						3.00E-05
4-n-Hexylphenol	2446-69-7		1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000		3.00E-05
4-n-Hexylphenol	2446-69-7		3.00E-05	RA _{E2}	Kawagoshi et al 2002		3.00E-05
4-Nitroquinoline-N-oxide	56-57-5	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
4-Nitrotoluene	99-99-0	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
4-n-Nonylphenol	104-40-5		2.00E-06	RA _{E2}	Kawagoshi et al 2002		2.00E-06
4-n-Octylphenol	1806-26-4						2.15E-06
4-n-Octylphenol	1806-26-4		4.00E-06	RA _{E2}	Kawagoshi et al 2002		4.00E-06
4-n-Octylphenol	1806-26-4	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000		3.00E-07
4-Nonylphenol	104-40-5						7.96E-04
4-Nonylphenol	104-40-5		4.60E-07	REC ₁₀ (M) ⁴	Kawamura et al 2003		7.39E-04

4-Nonylphenol	104-40-5		4.60E-07	REC ₁₀ (M) ³	Ogawa et al 2005	7.39E-04
4-Nonylphenol	104-40-5		3.00E-04	RA _{E2}	Kawagoshi et al 2002	3.00E-04
4-Nonylphenol	104-40-5	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
4-Nonylphenol	104-40-5		0.0022	RP ¹	Coldham et al 1997	2.20E-03
4-Nonylphenol (technical grade)			0.005	RP ¹	Coldham et al 1997	5.00E-03
4-Nonylphenol polyethoxylate (10)		>	3.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.00E-05
4-Nonylphenol polyethoxylate (15)		>	2.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.50E-05
4-Nonylphenol polyethoxylate (2)			1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	3.00E-07
4-Nonylphenol polyethoxylate (5)		>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-05
4-Nonylphenol polytheoxylate (23)		>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-05
4-n-Pentylphenol	14938-35-3					6.50E-05
4-n-Pentylphenol	14938-35-3		3.00E-06	REC ₁₀ (M) ¹	Nishihara et al 2000	1.00E-04
4-n-Pentylphenol	14938-35-3		3.00E-05	RA _{E2}	Kawagoshi et al 2002	3.00E-05
4-n-Propylphenol	645-56-7					2.64E-06
4-n-Propylphenol	645-56-7		1.00E-06	RA _{E2}	Kawagoshi et al 2002	1.00E-06
4-n-Propylphenol	645-56-7		7.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	4.29E-06
4-Octylphenol	1806-26-4					1.12E-01
4-Octylphenol	1806-26-4		0.003	RP ¹	Coldham et al 1997	3.00E-05
4-Octylphenol	1806-26-4		22.3	RIE	Fang et al 2000	2.23E-01
4-OH-Tamoxifen	68392-35-8		56	RIE	Fang et al 2000	5.60E-01
4-Phenylphenol [phenolic resin]	92-69-3					4.12E-05
4-Phenylphenol [phenolic resin]	92-69-3		4.70E-06	REC ₁₀ (M) ³	Ogawa et al 2005	7.23E-05
4-Phenylphenol [phenolic resin]	92-69-3		3.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	1.00E-05
4-sec-Butylphenol	99-71-8		1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	3.00E-05

4-tert-Butylbenzoic acid	98-73-7	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
4-tert-Butylphenol	98-54-4						6.00E-06
4-tert-Butylphenol	98-54-4		2.00E-06	RA _{E2}	Kawagoshi et al 2002		2.00E-06
4-tert-Butylphenol	98-54-4		3.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000		1.00E-05
4-tert-Butylphenylsalicylate	87-18-3					<	3.40E-07
4-tert-Butylphenylsalicylate	87-18-3	>	1.00E-03	REC ₁₀ (M) ⁴	Kawamura et al 2003	<	3.40E-07
4-tert-Butylphenylsalicylate	87-18-3	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
4-tert-Octylphenol	140-66-9						1.08E-01
4-tert-Octylphenol	140-66-9		2.00E-07	REC ₁₀ (M) ¹	Nishihara et al 2000		1.50E-03
4-tert-Octylphenol	140-66-9		0.00036	RP ¹	Coldham et al 1997		3.60E-06
4-tert-Octylphenol	140-66-9		4.00E-04	RA _{E2}	Kawagoshi et al 2002		4.00E-04
4-tert-Octylphenol	140-66-9		43	RIE	Fang et al 2000		4.30E-01
4-tert-Octylphenol polyethoxylate (10)		>	2.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.50E-05
4-tert-Octylphenol polyethoxylate (15)		>	2.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.50E-05
4-tert-Octylphenol polyethoxylate (2)			3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000		1.00E-06
4-tert-Octylphenol polyethoxylate (23)		>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-05
4-tert-Octylphenol polyethoxylate (5)		>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-05
4-tert-Pentylphenol	80-46-6						1.14E-04
4-tert-Pentylphenol	80-46-6		1.00E-06	REC ₁₀ (M) ¹	Nishihara et al 2000		3.00E-04
4-tert-Pentylphenol	80-46-6		3.08E-06	REC ₁₀ (M) ²	Shioji et al 2006		3.08E-06
4-tert-Pentylphenol	80-46-6		4.00E-05	RA _{E2}	Kawagoshi et al 2002		4.00E-05
4-Toluenesulfonamide	70-55-3	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
5,6,8,9-tetrahydrobenz[a]anthracen-11[10H]-one		<	1.00E-06	REP ²	Hayakawa et al 2011	<	1.00E-06

5,6-chrysenequinone		<	1.00E-06	REP ²	Hayakawa et al 2011	<	1.00E-06
5-hydroxybenz[a]anthracene	960-92-9	<	1.00E-04	REP	Hayakawa et al 2007	<	1.00E-04
5-hydroxybenzo[a]pyrene	24027-84-7					<	5.15E-05
5-hydroxybenzo[a]pyrene	24027-84-7	<	1.00E-04	REP	Hayakawa et al 2007	<	1.00E-04
5-hydroxybenzo[a]pyrene	24027-84-7	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
5-hydroxybenzo[c]phenanthrene		<	1.00E-04	REP	Hayakawa et al 2007	<	1.00E-04
6-Hydroxy-3,4-dichlorodibenzofuran		>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-05
6-hydroxybenzo[a]pyrene	33953-73-0					<	5.15E-05
6-hydroxybenzo[a]pyrene	33953-73-0	<	1.00E-04	REP	Hayakawa et al 2007	<	1.00E-04
6-hydroxybenzo[a]pyrene	33953-73-0	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
6-hydroxybenzo[b]fluoranthene	81824-09-1	<	1.00E-04	REP	Hayakawa et al 2007	<	1.00E-04
6-hydroxychrysene	37515-51-8	<	1.00E-04	REP	Hayakawa et al 2007	<	1.00E-04
6-hydroxyindeno[1,2,3-cd]pyrene	99520-67-9	<	1.00E-04	REP	Hayakawa et al 2007	<	1.00E-04
7-Hydroxy-1,2,3,6,8-pentachlorodibenzofuran		>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-05
7-Hydroxy-3,4-dichlorodibenzofuran			6.00E-06	REC ₁₀ (M) ¹	Nishihara et al 2000		5.00E-05
7-hydroxybenzo[a]pyrene	37994-82-4					<	5.15E-05
7-hydroxybenzo[a]pyrene	37994-82-4	<	1.00E-04	REP	Hayakawa et al 2007	<	1.00E-04
7-hydroxybenzo[a]pyrene	37994-82-4	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
7-hydroxybenzo[b]fluoranthene	81824-10-4	<	1.00E-04	REP	Hayakawa et al 2007	<	1.00E-04
8-Hydroxy-2,3,4-trichlorodibenzofuran	103124-63-6		1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000		3.00E-05
8-Hydroxy-2-monochlorodibenzofuran			1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000		3.00E-05
8-Hydroxy-3,4,6-trichlorodibenzofuran			1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000		3.00E-05
8-Hydroxy-3,4-dichlorodibenzofuran			5.00E-06	REC ₁₀ (M) ¹	Nishihara et al 2000		6.00E-05

8-Hydroxy-3-monochlorodibenzofuran			7.00E-06	REC ₁₀ (M) ¹	Nishihara et al 2000	4.29E-05
8-hydroxybenzo[a]pyrene	13345-26-1					< 5.15E-05
8-hydroxybenzo[a]pyrene	13345-26-1	<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
8-hydroxybenzo[a]pyrene	13345-26-1	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
8-hydroxybenzo[b]fluoranthene		<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
8-hydroxybenzo[k]fluoranthene		<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
8-hydroxyindeno[1,2,3-cd]pyrene	99520-58-8	<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
9,10-anthraquinone	84-65-1	<	1.00E-06	REP ²	Hayakawa et al 2011	< 1.00E-06
9,10-dihydrobenzo[a]pyrene-7[8H]-one	3331-46-2	<	1.00E-06	REP ²	Hayakawa et al 2011	< 1.00E-06
9,10-phenanthrenequinone	84-11-7	<	1.00E-06	REP ²	Hayakawa et al 2011	< 1.00E-06
9-fluorenone	486-25-9	<	1.00E-06	REP ²	Hayakawa et al 2011	< 1.00E-06
9-Hydroxy fluorene	1689-64-1					< 5.02E-05
9-Hydroxy fluorene	1689-64-1	<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
9-Hydroxy fluorene	1689-64-1	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
9-Hydroxy-2,6-dichlorodibenzofuran		>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-05
9-Hydroxy-3,4-dichlorodibenzofuran		>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-05
9-hydroxybenz[a]anthracene		<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
9-hydroxybenzo[a]pyrene	17573-21-6					< 5.15E-05
9-hydroxybenzo[a]pyrene	17573-21-6	<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
9-hydroxybenzo[a]pyrene	17573-21-6	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
9-hydroxybenzo[b]fluoranthene		<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
9-hydroxybenzo[e]pyrene		<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
9-hydroxybenzo[k]fluoranthene		<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04
9-hydroxyphenanthrene	484-17-3	<	1.00E-04	REP	Hayakawa et al 2007	< 1.00E-04

9-Octadecenoic acid amide	301-02-0	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
acenaphthoquinone	82-86-0	<	1.00E-06	REP ²	Hayakawa et al 2011	<	1.00E-06
Acephate	30560-19-1	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Acetaldehyde	75-07-0	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Acetamide	60-35-5	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Acetyleneugenol	93-28-7	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Acrylamide	79-06-1	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Acrylonitrile [polyacrylonitrile, AS resin, ABS resin, AB rubber]	107-13-1	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Adipic acid	124-04-9					<	3.20E-07
<i>Adipic acid</i>	124-04-9	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
<i>Adipic acid</i>	124-04-9	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Aflatoxin B1	1162-65-8	>	2.00E-06	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.50E-04
Alachlor	15972-60-8	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Aldicarb	116-06-3	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
Aldrin	309-00-2	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
Amitrole (3-Amino-1H-1,2,4-triazole)	61-82-5	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Androstenediol	521-17-5						1.55E-01
<i>Androstenediol</i>	521-17-5		0.023	RP ¹	Coldham et al 1997		2.30E-04
<i>Androstenediol</i>	521-17-5		31	RIE	Fang et al 2000		3.10E-01
Androstenedione	63-05-8		0	RP ¹	Coldham et al 1997		0.00E+00
Aniline	62-53-3	>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-05
Anthracene	120-12-7	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
anthrone	90-44-8	<	1.00E-06	REP ²	Hayakawa et al 2011	<	1.00E-06

Antimony(III) chloride	10025-91-9	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Apigenin	520-36-5		1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000		3.00E-05
Aplysiaterpenoid A	119945-08-3	>	10	REC ₁₀ (mg/l) ¹	Nishihara et al 2000	<	3.00E-11
Atrazine	1912-24-9	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Benz[a]anthracene	56-55-3	>	2.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.50E-06
Benzaldehyde	100-52-7	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
benzalkonium chloride	8001-54-5	>	100	REC ₁₀ (mg/l) ¹	Nishihara et al 2000	<	3.00E-12
benzanthrone	82-05-3	<	1.00E-06	REP ²	Hayakawa et al 2011	<	1.00E-06
Benzo[a]pyrene	50-32-8	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
benzo[a]pyrene[1,6]quinone	3067-13-8	<	1.00E-06	REP ²	Hayakawa et al 2011	<	1.00E-06
benzo[a]pyrene[11,12]quinone	60657-26-3	<	1.00E-06	REP ²	Hayakawa et al 2011	<	1.00E-06
benzo[a]pyrene[3,6]quinone	3067-14-9		2.30E-04	REP ²	Hayakawa et al 2011		2.30E-04
benzo[a]pyrene[4,5]quinone	42286-46-4	<	1.00E-06	REP ²	Hayakawa et al 2011	<	1.00E-06
benzo[a]pyrene[6,12]quinone	3067127	<	1.00E-06	REP ²	Hayakawa et al 2011	<	1.00E-06
benzo[a]pyrene[7,10]quinone		<	1.00E-06	REP ²	Hayakawa et al 2011	<	1.00E-06
benzo[a]pyrene[7,8]quinone	65199-11-3		2.00E-05	REP ²	Hayakawa et al 2011	<	2.00E-05
Benzo[b]fluoranthene	205-99-2	>	5.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	<	6.00E-06
benzo[c]phenanthrene[1,4]quinine		<	1.00E-06	REP ²	Hayakawa et al 2011	<	1.00E-06
benzo[c]phenanthrene[5,6]quinine		<	1.00E-06	REP ²	Hayakawa et al 2011	<	1.00E-06
Benzo[e]pyrene	192-97-2	>	2.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.50E-05
Benzo[g,h,i]perylene	191-24-2	>	2.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.50E-05
Benzo[k]fluoranthene	207-08-9	>	2.00E-06	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.50E-04
Benzoepinesulfate		>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
Benzoic acid	65-85-0	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07

Benzophenone	119-61-9					< 3.20E-07
<i>Benzophenone</i>	119-61-9	>	1.00E-03	REC ₁₀ (M) ⁴	Kawamura et al 2003	< 3.40E-07
<i>Benzophenone</i>	119-61-9	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
Benzoyl-peroxide	94-36-0	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
Benzyl alcohol	100-51-6	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
Bifenox	42576-02-3	>	5.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	< 6.00E-06
Biochanin A	491-80-5	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
Biphenyl	92-52-4	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
Bis(2,4-di- <i>tert</i> -butylphenyl)pentaerythritol diphosphate	26741-53-7	>	1.00E-04	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-06
Bis(2-chloroethyl) ether	111-44-4	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
Bis(2-ethylhexyl)azelate	103-24-2	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
Bis(3,5-di- <i>tert</i> -butyl-4-hydroxybenzylphosphoric acid ethyl)calcium	65140-91-2	>	1.00E-04	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-06
Bis(4-glycidyloxyphenyl)methane [epoxy resin]	2095036	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
Bis(4-hydroxyphenyl)methane	620-92-8					2.06E-05
<i>Bis(4-hydroxyphenyl)methane</i>	620-92-8		1.30E-05	REC ₁₀ (M) ³	Ogawa et al 2005	2.62E-05
<i>Bis(4-hydroxyphenyl)methane</i>	620-92-8		2.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	1.50E-05
Bis(4-hydroxyphenyl)sulfone	80-09-1	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	3.00E-07
Bisphenol A	80-05-7					8.50E-02
<i>Bisphenol A</i>	80-05-7		3.00E-06	REC ₁₀ (M) ¹	Nishihara et al 2000	1.00E-04
<i>Bisphenol A</i>	80-05-7		1.10E-05	REC ₁₀ (M) ⁴	Kawamura et al 2003	3.09E-05

<i>Bisphenol A</i>	80-05-7		1.10E-05	REC ₁₀ (M) ³	<i>Ogawa et al 2005</i>	3.09E-05
<i>Bisphenol A</i>	80-05-7		3.00E-05	RA _{E2}	<i>Kawagoshi et al 2002</i>	3.00E-05
<i>Bisphenol A</i>	80-05-7		0.005	RP ¹	<i>Coldham et al 1997</i>	5.00E-05
<i>Bisphenol A</i>	80-05-7		51	RIE	<i>Fang et al 2000</i>	5.10E-01
Bisphenol A bis(2,3-dihydroxypropyl)ether	5581-32-8	>	1.00E-03	REC ₁₀ (M) ³	<i>Ogawa et al 2005</i>	< 3.40E-07
Bisphenol A bis(3-chloro-2-hydroxyphenol)ether	4809-35-2	>	1.00E-03	REC ₁₀ (M) ³	<i>Ogawa et al 2005</i>	< 3.40E-07
Bisphenol-A-bischloroformate (BPA-GF)		>	1.00E-03	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 3.00E-07
Bisphenol-A-diglycidyl ether (BPA-GE)	1675-54-3					< 3.20E-07
<i>Bisphenol-A-diglycidyl ether (BPA-GE)</i>	1675-54-3	>	1.00E-03	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 3.00E-07
<i>Bisphenol-A-diglycidyl ether (BPA-GE)</i>	1675-54-3	>	1.00E-03	REC ₁₀ (M) ³	<i>Ogawa et al 2005</i>	< 3.40E-07
Bisphenol-A-dimethacrylate (BisDMA)	3253-39-2	>	1.00E-03	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 3.00E-07
Bisphenol-A-ethoxylate (BPA-E)		>	1.00E-03	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 3.00E-07
Bisphenol-A-ethoxylate diacrylate (BPA-ED)		>	1.00E-03	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 3.00E-07
Bisphenol-A-proxylate (BPA-P)		>	1.00E-03	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 3.00E-07
Bochanin A			0.0091	RP ¹	<i>Coldham et al 1997</i>	9.10E-05
Boric acid	10043-35-3	>	1.00E-04	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 3.00E-06
BPMC	3766-81-2	>	1.00E-04	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 3.00E-06
Bromobutide	74712-19-9	>	1.00E-05	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 3.00E-05
Bromodichloromethane	75-27-4	>	1.00E-03	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 3.00E-07
Bromoform	75-25-2	>	1.00E-03	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 3.00E-07
Butylated hydroxyanisole (BHA)	25013-16-5					< 3.20E-07
<i>Butylated hydroxyanisole (BHA)</i>	25013-16-5	>	1.00E-03	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 3.00E-07
<i>Butylated hydroxyanisole (BHA)</i>	25013-16-5	>	1.00E-03	REC ₁₀ (M) ³	<i>Ogawa et al 2005</i>	< 3.40E-07
Butylbenzyl phthalate	85-68-7					1.06E-02

<i>Butylbenzyl phthalate</i>	85-68-7		1.00E-08	RA _{E2}	<i>Kawagoshi et al 2002</i>	1.00E-08
<i>Butylbenzyl phthalate</i>	85-68-7		0.0004	RP ¹	<i>Coldham et al 1997</i>	4.00E-06
<i>Butylbenzyl phthalate</i>	85-68-7		5.00E-04	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	6.00E-07
<i>Butylbenzyl phthalate</i>	85-68-7	>	1.00E-03	REC ₁₀ (M) ³	<i>Ogawa et al 2005</i>	< 3.40E-07
<i>Butylbenzyl phthalate</i>	85-68-7		5.3	RIE	<i>Fang et al 2000</i>	5.30E-02
Cadmium chloride	10108-64-2	>	1.00E-04	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 3.00E-06
Camphorquinone	2767-84-2	>	1.00E-03	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 3.00E-07
Captans	133-06-2	>	1.00E-04	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 3.00E-06
Caravacrol	499-75-2	>	1.00E-04	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 3.00E-06
Carbaryl (NAC)	63-25-2	>	1.00E-04	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 3.00E-06
Carbendazim	10605-21-7	>	3.00E-04	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 1.00E-06
Carbofuran	1563-66-2	>	1.00E-04	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 3.00E-06
Catechol	120-80-9	>	1.00E-04	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 3.00E-06
Chinomethionat	2439012	>	3.00E-04	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 1.00E-06
Chlorhexidine gluconate	18472-51-0	>	1.00E-04	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 3.00E-06
Chlornitrofen (CNP)	1836-77-7	>	1.00E-05	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 3.00E-05
Chlorobenside	103-17-3	>	3.00E-04	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 1.00E-06
Chlorobenzene	108-90-7	>	1.00E-03	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 3.00E-07
Chlorobenzilate	510-15-6	>	3.00E-04	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 1.00E-06
Chlorodibromomethane	124-48-1	>	1.00E-03	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 3.00E-07
Chloropropham	101-21-3	>	3.00E-04	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 1.00E-06
Chlorothalonil (TPN)	1897-45-6	>	1.00E-04	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 3.00E-06
Chlorpyrifos-methyl	5598-13-0	>	3.00E-04	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 1.00E-06
Cholesterol	57-88-5		0	RP ¹	<i>Coldham et al 1997</i>	0.00E+00

<i>cis</i> -1,2,-Diphenylcyclobutane			3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	1.00E-06
<i>cis</i> -13-Docosenic acid amide	112-84-5	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
<i>cis</i> -Stilbene	645-49-8	>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-05
Clomiphene	911-45-5	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
Copper(II) sulfate	7758-98-7	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
Cortisol	50-23-7		0	RP ¹	Coldham et al 1997	0.00E+00
Coumaric acid	91-64-5	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
Coumestrin			1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	3.00E-05
Coumestrol	479-13-0					2.53E-01
<i>Coumestrol</i>	479-13-0		3.00E-07	REC ₁₀ (M) ¹	Nishihara et al 2000	1.00E-03
<i>Coumestrol</i>	479-13-0		0.67	RP ¹	Coldham et al 1997	6.70E-03
<i>Coumestrol</i>	479-13-0		75	RIE	Fang et al 2000	7.50E-01
Cucumechinoside D	125640-33-7	>	5.00E-08	REC ₁₀ (M) ¹	Nishihara et al 2000	< 6.00E-03
Cyanazin	21725-46-2	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
Cyclohexanol	108-93-0	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
Cyclohexanone	108-94-1	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
Cyclohexanone-iso-oxine <ε-Caprolactam> [polyamide]	105-60-2	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
Cyclohexylamine	108-91-8	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
Cyclosporin A	59865-13-3	>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-05
Cyfluthrin	68359-37-5	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.00E-06
Cyhalothrin	68085-85-8	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.00E-06
Cypermethrin	52315-07-8	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06

Daidzein	486-66-8					8.00E-06
<i>Daidzein</i>	486-66-8		1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	3.00E-06
<i>Daidzein</i>	486-66-8		0.0013	RP ¹	Coldham et al 1997	1.30E-05
Daidzin	552-66-9		3.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	1.00E-07
DDT	50-29-3					2.67E-03
<i>DDT</i>	50-29-3		0.00003	RP ¹	Coldham et al 1997	3.00E-07
<i>DDT</i>	50-29-3	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.00E-06
<i>DDT</i>	50-29-3		0.8	RIE	Fang et al 2000	8.00E-03
Dehydroepiandrosterone	53-43-0					6.01E-03
<i>Dehydroepiandrosterone</i>	53-43-0		0.0018	RP ¹	Coldham et al 1997	1.80E-05
<i>Dehydroepiandrosterone</i>	53-43-0		1.2	RIE	Fang et al 2000	1.20E-02
Dexamethasone	50-02-2	>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-05
Di(ethylene glycol)dibenzoate	120-55-8	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
Di(propylene glycol)dibenzoate	27138-31-4	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
Di-2-ethylhexyl adipate	103-23-1					< 3.00E-07
<i>Di-2-ethylhexyl adipate</i>	103-23-1	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
<i>Di-2-ethylhexyl adipate</i>	103-23-1	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
Di-2-ethylhexyl phthalate	117-81-7					< 2.45E-07
<i>Di-2-ethylhexyl phthalate</i>	117-81-7		0	RP ¹	Coldham et al 1997	0.00E+00
<i>Di-2-ethylhexyl phthalate</i>	117-81-7	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
<i>Di-2-ethylhexyl phthalate</i>	117-81-7	>	2.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.50E-07
Diacetyllauroyl glycerol	30899-62-8	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
Diazinon	333-41-5	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
Dibenz[<i>a,h</i>]anthracene	53-70-3	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06

Dibenzyl adipate	2451-84-5	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Dibenzyl ether	103-50-4	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Dibutyl adipate	105-99-7					<	5.17E-06
<i>Dibutyl adipate</i>	105-99-7	>	3.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-05
<i>Dibutyl adipate</i>	105-99-7	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Dibutyl maleate	105-76-0	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Dibutyl sebacate	109-43-3	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Dichlorvos (DDVP)	62-73-7	>	2.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.50E-06
Dicloran	99-30-9	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
Dicyclohexyl phthalate	84-61-7					<	6.70E-07
<i>Dicyclohexyl phthalate</i>	84-61-7	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
<i>Dicyclohexyl phthalate</i>	84-61-7	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Dicyclohexylamine	101-83-7	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Dicyclopentadiene	77-73-6	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Didecyldimethylammonium chloride	7173-51-5	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
Dieldrin	60-57-1	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
Dienestrol	84-17-3						5.47E-01
<i>Dienestrol</i>	84-17-3		25.4	RP ¹	Coldham et al 1997		2.54E-01
<i>Dienestrol</i>	84-17-3		84	RIE	Fang et al 2000		8.40E-01
Diethoxyleneglycol dimethacrylate		>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Diethyl adipate	141-28-6	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
Diethyl phthalate	84-66-2	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Diethyl sulfate	64-67-5	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Diethylbenzene, mixture	25340-17-4	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07

Diethylene glycol	111-46-6	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
Diethylstilbestrol (DES)	56-53-1					1.08E+00
<i>Diethylstilbestrol (DES)</i>	56-53-1		2.00E-10	REC ₁₀ (M) ¹	Nishihara et al 2000	1.50E+00
<i>Diethylstilbestrol (DES)</i>	56-53-1		74.3	RP ¹	Coldham et al 1997	7.43E-01
<i>Diethylstilbestrol (DES)</i>	56-53-1		100	RIE	Fang et al 2000	1.00E+00
Diflubenzuron	35367-38-5	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.00E-06
Diheptyl phthalate	3648-21-3					< 6.70E-07
<i>Diheptyl phthalate</i>	3648-21-3	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.00E-06
<i>Diheptyl phthalate</i>	3648-21-3	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
Dihydrogenistein			1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	3.00E-06
Dihydroglycitein		>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
Dihydrotestosterone (DHT)	521-18-6		5.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	6.00E-06
Di-iso-butyl adipate	141-04-8					< 5.17E-06
<i>Di-iso-butyl adipate</i>	141-04-8	>	3.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.00E-05
<i>Di-iso-butyl adipate</i>	141-04-8	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
Di-iso-butyl phthalate (DIBP)	84-69-5					< 1.67E-06
<i>Di-iso-butyl phthalate (DIBP)</i>	84-69-5	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
<i>Di-iso-butyl phthalate (DIBP)</i>	84-69-5	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
Diisodecyl adipate	27178-16-1	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
Diisodecyl phthalate	26761-40-0	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
Di-iso-decyl phthalate	26761-40-0	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.00E-06
Diisononyl adipate	33703-08-1	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
Diisononyl phthalate	28553-12-0					< 2.45E-07
<i>Diisononyl phthalate</i>	28553-12-0	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07

<i>Diisononyl phthalate</i>	28553-12-0	>	2.00E-03	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 1.50E-07
Diisooctyl phthalate	27554-26-3					< 2.45E-07
<i>Diisooctyl phthalate</i>	27554-26-3	>	1.00E-03	REC ₁₀ (M) ³	<i>Ogawa et al 2005</i>	< 3.40E-07
<i>Diisooctyl phthalate</i>	27554-26-3	>	2.00E-03	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 1.50E-07
Diisopropyl adipate	6938-94-9					< 6.70E-07
<i>Diisopropyl adipate</i>	6938-94-9	>	3.00E-04	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 1.00E-06
<i>Diisopropyl adipate</i>	6938-94-9	>	1.00E-03	REC ₁₀ (M) ³	<i>Ogawa et al 2005</i>	< 3.40E-07
Di-iso-propyl phthalate	605-45-8		2.00E-03	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	1.50E-07
Dimepiperate	61432-55-1	>	5.00E-05	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 6.00E-06
Dimethoate	60-51-5	>	1.00E-04	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 3.00E-06
Dimethyl adipate	627-93-0	>	3.00E-05	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 1.00E-05
Dimethyl phthalate	131-11-3					< 3.20E-07
<i>Dimethyl phthalate</i>	131-11-3	>	1.00E-03	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 3.00E-07
<i>Dimethyl phthalate</i>	131-11-3	>	1.00E-03	REC ₁₀ (M) ³	<i>Ogawa et al 2005</i>	< 3.40E-07
Dimethylsuccinate polymer with tetramethyl hydroxy-1-hydroxyethyl piperidine	65447-77-0	>	1.00E-04	REC ₁₀ (M) ³	<i>Ogawa et al 2005</i>	< 3.40E-06
Di-n-alkyl adipate (C=6,8,10)		>	1.00E-03	REC ₁₀ (M) ³	<i>Ogawa et al 2005</i>	< 3.40E-07
Di-n-butylphthalate	84-74-2					< 5.47E-07
<i>Di-n-butylphthalate</i>	84-74-2		0	RP ¹	<i>Coldham et al 1997</i>	0.00E+00
<i>Di-n-butylphthalate</i>	84-74-2	>	3.00E-04	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 1.00E-06
<i>Di-n-butylphthalate</i>	84-74-2	>	1.00E-03	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 3.00E-07
<i>Di-n-butylphthalate</i>	84-74-2	>	1.00E-03	REC ₁₀ (M) ³	<i>Ogawa et al 2005</i>	< 3.40E-07
Di-n-hexyl phthalate	84-75-3	>	5.00E-03	REC ₁₀ (M) ¹	<i>Nishihara et al 2000</i>	< 6.00E-08
Di-n-octyl adipate	123-79-5	>	1.00E-03	REC ₁₀ (M) ³	<i>Ogawa et al 2005</i>	< 3.40E-07

Di- <i>n</i> -octyl phthalate	117-84-0	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Dinonyl phthalate	84-76-4	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Di- <i>n</i> -pentyl phthalate	131-18-0	>	2.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.50E-07
Di- <i>n</i> -propyl adipate	106-19-4	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Di- <i>n</i> -propyl phthalate	131-16-8		3.00E-07	RA _{E2}	Kawagoshi et al 2002		3.00E-07
Dioctyl sebacate	122-62-3	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Diphenyl carbonate	102-09-0	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
Diphenylamine	122-39-4	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Diphenylcresyl phosphate	26444-49-5	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Diphenylmethane	101-81-5	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Diphenylmethane-4,4'-diisocyanate [urethane elastomer]	101-68-8	>	1.00E-04	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-06
Dipropyl phthalate	131-16-8	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
Distearyl pentaerythrityl diphosphite	3806-34-6	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Di- <i>tert</i> -butyl-peroxide	110-05-4	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Ditridecyl phthalate	119-06-2	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
<i>D</i> -Norgestrel	797-63-7		0.0004	RP ¹	Coldham et al 1997		7.50E-07
Docosanoic acid amide	3061-75-4	>	1.00E-04	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-06
Dodecamethylcyclohexanesiloxane	540-97-6	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Dodecylol polyethoxylate (15)		>	3.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-05
Dodecylol polyethoxylate (3)		>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-05
Dodecylol polyethoxylate (5)		>	3.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-05
Dodecylol polyethoxylate (9)		>	2.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.50E-05

Edifenfos (EDDP)	17109-49-8	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
Endosulfan (Benzoepin)	115-29-7	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
Endosulfan (α-Benzoepin)	959-98-8	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.00E-06
Endosulfan (β-Benzoepin)	33213-65-9	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.00E-06
Endrin	72-20-8	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.00E-06
Epichlorohydrin	106-89-8	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
EPN [<i>O</i> -Ethyl- <i>O</i> -(4-nitrophenyl)phenyl-phosphono thioate]	2104-64-5	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
Epoxidized soybean oil	8013078	>	1.00E-04	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-06
Equol	531-95-3					4.40E-04
<i>Equol</i>	531-95-3		1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	3.00E-05
<i>Equol</i>	531-95-3		0.085	RP ¹	Coldham et al 1997	8.50E-04
Esprocarb	85785-20-2	>	2.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.50E-05
Estriol	50-27-1					3.65E-03
<i>Estriol</i>	50-27-1		3.00E-07	REC ₁₀ (M) ¹	Nishihara et al 2000	1.00E-03
<i>Estriol</i>	50-27-1		0.63	RP ¹	Coldham et al 1997	6.30E-03
Estrone	53-16-7					4.99E-01
<i>Estrone</i>	53-16-7		3.00E-10	REC ₁₀ (M) ¹	Nishihara et al 2000	1.00E+00
<i>Estrone</i>	53-16-7		4.00E-01	RA _{E2}	Kawagoshi et al 2002	4.00E-01
<i>Estrone</i>	53-16-7		9.6	RP ¹	Coldham et al 1997	9.60E-02
Ethanolamine	141-43-5					< 3.00E-07
<i>Ethanolamine</i>	141-43-5	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
<i>Ethanolamine</i>	141-43-5	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
Ethyl 4-hydroxybenzoate	120-47-8		1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	3.00E-06

Ethyl benzene	100-41-4	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
Ethyl parathion	56-38-2	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.00E-06
Ethylcarbamate	51-79-6	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
Ethylene glycol	107-21-1	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
Ethylenediaminetetraacetic acid, 2Na (EDTA)	60-00-4	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
Eugenol	97-53-0	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
Fenbutatin oxide	13356-08-6	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.00E-06
Fenitrothion (MEP)	122-14-5	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
Fenobcarb	3766-81-2	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.00E-06
Fenoprop	93-72-1	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.00E-06
Fensulfothion	115-90-2	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.00E-06
Fenthion (MPP)	55-38-9	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
Fenvalerate	51630-58-1	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
Ferulic acid	1135-24-6	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
Flavone	525-82-6	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
Fluazifop-butyl	69806-50-4	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.00E-06
Flucythrinate	70124-77-5	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.00E-06
Fluvalinate	69409-94-5	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.00E-06
Formaldehyde	50-00-0	>	2.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.50E-07
Formononetin	485-72-3		0.0056	RP ¹	Coldham et al 1997	5.60E-05
Genistein	446-72-0					1.75E-03
Genistein	446-72-0		1.00E-07	REC ₁₀ (M) ¹	Nishihara et al 2000	3.00E-03
Genistein	446-72-0		0.049	RP ¹	Coldham et al 1997	4.90E-04
Genistin	529-59-9	>	1.00E-02	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-08

Glutaraldehyde	111-30-8	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Glycerol trilaurate <Trilaurin>	538-24-9	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Glycitein	40957-83-3	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Glycitin	40246-10-4	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Glycyrrhizic acid, 2K	1405-86-3	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
Glyoxal	107-22-2	>	5.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	6.00E-07
Heptachlor	76-44-8	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
Heptachlor epoxide	1024-57-3	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
Heptylnonyl adipate	68515-75-3	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Hexachloro-1,3-butadiene	87-68-3	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Hexachlorophene	70-30-4	>	10	REC ₁₀ (mg/l) ¹	Nishihara et al 2000		
Hexadecanoic acid amide	629-54-9	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Hexamethylenetetramine	100-97-0	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Hexestrol	84-16-2		30.6	RP ¹	Coldham et al 1997		3.06E-01
Hexestrol	84-16-2		89	RIE	Fang et al 2000		8.90E-01
Hinokitiol	499-44-5	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Hinokitiol acetylglucoside		>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Hinokitiol glucoside		>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Hippuric acid, Na	495-69-2	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
Hydroquinone	123-31-9	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Hydroxy-flutamide	52806-53-8	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Hydroxylamine sulfate	10039-54-0	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Hydroxy-tetrachlorobiphenyl		>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-05

Hydroxy-trichlorobiphenyl		>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-05
IBP	51146-56-6	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Iprodione	36734-19-7	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
Isoeugenol	97-54-1	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Isophorone	78-59-1	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Isopropyl benzene <Cumene>	98-82-8					<	3.00E-07
<i>Isopropyl benzene <Cumene></i>	98-82-8	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
<i>Isopropyl benzene <Cumene></i>	98-82-8	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.00E-07
Isoprothiolane	50512-35-1	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Isoxathion	18854-01-8	>	2.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.50E-05
ivermectin	70288-86-7	>	100	REC _{10m}	Eguchi et al 2002	<	3.00E-12
Kaempferol	520-18-3	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Kelthane (Dicofol)	115-32-2	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Kojic acid	501-30-4	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Lead nitrate	10099-74-8	>	2.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.50E-07
Linuron	330-55-2	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
Malaoxon	1634-78-2	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Malathion	121-75-5	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Maneb	12427-38-2	>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-05
Manzeb (Mancozeb)	8018017	>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-05
Marthasteroside A1 (20S-Acanthaglycoside E)	88434-24-6	>	2	REC ₁₀ (mg/l) ¹	Nishihara et al 2000	<	1.50E-10
m-Cresol	108-39-4		8.00E-08	RA _{E2}	Kawagoshi et al 2002		8.00E-08
Mefenacet	73250-68-7	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06

Melamine	108-78-1	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
MelQx	77500-04-0	>	2.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.50E-05
Menadione	58-27-5	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Mercury(II) chloride	7487-94-7	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Mestranol	72-33-3		7.3	RP ¹	Coldham et al 1997		7.30E-02
Metamitron	41394-05-2	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
Methidathion	950-37-8	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
Methomyl	16752-77-5	>	2.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.50E-06
Methoxychlor	72-43-5						1.70E-05
<i>Methoxychlor</i>	72-43-5		1.00E-06	RA _{E2}	Kawagoshi et al 2002		1.00E-06
<i>Methoxychlor</i>	72-43-5	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
<i>Methoxychlor</i>	72-43-5		0.0033	RP ¹	Coldham et al 1997		3.30E-05
Methyl 4-hydroxybenzoate	99-76-3		4.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000		7.50E-07
Methyl methacrylate (MMA)	80-62-6					<	3.00E-07
<i>Methyl methacrylate (MMA)</i>	80-62-6	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
<i>Methyl methacrylate (MMA)</i>	80-62-6	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.00E-07
Methylmercury chloride	115-09-3	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Metribuzin	21087-64-9	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
Microcystin RR	111755-37-4	>	1.34	REC ₁₀ (mg/l) ¹	Nishihara et al 2000	<	2.24E-10
Molinate	2212-67-1	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Monochloroacetic acid	79-11-8	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Monoethoxyleneglycol dimethacrylate		>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Morpholine	110-91-8	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07

<i>N,N'</i> -Di-2-naphthyl-4-phenylenediamine	93-46-9	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.00E-07
<i>N,N</i> -Dimethylaniline	121-69-7	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
<i>N,N</i> -Dimethylformamide	68-12-2	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Nafoxidine	1845-11-0		0	RP ¹	Coldham et al 1997		0.00E+00
Naphthalene	91-20-3	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Naringenin	480-41-1		3.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000		1.00E-05
<i>n</i> -Butyl 4-hydroxybenzoate	94-26-8		3.00E-06	REC ₁₀ (M) ¹	Nishihara et al 2000		1.00E-04
<i>n</i> -Butyl acrylate	141-32-2	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
<i>n</i> -Butylbenzene	104-51-8	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
<i>n</i> -Cyclohexyl-2-benzothiazolyl sulfenamide	95-33-0	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.00E-07
<i>n</i> -Decyl alcohol	112-30-1	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Nebron	555-37-3	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
Neophentylglycol dimethacrylate		>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
<i>N</i> -Ethylaniline	103-69-5	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Nickel(II) chloride	7718-54-9	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Nitrilotriacetic acid	139-13-9	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Nitrobenzene	98-95-3	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Nitrofen (NIP)	1836-75-5	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
<i>N</i> -Methylaniline	100-61-8	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
<i>N</i> -Nitrosodiethylamine	55-18-5	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
<i>N</i> -Nitrosodimethylamine	62-75-9	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
<i>N</i> -Nitrosodiphenylamine	86-30-6	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06

Nonoxynol iodide		>	100	REC ₁₀ (mg/l) ¹	Nishihara et al 2000	<	3.00E-12
Nonylphenol	25154-52-3		38.3	RIE	Fang et al 2000		3.83E-01
Nonylphenol ethoxylate	26027-38-3	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
N-Phenyl-1-naphthylamine	90-30-2					<	3.20E-07
N-Phenyl-1-naphthylamine	90-30-2	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
N-Phenyl-1-naphthylamine	90-30-2	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
N-Phenyl-2-naphthylamine	135-88-6	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
n-Propyl 4-hydroxybenzoate	94-13-3		1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000		3.00E-05
o,p'-DDD	53-19-0	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
o',p'-DDE	3424-82-6						4.00E-07
o',p'-DDE	3424-82-6		0.00004	RP ¹	Coldham et al 1997		4.00E-07
o',p'-DDE	3424-82-6	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
o',p'-DDT	789-02-6						1.10E-06
o',p'-DDT	789-02-6		0.00011	RP ¹	Coldham et al 1997		1.10E-06
o',p'-DDT	789-02-6	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
Octadecanoic acid amide	124-26-5	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Octadecyl-3,5-di-tert-butyl-4-hydroxyhydrocinnamate	2082-79-3	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Oleic acid	112-80-1	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Oleyl alcohol	143-28-2	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
o-Tolidine (3,3'-dimethylbenzidine)	119-93-7	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
p,p'-DDD	72-54-8	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
p,p'-DDE	72-55-9	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Paraquat	1910-42-5	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06

Pendimethalin	40487-42-1	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
Pentachloronitrobenzene (PCNB)	82-68-8	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Pentachlorophenol	87-86-5	>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-05
Pentachlorophenol (PCP)	87-86-5	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Permethrin	52645-53-1	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Phenol	108-95-2	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Phenthoate (PAP)	2597037	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Phenylhydrazine	100-63-0	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Phloretin	60-82-2	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
PhIP	105650-23-5	>	2.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.50E-05
Phosalone	2310-17-0	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
Phosphoric acid diphenyl 2-ethylhexyl ester	1241-94-7	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Phosphoric acid tris(3-methylphenyl)	563-04-2	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Phosphoric acid tris(4-methylphenyl)	78-32-0	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Piperidinium pentamethylenedithiocarbamate	98-77-1	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Poly(bisphenol A-co-epichlorohydrin)	25036-25-3	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Polyalkylpolyaminoethylglycine HCl		>	100	REC ₁₀ (mg/l) ¹	Nishihara et al 2000	<	3.00E-12
Potassium cyanide	151-50-8	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Potassium dichromate (VI)	7778-50-9	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Pretilachlor	51218-49-6	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Primiphos-methyl	29232-93-7	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
Procymidone	32809-16-8	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06

Progesterone	57-83-0		0	RP ¹	Coldham et al 1997		0.00E+00
Propanil (DCPA)	709-98-8	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Propazin	139-40-2	>	5.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	<	6.00E-06
Propoxur	114-26-1	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Propyzamide	23950-58-5	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
Pyrene	129-00-0	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Quercetin	117-39-5	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Quinoline	91-22-5	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Resorcinol	108-46-3	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Simazine (CAT)	122-34-9	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Simetryne	1014-70-6	>	2.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.50E-06
Sodium arsenite	7784-46-5	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Sodium dimethyldithiocarbamate dihydrate	72140-17-1	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Sodium lauryl sulfate (SDS)	151-21-3	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Sodium molybdate	7631-95-0	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Sodium selenate	13410-01-0	>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-05
Stigmasterol	83-48-7	>	1.00E-04	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-06
Styrenated phenol <di 93%, tri 7%>	61788-44-1	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Styrenated phenol <mono 74%, di 24%>	61788-44-1		2.90E-06	REC ₁₀ (M) ³	Ogawa et al 2005		1.17E-04
Styrenated phenol <mono or di or tri>	61788-44-1		3.40E-05	REC ₁₀ (M) ³	Ogawa et al 2005		1.00E-05
Styrene	100-42-5					<	3.20E-07
Styrene	100-42-5	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Styrene	100-42-5	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07

Tamoxifen	10540-29-1		0.0047	RP ¹	Coldham et al 1997	4.70E-05
Tefluthrin	79538-32-2	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.00E-06
Terephthalic acid	100-21-0	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
Testosterone	58-22-0					4.01E-03
Testosterone	58-22-0		0.001	RP ¹	Coldham et al 1997	1.00E-05
Testosterone	58-22-0		0.8	RIE	Fang et al 2000	8.00E-03
Tetrabromobisphenol A	79-94-7	>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-05
Tetrachlorobisphenol A	79-95-8	>	5.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	< 6.00E-06
Tetrachloroethylene	127-18-4	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
Tetrachlorofthalide		>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
Tetrachlorovinphos	961-11-5	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.00E-06
Tetraethylenepentamine	112-57-2	>	0.01	REC ₁₀ (ml/l) ¹	Nishihara et al 2000	< 3.00E-08
Tetraethylthiuram disulfide	97-77-8	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
Tetrakis [methylene-3-(3',5'-di- <i>tert</i> -butyl-4'-hydroxyphenyl)-propionate]methane	6683-19-8	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
Tetra- <i>n</i> -butylthiuram disulfide	1634-02-2	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
Thallium(I) chloride	7791-12-0	>	1.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-05
Thiabendazole	148-79-8	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.00E-06
Thiobencarb	28249-77-6	>	5.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 6.00E-07
Thiophanate-methyl	23564-05-8	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
Thiourea	62-56-6	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
Thiram	137-26-8	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
Thymol	89-83-8	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
Toluene	108-88-3	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
Toluene-2,4-diisocyanate [polyurethane]	584-84-9	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
Toxaphene (camphechlor)	8001-35-2	>	5.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000	< 6.00E-06
<i>trans</i> -1,2-Diphenylcyclobutane	20071-09-4	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07

<i>trans</i> -Stylbene	103-30-0	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
<i>trans-trans</i> -2,4,-Decadienal	25152-84-5	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.00E-07
Triadimefon	43121-43-3	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
Triadimenol	55219-65-3	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
Tributyl 2-acetylcitrate	77-90-7	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Tributyl phosphate	126-73-8	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Tributyltin(IV) chloride (TBT)	1461-22-9	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Triethoxylene glycol dimethacrylate	109-16-0	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Triethylamine	121-44-8	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Triethyleneglycolbis[3-(3- <i>tert</i> -butyl-5-methyl-4-hydroxyphenyl) propionate	36443-68-2	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Triethylenetetramine	112-24-3	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Trifluralin	1582-09-8	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Triforine	26644-46-2	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	1.00E-06
Trimellic acid tris(2-ethylhexyl)ester	3319-31-1	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.40E-07
Trimethylpropane triacrylate		>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Trimethylpropane trimethacrylate		>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Triphenyltin(IV) chloride (TPT)	639-58-7	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-07
Tris(2,4-di- <i>tert</i> -butylphenyl)phosphite	31570-04-4	>	1.00E-04	REC ₁₀ (M) ³	Ogawa et al 2005	<	3.00E-06
Tris(2-chloroethyl) phosphate	115-96-8	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.40E-06
Tris(butoxyethyl) phosphate	78-51-3	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	<	3.00E-06
Tris(nonylphenyl) phosphite	26523-78-4		1.00E-05	REC ₁₀ (M) ³	Ogawa et al 2005		3.40E-05
Trp-P-2	62450-07-1	>	2.00E-05	REC ₁₀ (M) ¹	Nishihara et al 2000		1.50E-05

Tyramine	51-67-2	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	1.00E-06
Tyrosine	60-18-4	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	1.00E-06
Urethane dimethacrylate	72869-86-4	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	3.00E-07
Vinclozolin	50471-44-8	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	3.00E-06
Vinylacetic acid	625-38-7	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	3.00E-06
Xylylcarb	2425107	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	1.00E-06
Zearalenol	5916-52-9		67	RIE	Fang et al 2000	6.70E-01
Zearalenone	17924-92-4		0.26	RP ¹	Coldham et al 1997	2.60E-03
Zineb	12122-67-7	>	40	REC ₁₀ (mg/l) ¹	Nishihara et al 2000	< 7.50E-12
Ziram	137-30-4	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
α-Hexachlorocyclohexane (HCH, BHC)	319-84-6	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.00E-06
α-Methylstyrene	98-83-9					< 3.20E-07
α-Methylstyrene	98-83-9	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07
α-Methylstyrene	98-83-9	>	1.00E-03	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-07
α-Zearalanol (zearanol)	26538-44-3		1.3	RP ¹	Coldham et al 1997	1.30E-02
α-Zearalenol	36455-72-8		8.7	RP ¹	Coldham et al 1997	8.70E-02
β-Estradiol-17-acetate	6045-67-6		5.00E-07	REC ₁₀ (M) ¹	Nishihara et al 2000	6.00E-04
β-Hexachlorocyclohexane (HCH, BHC)	319-85-7	>	3.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 1.00E-06
β-Sitosterol	83-46-5					< 3.20E-06
β-Sitosterol	83-46-5	>	1.00E-04	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-06
β-Sitosterol	83-46-5	>	1.00E-04	REC ₁₀ (M) ³	Ogawa et al 2005	< 3.40E-06
β-Zearalanol	42422-68-4		0.46	RP ¹	Coldham et al 1997	4.60E-03
β-Zearalenol	71030-11-0		0.066	RP ¹	Coldham et al 1997	6.60E-04
γ-Hexachlorocyclohexane (HCH, BHC)	58-89-9	>	1.00E-03	REC ₁₀ (M) ¹	Nishihara et al 2000	< 3.00E-07

Appendix D: Summary of Original Values and Normalization Assumptions for Economic Meta-analysis

Table D.1. Functional unit standardization.

Author	Functional unit	Capital cost of oil to biofuel in 2012 US dollar, \$/gal biofuel	Operating cost of oil to biofuel in 2012 US dollar, \$/gal biofuel	Conversion efficiency, fraction (biofuel / algae oil)
Davis	10 MM Gal biodiesel	3.03378		0.93
Callagher	Biodiesel of 500 ha open ponds	1.69686	0.71	
Stephenson	Algae oil of 200 ha open ponds			
kovacevic	Biodiesel of 400 ha open ponds	1.456458	0.34	
Benneman	Algae Oil of 300 ha open ponds			
New assumption	10 MM Gal biodiesel	2.062366	0.52	0.93

Table D.2. Financial assumption standardization

Author	Project life time, yr	Discount rate, %	Tax rate, %	Subsidy, \$/gal	Depreciation method	Money Currency
Davis	20	10	35		7 years MACRS	2011 US dollar
Callagher	20	10	34	1-1.5	15 years MACRS	2011 US dollar
Stephenson	30	15	30		30 years average	2010 US dollar
kovacevic	15	5	34		15 years average	2008 Europe dollar
Benneman						1982 US dollar
New Assumption	20	10%	30%	1	7 years MACRS	2012 US dollar

Table D.3. System boundary standardization

Author	Boundary	Distribution Cost, \$/gal (2012 US dollar)
Davis	Biodiesel at factory gate	
Callagher	Biodiesel at gactory gate	
Stephenson	Algal oil at gactory gate	
kovacevic	Biodiesel at gasoline pump station	0.27
Benneman	Algal oil at factory gate	
New Assumption	Biodiesel at gasoline pump station	0.27

Table D.4. Co-products standardization

Author	Co-product	AD, Capital cost, \$/kg digested algae biomass (2012 \$US)	AD, Operational cost, \$/kg digested algae biomass (2012 \$US)	Electricity productivity, kwh/kg digested algae biomass	Electricity sale price, \$/kwh
Davis	Anearobic digestion for electricity	0.180735888		0.62	0.066846
Callagher	No co-product				
Stephenson, base	High value product, algae cake				
Stephenson, projected	Algae cake sale				
Kovacevic	Anaerobic digestion for electricity	0.36782704	0.086030135	0.95	0.14064815
Benneman	Anaerobic digestion for methane	0.26272216			
New Assumption	Anaerobic digestion for electricity	0.270428363	0.086030135	0.785	0.066846

Table D.5. Technical input assumption for base case

Author	Algae yield productivity, g/m ² -day	Algae oil content, fraction	Lipid extract loss factor, fraction
Davis	25	0.25	0.15
Callagher	30	0.35	0
Stephenson	20	0.25	0.3
kovacevic	20	0.15	0
Benneman	30	0.5	0
New Assumption	25.00	0.30	0.10

Table D.6. Technical assumption for projected case

Author	Algae yield productivity, g/m ² -day	Algae oil content, fraction	Lipid extract loss factor, fraction
Callagher	40	0.4	0
Stephenson	50	0.5	0.1
kovacevic	30	0.3	0
Benneman	60	0.5	0.05
New Assumption	45	0.4	0.05