

Supporting Information for:
LIFE CYCLE COMPARISON OF ENVIRONMENTAL EMISSIONS FROM
THREE DISPOSAL OPTIONS FOR UNUSED PHARMACEUTICALS

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This document was prepared on April 9, 2012 for Environmental Science and Technology

Number of pages: 25

Number of figures: 7

Number of tables: 8

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Although this paper focuses on disposal options for unused pharmaceuticals, we also note that system improvements are needed to reduce the occurrence and impacts of active pharmaceutical ingredient (API) release to the environment from all sources. First, human and animal excretion is considered a major source of environmental API emissions,¹ and therefore pharmaceuticals should be designed to minimize excretion.² Second, the adoption of a waste prevention mentality by pharmaceutical companies, prescribing entities, and consumers would reduce the accumulation of unused pharmaceuticals. Third, pharmaceutical design should prioritize API susceptibility to waste treatment so once APIs are excreted or directly disposed of by toilet/trash, they are easily rendered harmless at end-of-life.² Until such developments occur, the immediate disposal of all unused pharmaceuticals in the trash will significantly reduce human health risks associated with pharmaceuticals accumulated in households, decrease current releases of APIs to the environment, and avoid significant increases in most other non-API emissions.

1) Disposal Options

This section outlines the main assumptions and sources of data used for each modeling disposal option, and it follows the layout of the freely accessible spreadsheet (available at deepblue.lib.umich.edu; file name “Unused Pharmaceutical Disposal”), which contains all values and calculations used in this study (see Figure S1). Figure S2 shows the waste treatment systems employed by each disposal option for both APIs and associated packaging.

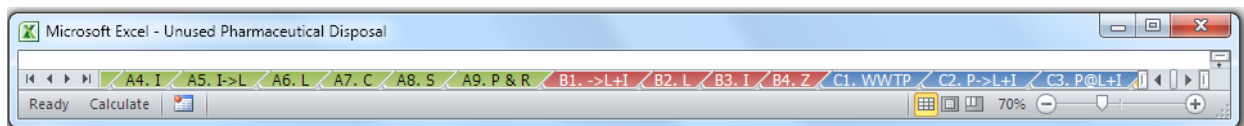


Figure S1. Spreadsheet “Unused Pharmaceutical Disposal” with worksheet labels that match the headings in this section.

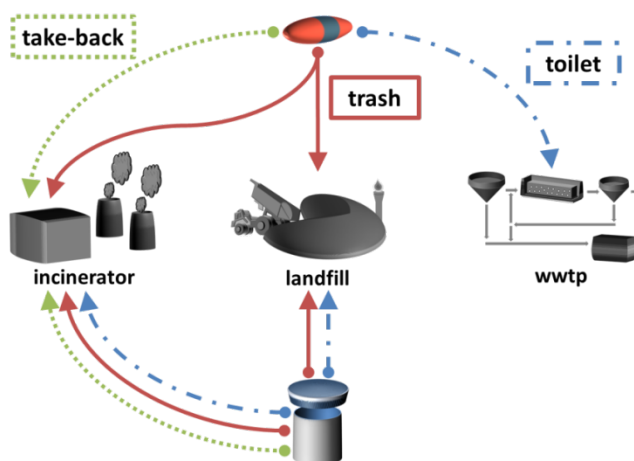


Figure S2. Waste treatment systems employed by each disposal option to manage the APIs from unused pharmaceuticals and associated packaging.
(wwtp = wastewater treatment plant)

A. Take-back

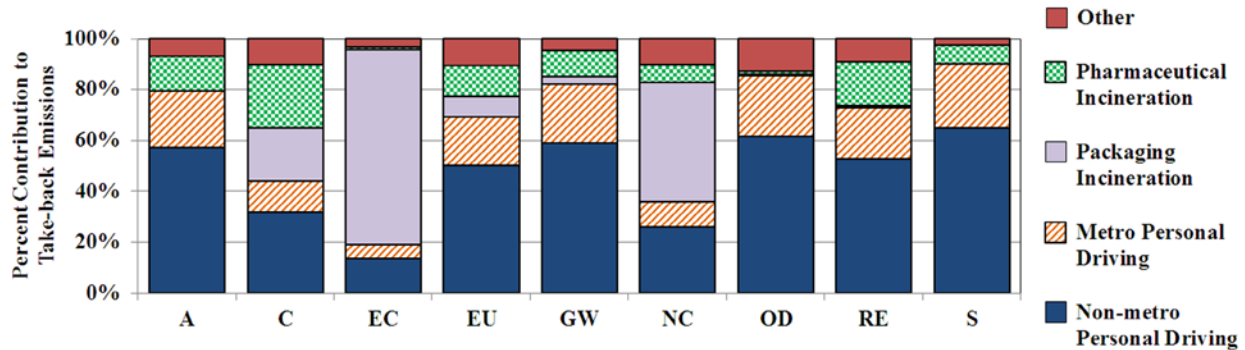


Figure S3. The contribution to overall take-back emissions by the materials and processes required by take-back disposal.

Abbreviations: A=acidification (H⁺ moles equivalent); C=carcinogenics (benzene equivalent); EC=ecotoxicity (kg 2,4-D equivalent); EU=eutrophication (kg nitrogen equivalent); GW=global warming (kg CO₂ equivalent); NC=non carcinogenics (toluene equivalent); OD=ozone depletion (kg CFC-11 equivalent); RE=respiratory effects (kg PM_{2.5} equivalent); and S=smog (kg NO_x equivalent).

A1. Personal driving to pharmacy

- Average distances from 50 random residences to the closest pharmacy are determined for nine cities that represent the U.S.'s nine rural-urban continuum codes³ (referred to as rurality categories)
- U.S. population (300 million) is distributed among these codes according to U.S. Census Bureau data³
- Types of personal vehicle are based on the 2008 vehicle market share,⁴ and all were assumed to use gasoline only
- Uncertainty parameters are used to calculate total personal driving emissions (Table S7):
 - Number of annual trips by each participant (#1)
 - Percentage of trips that are single-purpose vs. multi-purpose (#2)
 - Percentage of miles allocated to take-back during a multi-purpose trip (#3)
 - Vehicle fuel economy (#54 and #55)

A2. Hauling from pharmacy to secure storage facility

- Number of collection boxes is based on the mass of pharmaceutical waste returned and an assumed box capacity (Table S7 #4)
- Number of trips is based on the total mass hauled (pharmaceuticals, packaging, and boxes⁵) and a 21-ton⁶ truck load
- For each rurality category, Google Maps™ mapping service is used to estimate the average driving distance from a pharmacy to a secure storage facility

A3. Hauling from secure storage facility to incinerator

- Number of trips is based on a 21-ton truck load⁶ and the total mass hauled
- Driving distances from a secure storage facility to the closest commercial hazardous waste incinerator⁷ are estimated using Google Maps™ for two major pharmacy chains

A4. Incineration of APIs, packaging, & cardboard boxes

- Emissions from incinerating packaging and cardboard boxes are from life cycle inventory (LCI) databases (see Table S1)
- APIs' emissions are specific to each representative API (see Section 3C and Table S4)
- Energy recovery during hazardous waste incineration is based on the mass percent combusted with energy recovery (Table S7 #6) and the assumed energy density of 0.535 MWh electricity/ton combusted⁸

A5. Hauling API ash from incinerator to landfill

- Distances and the number of trips are based on the mass of ash generated (Table S7 #7), a 21-ton truck load,⁶ and the average driving distance from a commercial hazardous waste incinerator⁷ to the closest commercial hazardous waste landfill⁹

A6. Landfilling of API ash

- Emissions from general landfill processes are from LCI databases (see Table S1)

A7. Cardboard box production

- Emissions from cardboard production are from LCI databases (see Table S1)

A8. Steel bin production

- Total steel mass is based on a steel bin's mass¹⁰ and the number of U.S. pharmacies¹¹ (assuming each would have one steel bin if take-back is implemented nationally)
- Emissions from steel production are from LCI databases (see Table S1)
 - 60% by basic oxygen furnace and 40% by electric arc furnace¹²
 - A steel bin's lifetime is assumed to be 40 years, consistent with other LCI data and approaches^{13,14}

A9. Building infrastructure (pharmacy and secure storage facility)

- Dimensions of a steel bin¹⁰ were used to calculate the floor area required at a pharmacy
- Floor area required at a secure storage facility is based on 3 months of storage capacity, cardboard box dimensions,⁵ and assuming that boxes were stacked 25 high

B. Trash

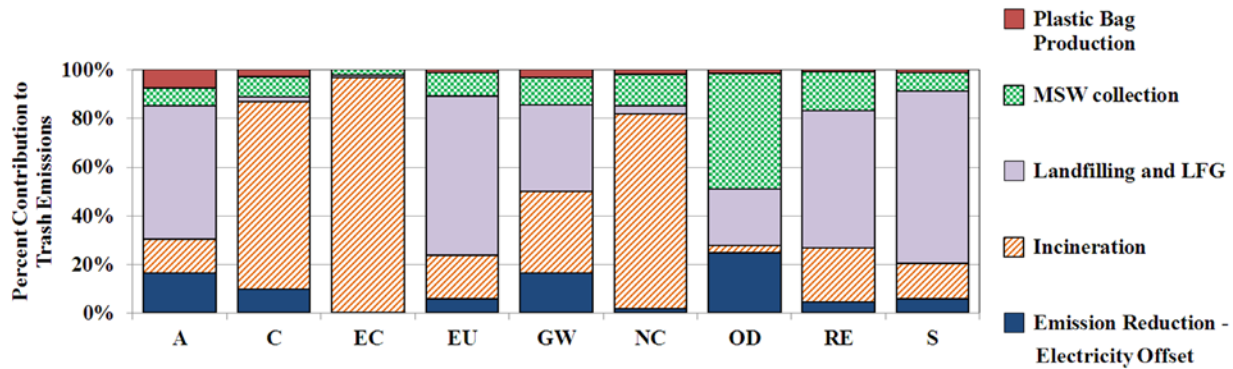


Figure S4. The contribution to overall trash emissions by the materials and processes required by trash disposal.

Note: recovery energy during incineration reduces emissions by offsetting electricity production.

B1. Trash collection and hauling APIs, packaging, and plastic bags with municipal solid waste (MSW)

- Trashed APIs, packaging, and plastic bags are landfilled (81%) and combusted with energy recovery (19%)¹⁵
- MSW collection assumed a 7-ton garbage truck load⁶ and distances for both collection (Table S7 #10) and hauling to an incinerator (Table S7 #9) or a landfill (Table S7 #8)

B2. Landfilling of APIs, packaging, and plastic bags with MSW

- Emissions from general landfill processes are from LCI databases (see Table S1)
- API landfill gas (LFG) emissions are specific to each representative API (see Section 2B and Table S3)
 - LFG has 3 fates: flared (28%), combusted for energy recovery (31%), or directly emitted (41%)¹⁶ (Table S7 #15)
- API contributions to leachate are specific to each representative API (see Section 2B)
 - Leachate is sent via piping (no energy required) to a wastewater treatment plant (WWTP)

B3. Incineration of APIs, packaging, and plastic bags with MSW

- Emissions from packaging and plastic bags are from LCI databases (see Table S1)
- APIs' emissions are specific to each representative API (see Section 3C and Table S4)
- API ash from an MSW incinerator is hauled to a MSW landfill
 - Distance is estimated using an uncertainty parameter (Table S7 #11)
 - Number of trips is based on a 21-ton truck load⁶ and total mass hauled
- Energy recovery assumes 0.535 MWh electricity/ton MSW combusted⁸

B4. Plastic bag production (LDPE film)

- The mass of low-density polyethylene (LDPE) needed plastic bags is based on the mass of a "sandwich-sized" bag
- Emissions from LDPE production are from LCI databases (see Table S1)

C. Toilet

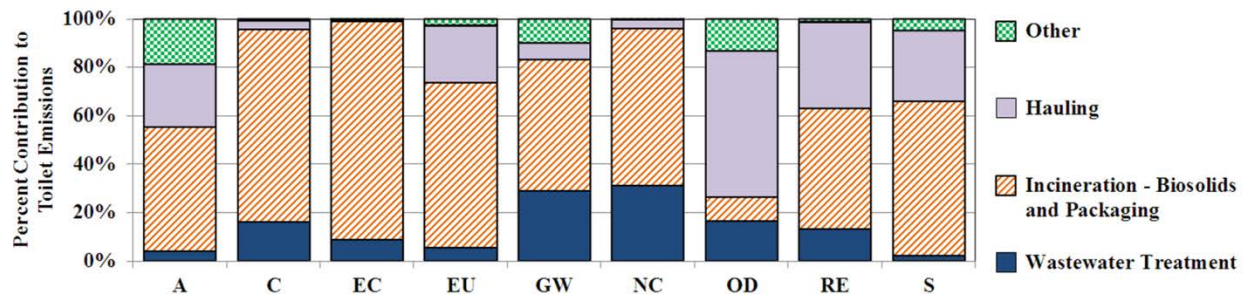


Figure S5. The contribution to overall toilet emissions by the materials and processes required by toilet disposal.

C1. Wastewater treatment of flushed APIs

- Amount of wastewater generated is based on typical volume of U.S. toilets (1.6 gallons/flush) and the number of times a person flushed APIs in a year (Table S7 #19)
- Amount of electricity used to treat this wastewater based on typical values (Table S7 #20)
 - Emissions from electricity are from LCI databases (see Table S1)
- API emissions and fate specific to each API (see Section 3A)
 - APIs sorbed to the biosolids and biosolids formed by the assimilation of API carbon are incinerated, landfilled, or land applied¹⁷
 - Incinerated biosolids and sorbed APIs generate emissions specific to the compound: air emissions (with flue gas scrubbing) and ash generation (with final disposal in a landfill)
 - Landfilled biosolids and sorbed APIs are retained in a landfill
 - Land applied biosolids have no further emissions
 - Land applied sorbed APIs are counted as API emissions

C2. Hauling packaging waste with MSW to a landfill and an incinerator

- Trashed packaging are combusted with energy recovery (19%) or landfilled (81%)¹⁵
- MSW collection assumed a 7-ton garbage truck load,⁶ a collection route distance (Table S7 #10), hauling distance to a landfill (Table S7 #8), and hauling distance to an incinerator (Table S7 #9)

C3. Packaging at landfill and incinerator

- Emissions from landfilling and incinerating packaging are from LCI databases (see Table S1)

2) Non-API Emissions

A. Life Cycle Inventory

Table S1 lists the unit processes considered in the life cycle inventory. Emissions are from three life cycle inventory databases: Ecoinvent,¹⁸ Franklin USA 1998,¹⁹ and U.S. LCI.²⁰ It also includes any modifications made to the original database's emissions (e.g. when U.S. data are substituted for European data).

Table S1. Unit processes in the life cycle inventory.

Unit Process	Source(s) of Emissions Data
Electricity generation and distribution (U.S. average)	Franklin USA 1998
Building infrastructure (30% wood and 70% steel)	Ecoinvent
Landfill process and infrastructure	Ecoinvent modified with U.S. electricity from Franklin USA 1998 database
Landfill emissions, compound specific (no APIs)	Ecoinvent
Incineration process and infrastructure	Ecoinvent
WWTP infrastructure	Ecoinvent
Cardboard production	Franklin USA 1998
Steel production (basic oxygen and electric air furnace)	Franklin USA 1998
Plastic bag production (low-density polyethylene film)	Franklin USA 1998
Gasoline production	Franklin USA 1998
Personal vehicle (car) emissions and infrastructure	Ecoinvent modified with emissions and fuel economy from EPA ²¹
Personal vehicle (light truck) emissions and infrastructure	Ecoinvent modified with emissions and fuel economy from EPA ²¹
Diesel production	Franklin USA 1998
Garbage truck emissions and infrastructure (full, load 7 tons)	Ecoinvent and modified with fuel economy from U.S. LCI
Garbage truck emissions and infrastructure (empty)	Ecoinvent modified with fuel economy from U.S. LCI and emissions from both the EPA ²² and Federal Highway Administration ²³
Semi-trailer truck emissions and infrastructure (full, load 21 tons)	Ecoinvent modified with emissions and fuel economy from U.S. LCI
Semi-trailer truck emissions and infrastructure (empty)	Ecoinvent modified with fuel economy from U.S. LCI and emissions from both the EPA ²² and Federal Highway Administration ²³

3) API Fates and Emissions

Table S2 shows the nine representative APIs used in this study and their physicochemical properties (octanol/water partition coefficient, acid dissociation constant, and Henry's law constant).

Table S2. API identification and physicochemical properties. (*n/a is not available*)

API	CAS#	log K _{ow} ^(citation)	pK _a ^(citation)	K _h ²⁴ (atm-L/mol)
Acetaminophen	103-90-2	0.46 ⁽²⁴⁾	9.4 ⁽²⁴⁾	6.42·10 ⁻¹⁰
Aspirin	50-78-2	1.2 ⁽²⁴⁾	3.5 ⁽²⁴⁾	1.30·10 ⁻⁶
Vitamin E	59-02-9	12 ⁽²⁴⁾	11 ⁽²⁵⁾	<i>n/a</i>
Prednisone	53-03-2	1.5 ⁽²⁴⁾	12 ⁽²⁵⁾	2.83·10 ⁻⁷
Ibuprofen	15687-27-1	4.0 ⁽²⁴⁾	4.9 ⁽²⁴⁾	1.50·10 ⁻⁴
Warfarin	81-81-2	2.6 ⁽²⁴⁾	5.1 ⁽²⁴⁾	2.77·10 ⁻⁶
Topiramate	97240-79-4	1.3 ⁽²⁶⁾	9.2 ⁽²⁵⁾	<i>n/a</i>
Etodolac	41340-25-4	3.9 ⁽²⁴⁾	4.7 ⁽²⁷⁾	<i>n/a</i>
Gabapentin	60142-96-3	-1.1 ⁽²⁴⁾	4.7 ⁽²⁵⁾	1.81·10 ⁻⁷

Further Description of Table 1 in the manuscript

Values presented in Table 1 are calculated in the following manner (all percentages are bounded by 0% and 100%).

The WWTP overall percent removal values from the literature indicate the mass removal of an API from the liquid phase. The minimum WWTP overall removal is the cited literature value minus 25%, and the maximum value is the cited literature value plus 25%.

The WWTP percent sorption values are calculated using one-parameter linear free energy relationships and each API's physicochemical properties (as described below in Section 2A). The minimum values are calculated using minimum WWTP overall removal values and a mixed liquor suspended solids (MLSS) concentration of 1 g/L. The maximum sorption values use the maximum WWTP overall removal values and an MLSS concentration of 4 g/L.

The WWTP percent biotransformation values are calculated as the difference between the overall percent removal and the percent removal by sorption. The minimum value subtracts the maximum sorption value from the minimum overall removal value. The maximum value subtracts the minimum sorption value from the maximum overall removal value.

The landfill biotransformation values are calculated by applying the anaerobic biotransformation potential parameter ($N_{LF/WWTP}$) to the average WWTP percent biotransformation values. The average WWTP percent biotransformation values are calculated using the literature WWTP overall removal values and the percent sorption values calculated with a MLSS concentration of 2.5 g/L. The minimum landfill biotransformation values are calculated when $N_{LF/WWTP}=0$. The maximum values are calculated when $N_{LF/WWTP}=1$.

Landfill sorption values are calculated with opLFERs. The minimum values are estimated by subtracting 25% from the sorption values calculated when $N_{LF/WWTP}=1$, the open leachate collection and removal system (LCRS) flowrate=10000 L/ha/d, the closed LCRS=1000 L/ha/d, and the landfill height=10m. The maximum values are calculated by adding 25% to the sorption values calculated when $N_{LF/WWTP}=0$, the open LCRS=100 L/ha/d, the closed LCRS=10 L/ha/d, and the landfill is 50 m high.

A. Wastewater Treatment Plant

Figure S6 shows how API removal from the liquid phase of wastewater at a WWTP is modeled. Each API's physicochemical properties (Table S2) and values for the overall percent removal during wastewater treatment (Table 1) are used to calculate the percent of an API's total mass that will both sorb and be biotransformed.

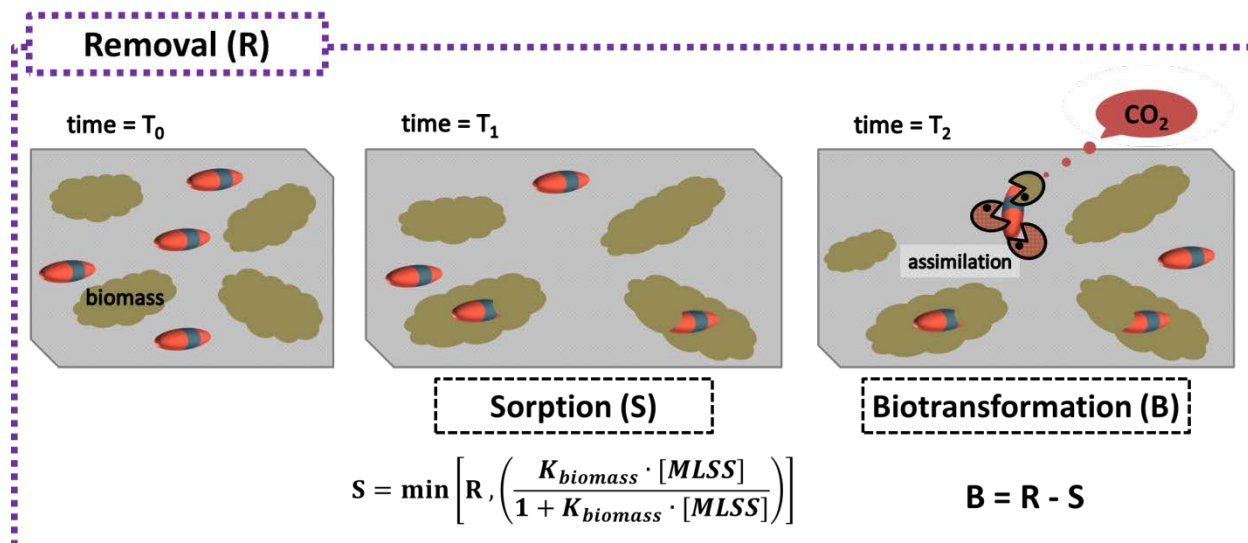


Figure S6. Removal is the overall WWTP percent removal for an API (R); sorption is to biomass (S); biotransformation is aerobic (B).

For sorption calculations, we assume that sorbed APIs are not bioavailable. Desorption is not included in these calculations but is later incorporated with uncertainty parameters used for the final sorption estimations (see Table S7 #31-39). Each API's biomass/wastewater partition coefficient ($K_{biomass}$) is estimated using its octanol/water partition coefficient (K_{ow}), its acid dissociation constant (pK_a), a wastewater pH of 7.5,²⁸ and the opLFER given below:²⁹

$$K_{biomass} \left(\frac{\text{liter}}{\text{gram}} \right) = \frac{\left(\frac{\text{mass of API sorbed}}{\text{mass of biomass}} \right)}{\left(\frac{\text{mass of API in liquid phase}}{\text{volume of solution}} \right)} = 10^{m \cdot \log \left(\frac{K_{ow}}{1 + 10 \cdot |pH - pK_a|} \right) + b} \quad (S1)$$

Where coefficients m and b are based on an API's functional groups.

The API mass percentage that sorbs to biomass is calculated using typical MLSS concentrations (Table S7 #40) and each API's $K_{biomass}$ coefficient with the following equation:³⁰

$$\% \text{ Sorbed} = \frac{C_{sorbed}}{C_{soluble} + C_{sorbed}} = \frac{K_{biomass} \cdot [MLSS]}{1 + K_{biomass} \cdot [MLSS]} \quad (S2)$$

Where C_{sorbed} is the concentration of API sorbed and $C_{soluble}$ is the concentration of API in the liquid phase.

For the final calculation of percent removal by sorption, the percentage was bound by an API's overall WWTP percent removal as shown by the following equation:

$$\begin{aligned} & (\% \text{ Removed by Sorption}) \\ & = \min \left[(\text{Overall \% Removal}), \left(\frac{K_{biomass} \cdot [MLSS]}{1 + K_{biomass} \cdot [MLSS]} \right) \right] \end{aligned} \quad (S3)$$

The remaining overall percent removal is assumed to be by biotransformation, shown here:

$$\begin{aligned} & (\% \text{ Removed by biotransformation}) \\ & = (\text{Overall WWTP \% Removal}) - (\% \text{ Removed by Sorption}) \end{aligned} \quad (S4)$$

Due to the lack of information about API transformation products (TPs), we assume that all aerobically biotransformed APIs are mineralized or assimilated into biomass. The mass of API carbon assimilated is based on observed yields for heterotrophs (Table S7 #17).

B. Landfill

Figure S7 shows the approach used to calculate the mass of APIs that anaerobically biotransform, sorb to MSW, or leave a landfill in the leachate.

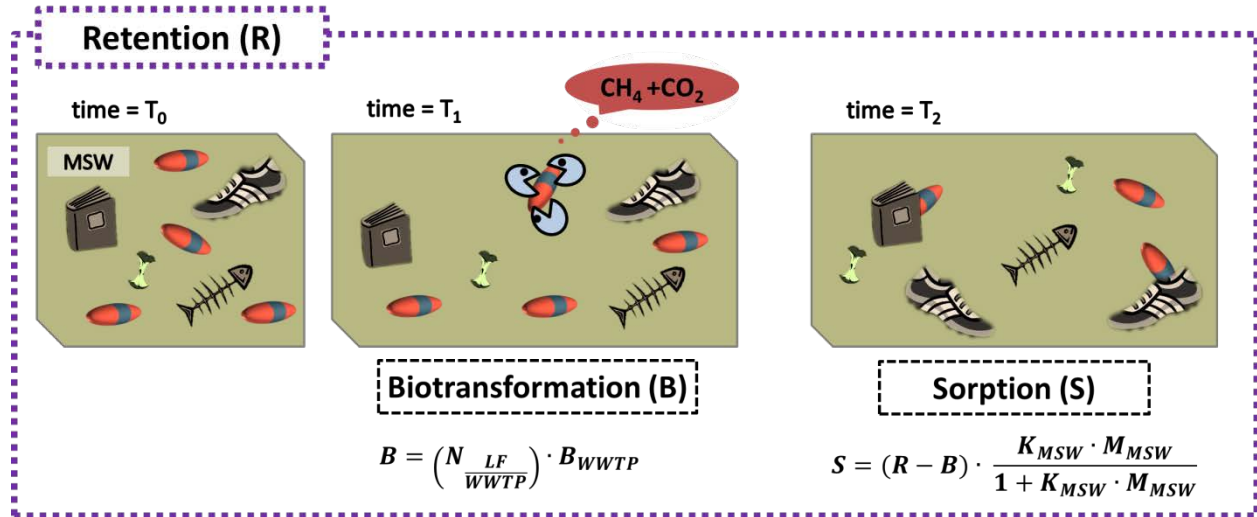


Figure S7. Landfill retention (R) is the total API mass that does not enter the leachate. It is the sum of APIs that are anaerobically biotransformed (B) and sorbed to MSW (S). Anaerobic biotransformation is based on the extent of aerobic biotransformation during wastewater treatment (B_{WWTP}).

The mass of API expected to anaerobically biotransform in a landfill is calculated using each API's aerobic wastewater biotransformation percentage with the following equation:

$$\begin{aligned} (\% \text{ Biotransformation in a Landfill}) \\ = \left(N_{\frac{LF}{WWTP}} \right) \cdot (\% \text{ Biotransformation in a WWTP}) \end{aligned} \quad (\text{S5})$$

Where the following is an uncertainty parameter (Table S7 #41):

$$N_{\frac{LF}{WWTP}} = \frac{\text{extent of landfill anaerobic biotransformation}}{\text{extent of wastewater aerobic biotransformation}} = [0,1]$$

Similar to wastewater treatment, due to the lack of information about API TPs, we assume that all anaerobically biotransformed APIs form LFG. Since all non-API emissions will be lower than baseline emissions if landfilled APIs do not produce LFG, the recommendation of trash disposal will not change if future research shows that LFG production from APIs is minimal. The LFG composition³⁷ is based on each API's chemical formula and the assumption that 45% of carbon forms CO₂ and 55% forms CH₄³² (see Table S3). Combusted LFG (31% for energy recovery and 28% flared¹⁶) is assumed to be completely oxidized.

Table S3. Landfill gas composition (mole compound/mole API) before flaring.

API	CO ₂	CH ₄	H ₂	H ₂ O	N ₂	H ₂ S
Acetaminophen	3.6	4.4	0.0	0.0	0.5	0.0
Aspirin	4.1	5.0	0.0	0.0	0.0	0.0
Vitamin E	13	16.0	0.0	0.0	0.0	0.0
Prednisone	9.5	12	0.0	0.0	0.0	0.0
Ibuprofen	5.9	7.2	0.0	0.0	0.0	0.0
Warfarin	8.6	11	0.0	0.0	0.0	0.0
Topiramate	5.4	6.6	0.0	0.0	0.5	1.0
Etodolac	7.7	9.4	0.0	0.0	0.5	0.0
Gabapentin	4.1	5.0	0.0	0.0	0.5	0.0

Sorption estimations are based on a MSW/leachate partition coefficient (K_{MSW}) for each API. These coefficients are calculated with the following opLFER that describes the sorption of organic compounds to MSW:³³

$$K_{MSW} \left(\frac{\text{liter}}{\text{gram}} \right) = \frac{\left(\frac{\text{mass of API sorbed}}{\text{net mass of MSW}} \right)}{\left(\frac{\text{mass of API in liquid phase}}{\text{volume of leachate}} \right)} = 10^{0.816 \cdot \log(K_{ow}) + 0.166} \quad (\text{S6})$$

The net mass of MSW and volume of leachate and are calculated using average values for landfills in the U.S.^{6,31,32,34} The net mass of MSW is calculated yearly over a 40 year period, which is the length of time that the leachate from a landfill is collected, removed, and treated.³² A landfill was assumed to accept MSW for 20 years.³² MSW degradation is calculated using the U.S. Environmental Protection Agency's (EPA) model³¹ with average parameter values.³² Leachate volume is calculated by estimating a typical height for landfills (Table S7 #44) and modeling a landfill to have one cell, 2-8 acres in size,³⁴ open at a time. An open cell is assumed to receive waste and be compacted and covered daily. After 2 years,³⁴ an open cell is assumed to be full and is closed by placing a permanent cover on top. Open and closed cells have different leachate collection and recovery system (LCRS) rates due to the differences in each cover's permeability,⁶ and these values are estimated with uncertainty parameters (Table S7 #42 and #43).

The API mass percentage that sorbs to MSW is calculated using the net mass of MSW in a landfill (M_{MSW}) and the API's K_{MSW} coefficient with the following equation:

$$(\% \text{ Sorbed}) = \frac{C_{\text{sorbed}}}{C_{\text{leachate}} + C_{\text{sorbed}}} = \frac{K_{MSW} \cdot M_{MSW}}{1 + K_{MSW} \cdot M_{MSW}} \quad (S7)$$

Finally, the API mass that does not biotransform or sorb is removed with the landfill leachate and sent to a WWTP for treatment.

C. Incinerator

Table S4 shows the air emissions assumed to result from API incineration before flue gas treatment. Before release to the atmosphere, a wet scrubber removes 90% of the sulfur dioxide mass^{35,36} and a catalytic converter removes 90% of the nitrogen dioxide mass³⁶ from the flue gas. The percentage of API mass that becomes incineration ash is based on average values for MSW (Table S7 #7). Incineration ash does not contain APIs and is hauled to a landfill.

Table S4. Emissions from the complete oxidation of APIs (incineration) based on each compound's chemical formula.

	CO ₂ (kg/kg API)	H ₂ O (kg/kg API)	NO ₂ (kg/kg API)	SO ₂ (kg/kg API)
Acetaminophen	2.0	0.4	0.3	0.0
Aspirin	1.9	0.3	0.0	0.0
Vitamin E	2.5	0.9	0.0	0.0
Prednisone	2.2	0.6	0.0	0.0
Ibuprofen	2.4	0.7	0.0	0.0
Warfarin	2.3	0.4	0.0	0.0
Topiramate	1.3	0.5	0.1	0.2
Etodolac	2.2	0.6	0.1	0.0
Gabapentin	2.0	0.8	0.2	0.0

4) Emissions Results

Table S5 describes the scenarios discussed in the research article. Table S6 lists emission magnitudes for all disposal scenarios. Table S7 describes all uncertainty parameters. Table S8 provides result from the sensitivity analysis.

Table S5. Disposal scenarios with participation rates and adjustments made to uncertainty parameters.

Disposal Scenarios	Participation				Uncertainty Parameters	
	Take-back (metro)	Take-back (non-metro)	Trash	Toilet	% Single purpose trips for take-back	% Miles allocated to take-back during multi-purpose trips
Baseline	0%	0%	60%	40%	0-100%	0-100%
Toilet	0%	0%	0%	100%		
Trash	0%	0%	100%	0%		
Take-back	100%	100%	0%	0%		
“Best-Case” Take-Back (I)	50%	0%	0%	0%	0%	0%
“Best-Case” Take-Back (II)	50%	0%	10%	7%		
43% Take-back	43%	43%	57%	0%		
43% Take-back without driving	43%	43%	57%	0%	0%	0%

A) Emissions Magnitudes

Table S6. The mean as well as the 10th, 25th, 50th, 75th, and 90th percentile values from each scenario's Monte Carlo simulation.
Abbreviations: A=acidification (H⁺ moles equivalent); C=carcinogenics (benzene equivalent); EC=ecotoxicity (kg 2,4-D equivalent); EU=eutrophication (kg nitrogen equivalent); GW=global warming (kg CO₂ equivalent); NC=non carcinogenics (toluene equivalent); OD=ozone depletion (kg CFC-11 equivalent); RE=respiratory effects (kg PM_{2.5} equivalent); and S=smog (kg NO_x equivalent).

		A	C	EC	EU	GW	NC	OD	RE	S	API
Baseline	Mean	5.3E+07	7.2E+04	1.9E+08	3.7E+04	8.4E+07	6.8E+08	4.7E-01	1.5E+05	7.6E+05	2.3E+07
	10%	1.2E+07	6.2E+04	1.3E+08	1.5E+04	6.0E+07	5.2E+08	3.0E-01	2.5E+04	2.5E+05	2.1E+07
	25%	2.0E+07	6.6E+04	1.5E+08	1.9E+04	6.8E+07	5.8E+08	3.8E-01	3.5E+04	3.5E+05	2.2E+07
	50%	3.9E+07	7.1E+04	1.8E+08	3.1E+04	7.9E+07	6.7E+08	4.7E-01	6.7E+04	6.1E+05	2.3E+07
	75%	7.1E+07	7.6E+04	2.2E+08	5.0E+04	9.6E+07	7.6E+08	5.6E-01	2.0E+05	1.0E+06	2.4E+07
	90%	1.2E+08	8.2E+04	2.4E+08	7.1E+04	1.2E+08	8.6E+08	6.4E-01	4.1E+05	1.5E+06	2.5E+07
Toilet	Mean	4.5E+06	7.4E+04	2.0E+08	8.2E+03	7.3E+07	8.1E+08	2.6E-01	1.1E+04	1.2E+05	5.3E+07
	10%	2.9E+06	6.0E+04	1.4E+08	6.4E+03	5.8E+07	5.5E+08	1.9E-01	7.7E+03	8.2E+04	4.9E+07
	25%	3.6E+06	6.5E+04	1.6E+08	7.2E+03	6.4E+07	6.3E+08	2.2E-01	9.0E+03	9.7E+04	5.1E+07
	50%	4.5E+06	7.1E+04	2.0E+08	8.2E+03	7.3E+07	7.4E+08	2.5E-01	1.1E+04	1.2E+05	5.3E+07
	75%	5.3E+06	7.9E+04	2.3E+08	9.2E+03	8.2E+07	8.9E+08	3.0E-01	1.2E+04	1.3E+05	5.5E+07
	90%	6.0E+06	9.4E+04	2.5E+08	1.0E+04	9.0E+07	1.2E+09	3.5E-01	1.4E+04	1.5E+05	5.7E+07
Trash	Mean	8.5E+07	7.0E+04	1.8E+08	5.7E+04	9.2E+07	6.0E+08	6.1E-01	2.4E+05	1.2E+06	2.7E+06
	10%	1.7E+07	6.1E+04	1.3E+08	1.9E+04	5.4E+07	4.7E+08	3.6E-01	3.4E+04	3.3E+05	1.1E+06
	25%	3.0E+07	6.5E+04	1.4E+08	2.7E+04	6.4E+07	5.2E+08	4.7E-01	5.1E+04	5.0E+05	1.8E+06
	50%	6.2E+07	7.0E+04	1.8E+08	4.6E+04	8.1E+07	5.9E+08	6.1E-01	1.0E+05	9.4E+05	2.6E+06
	75%	1.2E+08	7.5E+04	2.1E+08	7.8E+04	1.1E+08	6.8E+08	7.4E-01	3.3E+05	1.7E+06	3.5E+06
	90%	1.9E+08	7.9E+04	2.3E+08	1.1E+05	1.4E+08	7.3E+08	8.6E-01	6.7E+05	2.4E+06	4.4E+06
Take-back	Mean	3.5E+08	9.0E+05	1.2E+09	3.7E+05	1.9E+09	5.8E+09	9.5E+00	4.6E+05	1.4E+07	0.0E+00
	10%	1.5E+08	6.1E+05	8.6E+08	1.8E+05	7.8E+08	4.1E+09	3.6E+00	2.1E+05	4.7E+06	0.0E+00
	25%	2.1E+08	7.0E+05	1.0E+09	2.4E+05	1.1E+09	4.8E+09	5.5E+00	2.9E+05	7.5E+06	0.0E+00
	50%	3.3E+08	8.6E+05	1.2E+09	3.5E+05	1.8E+09	5.7E+09	8.8E+00	4.3E+05	1.3E+07	0.0E+00
	75%	4.8E+08	1.1E+06	1.4E+09	4.8E+05	2.6E+09	6.8E+09	1.3E+01	6.0E+05	1.9E+07	0.0E+00
	90%	6.0E+08	1.2E+06	1.5E+09	5.9E+05	3.3E+09	7.7E+09	1.7E+01	7.4E+05	2.5E+07	0.0E+00

Table S6 Continued.

		A	C	EC	EU	GW	NC	OD	RE	S	API
“Best Case” Take-back	Mean	1.1E+08	5.0E+05	8.7E+08	1.4E+05	5.3E+08	3.7E+09	2.6E+00	1.8E+05	3.0E+06	4.0E+06
	10%	7.1E+07	4.3E+05	6.3E+08	1.0E+05	3.5E+08	3.0E+09	1.6E+00	1.2E+05	1.6E+06	3.6E+06
	25%	8.4E+07	4.6E+05	7.2E+08	1.2E+05	4.1E+08	3.3E+09	2.0E+00	1.4E+05	2.0E+06	3.8E+06
	50%	1.1E+08	5.0E+05	8.7E+08	1.3E+05	5.1E+08	3.7E+09	2.5E+00	1.6E+05	2.8E+06	3.9E+06
	75%	1.3E+08	5.4E+05	1.0E+09	1.6E+05	6.3E+08	4.1E+09	3.2E+00	2.1E+05	3.8E+06	4.1E+06
	90%	1.6E+08	5.8E+05	1.1E+09	1.8E+05	7.4E+08	4.4E+09	3.7E+00	2.6E+05	4.6E+06	4.3E+06
43% Take-back	Mean	2.0E+08	4.3E+05	6.2E+08	1.9E+05	8.8E+08	2.9E+09	4.6E+00	3.3E+05	6.6E+06	1.5E+06
	10%	9.8E+07	3.1E+05	4.5E+08	1.1E+05	3.9E+08	2.2E+09	2.0E+00	1.5E+05	2.6E+06	6.4E+05
	25%	1.4E+08	3.5E+05	5.2E+08	1.4E+05	5.4E+08	2.5E+09	2.8E+00	2.0E+05	3.9E+06	1.0E+06
	50%	1.9E+08	4.2E+05	6.2E+08	1.8E+05	8.3E+08	2.9E+09	4.3E+00	2.9E+05	6.2E+06	1.5E+06
	75%	2.6E+08	5.1E+05	7.1E+08	2.4E+05	1.2E+09	3.3E+09	6.1E+00	4.1E+05	8.9E+06	2.0E+06
	90%	3.1E+08	5.8E+05	7.8E+08	2.9E+05	1.5E+09	3.8E+09	7.6E+00	5.9E+05	1.1E+07	2.5E+06
43% Take-back Without driving	Mean	8.0E+07	2.7E+05	5.2E+08	8.2E+04	2.0E+08	2.0E+09	1.1E+00	1.9E+05	1.3E+06	1.5E+06
	10%	4.1E+07	2.4E+05	3.7E+08	5.9E+04	1.7E+08	1.7E+09	8.6E-01	7.4E+04	7.7E+05	6.4E+05
	25%	4.9E+07	2.5E+05	4.3E+08	6.5E+04	1.9E+08	1.8E+09	9.5E-01	8.4E+04	8.7E+05	1.0E+06
	50%	6.7E+07	2.7E+05	5.2E+08	7.6E+04	2.0E+08	2.0E+09	1.1E+00	1.1E+05	1.1E+06	1.5E+06
	75%	9.8E+07	2.8E+05	6.2E+08	9.5E+04	2.2E+08	2.3E+09	1.2E+00	2.4E+05	1.5E+06	2.0E+06
	90%	1.4E+08	2.9E+05	6.8E+08	1.1E+05	2.4E+08	2.4E+09	1.3E+00	4.3E+05	2.0E+06	2.5E+06

B) Uncertainty Parameters

Table S7. The ranges and data sources of each uncertainty parameter.

Notes: OM=order of magnitude. All distances are one-way.

#	Uncertainty Parameters	Units	Low (L) Value	High (H) Value	Justification	Notes
1	Number of trips to pharmacy	trips/cap/yr	1	12	L=once a year H=once a month	Number of trips an individual makes to return unused medications
2	Single-purpose trips	% trips	0%	100%	L,H=total possible range	Percentage of trips with the sole purpose of returning medication
3	Take-back mile allocation for multi-purpose trips	% distance	0%	100%	L,H=total possible range	Percentage of a multi-purpose trip's distance allocated to take-back
4	Mass of full cardboard box	lbs	20	40	L=minus 10 lbs H=plus 10 lbs	Assumed 20-gallon box can hold 30 lbs (twice mass for 10-gallon box ⁵).
5	Mass packaging per pharmaceutical	% mass	10%	20%	L,H=cited range	Pilot take-back program found 10-20% of the collected waste was packaging ³⁷
6	Take-back incineration energy recovery	% mass	0%	100%	L,H=total possible range	Energy recovered during the incineration of hazardous waste
7	Incineration ash from APIs and biosolids	% mass	2%	20%	L=PE ¹⁴ H= MSW ¹⁴	Ash produced estimated as similar to polyethylene (PE) and average MSW
8	City to landfill	miles	10	100	L=half of ³⁸ H=OM more than L	EPA WARM default distance (20 miles) ³⁸
9	City to incinerator	miles	10	100	L=half of ³⁸ H=OM more than L	EPA WARM default distance (20 miles) ³⁸
10	Garbage truck collection route distance	miles	10	100	L=half of ³⁸ H=OM more than L	Assumed similar to WARM default distance
11	Incinerator to landfill	miles	10	100	L=half of ³⁸ H=OM more than L	Assumed similar to WARM default distance
12	WWTP to incinerator	miles	10	100	L=half of ³⁸ H=OM more than L	Assumed similar to WARM default distance
13	WWTP to landfill	miles	10	100	L=half of ³⁸ H=OM more than L	Assumed similar to WARM default distance

Table S7 Continued.

#	Uncertainty Parameters	Units	L	H	Justification	Notes
14	WWTP to land application site	miles	10	100	L=a third of ³⁹ H=OM more than L	A WWTP to a land application site is usually more than 30 miles ³⁹
15	Landfill gas (LFG) recovered for energy	% mass	31%	100%	L= ¹⁶ H=maximum	Currently 28% flaring, 31% energy recovery, and 41% direct emissions ¹⁶
16	Landfill gas energy content	kWh/short ton MSW	139	362	L,H=cited range	Energy content of landfill gas when combusted for electricity generation ⁴⁰
17	Aerobic, heterotroph observed yield	g cell COD/ g API COD	0.0	0.71	L=no growth H= ⁴¹	Typical activated sludge kinetic coefficients for heterotrophic bacteria ⁴¹
18	Mass of pharmaceutical per bag (trash disposal)	lbs	0.06	0.7	L=once a month H=once a year	Each person has 0.7 lbs of drugs thrown away at least once a year
19	Mass of pharmaceutical per flush (toilet disposal)	kg/flush	0.027	0.32	L=once a month H=once a year	Each person has 0.32 kg of drugs flushed away at least once a year
20	Wastewater treatment energy demand	kWh per 10 ⁶ gallons	530	1100	L=1200*(1-0.56) H=2500*(1-0.56)	WWTPs use 1200-2500 kWh/Mgal and 56% is for aeration ⁴²
21	WWTP biogenic electricity sources	% kWh	0%	100%	L,H=total possible range	Energy recovered from waste (with biogenic carbon emissions)
22-30	WWTP removal factors for all 9 APIs	% mass	-25%	+25%	L,H=(% overall removal) $\pm 25\%$	Factor applied to WWTP overall percent removal values ^{27,43-48}
31-39	WWTP sorption factors for all 9 APIs	% mass	-25%	+25%	L,H=(% sorption) $\pm 25\%$	Factor applied to the calculated percent sorption values
40	MLSS	g/L	1.0	4.0	L=conventional H=complete mix	Mixed liquor suspended solids (MLSS) typical concentrations and ranges ⁴¹
41	N _{LF/WWTP}	<i>dimensionless</i>	0.0	1.0	L,H=total possible range	Ratio of anaerobic to aerobic percent biotransformation
42	Daily cover LCRS	L/ha/d	100	10000	L=OM less than ³² H=OM more than ³²	Leachate collection and recovery systems (LCRS) rate for open landfill ³²
43	Final cover LCRS	L/ha/d	10	1000	L=OM less than ³² H=OM more than ³²	LCRS rate for closed landfill ³²
44	Final landfill height	m	10	50	L=shortest H=tallest	Total height for several landfills in the U.S. ³²

Table S7 Continued.

#	Uncertainty Parameters	Units	L	H	Justification	Notes
45-53	Landfill sorption factor – for all 9 APIs	% mass	-25%	+25%	L,H=(% sorption) $\pm 25\%$	Factor applied to the calculated percent sorption
54	Car mileage	miles per gal gas	19.4	26.9	$L=(^{21})*90\%$ $H=(^{21})*125\%$	Average car mileage, ²¹ assumed fuel economy will improve
55	Light truck mileage	miles per gal gas	15.5	21.5	$L=(^{21})*90\%$ $H=(^{21})*125\%$	Average car mileage, ²¹ assumed fuel economy will improve
56	Combination Truck Mileage	miles per gal diesel	4.9	6.8	$L=(^{49})*90\%$ $H=(^{49})*125\%$	Average combination truck mileage, ⁴⁹ assumed fuel economy will improve
57	Single-Unit Truck mileage	miles per gal diesel	4.0	5.5	$L=(^{50})*90\%$ $H=(^{50})*125\%$	Average mileage for garbage trucks less than 40,000 lbs (empty), ⁵⁰ assumed fuel economy will improve
58	Garbage Truck mileage	kg diesel per tkm	0.25	0.37	$L=(^{18})*75\%$ $H=(^{18})*110\%$	Average mileage for garbage trucks, ¹⁸ and assumed lower fuel economy due to stops during collection route
59	API Chemistry – Carbon	mole carbon	-10	10	L, H= average of range (8-29 moles C)	Number of moles added during API oxidation and reduction calculations (impacting non-API emissions)
60	API Chemistry – Hydrogen	mole hydrogen	-20	20	L, H= average of range (8-50 moles H)	Number of moles added during API oxidation and reduction calculations (impacting non-API emissions)
61	API Chemistry – Nitrogen	mole nitrogen	-1	1	L, H= average of range (0-1 moles N)	Number of moles added during API oxidation and reduction calculations (impacting non-API emissions)
62	API Chemistry – Sulfur	mole sulfur	-1	1	L, H= average of range (0-1 moles S)	Number of moles added during API oxidation and reduction calculations (impacting non-API emissions)

C) Sensitivity Analysis

The model results are sensitive to only 3 of the 62 uncertainty parameters (see Table S8): 1) the mass of packaging per mass of API; 2) the number of trips to a pharmacy in one year by each take-back participant; and 3) the heterotrophic yield observed when APIs are the substrate. While the disposal options are sensitive to these parameters, the emission trends of each disposal scenario is unaffected by uncertainty in these parameters.

Table S8. Emissions categories sensitive ($|\rho|>0.8$) to a particular uncertainty parameter. Negative and positive signs indicate correlation. Disposal scenarios include: baseline, 100% Trash, 100% Toilet, and 100% Take-back.*

		Uncertainty Parameters		
		Mass of packaging per mass API	Heterotroph Observed yield	Number of trips to pharmacy
Emissions Categories	Acidification			+Take-back
	Carcinogenics			+Take-back
	Ecotoxicity	+All (baseline, toilet, trash, Take-back)		
	Eutrophication			+Take-back
	Global Warming		-Toilet	+Take-back
	Non carcinogenics	+Trash		
	Ozone depletion			+Take-back
	Respiratory effects			+Take-back
	Smog			+Take-back
	API Emissions			

*An example for the 100% take-back disposal scenario (“Take-back”) that shows how to interpret this table: As the value of the uncertainty parameter “number of trips to a pharmacy” increases, so do acidification emissions because the acidification emissions category is strongly and positively correlated with the number of trips.

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