The Environmental and economic viability of chitosan production in Guayas-Ecuador: A robust investment and life cycle analysis

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Inventory Analysis of The Entire Processes in Chitosan Production

- ### Shrimp farming and processing

Table S1. Shrimp Farming (Semi-Intensive) and Processing- Inventory

Exchanges	Unit	Amount
Output of products/services:		
Shrimp meat	ton	0.7
Shrimp shell	ton	0.3
Input from nature (resources)		
Water, salt, ocean	m3	13
Water, fresh	m3	2.1
Input of products/services:		
Diesel, from crude oil, consumption mix, at refinery, 200 ppm sulphur EU-15 S	kg	7.08
Concrete block {RoW}| production | APOS, S	kg	1.42
Sodium hypochlorite/RER	kg	103
PVC pipe E	kg	1.3
Calcium oxide, flakes (GLO), market for | APOS, S	kg	318
Calcium carbonate, precipitated {RoW}| market for calcium carbonate, precipitated | APOS, U	kg	909
Feed	kg	970
Emissions to water:		
Phosphorus, total	kg	3.5
Nitrogen, total	kg	38
Ammonia	kg	-0.19
BOD5	kg	21
Suspended solids	kg	-8.19

Process

Table S2. Demineralization-Wastewater Inventory

Exchanges	Unit	Amount
Residue:		
Acid-Wastewater	kg	87
Avoided Products:		
Calcium chloride {RoW}| market for calcium chloride | APOS, S	kg	1.24
Magnesium chloride {RoW}| market for calcium chloride | APOS, S	kg	1.18
Sodium chloride, for chlor-alkali electrolysis, at plant/RER	kg	0.39
Input of products/services:		

Sodium bicarbonate {GLO}| market for sodium bicarbonate | APOS, S	kg	2.86
Emissions to air:		
Carbon dioxide	kg	0.084
Emissions to water for treatment:		
Wastewater, unpolluted {RoW}| market for wastewater, unpolluted | APOS, S	m3	0.085

Table S3. Deproteinization Wastewater Inventory

Exchanges	**Unit**	**Amount**
Residue:		
Basic-Wastewater	kg	87.5
Avoided Products:		
Sodium hydroxide, without water, in 50% solution state {GLO}| market for | APOS, S	kg	1.766
Input of products/services:		
Hydrochloric acid, without water, in 30% solution state {RoW}| market for | APOS, U	kg	0.03
Sodium bicarbonate {GLO}| market for sodium bicarbonate | APOS, S	kg	0.07
Emissions to air:		
Carbon dioxide	kg	1.72
Ammonia	kg	0.03059
Dinitrogen monoxide	kg	0.0014
Carbon dioxide, biogenic	kg	0.04
Emissions to water for treatment:		
Wastewater, unpolluted {RoW}| market for wastewater, unpolluted | APOS, S	m3	0.087
Sodium Hydroxide 50%, treatment	kg	1.766

Table S4. Ethanol Production Inventory

Exchanges	**Unit**	**Amount**
Product:		
Ethanol, 85%	kg	1000
Avoided product:		
Carbon Dioxide	m3	183
Natural resources:		
Water, river, RoW	m3	14.2
Input of products/services:		
Molasses	kg	4000
Electricity, high voltage {BR}| cane sugar production with ethanol by-product | APOS, S	kWh	12553
Vapor	kg	2400
Urea, as 100% CO(NH2)2 (NPK 46.6-0-0), at regional storehouse/RER Mass	kg	0.71
Emissions to air:		
Carbon dioxide	kg	6.3

Emissions to water for treatment:		
Wastewater, unpolluted {RoW}| market for wastewater, unpolluted | APOS, S	m3	0.087

Table S5. Chitosan Production Inventory

Exchanges	**Unit**	**Amount**
Product:		
Chitosan (Base Scenario-50% NaOH Solution)	kg	1
Avoided products:		
Urea, as N {GLO}| market for | APOS, S	kg	1.22
Natural resources:		
Water, process, unspecified natural origin/m3	m3	0.446
Occupation, industrial area, in ground	m2a	0.088
Input of products/services:		
Shrimp shell	kg	35
Sodium hydroxide, without water, in 50% solution state {GLO}| market for | APOS, U	kg	11.38
Natural gas, high pressure {GLO}| market group for | APOS, S	m3	2
Ethanol, 85%	kg	4.27
Hydrochloric acid, without water, in 30% solution state {GLO}| tetrafluoroethane production | APOS, U	kg	3.1
Electricity/heat:		
Electricity, medium voltage {EC}| market for electricity, medium voltage | APOS, S	kWh	0.07
Emissions to air:		
Carbon dioxide	kg	2
Carbon dioxide, biogenic	kg	-1.64
Emissions to water:		
Ethanol	kg	0.085

- Impact assessment results

Table S6. Chitosan Impact Assessment Results for 1 kg of Chitosan Production in Guayas-Ecuador by RECIPE Midpoint H Method.

Impact Category	Unit	Total	Chitosan-50%	Shrimp shell	NaOH	Natural gas	Ethanol	HCl	Electricity	Urea	NaOH, treatment	AcidWasteWater-Treatment	BasicWasteWater-Treatment
Global warming	kg CO_2 eq	59,2158202	2	23,1400182	15,7139295	0,83344732	18,5343368	0,37176825	0,0258885	-4,14838249	0,14893118	2,01399211	0,58189081
Stratospheric ozone depletion	kg CFC11 eq	4,0323E-05	0	7,3906E-06	1,6881E-05	6,9175E-07	1,7232E-06	2,9325E-07	1,9918E-08	-1,5356E-06	1,2076E-07	2,2948E-08	1,4715E-05
Ionizing radiation	kBq Co-60 eq	2,4654238	0	0,77068576	1,82587602	0,00821412	-0,02993441	0,03619998	0,0002306 4	-0,10848097	0,01067817	0,05405167	-0,10209716
Ozone formation, Human health	kg NOx eq	0,07981306	0	0,03880976	0,03972469	0,00153285	-0,01478291	0,00131437	7,2842E-05	-0,00594356	0,00029424	0,00525506	0,01353573
Fine particulate matter formation	kg PM2.5 eq	0,06073482	0	0,02778172	0,03613073	0,00097677	-0,01068273	0,00093651	4,3996E-05	-0,00717148	0,00022378	0,00519602	0,00729952
Ozone formation, Terrestrial ecosystems	kg NOx eq	0,08138323	0	0,03939858	0,04012006	0,00172091	-0,01448529	0,00153743	7,3584E-05	-0,00613349	0,00029733	0,00532338	0,01353074
Terrestrial acidification	kg SO2 eq	0,19720612	0	0,05956962	0,06079659	0,00293266	0,00516602	0,00194121	0,0001384 4	-0,02024954	0,0004902	0,02201719	0,06440373
Freshwater eutrophication	kg P eq	0,01394644	0	0,0049798	0,00908827	4,6026E-05	-0,00026119	0,00020579	8,7242E-07	-0,00073429	4,4494E-05	0,00118116	-0,00060449
Marine eutrophication	kg N eq	0,00314133	0	0,0003324	0,00083949	8,1083E-06	0,00208993	1,6238E-05	5,8317E-08	-0,00014903	4,5578E-06	4,9739E-05	-5,0172E-05

Terrestrial ecotoxicity	kg 1,4-DCB	105,874712	0,000222 7	85,825 3874	46,59734 39	0,196 23103	-21,0757 079	1,5444 5717	0,080 3059 6	-21,7877 383	0,35721114	14,7209209	-0,58592678
Freshwater ecotoxicity	kg 1,4-DCB	1,12532772	0,00053 465	0,5752 5481	0,552797 75	0,005 87889	-0,04485 112	0,0161 4965	0,000 3265 1	-0,08561 306	0,0033932	0,12412523	-0,02266879
Marine ecotoxicity	kg 1,4-DCB	1,55418783	1,9125E -05	0,7965 4646	0,775593	0,009 71199	-0,07198 541	0,0229 6879	0,000 4665 8	-0,13257 846	0,00482422	0,17919777	-0,03057623
Human carcinogenic toxicity	kg 1,4-DCB	1,3118754	0,00010 2	0,5356 2713	0,758787 96	0,012 52221	0,00490 478	0,0179 164	0,000 2262	-0,08753 946	0,00380803	0,11108903	-0,04556888
Human non-carcinogenic toxicity	kg 1,4-DCB	28,1797642	0	13,738 8335	15,82846 7	0,143 65521	-3,17541 545	0,5103 6481	0,003 7539	-2,90836 879	0,1086398	4,3641388	-0,43430463
Land use	m2a crop eq	5,69314884	0,06424	0,3763 6896	0,326260 61	0,001 81981	4,74071 968	0,0080 6689	5,750 4E-05	-0,04188 428	0,00368966	0,19681913	0,01699087
Mineral resource scarcity	kg Cu eq	0,10879267	0	0,0458 8393	0,045300 41	0,001 02525	0,01098 38	0,0015 9843	1,524 2E-05	-0,01243 858	0,00034274	0,01624634	-0,00016489
Fossil resource scarcity	kg oil eq	11,3095687	0	4,8371 0162	3,964190 65	1,901 09858	1,64994 862	0,1241 4726	0,008 0747 2	-1,61888 285	0,04040283	0,32941132	0,07407599
Water consumption	m3	34,4454749	0,46	0,2436 9174	0,397844 21	0,000 32659	33,5098 699	0,0091 4981	6,375 7E-05	-0,22562 695	0,01090143	-0,00158159	0,04083599

Table S7. Chitosan Production Scenarios' Comparison varying NaOH concentration (*wt.%*30-40-50% NaOH solution)

Impact Category	**Unit**	**Chitosan-30% (Scenario 3)**	**Chitosan-40% (Scenario 2)**	**Chitosan-50% (Scenario 1)**
Global warming	kg CO_2 eq	54,3828894	56,799355	59,2158203
Stratospheric ozone depletion	kg CFC11 eq	3,5131E-05	3,7727E-05	4,0323E-05
Ionizing radiation	kBq Co-60 eq	1,90386264	2,18464322	2,46542377

Ozone formation, Human health	kg NOx eq	0,06759545	0,07370426	0,07981306
Fine particulate matter formation	kg PM2.5 eq	0,04962256	0,05517869	0,06073482
Ozone formation, Terrestrial ecosystems	kg NOx eq	0,06904402	0,07521362	0,08138323
Terrestrial acidification	kg SO_2 eq	0,1785077	0,18785691	0,19720612
Freshwater eutrophication	kg P eq	0,01115128	0,01254886	0,01394644
Marine eutrophication	kg N eq	0,00288313	0,00301223	0,00314133
Terrestrial ecotoxicity	kg 1,4-DCB	91,5433669	98,7090396	105,874712
Freshwater ecotoxicity	kg 1,4-DCB	0,95531084	1,04031928	1,12532772
Marine ecotoxicity	kg 1,4-DCB	1,31564868	1,43491826	1,55418782
Human carcinogenic toxicity	kg 1,4-DCB	1,07850477	1,19519009	1,3118754
Human non-carcinogenic toxicity	kg 1,4-DCB	23,3116065	25,7456854	28,1797641
Land use	m2a crop eq	5,59280507	5,64297696	5,69314884
Mineral resource scarcity	kg Cu eq	0,09486021	0,10182644	0,10879267
Fossil resource scarcity	kg oil eq	10,0903537	10,6999613	11,3095687
Water consumption	m3	34,3231151	34,384295	34,4454749

- Sensitivity Analysis

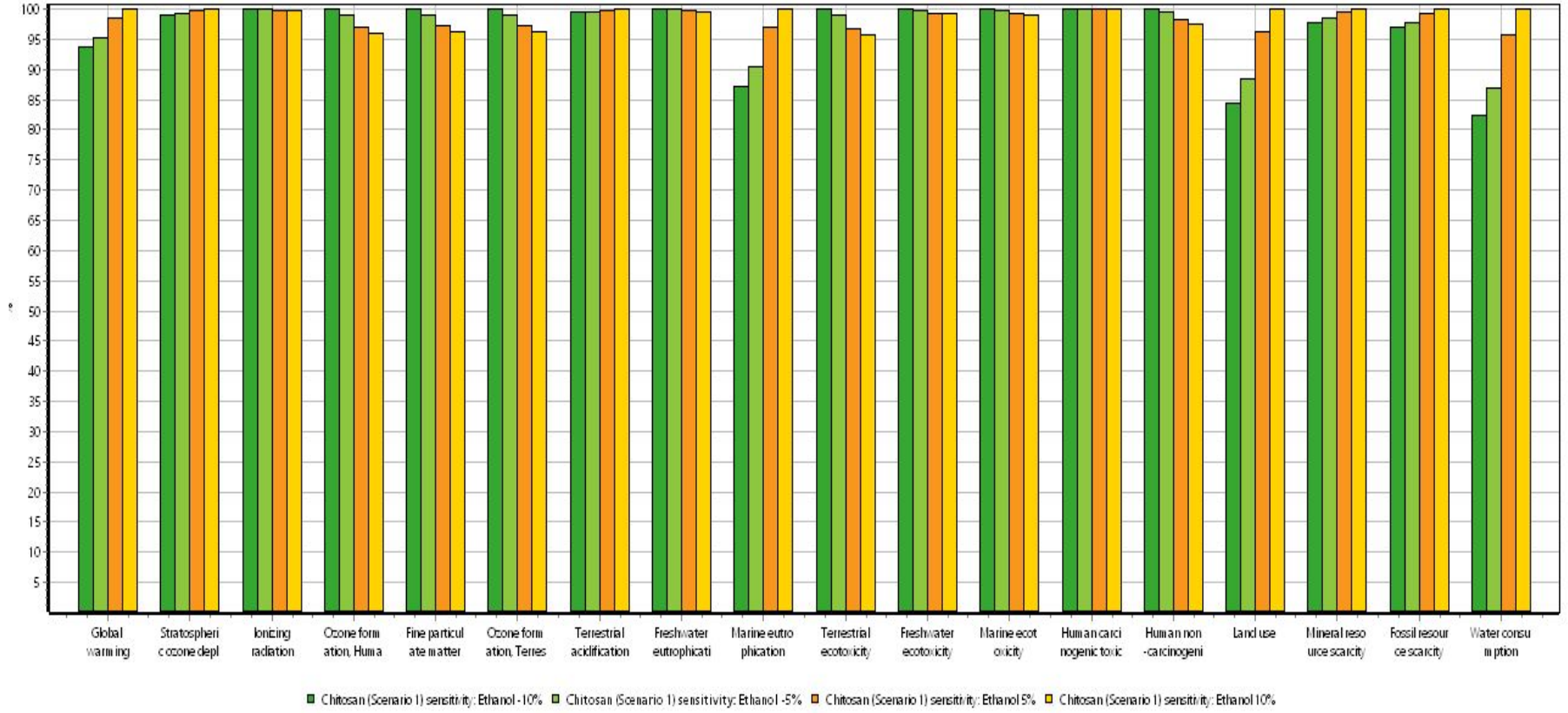

Figure S1. Sensitivity analysis results based-on different amounts of ethanol used.

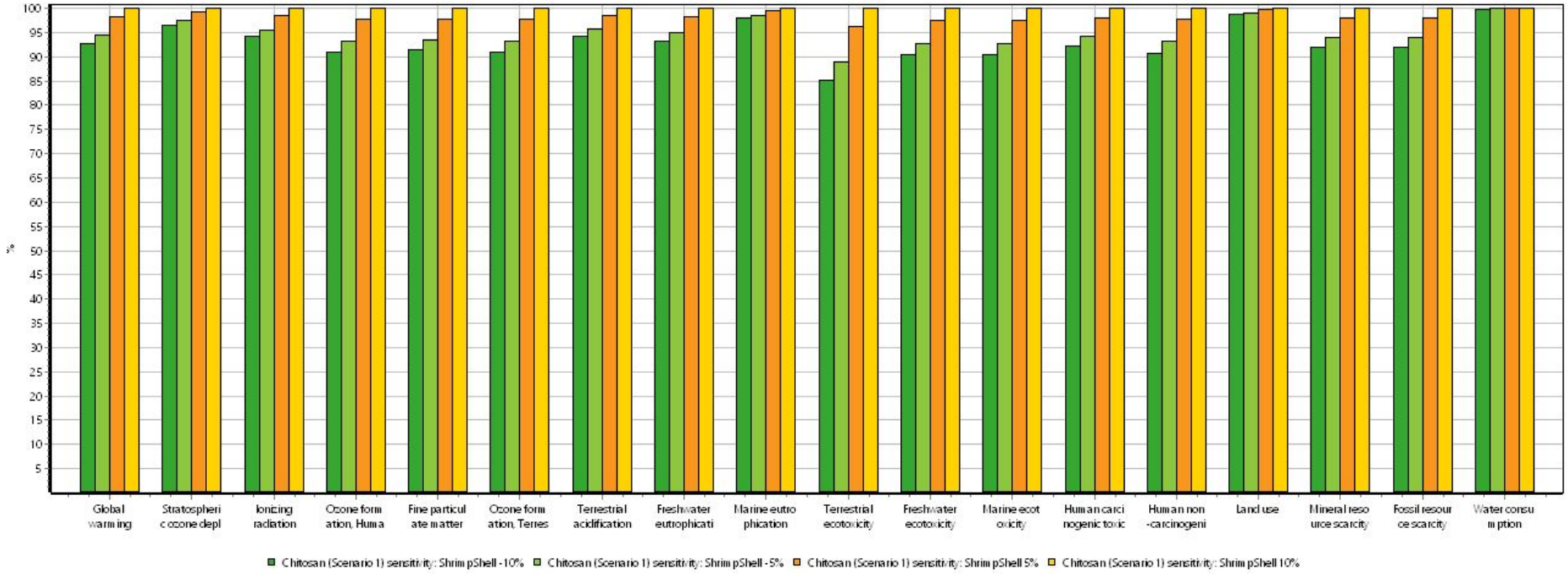

Figure S2. Sensitivity analysis results based-on different amounts of shrimp shell used.

Table S8. Normalized Sensitivity Analysis Results by Changing the Method used.

Impact (RECIPE Midpoint H)	Unit	Total	Impact (ILCD 2011+ Midpoint)	Unit	Total	Impact (TRACI 2.1)	Unit	Total
Global warming	kg CO2 eq	59,2158202	**Climate change**	kg CO2 eq	32,7155512	**Ozone depletion**	kg CFC-11 eq	1,0727E-05
Stratospheric ozone depletion	kg CFC11 eq	4,0323E-05	**Ozone depletion**	kg CFC-11 eq	1,0058E-05	**Global warming**	kg CO2 eq	57,4326198
Ionizing radiation	kBq Co-60 eq	2,4654238	**Human toxicity, non-cancer effects**	CTUh	1,1764E-05	**Smog**	kg O3 eq	2,2683187
Ozone formation, Human health	kg NOx eq	0,07981306	**Human toxicity, cancer effects**	CTUh	1,9451E-06	**Acidification**	kg SO2 eq	0,22572097
Fine particulate matter formation	kg PM2.5 eq	0,06073482	**Particulate matter**	kg PM2.5 eq	-0,01806157	**Eutrophication**	kg N eq	0,28803373
Ozone formation, Terrestrial ecosystems	kg NOx eq	0,08138323	**Ionizing radiation HH**	kBq U235 eq	3,321872 67	**Carcinogenics**	CTUh	1,9448E-06
Terrestrial acidification	kg SO2 eq	0,19720612	**Ionizing radiation E (interim)**	CTUe	3,5176E-05	**Non carcinogenics**	CTUh	1,1764E-05
Freshwater eutrophication	kg P eq	0,01394644	**Photochemical ozone formation**	kg NMVOC eq	0,10107147	**Respiratory effects**	kg PM2.5 eq	0,0272499
Marine eutrophication	kg N eq	0,00314133	**Acidification**	molc H+ eq	0,29647382	**Ecotoxicity**	CTUe	319,326053
Terrestrial ecotoxicity	kg 1,4-DCB	105,874712	**Terrestrial eutrophication**	molc N eq	0,84019483	**Fossil fuel depletion**	MJ surplus	53,3558104
Freshwater ecotoxicity	kg 1,4-DCB	1,12532772	**Freshwater eutrophication**	kg P eq	0,0603082			
Marine ecotoxicity	kg 1,4-DCB	1,55418783	**Marine eutrophication**	kg N eq	0,48815533			
Human carcinogenic toxicity	kg 1,4-DCB	1,3118754	**Freshwater ecotoxicity**	CTUe	320,806616			

Human non-carcinogenic toxicity	kg 1,4-DCB	28,1797642	**Land use**	kg C deficit	1449,65955			
Land use	m2a crop eq	5,69314884	**Water resource depletion**	m3 water eq	5,31191978			
Mineral resource scarcity	kg Cu eq	0,10879267	**Mineral, fossil & ren resource depletion**	kg Sb eq	0,00255691			
Fossil resource scarcity	kg oil eq	11,3095687						
Water consumption	m3	34,4454749						

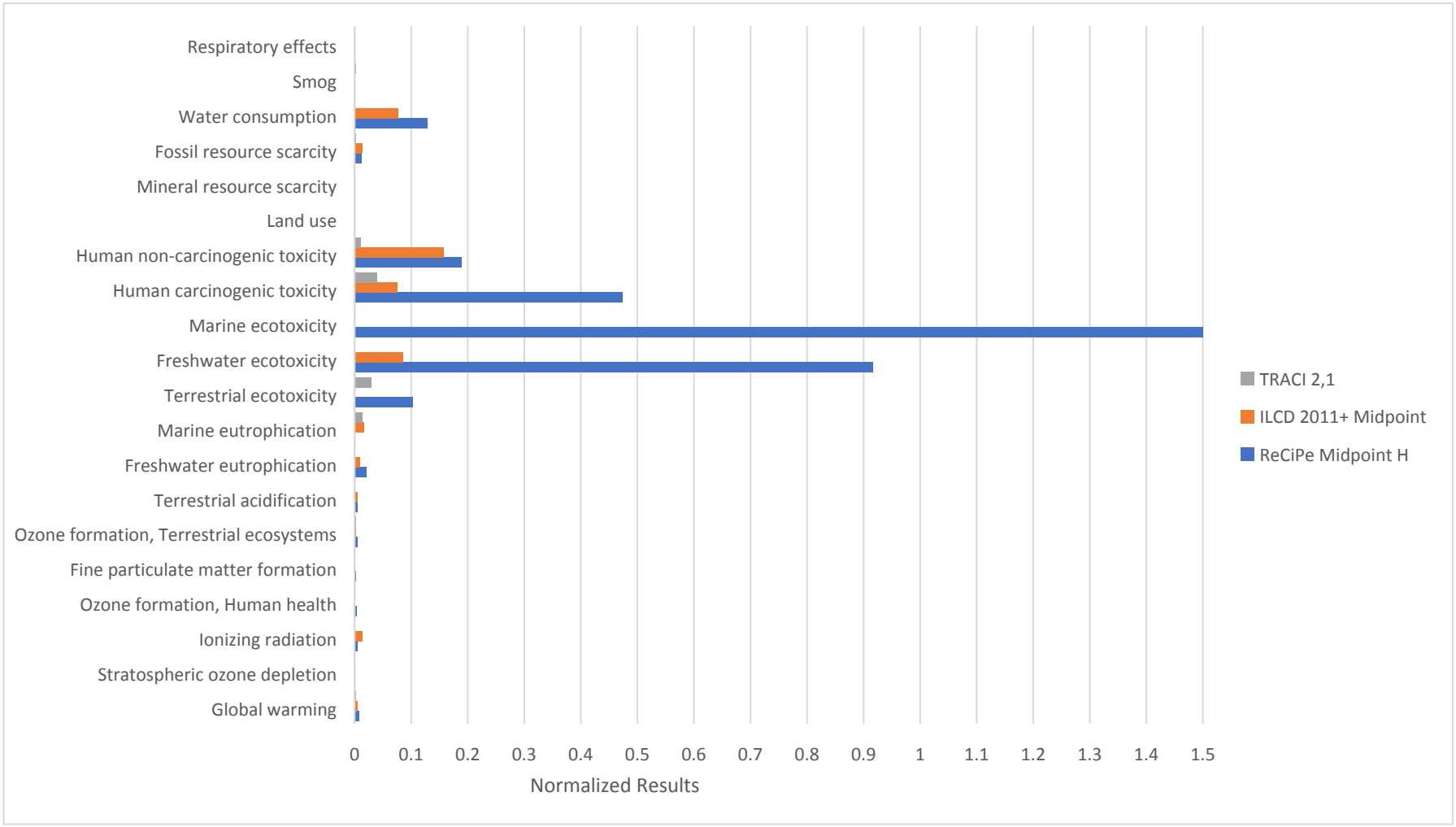

Figure S3. Sensitivity analysis of normalized results by changing LCIA method.