Photochemical Technologies Assessed.
The Case Of Rose Oxide.

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ELECTRONIC SUPPLEMENTARY INFORMATIONS

1. GENERAL

The environmental assessment has been carried out by using the software **EATOS** (**E**nvironmental **A**ssessment **T**ool for **O**rganic **S**yntheses; downloaded from Professor J. O. Metzger web site: http://www.chemie.uni-oldenburg.de/oc/metzger/eatos/) and the software **SimaPro** (version: 7; Eco-Indicator99 as the evaluation method; see http://www.pre.nl/simapro/ for details). Physical and environmental information (including risk and safety phrases, toxicity and ecological parameters) of considered compounds were obtained from the safety data sheets available on Sigma Aldrich web site (www.sigma-aldrich.com). The price of used compounds and materials (of reasonable purity) were obtained from Sigma Aldrich web site too, by chosing the largest quantity offered.

2. TABLE OF PARAMETERS FOR ROUTES #1-#6.

The following tables contain all the data used for both methods to carry out the assessments. As mentioned in the text, these values refers to a medium-scale process, viz. the isolation of 100 g of final product.

ROUTE #1

CHEMICALS*	
Citronellol - *Reagent*	188 g
Oxygen - *Reagent*	30.0 L
Bengal Rose - *Sensitizer*	750 mg
Methanol - *Solvent*	150 mL
Sodium Sulfite - *Reagent*	375 g
Water - *Solvent*	1.70 L
Water - *Solvent*	80.0 mL
Sulfuric Acid - *Reagent*	2.40 g
ENERGETIC CONTRIBUTIONS	
Lamp consumption (18 h @ 170 W) - *Irradiation*	3.0 kWh
Heater (1 h) - *Reduction step*	250 Wh
Vacuum pump (3 h @ 500 W) - *Distillation of glycols*	1.5 kWh
Heater (3 h) - *Distillation of glycols*	750 Wh
Heater (30 min) - *Cyclization step*	125 Wh
AUXILIARY MATERIALS	
Ice	1.00 kg
Cooling water - Lamp (18 h @ 500 mL/min)	540 L
Cooling water (3 h @ 500 mL/min)	90.0 L
Cooling water (0.5 h @ 500 mL/min)	15.0 L
Acetone - *Washing*	100 mL
EXTERNAL CONTRIBUTIONS	
Apparatus ageing	
Transports	
Waste Treatment	

* The references given for this process provide many examples. As far as the first Patent is concerned, the example #1 has been considered. On the other hand, for the second patent, the example #7 has been taken as reference. However, since in the database there was no data concerning "oxalic acid", the alternative presented in the example #4 has been taken into account. This is the reason why the cyclization step uses sulfuric acid.

ROUTE #2

CHEMICALS	
Citronellol - *Reagent*	188 g
Air - *Reagent*	160 L
Ruthenium complex - *Sensitizer*	9.00 g
Ethanol - *Solvent*	12.0 L
Sodium Sulfite - *Reagent*	375 g
Water - *Solvent*	1.70 L
Water - *Solvent*	80.0 mL
Sulfuric Acid - *Reagent*	2.40 g
ENERGETIC CONTRIBUTIONS	
LED consumption (65 h with 48000 LEDs @ 120 mW each) - *Irradiation*	374 kWh *
Heater (1 h) - *Reduction step*	250 Wh
Vacuum pump (3 h @ 500 W) - *Distillation of glycols*	1.5 kWh
Heater (3 h) - *Distillation of glycols*	750 Wh
Heater (30 min) - *Cyclization step*	125 Wh
AUXILIARY MATERIALS	
Ice	1.00 kg
Cooling water (3 h @ 500 mL/min)	90.0 L
Cooling water (0.5 h @ 500 mL/min)	15.0 L
Acetone - *Washing*	100 mL
EXTERNAL CONTRIBUTIONS	
Apparatus ageing	
Transports	
Waste Treatment	

* This value has been determined by assuming the use of the published number of LEDs scaled by the proper factor in order to obtain 100 g of rose-oxide, while maintaining the power of the LEDs and the irradiation time as previously reported. The nominal power of each LED has been taken from the technical data sheet of the article L-7113PBC-A. For details, see: www.kingbright.com.

ROUTE #3

CHEMICALS	
Citronellol - *Reagent*	203 g
Oxygen - *Reagent*	70.0 L
Bengal rose - *Sensitizer*	815 mg
iso-Propanol - *Solvent*	1.60 L
Sodium Sulfite - *Reagent*	405 g
Water - *Solvent*	1.84 L
Water - *Solvent*	86.4 mL
Sulfuric Acid - *Reagent*	2.60 g
ENERGETIC CONTRIBUTIONS	
Heater (1 h) - *Reduction step*	250 Wh
Vacuum pump (3 h @ 500 W) - *Distillation of glycols*	1.5 kWh
Heater (3 h) - *Distillation of glycols*	750 Wh
Heater (30 min) - *Cyclization step*	125 Wh
AUXILIARY MATERIALS	
Ice	1.00 kg
Cooling water - solar collector (18 h @ 1 L/min)	180 L
Cooling water (3 h @ 500 mL/min)	90.0 L
Cooling water (0.5 h @ 500 mL/min)	15.0 L
Acetone - *Washing*	100 mL
EXTERNAL CONTRIBUTIONS	
Apparatus ageing	
Transports	
Waste Treatment	

ROUTE #4

CHEMICALS	
Citronellol - *Reagent*	317 g
Hydrogen peroxide - *Reagent*	276 g
Sodium Molybdate - *Catalyst*	82.4 g
Methanol - *Solvent*	4.05 L
Sodium Sulfite - *Reagent*	634 g
Water - *Solvent*	2.87 L
Water - *Solvent*	135 mL
Sulfuric Acid - *Reagent*	4.06 g
ENERGETIC CONTRIBUTIONS	
Heater (1 h) - *Reduction step*	250 Wh
Vacuum pump (3 h @ 500 W) - *Distillation of glycols*	1.5 kWh
Heater (3 h) - *Distillation of glycols*	750 Wh
Heater (30 min) - *Cyclization step*	125 Wh
AUXILIARY MATERIALS	
Ice	1.00 kg
Cooling water (3 h @ 500 mL/min)	90.0 L
Cooling water (0.5 h @ 500 mL/min)	15.0 L
Acetone - *Washing*	100 mL
EXTERNAL CONTRIBUTIONS	
Apparatus ageing	
Transports	
Waste Treatment	

ROUTE #5

CHEMICALS	
Citronellol - *Reagent*	954 g
tert-Butyl hydroperoxide - *Reagent*	551 g
Cuprous chloride - *Catalyst*	30.6 g
Acetic acid - *Solvent*	1.47 kg
Water - *Solvent*	1.00 L
Sodium hydroxide - *Auxiliary material*	950 g
ENERGETIC CONTRIBUTIONS	
Heater (3 h) - *Reaction step*	750 Wh
Vacuum pump (3 h @ 500 W) - *Distillation step*	1.5 kWh
Heater (3 h) - *Distillation step*	750 Wh
AUXILIARY MATERIALS	
Cooling water (3 h @ 500 mL/min)	90.0 L
Acetone - *Washing*	100 mL
EXTERNAL CONTRIBUTIONS	
Apparatus ageing	
Transports	
Waste Treatment	

ROUTE #6

CHEMICALS	
Citronellol - *Reagent*	604 g
Lead oxide - *Reagent*	2.23 kg
Air - *Auxiliary material*	58,0 L
Acetic acid - *Solvent*	2.80 kg
Sodium hydroxide - *Auxiliary material*	1.10 kg
ENERGETIC CONTRIBUTIONS	
Heater (1 h) - *Reaction step*	250 Wh
Vacuum pump (3 h @ 500 W) - *Distillation step*	1.5 kWh
Heater (3 h) - *Distillation step*	750 Wh
AUXILIARY MATERIALS	
Cooling water (3 h @ 500 mL/min)	90.0 L
Acetone - *Washing*	100 mL
EXTERNAL CONTRIBUTIONS	
Apparatus ageing	
Transports	
Waste Treatment	

3. SOLVENT RECYCLING PROCEDURE MODELLING

The following table contains all the parameters used in the LCA modelling of the solvent recycling procedure.

CHEMICALS	
Alcoholic solvent (exhaust)	5 kg
ENERGETIC CONTRIBUTIONS	
Heater (6 h) – *Distillation procedure*	1.50 kWh
AUXILIARY MATERIALS	
Cooling water (6 h @ 500 mL/min)	180.0 L
EXTERNAL CONTRIBUTIONS	
Waste Treatment	
OUTPUT	
Alcoholic solvent (distilled - 95% yield)	4.75 kg

4. EATOS RESULTS

Table S1. The four EATOS indexes calculated for the processes considered.

Route (#)	**1**	**2**	**3**	**4**	**5**	**6**
S^{-1} [kg/kg]	25.03	118.76	39.10	77.63	47.82	81.57
E [kg/kg]	24.03	117.76	38.10	76.63	46.82	80.57
EI_{in} [PEI/kg]	30.75	168.44	54.12	200.99	99.10	267.33
EI_{out} [PEI/kg]	29.24	310.95	41.18	159.83	194.63	467.81

Table S2. Details for the **EI_{out}** EATOS indexes for the processes considered.

Route (#)	**1**	**2**	**3**	**4**	**5**	**6**
TOTAL EI_{out}	29.24	310.95	41.18	159.83	194.63	467.81
Solvents	21.35	302.21	31.78	125.83	73.42	83.55
Catalysts	0.08	0.90	0.08	4.53	1.62	--
Auxiliaries	0.12	0.12	0.43	2.80	50.44	88.84
Substrates	2.24	2.27	2.91	11.59	0.07	2.53
By-Products	3.03	3.03	3.56	12.43	67.76	248.14
Coupled Products	2.42	2.42	2.42	2.65	1.32	44.75

4. LCA RESULTS

In the following the details of the results of LCA assessment are reported for each procedure.

Table S3. LCA assessment for route #1.

Impact category	Total	Carcinogens	Respiratory organics	Respiratory inorganics	Climate change	Radiation	Ozone layer	Ecotoxicity	Acidification/ Eutrophication	Land use	Minerals	Fossil fuels
Unit	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt
Total	**7.79E-01**	**1.59E-02**	**9.45E-05**	**1.13E-01**	**7.84E-02**	**7.37E-04**	**1.51E-05**	**2.13E-02**	**4.95E-02**	**6.32E-03**	**4.01E-02**	**4.53E-01**
CITRONELLOL	1.78E-01	4.80E-03	3.61E-05	2.81E-02	3.99E-02	3.21E-04	2.94E-06	4.23E-03	1.05E-02	2.07E-03	7.22E-03	8.09E-02
OXYGEN	1.12E-03	2.49E-05	7.35E-08	1.92E-04	7.06E-05	5.98E-06	1.59E-08	7.83E-06	1.48E-05	5.81E-06	5.09E-05	7.48E-04
BENGAL ROSE	2.28E-04	7.92E-07	5.26E-08	1.22E-05	5.96E-06	6.98E-08	2.99E-09	1.79E-06	2.55E-06	4.25E-07	5.54E-06	1.99E-04
METHANOL	2.06E-02	2.11E-05	1.77E-06	3.83E-04	3.87E-04	2.91E-06	3.75E-07	2.17E-05	4.86E-05	5.66E-05	1.32E-04	1.95E-02
SODIUM SULFITE	5.99E-02	1.01E-03	3.52E-06	2.11E-02	2.26E-03	1.38E-04	8.55E-07	1.02E-03	1.44E-03	4.36E-04	4.34E-03	2.82E-02
WATER (solvent)	4.14E-05	2.38E-06	4.22E-09	7.38E-06	2.00E-06	1.67E-07	6.04E-10	5.18E-07	5.11E-07	1.67E-06	2.02E-06	2.48E-05
SULFURIC ACID	8.66E-05	8.80E-07	3.45E-09	5.46E-05	1.25E-06	3.72E-08	7.07E-10	1.53E-06	3.69E-06	5.74E-07	4.52E-06	1.95E-05
ELECTRICAL POWER (overall)	3.23E-01	1.61E-03	3.59E-05	4.19E-02	1.79E-02	3.90E-05	7.24E-06	3.40E-03	4.53E-03	1.74E-03	1.33E-02	2.39E-01
WATER (cooling)	1.50E-02	8.61E-04	1.53E-06	2.67E-03	7.25E-04	6.04E-05	2.19E-07	1.88E-04	1.85E-04	6.05E-04	7.31E-04	8.98E-03
ICE	2.75E-03	1.77E-08	0.00E+00	0.00E+00	0.00E+00	3.66E-08	0.00E+00	6.70E-07	0.00E+00	3.54E-06	9.39E-06	2.74E-03
ACETONE (washing)	1.49E-02	2.15E-04	2.53E-06	1.35E-03	1.10E-03	1.35E-05	3.89E-07	2.81E-04	9.85E-04	1.02E-04	5.13E-04	1.04E-02
APPARATUS AGEING	2.02E-02	3.49E-03	3.08E-07	2.95E-03	8.74E-05	3.86E-06	2.83E-08	4.51E-03	9.76E-05	3.65E-04	6.87E-03	1.79E-03
WASTE TREATMENT	1.37E-01	3.81E-03	1.17E-05	1.39E-02	1.59E-02	1.44E-04	2.84E-06	7.60E-03	3.16E-02	7.96E-04	6.68E-03	5.61E-02
TRANSPORTS	5.61E-03	5.25E-05	1.09E-06	4.10E-04	9.58E-05	7.53E-06	2.22E-07	7.02E-05	6.42E-05	1.37E-04	2.70E-04	4.50E-03

Table S4. LCA assessment for route #2.

Impact category	Total	Carcinogens	Respiratory organics	Respiratory inorganics	Climate change	Radiation	Ozone layer	Ecotoxicity	Acidification/ Eutrophication	Land use	Minerals	Fossil fuels
Unit	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt
Total	**2.46E+01**	**1.38E-01**	**3.45E-03**	**3.00E+00**	**1.36E+00**	**3.80E-03**	**5.09E-04**	**2.58E-01**	**4.17E-01**	**1.28E-01**	**9.74E-01**	**1.83E+01**
CITRONELLOL	1.78E-01	4.80E-03	3.61E-05	2.81E-02	3.99E-02	3.21E-04	2.94E-06	4.23E-03	1.05E-02	2.07E-03	7.22E-03	8.09E-02
RUTHENIUM COMPLEX	1.40E-02	1.68E-04	1.53E-06	1.77E-03	5.10E-04	1.28E-05	4.07E-07	3.36E-04	2.11E-04	8.87E-05	2.02E-04	1.07E-02
ETHANOL	2.17E+00	6.23E-03	9.49E-04	9.30E-02	5.16E-02	2.33E-04	7.83E-06	7.76E-03	4.20E-02	3.10E-03	3.51E-02	1.93E+00
SODIUM SULFITE	5.99E-02	1.01E-03	3.52E-06	2.11E-02	2.26E-03	1.38E-04	8.55E-07	1.02E-03	1.44E-03	4.36E-04	4.34E-03	2.82E-02
WATER (solvent)	4.14E-05	2.38E-06	4.22E-09	7.38E-06	2.00E-06	1.67E-07	6.04E-10	5.18E-07	5.11E-07	1.67E-06	2.02E-06	2.48E-05
SULFURIC ACID	8.66E-05	8.80E-07	3.45E-09	5.46E-05	1.25E-06	3.72E-08	7.07E-10	1.53E-06	3.69E-06	5.74E-07	4.52E-06	1.95E-05
ELECTRICAL POWER (overall)	2.17E+01	1.08E-01	2.40E-03	2.80E+00	1.20E+00	2.61E-03	4.85E-04	2.28E-01	3.04E-01	1.17E-01	8.89E-01	1.60E+01
WATER (cooling)	2.44E-03	1.40E-04	2.49E-07	4.35E-04	1.18E-04	9.84E-06	3.56E-08	3.05E-05	3.02E-05	9.86E-05	1.19E-04	1.46E-03
ICE	2.75E-03	1.77E-08	0.00E+00	0.00E+00	0.00E+00	3.66E-08	0.00E+00	6.70E-07	0.00E+00	3.54E-06	9.39E-06	2.74E-03
ACETONE (washing)	1.49E-02	2.15E-04	2.53E-06	1.35E-03	1.10E-03	1.35E-05	3.89E-07	2.81E-04	9.85E-04	1.02E-04	5.13E-04	1.04E-02
APPARATUS AGEING	5.20E-02	8.92E-03	1.04E-06	7.75E-03	2.61E-04	1.04E-05	7.25E-08	1.15E-02	2.81E-04	8.80E-04	1.75E-02	4.86E-03
WASTE TREATMENT	3.75E-01	7.78E-03	3.47E-05	3.90E-02	7.14E-02	3.14E-04	8.12E-06	3.99E-03	5.65E-02	2.06E-03	1.49E-02	1.78E-01
TRANSPORTS	1.01E-01	9.44E-04	1.95E-05	7.37E-03	1.72E-03	1.35E-04	3.99E-06	1.26E-03	1.15E-03	2.46E-03	4.86E-03	8.09E-02

Table S5. LCA assessment for route #3.

Impact category	Total	Carcinogens	Respiratory organics	Respiratory inorganics	Climate change	Radiation	Ozone layer	Ecotoxicity	Acidification/ Eutrophication	Land use	Minerals	Fossil fuels
Unit	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt
Total	**1.17E+00**	**1.72E-02**	**2.62E-04**	**1.30E-01**	**9.55E-02**	**1.02E-03**	**1.90E-05**	**2.10E-02**	**8.98E-02**	**7.22E-03**	**4.37E-02**	**7.68E-01**
CITRONELLOL	1.92E-01	5.18E-03	3.90E-05	3.04E-02	4.31E-02	3.47E-04	3.17E-06	4.57E-03	1.13E-02	2.24E-03	7.80E-03	8.74E-02
OXYGEN	2.62E-03	5.80E-05	1.71E-07	4.48E-04	1.65E-04	1.39E-05	3.72E-08	1.83E-05	3.46E-05	1.36E-05	1.19E-04	1.74E-03
BENGAL ROSE	2.48E-04	8.61E-07	5.72E-08	1.33E-05	6.47E-06	7.58E-08	3.25E-09	1.95E-06	2.77E-06	4.62E-07	6.02E-06	2.16E-04
ISOPROPANOL	4.17E-01	1.22E-03	1.61E-04	2.37E-02	1.02E-02	7.74E-05	2.09E-06	1.84E-03	3.84E-02	6.66E-04	7.67E-03	3.33E-01
SODIUM SULFITE	6.47E-02	1.09E-03	3.80E-06	2.27E-02	2.44E-03	1.49E-04	9.23E-07	1.11E-03	1.56E-03	4.71E-04	4.69E-03	3.05E-02
WATER (solvent)	4.49E-05	2.57E-06	4.56E-09	7.99E-06	2.17E-06	1.81E-07	6.54E-10	5.60E-07	5.53E-07	1.81E-06	2.18E-06	2.68E-05
SULFURIC ACID	9.38E-05	9.53E-07	3.73E-09	5.92E-05	1.35E-06	4.03E-08	7.66E-10	1.66E-06	4.00E-06	6.22E-07	4.90E-06	2.11E-05
ELECTRICAL POWER (overall)	1.51E-01	7.53E-04	1.67E-05	1.95E-02	8.33E-03	1.82E-05	3.38E-06	1.59E-03	2.12E-03	8.12E-04	6.20E-03	1.12E-01
WATER (cooling)	6.64E-03	3.81E-04	6.75E-07	1.18E-03	3.20E-04	2.67E-05	9.67E-08	8.29E-05	8.19E-05	2.67E-04	3.23E-04	3.97E-03
ICE	2.75E-03	1.77E-08	0.00E+00	0.00E+00	0.00E+00	3.66E-08	0.00E+00	6.70E-07	0.00E+00	3.54E-06	9.39E-06	2.74E-03
ACETONE (washing)	1.49E-02	2.15E-04	2.53E-06	1.35E-03	1.10E-03	1.35E-05	3.89E-07	2.81E-04	9.85E-04	1.02E-04	5.13E-04	1.04E-02
APPARATUS AGEING	1.33E-02	1.82E-03	3.89E-07	1.98E-03	2.07E-04	1.06E-05	6.86E-08	2.35E-03	9.68E-05	2.44E-04	3.74E-03	2.89E-03
WASTE TREATMENT	2.93E-01	6.30E-03	3.52E-05	2.75E-02	2.94E-02	3.44E-04	8.29E-06	9.00E-03	3.51E-02	2.03E-03	1.19E-02	1.72E-01
TRANSPORTS	1.50E-02	1.40E-04	2.90E-06	1.09E-03	2.56E-04	2.01E-05	5.91E-07	1.87E-04	1.71E-04	3.64E-04	7.20E-04	1.20E-02

Table S6. LCA assessment for route #4.

Impact category	Total	Carcinogens	Respiratory organics	Respiratory inorganics	Climate change	Radiation	Ozone layer	Ecotoxicity	Acidification/ Eutrophication	Land use	Minerals	Fossil fuels
Unit	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt
Total	**1.62E+00**	**2.08E-02**	**1.90E-04**	**1.71E-01**	**1.44E-01**	**1.34E-03**	**3.02E-05**	**2.09E-02**	**6.69E-02**	**1.11E-02**	**1.18E-01**	**1.07E+00**
CITRONELLOL	3.01E-01	8.11E-03	6.10E-05	4.76E-02	6.74E-02	5.43E-04	4.96E-06	7.15E-03	1.77E-02	3.51E-03	1.22E-02	1.37E-01
HYDROGEN PEROXIDE	6.63E-02	9.51E-04	1.79E-05	5.73E-03	2.90E-03	8.05E-05	1.34E-06	1.66E-03	7.63E-04	3.15E-04	8.02E-03	4.59E-02
SODIUM MOLYBDATE	8.98E-02	4.44E-04	8.29E-07	1.67E-02	5.35E-04	3.65E-05	1.74E-07	1.07E-03	1.76E-04	1.25E-03	6.35E-02	6.18E-03
METHANOL	5.56E-01	5.69E-04	4.78E-05	1.04E-02	1.05E-02	7.87E-05	1.01E-05	5.87E-04	1.31E-03	1.53E-03	3.56E-03	5.27E-01
SODIUM SULFITE	1.01E-01	1.71E-03	5.95E-06	3.56E-02	3.82E-03	2.34E-04	1.45E-06	1.73E-03	2.44E-03	7.37E-04	7.34E-03	4.77E-02
WATER (solvent)	7.00E-05	4.01E-06	7.12E-09	1.25E-05	3.38E-06	2.82E-07	1.02E-09	8.74E-07	8.63E-07	2.82E-06	3.41E-06	4.19E-05
SULFURIC ACID	1.46E-04	1.49E-06	5.83E-09	9.24E-05	2.11E-06	6.29E-08	1.20E-09	2.59E-06	6.25E-06	9.71E-07	7.65E-06	3.29E-05
ELECTRICAL POWER (overall)	1.51E-01	7.53E-04	1.67E-05	1.95E-02	8.33E-03	1.82E-05	3.38E-06	1.59E-03	2.12E-03	8.12E-04	6.20E-03	1.12E-01
WATER (cooling)	2.44E-03	1.40E-04	2.49E-07	4.35E-04	1.18E-04	9.84E-06	3.56E-08	3.05E-05	3.02E-05	9.86E-05	1.19E-04	1.46E-03
ICE	2.75E-03	1.77E-08	0.00E+00	0.00E+00	0.00E+00	3.66E-08	0.00E+00	6.70E-07	0.00E+00	3.54E-06	9.39E-06	2.74E-03
ACETONE (washing)	1.49E-02	2.15E-04	2.53E-06	1.35E-03	1.10E-03	1.35E-05	3.89E-07	2.81E-04	9.85E-04	1.02E-04	5.13E-04	1.04E-02
APPARATUS AGEING	8.33E-03	1.42E-03	1.26E-07	1.21E-03	3.82E-05	1.66E-06	1.26E-08	1.84E-03	4.02E-05	1.42E-04	2.84E-03	8.02E-04
WASTE TREATMENT	2.95E-01	6.13E-03	2.99E-05	2.98E-02	4.88E-02	2.75E-04	6.99E-06	4.54E-03	4.10E-02	1.75E-03	1.17E-02	1.51E-01
TRANSPORTS	3.40E-02	3.18E-04	6.59E-06	2.48E-03	5.80E-04	4.56E-05	1.34E-06	4.25E-04	3.89E-04	8.27E-04	1.64E-03	2.72E-02

Table S7. LCA assessment for route #5.

Impact category	Total	Carcinogens	Respiratory organics	Respiratory inorganics	Climate change	Radiation	Ozone layer	Ecotoxicity	Acidification/ Eutrophication	Land use	Minerals	Fossil fuels
Unit	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt
Total	**2.30E+00**	**4.84E-02**	**3.64E-04**	**2.76E-01**	**2.79E-01**	**3.31E-03**	**4.27E-05**	**5.04E-02**	**1.01E-01**	**2.03E-02**	**1.42E-01**	**1.38E+00**
CITRONELLOL	9.06E-01	2.44E-02	1.84E-04	1.43E-01	2.03E-01	1.63E-03	1.49E-05	2.15E-02	5.32E-02	1.06E-02	3.67E-02	4.11E-01
ACETIC ACID	3.57E-01	2.79E-03	3.61E-05	2.37E-02	8.83E-03	4.12E-04	8.80E-06	2.78E-03	3.42E-03	2.44E-03	1.61E-02	2.96E-01
CUPROUS CHLORIDE	6.92E-02	6.20E-03	9.07E-07	1.08E-02	4.71E-04	2.06E-05	1.85E-07	1.02E-02	4.31E-04	9.65E-04	3.40E-02	6.15E-03
PEROXIDE	2.49E-01	1.40E-03	6.61E-05	1.22E-02	5.82E-03	8.45E-05	1.59E-06	1.97E-03	1.50E-03	4.93E-04	1.08E-02	2.15E-01
WATER (solvent)	2.33E-05	1.34E-06	2.37E-09	4.15E-06	1.12E-06	9.37E-08	3.39E-10	2.91E-07	2.87E-07	9.39E-07	1.13E-06	1.39E-05
SODIUM HYDROXIDE	1.70E-01	4.32E-03	1.12E-05	2.78E-02	9.12E-03	7.26E-04	2.97E-06	3.21E-03	2.54E-03	1.40E-03	1.95E-02	1.01E-01
ELECTRICAL POWER (overall)	1.73E-01	8.60E-04	1.91E-05	2.23E-02	9.52E-03	2.08E-05	3.86E-06	1.81E-03	2.42E-03	9.28E-04	7.08E-03	1.28E-01
WATER (cooling)	2.10E-03	1.20E-04	2.13E-07	3.73E-04	1.01E-04	8.43E-06	3.06E-08	2.62E-05	2.59E-05	8.45E-05	1.02E-04	1.25E-03
ACETONE (washing)	1.49E-02	2.15E-04	2.53E-06	1.35E-03	1.10E-03	1.35E-05	3.89E-07	2.81E-04	9.85E-04	1.02E-04	5.13E-04	1.04E-02
APPARATUS AGEING	8.68E-03	1.47E-03	1.33E-07	1.25E-03	4.18E-05	1.78E-06	1.40E-08	1.89E-03	4.21E-05	1.47E-04	2.94E-03	8.93E-04
WASTE TREATMENT	2.99E-01	6.14E-03	3.39E-05	2.90E-02	4.00E-02	3.17E-04	7.95E-06	6.07E-03	3.58E-02	1.94E-03	1.18E-02	1.68E-01
TRANSPORTS	5.10E-02	4.78E-04	9.90E-06	3.73E-03	8.72E-04	6.85E-05	2.02E-06	6.39E-04	5.84E-04	1.24E-03	2.46E-03	4.09E-02

Table S8. LCA assessment for route #6.

Impact category	Total	Carcinogens	Respiratory organics	Respiratory inorganics	Climate change	Radiation	Ozone layer	Ecotoxicity	Acidification/ Eutrophication	Land use	Minerals	Fossil fuels
Unit	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt
Total	**1.44E+01**	**1.10E+01**	**2.99E-04**	**4.81E-01**	**2.27E-01**	**3.67E-03**	**5.13E-05**	**7.22E-01**	**2.87E-01**	**3.38E-02**	**1.29E-01**	**1.47E+00**
CITRONELLOL	5.73E-01	1.55E-02	1.16E-04	9.06E-02	1.28E-01	1.03E-03	9.45E-06	1.36E-02	3.37E-02	6.68E-03	2.33E-02	2.60E-01
LEAD OXIDE	1.23E+01	1.10E+01	2.01E-05	2.45E-01	6.08E-03	4.18E-04	3.81E-06	6.86E-01	1.91E-01	1.54E-02	2.31E-02	1.09E-01
ACETIC ACID	6.81E-01	5.32E-03	6.89E-05	4.53E-02	1.68E-02	7.86E-04	1.68E-05	5.30E-03	6.53E-03	4.66E-03	3.07E-02	5.66E-01
SODIUM HYDROXIDE	1.97E-01	5.01E-03	1.30E-05	3.22E-02	1.06E-02	8.41E-04	3.44E-06	3.72E-03	2.94E-03	1.62E-03	2.26E-02	1.17E-01
ELECTRICAL POWER (overall)	1.44E-01	7.17E-04	1.59E-05	1.86E-02	7.94E-03	1.73E-05	3.22E-06	1.51E-03	2.02E-03	7.74E-04	5.90E-03	1.06E-01
WATER (cooling)	2.10E-03	1.20E-04	2.13E-07	3.73E-04	1.01E-04	8.43E-06	3.06E-08	2.62E-05	2.59E-05	8.45E-05	1.02E-04	1.25E-03
ACETONE (washing)	1.49E-02	2.15E-04	2.53E-06	1.35E-03	1.10E-03	1.35E-05	3.89E-07	2.81E-04	9.85E-04	1.02E-04	5.13E-04	1.04E-02
APPARATUS AGEING	9.00E-03	1.52E-03	1.38E-07	1.30E-03	4.31E-05	1.83E-06	1.44E-08	1.97E-03	4.36E-05	1.53E-04	3.05E-03	9.16E-04
WASTE TREATMENT	4.30E-01	8.75E-03	5.01E-05	4.13E-02	5.45E-02	4.67E-04	1.17E-05	8.91E-03	4.88E-02	2.85E-03	1.68E-02	2.48E-01
TRANSPORTS	6.04E-02	5.65E-04	1.17E-05	4.42E-03	1.03E-03	8.11E-05	2.39E-06	7.56E-04	6.92E-04	1.47E-03	2.91E-03	4.85E-02

6. SOLVENT RECYCLING PROCEDURE RESULTS.

Table S9. LCA assessment variations by taking into account the solvent recycling procedure for routes #1-#4.

Impact category	Total	Carcinogens	Respiratory organics	Respiratory inorganics	Climate change	Radiation	Ozone layer	Ecotoxicity	Acidification/ Eutrophication	Land use	Minerals	Fossil fuels
Unit	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt	Pt
ROUTE 1												
OLD VALUE	7.79E-01	1.59E-02	9.45E-05	1.13E-01	7.84E-02	7.37E-04	1.51E-05	2.13E-02	4.95E-02	6.32E-03	4.01E-02	4.53E-01
Recycling PROCESS	-1.66E-02	1.85E-05	-1.37E-06	-5.58E-06	-1.94E-04	-1.17E-06	-2.91E-07	5.56E-05	1.61E-04	-3.38E-05	2.68E-06	-1.66E-02
NEW VALUE	**7.62E-01**	**1.59E-02**	**9.31E-05**	**1.13E-01**	**7.82E-02**	**7.36E-04**	**1.48E-05**	**2.14E-02**	**4.96E-02**	**6.29E-03**	**4.01E-02**	**4.37E-01**
ROUTE 2												
OLD VALUE	2.46E+01	1.38E-01	3.45E-03	3.00E+00	1.36E+00	3.80E-03	5.09E-04	2.58E-01	4.17E-01	1.28E-01	9.74E-01	1.83E+01
Recycling PROCESS	-1.83E+00	-2.84E-03	-8.77E-04	-5.96E-02	-3.51E-02	-9.33E-05	-2.20E-06	-1.27E-03	-2.33E-02	-1.34E-03	-2.31E-02	-1.68E+00
NEW VALUE	**2.28E+01**	**1.35E-01**	**2.57E-03**	**2.94E+00**	**1.33E+00**	**3.71E-03**	**5.07E-04**	**2.57E-01**	**3.93E-01**	**1.27E-01**	**9.51E-01**	**1.67E+01**
ROUTE 3												
OLD VALUE	1.17E+00	1.72E-02	2.62E-04	1.30E-01	9.55E-02	1.02E-03	1.90E-05	2.10E-02	8.98E-02	7.22E-03	4.37E-02	7.68E-01
Recycling PROCESS	-3.65E-01	-7.49E-04	-1.50E-04	-1.87E-02	-7.81E-03	-5.66E-05	-1.29E-06	-9.34E-04	-3.43E-02	-4.20E-04	-5.93E-03	-2.96E-01
NEW VALUE	**8.09E-01**	**1.64E-02**	**1.13E-04**	**1.11E-01**	**8.77E-02**	**9.65E-04**	**1.77E-05**	**2.01E-02**	**5.55E-02**	**6.80E-03**	**3.77E-02**	**4.72E-01**
ROUTE 4												
OLD VALUE	1.62E+00	2.08E-02	1.90E-04	1.71E-01	1.44E-01	1.34E-03	3.02E-05	2.09E-02	6.69E-02	1.11E-02	1.18E-01	1.07E+00
Recycling PROCESS	-4.49E-01	4.98E-04	-3.70E-05	-1.51E-04	-5.23E-03	-3.16E-05	-7.86E-06	1.50E-03	4.35E-03	-9.12E-04	7.24E-05	-4.49E-01
NEW VALUE	**1.17E+00**	**2.13E-02**	**1.53E-04**	**1.71E-01**	**1.39E-01**	**1.31E-03**	**2.24E-05**	**2.24E-02**	**7.13E-02**	**1.02E-02**	**1.18E-01**	**6.20E-01**