

ELECTRONIC SUPPLEMENTARY INFORMATION

Environmental sustainability assessment of a new degreasing formulation for the tanning cycle within leather manufacturing

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FIGURES

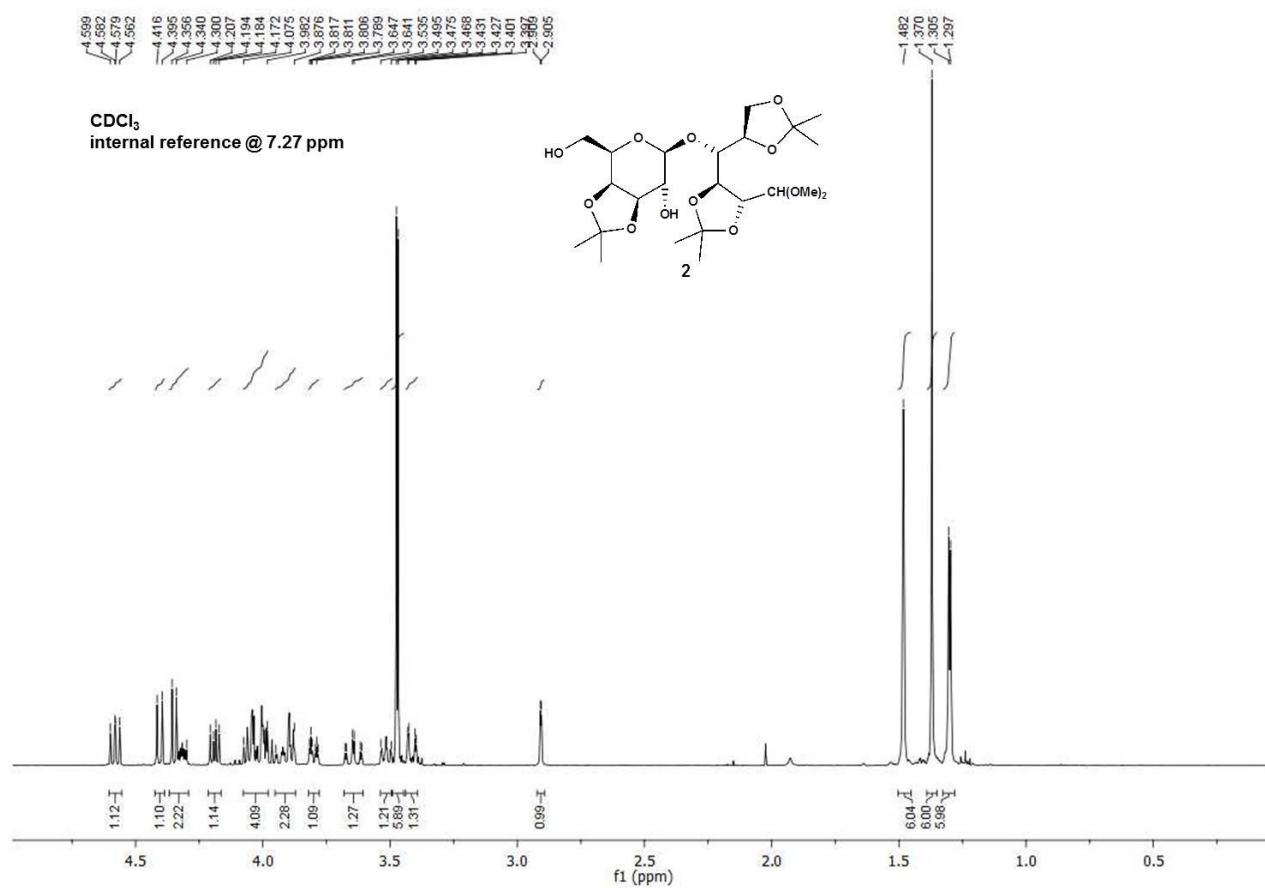


Figure 1 ESI ¹H-NMR spectrum of compound **2**.

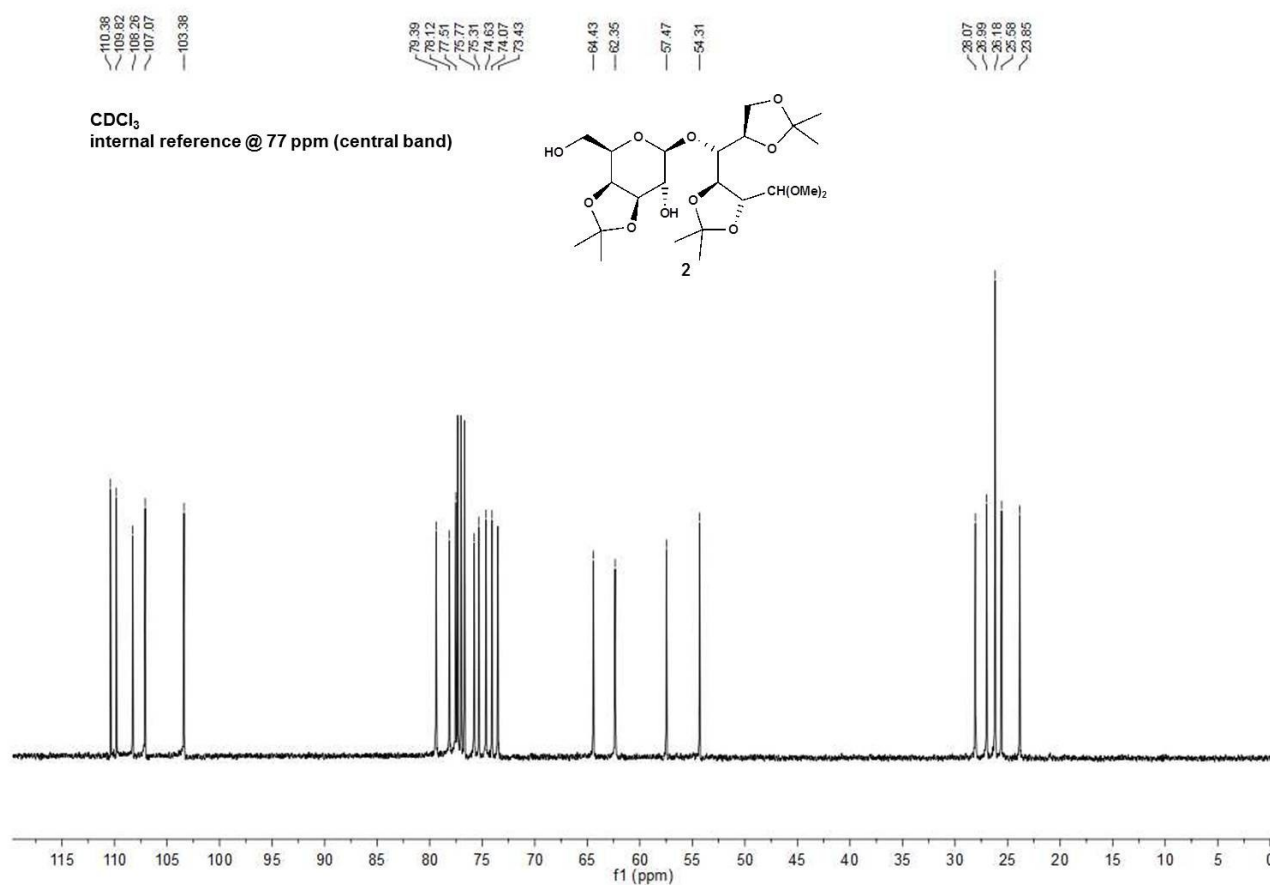


Figure 2 ESI ¹³C-NMR spectrum of compound 2.

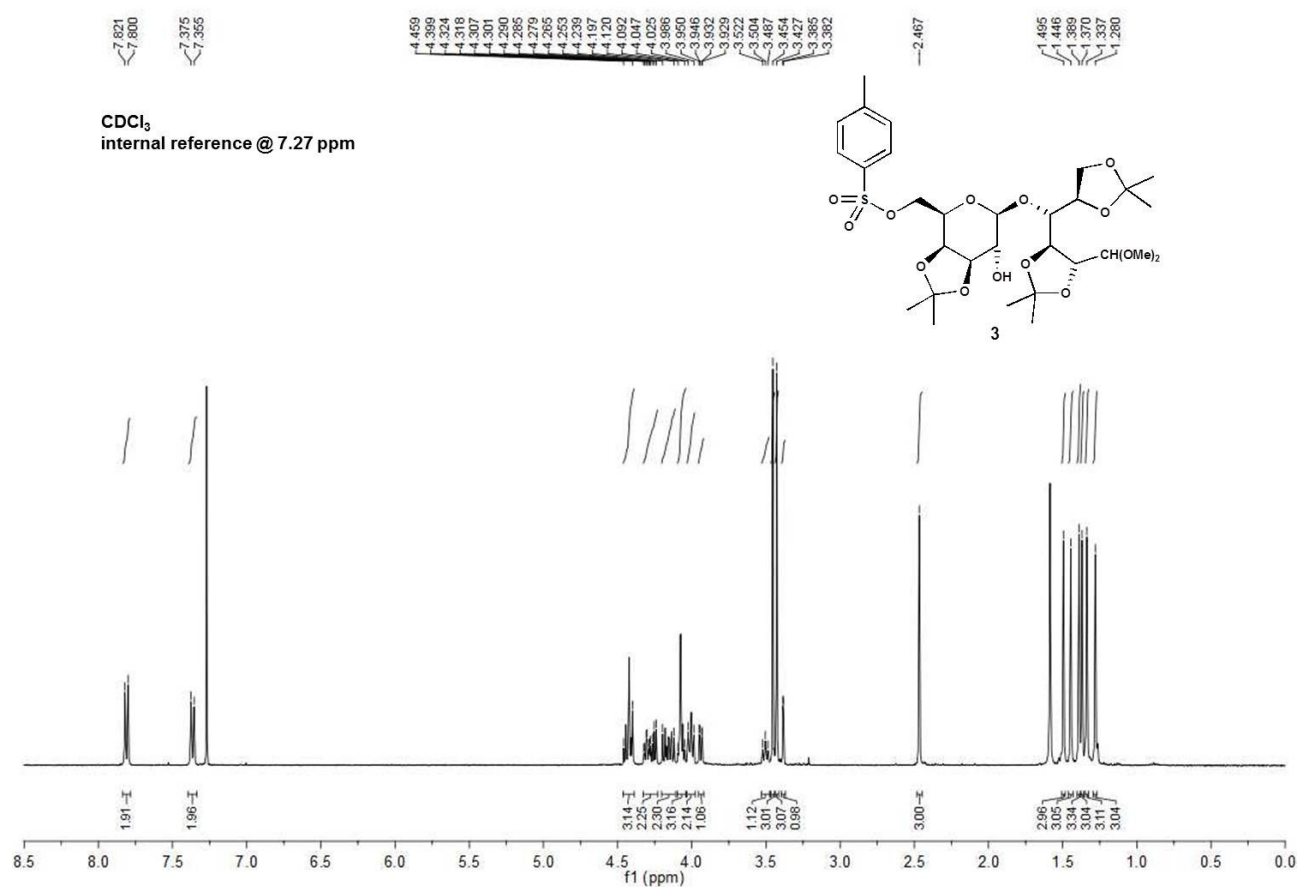


Figure 3 ESI ¹H-NMR spectrum of compound **3**.

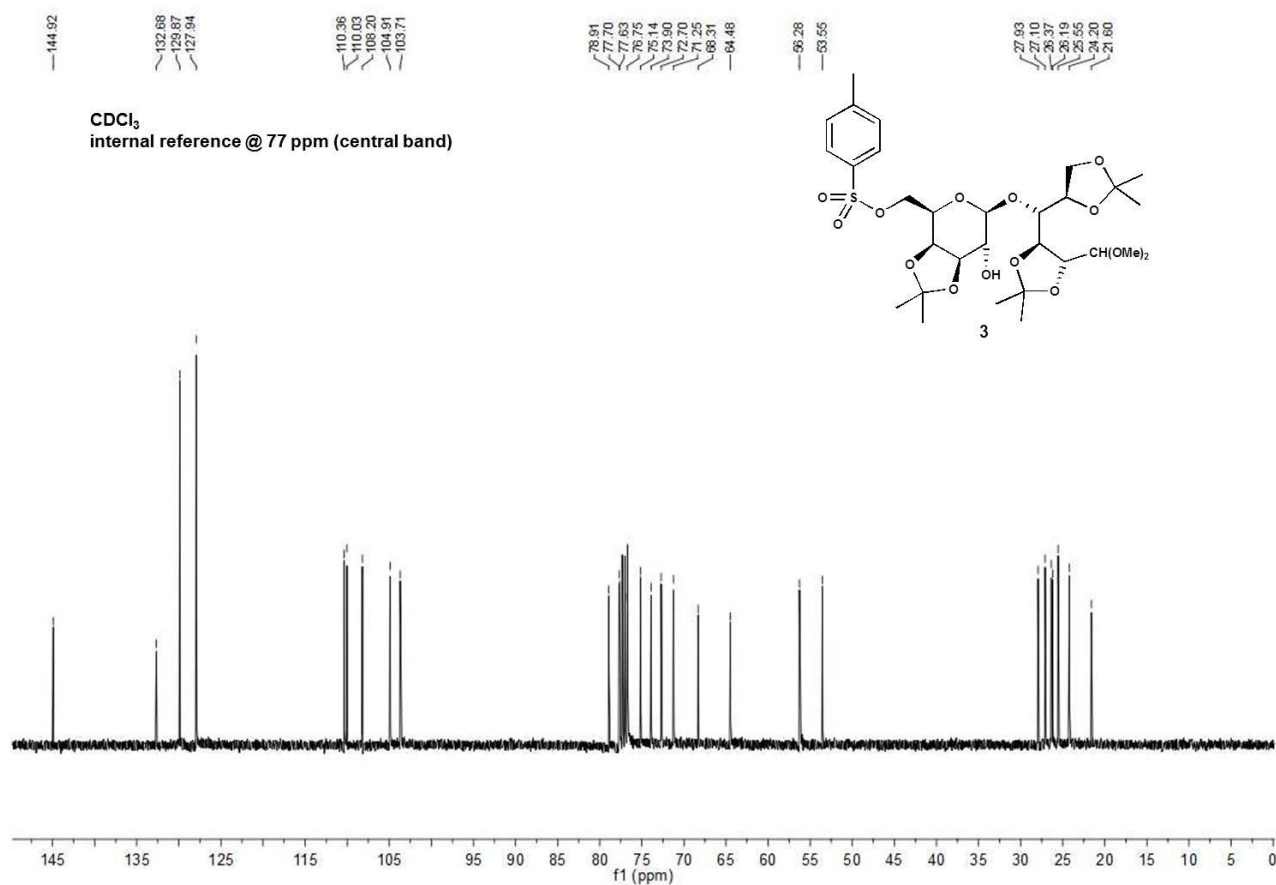


Figure 4 ESI ¹³C-NMR spectrum of compound **3**.

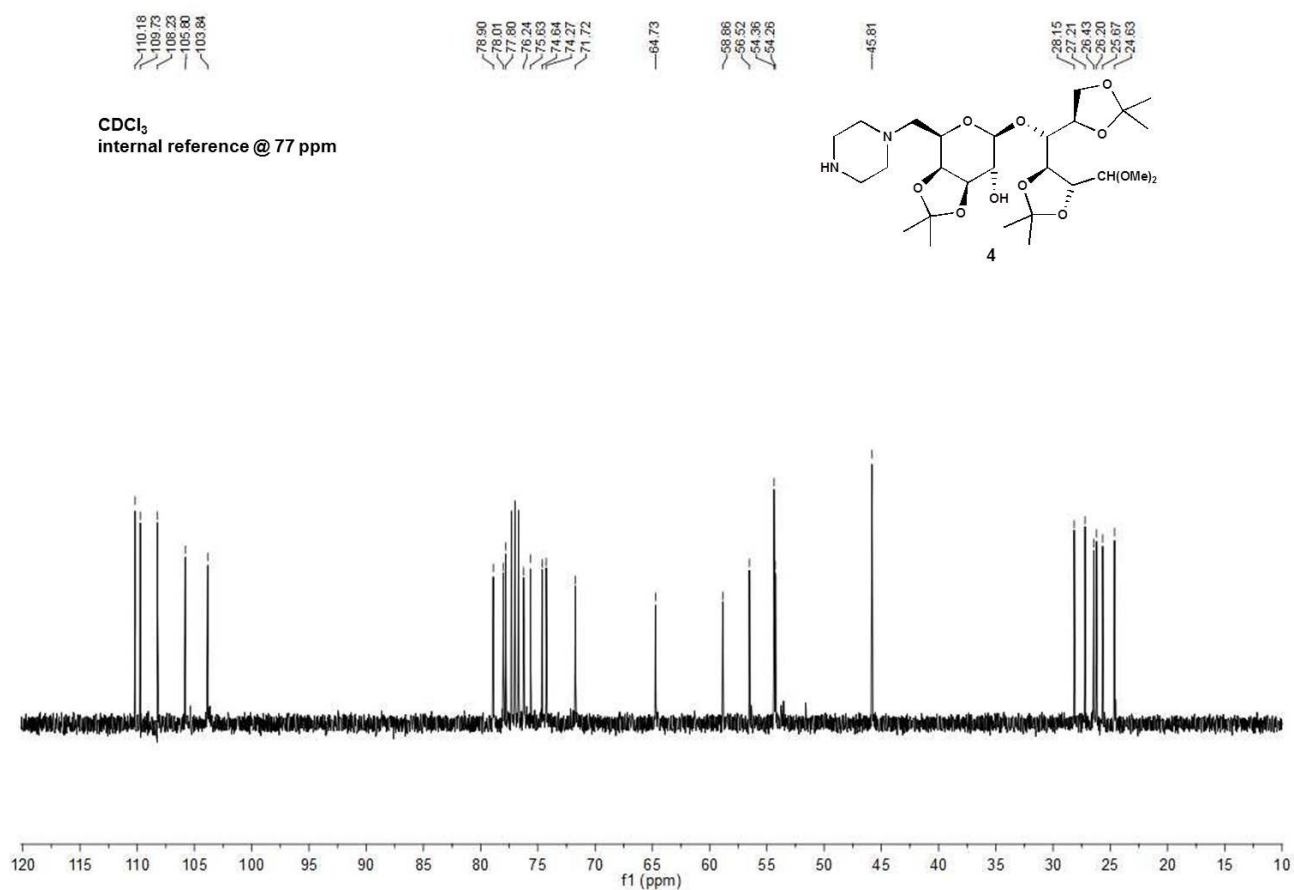


Figure 6 ESI ¹³C-NMR spectrum of compound 4.

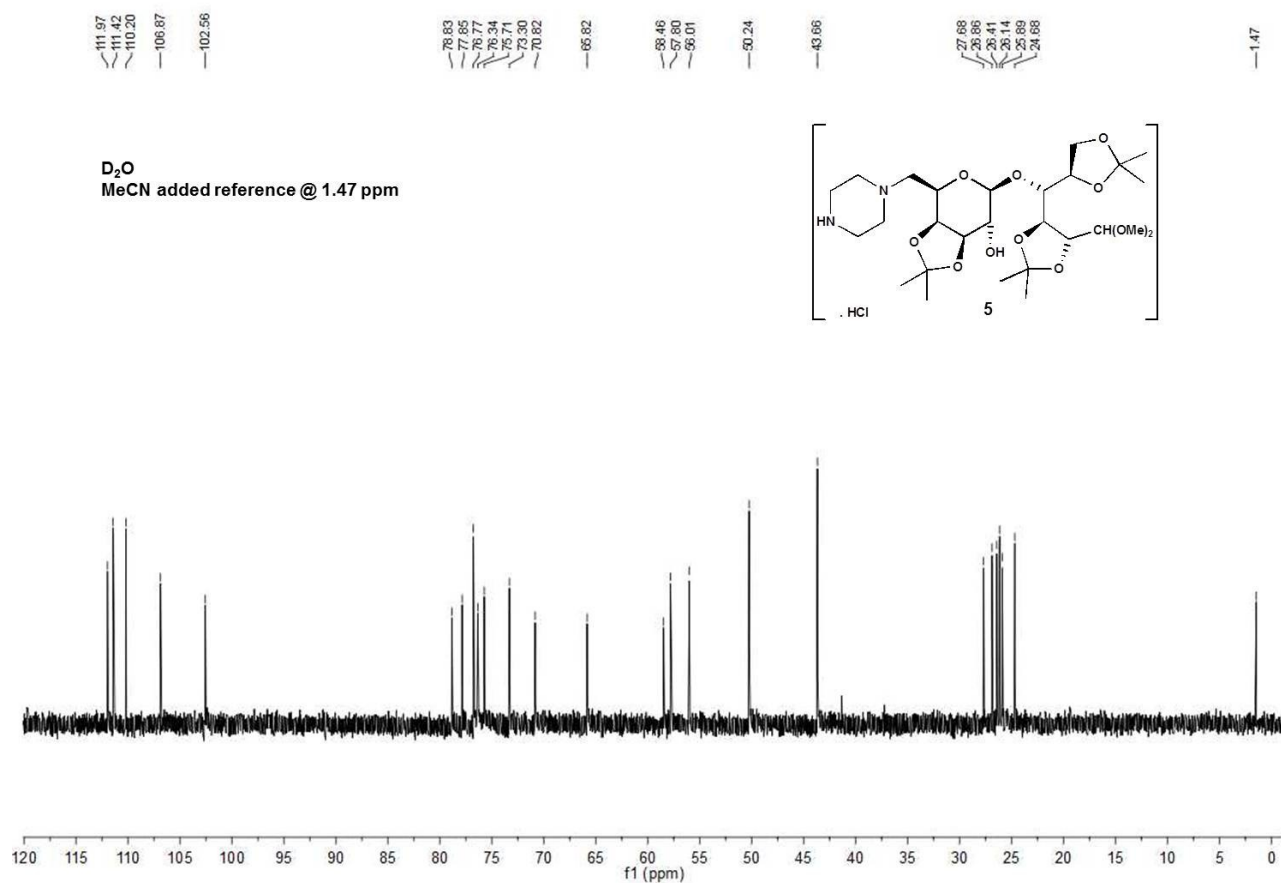


Figure 8 ESI ^{13}C -NMR spectrum of compound **5**.

TABLES

Table 1 ESI List of the substances considered in the EATOS assessment of the 4-steps chemical synthesis of compound **5**.

	Substance	Category	Quantity
Step 1	lactose	key substrate	170 g
	dimethoxypropane	substrate	1270 g
	<i>p</i> -toluenesulfonic acid	catalyst	7.2 g
	triethylamine	auxiliary material (reaction)	6.2 g
	dichloromethane	auxiliary material (isolation)	800 g
	hydrochloric acid	auxiliary material (reaction)	7.6 ml
	ammonium hydroxide	auxiliary material (reaction)	5.9 ml
	water	auxiliary material (isolation)	557 ml
	ethyl acetate	auxiliary material (isolation)	80 g
	PE	auxiliary material (isolation)	1050 g
	compound 2	product	170 g (Y: 67.3%)
	methanol	coupled product	according to Y
	water	coupled product	according to Y
Step 2	compound 2	key substrate	170 g
	<i>p</i> -toluenesulfonyl chloride	substrate	73 g
	dichloromethane	solvent	720 g
	dimethylaminopyridine	catalyst	4.1 g
	triethylamine	auxiliary material (reaction)	65.09 g
	sodium carbonate	auxiliary material (reaction)	39 g
	water	auxiliary material (isolation)	760 g
	citric acid	auxiliary material (isolation)	25.8 g
	acetonitrile	auxiliary material (isolation)	320 g
	compound 3	product	207 g (Y: 93.4%)
Step 3	HCl	coupled product	according to Y
	compound 3	key substrate	207 g
	piperazine	substrate	240 g
	dichloromethane	auxiliary (isolation)	2500 g
	water	auxiliary material (isolation)	950 g
	ethanol	auxiliary material (isolation)	1500 g
	compound 4	product	165 g (Y: 91.6%)
	<i>p</i> -toluenesulfonic acid	coupled product	according to Y
Step 4	compound 4	key substrate	165 g
	hydrochloric acid	substrate	28.4 g
	ethanol	solvent	95 g
	water	auxiliary (isolation)	1280 g
	compound 5	product	160 g (Y: 91.2%)

Table 2 ESI LCIA endpoint results of 3200g of EDF20 defatting agent (IMPACT 2002+ Method).

Damage category	Unit	Total	Step 1	Step 2	Step 3	Step 4	Step 5
Human Health	DALY	1.3E-05	8.7E-06	9.1E-06	-6.6E-06	-1.3E-06	3.3E-06
Climate Change	kg CO ₂ eq	15.0E00	12.3E00	6.4E00	-7.1E00	-1.0E00	4.4E00
Human Health, worker	DALY	8.6E-06	8.6E-06	7.2E-09	8.3E-09	3.4E-09	0.0E00
Ecosystem Quality	PDF*m2*yr	9.3E00	3.1E00	2.9E00	3.6E00	-3.7E00	3.4E00
Resources	MJ primary	8.7E00	179.2E00	112.1E00	-345.2E00	-14.4E00	7.7E01
Renewable Energy	MJ	110.0E00	33.0E00	27.5E00	52.1E00	-32.7E00	30.1E00

Table 3 ESI Detailed single score evaluation results referred to the different stages for the synthesis of compound **2**.

Impact category (mPt)	2,2- dimethoxy- propane	<i>p</i> -TsOH	Transport	Heating	Evaporation	Dissolution , partial deprot. and neutraliz.	Separation, washing and sep. aqueous phase 2	Evaporation 2	Dissolution, dilution and aging	Filtration	Washing
Carcinogens	9.6E-02	2.0E-04	3.1E-04	1.7E-02	-6.3E-02	5.9E-03	8.4E-03	3.6E-03	2.2E-01	1.8E-04	1.1E-04
Non-carcinogens	9.3E-03	2.1E-05	4.9E-04	5.5E-03	5.1E-02	7.5E-03	2.4E-02	-1.9E-03	1.2E-02	1.2E-05	5.5E-07
Respiratory inorganics	1.5E-01	4.9E-04	5.4E-03	1.4E-01	-3.3E-02	4.8E-01	7.2E-02	-2.6E-01	2.7E-01	4.5E-05	1.3E-05
Ionizing radiation	6.6E-05	1.8E-06	1.8E-05	8.6E-04	6.8E-04	2.7E-04	1.5E-04	2.8E-04	1.9E-03	1.3E-07	8.6E-08
Ozone layer depletion	1.4E-05	5.4E-08	2.0E-06	5.0E-05	1.8E-05	8.0E-03	1.4E-05	-5.8E-03	1.3E-04	9.4E-09	4.0E-09
Respiratory organics	6.1E-04	1.6E-06	9.8E-06	2.0E-04	-4.2E-04	3.4E-04	5.2E-05	-1.4E-04	6.3E-04	8.1E-08	4.7E-08
Aquatic ecotoxicity	3.2E-04	8.6E-07	2.1E-05	3.4E-04	1.3E-05	2.8E-04	3.2E-04	6.4E-07	9.2E-04	1.9E-07	3.8E-08
Terrestrial ecotoxicity	3.4E-03	1.8E-05	2.2E-03	1.4E-02	9.8E-03	8.4E-03	7.4E-03	3.8E-03	3.5E-02	4.7E-06	1.5E-06
Terrestrial acid/nutri	2.4E-03	7.1E-06	5.2E-05	1.7E-03	-7.2E-04	7.0E-03	9.9E-04	-3.5E-3	3.6E-03	6.0E-07	1.7E-07
Land occupation	3.3E-04	5.5E-06	2.7E-04	3.1E-02	1.6E-02	6.1E-03	4.4E-03	1.1E-02	6.1E-02	4.7E-06	3.8E-06
Aquatic acidification	0	0	0	0	0	0	0	0	0	0	0
Aquatic eutrophication	0	0	0	0	0	0	0	0	0	0	0
Global warming	1.8E-01	6.7E-04	7.5E-03	1.8E-01	-1.6E-02	2.8E-01	3.8E-01	-1.1E-01	3.4E-01	2.0E-04	1.8E-05
Non-renewable energy	4.9E-01	2.1E-03	7.8E-03	1.8E-01	-2.8E-01	2.7E-01	4.6E-02	-9.9E-02	5.6E-01	3.5E-05	1.9E-05
Mineral extraction	1.6E-04	8.6E-07	2.0E-05	1.2E-03	7.8E-04	3.9E-04	1.9E-04	3.9E-04	2.2E-03	1.8E-07	1.3E-07
Renewable Energy	0	0	0	0	0	0	0	0	0	0	0
Internal Costs	0	0	0	0	0	0	0	0	0	0	0
Respiratory inorganics indoor	0	0	0	0	0	8.3E-02	6.9E-02	0	0	0	0
Carcinogens, indoor	0	0	0	0	0	5.1E-08	4.2E-08	1.9E-07	1.1E00	6.5E-05	4.1E-05
Respiratory organics, indoor	0	0	0	8.4E-06	0	3.9E-05	3.2E-05	1.4E-04	4.1E-04	6.1E-08	8.6E-09
Non-carcinogens, indoor	0	0	0	3.5E-07	0	4.3E-07	3.5E-07	0	1.6E-07	9.8E-12	6.1E-12