materials

MDPI

Article

Evaluation of the Environmental Impact and Efficiency of N-Doping Strategies in the Synthesis of Carbon Dots

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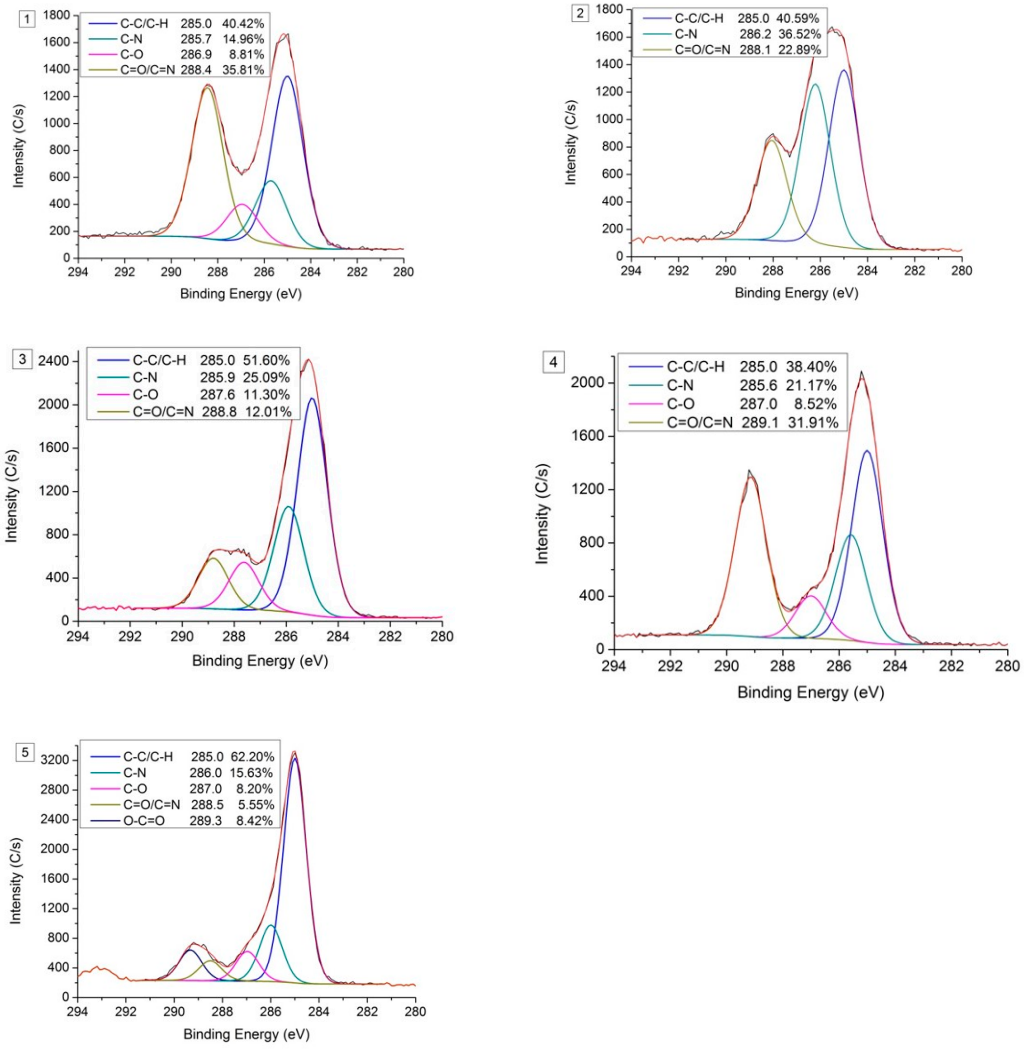


Figure S1. Detailed XPS spectra of C 1s (Carbon dots 1 to 5).

Table S1. Contributions (%) to C 1s peaks after deconvolution (CasaXPS software).

C 1s bond (BE)	1	2	3	4	5
C-C/C-H (~285 eV)	40	41	52	38	62

C-N (~286 eV)	15	37	25	21	16
C-O (~287 eV)	9	-	11	9	8
C=O/C=N (~288 eV)	36	23	12	32	6
O-C=O (~289 eV)	-	-	-	-	8

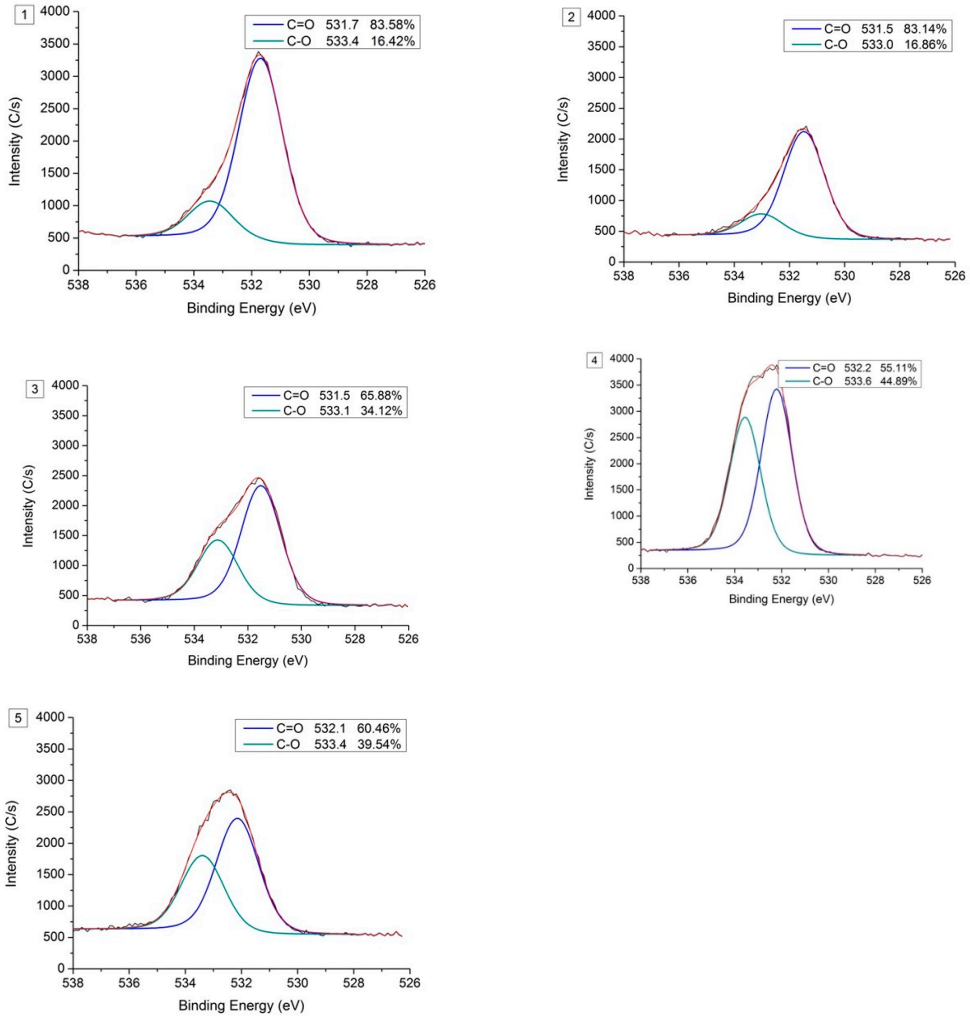


Figure S2. Detailed XPS spectra of O 1s (Carbon dots 1 to 5).

Table S2. Contributions (%) to O 1s peaks after deconvolution (CasaXPS software).

O 1s bond (BE)	**1**	**2**	**3**	**4**	**5**
C=O (~532 eV)	84	83	66	55	60
C-O (~533 eV)	16	17	34	45	40

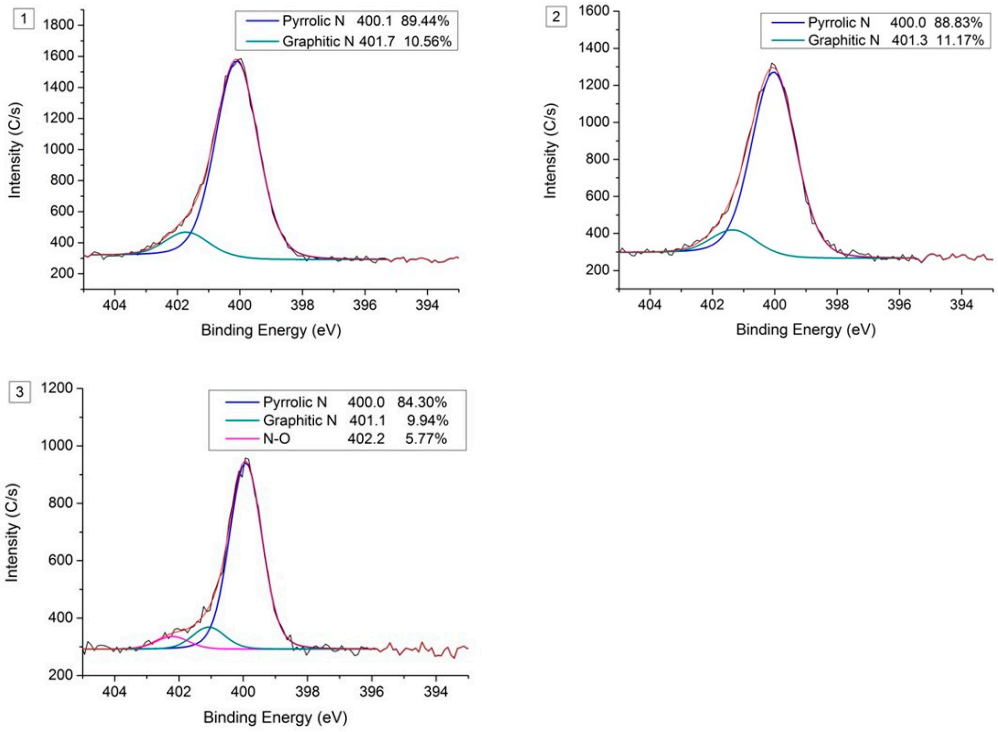


Figure S3. Detailed XPS spectra of N 1s (Carbon dots 1 to 3).

Table S3. Contributions (%) to N 1s peaks after deconvolution (CasaXPS software).

N 1s bond (BE)	1	2	3
Pyrrolic N (~400 eV)	89	89	84
Graphitic N (~401.5 eV)	11	11	10
N-O (~402 eV)	-	-	6

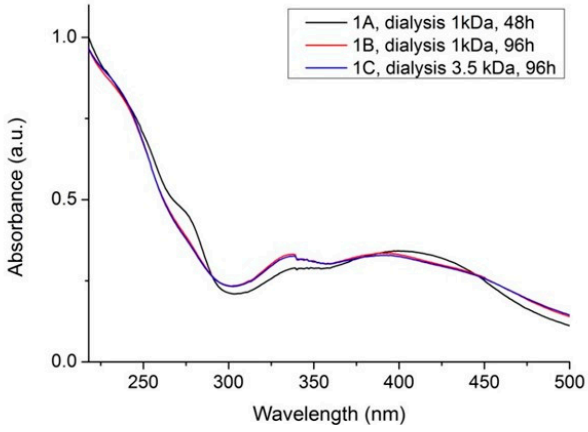


Figure S4. Absorbance spectra of carbon dots 1A, 1B and 1C.

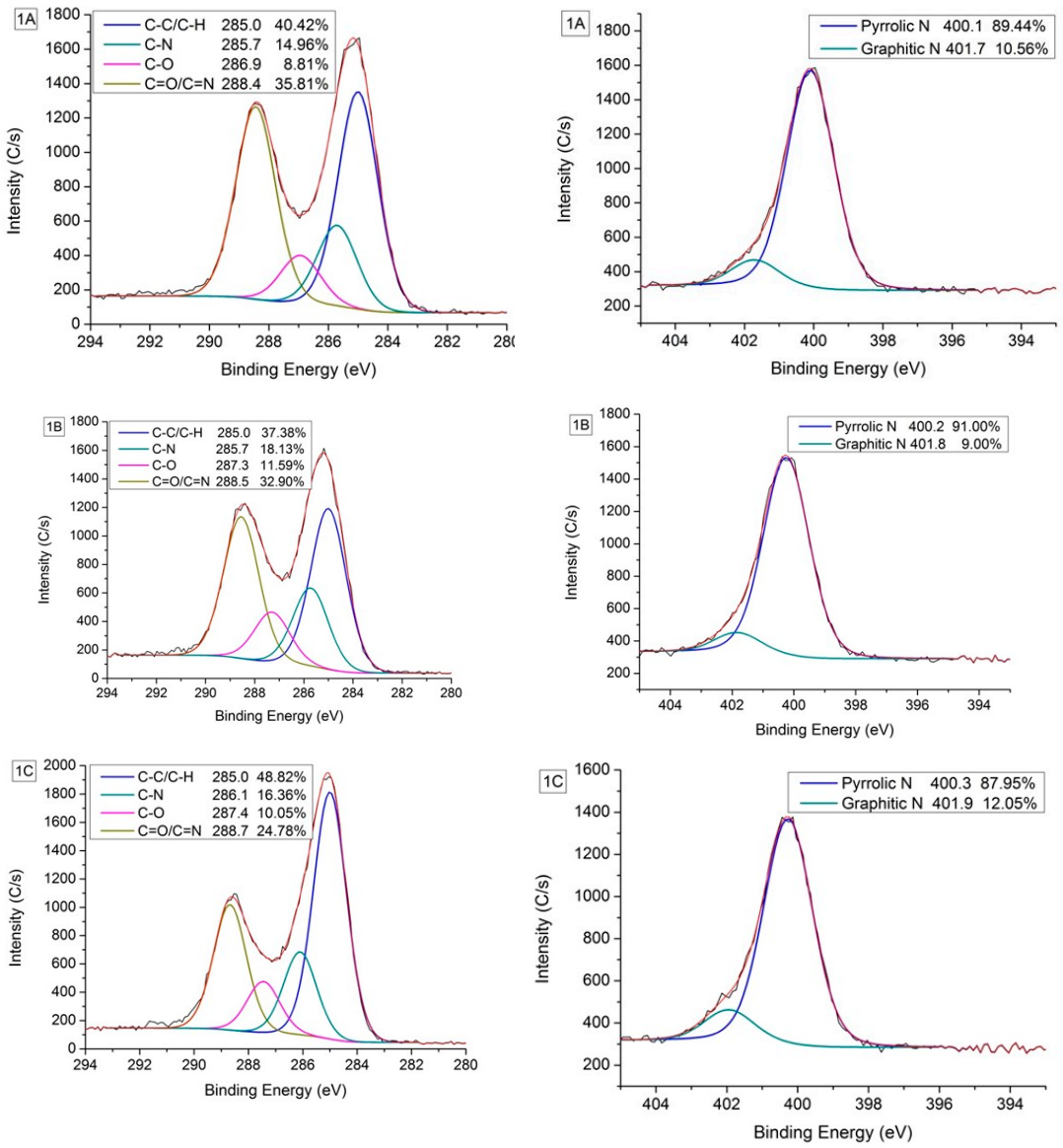


Figure S5. XPS spectra C 1s (left) and N 1s (right) for carbon dots 1A, 1B and 1C.

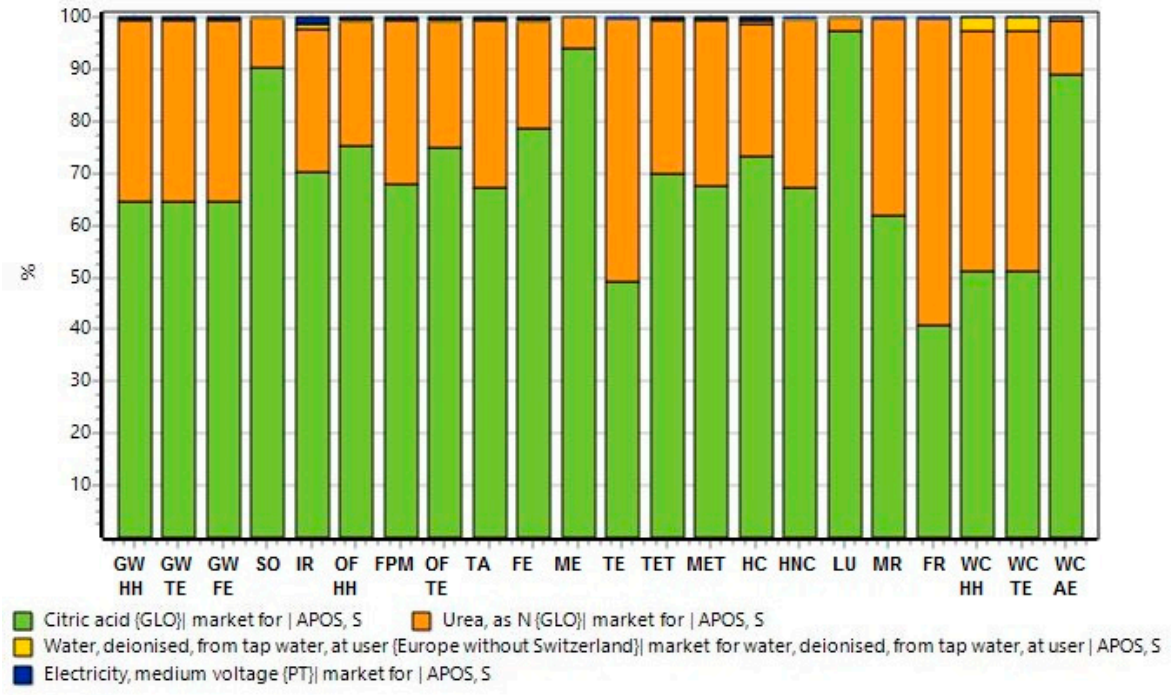
Table S4. Quantity of products required for the production of 1 kg of CDs (SimaPro software).

Carbon dots	Citric acid (kg)	Nitrogen source (kg)	Deionized water (kg)	Electricity (MJ)
1B	35	35	357	174
2	7.2	7.2	77.9	87.1
3	22.9	217	5.5	87.1
4	13.7	108	5.5	87.1
5	278	2720	5.5	87.1

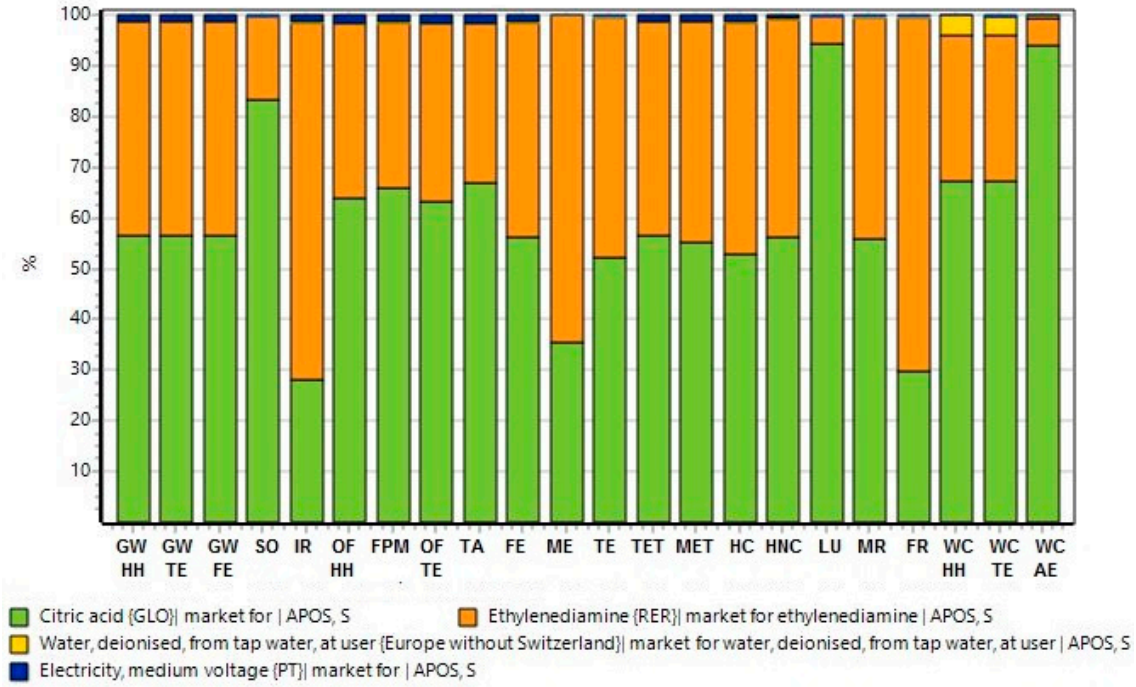
Table S5. Fluorescence quantum yields (QY_{FL}) and QY_{FL}-based functional units.

Carbon dots	QY_{FL} (%)	QY_{FL}-based functional unit (using 1B as reference)
1B	3.5	1.0

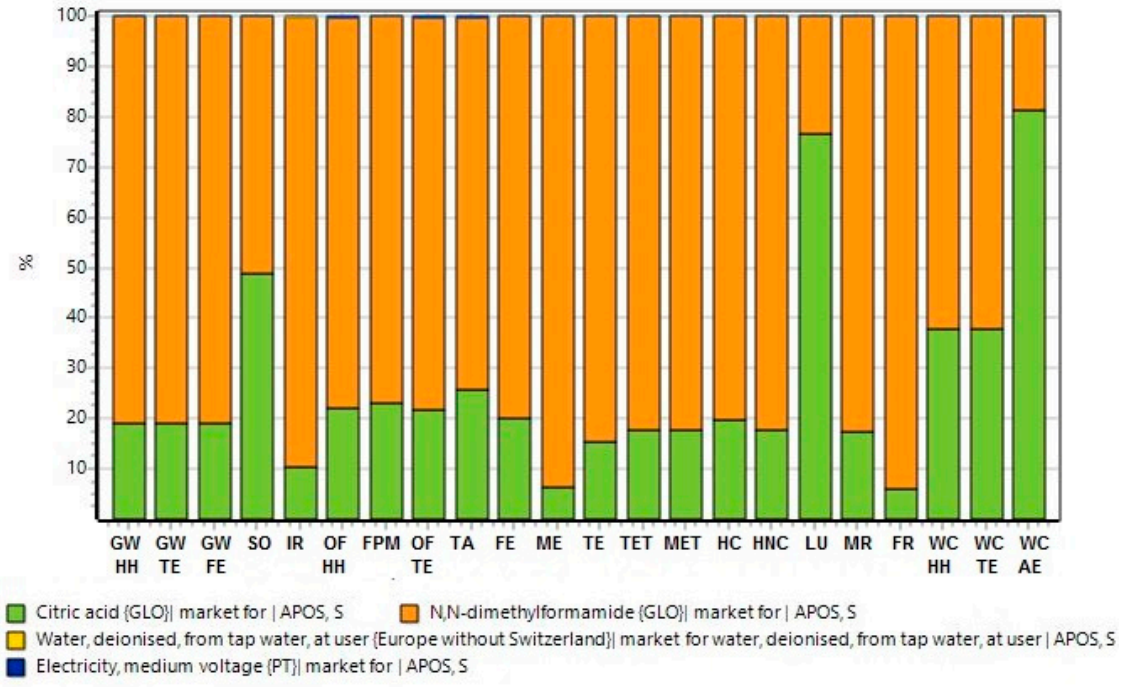
2	3.1	1.1
3	3.5	1.0
4	2.4	1.5
5	2.3	1.5



(**A**)



(**B**)


100
90
80
70
60
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40
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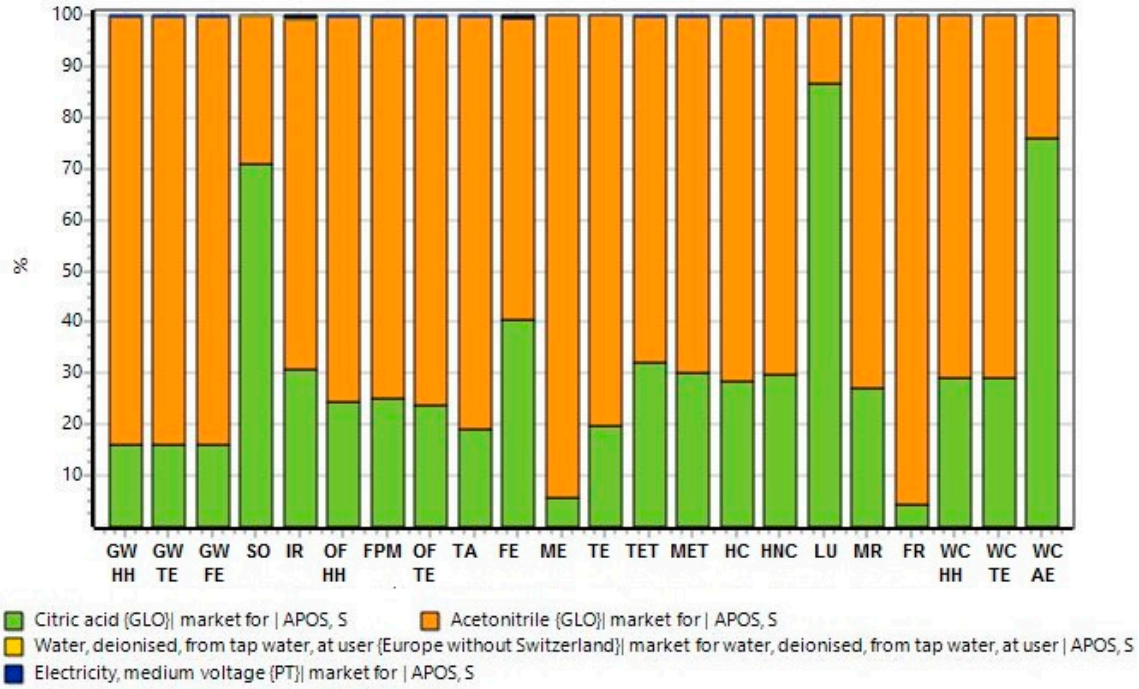
20
10
%
GW HH
GW TE
GW FE
SO
IR
OF HH
FPM
OF TE
TA
FE
ME
TE
TET
MET
HC
HNC
LU
MR
FR
WC HH
WC TE
WC AE
Citric acid {GLO}| market for | APOS, S
N,N-dimethylformamide {GLO}| market for | APOS, S
Water, deionised, from tap water, at user {Europe without Switzerland}| market for water, deionised, from tap water, at user | APOS, S
Electricity, medium voltage {PT}| market for | APOS, S

(**C**)


100
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40
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10
%
GW HH
GW TE
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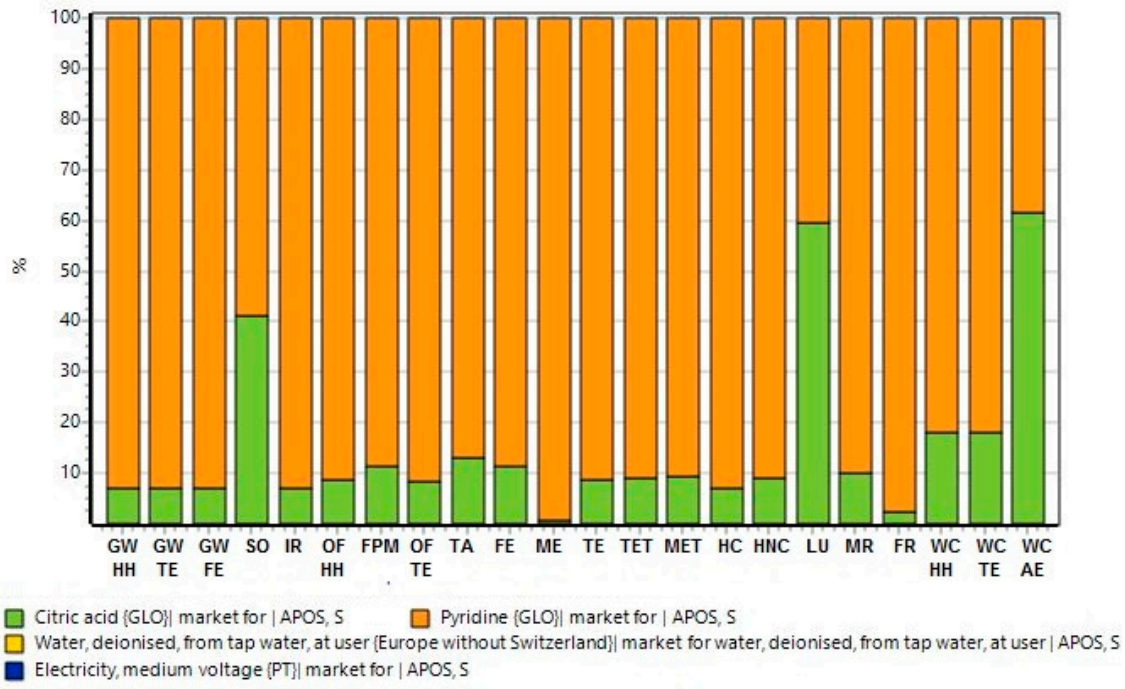
SO
IR
OF HH
FPM
OF TE
TA
FE
ME
TE
TET
MET
HC
HNC
LU
MR
FR
WC HH
WC TE
WC AE
Citric acid {GLO}| market for | APOS, S
Acetonitrile {GLO}| market for | APOS, S
Water, deionised, from tap water, at user {Europe without Switzerland}| market for water, deionised, from tap water, at user | APOS, S
Electricity, medium voltage {PT}| market for | APOS, S

(**D**)



(**E**)

Figure S6: Relative environmental impacts of each carbon dots solution with the ReCiPe2016 LCIA for: (**A**) CDs 1B, (**B**) CDs 2, (**C**) CDs 3, (**D**) CDs 4 and (**E**) CDs 5.