Supporting information for Green Chemistry

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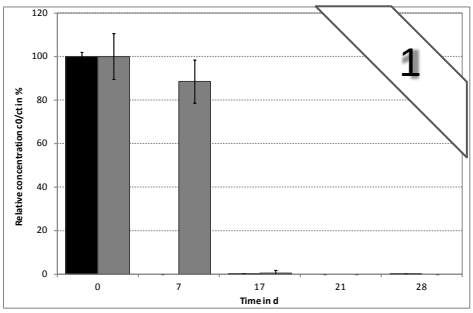
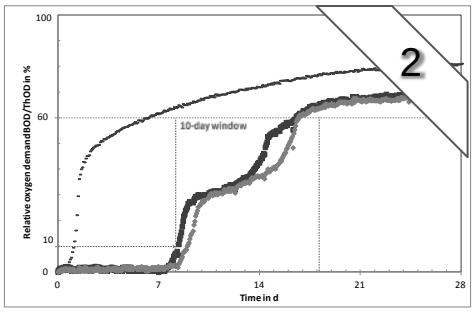
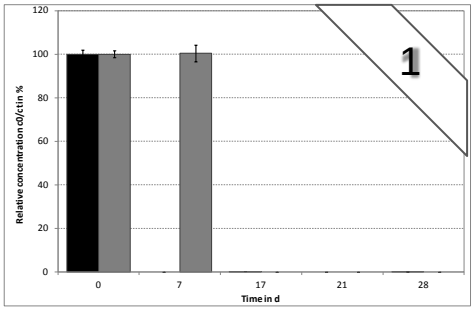
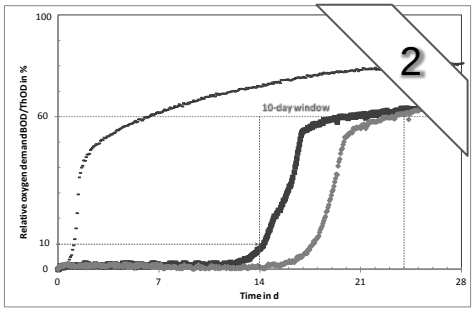
Biodegradability of 27 pyrrolidinium, morpholinium, piperidinium, imidazolium and pyridinium ionic liquid cations under aerobic conditions

Electronic supporting information

"Primarily and readily biodegradable"

Ionic liquid	Primary degradation test via specific analysis of the cation by ion chromatography (n = 2) Reference substance: aniline (black column)	Ready biodegradation test via biological oxygen demand by WTW Oxitop® devices (n = 2; both replicates shown) Reference substance: benzoic acid (n = 2; black dashes)
C_8mpyr Cl		
C_{3OH}mpyr Cl		

Classification

1 "Fully primarily degradable"

A 100 % decrease in relative concentration of the parent compound;
such a chemical is "potentially readily biodegradable"

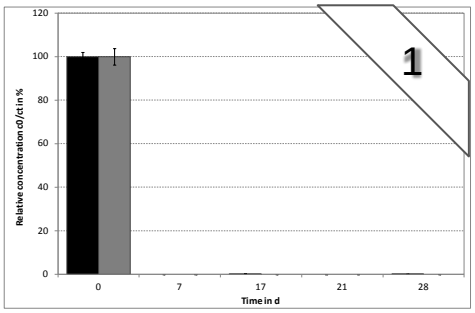
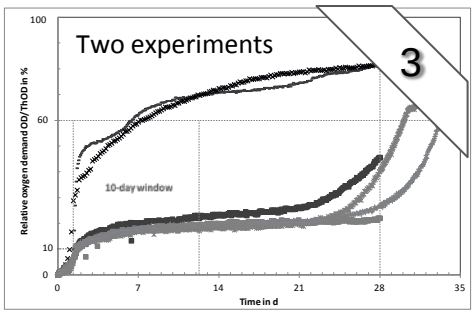
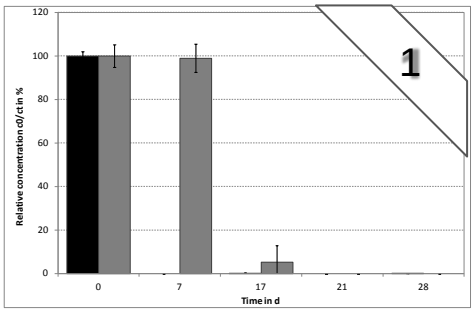
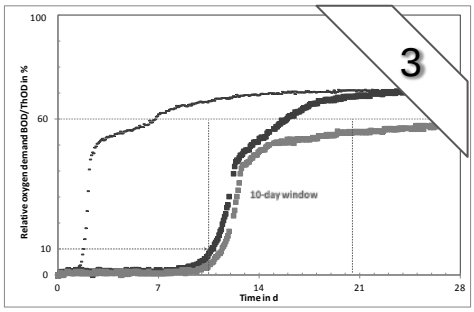
→ Further testing on "ready biodegradability" using measurements on biological oxygen demand

2 "Readily biodegradable"

The biological oxygen demand reaches 60 % of the theoretical oxygen demand within 28 d in a time window of 10 d (starting after 10 % relative oxygen demand is attained);
such a chemical is assumed to degrade rapidly and completely in aquatic environments under aerobic conditions, i.e. there is very low or no risk of persistency under the denoted conditions

→ No further testing in this study

"Primarily and inherently biodegradable"

Ionic liquid	Primary degradation test via specific analysis of the cation by ion chromatography (n = 2) Reference substance: aniline (black column)	Full mineralisation test via biological oxygen demand by WTW Oxitop® devices (n = 2; both replicates shown) Reference substance: benzoic acid (n = 2; black)
$C_{1COO2}mpyr$ Cl		
$C_{2OH}py$ I		

Classification

1 "Fully primarily degradable"

A 100 % decrease in relative concentration of the parent compound; such a chemical is "potentially readily biodegradable"

→ Further testing on "ready biodegradability" using measurements on biological oxygen demand

3 "Inherently biodegradable"

The chemical is not readily biodegradable, but there is unequivocally evidence of biodegradation in both tests of biodegradability (primary or full mineralisation); the chemical has potential for biodegradation under aerobic conditions; i.e. there is low risk of persistency under the denoted conditions

→ No further testing in this study

"Primarily and inherently biodegradable"

Ionic liquid

Primary degradation test

via specific analysis of the cation
by ion chromatography
(n = 2)

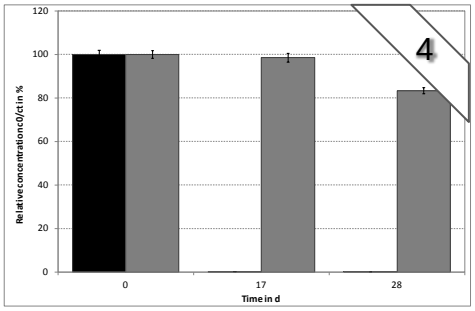
Reference substance: aniline (black column)

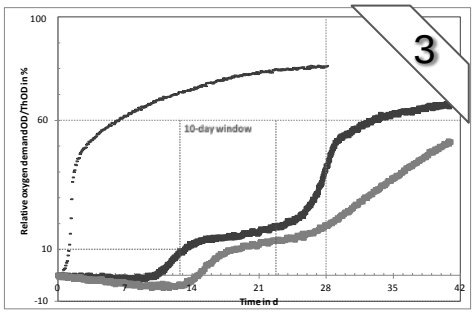
Full mineralisation test

via biological oxygen demand
by WTW Oxitop® devices
(n = 2; both replicates shown)

Reference substance: benzoic acid (n = 2; black)

$C_{3OH}mmor\ Cl$





Classification

4 "Partly primarily degradable"

No 100 % decrease in relative concentration at the end of the experimental run time

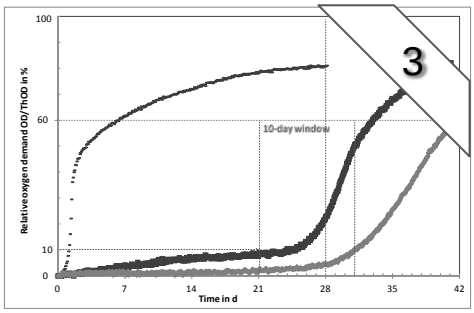
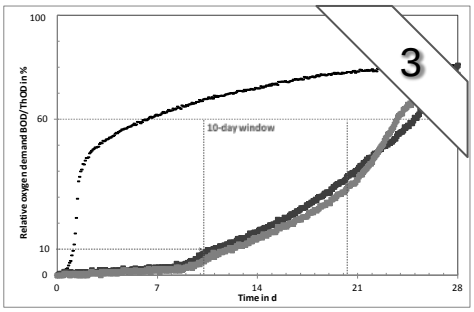
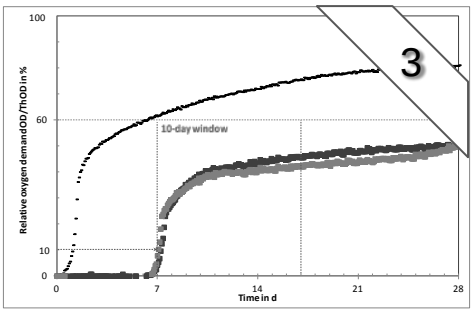
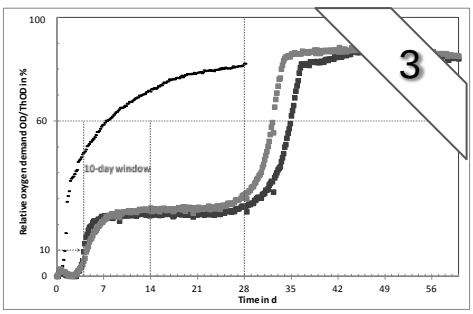
→ Further testing using measurements on biological oxygen demand

3 "Inherently biodegradable"

The chemical is not readily biodegradable, but there is unequivocally evidence of biodegradation in both tests of biodegradability (primary or full mineralisation); the chemical has potential for biodegradation under aerobic conditions; i.e. there is low risk of persistency under the denoted conditions

→ No further testing in this study

"Primarily and inherently biodegradable"

Ionic liquid	Primary degradation test via specific analysis of the cation by ion chromatography (n = 2) Reference substance: aniline (black column)	Full mineralisation test via biological oxygen demand by WTW Oxitop® devices (n = 2; both replicates shown) Reference substance: benzoic acid (n = 2; black)
C_4mpyr Br	Not tested	
C_{3OH}mpip Cl	Not tested	
C_{3OH}py Cl	Not tested	
C_{2OH}mpip Cl	Not tested	

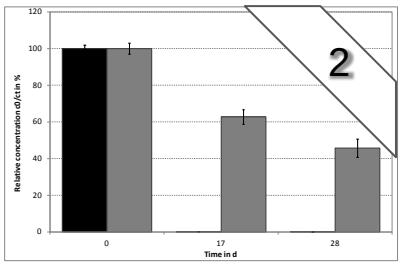
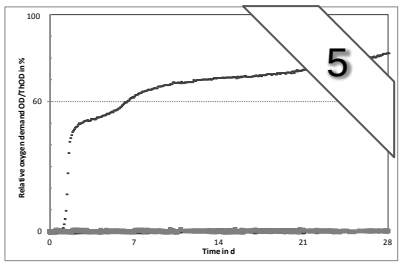
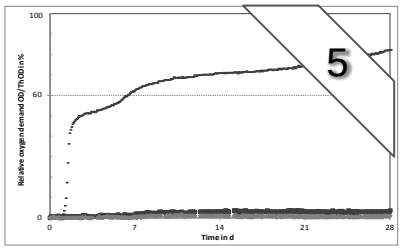
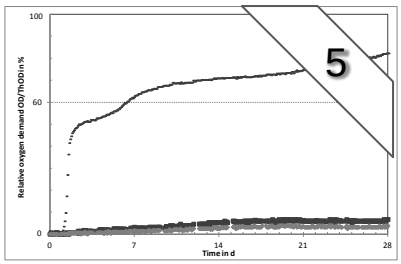
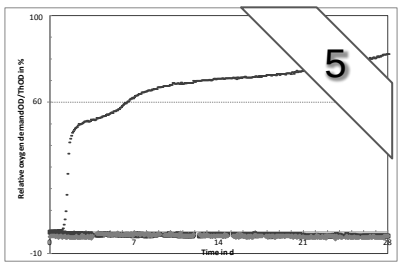
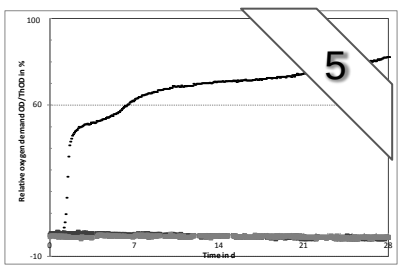
Classification

3 "Inherently biodegradable"

The chemical is not readily biodegradable, but there is unequivocally evidence of biodegradation in both tests of biodegradability (primary or full mineralisation); the chemical has potential for biodegradation under aerobic conditions; i.e. there is low risk of persistency under the denoted conditions

→ No further testing in this study

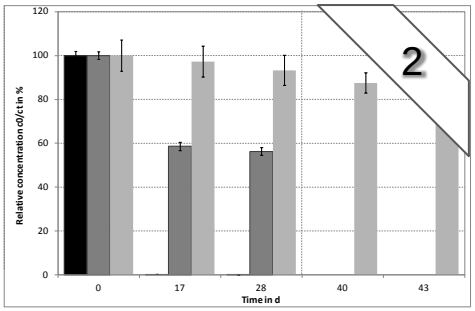
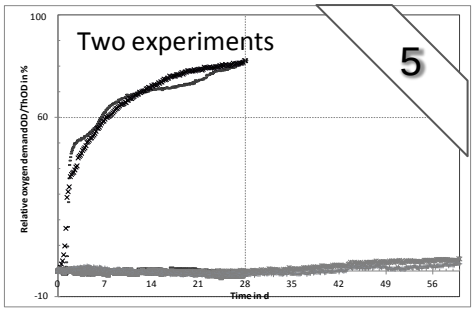
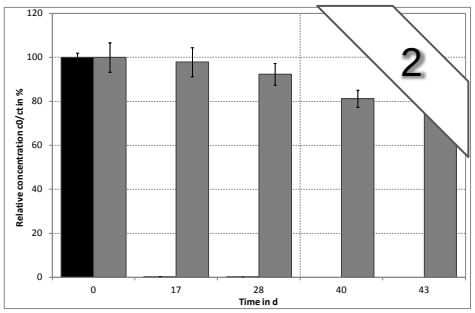
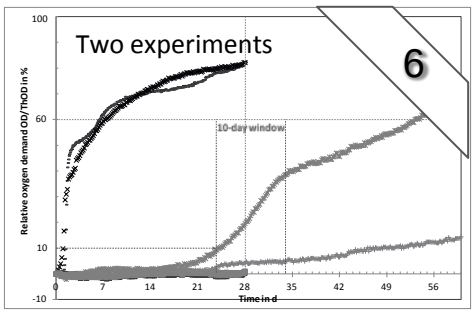
"Primarily, but not readily biodegradable"

Ionic liquid	Primary degradation test via specific analysis of the cation by ion chromatography (n = 2) Reference substance: aniline (black column)	Ready biodegradation test via biological oxygen demand by WTW Oxitop® devices (n = 2; both replicates shown) Reference substance: benzoic acid (n = 2; black dashes)
C_{1CN}mmor Cl		
C_{1CN}mpyr Cl	See discussion on C_{1CN}mmor Cl	
C_{1CN}mpip Cl	See discussion on C_{1CN}mmor Cl	
C_{1CN}py Cl	See discussion on C_{1CN}mmor Cl	
C_{1CN}mim Cl	See discussion on C_{1CN}mmor Cl	

Classification

4	"Partly primarily degradable"	No 100 % decrease in relative concentration at the end of the experimental run time → Further testing using measurements on biological oxygen demand and mass spectrometry
5	"Not readily biodegradable"	The chemical cannot be unequivocally classified as readily or inherently biodegradable under the experimental conditions → No further testing in this study

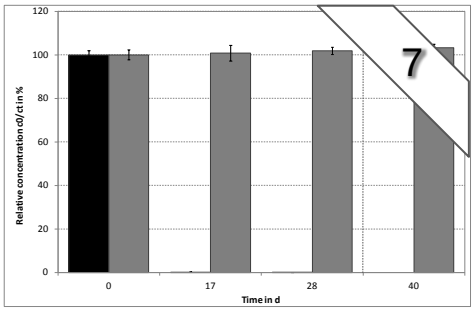
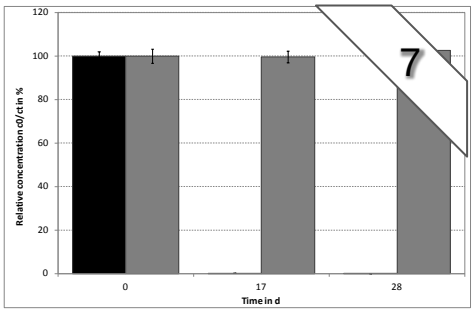
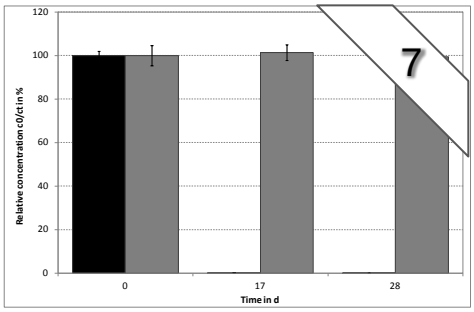
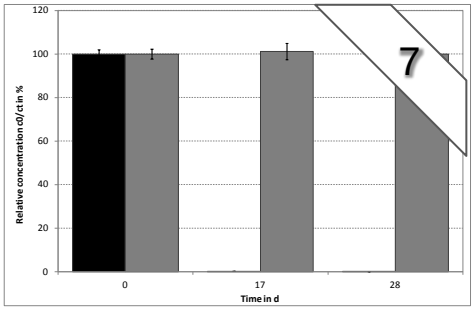
"Primarily, but not readily biodegradable"

Ionic liquid	Primary degradation test via specific analysis of the cation by ion chromatography (n = 2) Reference substance: aniline (black column)	Full mineralisation test via biological oxygen demand by WTW Oxitop® devices (n = 2; both replicates shown) Reference substance: benzoic acid (n = 2; black)
C_{2OH}mmor I		
C_{2OH}mpyr I		

Classification

4	"Partly primarily degradable"	No 100 % decrease in relative concentration at the end of the experimental run time → Further testing using measurements on biological oxygen demand and mass spectrometry
5	"Not readily biodegradable"	The chemical cannot be unequivocally classified as readily or inherently biodegradable under the experimental conditions → No further testing in this study
6	"Not readily biodegradable, but hints for being inherently biodegradable"	The chemical cannot be unequivocally classified as readily or inherently biodegradable under the experimental conditions, but showed in more than half of the experiments (primary and full mineralisation) a potential for being biodegradable → No further testing in this study

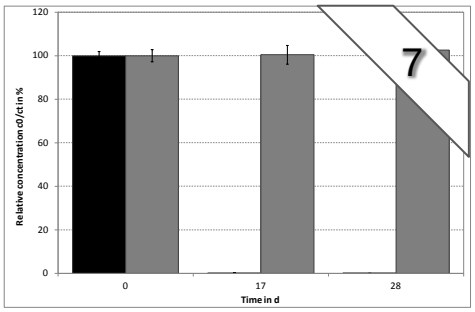
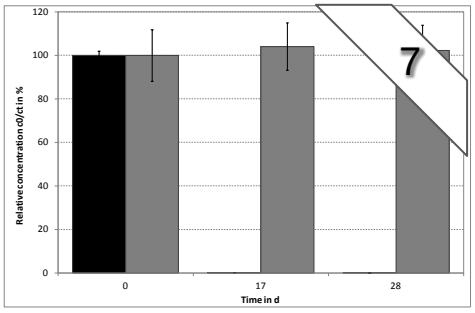
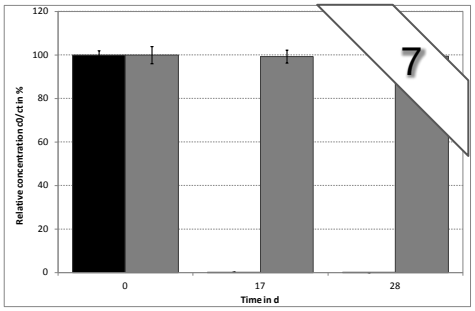
"Not primarily degradable"

Ionic liquid	Primary degradation test via specific analysis of the cation by ion chromatography (n = 2) Reference substance: aniline (black column)	Ready biodegradation test via biological oxygen demand by WTW Oxitop® devices (n = 2; both replicates shown) Reference substance: benzoic acid (n = 2; black dashes)
C_2mpyr C_2OSO_3		Not tested
$C_{1O2}mmor$ Cl		Not tested
$C_{2O1}mmor$ Cl		Not tested
$C_{2O2}mmor$ Br		Not tested

Classification

7	"Not primarily degradable"	No decrease in relative concentration → No further testing in this study

"Not primarily degradable"

Ionic liquid	Primary degradation test via specific analysis of the cation by ion chromatography (n = 2) Reference substance: aniline (black column)	Ready biodegradation test via biological oxygen demand by WTW Oxitop® devices (n = 2; both replicates shown) Reference substance: benzoic acid (n = 2; black dashes)
C_4mmor Br		Not tested
C_{1O2}mpip Cl		Not tested
C_{2O1}mpip Cl		Not tested

Classification

7	"Not primarily degradable"	No decrease in relative concentration → No further testing in this study

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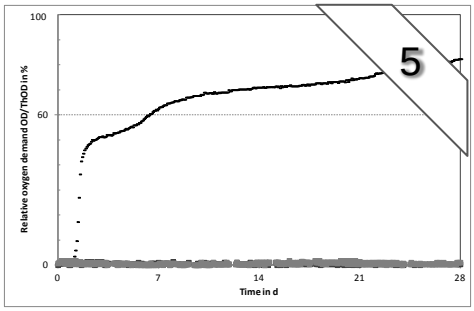
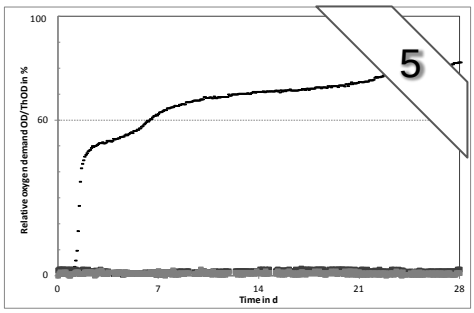
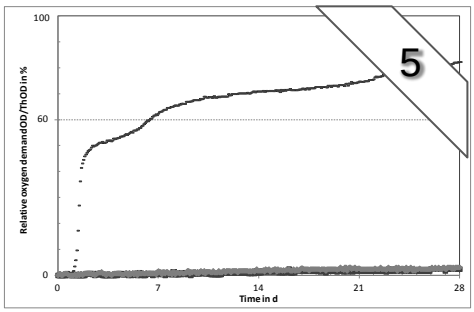
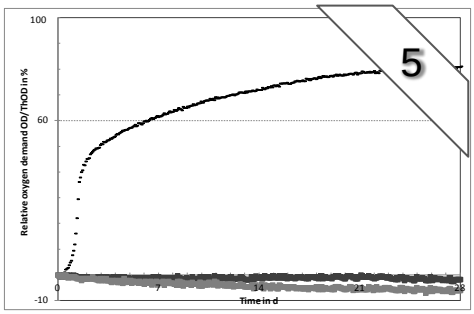
Ionic liquid	Primary degradation test via specific analysis of the cation by ion chromatography (n = 2) Reference substance: aniline (black column)	Ready biodegradation test via biological oxygen demand by WTW Oxitop® devices (n = 2; both replicates shown) Reference substance: benzoic acid (n = 2; black dashes)
C_3py Br	Not tested	
C_3mim PF_6	Not tested	
C_3mpip $(CF_3SO_2)_2N$	Not tested	
C_4mpip Br	Not tested	

Classification

5	"Not readily biodegradable"	The chemical cannot be unequivocally classified as readily biodegradable under the experimental conditions → No further testing in this study