

Electronic Supplementary Information

Authors: Qin-Tao Liu ^{*}, Rob I. Cumming, Alan D Sharpe

^{*} Correspondence to Dr. Qintao Liu, AstraZeneca Safety Health and Environment, Brixham, Devon, UK TQ5 8BA. Tel : +44 (0)1803 884 229, fax : +44 (0)1803 882 974, e-mail : Qintao.Liu@astrazeneca.com

Title: Photo-induced environmental depletion processes of β -blockers in river waters

Number of pages: 5 (including cover sheet)

Number of Figures: 2

Number of Tables: 3

Fig. 1 Sampling locations of river waters in UK

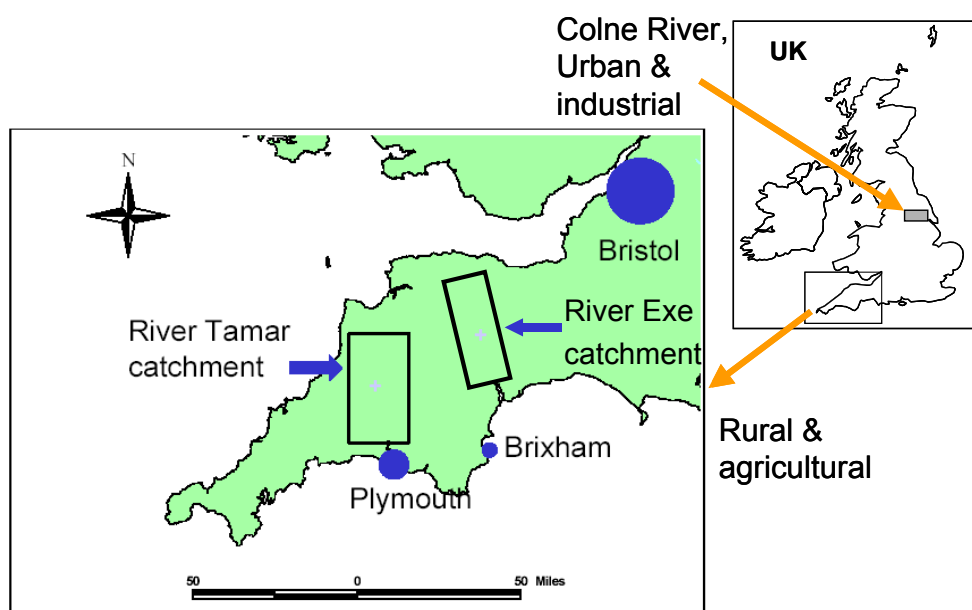


Fig. 2 Reaction vessels for the photo-induced studies

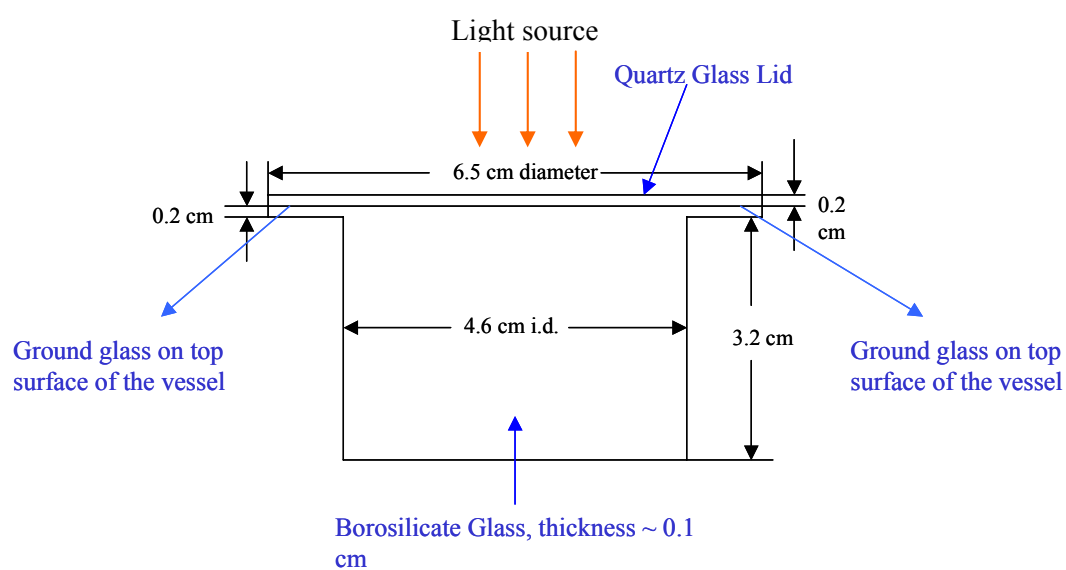


Table 1 Chemical analysis of fresh and frozen samples that were stored at -20 °C for 16 days (mg L⁻¹)

River Water Sample (0142)

m/z	24 h	24 h Frozen	48 h	48 h Frozen
276	0.022	0.013	0.015	0.012
292-1	0.600	0.606	0.356	0.257
292-2	0.139	0.156	0.158	0.154
308	0.251	0.260	0.228	0.222
310	0.075	0.131	0.166	0.131
264	0.200	0.170	0.211	0.172
258	0.018	0.019	0.038	0.030
Propranolol	0.246	0.310	0.036	0.032

Dark control River Water (Propranolol)

Original Value Frozen Sample

0hr	10.45	10.02
24hr	10.21	10.38
48hr	10.64	10.25

Table 2. River water parameters and measured 1st order degradation rate constants for propranolol, metoprolol and atenolol [§]

	Exe May 05 US	Exe May 05 DS	Tamar May 05 US	Tamar May 05 DS	Tamar Jul. 05 DS	Colne Aug. 05	Colne Nov. 05	Colne Aug. 06	Tamar Aug. 06 DS
Sampling T (°C)	12.58	12.67	12.49	12.11	18.22	14.14	6.2	15.46	
pH (field)	7.45	7.67	6.9	6.8	7.27	7.08	7.63	7.66	7.38
pH (lab)	6.77	6.82	6.79	6.79	6.89			7.96	8.01
Dissolved OC (as C) (mg L ⁻¹)	1.60	1.39	3.42	3.17	4.14	3.87		5.25	4.81
Nitrate as N (mg L ⁻¹)	2.692	2.272	2.497	2.378	1.175	2.548		2.993	1.024
Ammoniacal N ₂ as N (mg L ⁻¹)	<0.030	0.061	0.036	0.050	0.054	0.067		0.048	0.142
Nitrite as N (mg L ⁻¹)	0.028	0.018	0.013	0.012	0.005	0.052		0.017	0.066
N ₂ total oxidised as N (mg L ⁻¹)	2.720	2.290	2.510	2.390	1.180	2.600		3.010	1.090
Orthophosphate as P (mg L ⁻¹)	0.058	0.056	0.033	0.068	0.105	0.133		0.101	0.061
Redox potential (mV)	236.0	245.8	245.3	237.0	292.1	116.9		336.3	
Dissolved oxygen %	105.1	104.1	105.1	98.6	104.6	90.5	91.2	100	
Conductivity (us)	174	143	171	174	215	277	392	311	249
Suspended solids at 105 °C (mg L ⁻¹)					3.00	5.00		4.00	7.00
Solids, < 63 um (%)								80.79	94.37
Sorting coefficient								1.29	1.10
$k_{\text{propranolol}} (\text{h}^{-1})^{\text{§}}$	0.077	0.089	0.12	0.13					
$k_{\text{metoprolol}} (\text{h}^{-1})^{\text{§}}$					0.0078	0.0089	0.0082	0.021	0.015
$k_{\text{atenolol}} (\text{h}^{-1})^{\text{§}}$		0.021		0.020	0.011	0.013		0.013	0.0058

[§] All kinetics summarised in this Table was measured in non-sterilised river waters with replicates.

Table 3 Percentage of particles measured in three river water samples and statistical analysis of differences among samples

Particle size (microns)	% total suspended solids		
	Colne	Tamar Upper Stream	Tamar Down Stream
50.2-39	9.91	6.66	6.59
< 5.8	4.5	7.35	6.93
> 2000	0.00	0.00	0.00
11.4-9.1	5.17	7.60	7.60
112-84	5.67	2.07	1.30
14.5-11.4	7.24	10.83	11.05
160-112	3.93	0.62	1.04
18.5-14.5	8.88	13.10	13.48
2000-500	0.00	0.00	0.00
23.7-18.5	10.10	13.86	14.31
261-160	1.46	0.00	0.84
30.3-23.7	10.47	12.32	12.73
39-30.3	10.61	9.77	10.03
564-261	0.01	0.00	0.02
64-50	8.68	4.31	3.81
7.2-5.8	2.27	3.14	2.92
84-64	7.36	3.02	2.15
9.1-7.2	3.77	5.37	5.2
Inclusive Graphic Skewness (SKI)	-0.030	-0.050	-0.050
Particle Diameter, Mean (phi)	4.630	5.310	5.260
Particle Diameter, Median (phi)	5.130	5.690	5.690

Output from minitab;
series of paired t-tests undertaken on
arcsine square-root transformed data

Results indicate that there is no
significant difference between any of
the samples with respect to the
distribution of sediment sizes

19/06/2008 12:40:02			
Welcome to Minitab, press F1 for help.			
Paired T-Test and CI: Colne_trans, Tamar_US_trans			
Paired T for Colne_trans - Tamar_US_trans			
	N	Mean	StDev SE Mean
Colne_trans	20	0.2130	0.1076 0.0241
Tamar_US_trans	20	0.2035	0.1293 0.0289
Difference	20	0.0095	0.0649 0.0145
95% CI for mean difference: (-0.0209, 0.0399)			
T-Test of mean difference = 0 (vs not = 0): T-Value = 0.65 P-Value = 0.523			
Paired T-Test and CI: Colne_trans, Tamar_DS_trans			
Paired T for Colne_trans - Tamar_DS_trans			
	N	Mean	StDev SE Mean
Colne_trans	20	0.2130	0.1076 0.0241
Tamar_DS_trans	20	0.2068	0.1238 0.0277
Difference	20	0.0062	0.0643 0.0144
95% CI for mean difference: (-0.0238, 0.0363)			
T-Test of mean difference = 0 (vs not = 0): T-Value = 0.43 P-Value = 0.669			
Paired T-Test and CI: Tamar_US_trans, Tamar_DS_trans			
Paired T for Tamar_US_trans - Tamar_DS_trans			
	N	Mean	StDev SE Mean
Tamar_US_trans	20	0.2035	0.1293 0.0289
Tamar_DS_trans	20	0.2068	0.1238 0.0277
Difference	20	-0.00321	0.02412 0.00539
95% CI for mean difference: (-0.01450, 0.00808)			

