Supplementary Information (SI) for Environmental Science: Processes & Impacts.

Supporting information for

Linking water–sediment respiration to micropollutant biodegradation across aquatic environments

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S1. Supporting information for materials and methods

S1.1 Biochemical oxygen demand - respiration test

To avoid oxygen consumption due to the oxidation of reduced inorganic species, sediments were aerated before the start of the test. Aeration was performed by bubbling air through the sediments with the help of rubber tubes.

Dissolved Oxygen (DO) was measured in triplicate before and after the incubation using a HQ2200 multi-meter (Hach Lange GmbH, Düsseldorf, Germany) for which the DO probe had been calibrated the same day. The average DO before and after incubation was then utilized to calculate the BOD_3 of each replicate utilizing Equation S1.

$$BOD_3 = DO_{day0} - DO_{day3}$$

Equation S1. Formula for calculating three-day Biochemical Oxygen Demand (BOD_3).

S1.2 Modified OECD 309 biodegradation test

S1.2.1 Studied compounds

The test compounds used in this study were a sub-set of the compounds used by Tian et al.[1,2]. The subset of compounds was selected based on their ability to be identified and yield quantifiable degradation rate constants (k)[1,2]. Information about the preparation of the working solution used to spike samples for this study can be found in the supporting information of Tian et al 2024[2]. In brief, tested compounds were hydrophilic organic micropollutants which had previously been shown to be minimally impacted by sorption[2]. While the spiking mix contained a total of 129 compounds, a subset of 47 low sorption, easily quantified compounds, were selected for analysis in the study. The 47 compounds spanned a wide range of uses including pharmaceuticals, pesticides, food additives, personal care product and industrial chemicals, as well as functional groups including sulfonamides, carboxylic acids, phenylureas, and carbamates. The test chemicals were purchased from Sigma-Aldrich (Steinheim, Germany), Toronto Research Chemicals Inc. (North York, Canada), and CDN Isotopes (Pointe- Claire, Quebec, Canada). Some compounds were acquired as gifts from Unilever. The concentration of the chemicals in the working solution was 1.75 µg/mL in Milli-Q IQ 7000 water (Merck KGaA, Darmstadt, Germany). The internal standard working solution had a concentration of 1 µg/mL in methanol of LC/MS grade (VWR International, Rosny-sous-Bois, France).

Table S1. List of compounds in the spiking mixture. Compounds in brackets were included in the mixture but not analyzed in the study.

Compound name	Use	log D_{ow}[I]	pKa[II]	CAS Nr
Ethylhexylglycerin	Personal care products	2.4	13.64*[a]	70445-33-9
4-(4-nitrobenzyl)-pyridine	Laboratory chemical	2.6	5.51*[b]	1083-48-3
Anastrozole	Pharmaceutical	2.68	1.4[b]	33665-90-6
Acesulfame	Food additive	-2.77	2.0[a]	120511-73-1
Atrazine	Pesticide	2.66	4.2[b]	1912-24-9
Bezafibrate	Pharmaceutical	-0.11	3.83*[a]	41859-67-0
Bromoxynil	Pesticide	3.77	3.86[a]	1689-84-5
Caffeine	Natural product	0.28	-1.2[b]	1958-08-02
Candesartan	Pharmaceutical	0.04	2.45[b]	139481-59-7
Carbamazepine	Pharmaceutical	2.28	13.9[a]	298-46-4
Clofibric acid	Pharmaceutical	-0.88	NA	882-09-7
Climbazole	Personal care products	3.32	6.49[b]	38083-17-9
Chlortoluron	Pesticide	2.48	14.43*[a]	15545-48-9
Cyclamate	Food additive	-3.51	1.7[b]	100-88-9
Dicamba	Pesticide	1.24	1.97[b]	1918-00-9
Diclofenac	Pharmaceutical	1.37	1.97[a]	15307-86-5
Dimethenamid	Pesticide	2.45	1.16[b]	87674-68-8
Diuron	Pesticide	0.13	NA	330-54-1
Fluconazole	Pharmaceutical	0.7	1.76[b]	86386-73-4
Flufenacet	Pesticide	3.01	0.31*[a]	142459-58-3
Fenhexamid	Pesticide	4.17	7.3[a]	126833-17-8
Flecainide	Pharmaceutical	1.01	9.3[b]	54143-55-4
Furosemide	Pharmaceutical	-0.78	3.65[a]	54-31-9
Fluoxetine	Pharmaceutical	1.75	9.8*[b]	54910-89-3
Gabapentin	Pharmaceutical	-1.4	3.7[a]	60142-96-3
Gemfibrozil	Pharmaceutical	1.58	4.5[a]	25812-30-0
Hydroxy bupropion	Pharmaceutical (metabolite)	1.93	NA	357399-43-0
Iprovalicarb	Pesticide	3.29	11.41*[a]	140923-17-7
Isoproturon	Pesticide	2.45	15.06*[a]	34123-59-6
Ketoprofen	Pharmaceutical	0.06	3.98[a]	22071-15-4
MCPA	Pesticide	-1.09	3.13[a]	94-74-6
Mecoprop	Pesticide	-0.65	3.21[a]	7085-19-0
Mefenamic acid	Pharmaceutical	2.04	4.2[a]	61-68-7
Metformin	Pharmaceutical	-3.36	12.4[b]	657-24-9
Metolachlor	Pesticide	3.22	1.45[a]	51218-45-2
Metoprolol	Pharmaceutical	-0.25	9.56[b]	51384-51-1
Metoxuron	Pesticide	1.87	13.83[a]	19937-59-8
Naproxen	Pharmaceutical	0.45	4.15[a]	22204-53-1
p-toluenesulfonic acid	Laboratory chemical	-3.36	-1.34[a]	104-15-4
Sulfamethazine	Pharmaceutical	0.79	7.59[a]	57-68-1
Sulfadimethoxine	Pharmaceutical	-0.49	6.91*[a]	122-11-2
Sulfamethoxazole	Pharmaceutical	-0.56	6.16*[a]	723-46-6
Tamsulosin	Pharmaceutical	0.77	9.28*[b]	106133-20-4
Terbutryn	Pesticide	1.38	4.30[b]	886-50-0

Valsartan	Pharmaceutical	-0.89	3.6[a]	137862-53-4
Venlafaxine	Pharmaceutical	1.43	9.5[b]	93413-69-5
Zolpidem	Pharmaceutical	3.06	5.65[b]	82626-48-0
(1-Stearoyl-rac-glycerol)	Metabolite	2,6	-	123-94-4
(Butylhydroxytoluene)	Food preservative	5.07	11.6[*a]	128-37-0
(Alpha-isomethylionone)	Personal care products	4.22	-	127-51-5
(Chloroxylenol)	Household chemical	2.83	9.7[b]	88-04-0
(5-Methylbenzotriazole)	Industrial chemical	1.69	8.74[*b]	136-85-6
(Abacavir)	Pharmaceutical	1.32	5.8[*b]	136470-78-5
(Acetamiprid)	Pesticide	1.06	0.7[a]	135410-20-7
(Alachlor)	Pesticide	2.99	1.20[*a]	15972-60-8
(Amisulpride)	Pharmaceutical	-0.43	9.37[b]	71675-85-9
(Atazanavir)	Pharmaceutical	4.61	4.42[*b]	198904-31-3
(Atenolol)	Pharmaceutical	-1.85	9.58[b]	29122-68-7
(Azoxystrobin)	Pesticide	3.54	1.94[*b]	131860-33-8
(Benzotriazole)	Industrial chemical	1.5	8.37[b]	95-14-7
(Benzyl alcohol)	Laboratory chemical	4.85	15.4[a]	100-51-6
(Benzyl salicylate)	Personal care products	4.01	8.11[*b]	118-58-1
(Bisoprolol)	Pharmaceutical	0.12	9.67[*b]	66722-44-9
(C12 Isethionate)	Personal care products	-	-	7381-01-3
(Carbendazim)	Pesticide	1.51	4.29[b]	10605-21-7
(Chlorothiazide)	Pharmaceutical	-0.21	4.29[a]	58-94-6
(Chlorthalidone)	Pharmaceutical	0.41	6.85[a]	77-36-1
(Cilastatin)	Pharmaceutical	-1.9	9.14[*b]	82009-34-5
(Ciprofloxacin)	Pharmaceutical	-2.23	8.77[*b]	85721-33-1
(Citalopram)	Pharmaceutical	1.27	9.78[b]	59729-33-8
(Cocoamidopropyl betaine)	Personal care products	0.93	-	61789-40-0
(Decylamine)	Laboratory chemical	1.07	10.64[b]	2016-57-1
(Dibenzepin)	Pharmaceutical	1.24	8.23[b]	4498-32-2
(Diflufenican)	Pesticide	4.09	9.03[*b]	83164-33-4
(Dioctyl Sulfocinate Sodium Salt)	Industrial chemical	1.01	-0.75[*a]	10041-19-7
(Dodecyl sulfate sodium salt)	Personal care product	1.6	-1.5[a]	151-21-3
(Dodecylamine)	Laboratory chemical	1.86	10.63[*b]	124-22-1
(Dodecyltrimethylammonium chloride)	Industrial chemical	-	-	112-00-5
(Ethofumesate)	Pesticide	2.14	-	26225-79-6 2
(Ethylene glycol butyl ether)	Personal care products	0.77	14.42[*a]	111-76-2
(Ethylhexyl methoxycinnamate)	Personal care products	5.28	-4.8[*b]	5466-77-3
(Ethylparaben)	Food preservative	2.48	8.34[a]	120-47-8
(Fenofibrate)	Pharmaceutical	5.01	-4.9[*b]	49562-28-9
(Fipronil)	Pharmaceutical	3.71	-5.86[b]	120068-37-3
(Fludioxonil)	Pesticide	2.57	14.10[a]	131341-86-1
(Fluoxetine)	Pharmaceutical	1.75	9.8[*b]	54910-89-3
(Galaxolide)	Personal care products	5.93	-	1222-05-5
(Hexylene glycol)	Personal care products	0.23	15.10[a]	107-41-5
(Homosalate)	Personal care products	5.23	9.72[*a]	118-56-9
(Hydrochlorothiazide)	Pharmaceutical	-0.01	7.9[a]	58-93-5
(Imidacloprid)	Pesticide	-0.29	1.56[b]	138261-41-3
(Iodopropynyl butylcarbamate)	Personal care products	3.2	14.4[*a]	55406-53-6
(Irbesartan)	Pharmaceutical	1.24	5.85[*a]	138402-11-6
(Lamotrigine)	Pharmaceutical	1.68	5.7[b]	84057-84-1

(Levamisole)	Pharmaceutical	0.25	6.98[*b]	14769-73-4
(Levetiracetam)	Pharmaceutical	-0.74	-1.6[*b]	102767-28-2
(Lidocaine)	Pharmaceutical	1.26	7.95[b]	137-58-6
(Linezolid)	Pharmaceutical	0.82	1.8[b]	165800-03-3
(Losartan)	Pharmaceutical	1.29	5.5[a]	114798-26-4
(Ioxynil)	Pesticide	1.27	3.96[a]	1689-83-4
(Mefenamic acid)	Pharmaceutical	2.04	4.2[a]	61-68-7
(Methotrexate)	Pharmaceutical	-5.22	4.7[a]	59-05-2
(Methyl 4-hydroxybenzoate)	Food preservative	2.09	8.5[a]	99-76-3
(N-(3-dimethylaminopropyl)-octadecanamide)	Personal care products	6.12	16.29*[a]	7651-02-7
(N,N-bis(2hydroxyethyl) dodecanamide)	Personal care products	3.95	14.13[a]	120-40-1
(N,N-Bis(2-hydroxyethyl) tetradecanamide)	Personal care products	4.87	-	7545-23-5
(Naphthalene-2-carbonitrile)	Laboratory chemical	3.22	-	613-46-7
(Neostigmine)	Pharmaceutical	-2.77	-	59-99-4
(Nicotinamide)	Personal care products	-0.37	3.35[b]	98-92-0
(Novobiocin)	Pharmaceutical	-0.02	4.3[a]	303-81-1
(Oxazepam)	Pharmaceutical	1.5	1.55[b]	604-75-1
(Oxprenolol)	Pharmaceutical	0.19	9.57[b]	6452-71-7
(Paracetamol)	Pharmaceutical	0.4	9.38[b]	103-90-2
(Pargyline)	Pharmaceutical	2.31	8.05[*b]	555-57-7
(Picoxystrobin)	Pesticide	3.84	-1.09[*a]	117428-22-5
(Propachlor)	Pesticide	2.28	0.30[*a]	1918-16-7
(Propranolol)	Pharmaceutical	1.15	9.53[b]	525-66-6
(Propyl 4-hydroxybenzoate)	Personal care products	2.81	8.5[a]	94-13-3
(Ranitidine)	Pharmaceutical	-0.63	7.8[*b]	66357-35-5
(Rufinamide)	Pharmaceutical	0.42	12.64[a]	106308-44-5
(Sodium decyl sulfate)	Industrial chemical	-	-	142-87-0
(Sorbitan monolaurate)	Food additive	4.02	-	1338-39-2
(Sotalol)	Pharmaceutical	-1.63	9.76[a]	3930-20-9
(Sulfamethoxypyridazine)	Pharmaceutical	-0.29	6.84[*a]	80-35-3
(Sulfathiazole)	Pharmaceutical	0.03	7.2[a]	72-14-0
(Tartrazine)	Food additive	-10.17	-	1934-21-0
(Tetradecylamine)	Industrial chemical	3.05	10.62[a]	2016-42-4
(Tramadol)	Pharmaceutical	0.52	9.41[b]	27203-92-5
(Triethyl citrate)	Personal care products	1.09	11.82[a]	77-93-0
(Trimethoprim)	Pharmaceutical	-1.15	7.12[b]	738-70-5
(Trinexapac-ethyl)	Pesticide	-1.76	4.7[a]	95266-40-3

[I] Values for compound log D_{ow} were obtained from ChemSpider.
[II] Values of compound pKa were obtained from PubChem. If unavailable, predicted values were obtained from DrugBank or ChemBK, marked with *. Values are listed as: [a] acid pKa, or [b] base pKa.

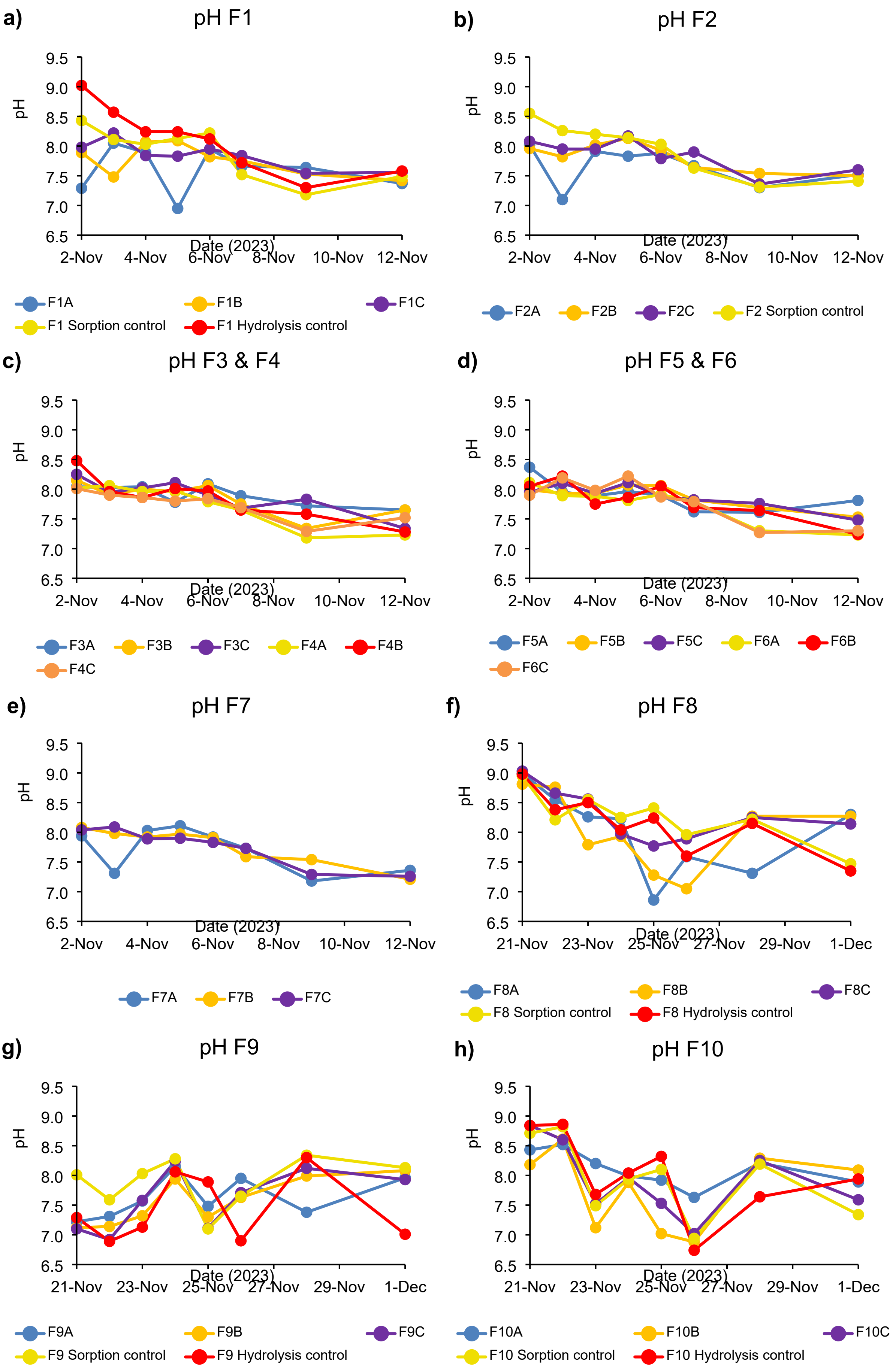
Table S2. List of the 15 compounds used as internal standards.

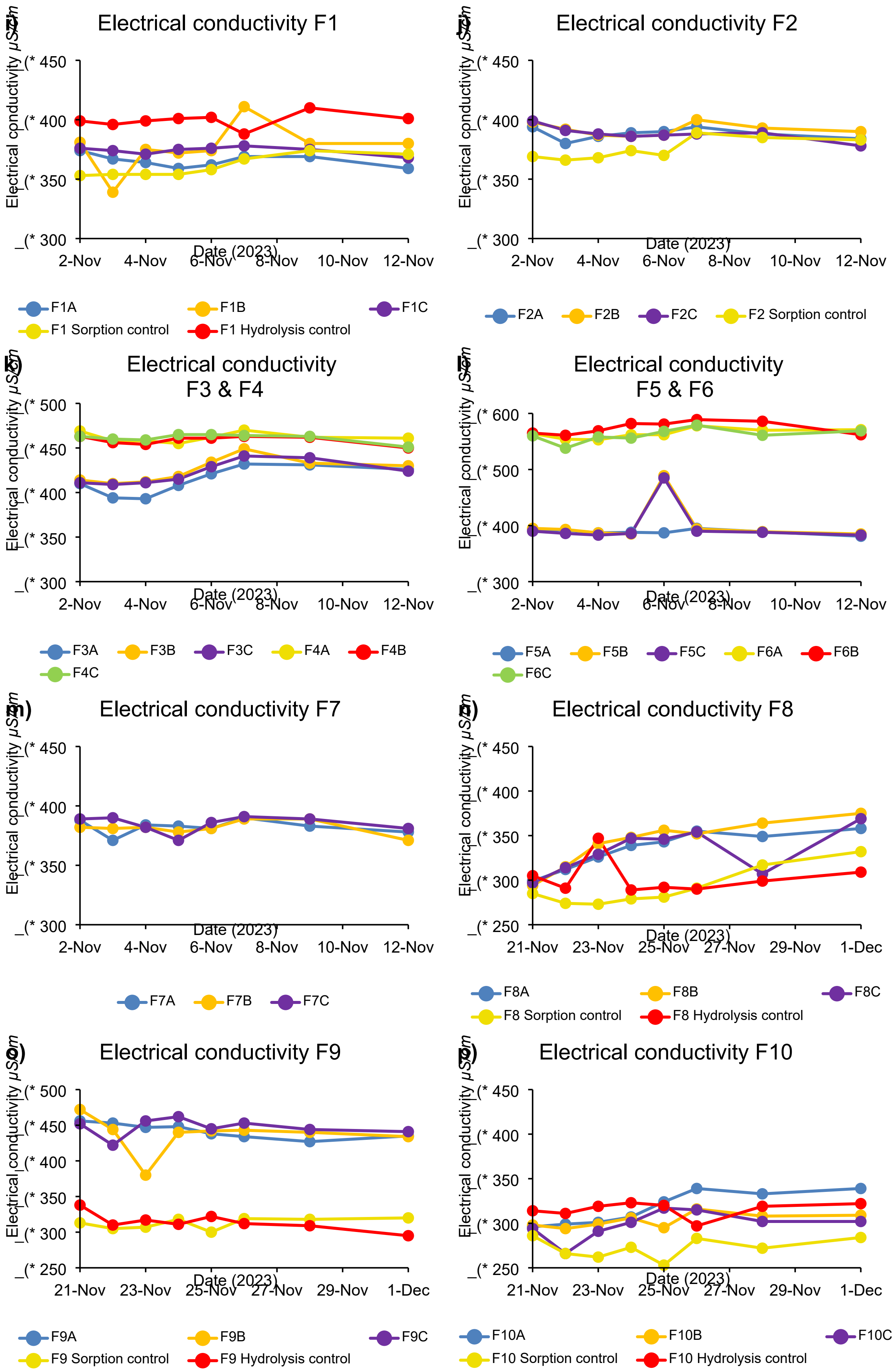
Internal Standard name
Acesulfame-d4
Bezafibrate-d4
Caffeine-d9
Carbamazepine-d8
Clofibric acid-d4
Fluconazole-d4
Gabapentin-d6
Mecoprop-d3
Metformin-d6
Metoprolol-d7
Naproxen-d3
Sulfamethoxazole-d4
Valsartan-d3
Venlafaxine-d6
Zolpidem-d6

S1.2.2 Incubation experiment procedure

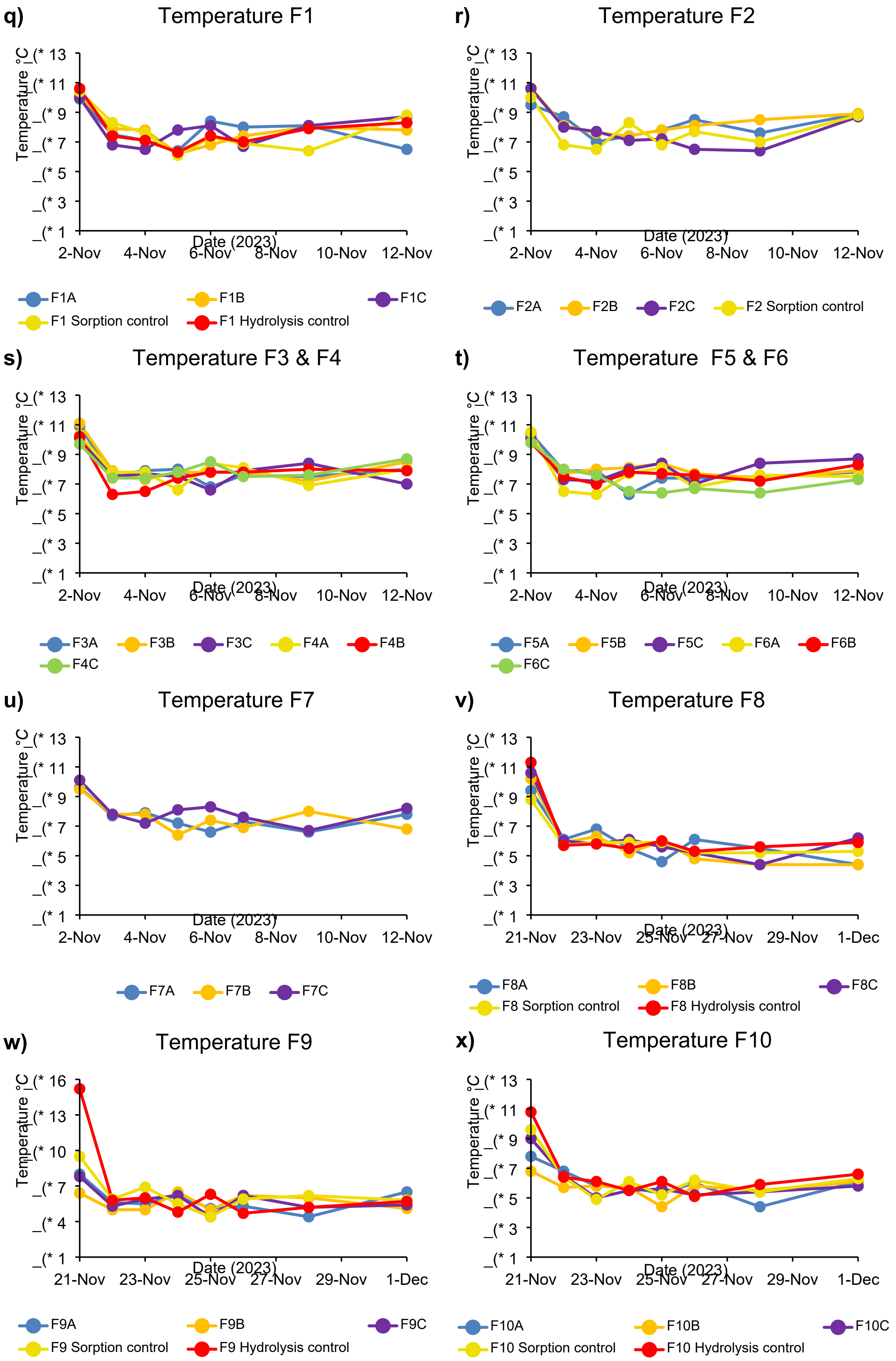
For biodegradation testing, the modified version of the OECD 309 protocol developed by Tian et al. was applied[1]. The protocol was altered slightly by increasing the spike concentration from 0.5 µg/L to 1 µg/L, as well as decreasing the water volume in the incubation flasks from 350 to 300 mL to match the capacity of the BOD bottles. The proportion of water to sediment was 50 g of wet sediment per L of water, the same proportion as was used by Tian et al.[1]. Approximately 15 g of sediment was weighed into 500 mL Erlenmeyer flasks. For sites F1, F2, F8, F9, and F10 sediment was weighed into a fourth flask to be used as a sorption control. 300 mL of water from the corresponding site was added to all flasks, and a fifth flask containing just 300 mL of water was prepared for sites F1, F8, F9, and F10 as hydrolysis controls. The sorption and hydrolysis control flasks were subsequently autoclaved for 30 min at 121°C to sterilize them. The opening of all flasks was covered with parafilm to prevent CO_2 outgassing during the incubation, which could impact sample pH.

After preparation the flasks were brought to a temperature-controlled room set to 4 °C and placed on a KS 501 digital orbital shaker (IKA-Werke GmbH & Co. KG, Staufen, Germany) at 100 rpm. The flasks were left on the shaker for 20 minutes to resuspend the sediment. Each flask was then spiked with a working solution of 129 micropollutants to a concentration of 1 µg/L. The degradation was monitored by taking 1.5 mL subsamples from each flask. The first time point, t0, was collected 20 min after spiking to ensure the compounds had been evenly mixed before subsampling. In total, subsamples were collected at 12 timepoints over 10 days. Subsamples were stored at -20 °C until analysis. The maximum storage time before analysis was approximately two months. During the incubation, DO, temperature, pH, and electrical conductivity were monitored in each flask using a HQ2200 multi-meter or a HQ40d multi-meter (Hach Lange GmbH, Düsseldorf, Germany), for which the probes had been calibrated the same day (Figure S1).


a)
pH F1
b)
pH F2
c)
pH F3 & F4
d)
pH F5 & F6
e)
pH F7
f)
pH F8
g)
pH F9
h)
pH F10
pH
Date (2023)
9.5
9.0
8.5
8.0
7.5
7.0
6.5
2-Nov
4-Nov
6-Nov
8-Nov
10-Nov
12-Nov
21-Nov
23-Nov
25-Nov
27-Nov
29-Nov
1-Dec
F1A
F1B
F1C
F1 Sorption control
F1 Hydrolysis control
F2A
F2B
F2C
F2 Sorption control
F3A
F3B
F3C
F4A
F4B
F4C
F5A
F5B
F5C
F6A
F6B
F6C
F7A
F7B
F7C
F8A
F8B
F8C
F8 Sorption control
F8 Hydrolysis control
F9A
F9B
F9C
F9 Sorption control
F9 Hydrolysis control
F10A
F10B
F10C
F10 Sorption control
F10 Hydrolysis control



i) Electrical conductivity F1
Electrical conductivity µS/m
Date (2023)
F1A
F1B
F1C
F1 Sorption control
F1 Hydrolysis control
j) Electrical conductivity F2
Electrical conductivity µS/m
Date (2023)
F2A
F2B
F2C
F2 Sorption control
k) Electrical conductivity F3 & F4
Electrical conductivity µS/m
Date (2023)
F3A
F3B
F3C
F4A
F4B
F4C
l) Electrical conductivity F5 & F6
Electrical conductivity µS/m
Date (2023)
F5A
F5B
F5C
F6A
F6B
F6C
m) Electrical conductivity F7
Electrical conductivity µS/m
Date (2023)
F7A
F7B
F7C
n) Electrical conductivity F8
Electrical conductivity µS/m
Date (2023)
F8A
F8B
F8C
F8 Sorption control
F8 Hydrolysis control
o) Electrical conductivity F9
Electrical conductivity µS/m
Date (2023)
F9A
F9B
F9C
F9 Sorption control
F9 Hydrolysis control
p) Electrical conductivity F10
Electrical conductivity µS/m
Date (2023)
F10A
F10B
F10C
F10 Sorption control
F10 Hydrolysis control



q)
Temperature F1
Temperature °C
Date (2023)
F1A
F1B
F1C
F1 Sorption control
F1 Hydrolysis control
r)
Temperature F2
Temperature °C
Date (2023)
F2A
F2B
F2C
F2 Sorption control
s)
Temperature F3 & F4
Temperature °C
Date (2023)
F3A
F3B
F3C
F4A
F4B
F4C
t)
Temperature F5 & F6
Temperature °C
Date (2023)
F5A
F5B
F5C
F6A
F6B
F6C
u)
Temperature F7
Temperature °C
Date (2023)
F7A
F7B
F7C
v)
Temperature F8
Temperature °C
Date (2023)
F8A
F8B
F8C
F8 Sorption control
F8 Hydrolysis control
w)
Temperature F9
Temperature °C
Date (2023)
F9A
F9B
F9C
F9 Sorption control
F9 Hydrolysis control
x)
Temperature F10
Temperature °C
Date (2023)
F10A
F10B
F10C
F10 Sorption control
F10 Hydrolysis control

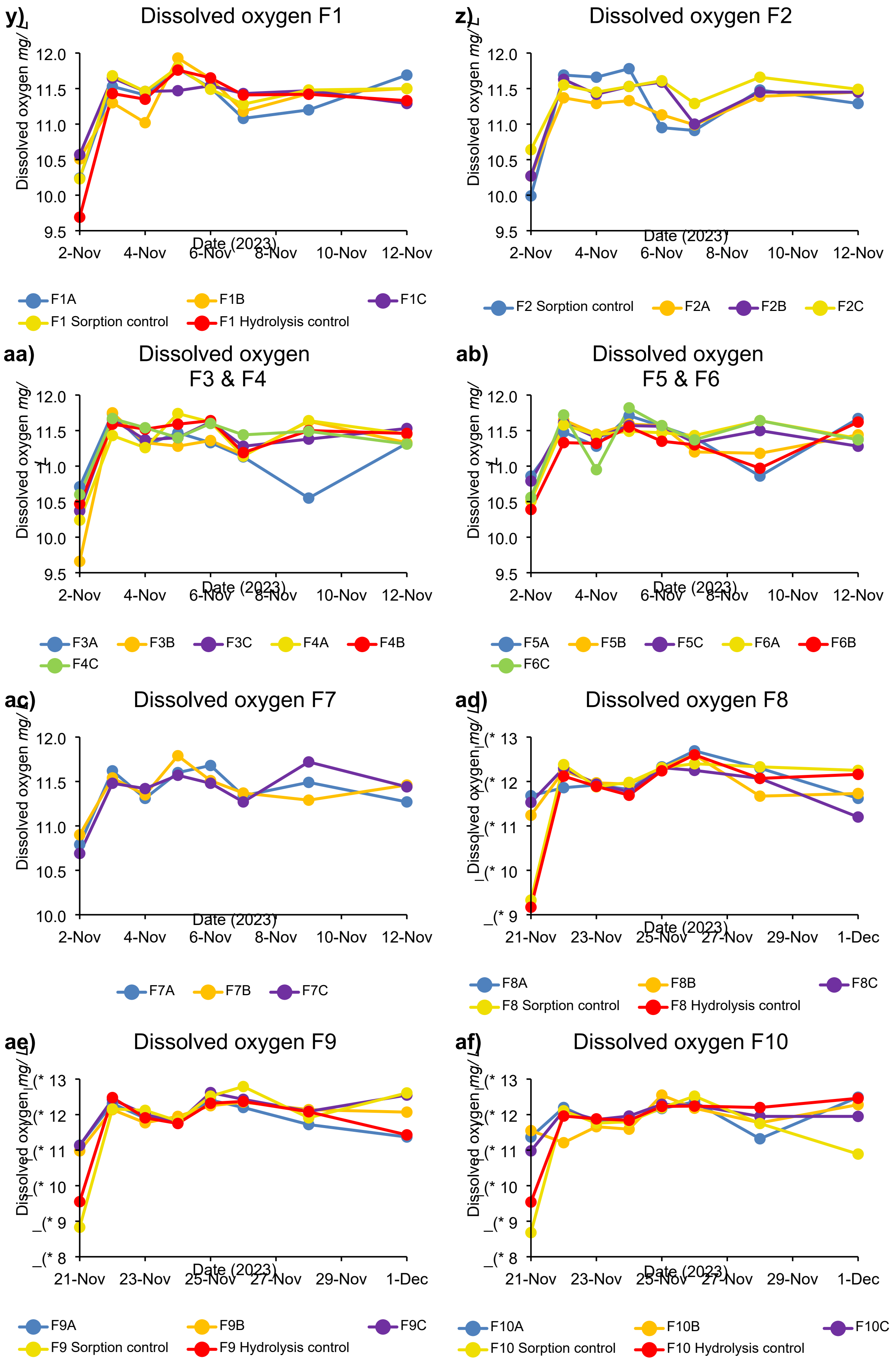

y)
Dissolved oxygen F1
Dissolved oxygen mg/L
Date (2023)
2-Nov 4-Nov 6-Nov 8-Nov 10-Nov 12-Nov
F1A F1B F1C
F1 Sorption control F1 Hydrolysis control
z)
Dissolved oxygen F2
F2 Sorption control F2A F2B F2C
aa)
Dissolved oxygen F3 & F4
F3A F3B F3C F4A F4B F4C
ab)
Dissolved oxygen F5 & F6
F5A F5B F5C F6A F6B F6C
ac)
Dissolved oxygen F7
F7A F7B F7C
ad)
Dissolved oxygen F8
21-Nov 23-Nov 25-Nov 27-Nov 29-Nov 1-Dec
F8A F8B F8C
F8 Sorption control F8 Hydrolysis control
ae)
Dissolved oxygen F9
F9A F9B F9C
F9 Sorption control F9 Hydrolysis control
af)
Dissolved oxygen F10
F10A F10B F10C
F10 Sorption control F10 Hydrolysis control

Figure S1. Measurements of pH, dissolved oxygen (DO), electrical conductivity (EC), and temperature during the OECD 309 batch incubation for each replicate. **A-H** shows the trends in pH over the experiment, **I-P** shows the trends in EC during the incubation, **Q-X** shows the temperature trends during the incubation, **Y-AF** shows the trends in DO for the replicates during the incubation.

S1.3 Instrumental analysis

Before analysis, the collected subsamples were thawed and vortexed, after which 800 µL of sample was transferred into a 1.5 mL SafeSeal reaction tube (SARSTEDT AG & Co. KG, Nümbrecht, Germany) together with 190 µL of methanol and 10 µL of Internal standard (IS) mixture (Table S2). The mixture was then thoroughly vortexed and filtered through a 0.45 µm PTFE filter (SARSTEDT AG & Co. KG, Nümbrecht, Germany) using a Henke-Ject syringe (Henke-Sass Wolf GmbH, Tuttlingen, Germany) into SureSTART 2 mL vials (Thermo Fisher Scientific, Langerwehe, Germany). The prepared samples were stored at -20 °C until analysis. Alongside the samples, blanks, quality control samples (QCs), and standards were prepared. Blanks were prepared similarly to samples, except the 800 µL of sample was replaced with 800 µL of Milli-Q water. For the quality control samples, the 800 µL of sample was replaced with water from site F1 that had been spiked in the same manner as the samples, but not incubated. A matrix matched standard curve was prepared for each sample site. The standards were prepared with water from the corresponding sample site, spiked with the same compound mixture as the samples (Table S1), and diluted to a concentration between 0.005 µg/L - 10 µg/L (0.005 µg/L, 0.01 µg/L, 0.02 µg/L, 0.04 µg/L, 0.06 µg/L, 0.08 µg/L, 0.1 µg/L, 0.25 µg/L, 0.5 µg/L, 1 µg/L, 2.5 µg/L, 5 µg/L, and 10 µg/L). As with the samples, blanks, and QCs, 190 µL of methanol and 10 µL of IS mixture were also added to each vial. The samples for each site were analysed as one batch, along with blanks, standards, and QCs. The utilized analytical instrumentation was ultrahigh performance liquid chromatography (UHPLC) coupled with a Q Exactive HF Hybrid Quadrupole-Orbitrap mass spectrometer (Orbitrap MS/MS, Thermo Fisher Scientific, Waltham, USA). 40 µL from each vial was injected into the instrument, with three QCs injections at the start and end of each sequence along with one QC injection after every six other injections. The injection order of the samples was randomized.

For the UHPLC, an Aquity UPLC HSS T3 1.8 µm 2.1x100 mm reversed-phase column with an Aquity UPLC HSS T3 VanGuard 1.8 µm 2.1x5 mm precolumn (both Waters Corporation, Milford, USA) was utilized along with two mobile phases. Mobile phase A consisted of Milli-Q IQ 7000 water (Merck KGaA, Darmstadt, Germany) with 10 mM acetic acid (Sigma Aldrich Chemie GmbH, Steinheim, Germany), while mobile phase B consisted of methanol (VWR International, Rosny-sous-Bois, France) with 10 mM acetic acid (se supplier above). A 17 min gradient was used, starting at 95% A and linearly increased to 95% B for 10 min, which was then kept constant for 2 min. The gradient was then shifted back to 95% A over 0.1 min and maintained for the final 2.9 min. The flow rate of the mobile phases was 0.4 mL/min, and the column temperature was 40 °C. The samples were kept in the autosampler compartment at 4 °C for a maximum of 92 h. After being separated on the UHPLC, the samples entered the Orbitrap

MS/MS and were ionized using ESI. Each sample was injected twice, once in ESI positive mode, and once in ESI negative mode. The instrument was calibrated before analysis of each batch. Further information on the Orbitrap MS/MS settings are available in Table S3. To get accurate retention times for the 47 focus compounds, a retention time standard was analysed after the last samples. The standard contained the working solution diluted to 1 ppb in 790 µL Milli-Q water, 190 µL methanol and 10 µL IS mixture.

Table S3. Mass spectrometer settings. **A** contains the settings for the MS and MS/MS scan. **B** contains the settings for the electrospray interface.

a)

Parameter	MS	MS/MS
Scan range *m/z*	70-900	-
Resolution *full width at half maximum*	120000	15000
Automatic gain control (AGC) target	3000000	20000
Maximum IT *ms*	150	20

b)

Parameter	Positive mode	Negative mode
Sheath gas flow rate	50	40
Auxiliary gas flow rate	13	10
Sweep gas flow rate	3	0
Spray voltage $\|kV\|$	3.5	3.5
Capillary temperature *°C*	320	320
S-lens RF-level	55	55
Auxiliary gas heater temperature *°C*	350	300

S1.4 Data processing and compound identification

S1.4.1 Compound identification

Raw files were processed using Compound Discoverer 3.3 (Thermo Fisher Scientific, Waltham, USA) to identify the target compounds. The Compound Discoverer workflow is the same as used by Tian et al, and is available in the supporting information of their 2023 paper[1]. Compounds were identified based on their MS/MS spectra and retention time (RT). The retention times were compared to the RTs of the retention time standard, with a difference of < ± 0.2 min considered a match. Some ISs could not be found in the RT standard; for these compounds the RT was instead compared to RT of the same compound measured previously using the same instrument and UHPLC method.

For compound identification, most targets were identified at a ≥ 70% MS/MS spectral match and a matching RT. Identification was also accepted in a few cases for compounds with a ≥

50% MS/MS spectral match and a matching RT. For two spiked compounds, fluoxetine and ethylhexylglycerin, no matches to spectra in the libraries were found. However, only a single peak was detected at their respective molecular weight. As these peaks appeared at the expected RT in all samples, they were assumed to have matched the two compounds in question. The identification of these two compounds is therefore somewhat uncertain. An overview of compound identification is provided in Table S4. Two compounds, metformin and acesulfame, along with their respective IS, were identified by Compound Discoverer 3.3, but not properly integrated. They were, therefore, integrated manually based on their RT and molecular weight using the software Xcalibur (Thermo Fisher Scientific, Waltham, USA).

Table S4. Overview of compound identification for each site. The legend for the colour scheme is provided at the top of the table.

≥70% spectral match and matching RT	≥50% spectral match and matching RT	No spectral match, matching molecular weight and RT	Not identified

Compound	Site									
	F1	**F2**	**F3**	**F4**	**F5**	**F6**	**F7**	**F8**	**F9**	**F10**
Ethylhexylglycerin										
4-(4-nitrobenzyl)-pyridine										
Acesulfame										
Anastrozole										
Atrazine										
Bezafibrate										
Bromoxynil										
Caffeine										
Candesartan										
Carbamazepine										
Chlortoluron										
Climbazole										
Clofibric acid										
Cyclamate										
Dicamba										
Diclofenac										
Dimethenamid										
Diuron										
Fenhexamid										
Flecainide										
Fluconazole										
Flufenacet										
Fluoxetine										
Furosemide										
Gabapentin										
Gemfibrozil										
Hydroxy bupropion										
Iprovalicarb										
Isoproturon										
Ketoprofen										
MCPA										
Mecoprop										
Mefenamic acid										
Metformin										
Metolachlor										
Metoprolol										

Metoxuron										
Naproxen										
p-toluenesulfonic acid										
Sulfadimethoxine										
Sulfamethazine										
Sulfamethoxazole										
Tamsulosin										
Terbutryn										
Valsartan										
Venlafaxine										
Zolpidem										
Mecoprop-d3										
acesulfame-d4										
clofibric acid-d4										
caffeine-d9										
naproxen-d3										
gabapentin-d6										
Metformin-d6										
fluconazole-d4										
carbamazepine-d8										
Zolpidem-d6										
Venlafaxine-d6										
metoprolol-d7										
Sulfamethoxazole-d4										
valsartan-d3										
Bezafibrate-d4										

S1.4.2 Quality control and data processing

For identified compounds, the peak areas were exported and corrected using an R-script called batchCorr developed by Brunius et al.[3]. It utilizes the repeatedly analysed QCs to correct for instrumental drift within a batch, thereby improving data quality. For site F4 and F5, one of the QCs had a much lower peak area than the others, possibly from instrumental errors or errors during preparation. As this would interfere with the batchCorr correction, the peak area of these QCs was replaced with the average peak area of the previous and following QC injections.

After running the data through batchCorr, the data quality was assured by checking that relative standard deviation (RSD) was below 25% in the QCs for spiked compounds and below 25% in all injections for IS compounds. A linear calibration curve was made for each spiked compound using the matrix-matched standards. The linear range was determined as the range of calibration standard concentrations for which the response factors of the calibration points had an RSD < 25%. The lowest concentration in the linear range was set as the limit of quantification (LOQ), and sample peak areas below the LOQ were removed. The peak areas were then transformed to the natural logarithm of the peak area relative to the peak area of the same compound at t_0 (Equation S2).

$$Transformed\ area = ln\frac{A_{sample}}{A_{t_0\ sample}}$$

Equation S2. Formula for calculating ln-transformed relative peak area.

The Chowclassifier script was utilized to calculate attenuation rate constants, k, from the slope of the linear regression of $\ln(A/A_{t0})$ against subsampling time[2]. Chowclassifier additionally performs a Chow test to check for breakpoints where the degradation trend changes. If the test detects a breakpoint at the selected significance level, 0.01 in this case, then the script will calculate two separate linear regressions for the timepoints before and after the breakpoint respectively. If no breakpoint is detected the script will create one linear regression for the whole dataset.

The measured BOD_3 and k were both normalized by dry weight to account for differences in sediment amounts between flasks. For the BOD_3 the dry weight was obtained directly from the experiment flasks by discarding excess water and drying the remaining sediment for 48h at 120°C. The dry weight of the sediment was then calculated by weighing the bottles and subtracting the weight of the bottles, which had been measured before sediment addition. The average BOD_3/g dry sediment, hereafter referred to as BOD_{3dry}, for each site was calculated from the values of the corresponding triplicates. The sediment dry weight of the OECD 309 experiments could not be measured directly, but was instead calculated by multiplying the sediment wet weight for each flask with the average dry content of the site's sediment, obtained from the mass ratio of the wet and dry sediment measured during the BOD experiment (Equation S3 & S4). The k values could then be normalized by the dry weight of the corresponding replicate, yielding k_{dry}.

$$Dry\ content = \frac{Average\ sediment\ dry\ weight}{Average\ sediment\ wet\ weight}$$

Equation S3. Formula for calculating the sediment dry content for each site.

$$Dry\ weight = Wet\ weight * Dry\ content$$

Equation S4. Formula for calculating sediment dry weight in biodegradation incubation flasks.

S1.4.3 Data processing for abiotic controls

For sites with abiotic controls, an abiotic-corrected version of k was produced. As abiotic processes had previously been shown to have little influence on the attenuation of the 47 selected compounds, the corrected and uncorrected data was expected to be similar. The correction was done by subtracting the natural logarithm of the relative peak area of the abiotic control from that of the replicate for each timepoint (Equation S5).

$$Area, tranformed\ and\ corrected = ln\frac{A_{sample}}{A_{to\ sample}} - ln\frac{A_{control}}{A_{to\ control}}$$

Equation S5. Formula for calculating sorption corrected ln-transformed relative peak area for a given timepoint.

As a second step, a correction for the dissolved fraction was performed. The purpose of this was to control for the buffering effect of sorption on the bioavailable concentration, which could cause an underestimation of k due to desorption as the dissolved fraction of the compound is degraded during the experiment. The dissolved fraction, *df*, of a compound was calculated by dividing the area of the abiotic control at t_0 with that of the hydrolysis control at t_0. For site F2 no hydrolysis control was available, and so the *df* of each compound was simulated based on the average *df* of that compound for the other sites. This was deemed appropriate as *df* generally varied little between sites (RSD < 25% for all compounds). The rate constants were then divided by their dissolved fraction before being divided by the sample dry weight (same as the non-abiotic corrected rate constants) to produce abiotic corrected dry weight normalized biodegradation rate constants k_{dryS}.

S1.4.4 Statistical testing

An analysis of variance (ANOVA) test was applied to test if the BOD_{3dry} differed between sites. Before the ANOVA test was applied, the normality and homogeneity of variances were tested with a Shapiro-Wilk test and Levene's test respectively. The pre-tests revealed that neither assumption was violated at a 0.05 significance level, and as such the ANOVA was performed. The result of the ANOVA test revealed that there were significant differences at a 0.05 significance level. Subsequently, a Tukey post-hoc test was applied to test which sites differed from each other regarding BOD_{3dry}.

A set of quality criteria was applied to the measured k_{dry}, which were only considered valid if they were based on a minimum of 5 timepoints and significantly different from 0, $p < 0.05$. The relationship between BOD_{3dry} and k_{dry} was assessed for all compounds which had 5 valid k_{dry} at a minimum of 3 sites using linear least squares regression. A positive or negative relationship between BOD_{3dry} and k_{dry} was considered significant if the p-value of the regression was smaller than 0.05. The same criteria and approach were applied to comparisons of BOD_{3dry} and k_{dryS}.

A paired t-test was used to assess if the standard deviation in k_{dry} decreased significantly after normalization by BOD_{3dry}. Before the test was employed, the assumption of normally distributed differences was tested using a Shapiro test, which indicated the assumption of normality could not be rejected ($p = 0.8279$). The effect size of the difference was subsequently tested using a paired sample Cohen's d test.

S2. Supporting information on study results

S2.1 Rate constants

Table S5. Dry weight–normalized attenuation rate constants, k_{dry}. The k_{dry} for each compound and site produced by the modified OECD 309 biodegradation test is shown blue. For sites with abiotic controls abiotic corrected rate constants, k_{dryS}, are also available in red. The three rows within each cell represent the observed kdry/kdryS for the three replicates of each site.

Compound	**F1**		**F2**		**F3**	**F4**	**F5**	**F6**	**F7**	**F8**		**F9**		**F10**	
	k_{dry}	k_{dryS}	k_{dry}	k_{dryS}	k_{dry}	k_{dry}	k_{dry}	k_{dry}	k_{dry}	k_{dry}	k_{dryS}	k_{dry}	k_{dryS}	k_{dry}	k_{dryS}
4-(4-Nitrobenzyl) pyridine			0.026									0.016			
	0.022	-0.065	0.022												
	0.019		0.018												
Acesulfame	0.002	0.002	0.002	0.002		-0.004									-0.001
	0.001		0.002	0.001											
	0.002	0.001	0.002	0.001						-0.001		0.001			-0.001
Anastrozole	0.012		0.004		0.016	0.019	0.003					0.004		0.011	0.015
	0.010		0.003		0.011		0.002			0.003	0.005			0.007	0.010
	0.010		0.003		0.011	0.033	0.002					0.006		0.009	0.012
Atrazine			0.002												
			0.001									0.002	0.022		
												0.002	0.017		
Bezafibrate										0.028	0.032			0.014	
	0.001									0.041	0.044			0.015	
	0.001							0.011		0.043	0.046	0.002		0.012	0.018
Bromoxynil															
	0.018								-0.012						
Caffeine			0.022	0.022			0.005								0.105
			0.016	0.002											0.133
			0.015	0.017			0.005								0.149
Candesartan			0.001							0.002					
			0.001			0.007									

						0.008								0.005	
Carbamazepine	0.003 0.002		0.002		0.005 0.005 0.003	0.007 0.007		0.006				0.001 0.002 0.002		0.004 0.002	0.007
Chlortoluron	0.005		0.004 0.003		0.005	0.012 0.011	0.002					0.004 0.005		0.008 0.007 0.006	0.010 0.009 0.008
Clofibric acid			0.001 0.001					0.004		0.001				0.001 0.004 0.001	
Diclofenac	0.011							0.010							
Dimethenamid			0.003		0.003	0.007 0.009	0.001		-0.001			0.004	0.004		
Diuron	0.012 0.006		0.005 0.004					0.011				0.007		0.012 0.011 0.012	0.034 0.032 0.033
Ethylhexylglycerine					0.025		0.075 0.060 0.063		0.119 0.103 0.042	0.084 0.130 0.119				0.058	
Fenhexamid						0.09	0.002	0.178	0.009					0.014	
Flecainide*	0.016 0.021 0.017	0.023	0.005 0.005 0.004			0.021 0.020	0.007 0.006 0.006			0.007	0.009		-0.044	0.012	0.025 0.027 0.031
Fluconazole*	0.002 0.001	0.002 0.001	0.001 0.001	0.001	0.006 0.004	0.007 0.010		0.009						0.003 0.003	0.004 0.003 0.004

flufenacet			0.006												
Furosemide	0.007 0.004 0.004	0.004	0.005 0.005 0.003	0.004 0.004 0.002	0.013 0.013 0.011			0.009 0.009 0.012				0.004	0.004	0.008 0.010 0.010	0.008
Gabapentin			0.003 0.002 0.003	0.015 0.021			0.001 0.000								0.014
Gemfibrozil			0.002 0.001		0.008 0.010					0.011 0.017 0.023	0.010 0.016 0.022			0.016 0.008	
Hydroxy bupropion	0.002 0.002		0.003 0.003 0.003		0.006 0.004	0.005 0.006	0.001 0.001 0.001					0.002	-0.002	0.004 0.003 0.004	0.009 0.007 0.010
Iprovalicarb			0.004 0.002	0.003	0.007 0.007 0.004	0.006 0.007	0.001 0.002					0.003		0.014	0.025 0.028
Isoproturon	0.003		0.003 0.003 0.002		0.002	0.008 0.007		0.005 0.007				0.002		0.003	0.005 0.004 0.004
Ketoprofen	0.003 0.002		0.005 0.003 0.003	0.004 0.003 0.003	0.009 0.009 0.008		0.002 0.002 0.003	0.006	0.002	0.007 0.010 0.007	0.009 0.012 0.009	0.002 0.002 0.003		0.014 0.016 0.009	0.015 0.017 0.010
MCPA	0.002	0.002	0.002 0.001 0.001	0.001 0.001	0.003 0.002	0.005 0.005		0.004	0.000	0.003 0.003 0.003	0.003 0.004 0.004			0.004 0.003 0.002	0.005 0.005 0.004
Mecoprop		0.001	0.001 0.001			-0.003				0.001				0.002 0.002	0.003 0.003 0.002
Mefenamic acid			0.005												
Metformin			0.005	0.005	0.009	0.007		0.006							

			0.004 0.003	0.004 0.003	0.008	0.007 0.007				0.007				-0.010 -0.005	-0.011
Metolachlor	0.006		0.004			0.017						0.003		0.012	
Metoprolol	0.009 0.008 0.009		0.002 0.002 0.002		0.011 0.007	0.013 0.015 0.046	0.003 0.003 0.003	0.012 0.010		0.003 0.007	0.010	0.003 0.004		0.008	0.019 0.025
Metoxuron	0.004		0.003 0.002		0.006 0.004 0.004	0.012 0.013 0.016						0.002 0.003 0.002	0.003 0.004 0.003	0.004 0.004 0.005	0.010 0.010 0.011
Naproxen			0.002		0.013		0.003 0.002	0.007 0.011		0.013	0.011			0.014 0.008 0.010	0.019 0.015 0.012
p-Toluenesulfonic acid			0.016 0.015 0.014	0.017 0.016 0.016	0.016 0.010		0.007		0.003 0.007 0.006	0.015 0.037 0.023	0.015 0.023	0.002		0.008 0.014 0.005	0.006 0.012
Sulfadimethoxine	0.011 0.005 0.007		0.004 0.002		0.032 0.031	0.042 0.050 0.043	0.002 0.002	0.016 0.015 0.017		0.006 0.010 0.008	0.007 0.011 0.009			0.017 0.017 0.012	0.014 0.014 0.010
Sulfamethazine	0.022 0.013 0.013		0.005 0.004 0.003			0.177 0.180	0.004 0.002 0.003			0.012 0.018 0.013	0.010 0.017 0.011			0.185 0.182 0.160	0.172 0.168 0.146
Sulfamethoxazole	0.004				0.022 0.021 0.016	0.017 0.030 0.027	0.002			0.008 0.012 0.007	0.008 0.012 0.008			0.011 0.013 0.008	0.008 0.011 0.006
Tamsulosin	0.009										0.014				0.031 0.021 0.019
Terbutryn			0.007 0.005									0.009			0.008 0.003 0.002
Valsartan	0.003	0.004	0.006 0.003 0.004	0.006 0.003 0.004	0.009 0.005 0.006		0.002 0.001			0.008 0.012 0.010	0.006 0.010 0.008			0.011	

Venlafaxine			0.008 0.008 0.007		0.014	0.017 0.016	0.011 0.010 0.010		0.005			0.005		0.007	0.086 0.100
Zolpidem	0.017 0.012 0.013		0.008 0.008 0.004	-0.005	0.018	0.019 0.017 0.022	0.005 0.005 0.004			0.007	0.010	0.006	-0.009 -0.009	0.010 0.008 0.017	0.020 0.017 0.030

S2.2 Relationship between respiration and attenuation

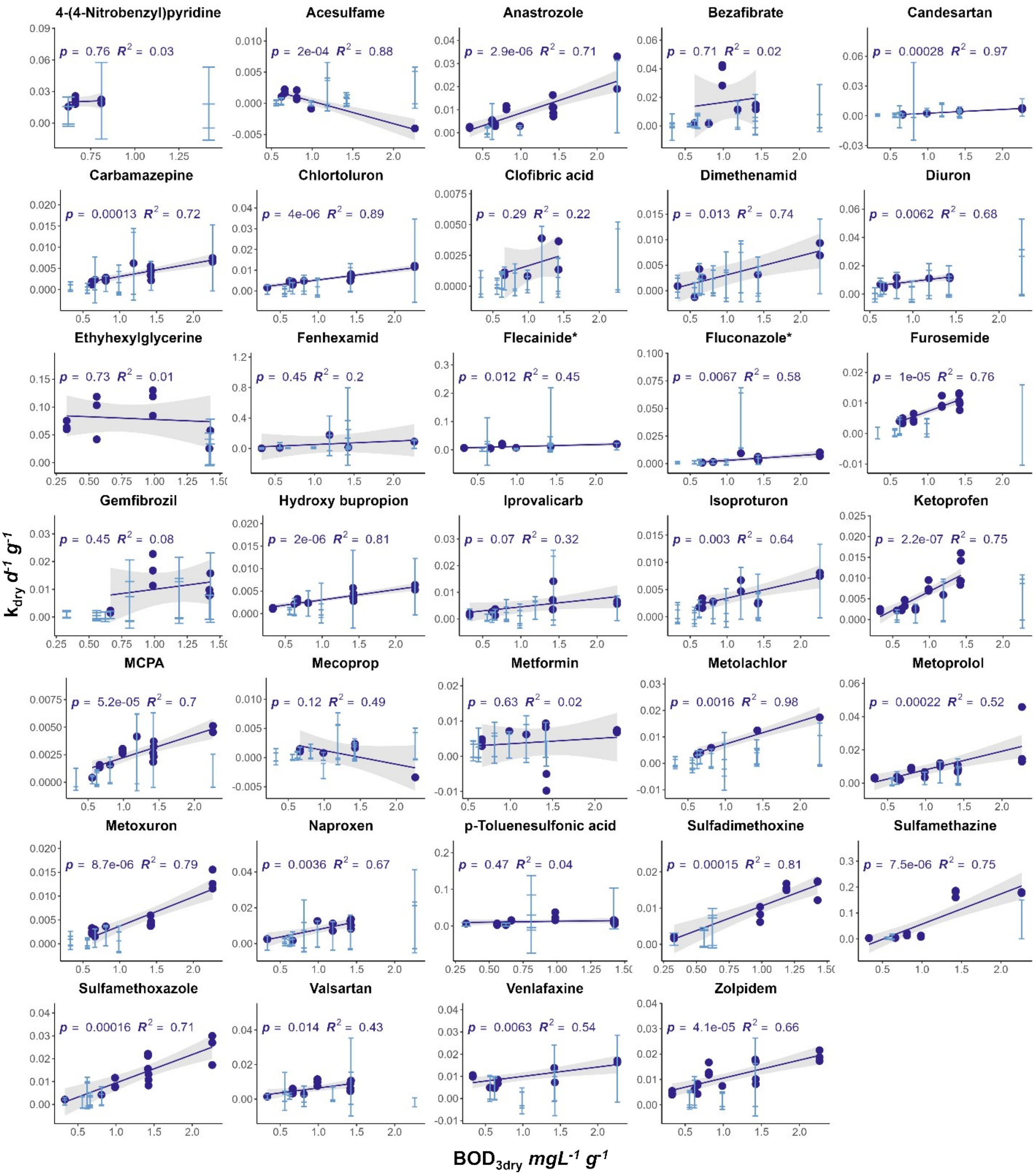
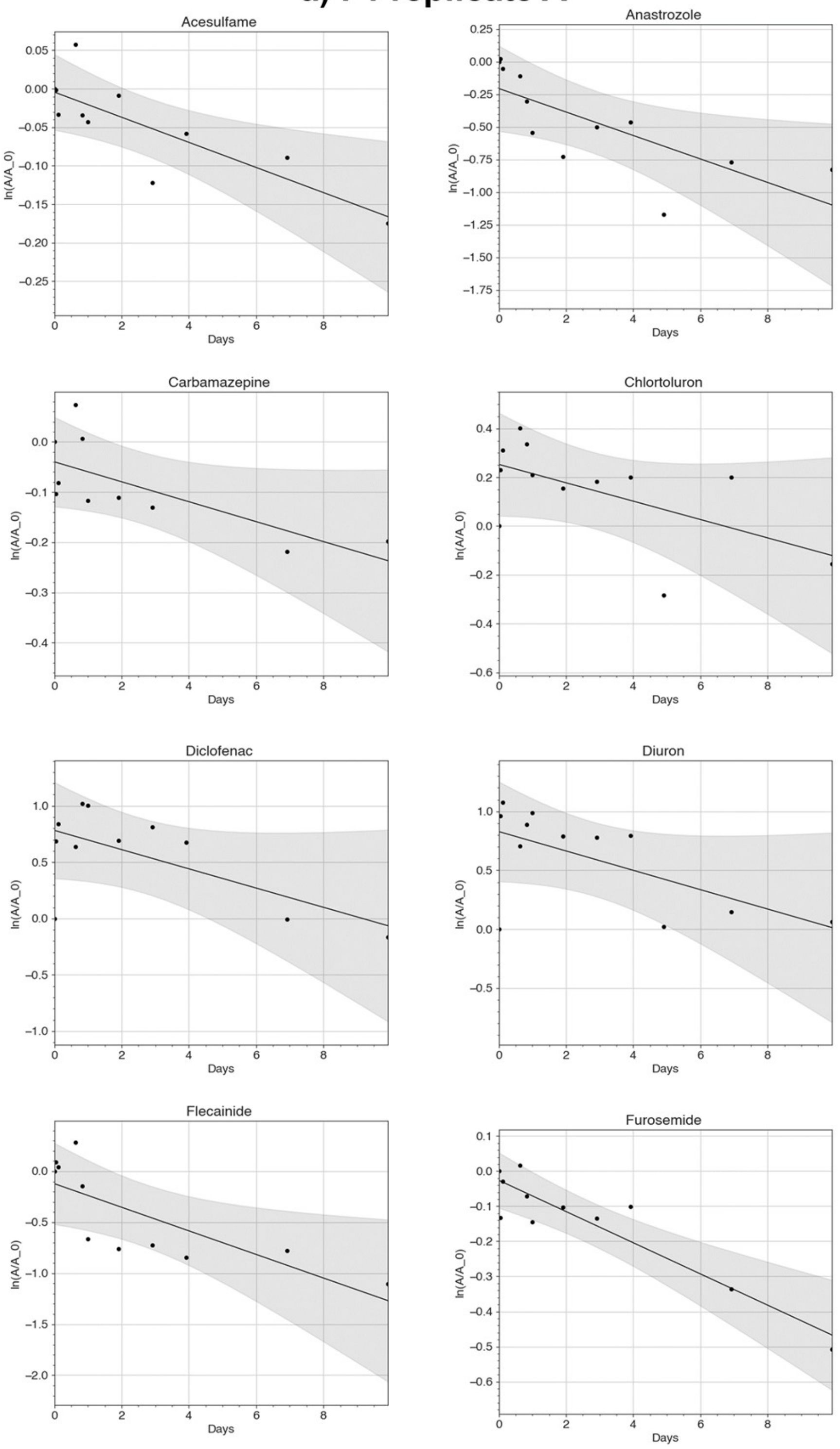


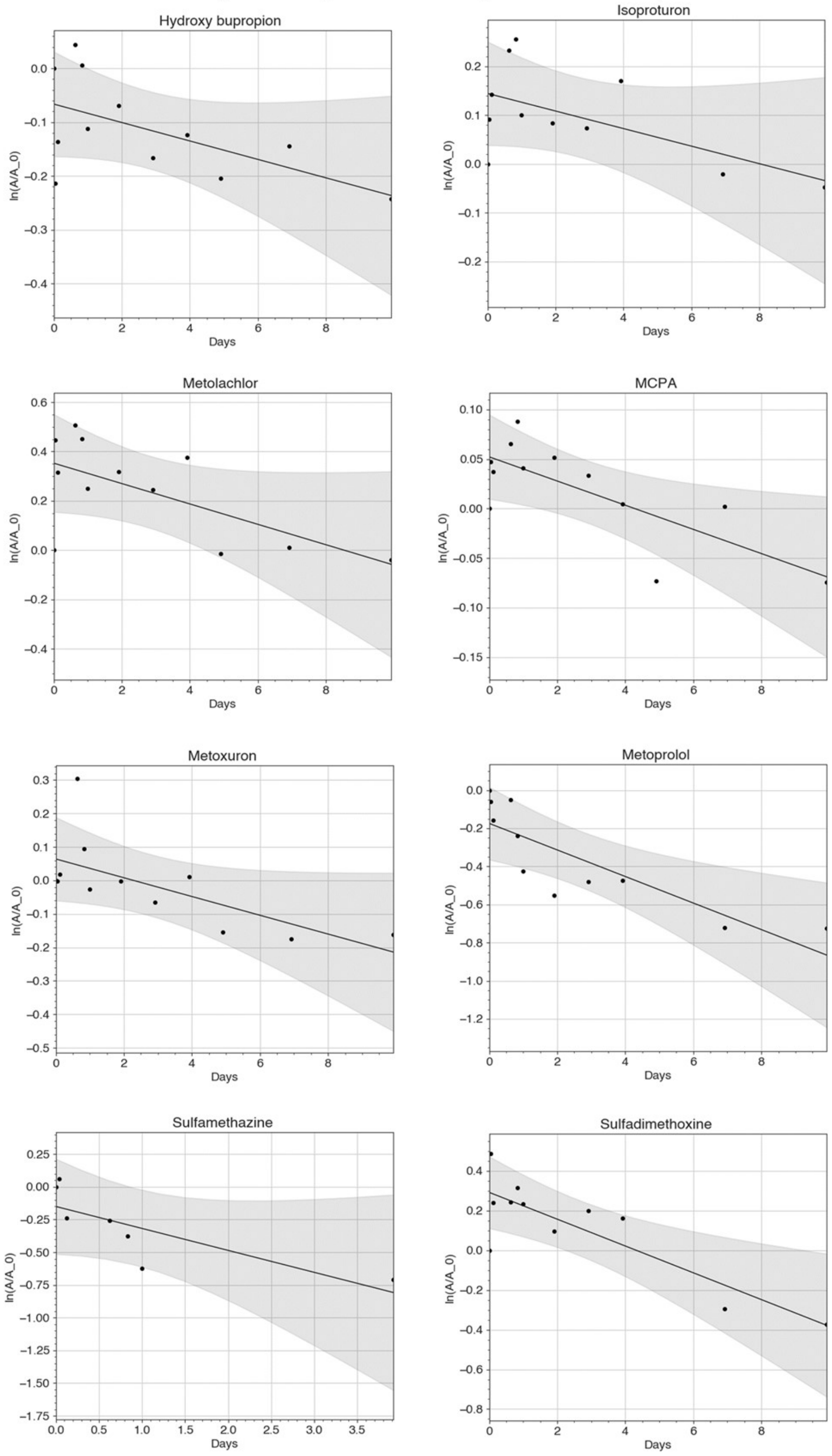
Figure S2. Relationship between BOD_{3dry} and k_{dry} for all datapoints. The figure displays the linear regression between BOD_{3dry} and k_{dry} as calculated from only the datapoints which passed data quality criteria (blue dots), the shaded areas represent the 95% confidence interval of each slope. Light blue bars represent the 95% confidence interval of datapoints which did not pass data quality criteria. Compounds marked with * were subject to outlier removal (see Materials and Methods – Data processing).

S2.3 Peak area timeseries

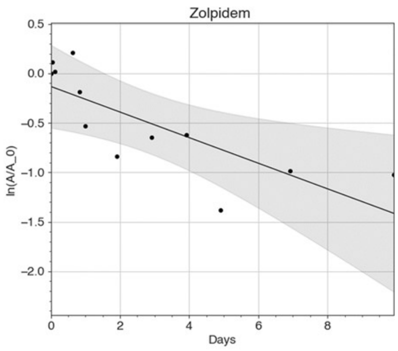
a) F1 replicate A



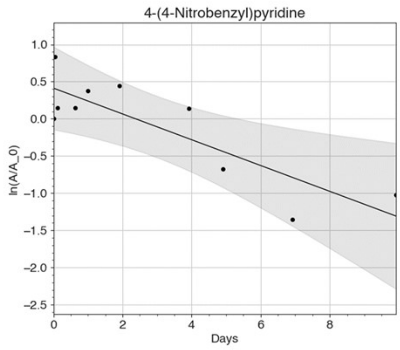
a) F1 replicate A (continued)

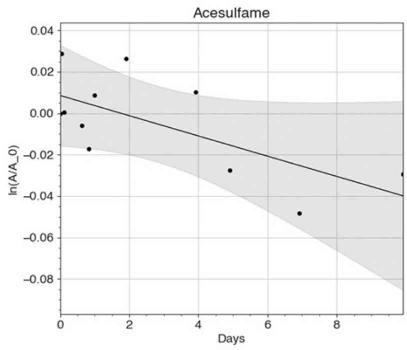


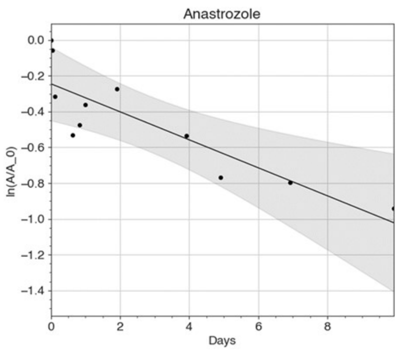
a) F1 replicate A (continued)

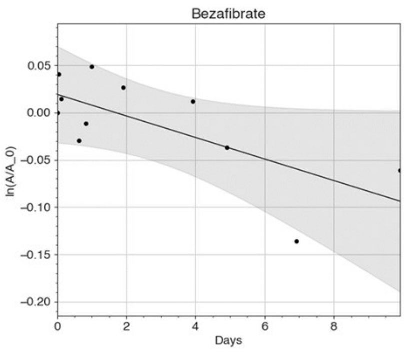


b) F1 replicate B

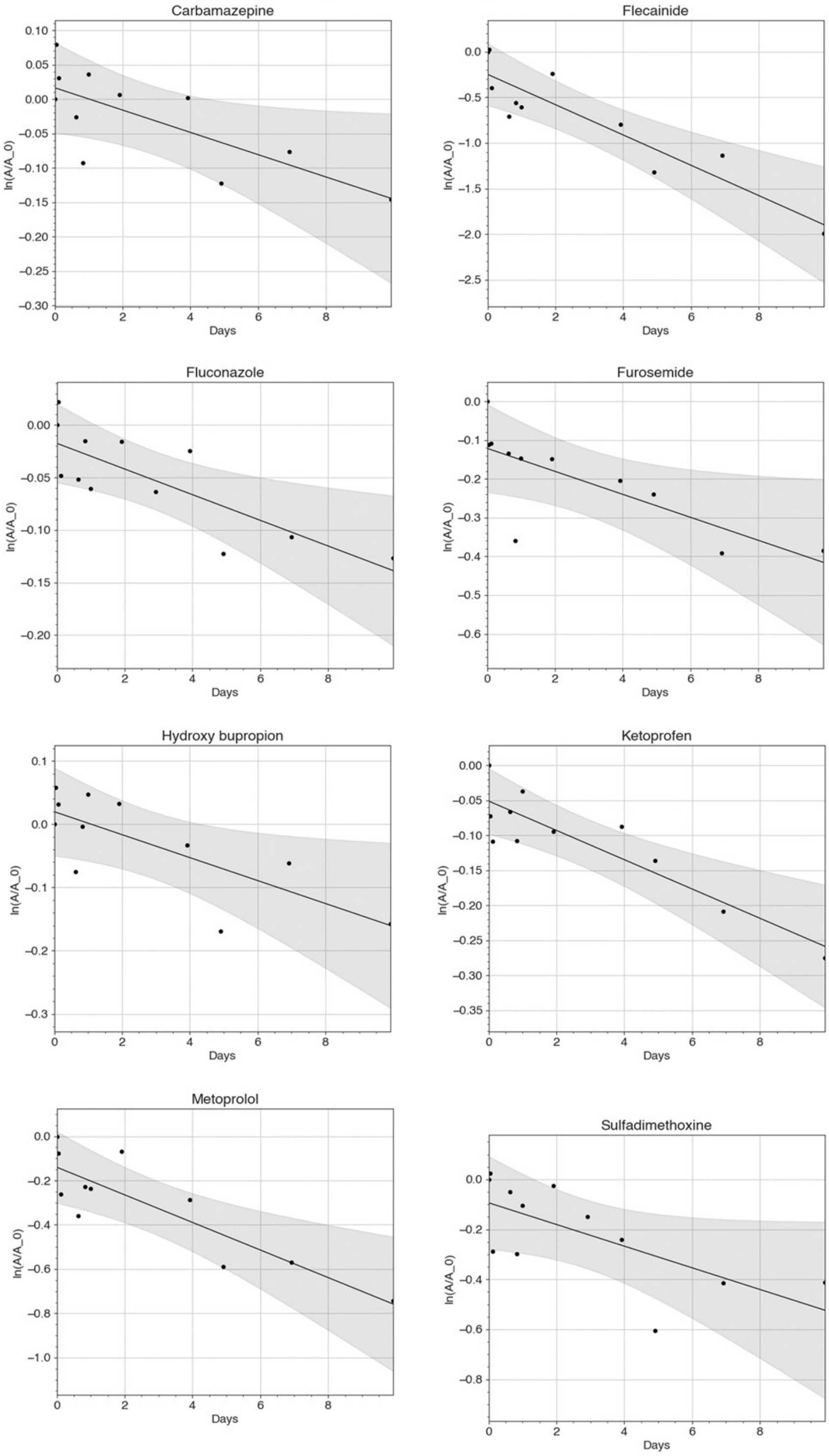




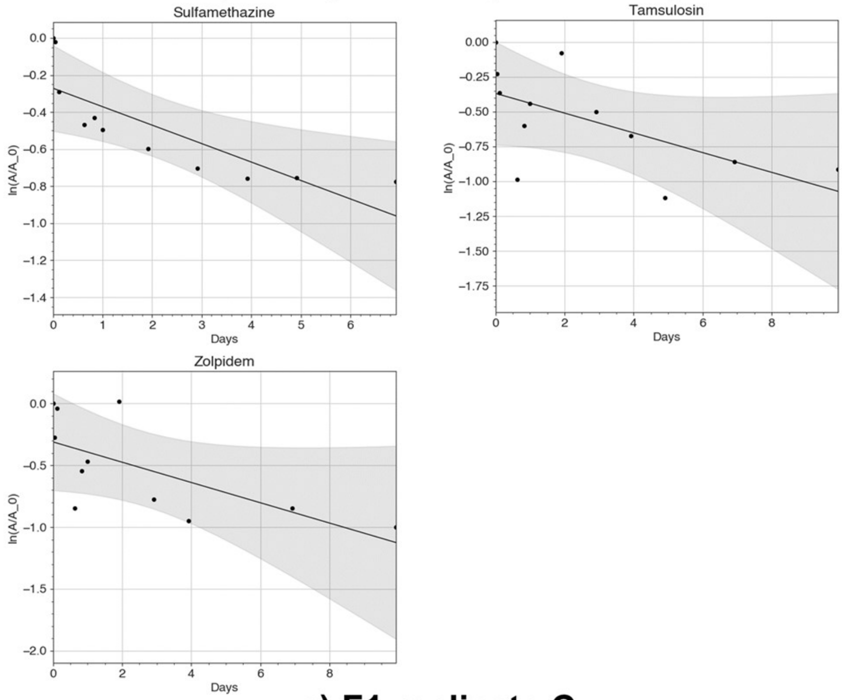




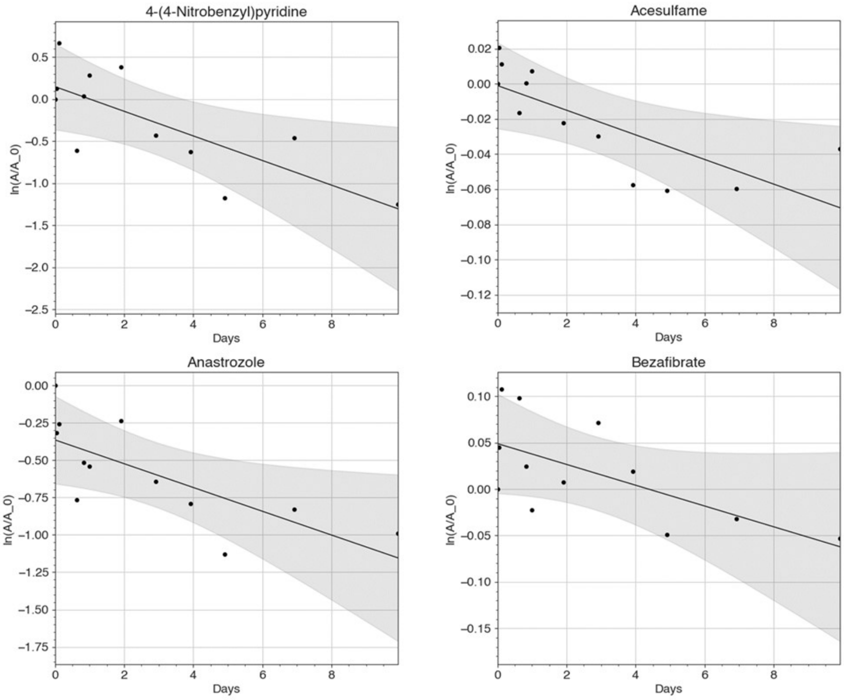
b) F1 replicate B (continued)



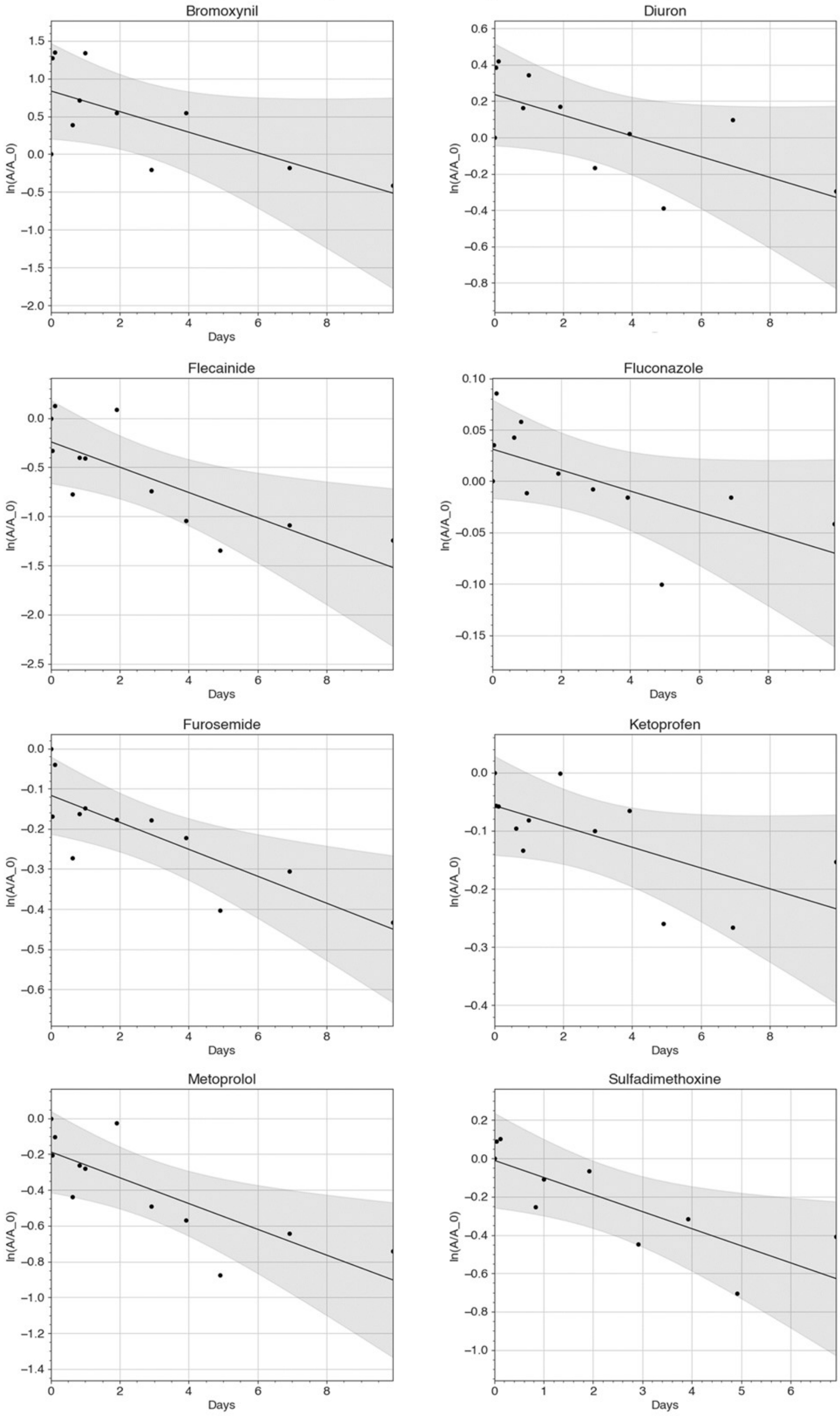
b) F1 replicate B (continued)



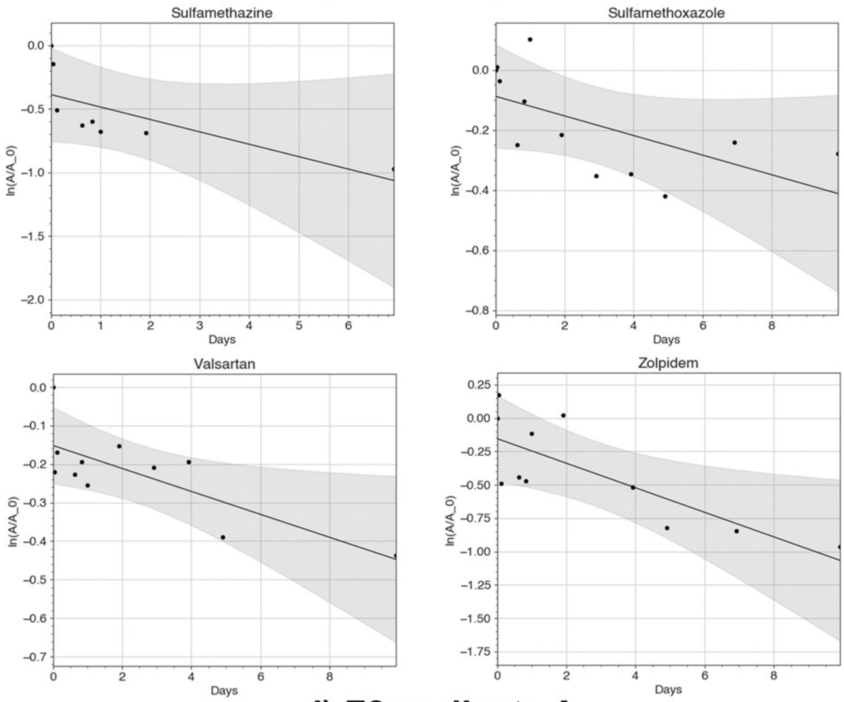
c) F1 replicate C



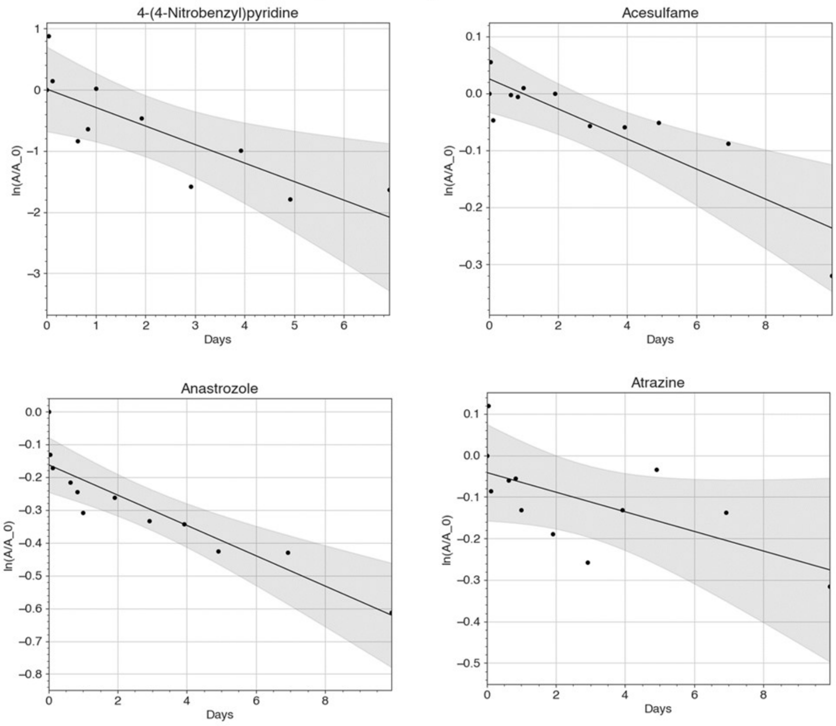
c) F1 replicate C (continued)



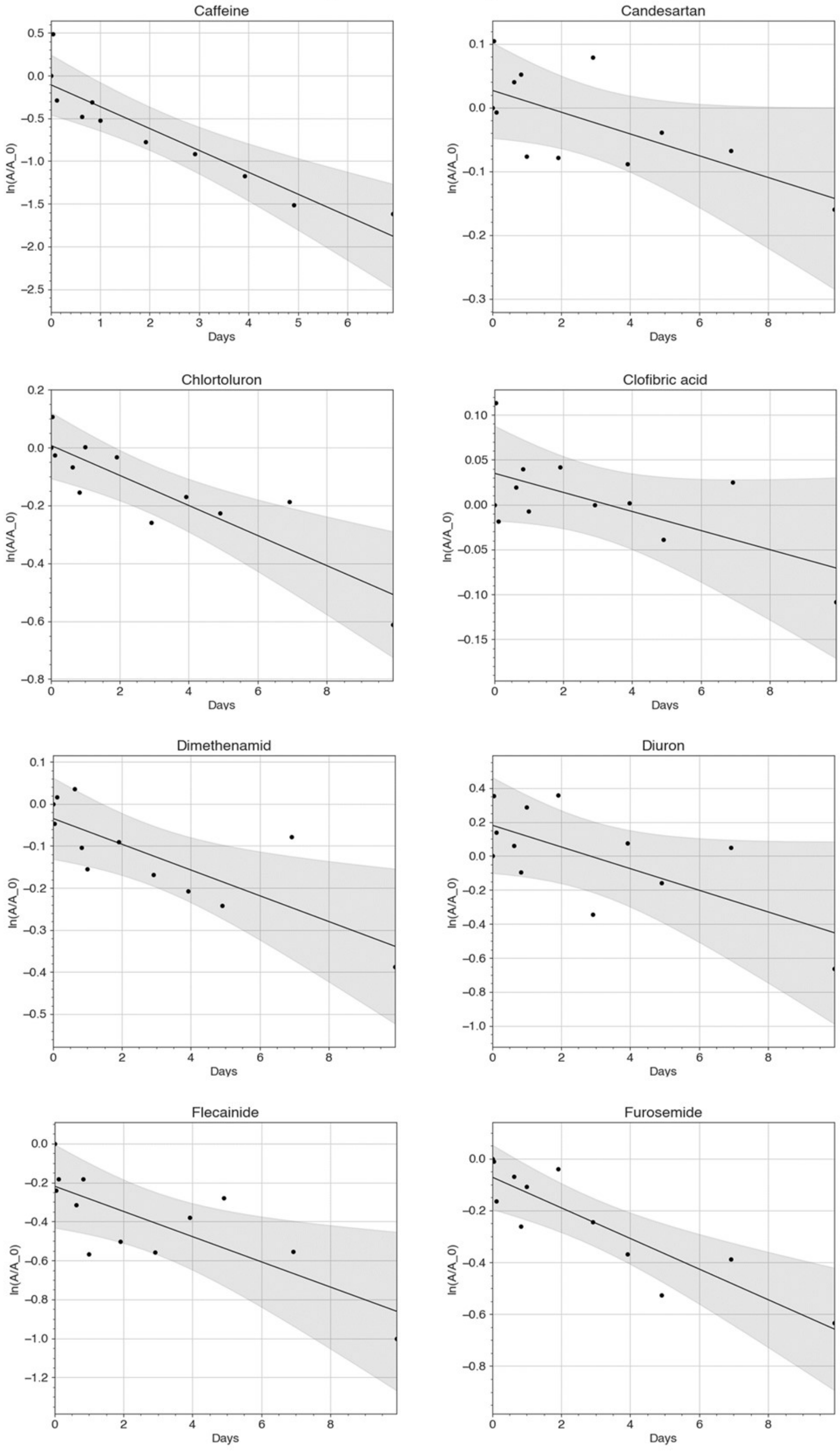
c) F1 replicate C (continued)



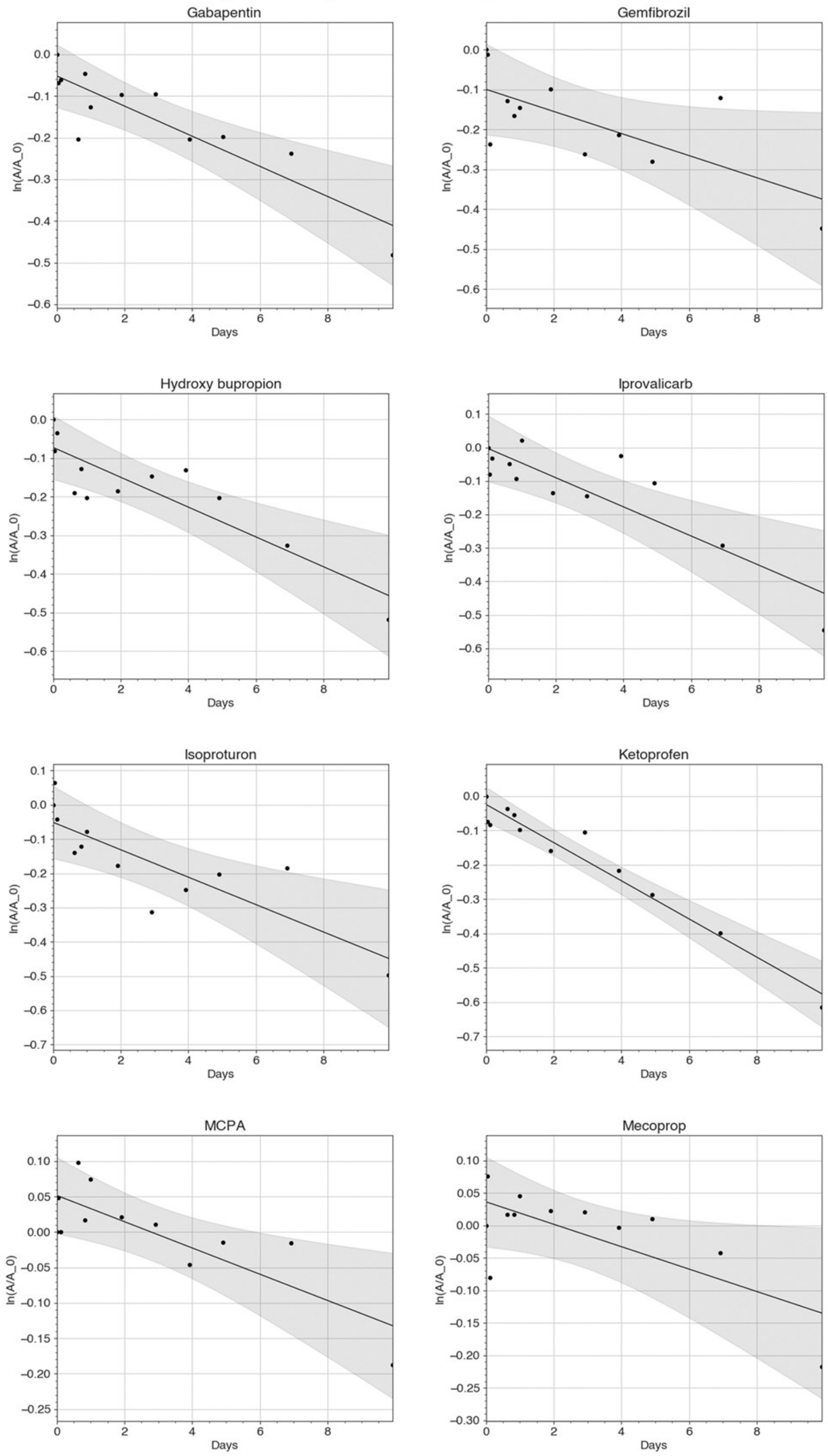
d) F2 replicate A



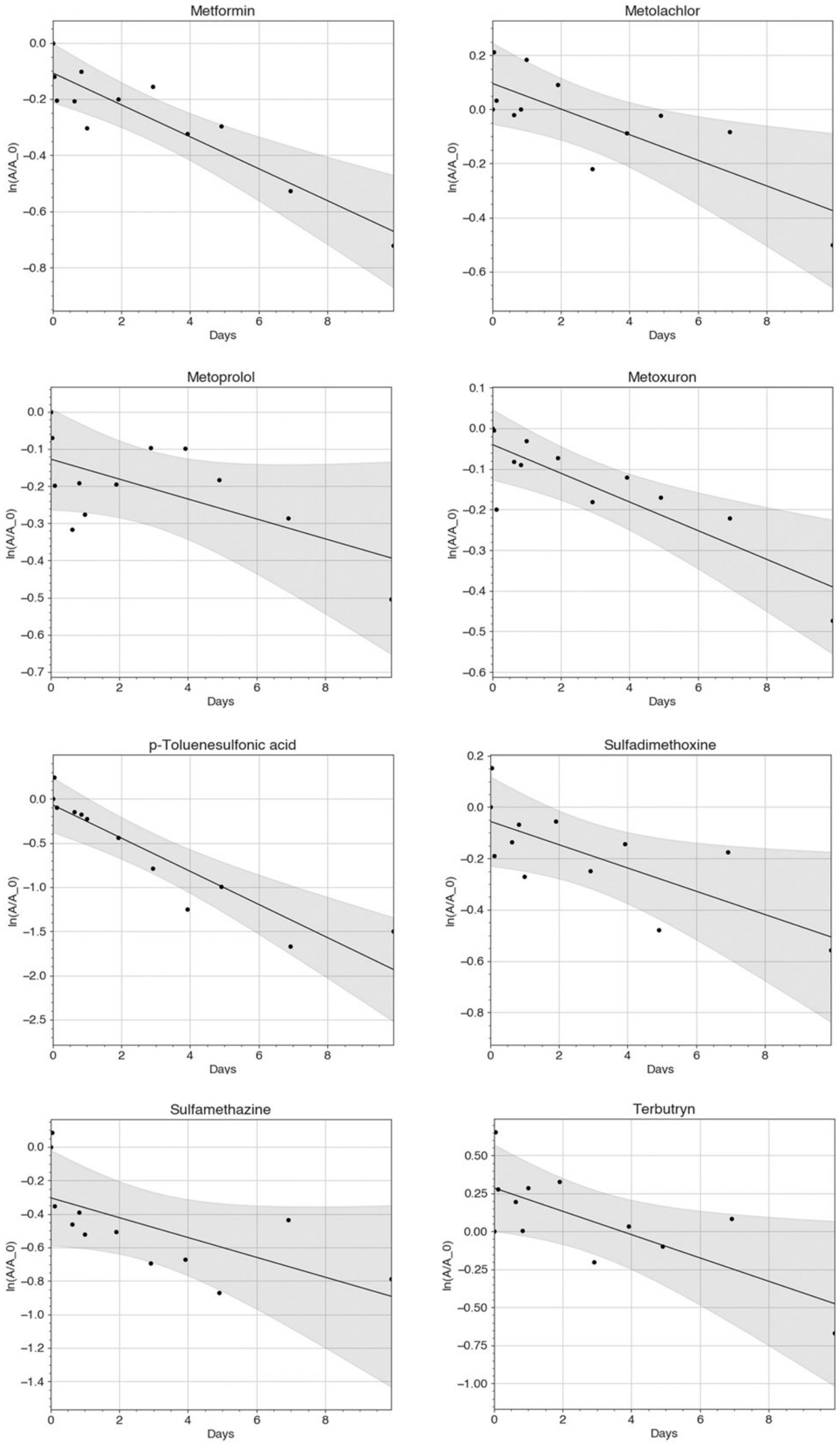
d) F2 replicate A (continued)



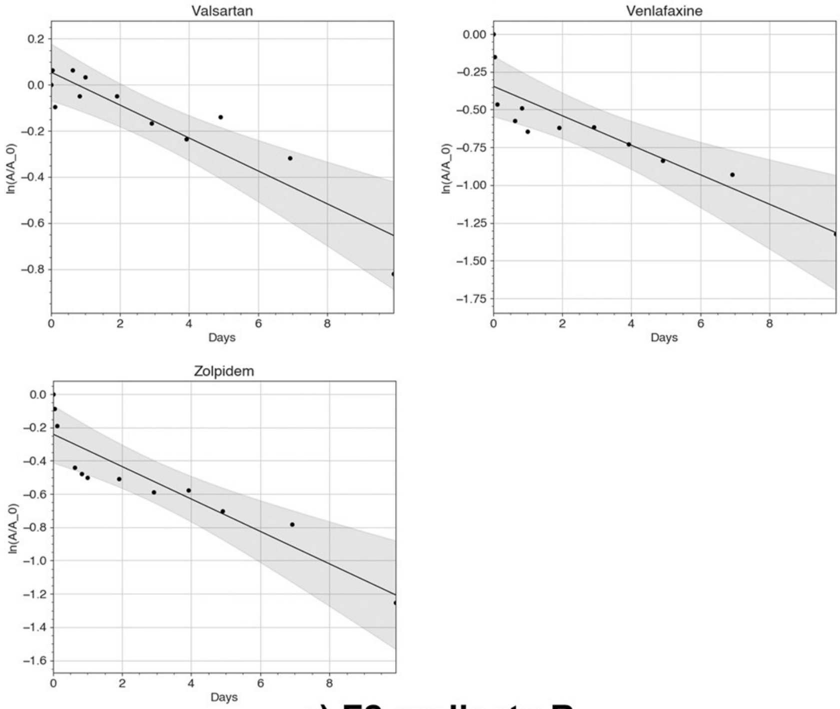
d) F2 replicate A (continued)



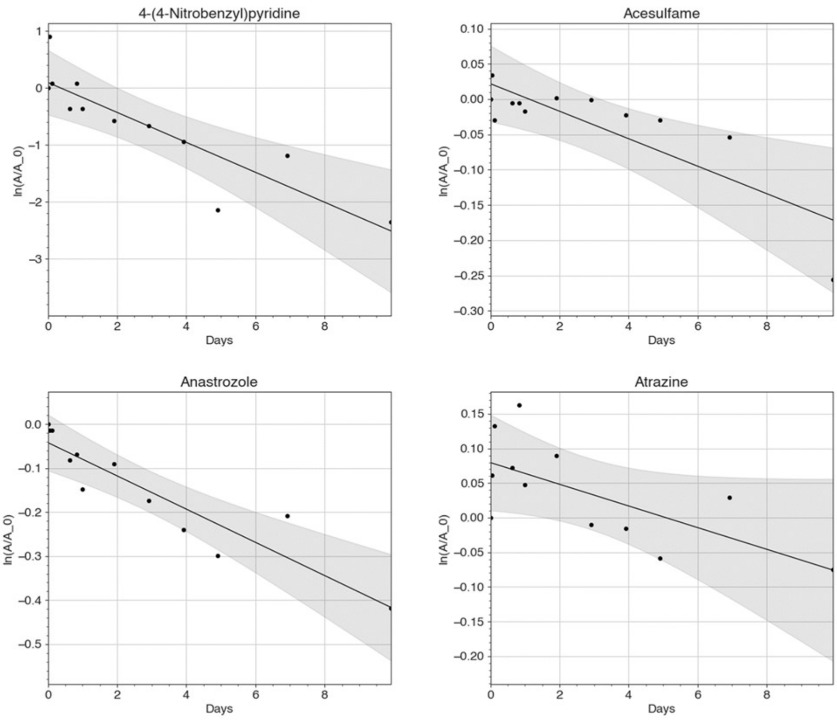
d) F2 replicate A (continued)



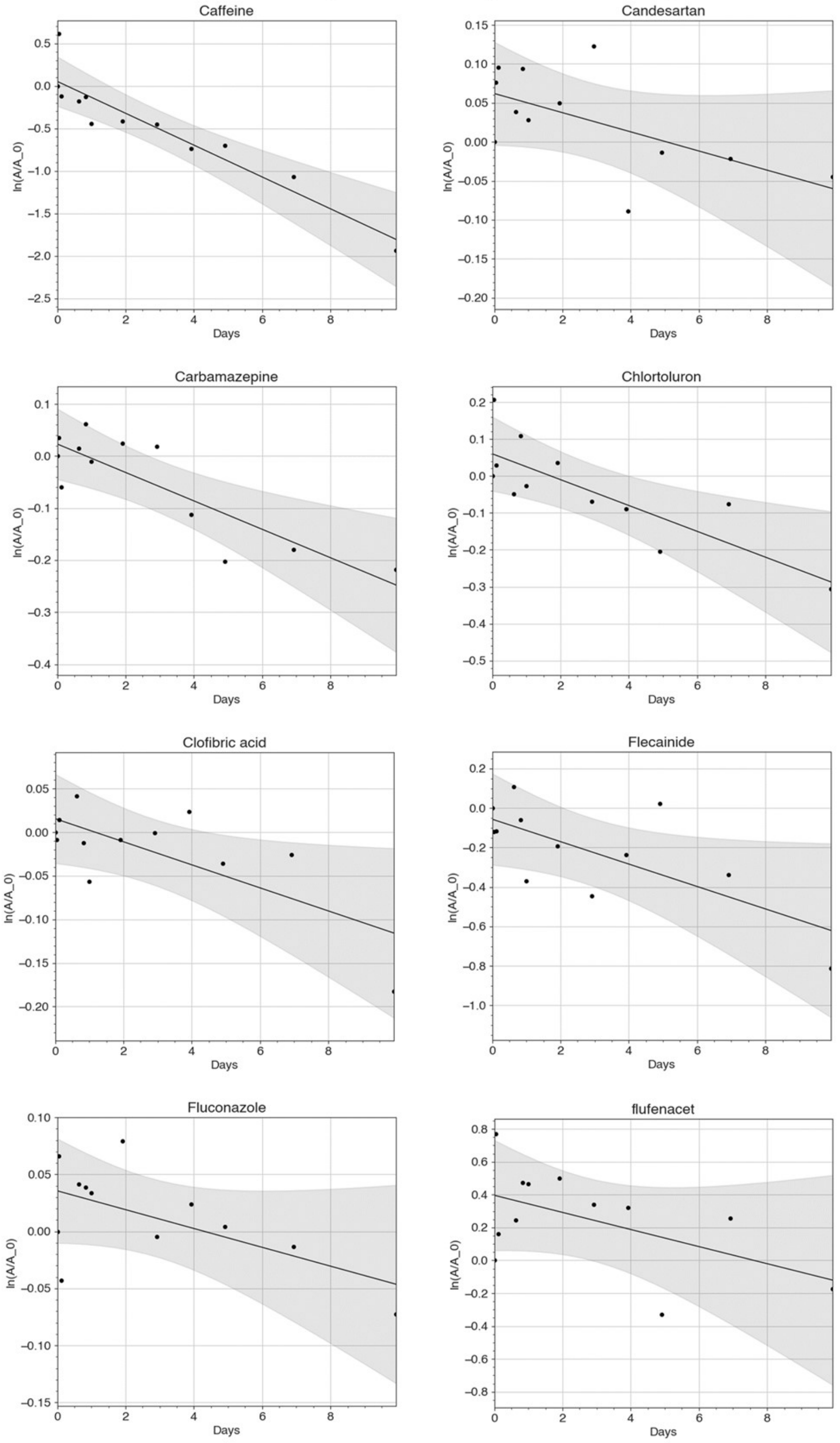
d) F2 replicate A (continued)



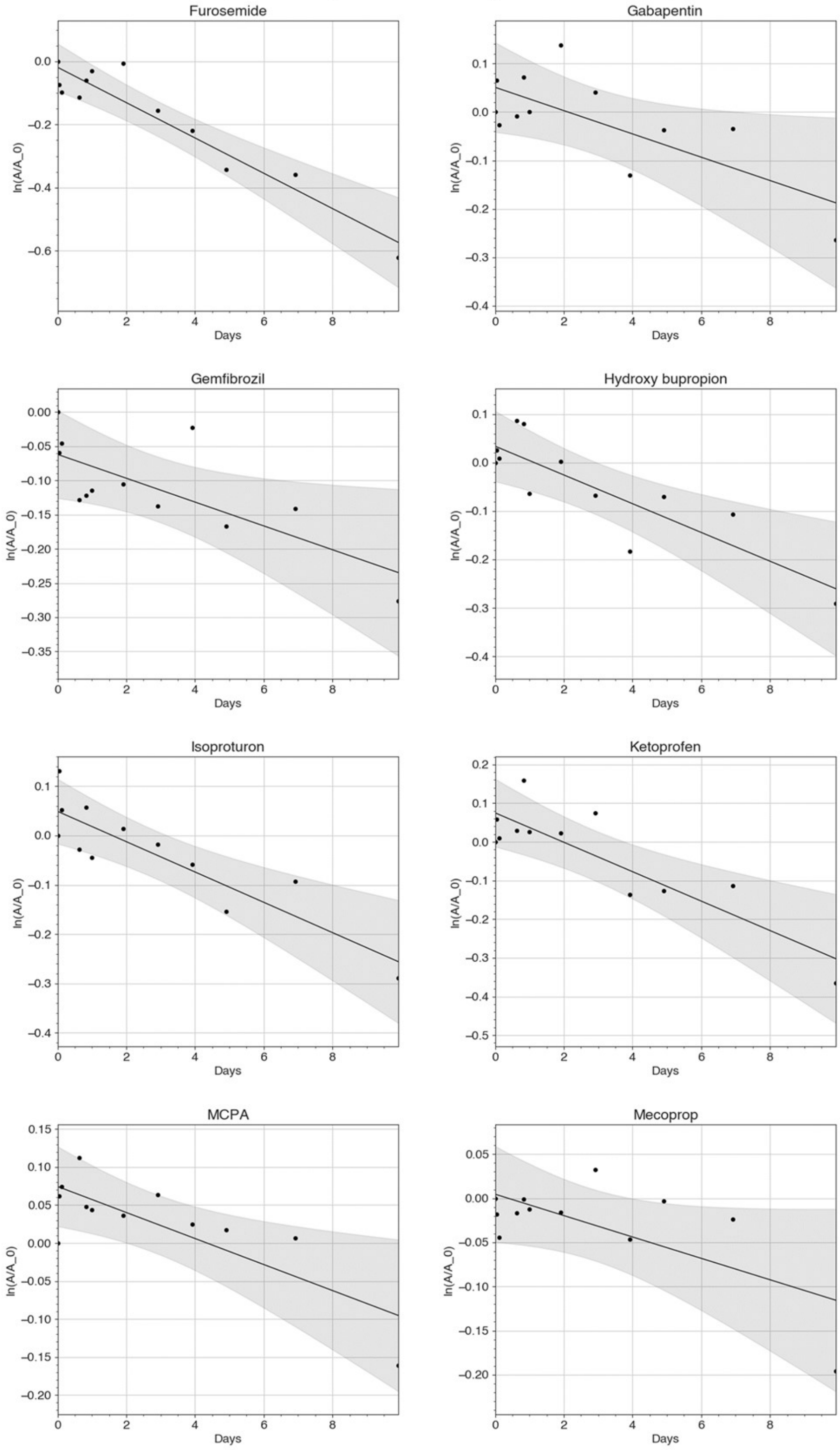
e) F2 replicate B



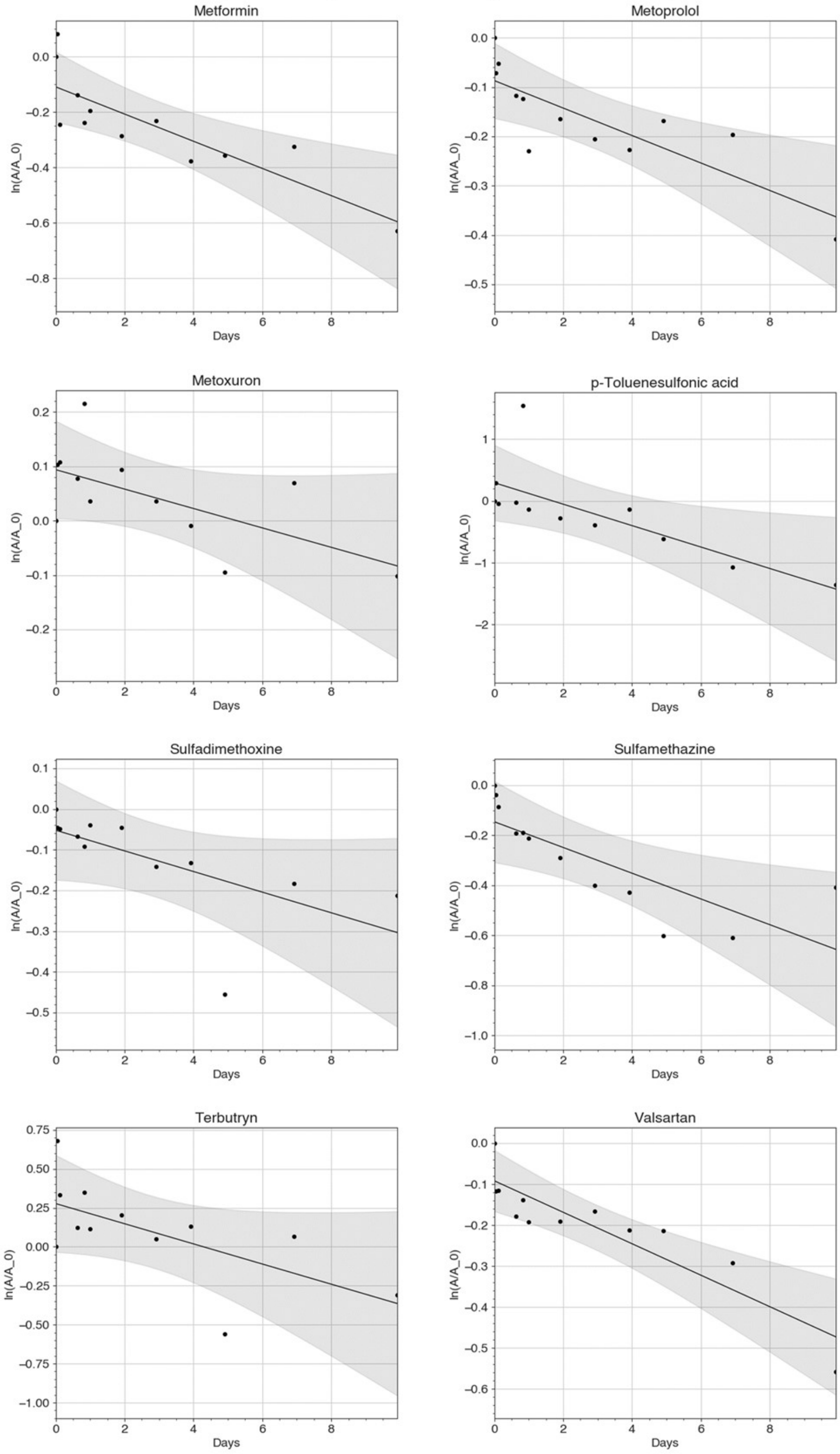
e) F2 replicate B (continued)



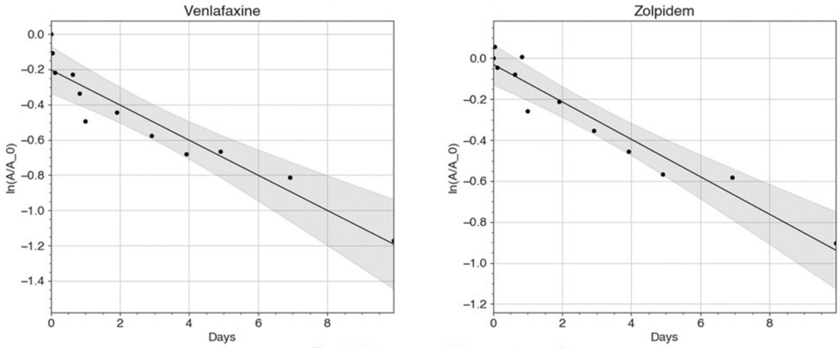
e) F2 replicate B (continued)



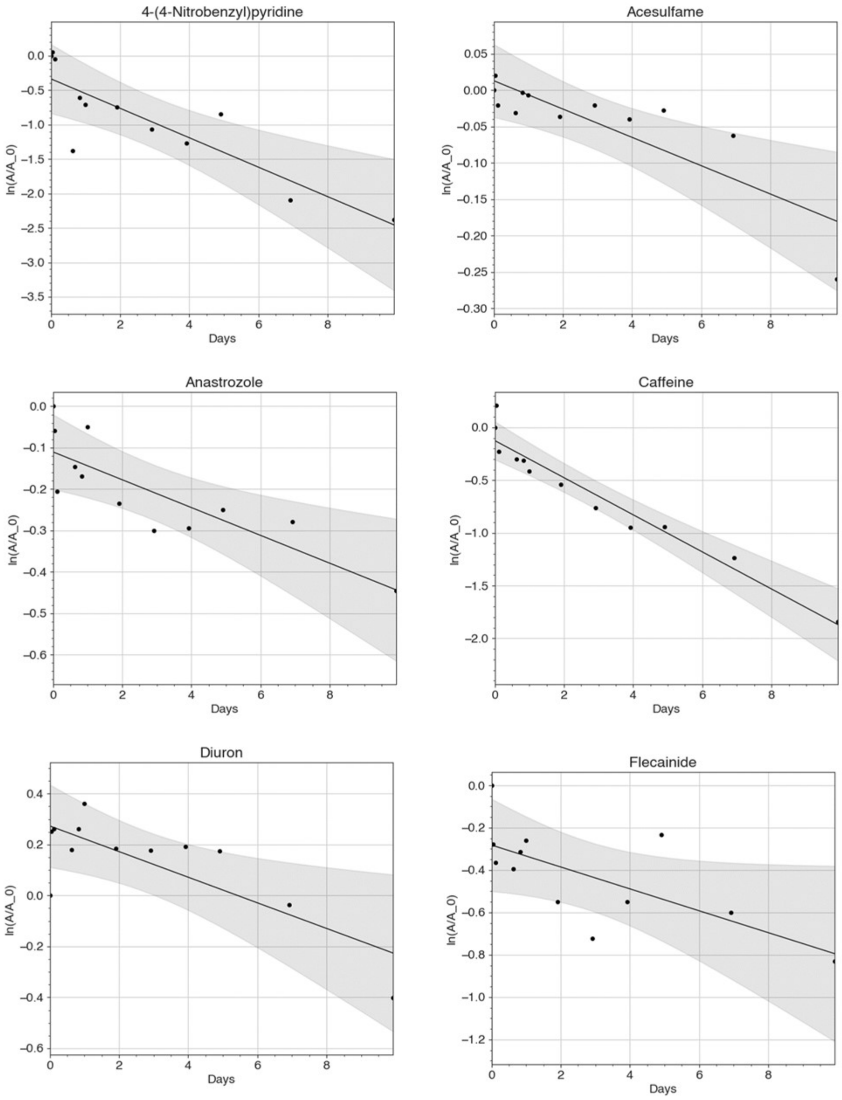
e) F2 replicate B (continued)



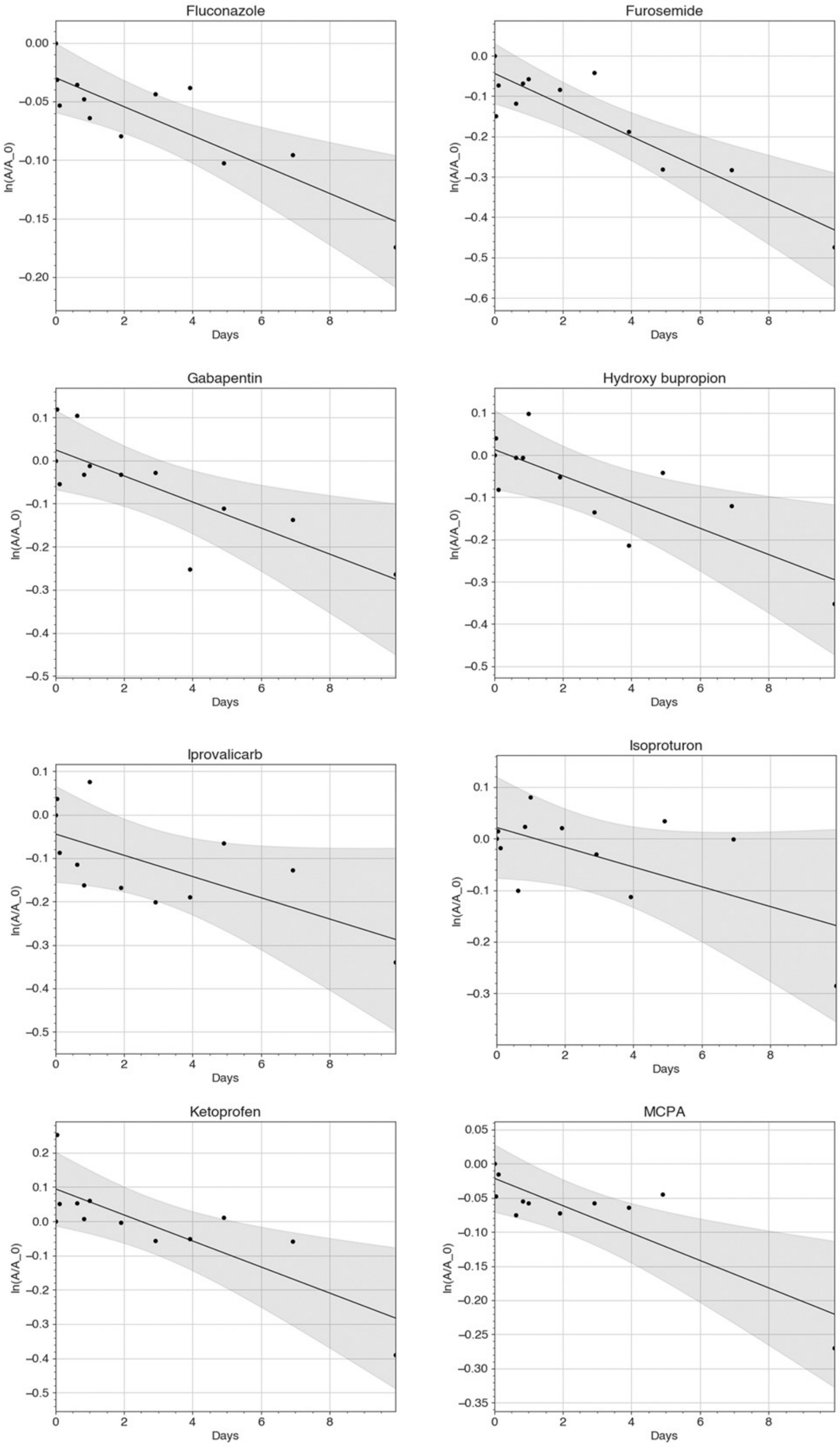
e) F2 replicate B (continued)



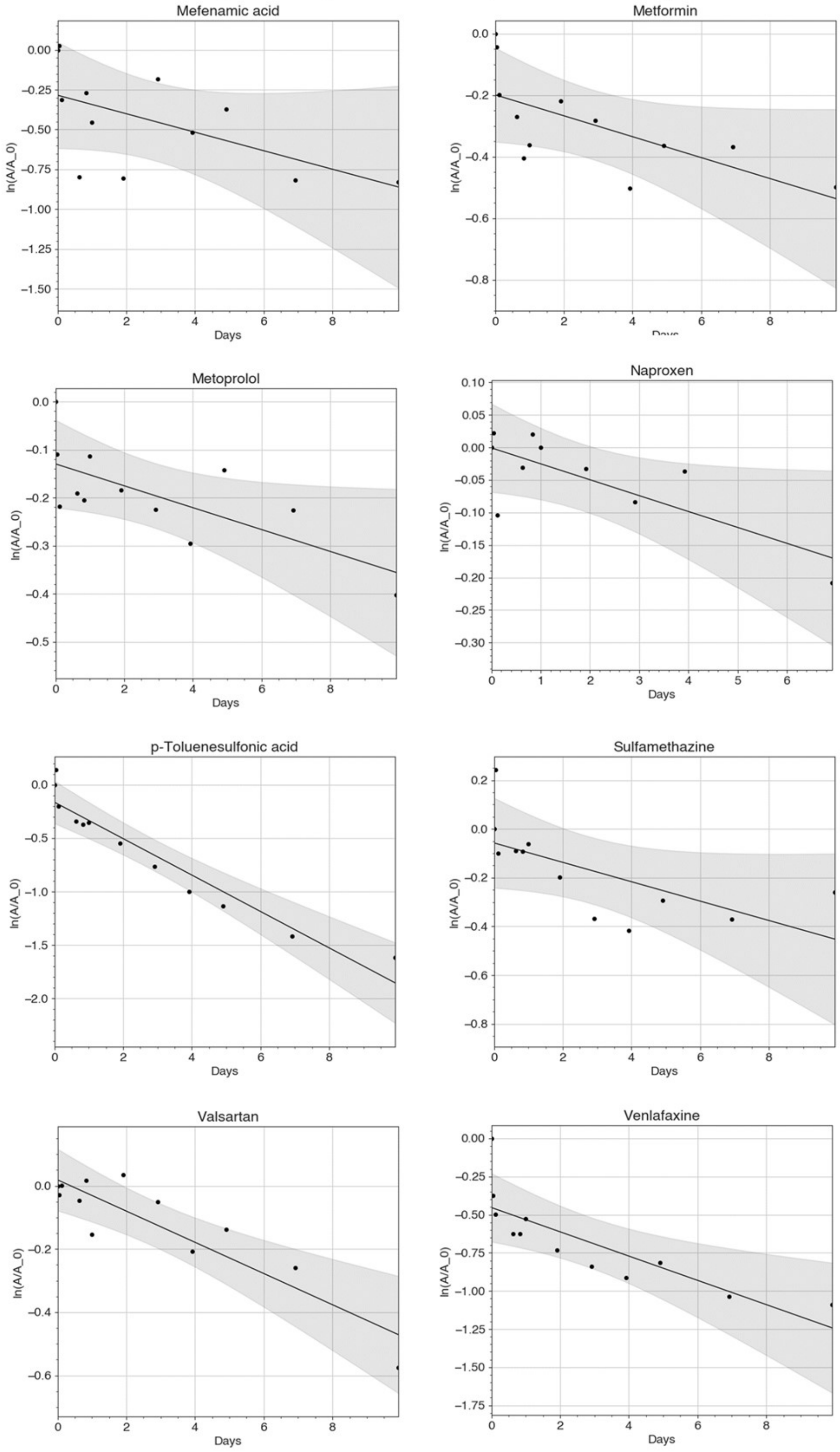
f) F2 replicate C



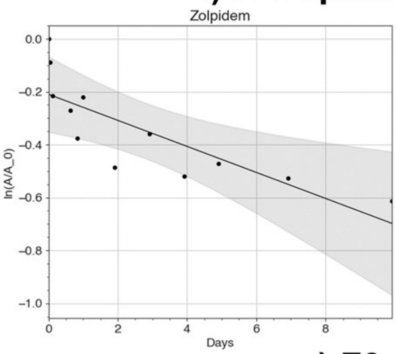
f) F2 replicate C (continued)



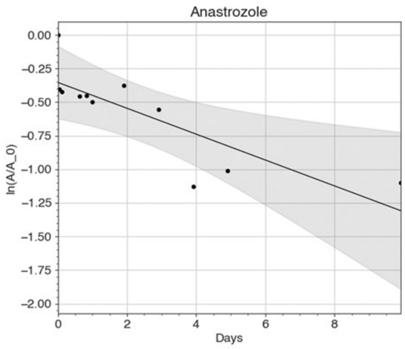
f) F2 replicate C (continued)

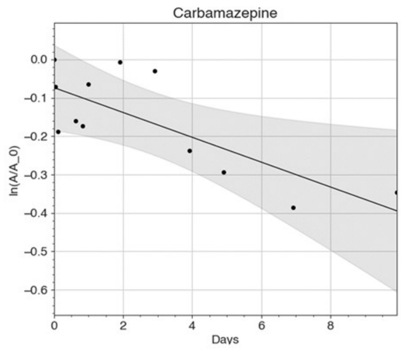


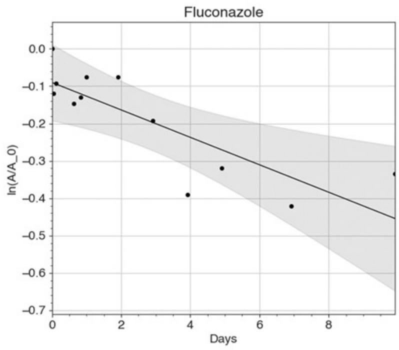
f) F2 replicate C (continued)

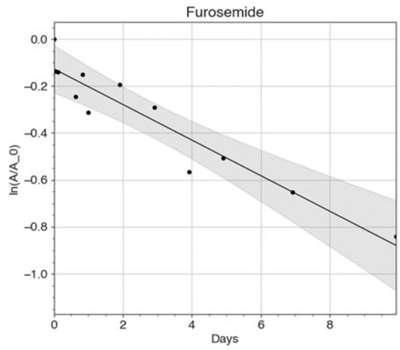


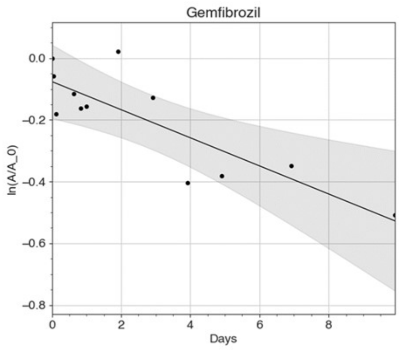
g) F3 replicate A

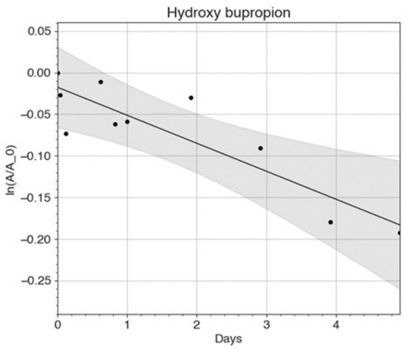




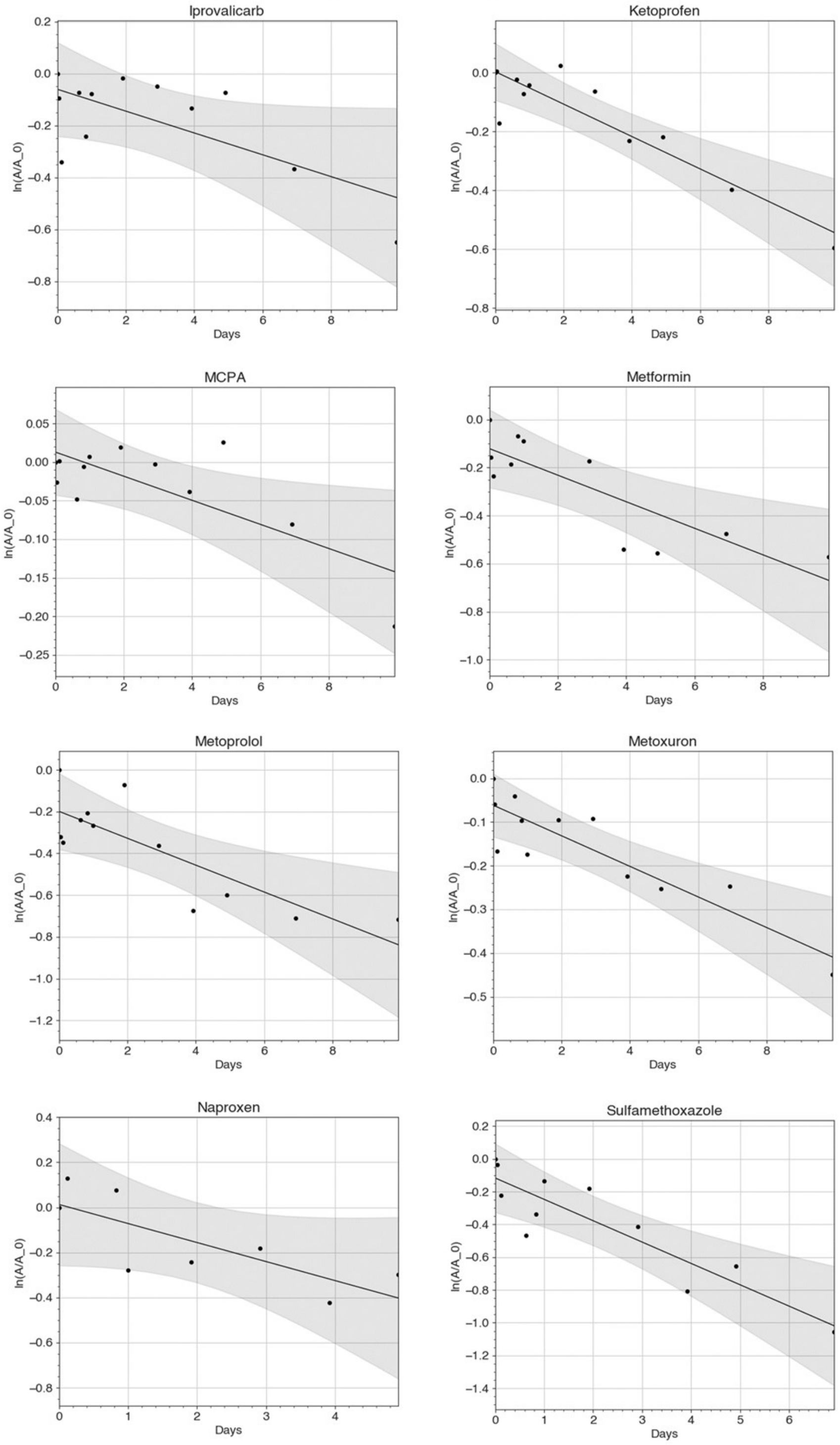




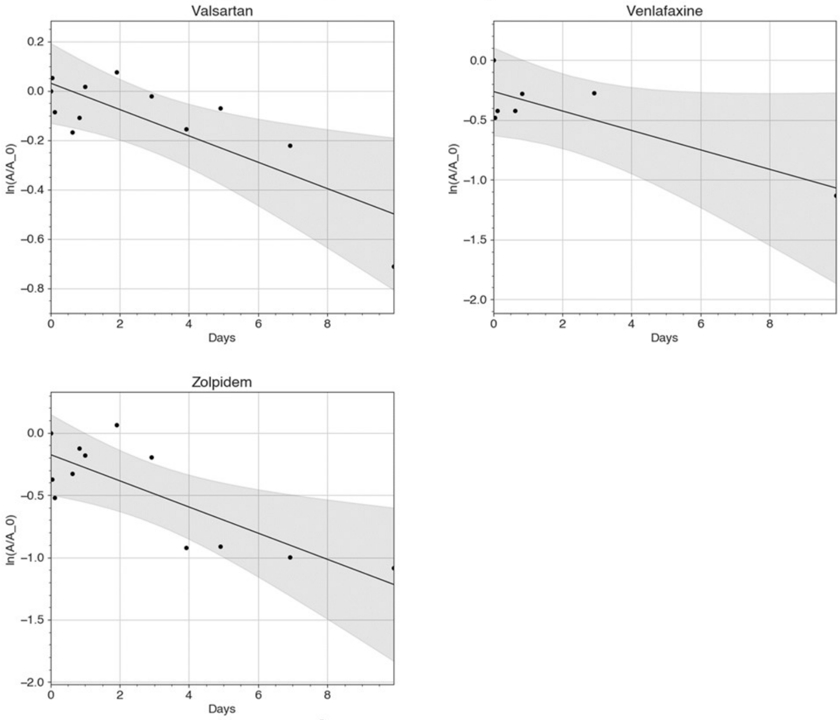




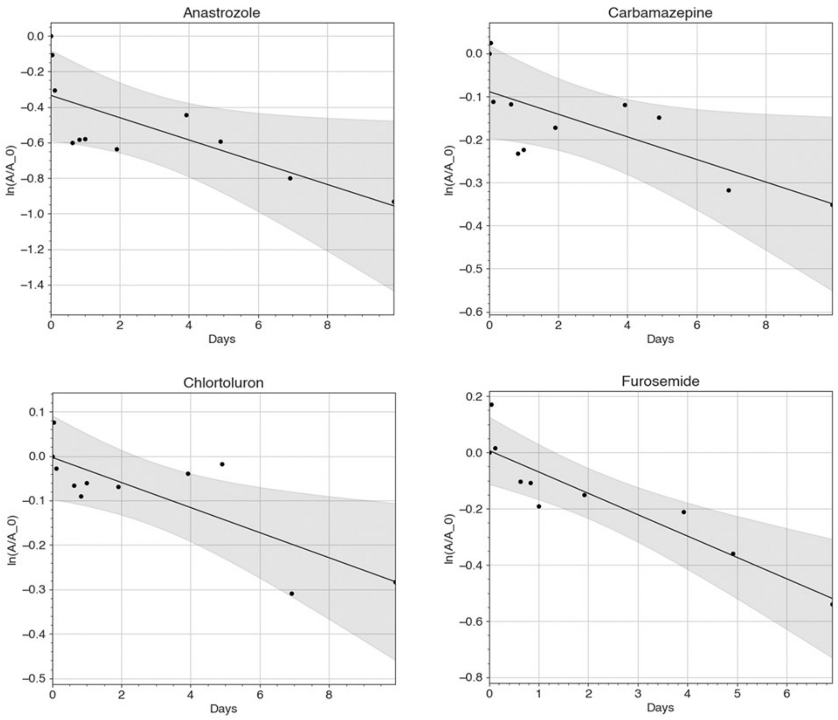
g) F3 replicate A (continued)



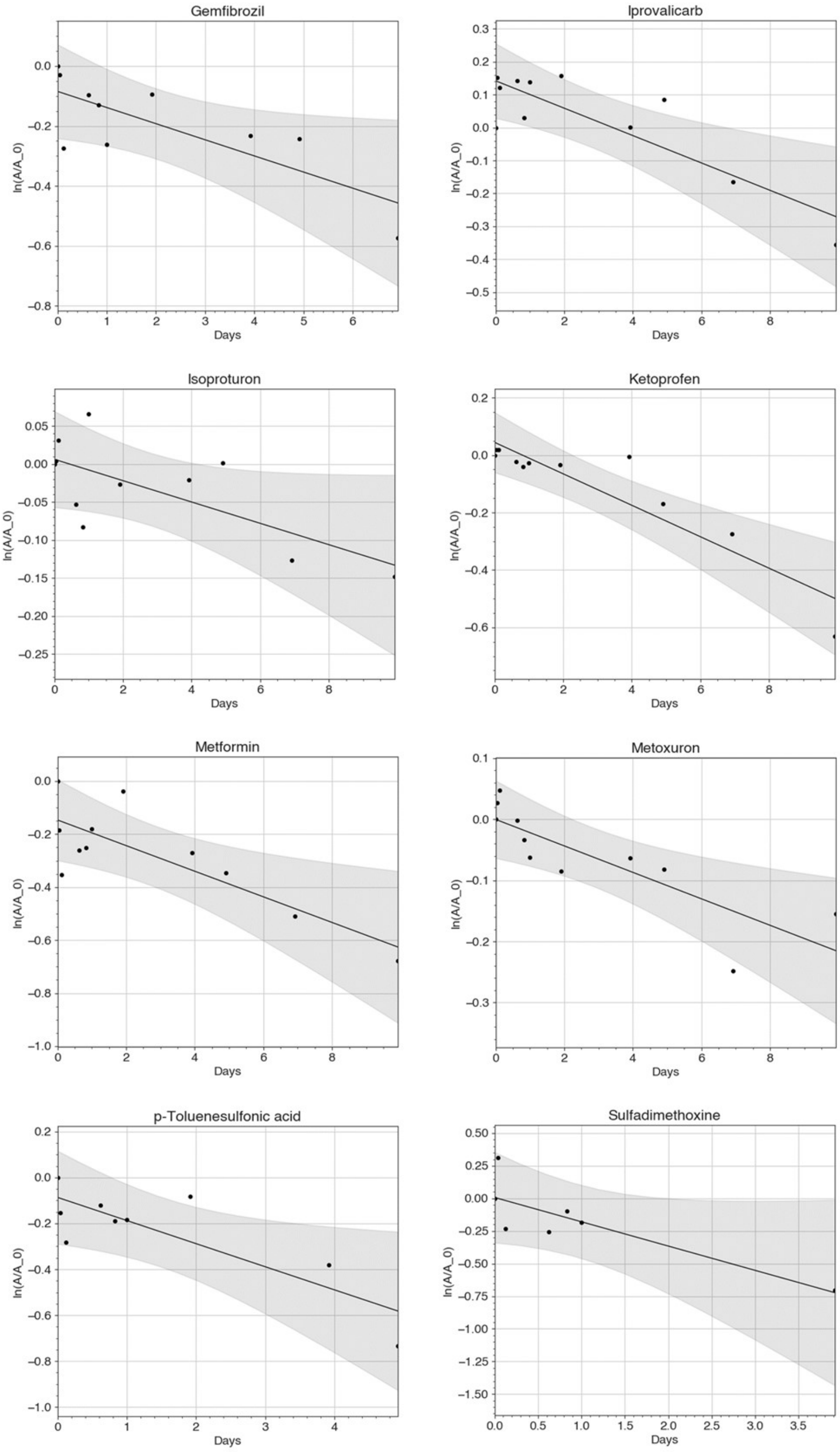
g) F3 replicate A (continued)



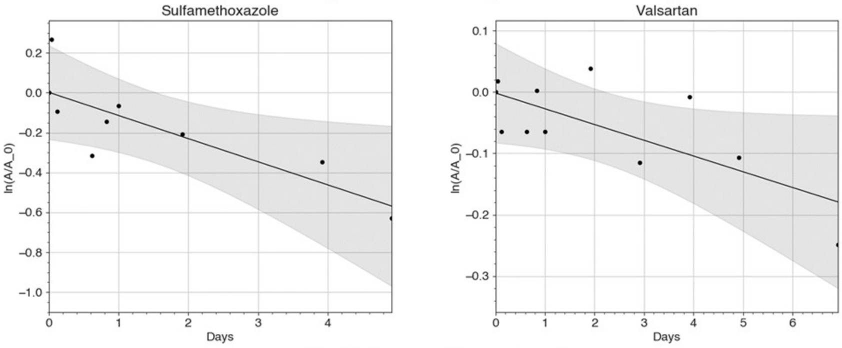
h) F3 replicate B



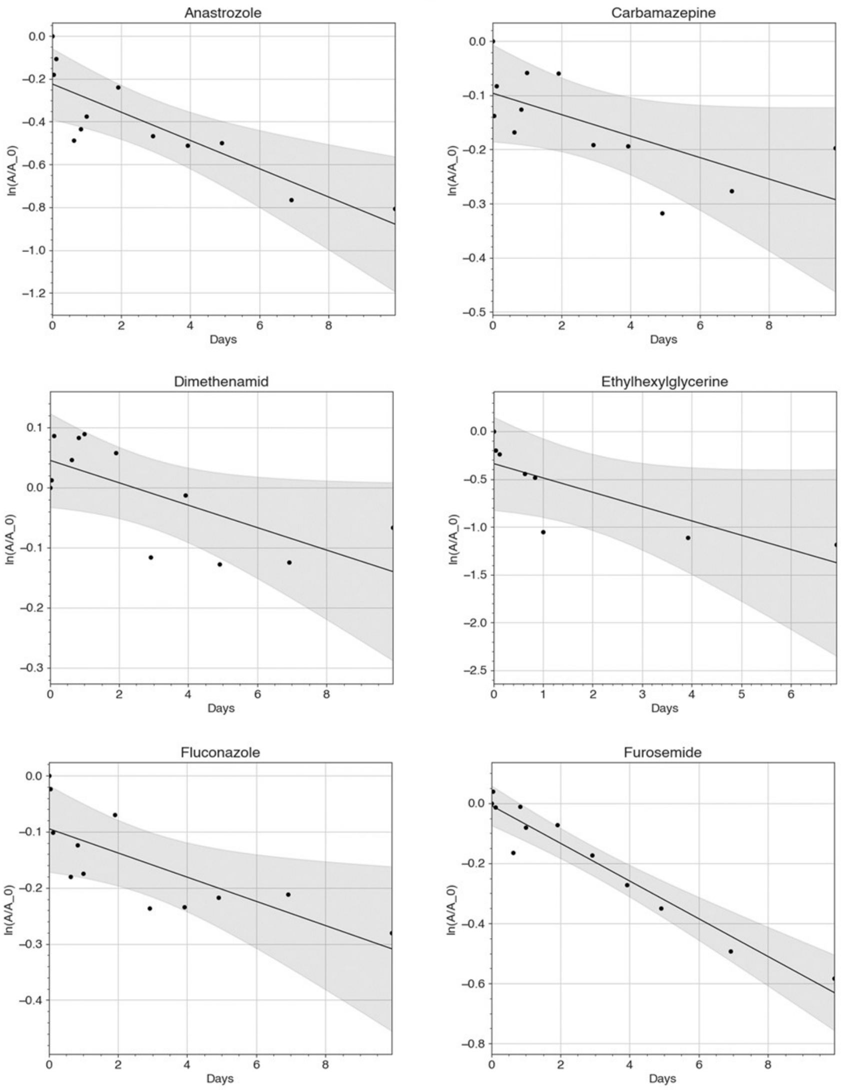
h) F3 replicate B (continued)



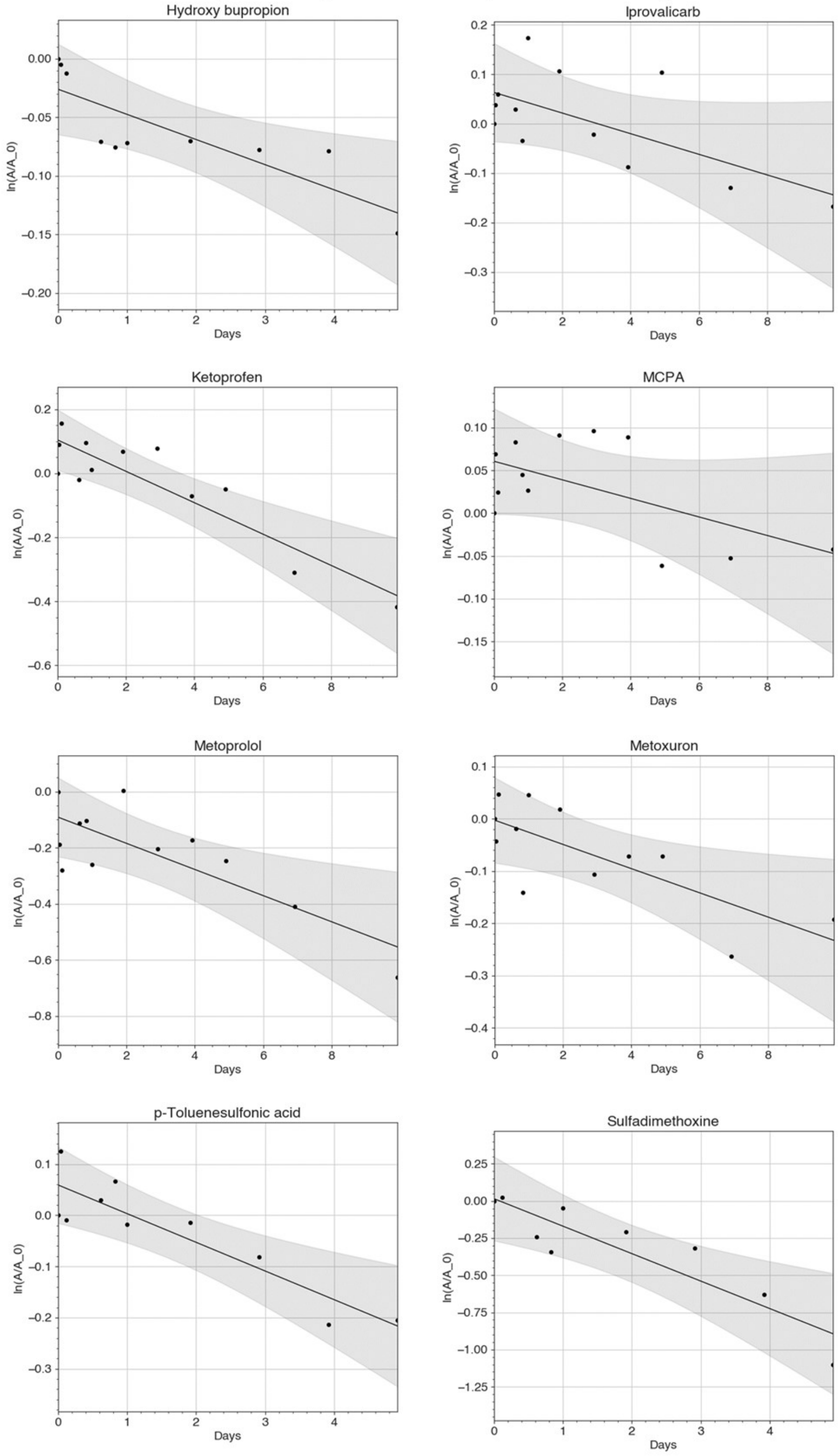
h) F3 replicate B (continued)



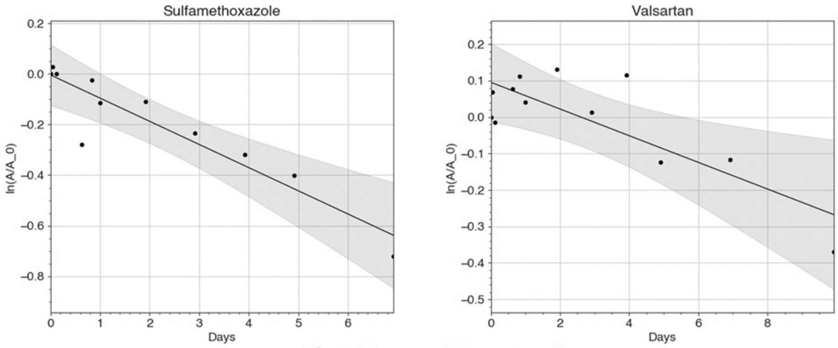
i) F3 replicate C



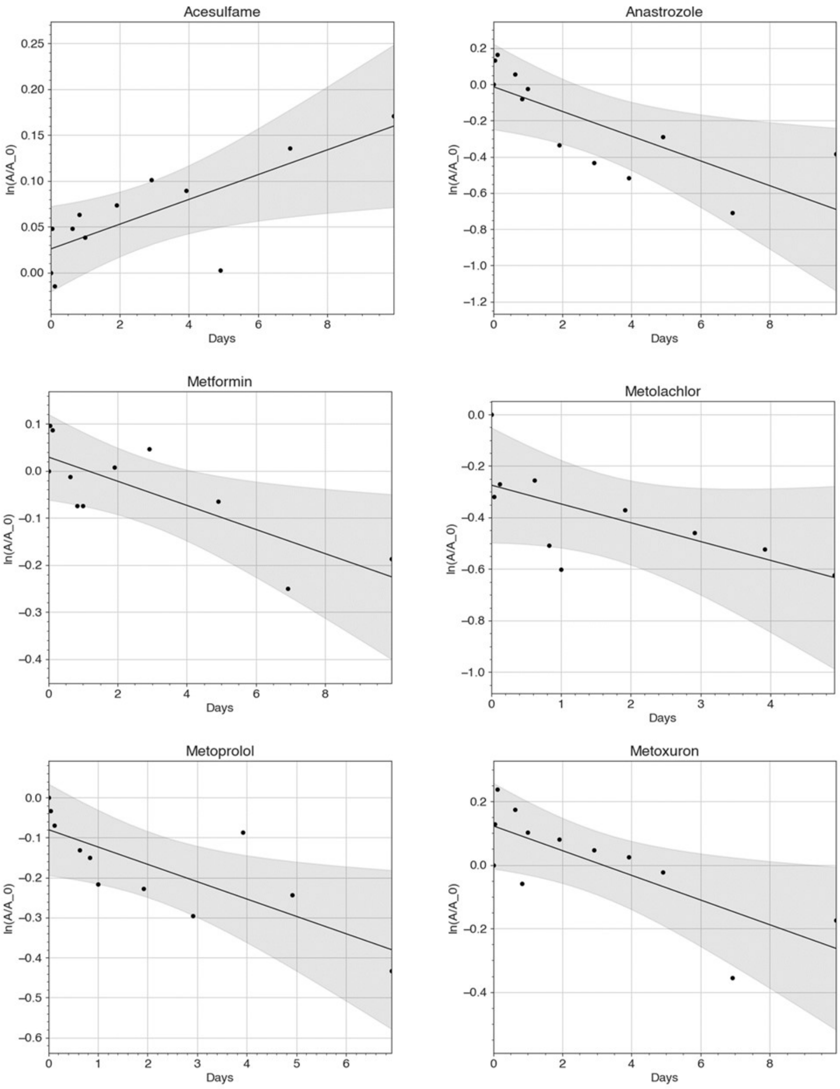
i) F3 replicate C (continued)



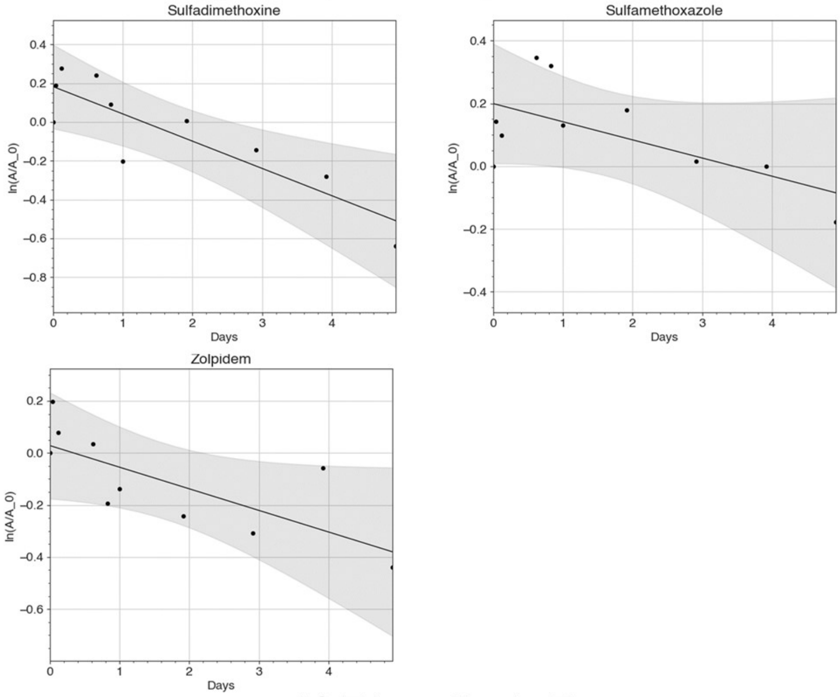
i) F3 replicate C (continued)



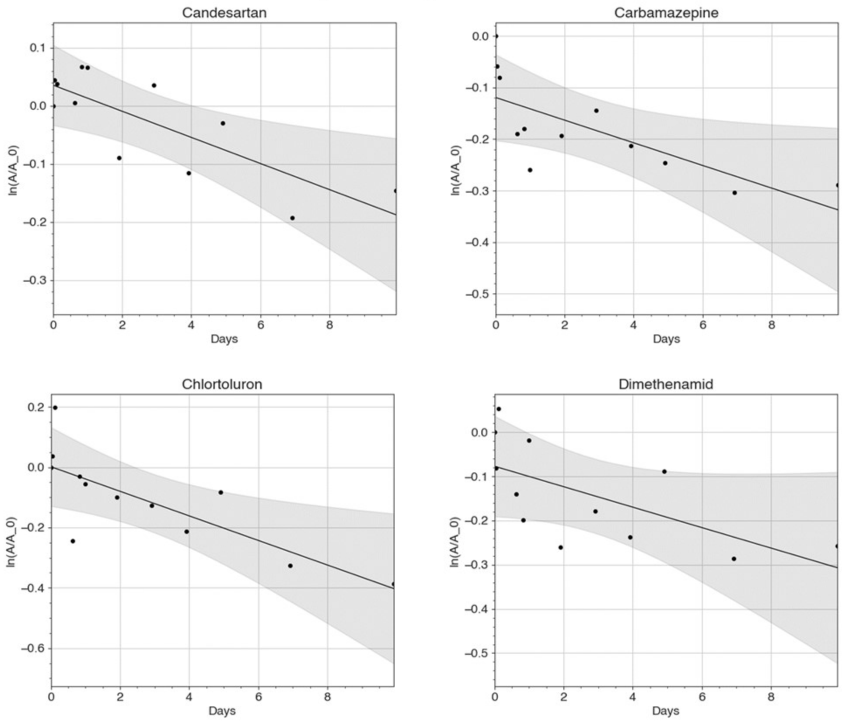
j) F4 replicate A



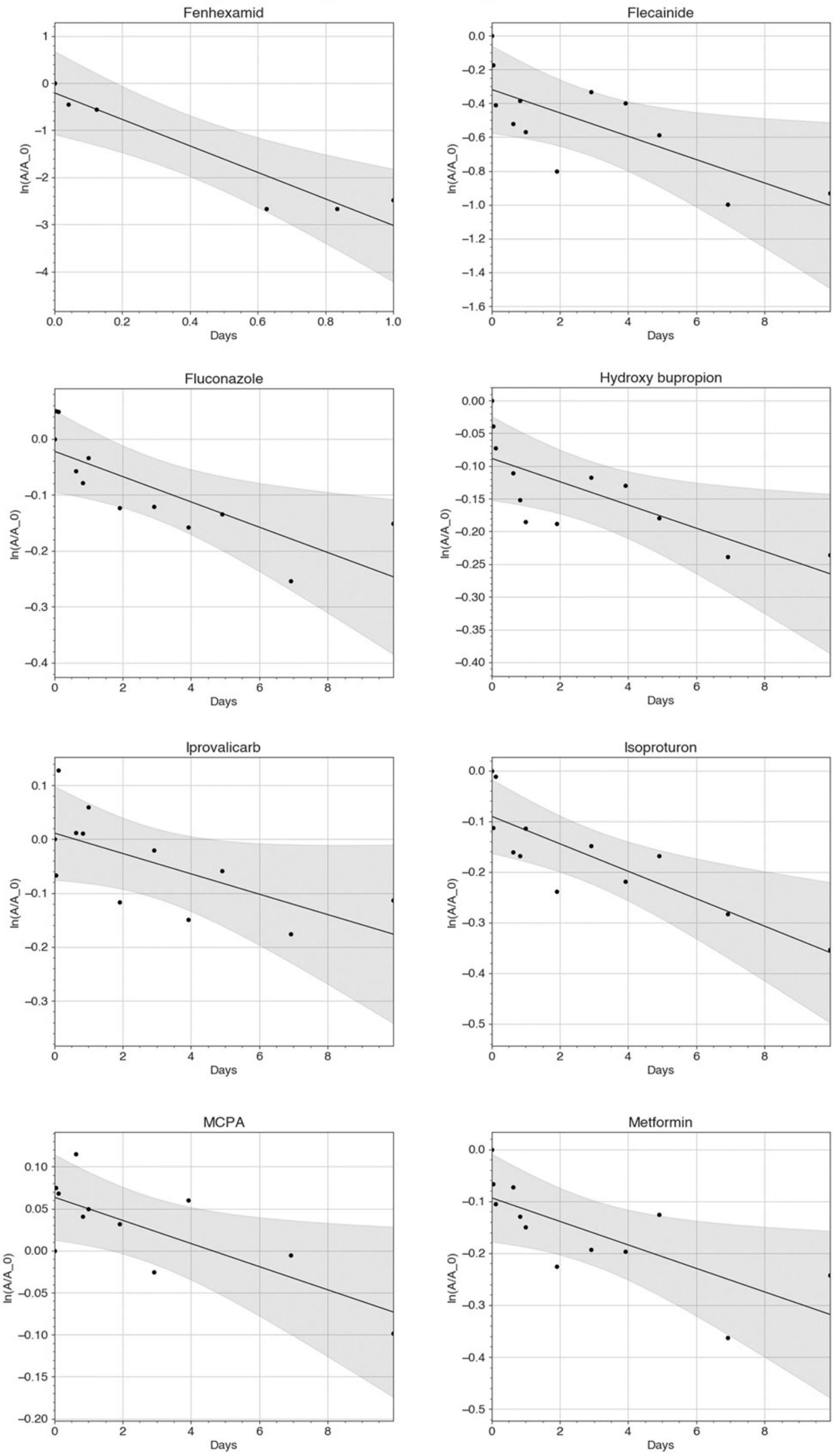
j) F4 replicate A (continued)



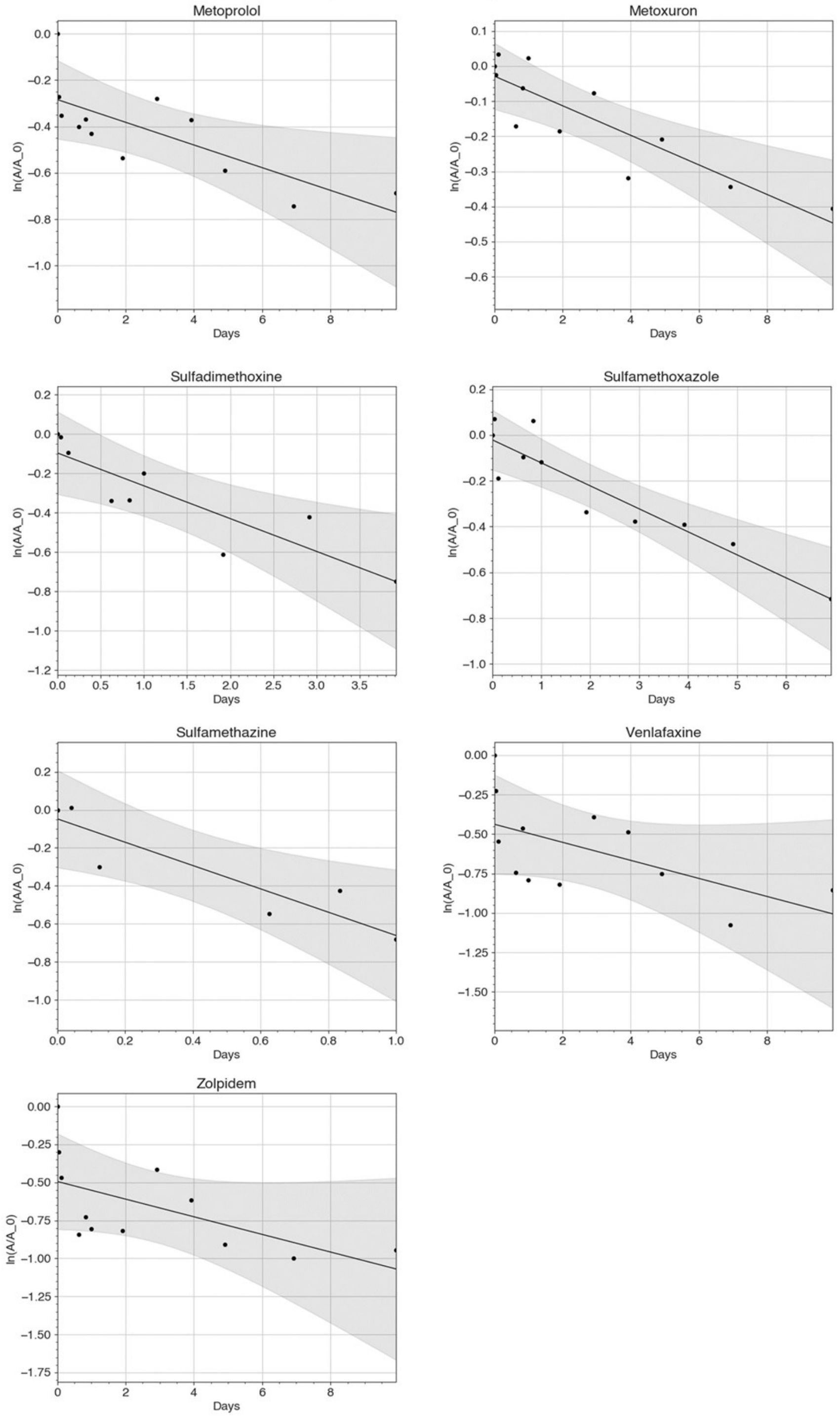
k) F4 replicate B



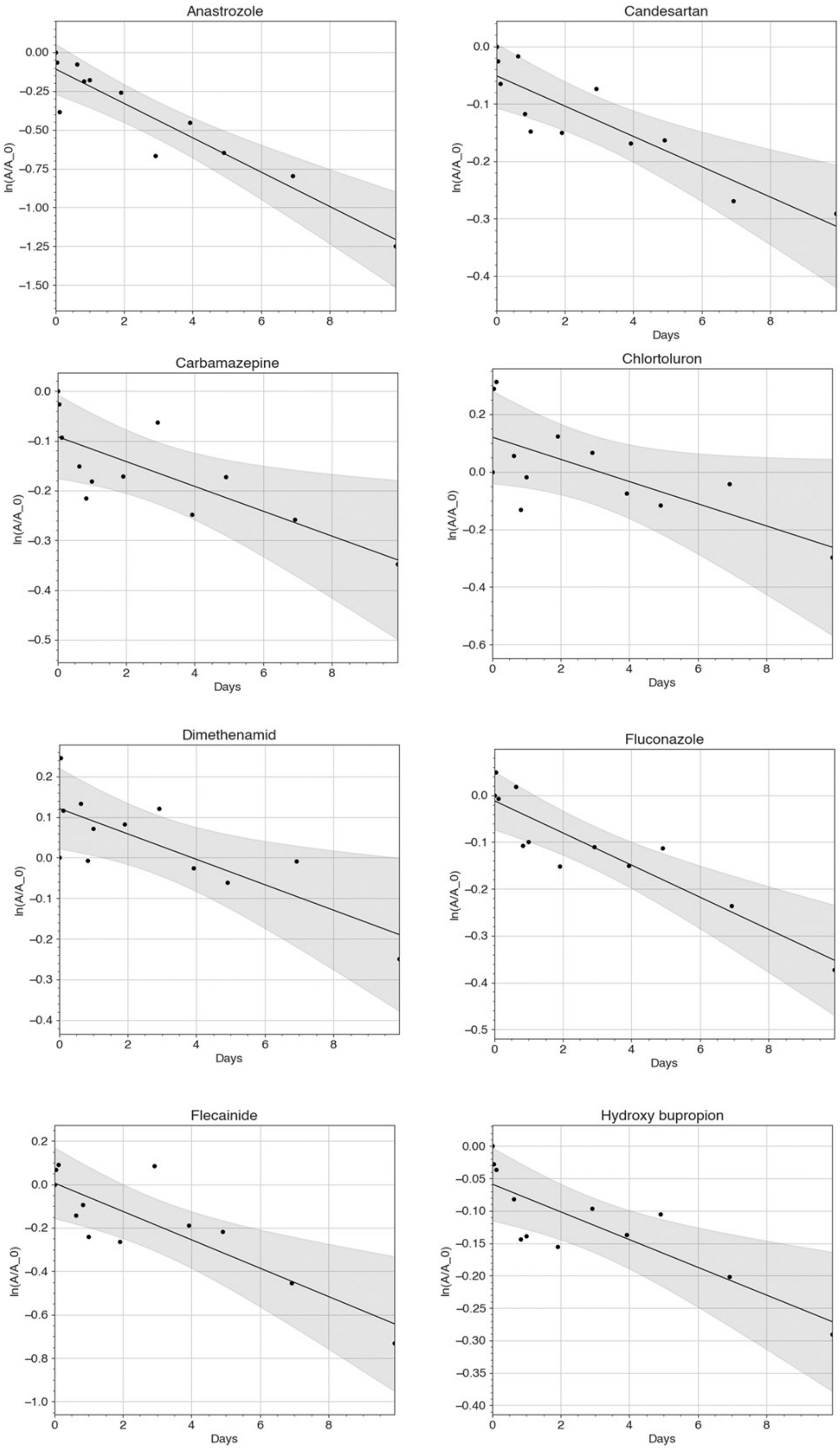
k) F4 replicate B (continued)



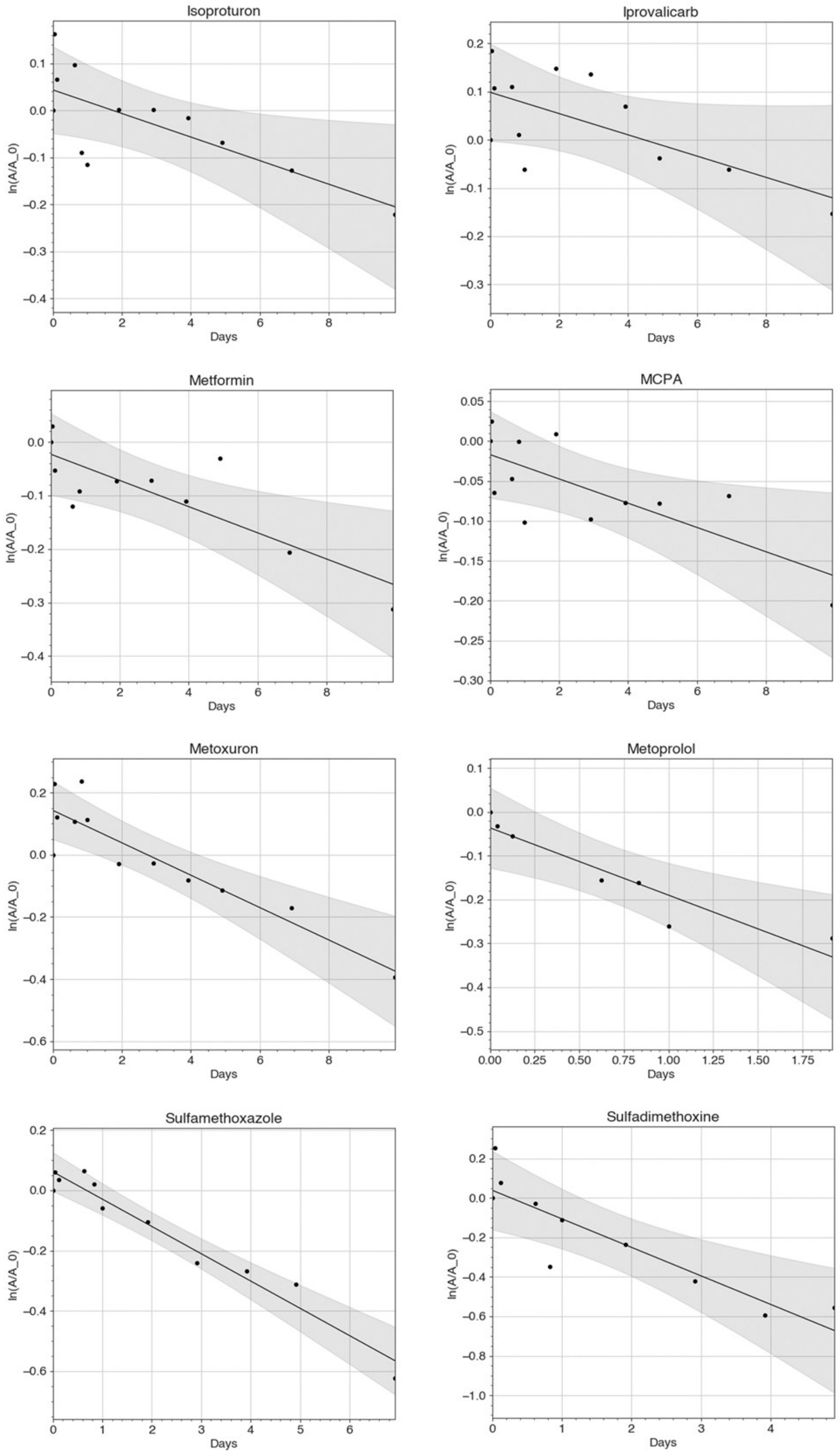
k) F4 replicate B (continued)



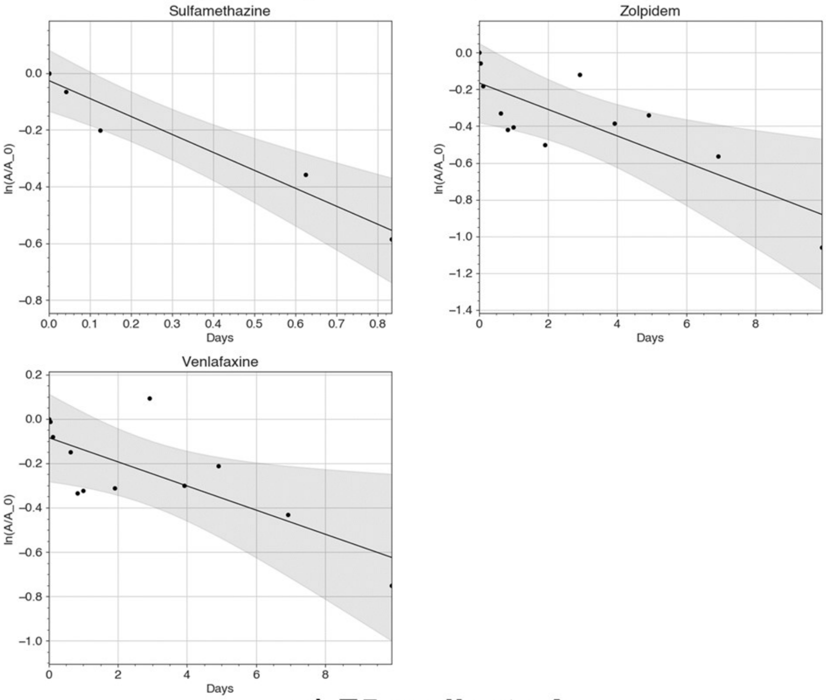
I) F4 replicate C



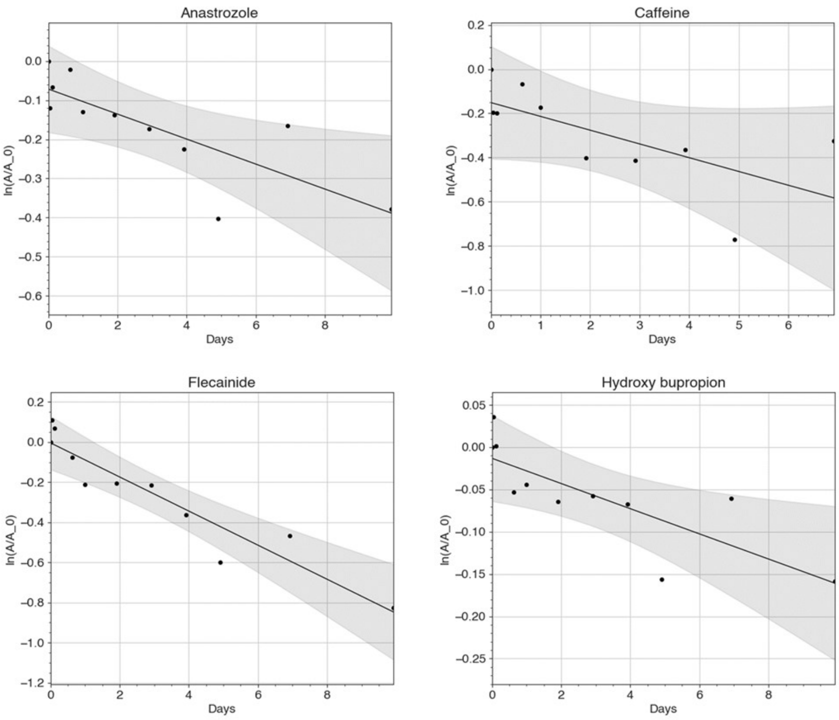
l) F4 replicate C (continued)



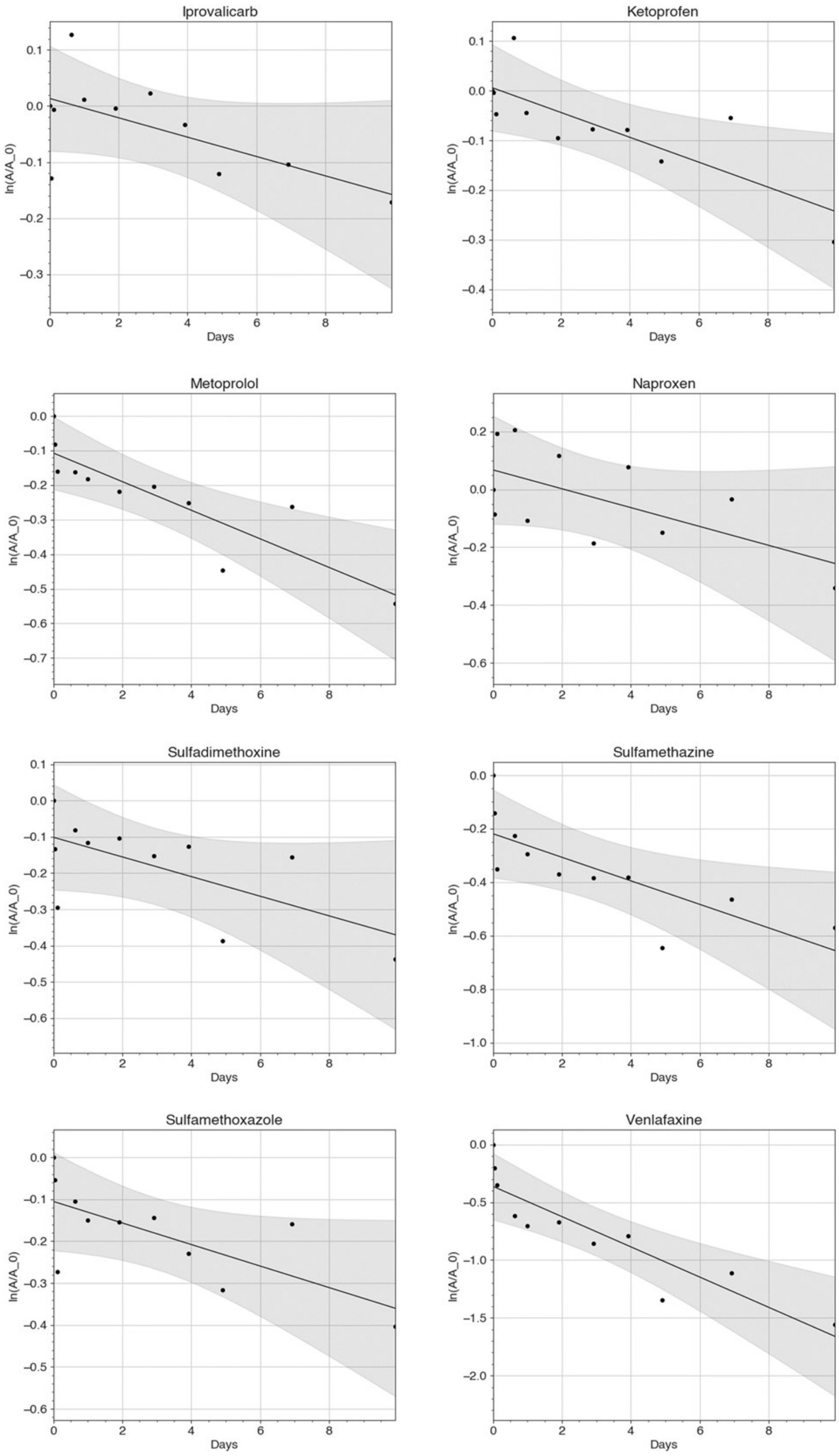
l) F4 replicate C (continued)



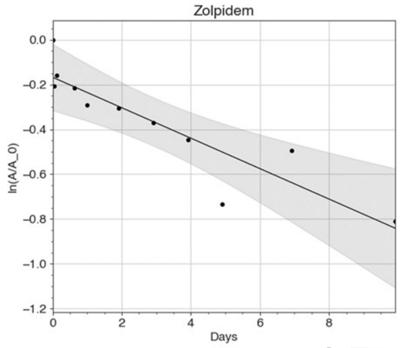
m) F5 replicate A



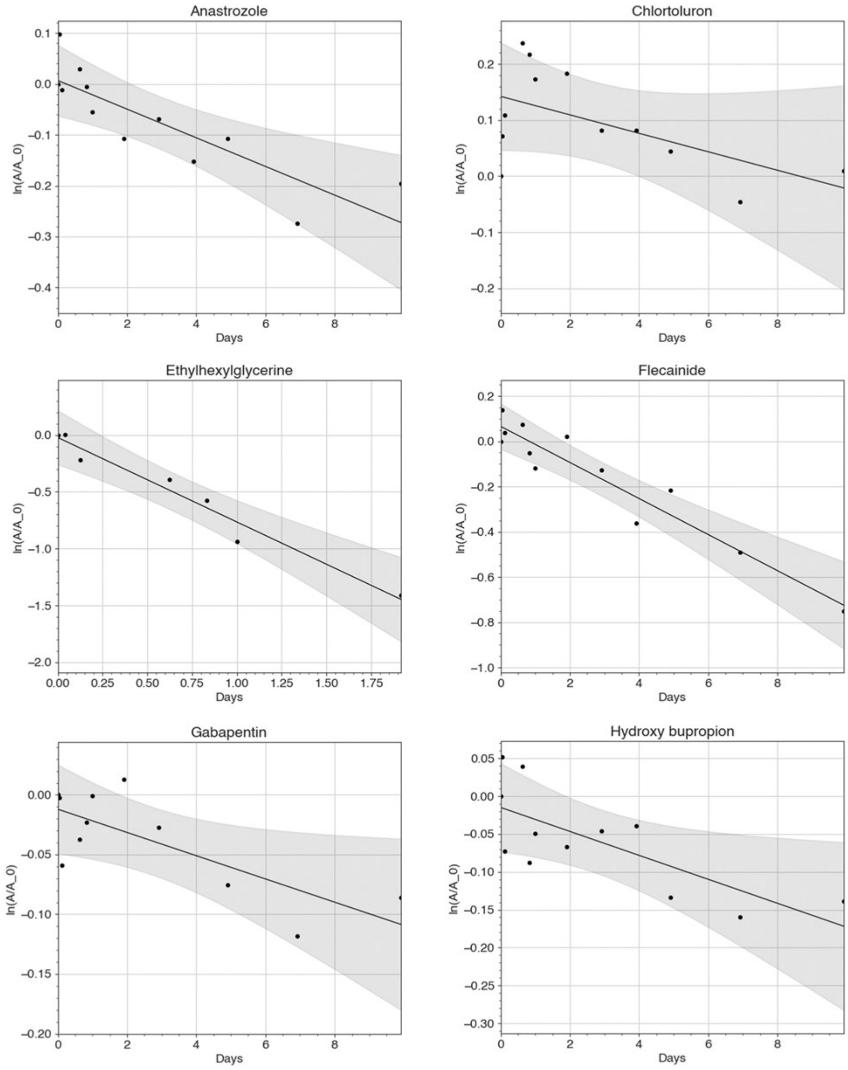
m) F5 replicate A (continued)



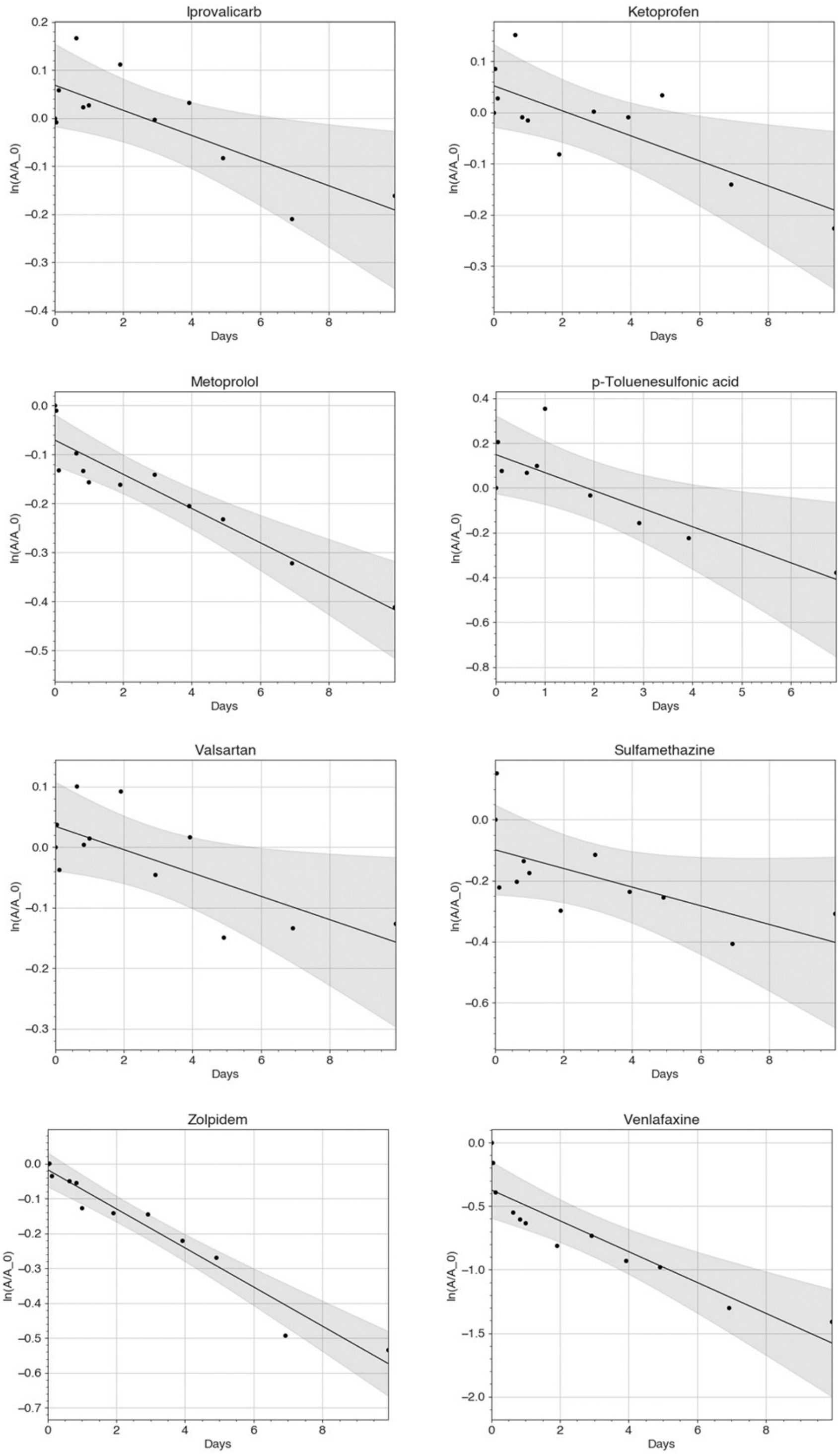
m) F5 replicate A (continued)



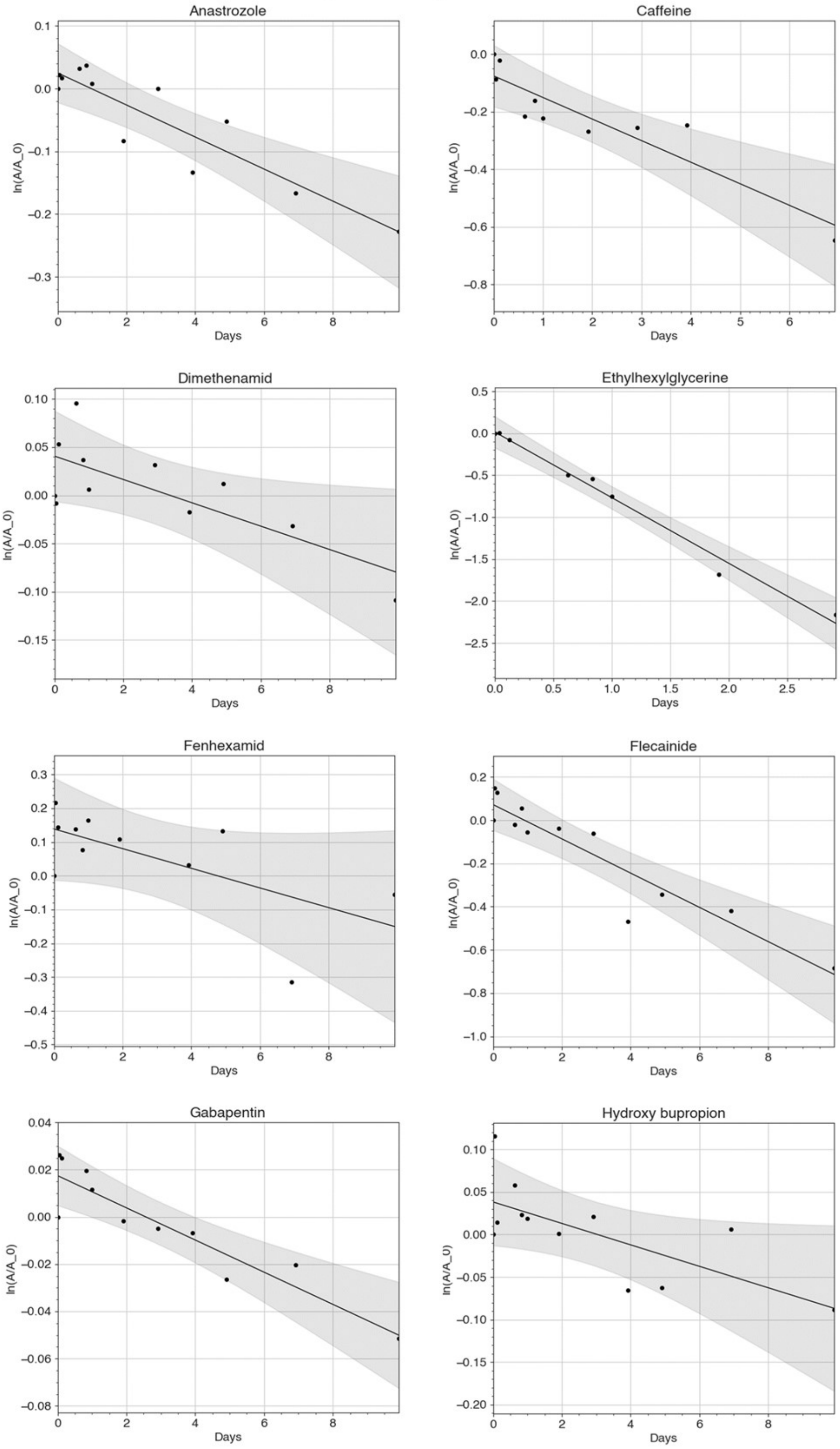
n) F5 replicate B



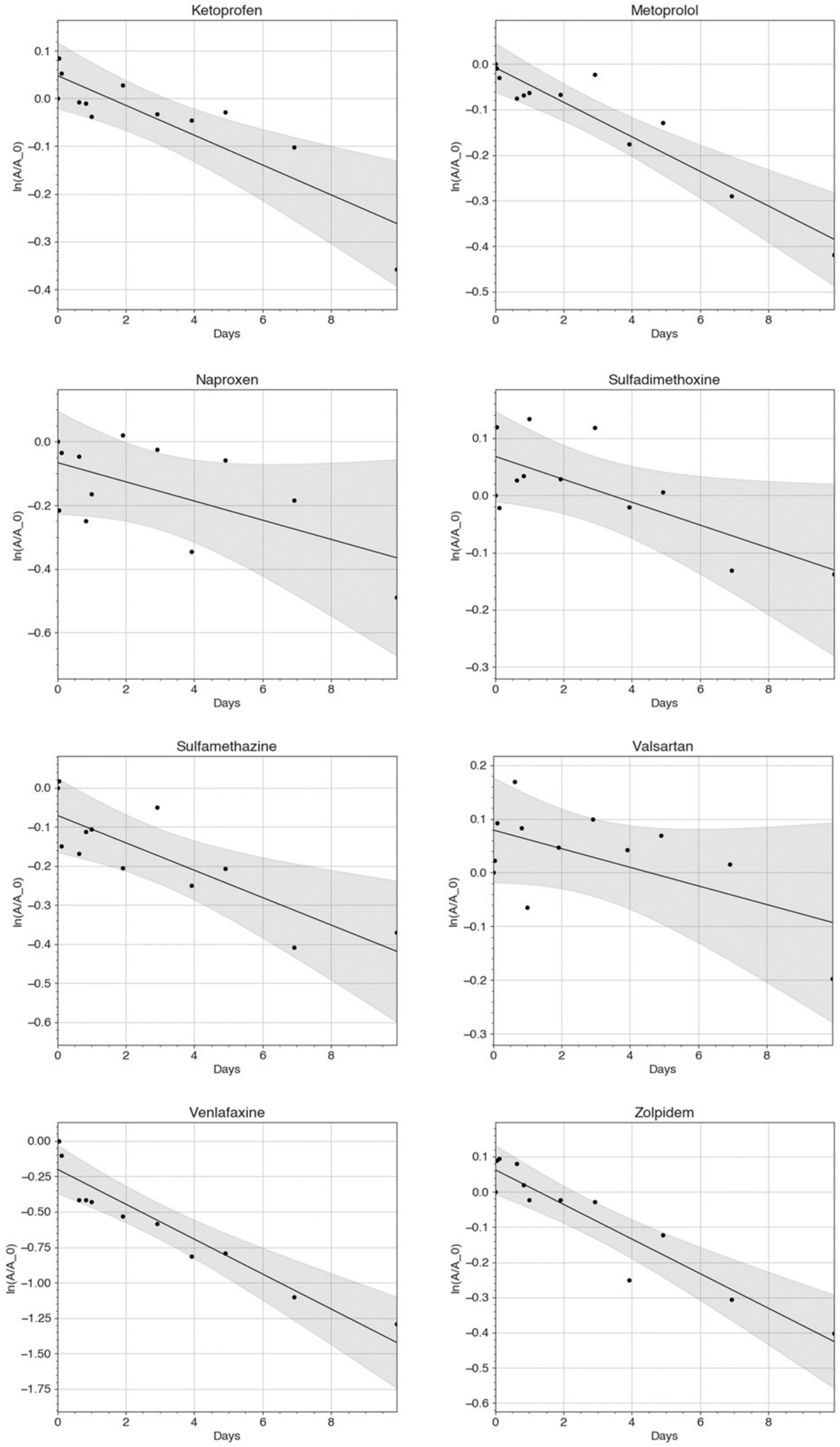
n) F5 replicate B (continued)



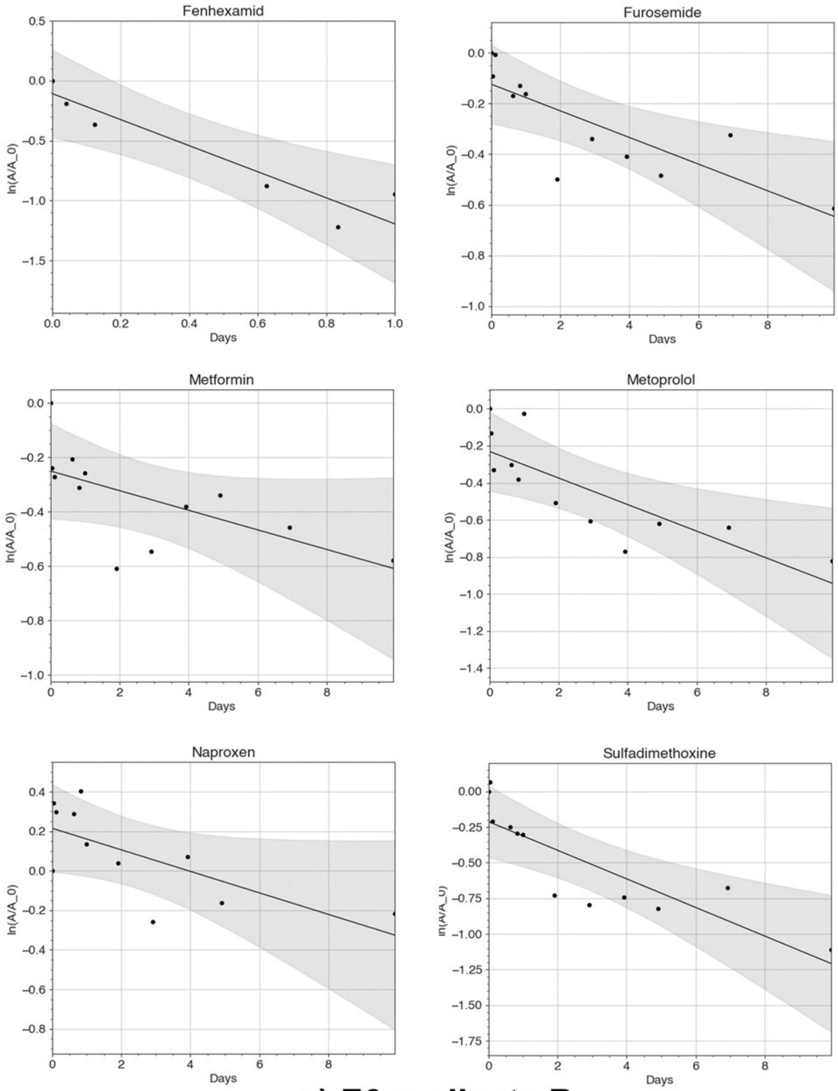
o) F5 replicate C



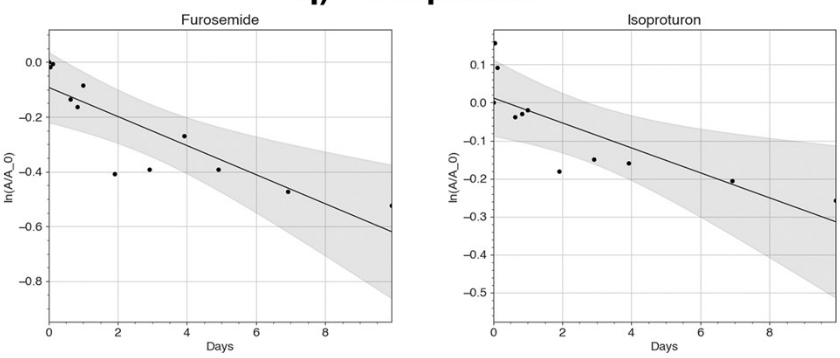
o) F5 replicate C (continued)



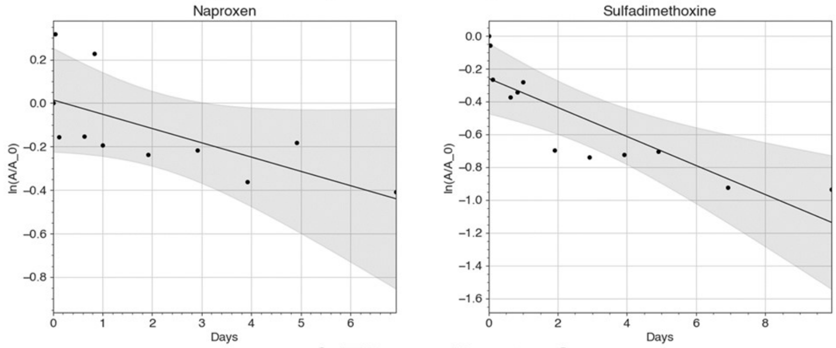
p) F6 replicate A



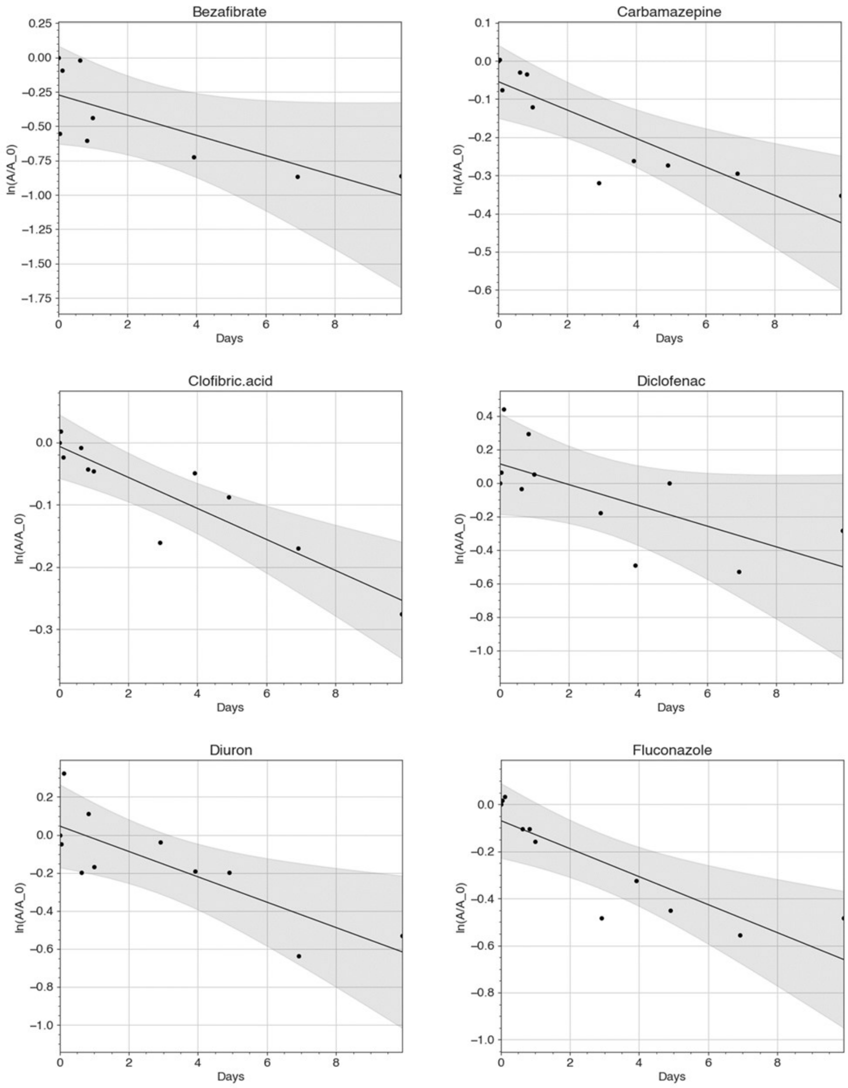
q) F6 replicate B



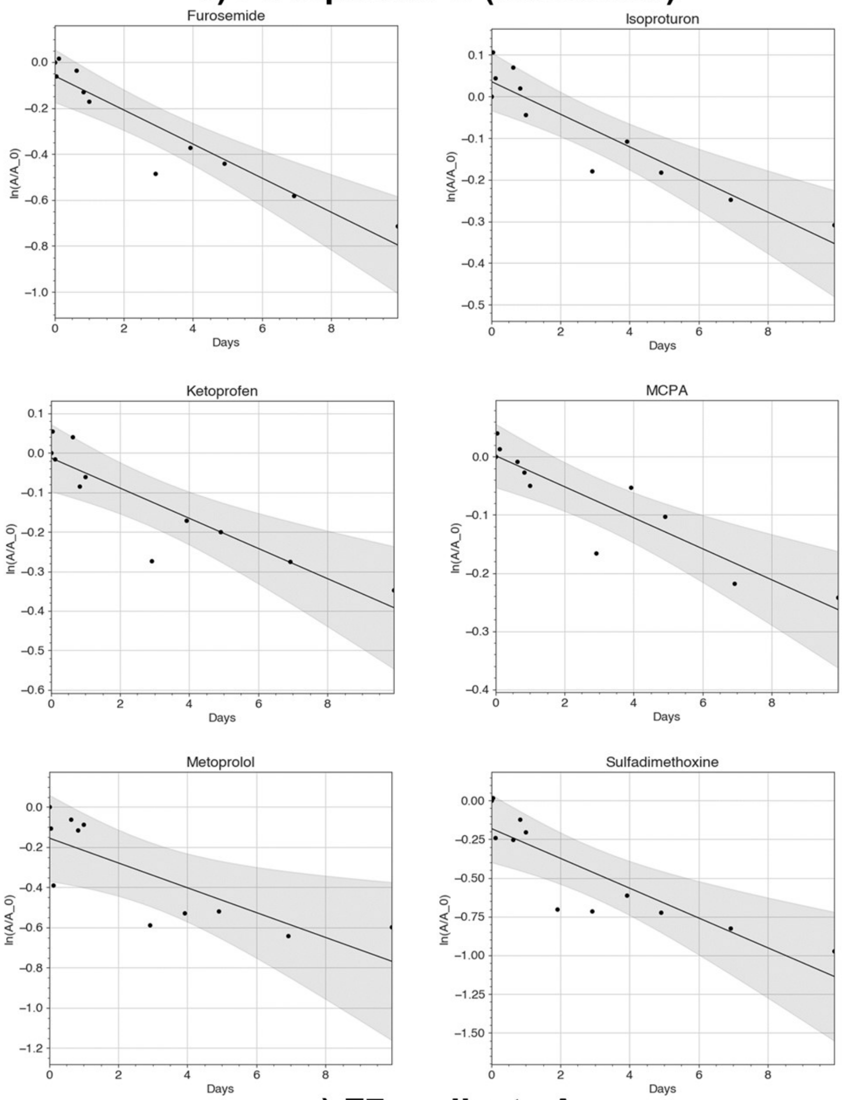
q) F6 replicate B (continued)



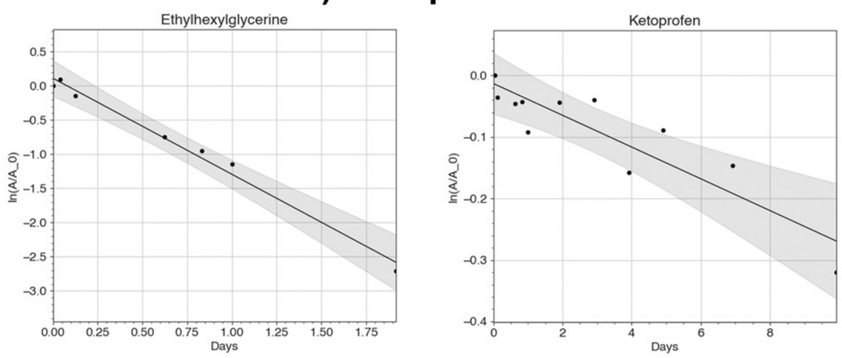
r) F6 replicate C



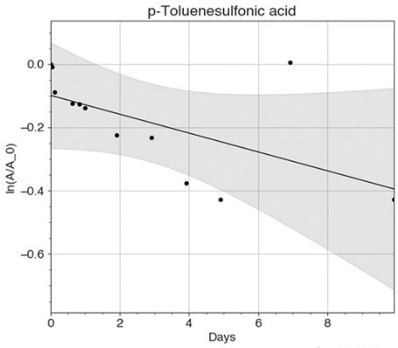
r) F6 replicate C (continued)



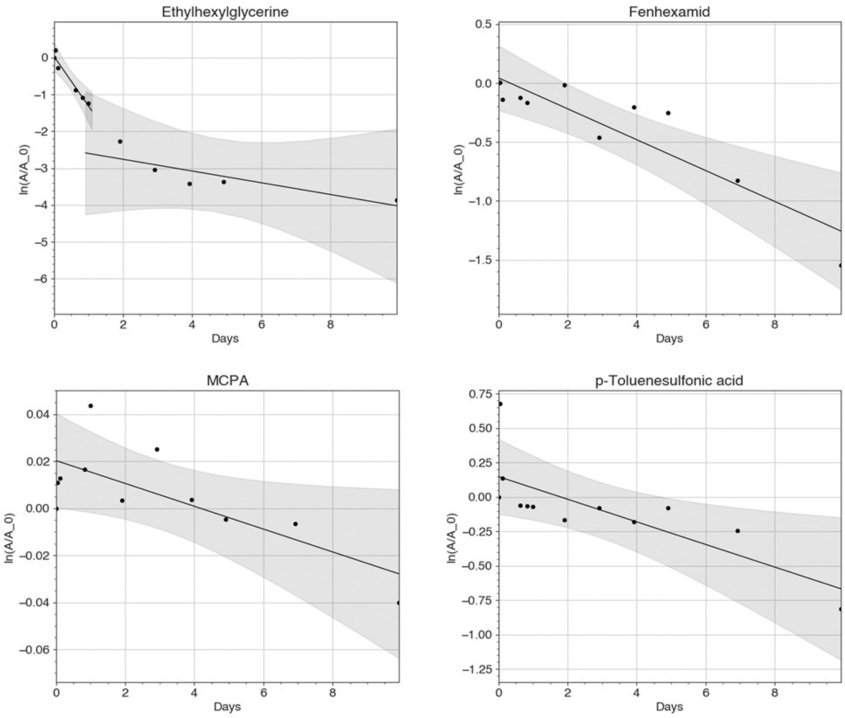
s) F7 replicate A



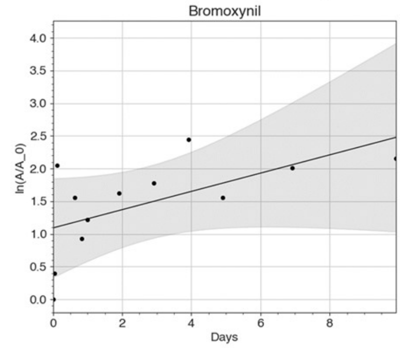
s) F7 replicate A (continued)

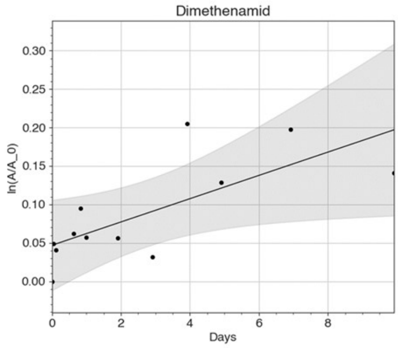


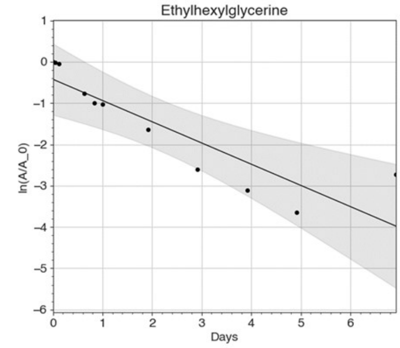
t) F7 replicate B

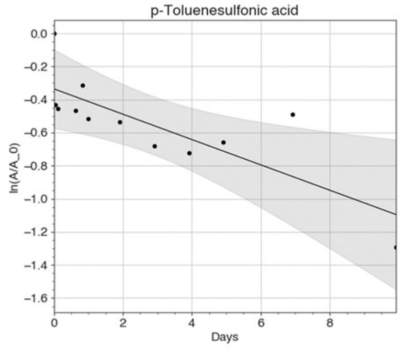


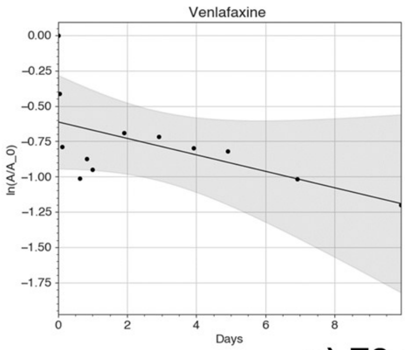
u) F7 replicate C



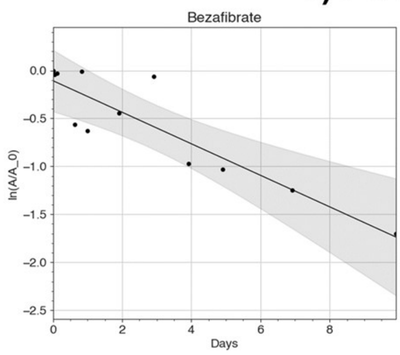


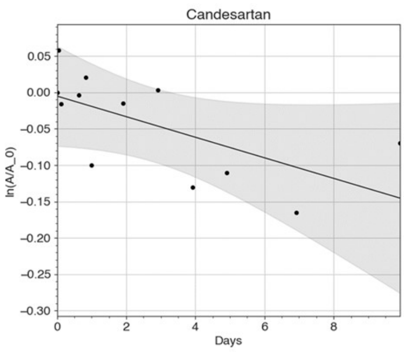




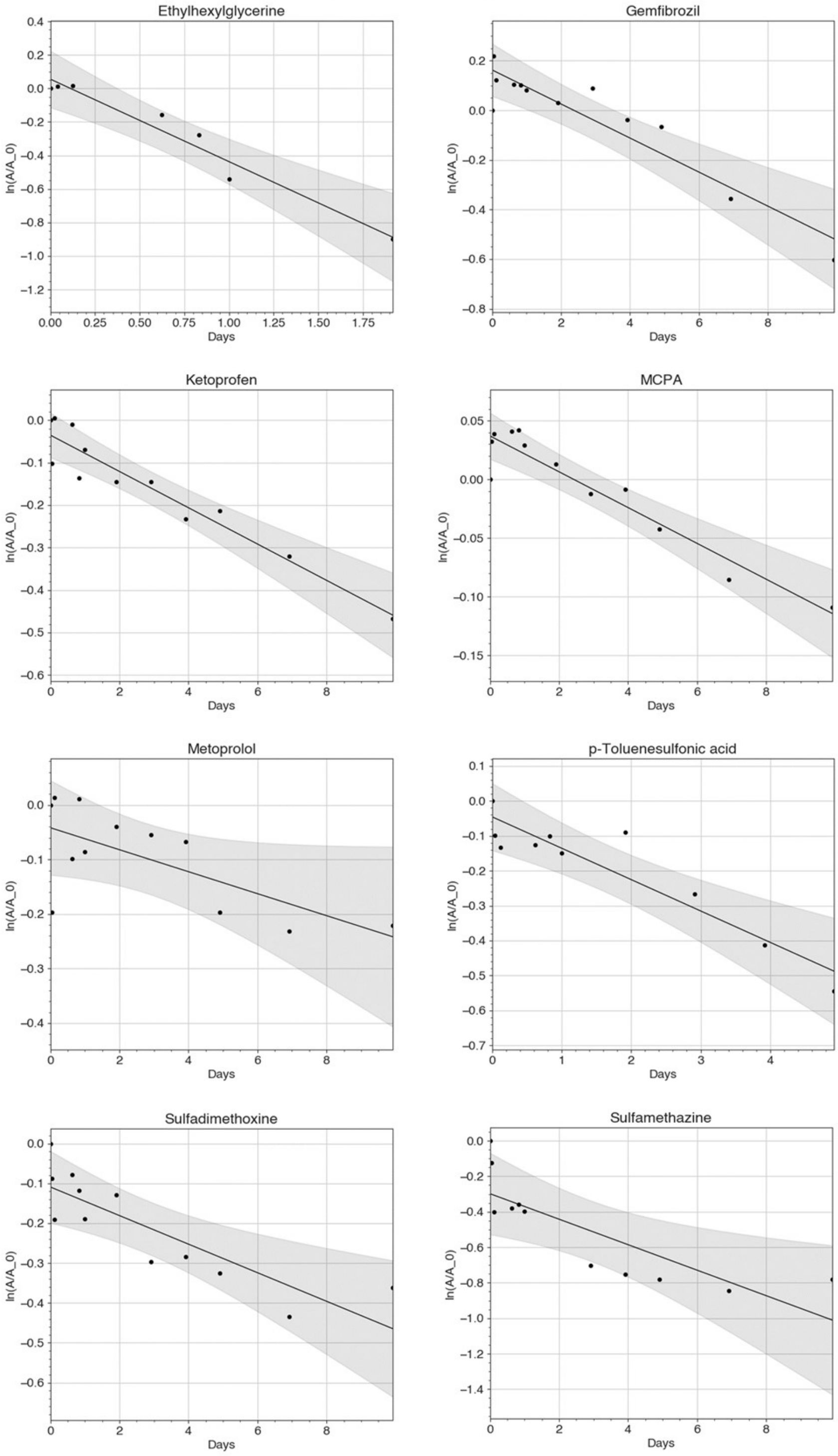


v) F8 replicate A

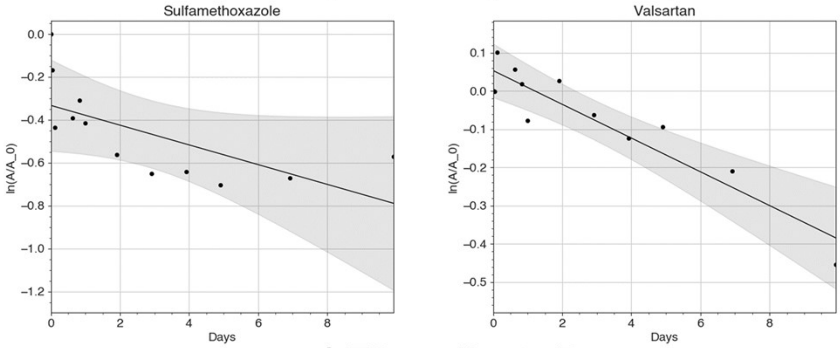




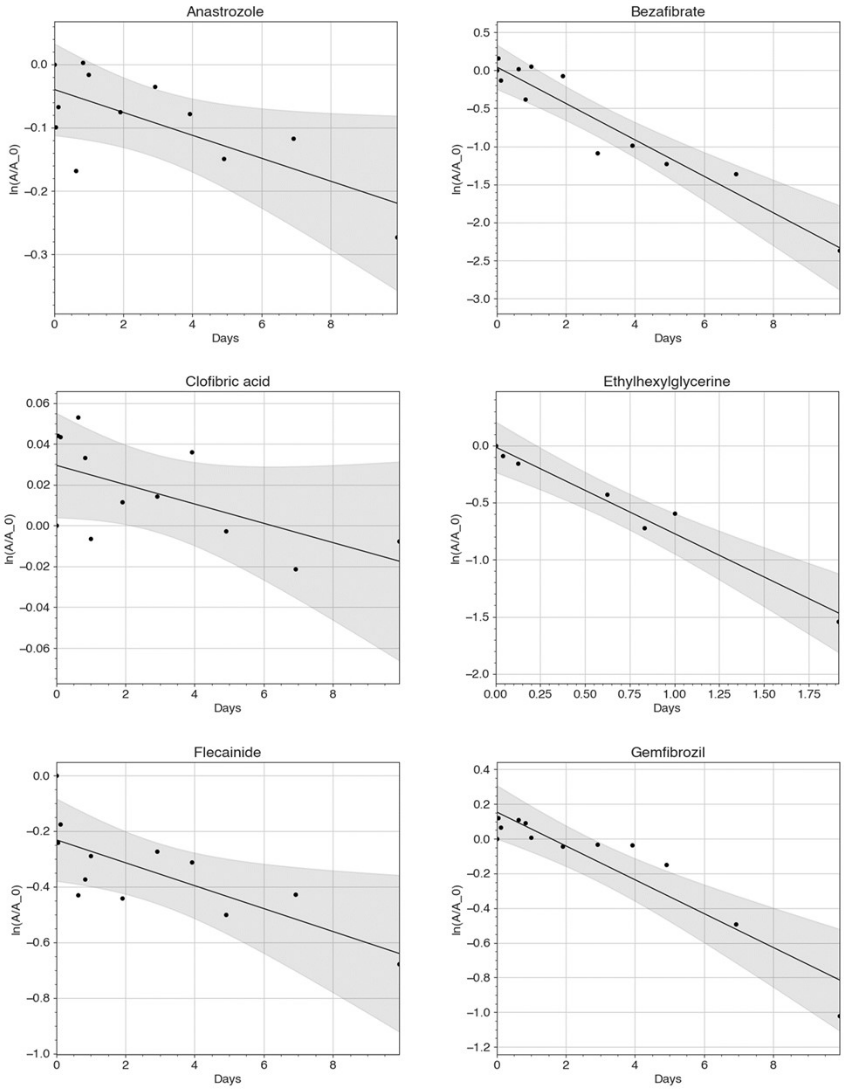
v) F8 replicate A (continued)



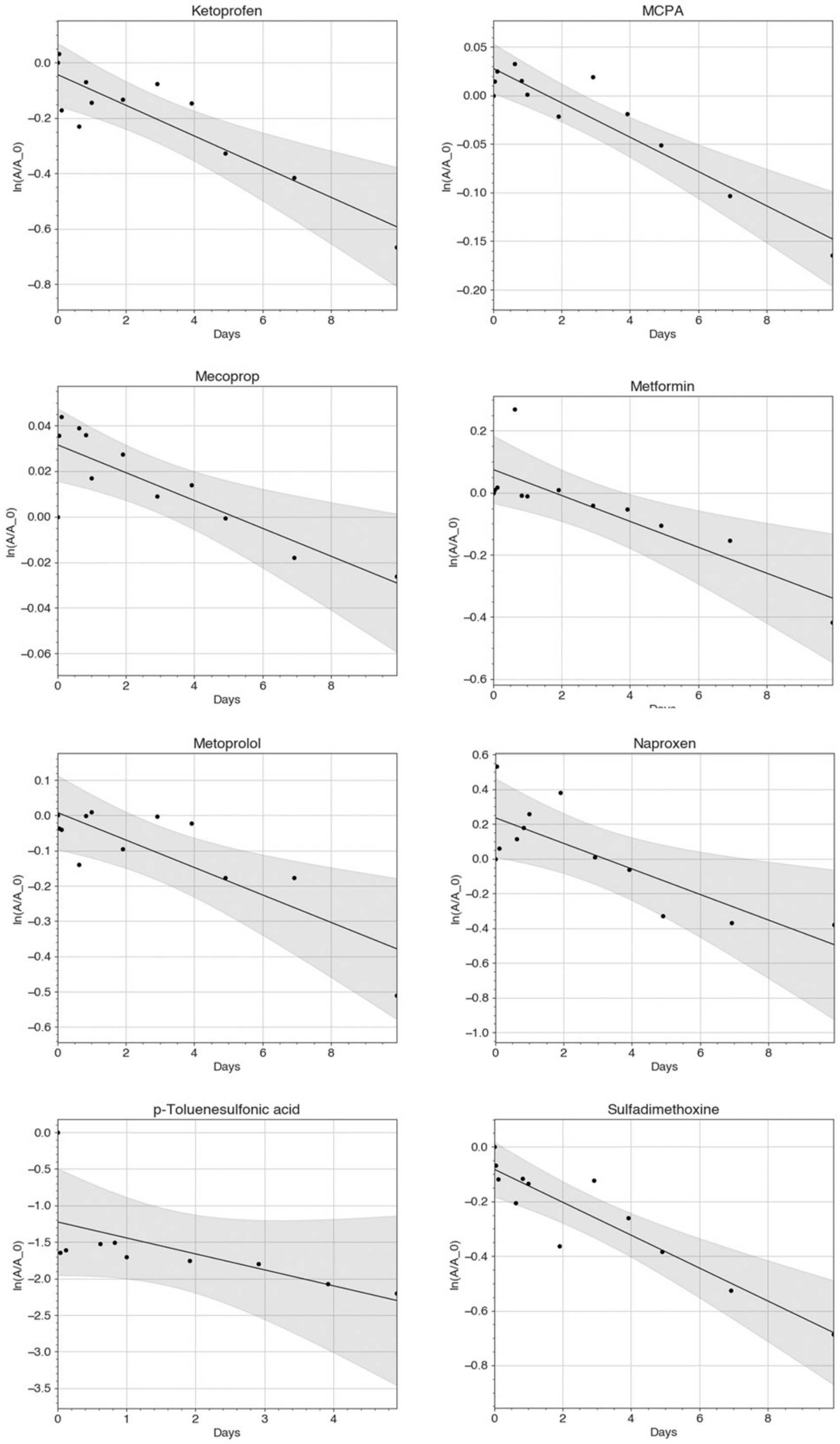
v) F8 replicate A (continued)



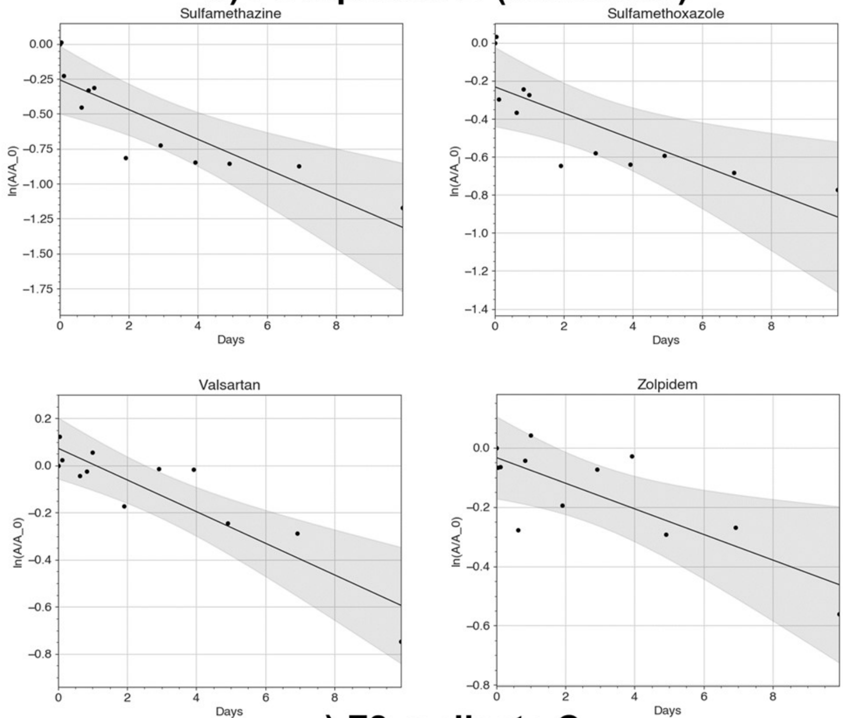
w) F8 replicate B



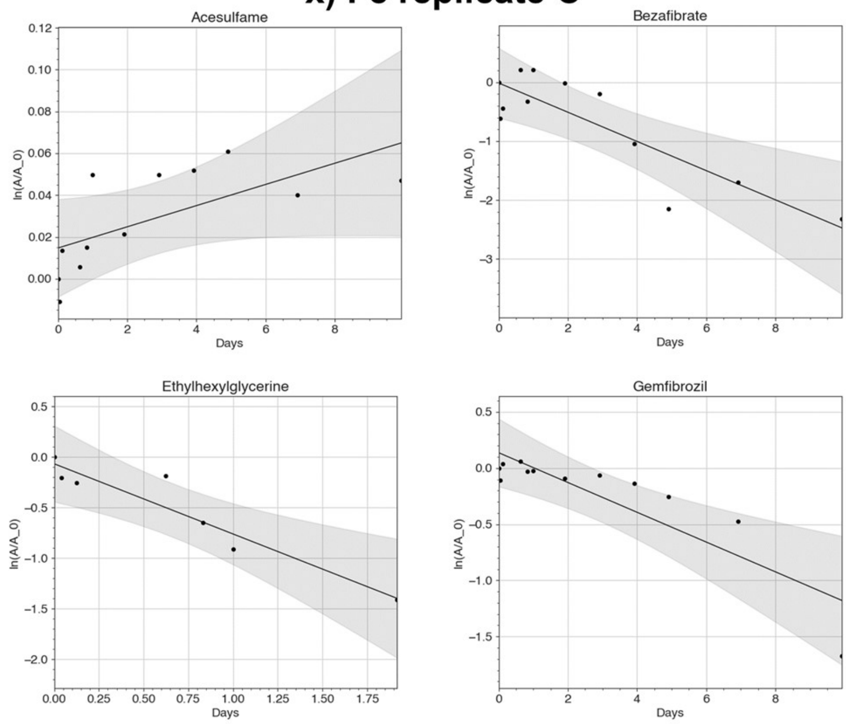
w) F8 replicate B (continued)



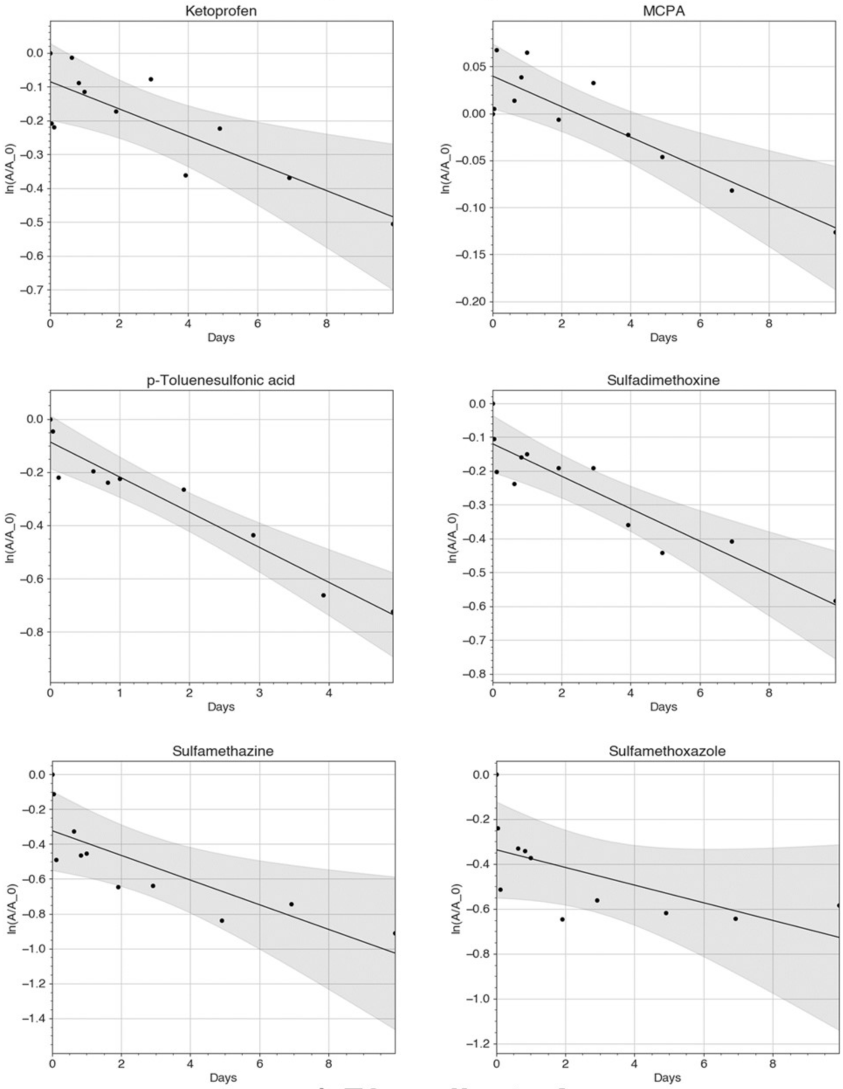
w) F8 replicate B (continued)



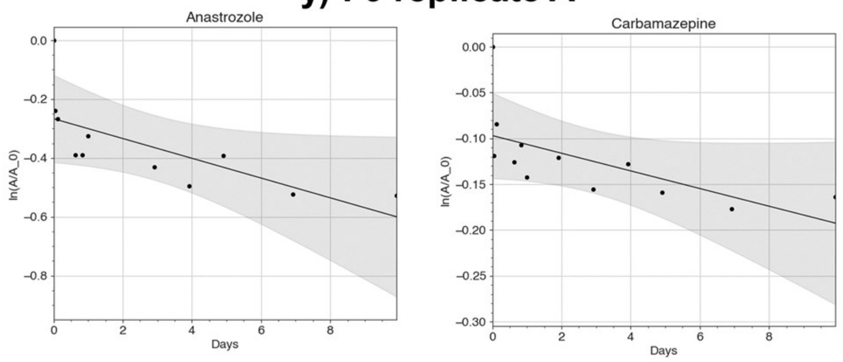
x) F8 replicate C



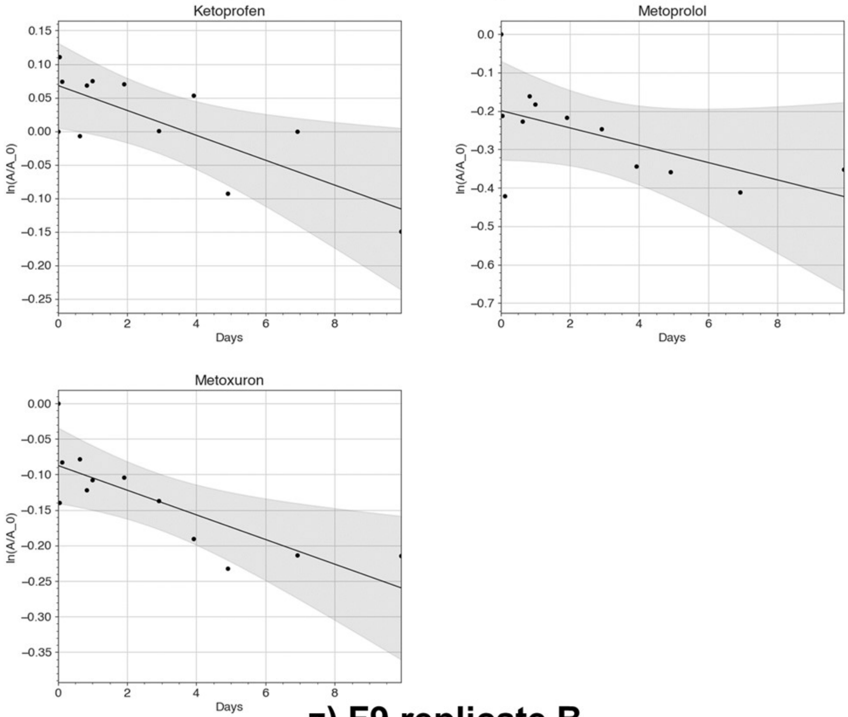
x) F8 replicate C (continued)



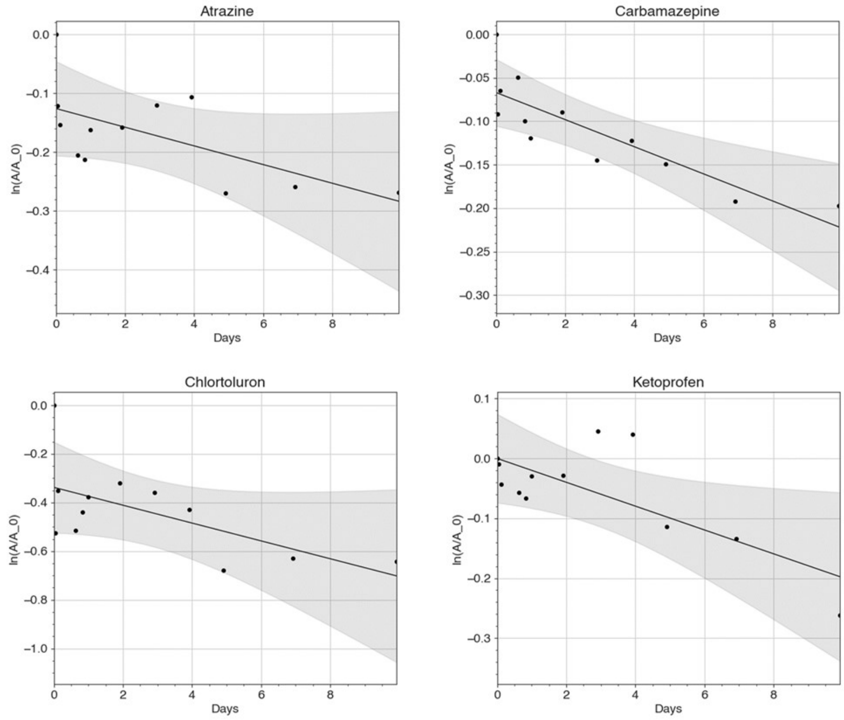
y) F9 replicate A



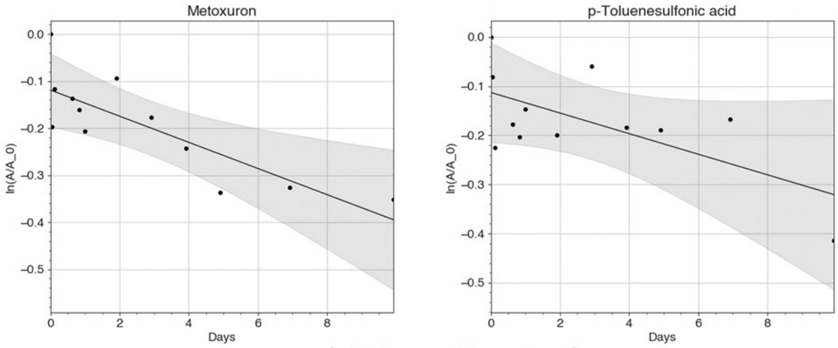
y) F9 replicate A (continued)



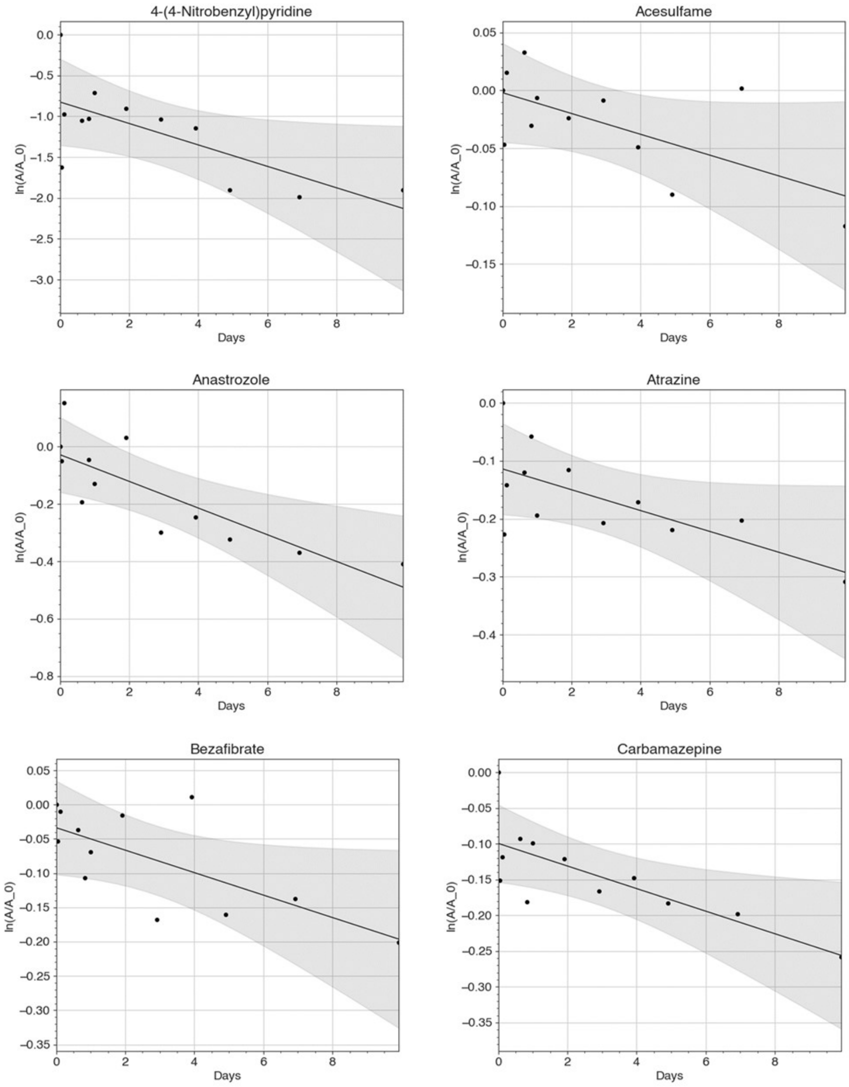
z) F9 replicate B



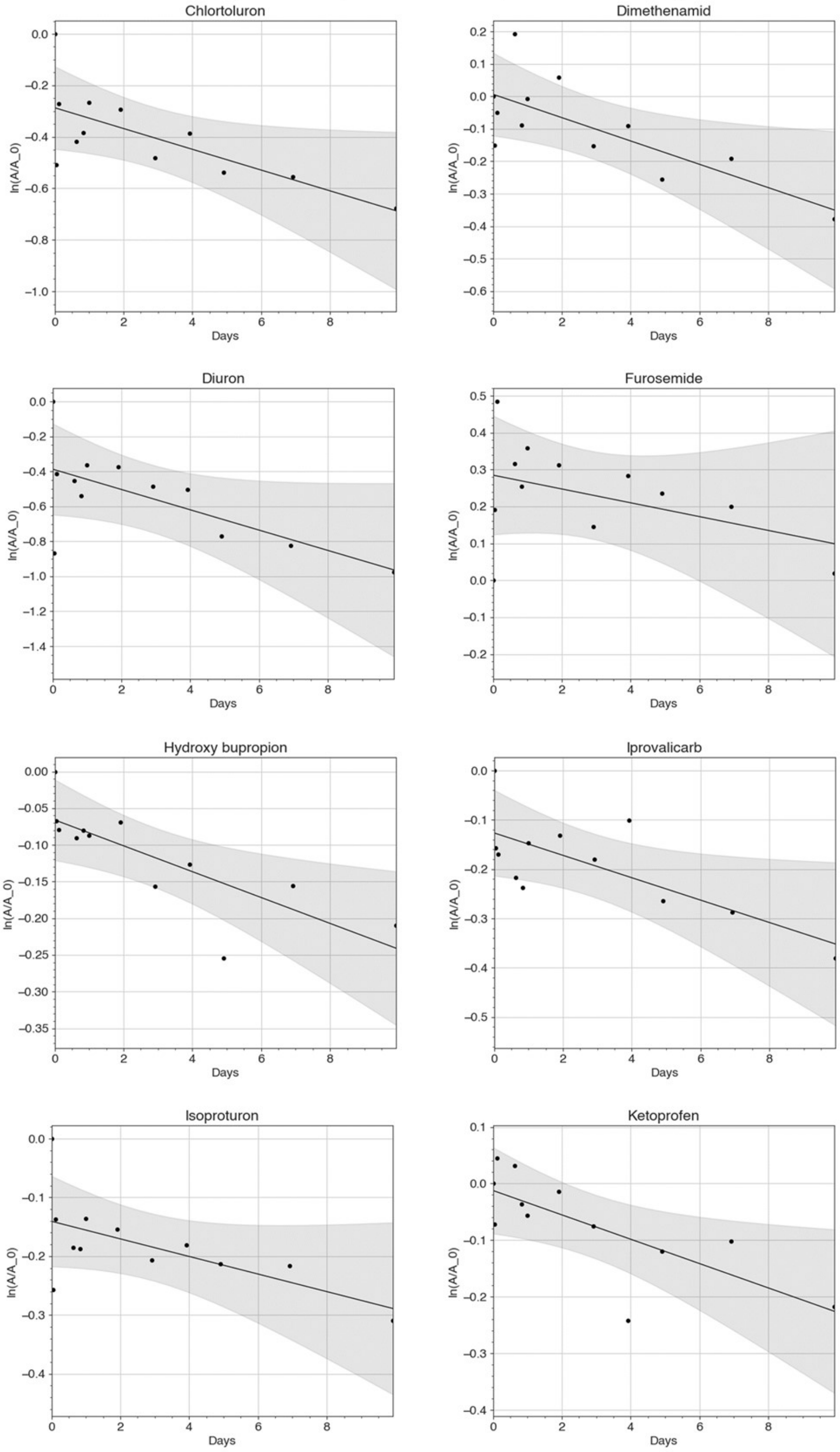
z) F9 replicate B (continued)



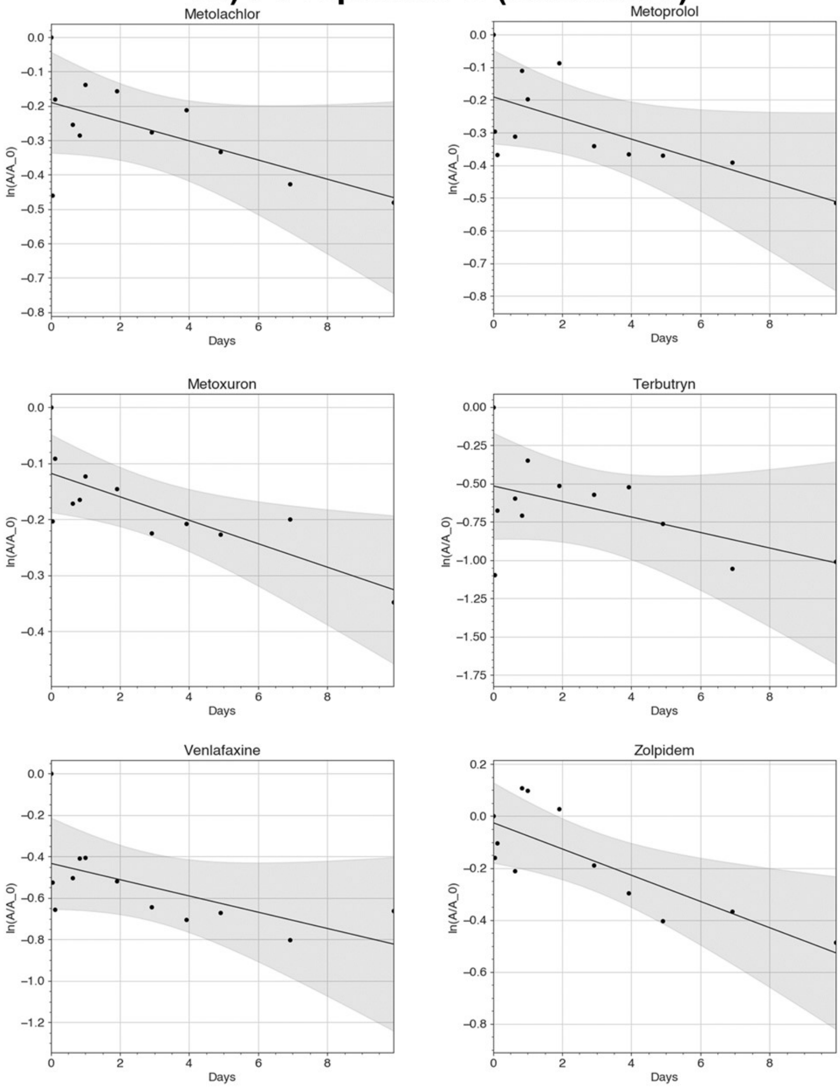
aa) F9 replicate C



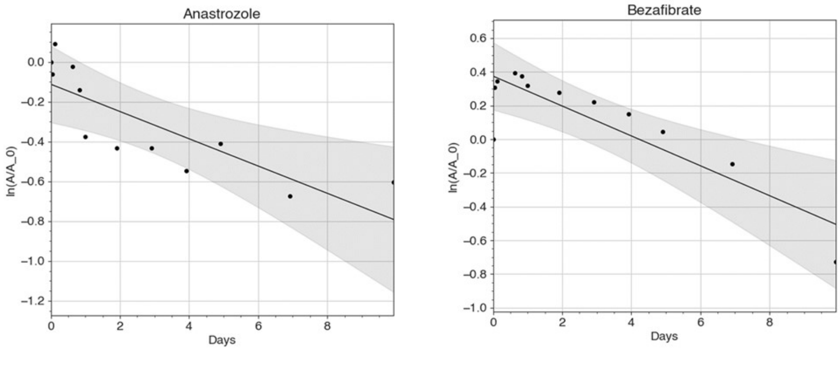
aa) F9 replicate C (continued)



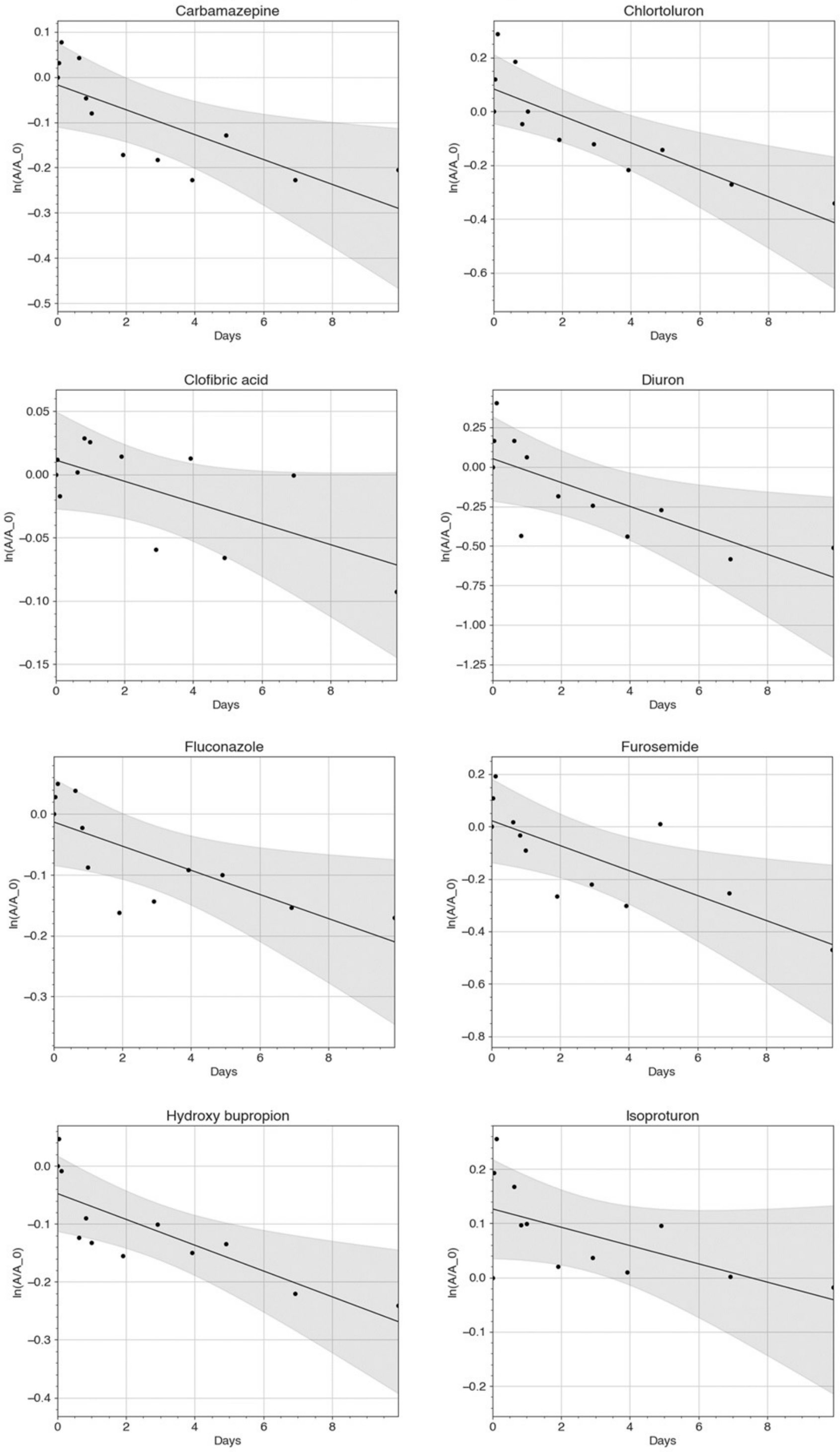
aa) F9 replicate C (continued)



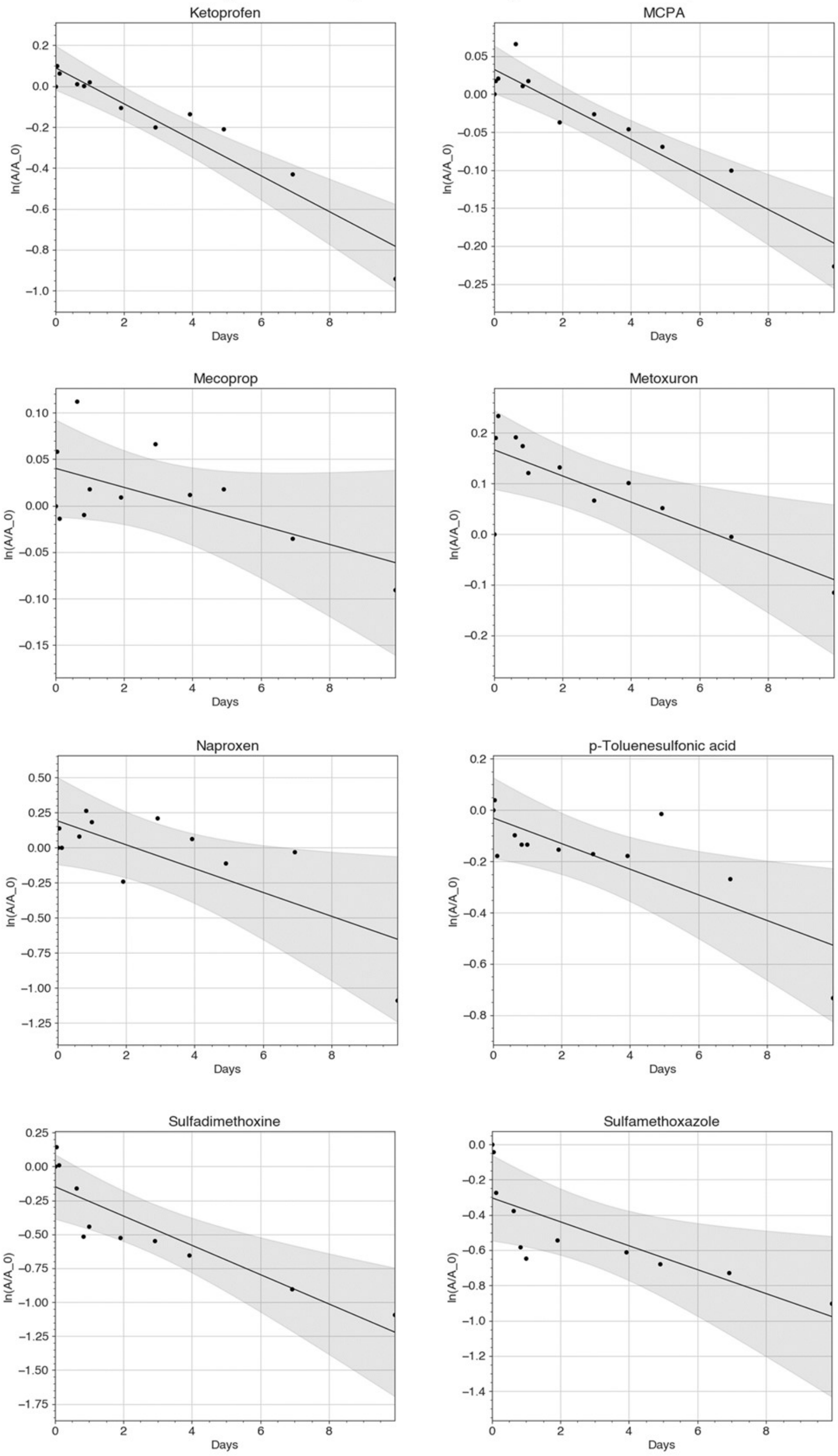
ab) F10 replicate A



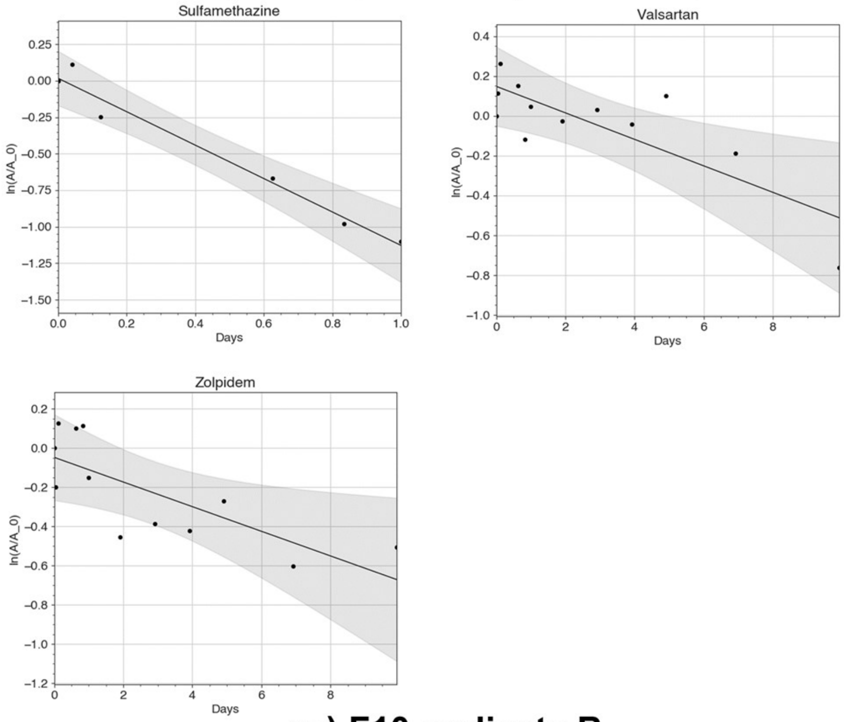
ab) F10 replicate A (continued)



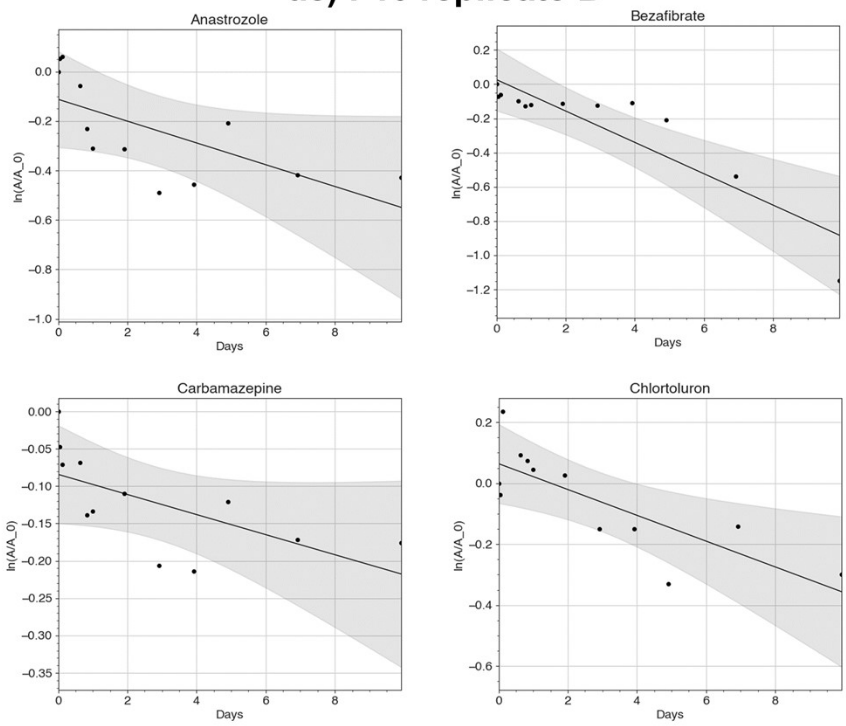
ab) F10 replicate A (continued)



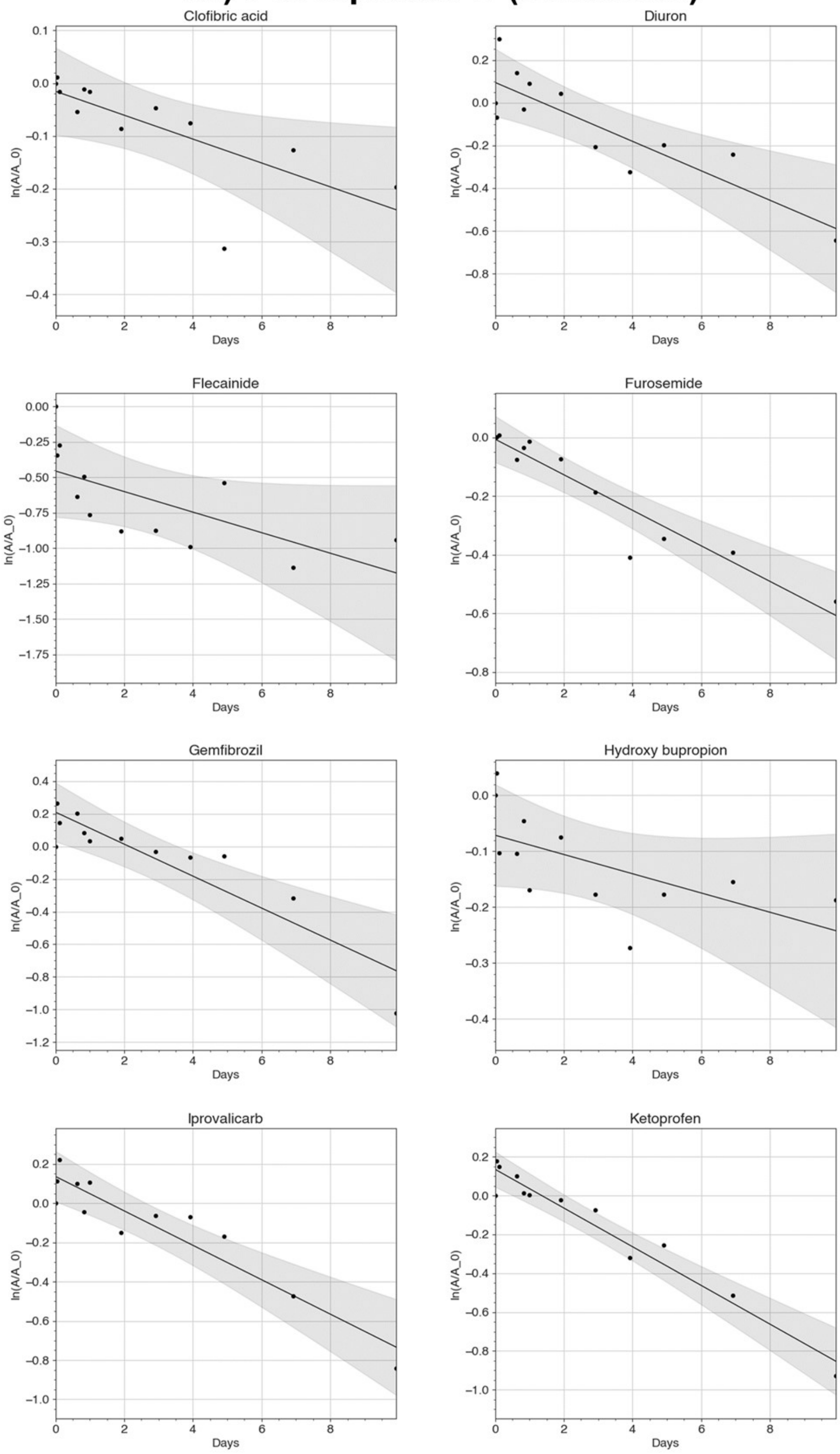
ab) F10 replicate A (continued)



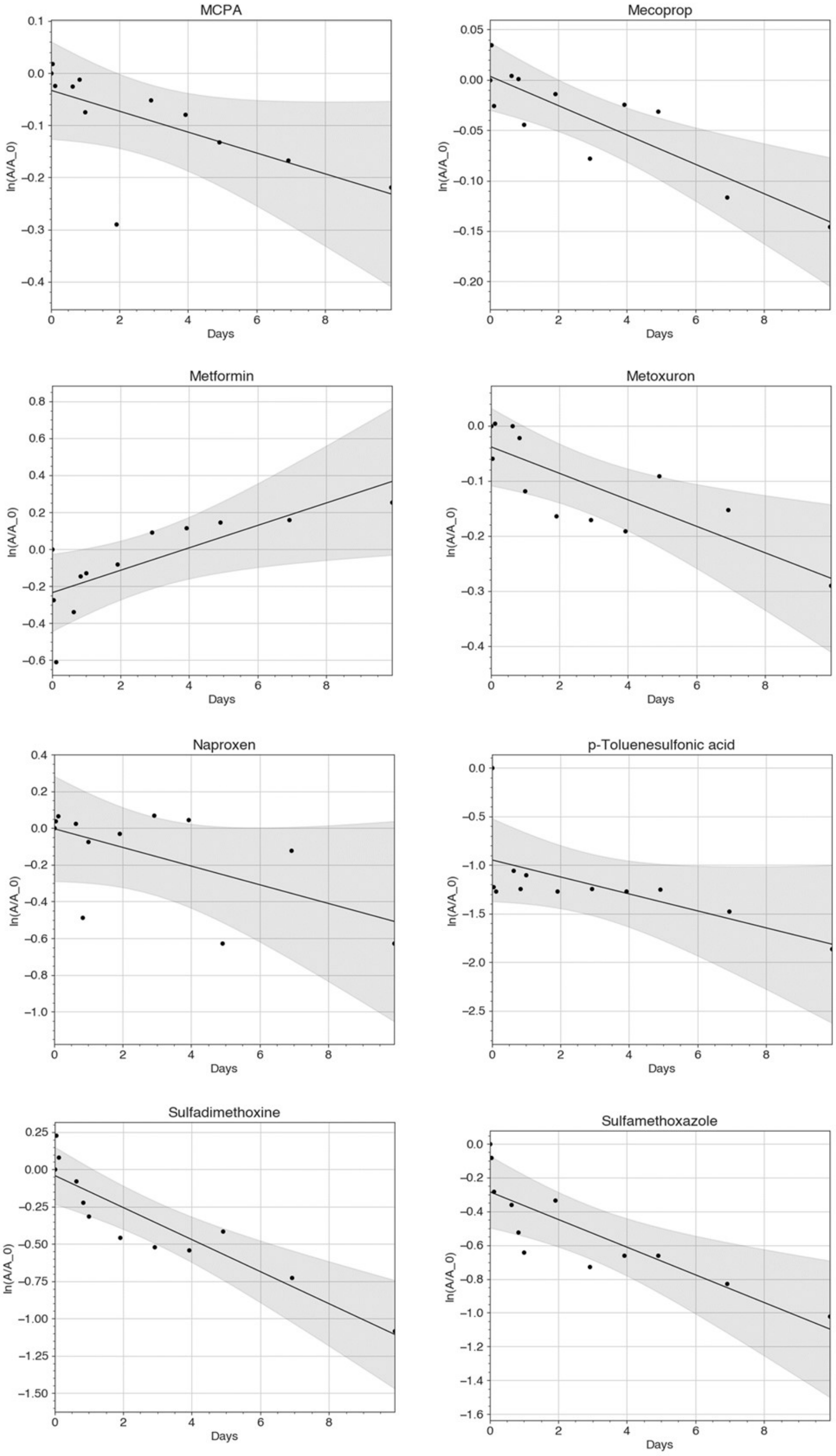
ac) F10 replicate B



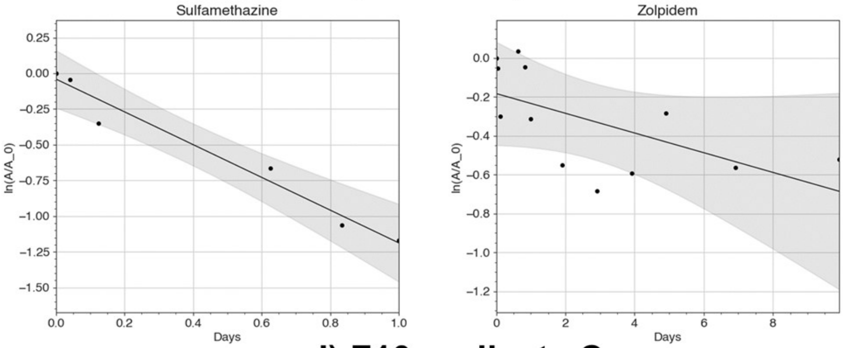
ac) F10 replicate B (continued)



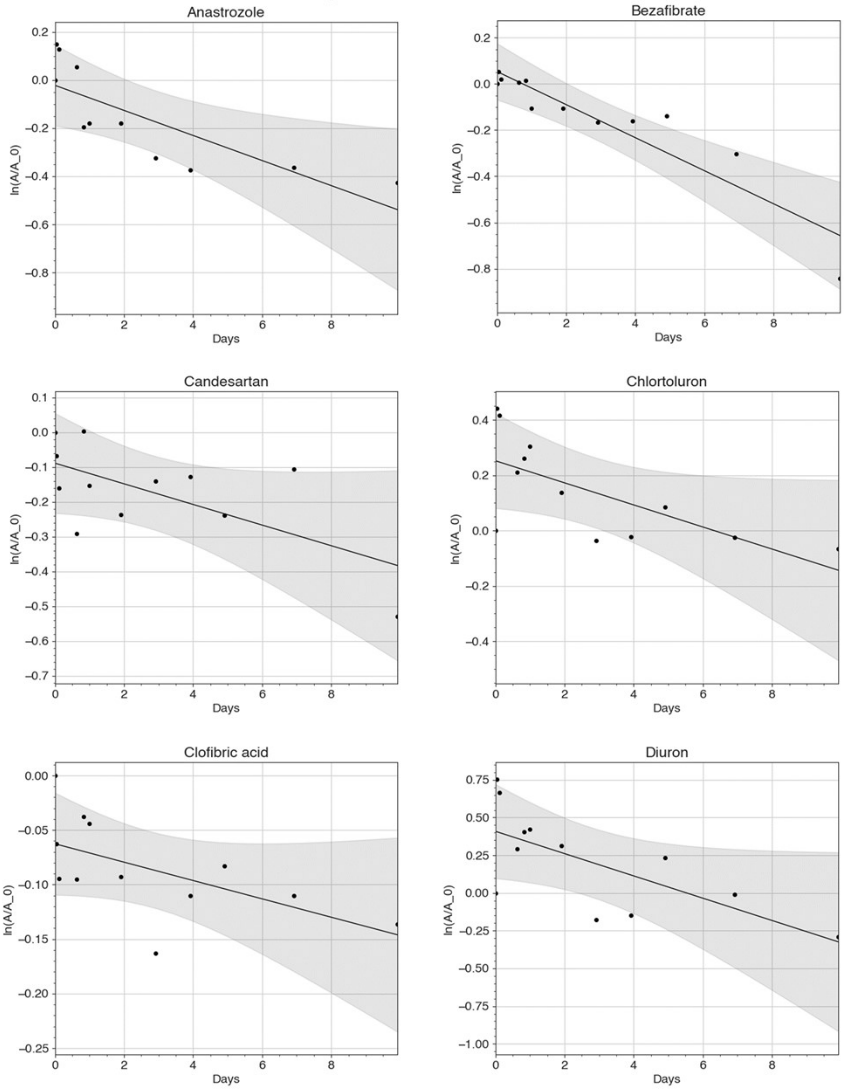
ac) F10 replicate B (continued)



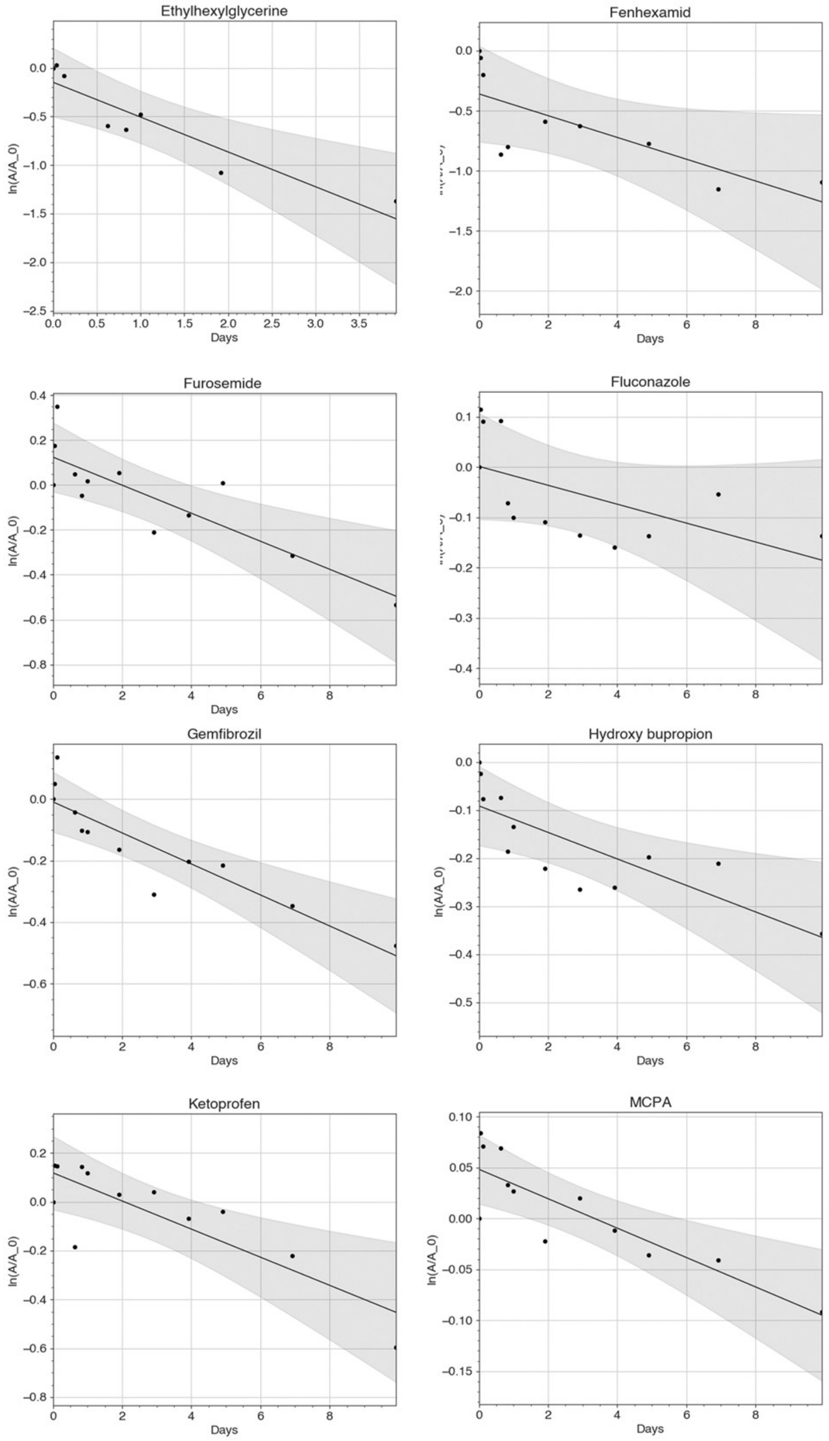
ac) F10 replicate B (continued)



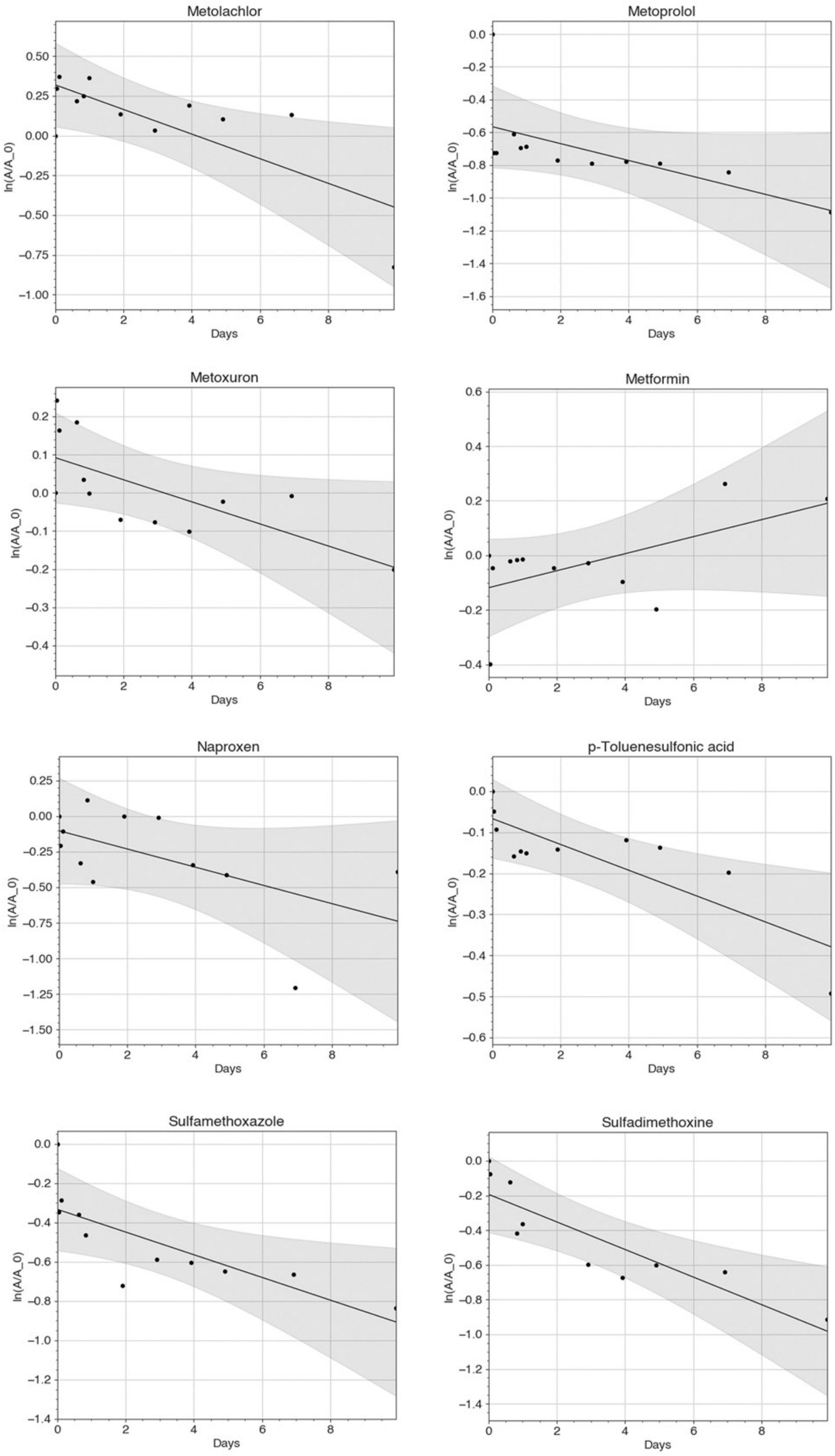
ad) F10 replicate C



ad) F10 replicate C (continued)



ad) F10 replicate C (continued)



ad) F10 replicate C (continued)

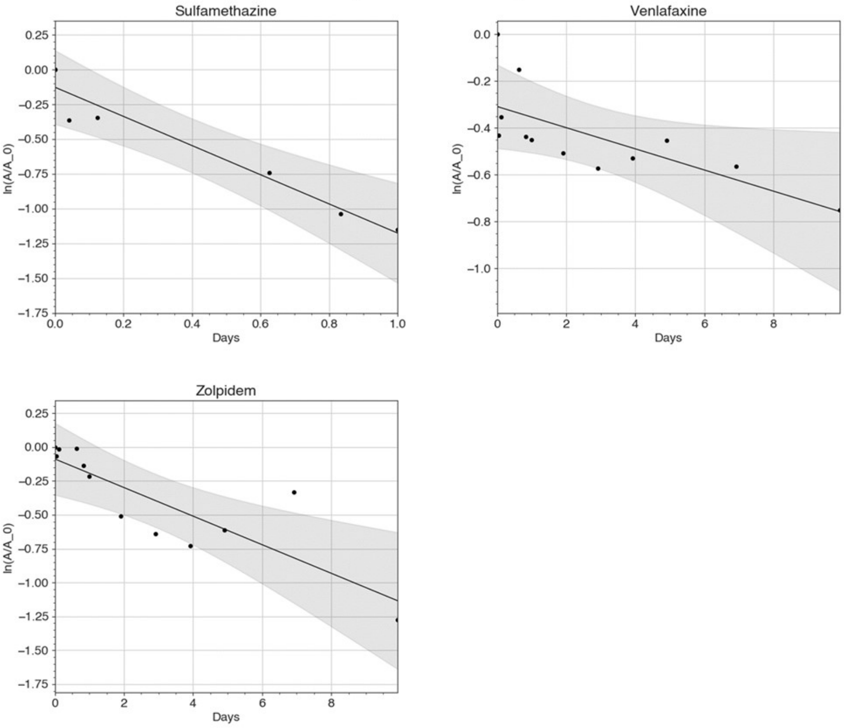
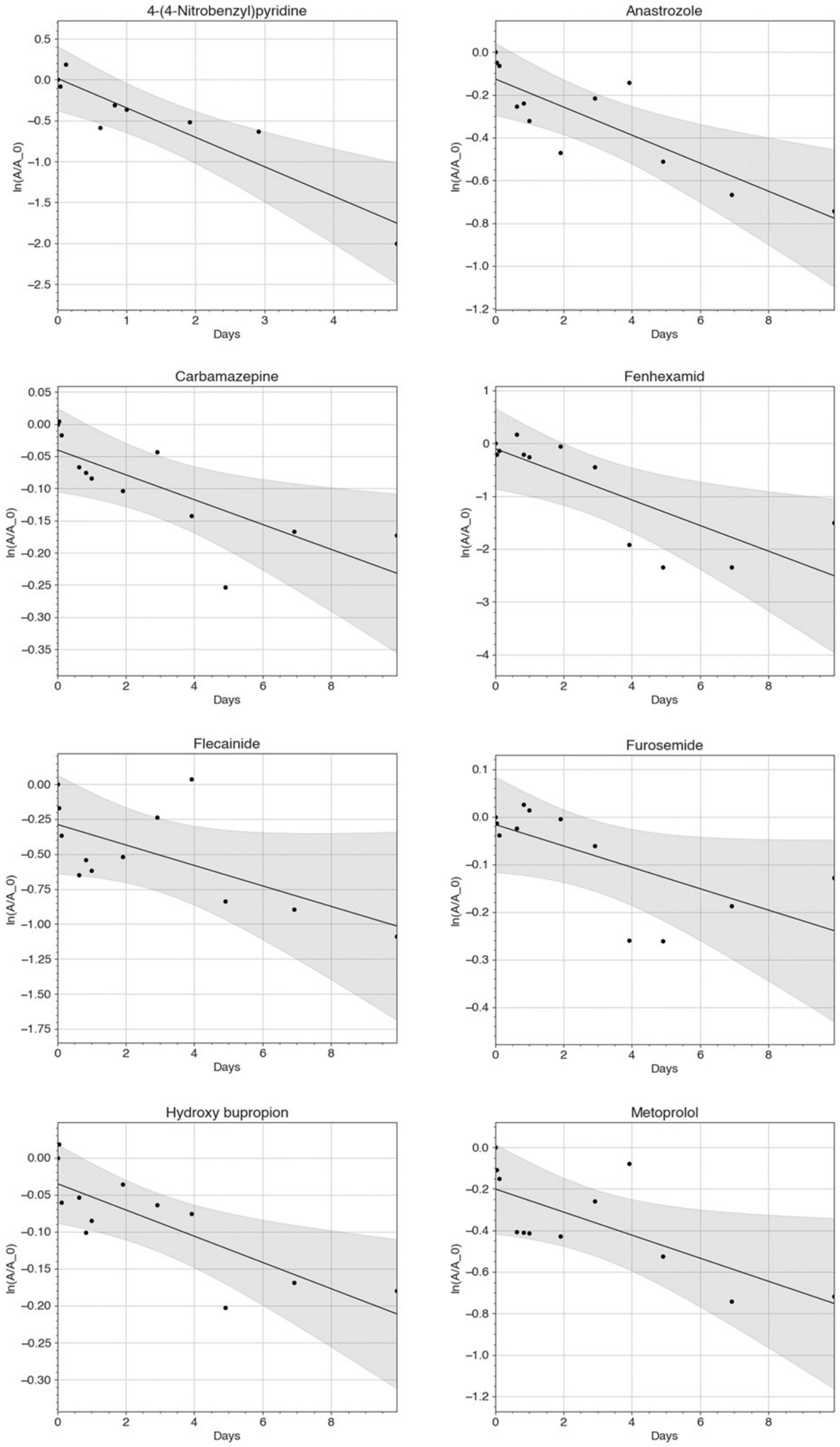


Figure S3. Relative peak area timeseries of the compounds with significant ($p < 0.05$) dissipation for each replicate. Shaded area represents 99% confidence interval of the slope.

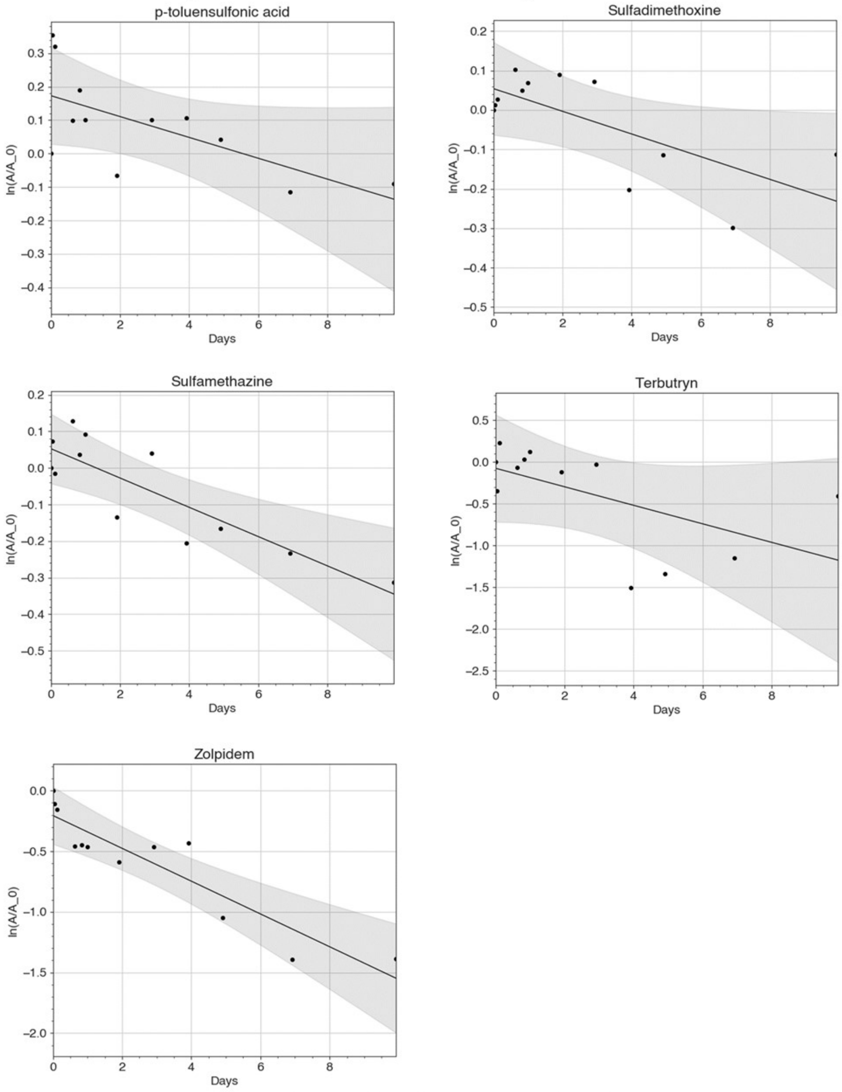
S2.4 Dissipation in abiotic controls

Some dissipation in at least one abiotic control was observed for 19 of the tested compounds. However, no compound dissipated in more than 3/5 abiotic controls, with most (11) compounds showing dissipation in only a single control. Combined with the fact that several of the compounds dissipating in the abiotic controls had very low log D_{ow} (e.g., metoprolol, sulfadimethoxine, acesulfame), while some compounds that didn't dissipate in any abiotic control had a relatively high log Dow (e.g., iprovalicarb, dimethenamid) leads us to suspect this dissipation might be the result of residual biodegradation due to unsuccessful sterilization rather than sorption. Residual biodegradation was noted as a problem in a previous version of the modified OECD 309 method with sodium azide as the sterilization tool[4]. Autoclaving was attempted for this study as an alternative sterilization tool, but has since been noted here as well as in other not yet published experiments to appear unsuccessful at fully sterilizing the controls. Still, for the few compounds with a high log D_{ow} that dissipated in several sorption controls (e.g Anastrozole, Zolpidem) sorption may have played a role.

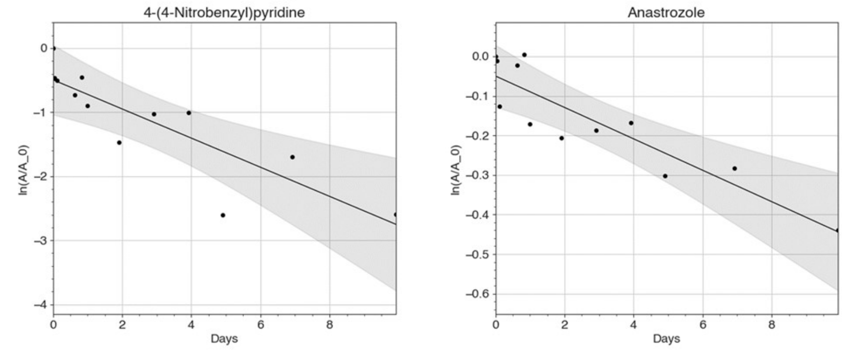
a) F1 Abiotic control



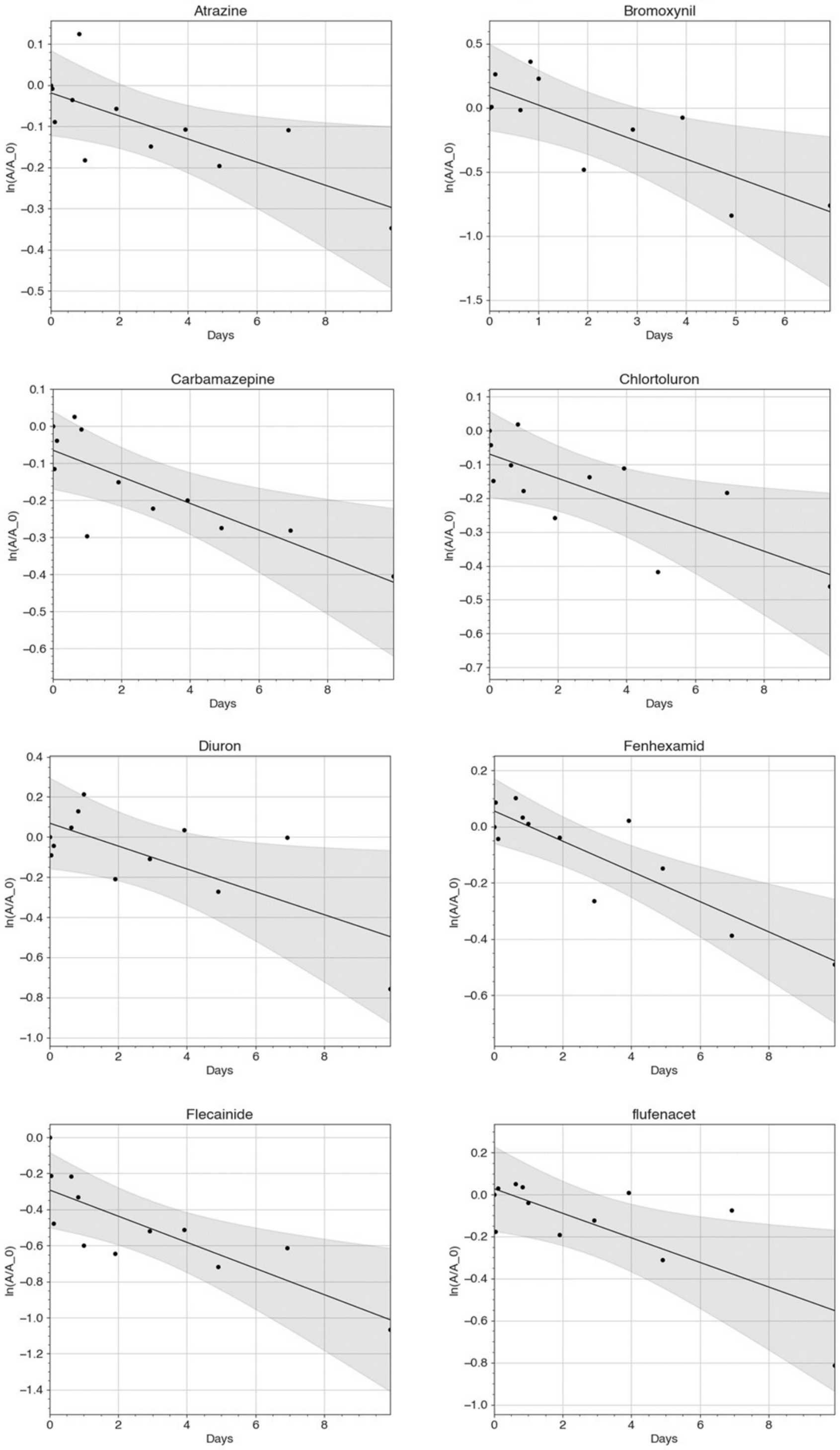
b) F1 Abitoic control (continued)



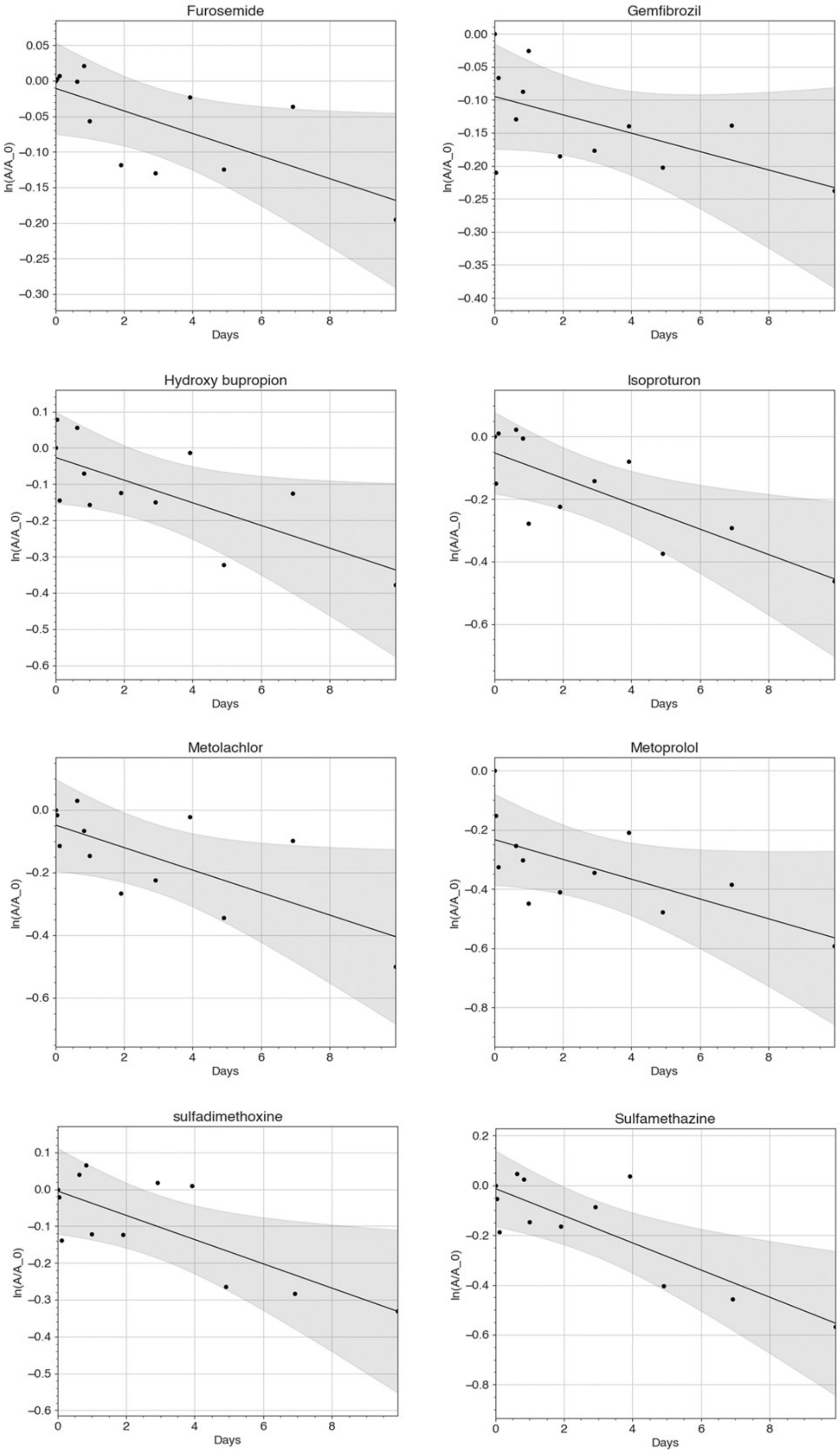
a) F2 Abitoic control



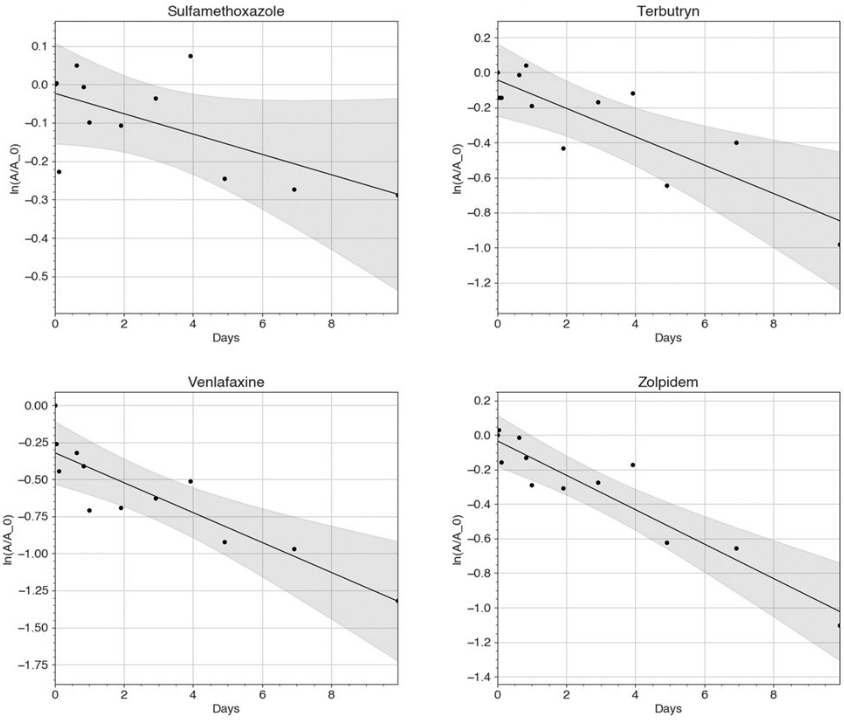
b) F2 Abiotic control (continued)



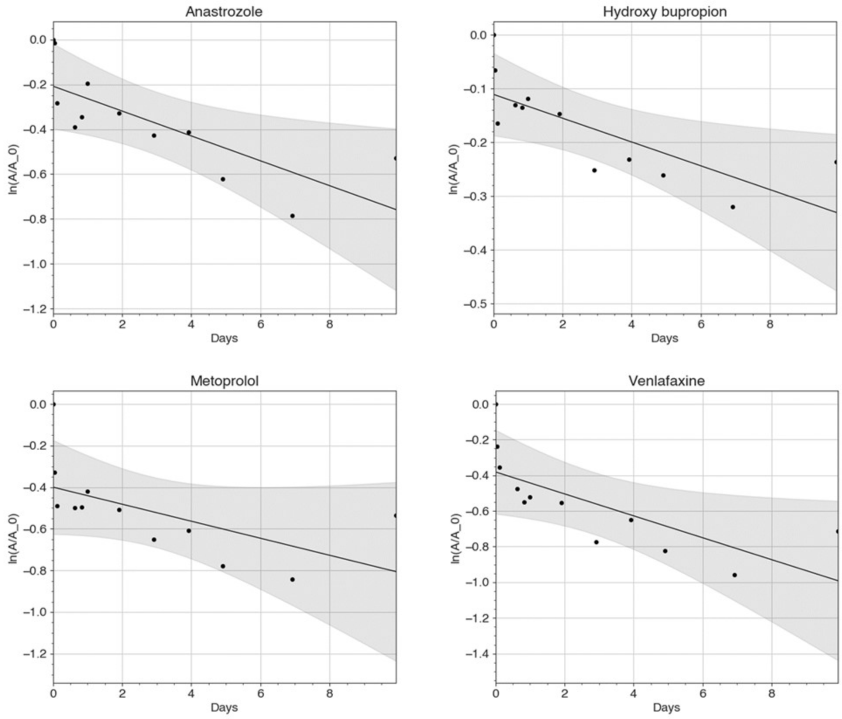
b) F2 Abiotic control (continued)



b) F2 Abiotic control (continued)



b) F9 Abiotic control



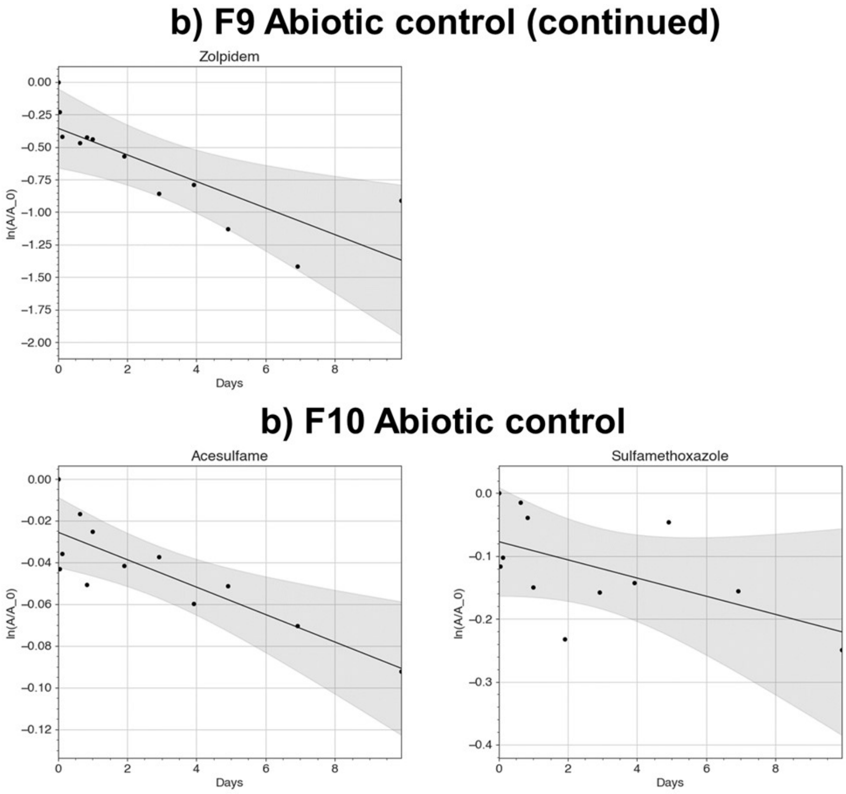


Figure S4. Relative peak area timeseries of the compounds with significant ($p < 0.05$) dissipation in each abiotic control. No compound had significant dissipation in the abiotic control of site F8. Shaded area represents 99% confidence interval of the slope.

S3. References

1. Tian, R., Posselt, M., Fenner, K. & McLachlan, M. S. Increasing the Environmental Relevance of Biodegradation Testing by Focusing on Initial Biodegradation Kinetics and Employing Low-Level Spiking. *Environ. Sci. Technol. Lett.* **10**, 40–45 (2023).
2. Tian, R., Posselt, M., Miaz, L. T., Fenner, K. & McLachlan, M. S. Influence of Season on Biodegradation Rates in Rivers. *Environ. Sci. Technol.* **58**, 7144–7153 (2024).
3. Brunius, C., Shi, L. & Landberg, R. Large-scale untargeted LC-MS metabolomics data correction using between-batch feature alignment and cluster-based within-batch signal intensity drift correction. *Metabolomics Off. J. Metabolomic Soc.* **12**, 173 (2016).
4. Weir, L. M., Tian, R., Posselt, M., Mueller, J. F. & McLachlan, M. S. From Freshwater to

Marine Environments: Spatial Variation in Chemical Biodegradation Rates Applying a Modified OECD 309-Type Experiment. *Environ. Sci. Technol.* **60**, 1141–1152 (2026).