



Supplementary Material

Degradation of a New Herbicide Florpyrauxifen-benzyl in Water: Kinetics, Various Influencing Factors and Its Reaction Mechanisms

Rendan Zhou ¹, Zemin Dong ^{1,2}, Long Wang ¹, Wenwen Zhou ³, Weina Zhao ², Tianqi Wu ¹, Hailong Chang ¹, Wei Lin ¹ and Baotong Li ^{1,*}

Table S1. Temperature effect coefficient (Q), activation energy (E_a), activation enthalpy (ΔH), activation entropy (ΔS) and Gibbs free energy (ΔG) of florpyrauxifen-benzyl hydrolysis.

Temperatur e/K	Rate Constant (k)/d ⁻¹	Q	E_a / kJ mol ⁻¹	ΔH / kJ mol ⁻¹	ΔS / kJ (mol K) ⁻¹	ΔG / kJ mol ⁻¹
288	0.0086	/	140.0197	137.6253	0.2960	52.3798
298	0.0529	6.1739	140.0197	137.5421	0.2957	49.4213
308	0.3573	6.7530	140.0197	137.4590	0.2954	46.4656
323	4.6981	/	140.0197	137.3343	0.2950	42.0371

Table S2. Information on the disposable face masks (DFMs).

Brand	Mass/g	Retail Price/CNY ^a	Production Date	Executive Standard	Materials
JIEMIAN	2.8126~2.9325	0.3	2022.03	YY0469-2011	PP/PET
Size / cm	Color				
17.5× 9.5- three layers	Blue/White				

Note: a: We divided the total purchase price by the number of the masks.

Table S3. Composition of artificial seawater.

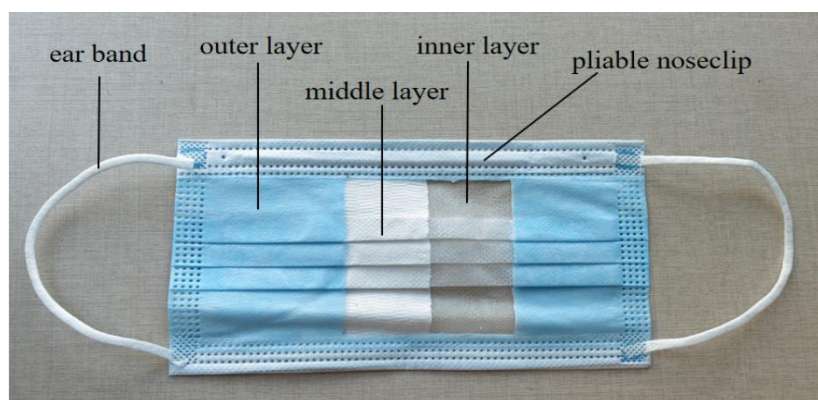
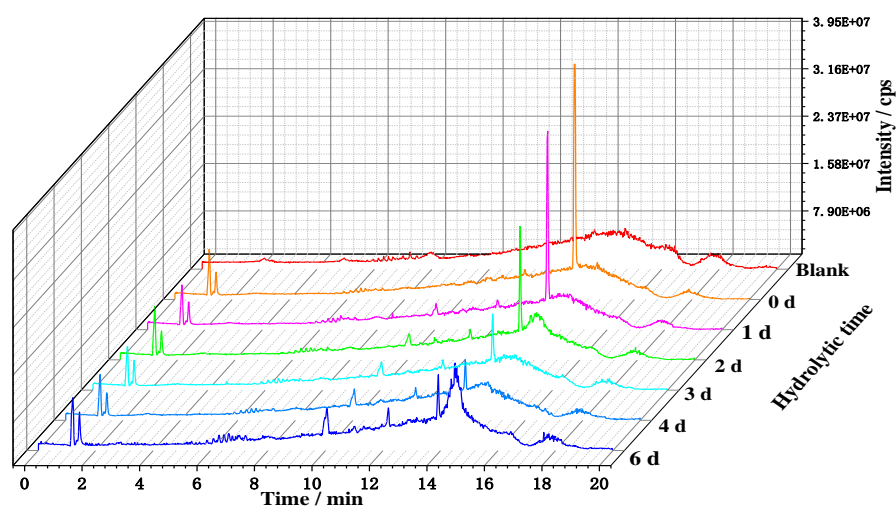
Metal Salts	Amount/mg L ⁻¹
Sodium chloride, NaCl	24.3200
Magnesium chloride, MgCl ₂	5.1400
Calcium chloride anhydrous, CaCl ₂	1.1400
Potassium chloride, KCl	0.6900
Sodium bicarbonate, NaHCO ₃	0.2000
Potassium bromide, KBr	0.1000
Boric acid, H ₃ BO ₃	0.0270
Strontium chloride hexahydrate, SrCl ₂ ×6H ₂ O	0.0260
Ammonium chloride, NH ₄ Cl	0.0064
Sodium fluoride, NaF	0.0030
Sodium metasilicate, Na ₂ SiO ₃	0.0020
Iron(III) phosphate tetrahydrate, FePO ₄ ×4H ₂ O	0.0010

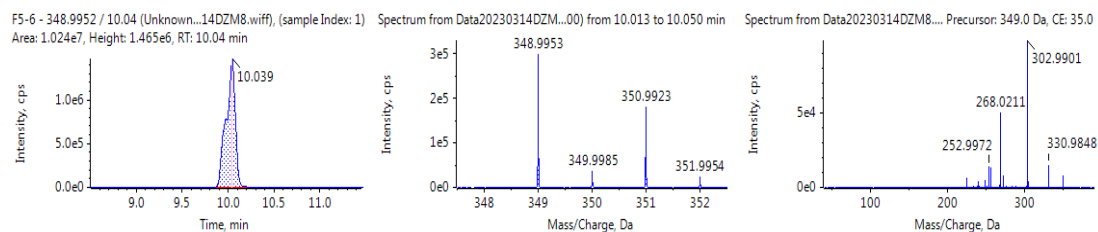
The artificial seawater solution pH is 8.18.

Table S4. The mass spectrometry conditions for the chromatographic analysis of florpyrauxifen-benzyl.

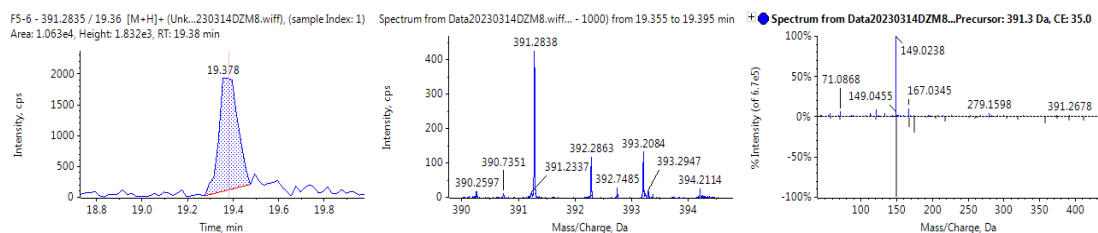
Compound	Retention Time/min	Selected Ion	Precursor Ion/m/z	Extracted Fragment Ion/m/z	DP/V	CE/eV	Ionization Mode
florpyrauxifen-benzyl	5.62	[M+H] ⁺	439.0422	50.0157	90	145	+
				51.0235	90	145	
				63.0236	90	140	
				65.0387	90	95	
				91.0551*	90	95	
Ion source temperature	Spray voltage	Capillary temperature	Gas1	Gas2	Curtain Gas	EPI scan speed	Acquisition time
/°C	/V	/°C	/psi	/psi	/psi	/Da/s	/ms
550	5500	320	50	55	35	10000	100

where “*” represented quantitative ion, DP represented declustering potential and CE represented collision energy.

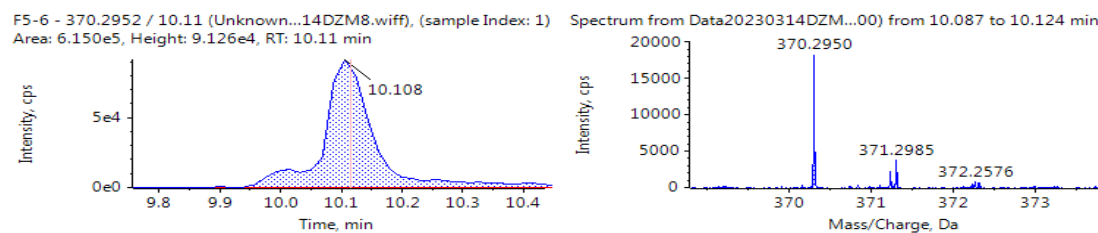
**Figure S1.** The components of disposable face masks (DFMs).**Figure S2.** The total ion chromatograms of florpyrauxifen-benzyl degradation solution performed by QTOF-MS/MS.



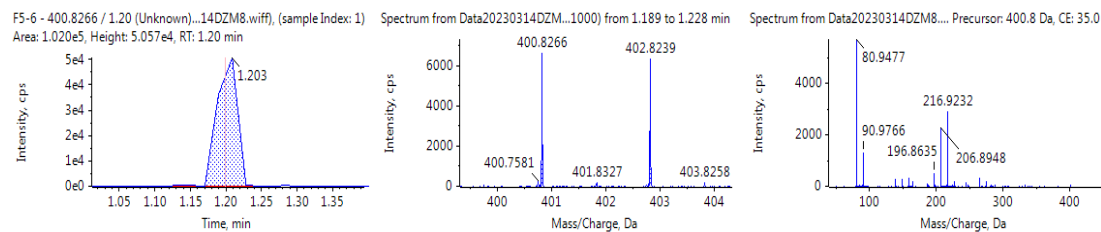
Product a:



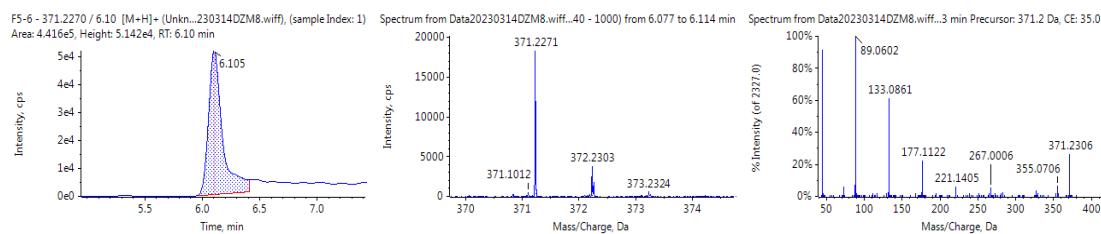
Product b:



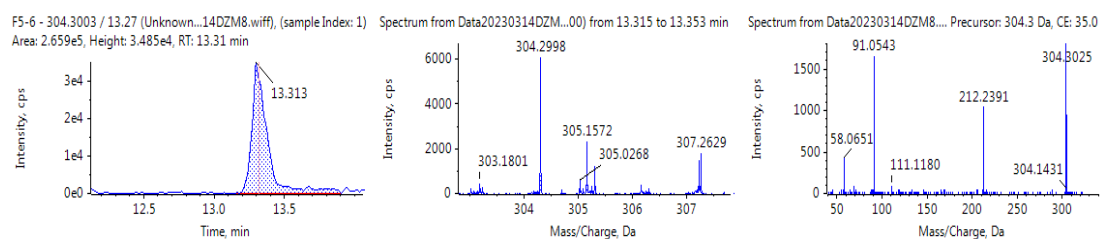
Product c:



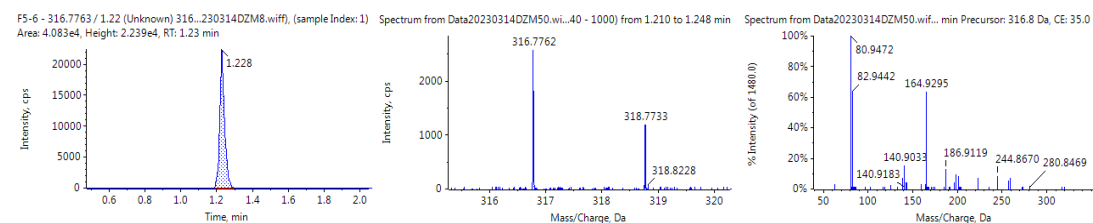
Product d:



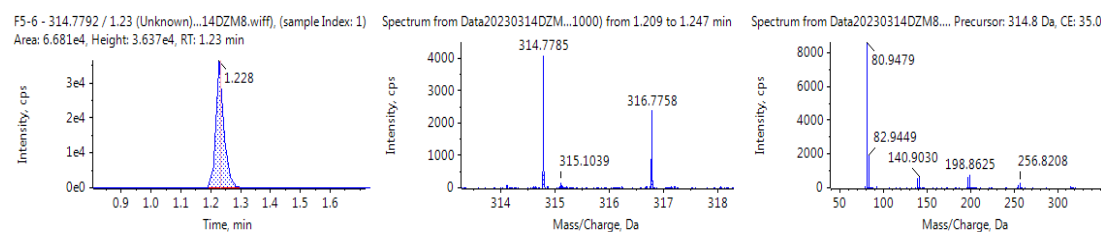
Product e:



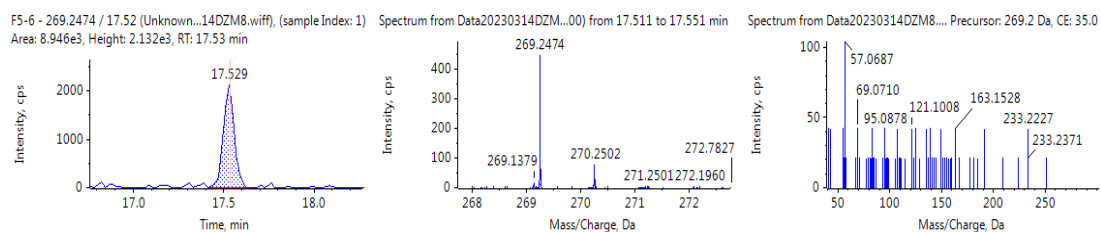
Product g:



Product h:



Product i:



Product j:

Figure S3. The primary and secondary mass spectrograms of the hydrolytic products.

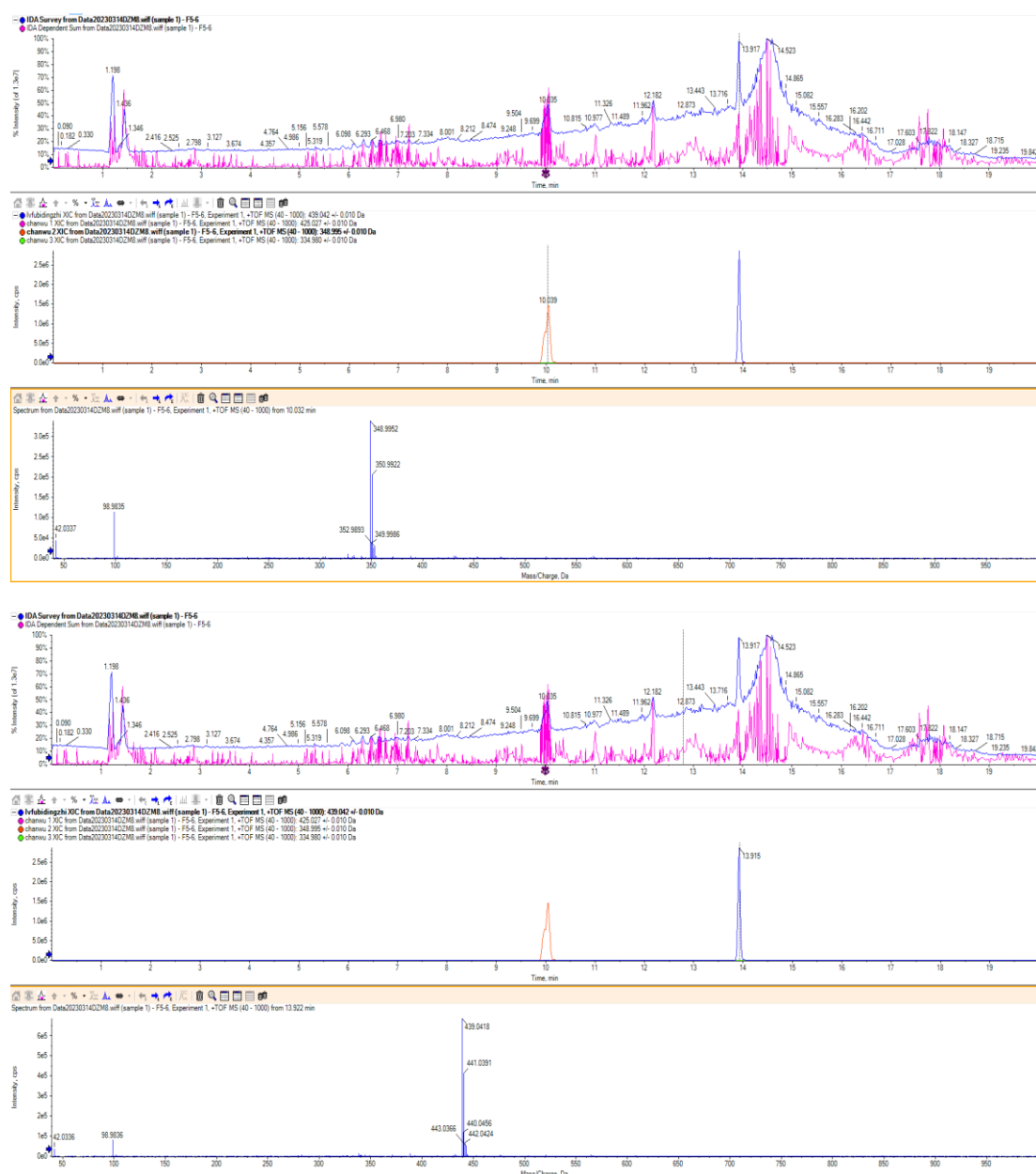


Figure S4. The total ion chromatograms and extraction ion chromatograms of florpyrauxifen-benzyl hydroxy and florpyrauxifen-hydroxy acid, primary mass spectrograms of florpyrauxifen (10.039 min) and florpyrauxifen-benzyl (13.915 min).