UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, D.C. 20460

OFFICE OF CHEMICAL SAFETY
AND POLLUTION PREVENTION

**MEMORANDUM**

**DATE:** November 1, 2016

**SUBJECT:** Drinking Water Assessment for the New Chemical Florpyrauxifen-benzyl (XDE-848 Benzyl Ester, Rinskor™), in Support of the Health Effects Division's Human Health Risk Assessment
(PC Code 030093; DP Barcode D429727)

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This memo presents the Environmental Fate and Effects Division's (EFED) Tier I Estimated Drinking Water Concentrations (EDWCs) for florpyrauxifen-benzyl (CAS No. 1390661-72-9; alternate names: XDE-848 benzyl ester, XDE-848 BE, Rinskor™), calculated using the Tier I Rice Model v.1.0 (for the rice use), or based on the maximum proposed application rate (for the aquatics use pattern), for use in the human health risk assessment by the Health Effects Division (HED). The registrant seeks registration for the new uses of the chemical on rice and aquatics.

Based on the degradation profile and the available data on the major degradates of florpyrauxifen-benzyl, the majority of the mass of parent is expected to reach paddy water/soil, while a smaller amount is expected to reach adjacent surface water by drift. The majority of parent reaching paddy water/soil is expected to partition into the soil and in the paddy environment and degrade rather quickly [$t_{½}$ = 12-31 days in aerobic soil (flooded system), and 15-46 days in anaerobic soil environments; if the test substance is applied to dry soils, the half-lives will range from 8.9-348 days]. Parent reaching water bodies by drift or applied directly to water (aquatics use), is expected to degrade rather quickly ($t_{½}$ = 4.0-6.2 days in aerobic aquatic, and 2.1-2.4 days in anaerobic aquatic environments). These half-life values were selected based on the process involved in the field. The soils studies were considered representative of the paddy and the sediment studies were considered representative of an aquatics site (*e.g.*, a pond).

The Tier I Estimated Drinking Water Concentrations (EDWCs) for florpyrauxifen-benzyl for use in the human health risk assessment by HED, based on the maximum application rate for the aquatics use pattern, were as follows: for florpyrauxifen-benzyl in surface water, the acute and chronic surface waters EDWC should not exceed 150 ppb. In an email communication from HED to EFED on October 25, 2016, EFED was notified that HED will perform a qualitative assessment for florpyrauxifen-benzyl, which is the only chemical included in this DWA. Should any questions arise, please contact José Meléndez at melendez.jose@epa.gov.

### Identification of Data Gaps

The environmental fate database for florpyrauxifen-benzyl is considered substantially complete. Several of the fate studies were considered supplemental, since certain deficiencies were observed; however, given the high number of studies pointing towards similar conclusions, including the field studies, it is believed that the environmental fate of this compound is relatively well understood. There is uncertainty in the fate studies conducted with soils and sediments, since high levels of unextracted radioactivity were observed. In the laboratory studies, the extractions were conducted with a relatively polar solvent in all instances. However, a supplemental study was conducted in which three additional solvents with a wide range of dielectric constants were used. No secondary extraction with acetone, hexane and ethyl acetate, at room temperature, yielded >3% of the applied. Additionally, for the benzyl-labeled florpyrauxifen-benzyl, the total recoveries were below guideline requirements (90-110% AR) in many studies. The main products of this labeled substance were benzoic acid and benzyl alcohol (depending on the study), both of which the registrant claims are of low toxicological concern.

## EXECUTIVE SUMMARY

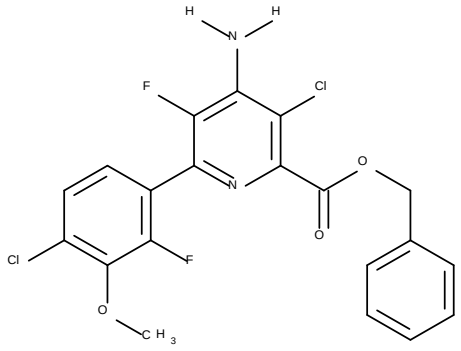
Florpyrauxifen benzyl (XDE-848 benzyl ester; PC Code 030093; CAS No. 1390661-72-9, **Table 1**) is a new systemic auxin herbicide (WSSA Group 4; HRAC Group O) currently proposed only for uses on rice fields (in AR, FL, LA, MS, MO, SC, TN and TX[1]) for post-emergence grass, sedge, and broadleaf weed control; and for aquatics applications, for management of freshwater aquatic vegetation in ponds, lakes, reservoirs, marshes, wetlands, bayous, drainage ditches, canals,

[1] These are most of the major rice producing states in the U.S., with the notable exception of California.

and other aquatic sites, including vegetation control on shoreline and riparian areas within or adjacent to these sites (includes both, direct in water applications or foliar applications to aquatic vegetation).

In addition to the technical product, four end use products (GF-3206, GF-3301, GF-3480, and GF-3565) are proposed for registration in the U.S. Two of the proposed end-use products contain an additional active ingredients, including cyhalofop or penoxsulam. Florpyrauxifen-benzyl may be applied as a foliar spray twice per year via aerial or ground equipment at a maximum single application rate of 0.0300 kg a.i./ha for the rice use (two applications allowed per season) or 0.0591 kg a.i./ha for the aquatic foliar use (two applications allowed per annual growth cycle) according to the proposed label. For direct in water applications, the maximum application rate is 150 µg/L (ppb) of active ingredient (one application allowed at this rate).

**Table 1: Structure of Florpyrauxifen-benzyl**

| Structure | Mass [g/mole] | Chemical name |
|---|---|---|
|  | 439.24 | **IUPAC:** Benzyl 4-amino-3-chloro-6-(4-chloro-2-fluoro-3-methoxy-phenyl)-5-fluoro-pyridine-2-carboxylate<br><br>**Formula:** $C_{20}H_{14}Cl_2F_2N_2O_3$<br><br>**SMILES Code:** [H]N([H])c1c(c(nc(c1Cl)C(=O)OCc2ccccc2)c3ccc(c(c3F)OC)Cl)F |

This drinking water assessment is related to a Section 3 (new chemical) for florpyrauxifen-benzyl. There are four proposed products containing florpyrauxifen-benzyl: GF-3301, GF-3206, GF-3480, and GF-3565, which are liquid formulations. The maximum seasonal application rate is 0.060 kg a.i./ha for the use on rice and 150 ppb for the aquatics use pattern. The chemical may be applied by air or ground equipment, or directly in water (for the aquatics use pattern).

The model used for this Tier 1 screening level drinking waters assessment is the Tier 1 Rice Model v.1.0 (rice use). For the aquatics uses, the maximum application rate was assumed. No degradates were modelled.

Florpyrauxifen-benzyl degradation is dependent on the environmental conditions, and it degrades from rapidly to slowly in different environments; further, it yields several degradates. Major degradates differ when the test substance is exposed to light, compared to soil/sediment metabolism studies. Levels of unextracted radioactivity were high in most of the metabolism studies. In the field, it appears that a combination of routes of dissipation takes place. The majority of the mass of parent is expected to reach paddy water/soil, while a smaller amount is expected to

reach adjacent surface water by drift. Parent reaching paddy water/soil is expected to partition into the soil and in the paddy environment and degrade rather quickly [$t_{½}$ = 12-31 days in aerobic soil (flooded system), and 15-46 days in anaerobic soil environments; if the test substance is applied to dry soils, the half-lives will range from 8.9-67.2 days]. The following degradates are expected to form in the aquatic environments (based on the aerobic flooded and anaerobic soil metabolism studies): XDE-848 acid (73.5% maximum, with a half-life of 14 days under aerobic conditions); XDE-848 benzyl hydroxy (15.9% maximum, with a half-life of 87 days); and XDE-848 hydroxy acid (68.9% maximum, with a half-life of 127-729 days). Parent reaching water bodies by drift or applied directly to water (aquatics use), is expected to degrade rather quickly ($t_{½}$ = 4.0-6.2 days in aerobic aquatic, and 2.1-2.4 days in anaerobic aquatic environments), forming the following degradates: XDE-848 acid (46.9% maximum, with a half-life of 6.3-18 days under aerobic aquatic metabolism conditions); XDE-848 benzyl hydroxy (43.1% maximum, with a half-life of 6-14 days); and XDE-848 hydroxy acid (104.4% maximum, with a half-life of 53-121 days aerobic aquatic conditions, while it was the terminal degradate under anaerobic aquatic metabolism conditions).

A more definitive assessment could be conducted, using the more refined Tier II aquatic surface water model Pesticides in Flooded Application Model (PFAM v.2.0), if the HED requested it. A summary of the results obtained of Tier I modeled drinking water concentrations, is tabulated below (**Table 2**).

**Table 2. Maximum surface waters Estimated Drinking Water Concentrations (EDWCs) for drinking water risk assessment based on in-water application of florpyrauxifen-benzyl for the aquatics uses**

| Use | Acute (ppb) | Chronic (ppb) |
|---|---|---|
| Aquatics, 150 ppb/season | 150 | ≤150 |

While water in rice paddies may leach into the subsurface, the degree of leaching is limited by the presence of impervious claypan soils. Although pesticides have been found in groundwater near rice paddies, rice growing areas are not considered to be highly vulnerable to movement of pesticides into groundwater. Rice paddies are designed to hold water for extended periods of time, and the amount of leaching is expected to be low compared to that of vulnerable areas. Surface water concentrations of pesticides are also expected to be higher than groundwater concentrations[2]. Therefore, groundwater simulations will not be completed for use of florpyrauxifen-benzyl on rice.

## PROBLEM FORMULATION

*This is a Tier I drinking water assessment that uses modeling to estimate the surface water concentrations of florpyrauxifen-benzyl, in drinking water source water (pre-treatment) resulting from pesticide use on rice and aquatics use sites. This initial tier screens out chemicals with low potential risk and provides estimated exposure concentrations for the human health dietary risk assessment.*

[2] CRC. 2013. *Rice-Specific Groundwater Assessment Report*. July 2013. Central Valley Regional Water Quality Control Board. California Rice Commission. Available at the following URL (accessed May 21, 2016): http://www.waterboards.ca.gov/centralvalley/water_issues/irrigated_lands/regulatory_information/rice_growers_sacvalley_wdrs/2013july_crc_gar_final.pdf.

# ANALYSIS

## Use Characterization

There are four products containing florpyrauxifen-benzyl (**Tables 3 and 4**). Two of the products have only florpyrauxifen-benzyl as the sole active ingredient, while two of the products are coformulated with penoxsulam and cyhalofop, respectively. While all of the products can be used on rice crops (**Table 3**), the only product that can be used in aquatics use sites is GF-3301 (**Table 4**). The aquatics uses for the product GF-3301, are for the "management of freshwater aquatic vegetation in ponds, lakes, reservoirs, marshes, wetlands, bayous, drainage ditches, canals, and other aquatic sites, including vegetation control on shoreline and riparian areas within or adjacent to these sites."

**Table 3. Summary of Florpyrauxifen-benzyl Proposed Products/Labels – *Rice Use***

| Product Name | GF-3301 | GF-3206 | GF-3480 | GF-3565 |
|---|---|---|---|---|
| A.I.s by weight | 26.5% florpyrauxifen-benzyl | 2.7% florpyrauxifen-benzyl | 2.13% florpyrauxifen-benzyl; 10.64% cyhalofop | 1.3% florpyrauxifen-benzyl; 2.1% penoxsulam |
| A.I.s by volume | 2.50 lb a.i./gal florpyrauxifen-benzyl | 0.21 lb a.i./gal florpyrauxifen-benzyl | 0.17 lb a.i./gal florpyrauxifen-benzyl; 0.83 lb a.i./gal cyhalofop | 0.10 lb a.i./gal florpyrauxifen-benzyl; 0.17 lb a.i./gal penoxsulam |
| Uses | Rice | | | |
| Geographic Restrictions | Only in AR; FL; LA; MO; MS; SC; TN; TX | | | |
| Single Rate (based on florpyrauxifen-benzyl) | 0.5–1.37 fl oz/acre/app[1]; maximum rate is 0.0268 lb a.i./A or 0.0300 kg a.i./ha | 6–16 fl oz/acre/app[1]; maximum rate is 0.0263 lb a.i./A or 0.0294 kg a.i./ha | 20.5 fl oz/acre; 0.0272 lb a.i./A or 0.0305 kg a.i./ha | 27.4 fl oz/acre; 0.0214 lb a.i./A or 0.0240 kg a.i./ha |
| Max. No. of Apps | 2 | | 1 | |
| Int. between Apps (days) | 14 | | Not Applicable | |
| Timing of App | From 2 leaf stage (drill-seeded rice or water-seeded rice) with no exposed roots up to 60 days before harvest. | | | |
| Pre-harvest Interval (days) | 60 | | | |

[1] Rate depends on weed controlled.

**Table 4. Summary of Florpyrauxifen-benzyl Proposed Product/Label – *Aquatics Use***

| Product Name | GF-3301 only | |
|---|---|---|
| Uses | Aquatics | |
| Geographic Restrictions | Ponds, lakes, reservoirs, marshes, wetlands, bayous, drainage ditches, canals, and other aquatic sites (freshwater aquatic vegetation) | |
| Type of Application | Direct application to water | Foliar applications or foliar spot treatments: by boat or with ground equipment, or aerial |

| Product Name | GF-3301 only | |
|---|---|---|
| Application Rate | 10-150 ppb (or 150 ppb per annual growth cycle);<br>50 ppb or less is the typical rate; 150 ppb is the maximum rate | 1.4–2.7 fl oz/acre/app;<br>maximum single app rate is 0.0527 lb a.i./A/app or 0.0591 kg a.i./ha/app;<br>5.4 fl oz/acre/annual growing cycle;<br>0.105 lb a.i./A or 0.118 kg a.i./ha/ annual growing cycle |
| Max. No. of Apps | 1 at maximum rate | 2 at maximum rate |
| Int. between Apps (days) | 10 days, if less than the maximum rate is used | Not specified, assume 10 days |

The products GF-3301 and 3206 do not provide residual weed control. The use of an agriculturally approved methylated seed oil (MSO) adjuvant is recommended for GF-3301 and GF-3206. The GF-3480 and GF-3562 formulations have adjuvant built-in. GF-3301, GF-3206, GF-3480, and GF-3565 can be tank mixed with a number of other herbicides as listed in each label. The most restrictive instructions of tank mixed products should be followed. The products GF-3301, GF-3206, GF-3480, and GF-3565 are not for use on wild rice.

For the rice use (all four products), the minimum spray volume is 10 gallons per acre (gpa) for both aerial and ground applications. Applications at wind speeds below 2 mph should be avoided (it is stated that drift potential is lowest at wind speeds of 2-10 mph). These products should not by applied under conditions of a low level air temperature inversion. Further, it is instructed to use coarse droplet category per S- 572 ASABE standard at spray boom pressure no greater than 30 psi for aerial applications, in order to minimize spray drift. For the aerial applications, the boom height should not be greater than 10 feet above the top of the largest plants, unless a greater height is required for aircraft safety. For ground applications, the use of coarse or coarser nozzle spray quality per S-572 ASABE standard is instructed.

Florpyrauxifen-benzyl in these products can be applied pre-flood and post-flood. For post-flood applications, the flood water should be lowered to expose at least 70% of the weed foliage (*e.g.*, 1 to 2 inches deep). Normal flood should be re-established, beginning within 3 hours after application, preventing germination of new weeds. Per the labels, establishing permanent flood <5 days after application of product can benefit weed control. According to the labels, all four products GF-3301, GF-3206, GF-3480 and GF-3565 are rainfast in 2 hours. Resistance management language is also added to the labels, and the products should be used as part of an Integrated Pest Management (IPM) programs.

For the aquatics uses of GF-3301, a permit is required prior to chemical application. There are certain restrictions for using treated water for irrigation. For the in-water applications (to submersed or floating aquatic weeds), the product can be applied undiluted, or diluted with water. For post-emergent foliar applications (to floating and emergent weeds), an approved surfactant for aquatics uses should be used and product should be diluted with water to achieve proper coverage of treated plants. Spray volumes up to 100 gpa are recommended for the ground foliar applications. A coarse or coarser nozzle spray quality per S-572 ASABE standard is recommended. For spot treatments, product should be diluted 0.01 to 0.02% GF-3301 plus an adjuvant added. Spray coverage should be sufficient to moisten the leaves of the target vegetation but not to the point of runoff. For the aerial foliar applications, the spray volume should be 15 gpa or more and a coarse

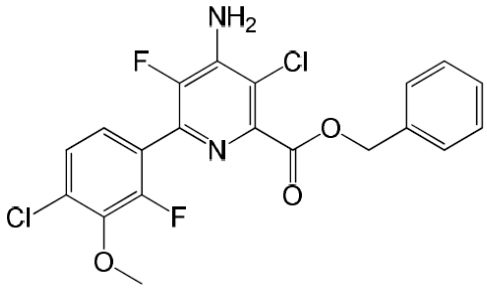
droplet category per S-572 ASABE standard should be used. GF-3301 may be mixed with other herbicides or algaecides registered for aquatic use (unless prohibited by the label).

## Fate and Transport Characterization

Florpyrauxifen benzyl degradation is dependent on the environmental conditions, and it degrades from rapidly to slowly in different environments; further, it yields several degradates. Major degradates differ when the test substance is exposed to light, when compared to soil/sediment metabolism studies. Levels of unextracted radioactivity were high in most of the metabolism studies. In the field, it appears that a combination of routes of dissipation takes place.

**Table 5** gives a summary of physicochemical properties of florpyrauxifen-benzyl. **Table 6** provides a summary of environmental fate properties of the chemical, along with some fate information about its transformation products.

**Table 5. Physicochemical Properties of Florpyrauxifen Benzyl (XDE-848 Benzyl Ester)**

| Property | Value and units | MRID or Source |
|---|---|---|
| Molecular Weight | **439.2 g/mole** | 49677702 |
| Chemical Formula | $C_{20}H_{14}Cl_2F_2N_2O_3$ | 49677702 |
| CAS No. | 1390661-72-9 | 49677702 |
| Structure |  | 49677702 |
| Physical State | Powder (as manufactured) @ 21.3°C | 49677702 |
| Relative Density<br>Bulk Density | Relative density 1.39<br>Bulk Density 0.202 g/mL at 23.4°C<br>Tap Density 0.320 g/mL at 23.4°C | 49677702 |
| Vapor Pressure | 4.6 x $10^{-5}$ Pa (**3.5 x $10^{-7}$ torr**) at 25°C<br>3.2 x $10^{-5}$ Pa (2.4 x $10^{-7}$ torr) at 20°C<br>Classified as<br>'Non-volatile under field conditions.' **(1)(3)** | 49677702 |
| Henry's Law Constant | 9.2 x $10^{-6}$ atm-$m^3$/mole at 20°C<br>---<br>1.3 x $10^{-5}$ atm-$m^3$/mole, using VP at 25°C and S at 20°C | Estimated from water solubility and vapor pressure |
| Water Solubility | Purified Water: 0.015 mg/L at 20°C<br>pH 5 buffer solution: 0.014 mg/L<br>pH 7 buffer solution: **0.011 mg/L**<br>pH 9 buffer solution: 0.012 mg/L | 49677702 |

| Property | Value and units | MRID or Source |
|---|---|---|
| Solubility in Organic Solvents | All at 20°C: methanol 13 g/L<br>acetone 210 g/L<br>xylene 14 g/L<br>1,2-dichloroethane 95 g/L<br>ethyl acetate 120 g/L<br>n-heptane 0.053 g/L<br>n-octanol 4.9 g/L | 49677702 |
| Octanol – water partition coefficient ($K_{OW}$) | pH 5: $\log_{10} P_{OW} = 5.4 \pm 0.1$ at 20°C<br>pH 7: $\log_{10} P_{OW} = 5.5 \pm 0.04$ at 20°C<br>pH 9: $\log_{10} P_{OW} = 5.5 \pm 0.1$ at 20°C | 49677702 |
| Air-water partition coefficient ($K_{AW}$) | $K_{AW} = C_{air}/C_{water}$ =<br>HLC/(RT) = $3.84 \times 10^{-4}$ (unitless) at 20°C<br>Classified as<br>'Slightly volatile from a water surface.' (1) | Calculated<br><br>HLC = Henry's Law Constant |
| Octanol-air partition coefficient ($K_{OA}$) | $K_{OA} = K_{OW}/K_{AW} = 8.2 \times 10^{8}$ (unitless) | Calculated |
| $C_{water+soil}/C_{air}$ | $C_{water+soil}/C_{air} = (C_{water}/C_{air})(1/r + K_d)$ =<br>(2604) (1/6 + 796.5) = $2.07 \times 10^{6}$ (3)<br>Classified as 'Non-volatile from a moist soil.' (1)(2)(3) | Calculated |
| Dissociation Constant | Does not dissociate in the environmental pH range (pH 4 to 10) | 49677702 |
| pH | 6.58 at 23.4 °C (1% dilution in water) | 49677702 |
| UV/Visible light absorption | Neutral: λ max at 212, 245 nm<br>Acidic: λ max at 212, 245 nm<br>Alkaline: λ max at 217, 241 nm | 49677702 |

(1) For classification scheme, see "Guidance for Reporting on the Environmental Fate and Transport of the Stressors of Concern in Problem Formulations," available at (accessed 07/07/2016): https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/guidance-reporting-environmental-fate-and-transport.

(2) Assuming 2% organic carbon, soil to soil water ratio (w/w) = 6, and soil water to soil air (v/v) = 1.

(3) Note that all chemicals may volatilize to some extent; this classification simply indicates that the volatility potential is very low.

### *Degradation and Metabolism*

Florpyrauxifen benzyl undergoes base-catalyzed hydrolysis (faster hydrolysis at pH 9, relatively stable at pH 4). At neutral pH, the $t_{1/2}$ = 111 days, indicating relatively slow hydrolysis in neutral water. Based on the available data, it appears that aqueous photolysis is the major route of degradation of this chemical (environmental $t_{1/2}$ <0.2 days). It should be noted, however, that this mechanism of dissipation occurs mainly in the uppermost layer of a surface body of water and might occur in the shallow/not so turbid rice paddy when applied at the early stage of rice development when the rice plant shadowing effect is low. It is less important in turbid waters following the release of contaminated water outside the paddy. In contrast to the aqueous photolysis, it is noted that florpyrauxifen benzyl degrades much more slowly in the soil photolysis study (environmental $t_{1/2}$ = 50 days).

In soils, under aerobic conditions, the range of half-lives was very wide, with representative half-lives 8.9-67.2 days. In the study, there was no clear relationship of degradation and soil pH values. Under aerobic soil flooded conditions, the representative half-lives were 12-31 days in two soils tested. In the anaerobic soil metabolism study, the representative half-lives were 14.8-46.2 days, in four soils tested.

In contrast, in the two aquatic metabolism studies, the half-lives for florpyrauxifen-benzyl were lower than in the soil studies described above. The aerobic aquatic metabolism SFO representative half-lives were 4-6 days, and the anaerobic aquatic metabolism SFO representative half-lives ~2 days in both sediments tested. In the aquatic metabolism studies, the pH of the sediments/water systems were relatively high (especially the anaerobic study), which may have promoted hydrolysis of the parent compound.

**Table 6. Environmental Fate Properties of Florpyrauxifen-benzyl (XDE-848 Benzyl Ester)**

| Study | Value and unit | Major Degradates; *Minor Degradates* | MRID or Citation | Study Classification, Comment |
|---|---|---|---|---|
| Abiotic Hydrolysis | XDE-848 BE SFO half-life at 25°C =<br>pH 4 = Stable<br>**pH 7 = 111 days**<br>pH 9 = 1.23 days<br>---<br>**XDE-848 acid was stable** at 50°C and pH's of 4, 7 and 9 for 5 days. | **Major** at pH 7:<br>XDE-848 acid;<br>Benzyl alcohol | 49677711 | Acceptable;<br><br>Note: Additional studies were conducted for XDE-848 BE at 10°C, 35°C and 50°C, but they are not reported in this table. |
| Atmospheric Degradation | XDE-848 BE half-life =<br>1.12 days, estimated for OH radical reaction;<br>No ozone reaction estimation. | Not Available | 49677713<br>EPI Suite v.4.11 Estimates;<br>AOPWIN v.1.92 | Supplemental;<br><br>Hydroxyl radical reaction assumptions: at $25^0$C and 12-hr day; $1.5x10^6$ OH/$cm^3$ |
| Direct Aqueous Photolysis | pH 4 buffered solution:<br><br>Corrected to natural summer sunlight (40°N) environmental photolysis SFO half-life =<br><br>XDE-848 BE **$t_{1/2}$ = 0.0786 days** | **Major:**<br>Des-chloro XDE-848 acid;<br>Des-chloro XDE-848 Benzyl ester;<br>Benzyl alcohol<br><br>***Minor*:**<br>X12421263 | 49677712 | Supplemental;<br><br>In pH 4 buffer:<br>XDE-848 Benzyl Ester was stable in the dark control. |
| | Natural water:<br><br>Corrected to natural summer sunlight (40°N) environmental photolysis SFO half-life =<br><br>XDE-848 BE **$t_{1/2}$ = 0.161 days** | **Major:**<br>Des-chloro XDE-848 Benzyl ester;<br>Benzyl alcohol<br><br>***Minor*:**<br>Des-chloro XDE-848 acid;<br>XDE-848 acid | | In natural water:<br>XDE-848 Benzyl Ester shows an SFO $DT_{50}$ = 5.87 days in the dark controls.<br><br>XDE-848 acid was higher in the dark control than in the irradiated samples and it was not considered a phototransformation product. |

| Study | Value and unit | Major Degradates; *Minor Degradates* | MRID or Citation | Study Classification, Comment |
|---|---|---|---|---|
| Soil Photodegradation | Natural summer sunlight (40°N)<br>SFO environmental half-life for XDE-848 BE<br>$t_{1/2}$ = 50 days, German loam (Speyer 2.4);<br><br>The degradation appeared to slow down with time. | **Major:**<br>Unextracted Residues<br><br>***Minor*:**<br>Des-chloro XDE-848 Benzyl Ester;<br>Des-chloro XDE-848 acid;<br>XDE-848 acid | 49677714 | Supplemental;<br><br>The preferred kinetics model from PestDF is DFOP instead of SFO. The uncorrected DFOP slow $t_{1/2}$ = 46.3 days. |
| Aerobic Soil Metabolism (20°C) | XDE-848 BE half-life =<br>348 days (DFOP), Yolo loam soil (CA), pH 7.2;<br>129 days (DFOP), loam (Germany), pH 6.2;<br>34 days (IORE), silt loam (UK), pH 5.9;<br>8.91 days (IORE), loamy sand (UK), pH 7.4;<br>*and*,<br>182 days (IORE), *sterile* (via gamma irradiation) sandy loam (UK);<br><br>90th percentile confidence bound on the mean half-life value<br>**$t_{input}$ = 55.3 days** | **Major:**<br>Unextracted Residues;<br>XR-848 acid;<br>Nitro hydroxy acid (or X12483137)<br><br>***Minor*:**<br>XR-848 Hydroxy acid;<br>XR-848 Benzyl hydroxy | 49677715 | Supplemental;<br><br>Estimated SFO half-lives for XR-848 acid:<br>64.1 days;<br>57.9 days;<br>121 days;<br>40.8 days |
| Aerobic Soil Metabolism (Flooded System) (20°C) | XDE-848 BE half-life =<br>31.3 days (IORE), loam (Italy);<br>11.6 days (IORE), sandy loam (Italy)<br><br>90th percentile confidence bound on the mean half-life value:<br>**$t_{input}$ = 44.6 days** | **Major:**<br>Unextracted Residues;<br>XR-848 Hydroxy acid;<br>XR-848 Acid;<br>XR-848 Benzyl hydroxy | 49677716 | Supplemental;<br><br>Estimated SFO half-lives:<br>XR-848 Hydroxy acid: 127, and 729 days;<br>XR-848 acid: 14 days;<br>XR-848 benzyl hydroxy: 86.9 days |
| Anaerobic Soil Metabolism (Flooded) (20°C) | XDE-848 BE half-life =<br>37.6 days (IORE), Yolo clay loam (CA);<br>14.8 days (IORE), loam (Germany);<br>16.9 days (IORE), silt loam (UK);<br>46.2 days (IORE), Site I2 sandy loam (UK);<br><br>90th percentile confidence bound on the mean half-life value =<br>**$t_{input}$ = 41.5 days** | **Major:**<br>Unextracted Residues;<br>XR-848 Hydroxy acid;<br>XR-848 Acid | 49677718 | Supplemental |

| Study | Value and unit | Major Degradates; *Minor Degradates* | MRID or Citation | Study Classification, Comment |
|---|---|---|---|---|
| Aerobic Aquatic Metabolism (20°C) | XDE-848 BE representative half-life =<br>4.04 days (SFO), loam sediment (France), water pH 7.8, sediment pH 7.1;<br>6.16 days (SFO), loamy sand sediment (England), water pH 6.6, sediment pH 6.2;<br><br>90$^{th}$ percentile confidence bound on the mean half-life value:<br>**$t_{input}$ = 8.36 days** at 20°C. | **Major:**<br>Unextracted Residues;<br>XR-848 Hydroxy acid;<br>XR-848 Acid;<br>XR-848 Benzyl hydroxy;<br>Benzoic acid | 49677719 | Supplemental;<br><br>Estimated SFO half-lives:<br>XR-848 Hydroxy acid: 121 and 52.5 days;<br>XR-848 acid: 6.32 and 18 days;<br>XR-848 benzyl hydroxy: 5.65 and 14 days |
| Anaerobic Aquatic Metabolism (20°C) | XDE-848 BE representative half-life =<br>2.37 days (SFO), loamy sand sediment (Switzerland), water pH 8.14, sediment pH 7.35;<br>2.1 days (SFO), silt loam sediment (Switzerland), water pH 7.42, sediment pH 7.15;<br><br>90$^{th}$ percentile confidence bound on the mean half-life value:<br>**$t_{input}$ = 2.65 days** | **Major:**<br>Unextracted Residues;<br>Hydroxy acid;<br>XDE-848 acid;<br>Benzyl hydroxy;<br>Benzoic acid<br><br>***Minor:***<br>Benzyl alcohol | 49677720 | Supplemental;<br><br>Alkaline pH may have promoted base-catalyzed hydrolysis of the parent compound.<br><br>Hydroxy acid was the terminal degradate |
| Mobility/ Batch Equilibrium for the parent XDE-848 BE | XDE-848 BE mean **$K_{OC}$ = 32280 L/kg$_{OC}$**<br><br>(See tables below.) | N/A | 49677710 | Supplemental |
| Mobility/ Batch Equilibrium for three degradates | XDE-848 Acid mean **$K_{OC}$ = 71.8 L/kg$_{OC}$** (mobile, based on FAO 2000);<br><br>XDE-848 Hydroxy Acid mean **$K_d$ = 1.91 L/kg**;<br><br>XDE-848 hydroxy benzyl ester mean **$K_d$ = 118 L/kg**. | N/A | 49677709 | Supplemental |

| Study | Value and unit | Major Degradates; *Minor Degradates* | MRID or Citation | Study Classification, Comment |
|---|---|---|---|---|
| Aquatic Field Dissipation (***Rice use***) | Range of values provided for two applications, XDE-848 BE dissipation half-lives[2] =<br><br>CA clay loam EC formulation:<br>Water: 0.159-0.199 days (SFO);<br>Soil: 1.45 days (SFO); 22.6 days (IORE);<br><br>CA clay loam GR formulation:<br>Water: 0.15-0.343 days (SFO);<br>Soil: 17, 24.2 days (DFOP);<br><br>TX sandy loam:<br>Water: N/A, 0.791 days (SFO);<br>Soil: 8.11 days (SFO), ND | **Major:**<br>XDE-848 Acid;<br>XDE-848 Hydroxy Acid;<br>XDE-848 Hydroxy BE was major only in the GR formulation applications.<br><br>***Minor*** (comparatively):<br>Des-chloro XDE-848 BE;<br>Des-chloro XDE-848 acid | 49677721 | Supplemental |
| Aquatic Field Dissipation (***Aquatics use***) | XDE-848 BE dissipation half-life[2]=<br><br>Water half-lives:<br>Two sites at 50 ppb:<br>FL site $t_{1/2}$ = 1.4 days (SFO);<br>NC site $t_{1/2}$ = 2.3 days (SFO);<br><br>One site at 150 ppb:<br>FL site $t_{1/2}$ = 6.4 days (SFO);<br><br>Sediment half-lives could not be calculated. | **Major:**<br>XDE-848 acid – 35.2% (22 days)<br><br>***Minor:***<br>XDE-848 benzyl hydroxy – 1.0% (22 and 28 days)<br>XDE-848 hydroxy acid – 4.7% (22 days)<br>Des-chloro XDE-848 benzyl ester – 0.2% (0.5, 1.5 and 2 days)<br>Des-chloro XDE-848 acid – 0.2% (7, 14 and 22 days) | 49677722 & 49677723 | Supplemental;<br><br>Percentages presented are based on the study conducted at 150 ppb. |
| Bioconcentration Factor (BCF) – Bluegill Sunfish (*Lepomis macrochirus*) (22°C) | Maximum steady state BCF obtained at the highest concentration, and based on TRR=<br><br>356 L/kg wet wt whole fish;<br>55 L/kg wet wt edible tissue;<br>686 L/kg wet wt non-edible tissue;<br><br>Depuration $t_{1/2}$ = 0.2-0.4 days | **Major:**<br>XDE-848 acid;<br>Taurine conjugate of XDE-848 acid;<br><br>***Minor:***<br>XDE-848 deschloro acid;<br>Other degradates ≤1.2% TRR | 49677749 | Supplemental |

ND = Not Determined; TRR = Total Radioactive Residues; GR = Granular.

(1) 90th percentile confidence bound on the mean calculated using the following equation:

$$t_{input} = \overline{t_{1/2}} + \frac{t_{90,n-1}s}{\sqrt{n}}$$

(2) The value may reflect both dissipation and degradation processes.

### *Degradation Pathway*

**Figure 1** shows the registrant-proposed degradation pathway for florpyrauxifen-benzyl. Based on this pathway, de-esterification is an important process in the degradation of

florpyrauxifen benzyl, since all the terminal products are carboxylic acids. Since this is a new chemical, there is no monitoring data available at this time.

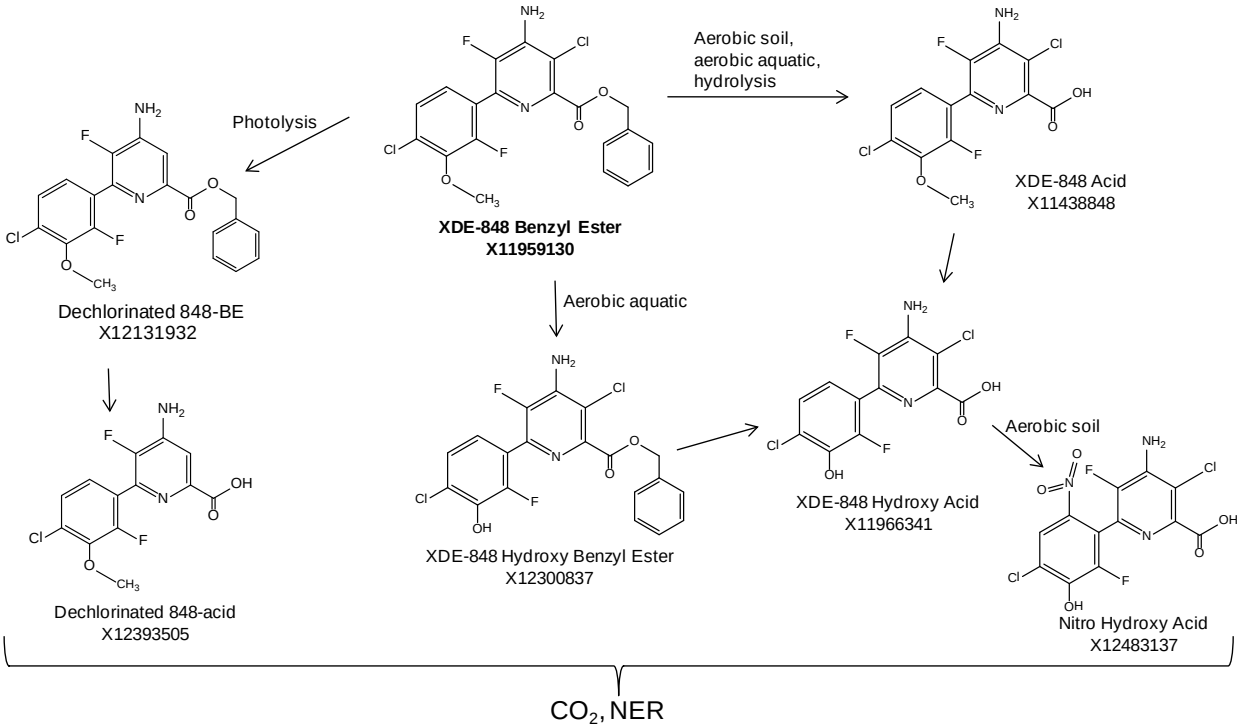



**Figure 1. Registrant-Proposed Degradation Pathway for Florpyrauxifen Benzyl (XDE-848 BE)**

Depending on the route of degradation (*i.e.*, photolysis vs. metabolism), florpyrauxifen-benzyl displays differing major degradates (refer also to **Table A-4**, for structures and maximum percentages observed in the laboratory fate studies, in the **Appendix A**).

### *Mobility*

The mean $K_{OC}$ for florpyrauxifen-benzyl is 32,280 ml/$g_{OC}$ (hardly mobile). The relatively high $K_{OC}$ displayed by this test substance suggests that it is more likely to partition with soils and sediments, especially if they are organic carbon-rich (**Tables 7 and 8**). The vapor pressure and Henry's Law constant for florpyrauxifen-benzyl are indicative of a test substance with relatively low potential to volatilize ($2.4 \times 10^{-7}$ torr and $9.2 \times 10^{-6}$ atm-$m^3$/mole at 20°C, respectively). The water solubility of florpyrauxifen-benzyl is relatively low, compared to the application rates in the field of up to 150 µg/L for the in water aquatics uses (solubility in water is 15 µg/L at 20°C). It appears that the formulation improves the chemical's solubility in water.

**Table 7. <u>Adsorption</u> Coefficients for Florpyrauxifen benzyl (XDE-848 Benzyl Ester) in Six Soils (MRID 49677710)**

| Soil | $K_d$ (L/kg) | $K_{OC}$ | $K_F$ (L/kg) | $K_{FOC}$ |
|---|---|---|---|---|
| Yolo Clay loam | 248.96 | 31120 | 130.84 | 16354 |
| RefSol 03G Loam | 1221.64 | 24931 | 853.13 | 17411 |

| Soil | $K_d$ (L/kg) | $K_{OC}$ | $K_F$ (L/kg) | $K_{FOC}$ |
|---|---|---|---|---|
| Site E1 Silt loam | 1358.55 | 30876 | 1474.08 | 33502 |
| Site I2 Sandy loam | 479.08 | 21777 | 337.90 | 15359 |
| Casalino Sandy loam | 575.61 | 44278 | 377.67 | 29051 |
| Ogori Clay loam | 895.37 | 40699 | 542.17 | 24644 |
| **Mean** | 796.54 | **32280.17** | 619.30 | 22720.17 |
| Standard Deviation | 437.21 | 8746.08 | 483.21 | 7522.37 |
| Coefficient of Variation | 54.89 | 27.09 | 78.02 | 33.11 |

**Table 8. Desorption Coefficients for Florpyrauxifen benzyl (XDE-848 Benzyl Ester) in Six Soils (MRID 49677710)**

| Soil | $K_{d\text{-}des}$ (L/kg) | $K_{OC\text{-}des}$ |
|---|---|---|
| Yolo Clay loam | 539.06 | 67382 |
| RefSol 03G Loam | 2488.81 | 50792 |
| Site E1 Silt loam | 2094.81 | 47609 |
| Site I2 Sandy loam | 854.83 | 38856 |
| Casalino Sandy loam | 1642.13 | 126318 |
| Ogori Clay loam | 1291.45 | 58702 |

Freundlich desorption coefficients $K_F$ and $K_{FOC}$ were not determined, since separate samples were prepared for the desorption study using a single nominal test concentration of 0.005 µg/mL.

### *Field Dissipation*

Three aquatic field dissipation studies appear to confirm what is predicted from the laboratory studies. In one study, rice plots in California[3] (water seeded) and Texas (dry seeded) were used. In California, an emulsifiable concentrate and a granular formulation (not currently proposed in any label) were studied; in Texas, only the EC formulation was tested. Each of the three plots received two applications of florpyrauxifen-benzyl at a rate which was at least twice the currently proposed label/application. In California, both applications occurred to the rice field on a clay loam soil, when it was wet (*i.e.*, flooded). In Texas, the florpyrauxifen-benzyl was firstly applied to dry soil, while the second application was on a wet soil (flooded). The soil was a sandy loam. The estimated half-lives in water for both applications of the EC formulation in CA were ~0.2 days. For the granular formulation, the water half-lives were 0.15-0.34 days. In soils, for the EC formulation, the first application half-life was 1.5 days and for the second application it was 23 days. For the granular formulation, the soil half-lives were 17-24 days. For the first application in TX, the water half-life does not apply (dry seeded), but for the soil, the half-life was 8.1 days. For the second application, the water half-life was 0.79 days, while the soil half-life could not be determined.

In addition, there are two field dissipation studies, representing the aquatics proposed use pattern. In the first study, conducted in Florida and North Carolina, applications of florpyrauxifen-benzyl were performed at 50 ppb. It is apparent that 50 ppb will be a typical rate of application directly to water for the aquatics use. In another study, the maximum proposed rate of 150 ppb was used; the study was conducted only in Florida. The water half-lives in FL and NC at 50 ppb for the parent compound were 1.4-2.3 days, which appears to confirm the results of the aerobic and anaerobic aquatic metabolism studies, which predicted half-lives for florpyrauxifen-benzyl on the order of about 2-6 days, depending on the testing conditions. Further, at 150 ppb, the parent's

[3] Note that according to the proposed labels, florpyrauxifen-benzyl *is not intended for use in California*.

half-life was about three times as high, with 6.4 days. Sediment half-lives could not be determined, due to variability and/or the small percentage of the total applied observed in the sediments.

### *Fish BCF*

Although the octanol/water partition coefficient (Log $K_{OW}$) for florpyrauxifen-benzyl is 5.5 at pH 7 and 20°C, and considered high, the fish BCF study yielded maximum BCF values of only 356 L/Kg wet weight (for whole fish), based on the total recovered radioactivity. Although the BCF for the parent only was not reported, it will be less than 356 L/kg. Further, the depuration $t_{1/2}$ was only 0.2-0.4 days for the total recovered residues, which means that the test substance is unlikely to remain in fish tissue for extended periods of time once exposure is stopped.

### *Transport / Water Exposure Summary*

Based on the degradation profile and the available data on the major degradates of florpyrauxifen-benzyl, the majority of the mass of parent is expected to reach paddy water/soil, while a smaller amount is expected to reach adjacent surface water by drift (maximum default value for modeling is 13.5%). The majority of parent reaching paddy water/soil is expected to partition into the soil and in the paddy environment and degrade rather quickly [$t_{½}$ = 12-31 days in aerobic soil (flooded system), and 15-46 days in anaerobic soil environments; if the test substance is applied to dry soils, the half-lives will range from 8.9-67 days]. The following degradates are expected to form in the aquatic environments (based on the aerobic flooded and anaerobic soil metabolism studies): XDE-848 acid (estimated half-life of 14 days under aerobic conditions); XDE-848 benzyl hydroxy (estimated half-life of 87 days); and XDE-848 hydroxy acid (estimated half-lives of 127-729 days). Undegraded parent along with degradates listed above are expected to cause exposure to surface waters upon the release of paddy waters into surface water bodies.

Parent reaching water bodies by drift or applied directly to water (aquatics use), is expected to degrade rather quickly ($t_{½}$ = 4.0-6.2 days in aerobic aquatic, and 2.1-2.4 days in anaerobic aquatic environments), forming the following degradates (based on the aerobic and anaerobic aquatic metabolism): XDE-848 acid (estimated half-life of 6.3-18 days under aerobic conditions); XDE-848 benzyl hydroxy (estimated half-life of 6-14 days); and XDE-848 hydroxy acid (estimated half-life of 53-121 days aerobic; it was the terminal degradate under anaerobic conditions). Undegraded florpyrauxifen-benzyl, along with degradates listed above are expected to cause exposure to surface bodies of water impacted.

In cases where the surface water is clear, the following degradates may be observed (based on the aquatic photolysis study (pH 4 and sterilized natural water): Des-chloro XDE-848 benzyl ester (it did not further degrade in pH 4 water), and Des-chloro XDE-848 acid (no estimated half-life available). It should be noted that in the field, these dechlorinated degradation products were found to be minor in three aquatic field dissipation studies (representing rice use in two sites, and aquatics uses in two sites).

While water in rice paddies may leach into the subsurface, the degree of leaching is limited by the presence of impervious claypan soils. Rice growing areas are not considered to be highly

vulnerable to movement of pesticides into groundwater. Rice paddies are designed to hold water for extended periods of time, and the amount of leaching is expected to be low compared to that of vulnerable areas.

## Drinking Water Exposure Modeling

### *Model Description*

The Tier I Rice Model v1.0 relies on an equilibrium partitioning concept to provide conservative estimates of environmental concentrations resulting from application of pesticides to rice paddies. When a pesticide is applied to a rice paddy, the model assumes that it will instantaneously partition between a water phase and a sediment phase. The Tier I rice conceptual model is simplified to the Tier I Rice Model v1.0 (see Appendix I for derivation):

$$C_w = \frac{m_{ai}'}{0.00105 + 0.00013K_d} \quad (1)$$

Where, in this case:

$C_w$ = water concentration [µg/L]
$m_{ai}'$ = mass applied per unit area [kg/ha]
$K_d$ = water-sediment partitioning coefficient [L/kg]

Model input values for the water-sediment partitioning coefficient ($K_d$) should represent a mean $K_d$ of relevant soil (or sediment). A mean $K_{oc}$ value should be used to generate model input values for $K_d$ in cases where sorption $K_d$ values correlate with soil organic matter content. In these cases, $K_d$ model input values should be calculated from the mean $K_{oc}$ using a fraction of organic carbon ($f_{oc}$) of 0.01. $K_d$ can thus be estimated by the following equations:

$$K_d = f_{oc}K_{oc} \quad (2)$$

$$K_d = 0.01K_{oc} \quad (3)$$

Alternatively, mean $K_{OC}$ values can be directly entered into equation (4):

$$C_w = \frac{m_{ai}'}{0.00105 + 0.0000013K_{oc}} \quad (4)$$

### *Modeling Approach and Input Parameters*

**Table 9** lists the input parameters for florpyrauxifen-benzyl, for the use on rice.

**Table 9. Tier I Rice Model v1.0 input parameters for Florpyrauxifen-benzyl**

| Input Parameter | Value | Justification | Source |
|---|---|---|---|
| Application Rate (kg a.i./ha) | 0.0600 | 0.0300 kg a.i./ha x 2 applications/year | Proposed label |
| Soil-to-Water Partition Coefficient ($K_d$) (L/kg) | 322.8 | Mean $K_{OC}$ (32,280 L/kg$_{OC}$) x 1% organic carbon content = 322.8 L/kg | MRID 49677710 |

### *Modeling Results*

Using **Equation 1**, for the rice use, the Tier 1 Rice Model v.1.0 EDWC is 1.4 ppb of florpyrauxifen-benzyl, which can be used for both acute and chronic exposure. For the aquatics use, the EDWC is 150 ppb, based on the maximum application rate in aquatics use sites (**Table 9**).

**Table 10. Maximum surface waters Estimated Drinking Water Concentrations (EDWCs) for drinking water risk assessment based on aerial application of florpyrauxifen-benzyl on rice and in water application to aquatics use sites**

| Use | Acute (ppb) | Chronic (ppb) |
|---|---|---|
| Rice at maximum rate of 0.060 kg a.i./ha/season (Tier 1 Rice Model v.1.0) | 1.4 | ≤1.4 |
| Aquatics use pattern at maximum rate of 150 ppb/season | 150 | ≤150 |

The estimated concentrations provided in this assessment are conservative estimates of concentrations in drinking water. If dietary risks require refinement, higher tiered crop-specific and location-specific models and modeling scenarios can be used.

### *Monitoring Data*

Since this is a new chemical, no monitoring data would be found.

## CONCLUSIONS

This is a Tier 1 drinking water assessment for the residues of florpyrauxifen-benzyl. Should any degradates need to be included, the EDWCs for the rice use may be expressed as a range of values, representing the included degradates. For the aquatics use pattern, the EDWCs were based on the maximum application rate allowed in the label. For the rice use pattern, the Tier 1 Rice Model v.1.0 was used. A more definitive drinking surface water assessment may be performed with the use of the Tier 2 aquatic model PFAM v.2.0.

For the aquatics use pattern, the EDWCs are unrefined/very rough estimates, given that EFED was told that HED is going to perform a qualitative assessment for florpyrauxifen-benzyl.

The following notes and/or uncertainties are cited by the Tier 1 Rice Model v.1.0 guidance. It should be noted that the results of the rice model were based on the parent compound only: Neither the degradation of the pesticide nor the mass transfer from the aqueous phase to the

sediment is considered in this conceptualization, which greatly simplifies the model. The absence of degradation adds conservatism to the model (*i.e.*, estimated concentrations should be higher than those usually found in rice paddies). The absence of mass transfer processes can either add or reduce conservatism depending on numerous conditions such as whether the pesticide is soil or water applied and whether actual degradation occurs preferentially in the sediment or the water compartment; however, consideration of this parameter is a refinement beyond a Tier I conceptualization. Most of the assumptions used in this model help ensure that the outputs are protective of most environments associated with rice agriculture. The model assumptions include the following:

1. Movement of pesticide on suspended sediment is not considered.
2. Degradation does not occur.
3. Volatilization and other dissipation processes are not considered.
4. Partitioning to sediment is instantaneous.
5. Water is available for human or wildlife exposure instantaneously.
6. Water column depth is 10 cm.
7. Sediment depth is 1 cm.
8. All pore space is saturated with water.
9. Organic carbon fraction is 0.01.
10. Bulk density is 1300 $kg/m^3$.
11. Grain density is 2650 $kg/m^3$.

Tier I model estimates are screening estimates and, as such, are expected to exceed peak values found in the environment in most cases. This expectation is due to the protective assumptions of the model listed above, such as exclusion of degradation as well as dilution with uncontaminated water outside the paddy. Evaluation of the Tier I Rice Model v1.0 indicates that modeled within-paddy estimates are conservative, exceeding peak measured concentrations of pesticides in water bodies well downstream of rice paddies by less than one order of magnitude to multiple orders of magnitude. The range of modeled estimate exceedances over measured concentrations is most likely in response to chemical, environmental, and study-specific factors.

Estimates from the Tier I model generally do not represent typical concentrations found in human drinking water, as they represent paddy discharge water. However, these concentrations may be a reasonable estimate of acute concentrations for use in ecological assessment where exposure occurs at or near the rice paddy. In both cases, human drinking water and ecological exposure, the chronic concentrations as well as offsite concentrations are expected to be conservative. A higher tier rice model should be used to estimate chronic exposure to compounds that degrade rapidly into degradates that are not of risk concern. For florpyrauxifen-benzyl under aquatic conditions, the parent alone degrades at moderate rates; however, if XDE-848 acid and/or other degradates are to be included, the degradation of the total toxic residues would proceed more slowly.

If Tier I estimates calculated by this screening method do not exceed the level of concern in a risk assessment, there is high confidence that there will be little or no risk above the level of concern from exposure through water resources. However, because of the uncertainties associated with a screening method, when a level of concern is exceeded it cannot be determined whether the

exceedance will in fact occur or whether this method has overestimated the exposure.

### *Water Treatment*

It is likely that primary treatment *may* reduce the levels of florpyrauxifen-benzyl due to its tendency to bind. However, there is no information available at this time to determine the levels of reduction. Furthermore, the softening of drinking water will generally result in an increase in pH. Florpyrauxifen-benzyl is more susceptible to hydrolysis under alkaline conditions; therefore, softening *may* result in increased dissipation from hydrolysis, and consequently possible formation of XDE-848 acid (USEPA 2011).

## REFERENCES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## Appendix A. Structures and Further Information of Florpyrauxifen-benzyl and its Transformation Products

### *Major Degradation Products*

XDE-848 acid (maximum observed: up to 99.5% in the pH 9 hydrolysis study at 35°C): This compound results from the hydrolysis of the ester moiety of the parent compound (which results in an acid and an alcohol). It does not have the benzyl ring from the parent in its structure. This compound was a major degradate in many of the studies, including hydrolysis and metabolism. It was also an important component in fish tissue. XDE-848 acid was found to be stable to hydrolysis at a range of pH values. *Estimated* decline half-lives from the available studies are: 41-121 days in the aerobic soil metabolism study; 14 days in one of the soils of the aerobic soil flooded metabolism study; and 6-18 days in the aerobic aquatic metabolism study.

There is a batch equilibrium study that gives information on the mobility of three of the degradates of florpyrauxifen benzyl: for XDE-848 acid the mean $K_{OC}$ = 71.8 L/kg$_{OC}$; for XDE-848 hydroxy acid the mean $K_d$ = 1.91 L/kg; and for XDE-848 hydroxy benzyl ester (or benzyl hydroxy) the mean $K_d$ = 118 L/kg. All three degradates appear to be more mobile than the parent compound.

**Table A-1. Adsorption Coefficients for XDE-848 Acid (MRID 49677709)**

| Soil | $K_d$ (L/kg) | $K_{OC}$ (L/kg$_{OC}$) | $K_F$ (L/kg) | $K_{FOC}$ (L/kg$_{OC}$) |
|---|---|---|---|---|
| Yolo Clay loam | 0.38 | 48 | 0.49 | 62 |
| Ogori clay loam | 2.82 | 128 | 3.02 | 137 |
| RefSol 03-G Loam | 1.38 | 28 | 1.48 | 30 |
| Site E1 Silt loam | 1.56 | 35 | 1.73 | 39 |
| RefSol 01-A Loamy sand | 0.71 | 65 | 0.83 | 76 |
| Site K Loam | 1.64 | 50 | 1.83 | 56 |
| San Pietro Loam | 2.18 | 136 | 2.37 | 148 |
| Casalino Sandy loam | 2.27 | 174 | 2.54 | 196 |
| Site I2 Sandy loam | 0.55 | 25 | 0.67 | 31 |
| Centerville Clay loam | 0.21 | 41 | 0.26 | 52 |
| Bernard-Edna Sandy clay loam | 0.36 | 89 | 0.45 | 113 |
| Site Fr3 Sandy loam | 0.86 | 45 | 0.99 | 52 |
| Site Sp4 Silty clay | 2.39 | 68 | 2.51 | 72 |
| **Mean** | 1.33 | **71.8** | 1.48 | 81.8 |
| Standard Deviation | 0.89 | 46.9 | 0.93 | 51.2 |
| Coefficient of Variation (%) | 86.6 | 65.3 | 63.0 | 62.7 |

XDE-848 benzyl hydroxy (maximum observed: 43.1% AR in one of the anaerobic aquatic metabolism studies): This compound results from the loss of a methyl group, but it keeps the ester moiety of the parent compound (*i.e.*, it has the benzyl ring in its structure). It was a major degradate in metabolism studies involving flooded soils or sediments (aerobic or anaerobic). Estimated decline half-lives were 87 days for one of the aerobic soil metabolism study (flooded system) and 6-14 days in the aerobic aquatic metabolism study.

**Table A-2. Adsorption Coefficients for XDE-848 Hydroxy Benzyl Ester (MRID 49677709)**

| Soil | $K_d$ (L/kg) | $K_{OC}$ (L/kg$_{OC}$) | $K_F$ (L/kg) | $K_{FOC}$ (L/kg$_{OC}$) |
|---|---|---|---|---|
| Yolo Clay loam | 10.14 | 1268 | 10.51 | 1314 |
| Ogori clay loam | 149.34 | 6788 | 123.72 | 5624 |
| RefSol 03-G Loam | 330.65 | 6748 | 285.97 | 5836 |
| Site E1 Silt loam | 272.64 | 6196 | 226.77 | 5154 |
| RefSol 01-A Loamy sand | 72.39 | 6581 | 67.91 | 6174 |
| Site K Loam | 26.51 | 803 | 25.68 | 778 |
| San Pietro Loam | 368.38 | 23024 | 273.06 | 17066 |
| Casalino Sandy loam | 184.87 | 14221 | 160.61 | 12355 |
| Site I2 Sandy loam | 33.56 | 1525 | 30.00 | 1364 |
| Centerville Clay loam | 3.85 | 770 | 4.22 | 845 |
| Bernard-Edna Sandy clay loam | 10.15 | 2538 | 10.21 | 2552 |
| Site Fr3 Sandy loam | 19.59 | 1031 | 19.42 | 1022 |
| Site Sp4 Silty clay | 52.67 | 1505 | 49.07 | 1402 |
| **Mean** | **118.1** | 5615.2 | 99.0 | 4729.6 |
| Standard Deviation | 130.7 | 6523.6 | 104.3 | 4882.4 |
| Coefficient of Variation (%) | 110.7 | 116.2 | 105.4 | 105.3 |

XDE-848 hydroxy acid (maximum observed: up to 104.4% AR at 80 days in the anaerobic aquatic metabolism study): This compound results from the hydrolysis of the ester moiety of XDE-848 benzyl hydroxy. It does not have the benzyl ring in its structure and keeps two of the rings of the parent compound. It was a major degradate in all the metabolism studies involving flooded soils or aquatic sediments. This degradate appeared to persist longer than other degradates in the studies where decline could be calculated: 127-729 days in the aerobic soil metabolism (flooded), 51-121 days in the aerobic aquatic metabolism study, and it appears to be the terminal degradate of the anaerobic soil and aquatic metabolism test systems.

**Table A-3. Adsorption Coefficients for XDE-848 Hydroxy Acid (MRID 49677709)**

| Soil | $K_d$ (L/kg) | $K_{OC}$ (L/kg$_{OC}$) | $K_F$ (L/kg) | $K_{FOC}$ (L/kg$_{OC}$) |
|---|---|---|---|---|
| Yolo Clay loam | 0.14 | 18 | 0.20 | 25 |
| Ogori clay loam | 5.19 | 236 | 4.38 | 199 |
| RefSol 03-G Loam | 1.41 | 29 | 1.40 | 29 |
| Site E1 Silt loam | 2.21 | 50 | 2.10 | 48 |
| RefSol 01-A Loamy sand | 1.20 | 109 | 1.20 | 109 |
| Site K Loam | 0.47 | 14 | 0.50 | 15 |
| San Pietro Loam | 4.07 | 255 | 3.63 | 227 |
| Casalino Sandy loam | 3.51 | 270 | 3.21 | 247 |
| Site I2 Sandy loam | 0.46 | 21 | 0.47 | 21 |
| Centerville Clay loam | 0.15 | 30 | 0.15 | 31 |
| Bernard-Edna Sandy clay loam | 0.46 | 116 | 0.49 | 121 |
| Site Fr3 Sandy loam | 3.11 | 164 | 2.96 | 156 |
| Site Sp4 Silty clay | 2.48 | 71 | 2.43 | 69 |
| **Mean** | **1.91** | 106.3 | 1.78 | 99.8 |
| Standard Deviation | 1.66 | 95.2 | 1.44 | 83.5 |
| Coefficient of Variation (%) | 86.8 | 89.6 | 80.8 | 83.7 |

Des-chloro XDE-848 benzyl ester (maximum observed: 30.8% AR in the pH 4 aqueous photolysis study): Results from the photolysis of the parent compound. It loses a Cl atom in the structure, which is substituted by a hydrogen atom. Its structure keeps all three rings from the

parent compound. This transformation product was observed in both the aqueous and soil photolysis studies, but it was only a minor component in the soil photolysis study.

*Other Degradation Products*

Des-chloro XDE-848 acid (maximum observed: 10.4% in the aqueous photolysis study at pH 4): It is the product of the hydrolysis of Des-chloro XDE-848 benzyl ester, resulting in an acid moiety. Its structure keeps only two of the three rings from the parent compound. This degradate was observed in the aqueous and soil photolysis studies, but it exceeded 10% AR only in the pH 4 aqueous photolysis study.

Nitro hydroxy acid (X12483137) (maximum observed: 11.1% in one of the soils of the aerobic soil metabolism studies): It is a major product of the aerobic soil metabolism study (one of the soils, and minor in the remaining soils).

Benzyl alcohol (maximum observed: 100% in pH 9 hydrolysis study at 25°C): Major product of the hydrolysis and the aqueous photolysis studies. Appeared to be the terminal degradate of the hydrolysis study.

Benzoic acid (maximum observed: 21.3% in the aerobic aquatic metabolism study): Major product of the aerobic and anaerobic aquatic metabolism studies. For the benzyl labeled studies, oftentimes the recovered radioactivity fell below guideline criteria (<90% AR), and the study author attributed it to possible loss of carbon dioxide.

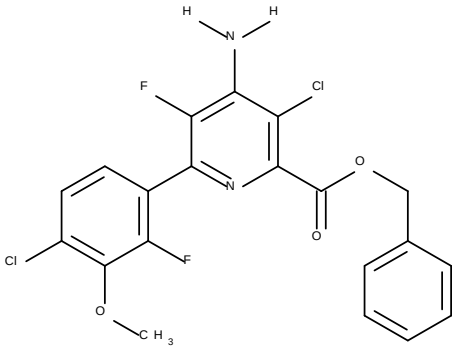
X12421263 (maximum observed: 6.1% in the pH 4 aqueous photolysis study): Minor product in the aqueous photolysis study at pH 4 (not observed in natural water, and not detected by the end of the pH 4 study).

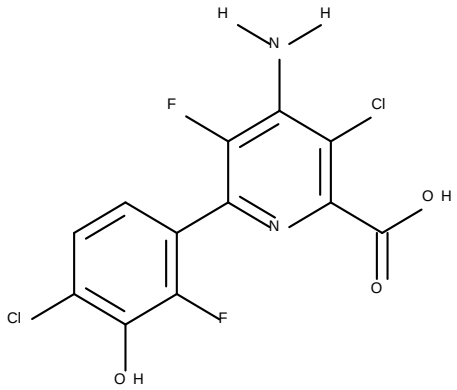
Taurine conjugate of XDE-848 acid: It was observed in minor amounts in fish tissue in the Fish BCF study.

Four unidentified degradates (at ~10-13% AR): Two of which were observed in the aqueous photolysis study, and the other two were observed in the anaerobic aquatic metabolism study.

Carbon dioxide: It was a major product in many of the metabolism studies, especially for the benzyl labeled test substance.

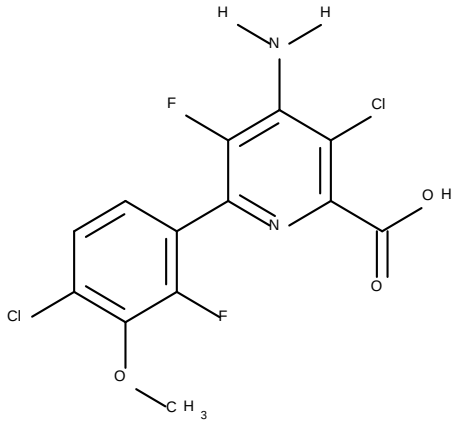
**Table A-4. Florpyrauxifen-benzyl (XDE-848 Benzyl Ester, Rinskor™) and Its Environmental Transformation Products[A]**

| Code Name/Synonym | Chemical Name | Chemical Structure | Study Type | MRID | Maximum %AR (day) | Final %AR (study length) |
|---|---|---|---|---|---|---|
| **PARENT** | | | | | | |
| **Florpyrauxifen-benzyl (XDE-848 Benzyl Ester, Rinskor™, XR-848-BE, XR-848 Benzyl, X11959130, TSN301734)** | **IUPAC:** Benzyl 4-amino-3-chloro-6-(4-chloro-2-fluoro-3-methoxy-phenyl)-5-fluoro-pyridine-2-carboxylate<br><br>**Formula:** $C_{20}H_{14}Cl_2F_2N_2O_3$<br>**MW:** 439.24 g/mol<br>**SMILES:** [H]N([H])c1c(c(nc(c1Cl)C(=O)OCc2ccccc2)c3ccc(c(c3F)OC)Cl)F |  | 835.2120 Hydrolysis | 49677711 | PRT | PRT |
| | | | 835.2240 Aqueous photolysis | 49677712 | | |
| | | | 835.2410 Soil photolysis | 49677714 | | |
| | | | 835.4100 Aerobic soil metabolism | 49677715 | | |
| | | | 835.4200 Anaerobic soil metabolism | 49677718 | | |
| | | | 835.4300 Aerobic aquatic metabolism | 49677716 | | |
| | | | | 49677719 | | |
| | | | 835.4400 Anaerobic aquatic metabolism | 49677720 | | |
| | | | 835.1230 Batch equilibrium | 49677710 | | |

| Code Name/Synonym | Chemical Name | Chemical Structure | Study Type | MRID | Maximum %AR (day) | | Final %AR (study length) |
|---|---|---|---|---|---|---|---|
| | | | 835.6200 Aquatic field dissipation | 49677721 | | | |
| | | | | 49677722 | | | |
| | | | | 49677723 | | | |
| | | | 850.1730 Fish BCF | 49677749 | | | |
| **MAJOR (>10%) TRANSFORMATION PRODUCTS** | | | | | | | |
| **Hydroxy acid (XDE-848 hydroxy acid, XR-848 hydroxy acid, X11966341, TSN301668, TSN305649, TSN306022, OHA)** | **IUPAC:** 4-Amino-3-chloro-6-(4-chloro-2-fluoro-3-hydroxy-phenyl)-5-fluoro-pyridine-2-carboxylic acid<br><br>**Formula:** $C_{12}H_6Cl_2F_2N_2O_3$<br>**MW:** 335.09 g/mol<br>**SMILES:** [H]N([H])c1c(c(nc(c1Cl)C(=O)O)c2ccc(c(c2F)O)Cl)F |  | 835.4100 Aerobic soil metabolism | 49677715 | California loam | 3.30% (59 d) | 3.11% (120 d) |
| | | | | | Germany Loam | 7.80% (30 d) | 1.41% (120 d) |
| | | | | | Silt loam | 6.38% (30 d) | 1.48% (120 d) |
| | | | | | Loamy sand | 4.10% (45 d) | 1.00% (120 d) |
| | | | 835.4200 Anaerobic soil metabolism | 49677718 | Clay loam | **58.3%** (126 d) | **58.3%** (126 d) |
| | | | | | Loam | **64.4%** (106 d) | **63.0%** (126 d) |
| | | | | | Silt loam | **61.5%** (106 d) | **61.4%** (126 d) |

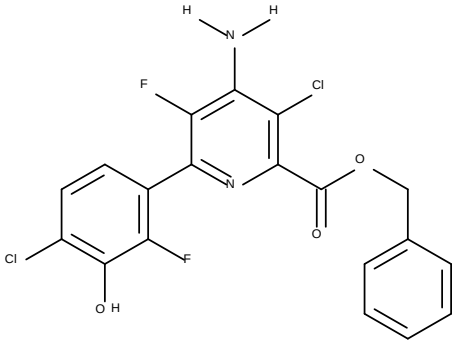
| Code Name/Synonym | Chemical Name | Chemical Structure | Study Type | MRID | Maximum %AR (day) | | | Final %AR (study length) |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | | |
| | | | | | Sandy loam | | **68.9%** (126 d) | **68.9%** (126 d) |
| | | | 835.4300 Aerobic aquatic metabolism | 49677716 | Water:loam | | **26.3%** (58 d) | **16.4%** (156 d) |
| | | | | | Water:sandy loam | | **64.2%** (72 d) | **57.8%** (156 d) |
| | | | | 49677719 | Lagoon water:loam | | **75.2%** (31 d) | **47.2%** (105 d) |
| | | | | | Lake water:loamy sand | | **78.3%** (59 d) | **44.8%** (105 d) |
| | | | 835.4400 Anaerobic aquatic metabolism | 49677720 | River water:loamy sand | | **104.4%** (80 d) | **97.4%** (105 d) |
| | | | | | Pond water:silt loam | | **100.0%** (13 d) | **94.3%** (105 d) |
| | | | 835.6200 Aquatic field dissipation | 49677721 | California EC formulation | Soil | **34.7%** (3 d, 1st Appl) | 0.8% (181 d) |
| | | | | | | Water | 0.1% (42 d, 2nd Appl) | NS (181 d) |
| | | | | | California Granular formulation | Soil | **12.2%** (3 d, 2nd Appl) | 1.0% (181 d) |

| Code Name/Synonym | Chemical Name | Chemical Structure | Study Type | MRID | Maximum %AR (day) | | | Final %AR (study length) |
|---|---|---|---|---|---|---|---|---|
| | | | | | | Water | 0.2% (1 d, 1st Appl) | NS (181 d) |
| | | | | | Texas | Soil | **13.4%** (28 d, 2nd Appl) | 0.0% (184 d) |
| | | | | | | Water | 0.1% (1, 3, 15 d, 2nd Appl) | NS (184 d) |
| | | | | 49677722 | Florida | Water | 6.8% (14 d) | 0.0% (282 d) |
| | | | | | North Carolina | Sediment | 0.37% (43 d) | Not analyzed (246 d) |
| | | | | | | Water | 2.7% (22 d) | 0.0% (246 d) |
| | | | | 49677723 | North Carolina | Sediment | 1.72% (92 d) | 0.0% (246 d) |
| | | | | | | Water | 3.7% (22 d) | 0.0% (246 d) |
| **XDE-848 acid (X11438848, TSN304667, TSN301691, 1552-A)** | **IUPAC:** 4-Amino-3-chloro-6-(4-chloro-2-fluoro-3-methoxy-phenyl)-5-fluoro-pyridine-2-carboxylic acid<br>**Formula:** $C_{13}H_8Cl_2F_2N_2O_3$<br>**MW:** 349.12 g/mol<br>**SMILES:** [H]N([H])c1c(c(nc(c1Cl)C(=O)O)c2ccc(c(c2F)OC)Cl)F | | 835.2120 Hydrolysis | 49677711 | pH 7 (10°C) | | 1.7% (30 d) | 1.7% (30 d) |
| | | | | | pH 9 (10°C) | | **89.6%** (30 d) | **89.6%** (30 d) |
| | | | | | pH 4 (25°C) | | 2.9% (30 d) | 2.9% (30 d) |

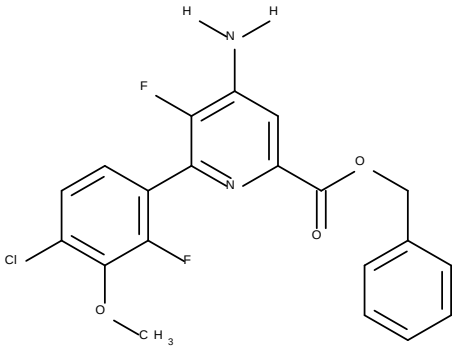
| Code Name/Synonym | Chemical Name | Chemical Structure | Study Type | MRID | Maximum %AR (day) | | Final %AR (study length) |
|---|---|---|---|---|---|---|---|
| | |  | | | pH 7 (25°C) | **16.6%** (30 d) | **16.6%** (30 d) |
| | | | | | pH 9 (25°C) | **98.5%** (30 d) | **98.5%** (30 d) |
| | | | | | pH 4 (35°C) | 5.9% (22 d) | 5.7% (30 d) |
| | | | | | pH 7 (35°C) | **41.1%** (30 d) | **41.1%** (30 d) |
| | | | | | pH 9 (35°C) | **99.5%** (30 d) | **99.5%** (30 d) |
| | | | | | pH 4 (50°C) | 5.1% (5 d) | 5.1% (5 d) |
| | | | | | pH 7 (50°C) | **46.6%** (5 d) | **46.6%** (5 d) |
| | | | | | pH 9 (50°C) | **98.6%** (5 d) | **98.6%** (5 d) |
| | | | 835.2240 Aqueous photolysis | 49677712 | Natural water | 8.9% (0.17 d) | 0.8% (15.91 d) |
| | | | 835.2410 Soil photolysis | 49677714 | Loam | 7.0% (10 d) | 6.7% (17 d) |
| | | | 835.4100 Aerobic soil metabolism | 49677715 | California loam | **39.71%** (30 d) | **19.67%** (120 d) |

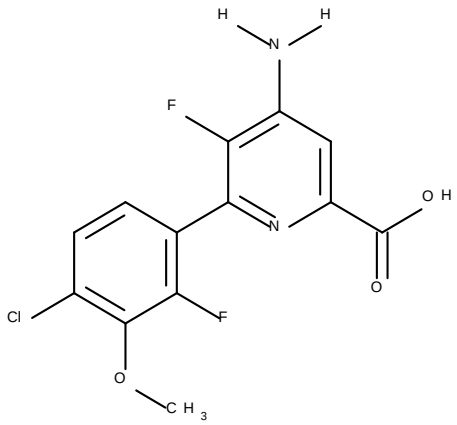
| Code Name/Synonym | Chemical Name | Chemical Structure | Study Type | MRID | Maximum %AR (day) | | Final %AR (study length) |
|---|---|---|---|---|---|---|---|
| | | | | | Germany Loam | **32.95%** (9 d) | 8.08% (120 d) |
| | | | | | Silt loam | **37.67%** (15 d) | **23.50%** (120 d) |
| | | | | | Loamy sand | **62.40%** (7 d) | 5.66% (120 d) |
| | | | 835.4200 Anaerobic soil metabolism | 49677718 | Clay loam | **61.3%** (26 d) | **22.2%** (126 d) |
| | | | | | Loam | **39.2%** (18 d) | 3.1% (126 d) |
| | | | | | Silt loam | **25.2%** (18 d) | 1.1% (126 d) |
| | | | | | Sandy loam | **73.5%** (26 d) | **16.8%** (126 d) |
| | | | 835.4300 Aerobic aquatic metabolism | 49677716 | Water:loam | 8.1% (6 d) | 0.4% (156 d) |
| | | | | | Water:sandy loam | **33.1%** (20 d) | 0.7% (156 d) |
| | | | | 49677719 | Lagoon water:loam | **30.6%** (3 d) | 1.6% (105 d) |
| | | | | | Lake water:loamy sand | **45.2%** (21 d) | 1.2% (105 d) |

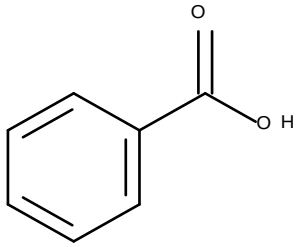
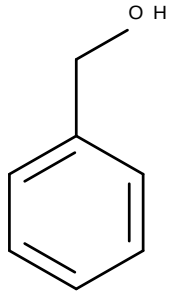
| Code Name/Synonym | Chemical Name | Chemical Structure | Study Type | MRID | Maximum %AR (day) | | | Final %AR (study length) |
|---|---|---|---|---|---|---|---|---|
| | | | 835.4400 Anaerobic aquatic metabolism | 49677720 | River water:loamy sand | | **27.9%** (7 d) | ND (105 d) |
| | | | | | Pond water:silt loam | | **46.9%** (3 d) | ND (105 d) |
| | | | 835.6200 Aquatic field dissipation | 49677721 | California EC formulation | Soil | **21.6%** (3 d, 1st Appl) | 0.9% (181 d) |
| | | | | | | Water | 3.9% (3 d, 1st Appl) | NS (181 d) |
| | | | | | California Granular formulation | Soil | **6.8%** (3 d, 1st Appl) | 0.5% (181 d) |
| | | | | | | Water | **13.7%** (1 d, 1st Appl) | NS (181 d) |
| | | | | | Texas | Soil | **12.3%** (7 d, 1st Appl) | 0.0% (184 d) |
| | | | | | | Water | 6.6% (1 d, 2nd Appl) | NS (184 d) |
| | | | | 49677722 | Florida | Sediment | 0.42% (14 d) | Not analyzed (282 d) |

| Code Name/Synonym | Chemical Name | Chemical Structure | Study Type | MRID | Maximum %AR (day) | | | Final %AR (study length) |
|---|---|---|---|---|---|---|---|---|
| | | | | | | Water | **17.4%** (14 d) | 0.0% (282 d) |
| | | | | | North Carolina | Water | **33.0%** (14 d) | 0.0% (246 d) |
| | | | | 49677723 | North Carolina | Water | **35.2%** (22 d) | 0.0% (246 d) |
| | | | 850.1730 Fish BCF | 49677749 | NA | | | NA |
| **Benzyl hydroxy (XDE-848 Hydroxy BE, X12300837, TSN302111, TSN305650, OHBE)** | **IUPAC:** Benzyl 4-amino-3-chloro-6-(4-chloro-2-fluoro-3-hydroxy-phenyl)-5-fluoro-pyridine-2-carboxylate<br><br>**Formula:** $C_{19}H_{12}Cl_2F_2N_2O_3$<br>**MW:** 425.21 g/mol<br>**SMILES:** [H]N([H])c1c(c(nc(c1Cl)C(=O)OCc2ccccc2)c3ccc(c(c3F)O)Cl)F |  | 835.4100 Aerobic soil metabolism | 49677715 | California loam | | 2.45% (0 d) | 1.11% (120 d) |
| | | | | | Germany Loam | | 2.49% (0 d) | 0.74% (120 d) |
| | | | | | Silt loam | | 2.50% (0 d) | 0.59% (120 d) |
| | | | | | Loamy sand | | 2.44% (0 d) | ND (120 d) |
| | | | 835.4300 Aerobic aquatic metabolism | 49677716 | Water:loam | | **15.9%** (30 d) | 6.8% (156 d) |
| | | | | | Water:sandy loam | | 6.5% (20 d) | 0.6% (156 d) |

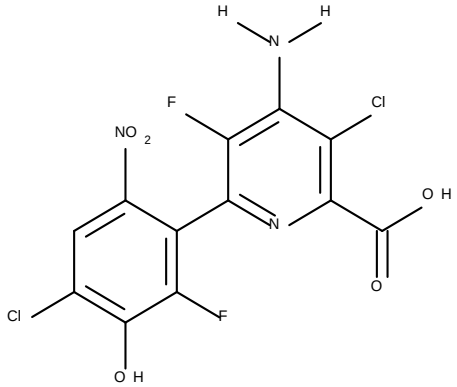
| Code Name/Synonym | Chemical Name | Chemical Structure | Study Type | MRID | Maximum %AR (day) | | | Final %AR (study length) |
|---|---|---|---|---|---|---|---|---|
| | | | | 49677719 | Lagoon water:loam | | **22.8%** (7 d) | 0.2% (105 d) |
| | | | | | Lake water:loamy sand | | **13.2%** (14 d) | 0.1% (105 d) |
| | | | 835.4400 Anaerobic aquatic metabolism | 49677720 | River water:loamy sand | | **21.5%** (10 d) | ND (105 d) |
| | | | | | Pond water:silt loam | | **43.1%** (10 d) | ND (105 d) |
| | | | 835.6200 Aquatic field dissipation | 49677721 | California EC formulation | Soil | 0.5% (3 d, 1st Appl) | 0.0% (181 d) |
| | | | | | California Granular formulation | Soil | **10.0%** (14 d, 2nd Appl) | 1.5% (181 d) |
| | | | | | | Water | 0.1% (1 d, 1st Appl) | NS (181 d) |
| | | | | | Texas | Water | 0.1% (1 d, 2nd Appl) | NS (184 d) |
| | | | | 49677722 | Florida | Water | 1.5% (14 d) | 0.0% (282 d) |
| | | | | | North Carolina | Sediment | 0.18% (125 d) | Not analyzed (246 d) |

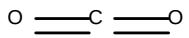
| Code Name/Synonym | Chemical Name | Chemical Structure | Study Type | MRID | Maximum %AR (day) | | | Final %AR (study length) |
|---|---|---|---|---|---|---|---|---|
| | | | | | | Water | 0.3% (7 d) | 0.0% (246 d) |
| | | | | 49677723 | North Carolina | Sediment | 0.52% (28 d) | 0.0% (246 d) |
| | | | | | | Water | 0.5% (22 d) | 0.0% (246 d) |
| **Des-chloro XDE-848 Benzyl Ester (De-Chloro BE, X12131932, TSN304946, DBE)** | **IUPAC:** Benzyl 4-amino-6-(4-chloro-2-fluoro-3-methoxy-phenyl)-5-fluoro-pyridine-2-carboxylate<br><br>**Formula:** $C_{20}H_{15}ClF_2N_2O_3$<br>**MW:** 404.79 g/mol<br>**SMILES:** [H]N([H])c1cc(nc(c1F)c2ccc(c(c2F)OC)Cl)C(=O)OCc3ccccc3 |  | 835.2240 Aqueous photolysis | 49677712 | pH 4 | | **30.8%** (0.17 d) | ND (17.99 d) |
| | | | | | Natural water | | **28.4%** (0.17 d) | ND (15.91 d) |
| | | | 835.2410 Soil photolysis | 49677714 | Loam | | 3.4% (1 d) | 2.9% (17 d) |
| | | | 835.6200 Aquatic field dissipation | 49677721 | California EC formulation | Water | 0.1% (0 d, 1st Appl) | NS (181 d) |
| | | | | | Texas | Water | 0.1% (0 d, 2nd Appl) | NS (184 d) |
| | | | | 49677722 | Florida | Water | 0.2% (0.04, 0.25, 0.5 d) | 0.0% (282 d) |
| | | | | | North Carolina | Sediment | 0.29% (125 d) | Not analyzed (246 d) |
| | | | | | | Water | 0.1% (0.04, 0.25, 0.5, 1, 1.5 d) | 0.0% (246 d) |
| | | | | 49677723 | North Carolina | Water | 0.2% (0.5, 1.5, 2 d) | 0.0% (246 d) |

| Code Name/Synonym | Chemical Name | Chemical Structure | Study Type | MRID | Maximum %AR (day) | | | Final %AR (study length) |
|---|---|---|---|---|---|---|---|---|
| **Des-chloro XDE-848 acid (De-Chloro Acid, X12393505, TSN304479, DA)** | **IUPAC:** 4-Amino-6-(4-chloro-2-fluoro-3-methoxy-phenyl)-5-fluoro-pyridine-2-carboxylic acid<br><br>**Formula:** $C_{13}H_9ClF_2N_2O_3$<br>**MW:** 314.67 g/mol<br>**SMILES:** [H]N([H])c1cc(nc(c1F)c2ccc(c(c2F)OC)Cl)C(=O)O |  | 835.2240 Aqueous photolysis | 49677712 | pH 4 | | **10.4%** (0.99 d) | ND (17.99 d) |
| | | | | | Natural water | | 8.4% (1.00 d) | 2.4% (15.91 d) |
| | | | 835.2410 Soil photolysis | 49677714 | Loam | | 2.8% (7 d) | 2.1% (17 d) |
| | | | 835.6200 Aquatic field dissipation | 49677721 | California EC formulation | Water | 0.2% (3 d, 1st Appl) | NS (181 d) |
| | | | | | California Granular formulation | Water | 0.4% (1 d, 1st Appl) | NS (181 d) |
| | | | | | Texas | Water | 0.1% (1-7 d, 2nd Appl) | NS (184 d) |
| | | | | 49677722 | Florida | Water | 0.2% (1.5, 3, 8 d) | 0.0% (282 d) |
| | | | | | North Carolina | Water | 0.2% (3, 7 d) | 0.0% (246 d) |
| | | | | 49677723 | North Carolina | Water | 0.2% (7, 14, 22 d) | 0.0% (246 d) |

| Code Name/Synonym | Chemical Name | Chemical Structure | Study Type | MRID | Maximum %AR (day) | | Final %AR (study length) |
|---|---|---|---|---|---|---|---|
| | | | 850.1730 Fish BCF | 49677749 | NA | | NA |
| **Benzoic acid (X194973)** | **IUPAC:** Benzoic acid<br><br>**Formula:** $C_7H_6O_2$<br>**MW:** 122.12 g/mol<br>**SMILES:** c1ccc(cc1)C(=O)O |  | 835.4300 Aerobic aquatic metabolism | 49677719 | Lagoon water:loam | **21.3%** (10 d) | ND (105 d) |
| | | | | | Lake water:loamy sand | **10.7%** (14 d) | ND (105 d) |
| | | | 835.4400 Anaerobic aquatic metabolism | 49677720 | River water:loamy sand | 7.4% (7 d) | ND (105 d) |
| | | | | | Pond water:silt loam | **20.2%** (10 d) | ND (105 d) |
| **Benzyl alcohol (Phenyl methanol, X195023, TSN305834)** | **IUPAC:** Benzyl alcohol<br><br>**Formula:** $C_7H_8O$<br>**MW:** 108.14 g/mol<br>**SMILES:** c1ccc(cc1)CO |  | 835.2120 Hydrolysis | 49677711 | pH 7 (10°C) | 2.7% (30 d) | 2.7% (30 d) |
| | | | | | pH 9 (10°C) | **90.7%** (30 d) | **90.7%** (30 d) |
| | | | | | pH 4 (25°C) | 2.0% (30 d) | 2.0% (30 d) |
| | | | | | pH 7 (25°C) | **20.1%** (30 d) | **20.1%** (30 d) |

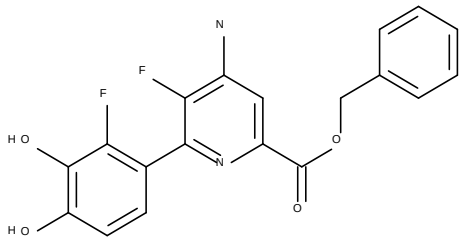
| Code Name/Synonym | Chemical Name | Chemical Structure | Study Type | MRID | Maximum %AR (day) | | Final %AR (study length) |
|---|---|---|---|---|---|---|---|
| | | | | | pH 9 (25°C) | **100.0%** (30 d) | **100.0%** (30 d) |
| | | | | | pH 4 (35°C) | 5.3% (30 d) | 5.3% (30 d) |
| | | | | | pH 7 (35°C) | **51.5%** (30 d) | **51.5%** (30 d) |
| | | | | | pH 9 (35°C) | **100.0%** (30 d) | **100.0%** (30 d) |
| | | | 835.2240 Aqueous photolysis | 49677712 | pH 4 | **67.5%** (7.01 d) | **59.7%** (17.93 d) |
| | | | | | Natural water | **81.5%** (6.90 d) | **75.7%** (15.88 d) |
| | | | 835.4400 Anaerobic aquatic metabolism | 49677720 | River water:loamy sand | 8.2% (7 d) | ND (105 d) |
| **X12483137 (TSN307911, Nitro hydroxy acid, or 6-Nitro hydroxy acid)** | **IUPAC:** 4-Amino-3-chloro-6-(4-chloro-2-fluoro-3-hydroxy-6-nitro-phenyl)-5-fluoro-pyridine-2-carboxylic acid<br><br>**Formula:** $C_{12}H_5Cl_2F_2N_3O_5$<br>**MW:** 380.09 g/mol<br>**SMILES:** [H]N([H])c1c(c(nc(c1Cl)C(=O)O)c2c(cc(c(c2F)O)Cl)[N+](=O)[O-])F | | 835.4100 Aerobic soil metabolism | 49677715 | California loam | 8.26% (120 d) | 8.26% (120 d) |
| | | | | | Germany Loam | 8.33% (120 d) | 8.33% (120 d) |

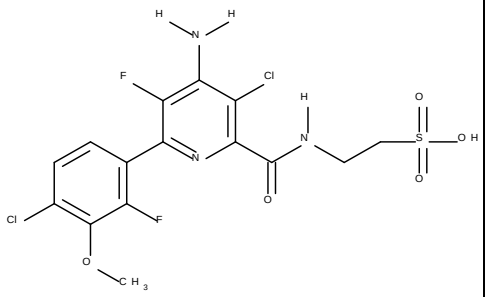
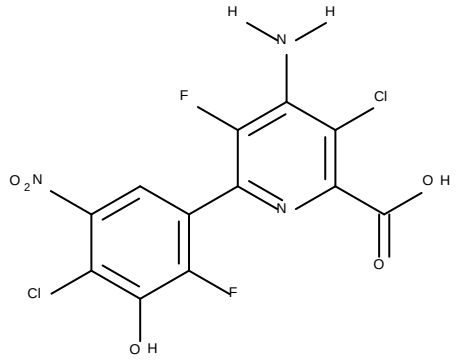
| Code Name/Synonym | Chemical Name | Chemical Structure | Study Type | MRID | Maximum %AR (day) | | Final %AR (study length) |
|---|---|---|---|---|---|---|---|
| | |  | | | Silt loam | **11.14%** (80 d) | **10.18%** (120 d) |
| **Unknown (Rt 12:20-12:40)** | NA | Structure not provided | 835.2240 Aqueous photolysis | 49677712 | pH 4 | **13.0%** (1.08, 2.01 d) | 8.0% (17.93 d) |
| **Unknown (Rt 22:50-23:00)** | NA | Structure not provided | 835.2240 Aqueous photolysis | 49677712 | pH 4 | **12.7%** (4.01 d) | 8.8% (17.93 d) |
| **Unknown M7** | NA | Structure not provided | 835.4400 Anaerobic aquatic metabolism | 49677720 | River water:loamy sand | **9.6%** (0.33 d) | ND (105 d) |

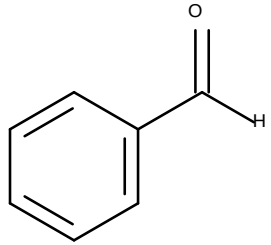
| Code Name/Synonym | Chemical Name | Chemical Structure | Study Type | MRID | Maximum %AR (day) | | Final %AR (study length) |
|---|---|---|---|---|---|---|---|
| **Unknown M10** | NA | Structure not provided | 835.4400 Anaerobic aquatic metabolism | 49677720 | Pond water:silt loam | **12.9%** (10 d) | ND (105 d) |
| **Carbon dioxide** | **IUPAC:** Carbon dioxide<br><br>**Formula:** $CO_2$<br>**MW:** 44 g/mol<br>**SMILES:** C(=O)=O |  | 835.2240 Aqueous photolysis | 49677712 | pH 4 | **44.0%** (17.99 d) | **44.0%** (17.99 d) |
| | | | | | Natural water | **37.5%** (15.91 d) | **37.5%** (15.91 d) |
| | | | 835.2410 Soil photolysis | 49677714 | Loam | **13.2%** (17 d) | **13.2%** (17 d) |
| | | | 835.4100 Aerobic soil metabolism | 49677715 | California loam | **46.58%** (120 d) | **46.58%** (120 d) |
| | | | | | Germany Loam | **59.13%** (120 d) | **59.13%** (120 d) |
| | | | | | Silt loam | **64.06%** (120 d) | **64.06%** (120 d) |
| | | | | | Loamy sand | **64.25%** (120 d) | **64.25%** (120 d) |
| | | | 835.4200 Anaerobic soil metabolism | 49677718 | Clay loam | **47.2%** (106 d) | **14.5%** (126 d) |
| | | | | | Loam | **41.0%** (126 d) | **41.0%** (126 d) |

| Code Name/Synonym | Chemical Name | Chemical Structure | Study Type | MRID | Maximum %AR (day) | | Final %AR (study length) |
|---|---|---|---|---|---|---|---|
| | | | | | Silt loam | **45.8%** (126 d) | **45.8%** (126 d) |
| | | | | | Sandy loam | **45.0%** (106 d) | **44.4%** (126 d) |
| | | | 835.4300 Aerobic aquatic metabolism | 49677716 | Water:loam | **37.6%** (156 d) | **37.6%** (156 d) |
| | | | | | Water:sandy loam | **71.5%** (156 d) | **71.5%** (156 d) |
| | | | | 49677719 | Lagoon water:loam | **67.34%** (105 d) | **67.34%** (105 d) |
| | | | | | Lake water:loamy sand | **80.67%** (91 d) | **75.61%** (105 d) |
| | | | 835.4400 Anaerobic aquatic metabolism | 49677720 | River water:loamy sand | **49.1%** (105 d) | **49.1%** (105 d) |
| | | | | | Pond water:silt loam | **55.1%** (82 d) | **52.5%** (105 d) |
| **Unextracted residues** | NA | NA | 835.2410 Soil photolysis | 49677714 | Loam | **15.3%** (17 d) | **15.3%** (17 d) |
| | | | 835.4100 Aerobic soil metabolism | 49677715 | California loam | **32.92%** (120 d) | **32.92%** (120 d) |

| Code Name/Synonym | Chemical Name | Chemical Structure | Study Type | MRID | Maximum %AR (day) | | Final %AR (study length) |
|---|---|---|---|---|---|---|---|
| | | | | | Germany Loam | **56.84%** (120 d) | **56.84%** (120 d) |
| | | | | | Silt loam | **53.09%** (80 d) | **52.69%** (120 d) |
| | | | | | Loamy sand | **80.58%** (120 d) | **80.58%** (120 d) |
| | | | 835.4200 Anaerobic soil metabolism | 49677718 | Clay loam | **19.9%** (18 d) | 9.2% (126 d) |
| | | | | | Loam | **40.0%** (81 d) | **23.9%** (126 d) |
| | | | | | Silt loam | **31.3%** (81 d) | **29.4%** (126 d) |
| | | | | | Sandy loam | **35.0%** (12 d) | **24.0%** (126 d) |
| | | | 835.4300 Aerobic aquatic metabolism | 49677716 | Water:loam | **61.0%** (156 d) | **61.0%** (156 d) |
| | | | | | Water:sandy loam | **36.3%** (93 d) | **33.1%** (156 d) |
| | | | | 49677719 | Lagoon water:loam | **42.12%** (105 d) | **42.12%** (105 d) |

| Code Name/Synonym | Chemical Name | Chemical Structure | Study Type | MRID | Maximum %AR (day) | | Final %AR (study length) |
|---|---|---|---|---|---|---|---|
| | | | | | Lake water:loamy sand | **44.27%** (91 d) | **38.93%** (105 d) |
| | | | 835.4400 Anaerobic aquatic metabolism | 49677720 | River water:loamy sand | **12.8%** (3, 10 d) | 8.8% (105 d) |
| | | | | | Pond water:silt loam | **11.8%** (41 d) | **9.9%** (105 d) |
| **MINOR (<10%) TRANSFORMATION PRODUCTS** | | | | | | | |
| **X12421263 (TSN305953)** | **IUPAC:** Benzyl 4-amino-5-fluoro-6-(2-fluoro-3,4-dihydroxy-phenyl)pyridine-2-carboxylate<br><br>**Formula:** $C_{19}H_{14}F_2N_2O_4$<br>**MW:** 372.32 g/mol<br>**SMILES:** c1ccc(cc1)COC(=O)c2cc(c(c(n2)c3ccc(c(c3F)O)O)F)N |  | 835.2240 Aqueous photolysis | 49677712 | pH 4 | 6.1% (0.17 d) | ND (17.99 d) |

| Code Name/Synonym | Chemical Name | Chemical Structure | Study Type | MRID | Maximum %AR (day) | Final %AR (study length) |
|---|---|---|---|---|---|---|
| **Taurine conjugate of XDE-848 acid (Taurine conjugate of X11433848)** | **IUPAC:** 2-[[4-Amino-3-chloro-6-(4-chloro-2-fluoro-3-methoxy-phenyl)-5-fluoro-pyridine-2-carbonyl]amino]ethanesulfonic acid<br><br>**Formula:** $C_{15}H_{13}Cl_2F_2N_3O_5S$<br>**MW:** 456.25 g/mol<br>**SMILES:** [H]N([H])c1c(c(nc(c1Cl)C(=O)N([H])CCS(=O)(=O)O)c2ccc(c(c2F)OC)Cl)F |  | 850.1730 Fish BCF | 49677749 | NA | NA |
| **REFERENCE COMPOUNDS NOT IDENTIFIED** | | | | | | |
| **YC7-146847-39** | **IUPAC:** 4-Amino-3-chloro-6-(4-chloro-2-fluoro-3-hydroxy-5-nitro-phenyl)-5-fluoro-pyridine-2-carboxylic acid<br><br>**Formula:** $C_{12}H_5Cl_2F_2N_3O_5$<br>**MW:** 380.09 g/mol<br>**SMILES:** [H]N([H])c1c(c(nc(c1Cl)C(=O)O)c2cc(c(c(c2F)O)Cl)[N+](=O)[O-])F |  | 835.4100 Aerobic soil metabolism | 49677715 | NA | NA |

| Code Name/Synonym | Chemical Name | Chemical Structure | Study Type | MRID | Maximum %AR (day) | Final %AR (study length) |
|---|---|---|---|---|---|---|
| **Benzaldehyde** | **IUPAC:** Benzaldehyde<br><br>**Formula:** $C_7H_6O$<br>**MW:** 106.12 g/mol<br>**SMILES:** [H]C(=O)c1ccccc1 |  | 835.4400 Anaerobic aquatic metabolism | 49677720 | NA | NA |

[A] AR means “applied radioactivity”. MW means “molecular weight”. PRT means “parent”. ND means “not detected”. NA means “not applicable”. EC means “emulsifiable concentrate”. Appl means “Application”. BCF means “bioconcentration factor”. NS means “no sample”.