ENVIRONMENTAL ASSESSMENT

1. **Date:** February 12, 2016

2. **Name of Applicant/Petitioner:** Biosan LLC

3. **Address:**
   - 3 Duplainville Road
   - Saratoga Springs, New York 12866
   - Lewis & Harrison LLC (Agent)
   - 122 C Street NW Suite 505
   - Washington DC 20001

4. **Description of Proposed Action:**

   **A. Requested Action**

   This Food Contact Notification (FCN) requests the clearance of a food-contact substance (FCS) that is an aqueous solution containing peroxyacetic acid (PAA), hydrogen peroxide (HP), acetic acid (AA), hydroxyethylidene 1,1-diphosphonic acid (HEDP), dipicolinic acid (DPA), and optionally, sulfuric acid. The FCS will be used in food processing facilities as an antimicrobial agent used in:

   (1) Process water applied as a spray, wash, rinse, dip, chiller water, low-temperature (e.g., less than 40°F) immersion baths, or scald water for whole or cut poultry carcasses, parts, trim, and organs.
   (2) Process water or ice used for washing, rinsing, or cooling whole or cut meat, including carcasses, parts, trim, and organs;
   (3) Process water, ice, or brine used for washing, rinsing, or cooling of processed and pre-formed meat as defined in 21 CFR § 170.3(n)(29) and poultry as defined in 21 CFR § 170.3(n)(34); and,
   (4) Process water for washing or chilling fruits and vegetables in food processing facilities.

   The FCS is a concentrate that must be diluted prior to use. The concentrations of the FCS components in process water are summarized below:

   - For use in spray, wash, rinse, dip, chiller water, low-temperature (e.g., less than 40°F) immersion baths and scald water for whole or cut poultry carcasses, parts, trim, skin on or off, and organs, the maximum concentrations requested are 2000 ppm.
peroxyacetic acid, 933 ppm hydrogen peroxide, 120 ppm HEDP, and 0.5 ppm DPA. The FCS also contains acetic acid as required to stabilize the solution and optionally sulfuric acid.

- For whole or cut meat applications, the maximum concentrations requested are 400 ppm peroxyacetic acid, 187 ppm hydrogen peroxide, 24 ppm HEDP and 0.5 ppm DPA. The FCS also contains acetic acid as required to stabilize the solution and optionally sulfuric acid.

- For processed and pre-formed meat as defined in 21 CFR 170.3(n)(29) and poultry as defined in 21 CFR 170.3(n)(34), the maximum concentrations requested are 230 ppm peroxyacetic acid, 107 ppm hydrogen peroxide, 14 ppm HEDP, and 0.1 ppm DPA. The FCS also contains acetic acid as required to stabilize the solution and optionally sulfuric acid.

- For fruits and vegetables in food processing facilities, the maximum concentrations requested are 80 ppm peroxyacetic acid, 37 ppm hydrogen peroxide, 5 ppm HEDP and 0.25 ppm DPA. The FCS also contains acetic acid as required to stabilize the solution and optionally sulfuric acid.

B. Need for Action

The FCS is a well-known antimicrobial agent that effectively reduces or eliminates pathogenic and non-pathogenic microorganisms that may be present on food. As a result, the FCS will contribute to increasing the safety and shelf-life of poultry, meat, fruits and vegetables.

The USDA has imposed additional testing for the poultry industry for Campylobacter spp.¹ For many processing plants, an additional treatment using higher concentrations of peroxyacetic acid (400-2000 ppm) for a short time interval can result in the satisfactory reduction of the Campylobacter spp identified by USDA. In addition, the USDA is looking to expand monitoring to more processing areas, to other meats, and to newer species of bacteria, such as Shiga Toxin-Producing Escherichia coli (STEC). Finally, the Food Safety Modernization Act (FSMA) will create pressure for more effective antimicrobial treatments for FDA inspected facilities.

The action requested by this FCN addresses current and future needs for processors and governmental agencies by responding to increased pressure to improve food safety. For the poultry industry, the use of peroxyacetic acid at higher concentrations for relatively short periods of time, and in smaller total volumes, enhance the capacity of processors to improve techniques (i.e., more flexibility in terms of time, concentrations, spray vs immersion, etc.) so that food pathogens are better controlled.

C. **Locations of Use and/or Disposal**

The FCS is intended for use in meat, poultry, and fruit and vegetable processing plants throughout the United States. All waste process water containing the FCS at these plants is expected to enter the wastewater treatment unit at the plants. For the purposes of this Environmental Assessment, it is assumed that treated wastewater will be discharged directly to surface waters in accordance with the plants’ National Pollutant Discharge Elimination System (NPDES) permit. This assumption can be considered a “worst-case” scenario since it does not take into account any further treatment that may occur at a POTW. It is further assumed that very minor or negligible quantities of the FCS are lost via evaporation.

5. **Identification of Substances that are the Subject of the Proposed Action:**

The FCS is an aqueous mixture of hydrogen peroxide, peroxyacetic acid (PAA), acetic acid, hydroxyethylidene 1,1-diphosphonic acid (HEDP), dipicolinic acid (DPA) and sulfuric acid (optionally). It is produced by blending acetic acid, hydrogen peroxide, HEDP and water. During the blending process, peroxyacetic acid is formed, *in situ*, as a result of an equilibrium reaction between hydrogen peroxide and acetic acid. Sulfuric acid is optionally added as a catalyst in the reaction process.

The aqueous mixture is provided to users as a concentrate which is then diluted, prior to use, on-site. The chemical structures for the components of the FCS and associated chemical identification information is provided below:

**Hydrogen Peroxide**
CASRN: 7722-84-1  
Molecular Formula: \( \text{H}_2\text{O}_2 \)  
Molecular Weight: 34.01  
Structure:

\[
\begin{array}{c}
\text{H} \\
\text{O} \\
\text{O} \\
\text{H}
\end{array}
\]

**Peroxyacetic Acid**
CASRN: 79-21-0  
Molecular Formula: \( \text{CH}_3\text{CO}_3\text{H} \)  
Molecular Weight: 76.05  
Structure:

\[
\begin{array}{c}
\text{O} \\
\text{C} \\
\text{O} \\
\text{O} \\
\text{H}
\end{array}
\]
**Acetic Acid**  
CASRN: 64-19-7  
Molecular Formula: CH₃CO₂H  
Molecular Weight: 60.05  
Structure:

\[
\overset{\text{O}}{\text{C}}\overset{\text{O}}{\text{H}}
\]

**Hydroxyethylidene 1,1-diphosphonic acid**  
CASRN: 2809-21-4  
Molecular Formula: C₂H₆O₇P₂  
Molecular Weight: 206.02  
Structure:

**Dipicolinic acid**  
CASRN: 499-83-2  
Molecular Formula: C₇H₅NO₄  
Molecular Weight: 167.12  
Structure:

\[
\overset{\text{O}}{\overset{\text{N}}{\text{O}}}
\overset{\text{O}}{\text{C}}\overset{\text{O}}{\text{H}}
\]

**Sulfuric Acid**  
CASRN: 7664-93-9  
Molecular Formula: H₂SO₄  
Molecular Weight: 98.079  
Structure:

\[
\overset{\text{O}}{\overset{\text{O}}{\text{S}}}
\overset{\text{O}}{\text{H}}\overset{\text{O}}{\text{H}}
\]

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Environmental Assessment for Food Contact Notification FCN 1639  
http://www.fda.gov/Food/IngredientsPackagingLabeling/EnvironmentalDecisions/default.htm
6. **Introduction of the Substances into the Environment:**

A. **Introduction of Ingredient Substances into the Environment as a Result of Manufacture:**

The FCS is currently manufactured at facilities which meet all applicable federal, state and local environmental regulations. The notifier is responsible for all effluent, solid, and airborne discharges from these facilities.

The notifier asserts that there are no extraordinary circumstances pertaining to the manufacture of the FCS such as: 1) unique emission circumstances that have not already been addressed by general or specific emission requirements (including occupational) imposed by Federal, State and local environmental agencies and the emissions may harm the environment; 2) a proposed action that threatens a violation of Federal, State or local environmental laws or requirements (40 CFR §1508.27(b)(10)); 3) production associated with a proposed action that may adversely affect a species or the critical habitat of a species determined under the Endangered Species Act or the Convention of International Trade in Endangered Species of Wild Fauna and Flora to be endangered or threatened, or wild fauna or flora that are entitled to special protection under some other Federal law.

B. **Introduction of substances into the environment as a result of use/disposal:**

The FCS mixture is provided as a concentrate that is diluted on site. When diluted for use, the target levels of PAA in the process water will vary depending on the application. The resulting maximum concentration of PAA, hydrogen peroxide, HEDP, and DPA for each application will be as follows:

<table>
<thead>
<tr>
<th>Use</th>
<th>PAA</th>
<th>H2O2</th>
<th>HEDP</th>
<th>DPA</th>
</tr>
</thead>
<tbody>
<tr>
<td>Whole or cut poultry carcasses, parts, trim, and</td>
<td>2000</td>
<td>933</td>
<td>120</td>
<td>0.5</td>
</tr>
<tr>
<td>Whole or cut meat, including carcasses, parts, trim, and organs</td>
<td>400</td>
<td>187</td>
<td>24</td>
<td>0.5</td>
</tr>
<tr>
<td>Processed and pre-formed meat and poultry products</td>
<td>230</td>
<td>107</td>
<td>14</td>
<td>0.1</td>
</tr>
<tr>
<td>Fruits and vegetables</td>
<td>80</td>
<td>37</td>
<td>5</td>
<td>0.25</td>
</tr>
</tbody>
</table>

Treatment of the process water at an on-site waste water treatment facility is expected to result in complete degradation of peroxyacetic acid, hydrogen peroxide, and acetic acid. Specifically, the peroxyacetic acid will breakdown into oxygen and acetic acid, while hydrogen peroxide will breakdown into oxygen and water. All three compounds are rapidly degraded on contact with organic matter, transition metals, and upon exposure to sunlight. As cited in the Joint Assessment of Commodity Chemicals report on PAA Mucke suggested that hydrolysis of PAA occurs almost exclusively by hydrolytic cleavage. He showed hydrolysis half-lives at 20°C for a 2% PAA solution of about 1 week at pH 4.4 and less than 1 day at pH 7. As cited in the Joint Assessment of Commodity Chemicals report on hydrogen

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4 Ibid.
peroxide\(^5\), the half-life of hydrogen peroxide in natural river water ranged from 2.5 days when initial concentrations were 10,000 ppm, and increased to 15.2 days when the concentration decreased to 250 ppm.\(^6\) In biodegradation studies of acetic acid, 99% degraded in 7 days under anaerobic conditions.\(^7\) Acetic acid it is not expected to concentrate in the wastewater discharged to the POTW. In wastewater, sulfuric acid will completely dissociate into sulfate ions and hydrated protons, neither of which are a toxicological or environmental concern at the proposed use levels. Therefore, peroxyacetic acid, hydrogen peroxide, acetic acid and sulfuric acid are not expected to be introduced into the environment to any significant extent as a result of the proposed use of the FCS.

The remainder of this section will consider only the environmental introduction of HEDP and DPA

Assuming in the very worst-case, that all the water used in a processing plant is treated with the FCS, the HEDP and DPA environmental introduction concentrations (EICs) would be as shown below.

<table>
<thead>
<tr>
<th>Use</th>
<th>HEDP EIC</th>
<th>DPA EIC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Whole or cut poultry, carcasses, parts, trim, and organs</td>
<td>120 ppm</td>
<td>0.5 ppm</td>
</tr>
<tr>
<td>Whole or cut meat carcasses, parts, trim and organs</td>
<td>24 ppm</td>
<td>0.5 ppm</td>
</tr>
<tr>
<td>Processed and pre-formed meat and poultry products</td>
<td>14 ppm</td>
<td>0.1 ppm</td>
</tr>
<tr>
<td>Fruits and Vegetables</td>
<td>5 ppm</td>
<td>0.25 ppm</td>
</tr>
</tbody>
</table>

In sum, as large-scale facilities do not typically process more than one type of food, we will use the EIC for poultry processing of 120 ppm and 0.5 ppm for DPA as the worst-case concentration for all processing facilities using the FCS in the intended applications. Therefore, the discussion of impacts in Items 7 and 8 will focus on poultry processing facilities.

7. **Fate of Emitted Substances in the Environment:**

HEDP is expected to partition between water and sludge so the EIC for HEDP needs to be refined. Based on information from a report issued by the Human and Environmental Risk Assessment (HERA) project, we expect HEDP will significantly partition to sewage sludge. According to the HERA report, the treatment steps at an onsite treatment facility will remove or decompose at least a portion of any HEDP that remains.\(^8\) The HERA report cites 80% adsorption of HEDP to sewage treatment sludge. Therefore, the EIC for HEDP has been adjusted by applying the 20:80 (water: sludge) partition factor from the HERA report to

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\(^6\) Ibid.


estimate the concentrations in water and sewage sludge, as shown in the table below.

No refinement was necessary for DPA since, as discussed below, this substance is anticipated to remain solely with water and not partition into sludge

As previously mentioned, PAA, HP, and AA are not expected to survive treatment at the primary wastewater treatment facilities; therefore, Expected Environmental Concentrations (EECs) have not been calculated for these substances. The EEC for sulfuric acid has also not been calculated since, as noted above, no environmental impact is expected for this substance.

The EECs for HEDP and DPA in surface water has been calculated by applying a 10-fold dilution factor to the estimated EIC. This dilution factor accounts for the expected dilution in surface waters of effluent from an onsite treatment facility as supported by data reported by Rapaport. Finally, we note that the EEC for sludge is a maximum for terrestrial impacts as any sludge used as a soil amendment will likely be significantly diluted by soil or sludge from other sources.

<table>
<thead>
<tr>
<th>EICs and EECs for HEDP and DPA</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Use</strong></td>
</tr>
<tr>
<td>Whole or cut poultry, carcasses, parts, trim, and organs</td>
</tr>
</tbody>
</table>

* Calculations:
  
  HEDP-EICwater = max. use x water partition = 120 ppm x 20% = 24 ppm
  
  HEDP-EICsludge = max. use x sludge partition = 120 ppm x 80% = 96 ppm
  
  HEDP-EECsludge = 96 ppm (assume that the EIC = EEC since there is no dilution)
  
  HEDP-EECwater = EICwater ÷ dilution in aqueous receiving body = 24 ppm ÷ 10 = 2.4 ppm
  
  DPA-EECwater = EICwater ÷ dilution in aqueous receiving body = 0.5 ppm ÷ 10 = 0.05 ppm

No further adjustment of the calculated EEC is appropriate for HEDP since this substance is relatively stable in the environment. According to the published literature, decomposition of HEDP occurs at a moderately slow pace in water; 33% in 28 days. Regarding soil biodegradation, the HERA report estimates a half-life in soil of 373 days. Therefore, any aquatic or soil biodegradation of HEDP is not expected to significantly lower the estimated EECs for HEDP provided in Table 1.

Studies concerning the environmental fate of DPA were not available from the published literature or proprietary sources. In the absence of environmental fate studies, a USEPA model (EPI Suite) was used to provide information on the environmental fate of DPA. The EPI Suite model uses the chemical structure of a substance to estimate chemical/physical properties and environmental fate characteristics.

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10 Ibid

The EPI Suite (v 4.11) results for DPA are shown in Attachment 1 and the key findings are summarized below.

- DPA is soluble in water, with the estimated water solubility ranging from 990 mg/L to 20,790 mg/L. The partition coefficient (Log $K_{ow}$) is estimated to be 0.57.

- The biodegradation of DPA was evaluated using seven different Quantitative Structure Activity Relationship (QSAR) methods. The methods that are relevant to the expected environmental pathway of DPA (discharge to POTW’s) are the MITI linear and nonlinear methods. Both of these methods, predict that DPA is readily biodegradable.

Based on EPI Suite estimates for DPA, it is reasonable to conclude that DPA will substantially remain with water and not be absorbed to sludge and that DPA will be readily biodegraded in POTW’s. Since this Environmental Assessment assumes direct discharge of treated wastewater (containing the FCS) to surface waters, the expected biodegradation of DPA is not being considered.

8. **Environmental Effects of Released Substances:**

A. **Terrestrial Toxicity:**

The No-Observable Effect Concentration (NOEC) for HEDP toxicity to terrestrial organisms is greater than 1000 mg/kg soil dry weight for *Eisenia fetida*). The maximum estimated concentration in sludge (96 ppm) is approximately 10-fold lower than the NOEC level and the maximum concentration in soil when used as a soil amendment should have an even larger margin of safety with respect to the NOEC level. Therefore, HEDP is not expected to have any terrestrial environmental toxicity concerns at levels at which it is expected to be present in sludge. Moreover, the much smaller level of HEDP present in the surface water is not expected to have any adverse environmental impact with respect to sedimentation based on the terrestrial toxicity endpoints available for plants, earthworms, and birds. When the wastewater encounters the land, any increase in phosphates in soil will be only a minimal amount of the total phosphorus concentrations that already exist in the environment.

As noted above in Section 7, DPA is soluble in water and very little, if any, DPA is expected to partition to sludge. Accordingly, terrestrial releases of DPA from the intended uses of the FCS are anticipated to be negligible and no toxicity concerns are expected.

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13 Ibid
B. Aquatic Toxicity

HEDP

An extensive database has been compiled on the toxicity of HEDP to aquatic organisms. Studies have been conducted on the toxicity of HEDP to freshwater and marine organisms and algae. The test results from the studies is shown in the following table:

### Aquatic Toxicity Data for HEDP

<table>
<thead>
<tr>
<th>Species</th>
<th>Endpoint</th>
<th>(mg/l)=ppm</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Short Term</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td><em>Lepomis macrochirus</em></td>
<td>96h LC50</td>
<td>868</td>
</tr>
<tr>
<td><em>Oncorhynchus mykiss</em></td>
<td>96h LC50</td>
<td>360</td>
</tr>
<tr>
<td><em>Cyprinodon variegatus</em></td>
<td>96h LC50</td>
<td>2180</td>
</tr>
<tr>
<td><em>Lctalurus punctatus</em></td>
<td>96h LC50</td>
<td>695</td>
</tr>
<tr>
<td><em>Leuciscus idus melonatus</em></td>
<td>48h LC50</td>
<td>207-350</td>
</tr>
<tr>
<td><em>Daphnia magna</em></td>
<td>24 - 48h EC50</td>
<td>165-500</td>
</tr>
<tr>
<td><em>Palaemonetes pugio</em></td>
<td>96 h EC50</td>
<td>1770</td>
</tr>
<tr>
<td><em>Crassostrea virginica</em></td>
<td>96h EC50</td>
<td>89</td>
</tr>
<tr>
<td><em>Selenastrum capricornutum</em></td>
<td>96h LC50</td>
<td>3</td>
</tr>
<tr>
<td><em>Selenastrum capricornutum</em></td>
<td>96h NOEC</td>
<td>1.3</td>
</tr>
<tr>
<td>Algae</td>
<td>96h NOEC</td>
<td>0.74</td>
</tr>
<tr>
<td><em>Chiarella vulgaris</em></td>
<td>48h NOEC</td>
<td>&gt;100</td>
</tr>
<tr>
<td><em>Pseudomonas putida</em></td>
<td>30 minute NOEC</td>
<td>1000</td>
</tr>
<tr>
<td><strong>Long Term</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td><em>Oncorhynchus mykiss</em></td>
<td>14 d NOEC</td>
<td>60-180</td>
</tr>
<tr>
<td><em>Daphnia magna</em></td>
<td>28 d NOEC</td>
<td>10 - &lt;12.5</td>
</tr>
<tr>
<td>Algae</td>
<td>14 day NOEC</td>
<td>13</td>
</tr>
</tbody>
</table>


The aquatic toxicity data on HEDP needs to be assessed in the context of the known chelation effects of HEDP. Work by Jaworska et al. showed that the primary adverse effects of HEDP result from chelation of nutrients rather than direct toxicity of HEDP. Chelation is not toxicologically relevant to wastewater discharges containing HEDP from food processing plants since eutrophication, not nutrient depletion, has been demonstrated to be the controlling toxicological mode for this type of wastewater discharge. The lowest short-term or acute LC50 values published for algae (Selenastrum capricornutum - 3 ppm), freshwater invertebrate (Daphnia magna -165 ppm), and mollusks Crassostrea virginica (89 ppm) are acute toxicity endpoints considered to result from this chelation.

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effect. These values are not relevant when excess nutrients are present as expected in food processing wastewaters.

The lowest relevant endpoint for food processing uses was determined to be the chronic NOEC of 10 ppm for *Daphnia magna*. Although FDA has previously noted that uncertainties intrinsic to its derivation make the usefulness of the NOEC/NOEL debatable, the agency has previously indicated that a NOEC for *Daphnia magna* is an appropriate benchmark for environmental toxicology. The EEC of 2.4 ppm is approximately 4-fold lower than the 10 ppm chronic NOEC for *Daphnia magna*.

**DPA**

No test data concerning the aquatic toxicity of DPA was found in the published literature. An alternative approach is to use a well-established Quantitative Structure Activity Relationship or “QSAR” model to predict the aquatic toxicity of DPA. For this Environmental Assessment, USEPA’s ECOSAR model was used to provide estimates of the aquatic toxicity of DPA. ECOSAR (Ecological Structure Activity Relationships) estimates the aquatic toxicity of untested compounds using structure-activity relationships (SARs). The toxicity data used to build the SARs are collected from publically available experimental studies and confidential submissions provided to the U.S. EPA New Chemicals Program. The ECOSAR results for DPA are shown in Attachment 2. The results show that DPA is practically non-toxic to fish (LC50 = 322 mg/1), freshwater invertebrates (LC50 = 89 mg/1 for the Daphnid) and algae (EC50 = 111 mg/1 for green algae).

The highest calculated EEC for DPA is 0.05 ppm. This value is more than 100-fold lower than the predicted toxicity values for DPA. Therefore, the aquatic risks for the intended uses of DPA are expected to be negligible.

9. **Use of Resources and Energy:**

No net increase in the use of energy and resources is expected from the use of this FCS since it is expected to substitute for other products (e.g. the FCS identified in FCN Nos. 140, 1501 and 1522) that are currently being utilized for the same uses as proposed in this FCN and contain the same components as this FCS at the same maximum concentrations.

In addition, the manufacture of the FCS will consume comparable amounts of energy and resources as similar products, and the raw materials used in the product of the FCS are commercially manufactured materials that are produced for use in a variety of chemical reactions and processes. Energy used specifically for the production of the FCS is not significant.


17 See e.g. Food and Drug Administration, 2014, Environmental Decision Memo for FCN 1379 and 1419.
10. **Mitigation Measures:**

As discussed above, no significant adverse environmental impacts are expected to result from the use and disposal of the dilute FCS mixture. Thus, the use of the solution is not reasonably expected to result in any new environmental problems requiring mitigation measures of any kind.

11. **Alternatives to the Proposed Action:**

There are no potential adverse environmental effects identified that would necessitate alternative actions to that proposed in this FCN. The alternate of not approving this FCN would simply result in the continued use of nearly identical products by the beef, poultry, pork and fruits and vegetables processing industry; such action would therefore have no environmental impact. The addition of the concentrated FCS mixture to the options that are currently available to meat processors is not expected to greatly increase the use of peroxyacetic acid products.

12. **List of Preparers:**

This Environmental Assessment was prepared on behalf of Biosan, LLC, by Wendy A. McCombie of Lewis & Harrison, LLC. Ms. McCombie has a B.S. in Biology with 23 years of experience providing consulting services for chemical regulations.

13. **Certification:**

The undersigned official certifies that the information provided herein is true, accurate, and complete to the best of his knowledge.

Name: Wendy A. McCombie, Lewis & Harrison LLC

Title: Agent for Biosan, LLC

Date: February 12, 2016
14. **List of References:**

Environmental Protection Agency, Reregistration Eligibility Decision: Peroxy Compounds (December 1993)  

European Centre for Ecotoxicology and Toxicology of Chemicals, January 2001 Peracetic Acid (CAS No. 79-21-0) and its Equilibrium Solutions. JACC No. 40.  

European Centre for Toxicology and Toxicology of Chemicals, January, 1993 Joint Assessment of Commodity Chemicals No. 22. Hydrogen Peroxide. CAS No. 7722-84-1  

Food and Drug Administration, 2014, Environmental Decision Memo for Food Contact Notification 1379, available at  

Food and Drug Administration, 2014, Environmental Decision Memo for Food Contact Notification 1419, available at  


Rapaport, Robert A., 1988. Prediction of consumer product chemical concentrations as a function of publically owned treatment works treatment type and riverine dilution. Environmental Toxicology and Chemistry 7(2), 107-115. Found online at:  
http://onlinelibrary.wiley.com/doi/10.1002/etc.5620070204/abstract

15. **List of Attachments:**

Attachment 1: Formulation
Attachment 2: ECOSAR and EPI
ATTACHMENT 1
FORMULATION
<table>
<thead>
<tr>
<th>Ingredient</th>
<th>Minimum Concentration</th>
<th>Maximum Concentration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Peroxyacetic acid</td>
<td>5.3%</td>
<td>22.0%</td>
</tr>
<tr>
<td>Hydrogen Peroxide</td>
<td>3.0%</td>
<td>22.5%</td>
</tr>
<tr>
<td>HEDP</td>
<td>0.05%</td>
<td>0.9%</td>
</tr>
<tr>
<td>DPA</td>
<td>0.01%</td>
<td>0.02%</td>
</tr>
<tr>
<td>Acetic Acid</td>
<td>10.0%</td>
<td>35.0%</td>
</tr>
<tr>
<td>Water (potable)</td>
<td>Q.S.</td>
<td>Q.S.</td>
</tr>
<tr>
<td>Sulfuric Acid</td>
<td>---</td>
<td>0.95%</td>
</tr>
</tbody>
</table>
ECOSAR Version 1.11 Results Page

SMILES : clcc(nc(c1)(C(=O)O)c(=O)O)
CHEM :
CAS Num: 
ChemID1:
MOL FOR: C7 H5 N1 O4
MOL WT : 167.12
Log Kow: 0.567 (EPISuite Kowwin v1.68 Estimate)
Log Kow: (User Entered)
Melt Pt: 249.00 (deg C, PhysProp DB exp value for Melt Sol est, 249 deg)
Wet Sol: 4829 (mg/L, EPISuite WSKowwin v1.43 Estimate)
Wet Sol: (User Entered)
Wet Sol: 5000 (mg/L, PhysProp DB exp value)

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Values used to Generate ECOSAR Profile

Log Kow: 0.567 (EPISuite Kowwin v1.68 Estimate)
Wet Sol: 5000 (mg/L, PhysProp DB exp value)

Available Measured Data from ECOSAR Training Set

<table>
<thead>
<tr>
<th>CAS No</th>
<th>Organism</th>
<th>Duration</th>
<th>End Pt</th>
<th>Measured</th>
<th>Ecosar Class</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>000499-83-2</td>
<td>Fish</td>
<td>96-hr</td>
<td>LC50</td>
<td>322</td>
<td>Pyridine alpha-acid</td>
<td>DGL</td>
</tr>
</tbody>
</table>

ECOSAR v1.1 Class-specific Estimations

Pyridine-alpha-Acid

<table>
<thead>
<tr>
<th>ECOSAR Class</th>
<th>Organism</th>
<th>Duration</th>
<th>End Pt</th>
<th>Predicted mg/L (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pyridine-alpha-Acid</td>
<td>Fish</td>
<td>96-hr</td>
<td>LC50</td>
<td>323.608</td>
</tr>
<tr>
<td>Pyridine-alpha-Acid</td>
<td>Fish</td>
<td>96-hr</td>
<td>ChV</td>
<td>29.342</td>
</tr>
</tbody>
</table>

Neutral Organic SAR (Baseline Toxicity)

<table>
<thead>
<tr>
<th>Organism</th>
<th>Duration</th>
<th>End Pt</th>
<th>Predicted mg/L (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fish</td>
<td>96-hr</td>
<td>LC50</td>
<td>2656.694</td>
</tr>
<tr>
<td>Daphnid</td>
<td>48-hr</td>
<td>LC50</td>
<td>1321.570</td>
</tr>
<tr>
<td>Green Algae</td>
<td>96-hr</td>
<td>EC50</td>
<td>509.703</td>
</tr>
<tr>
<td>Fish</td>
<td></td>
<td>ChV</td>
<td>222.185</td>
</tr>
<tr>
<td>Daphnid</td>
<td></td>
<td>ChV</td>
<td>89.187</td>
</tr>
<tr>
<td>Green Algae</td>
<td></td>
<td>ChV</td>
<td>111.124</td>
</tr>
</tbody>
</table>

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect. If the effect level exceeds the water solubility by 10X, typically no effects at saturation (MES) are reported.

NOTE: ! = exclamation designates: The toxicity value was estimated through application of acute-to-chronic ratios per methods outlined in the ECOSAR Methodology Document provided in the ECOSAR Help Menu.

Class Specific LogKow Cut-Offs

If the log Kow of the chemical is greater than the endpoint specific cut-offs presented below, then no effects at saturation are expected for those endpoints.
Pyridine-alpha-Acid:

Maximum LogKow: 5.0 (LC50)
Maximum LogKow: 6.4 (EC50)
Maximum LogKow: 8.0 (ChV)

Baseline Toxicity SAR Limitations:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50)
Maximum LogKow: 6.4 (Green Algae EC50)
Maximum LogKow: 8.0 (ChV)