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OFFICE OF
PREVENTION, PESTICIDES AND
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**MEMORANDUM**

**DATE:** March 30, 2004

**SUBJECT:** *Amended* Environmental Fate and Effects Risk Assessment for the Reregistration of 1-Naphthaleneacetic acid (NAA) and Related Compounds as a Low Toxicity Substance.

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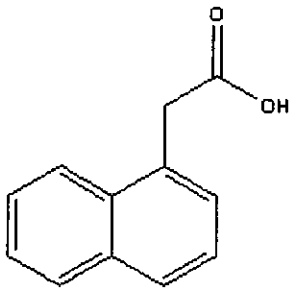
This memorandum characterizes the exposure, toxicity, and exceedances of the Agency's levels of concern for terrestrial and aquatic organisms from the use of the herbicide naphthaleneacetic acid (NAA) and related compounds. NAA will be considered by the Low Toxicity Pesticide Chemical FOCUS Group as a "low toxicity" compound.

Based on the limited data set available, EFED believes that NAA and related compounds present little or no potential for risks to nontarget organisms, including mammals, birds, aquatic organisms, and nontarget plants. Risks to terrestrial insects cannot be quantified but the available data do not suggest a substantial potential for adverse effects.

Tier I Estimated Drinking Water Concentrations (EDWCs) for 1-naphthaleneacetic acid were calculated using FIRST V. 1.0 (surface water) and SCIGROW V. 2.3 (ground water) for use in the human health risk assessment. The acute (peak) surface water concentration was **12.9 ppb**, the annual average surface water concentration was **0.71 ppb**, and the ground water concentration, suitable for both acute and chronic is **<0.006 ppb**. These values generally represent upper-bound estimates of the concentrations of 1-naphthaleneacetic acid equivalents that might be found in surface and ground water due to the use of 1-naphthalenacetic acid (sodium salt) on apples, which represents the highest use rate scenario. Both models provide estimates suitable for screening purposes. Additional refinements may be developed should they be needed by HED (Refer to copy of drinking water memorandum attached in appendix E).

# Environmental Fate and Ecological Risk Assessment for the Reregistration of NAPHTHALENEACETIC ACID and related compounds

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## Environmental Risk Conclusions

EFED has considered available information on the toxicity of naphthaleneacetic acid (NAA) and related compounds, the registered uses and areas in which these compounds are applied, fate properties, and application methods in characterizing environmental exposures and ecological risks related to labeled uses. EFED relied on studies conducted on NAA, 1-naphthaleneacetamide, and the ethyl 1-naphthaleneacetate ester, as well as the sodium, potassium, and ammonium salts of NAA. Data gaps were addressed using structure activity relationships (SAR). Upon review and synthesis of this information, EFED believes NAA and related compounds do not present significant potential for risks to nontarget species (mammals, birds, aquatic organisms, and plants). Risks to terrestrial insects cannot be quantified, but the available data do not suggest a significant potential for adverse effects.

Very little experimental data are available on the physical and chemical properties or the environmental fate of NAA and related compounds. The major routes of dissipation and degradation appear to be volatilization (at least from plant surfaces) and photolysis, respectively. Substantial volatilization from water is probably not important. Biodegradation may also be important, but quantitative data are not available. While no experimental data are available on soil mobility, the chemical and physical properties of NAA suggest moderate to low mobility in soil.

Tier I (FIRST) modeling for drinking water determined when NAA is applied at the maximum labeled rate of 0.134 lb a.i./A for two applications in a 5-day interval, the residues in surface water are **12.9 µg/L** for the annual peak concentration, and **0.712 µg/L** for the annual mean concentration. Estimates of peak concentrations in ambient surface water (GEENEC2) are somewhat lower – i.e., **9.09 µg/L**. The concentration of NAA in shallow ground water predicted based on SCIGROW2.3 is **<0.006 µg/L** (Table 1).

**Table 1. Estimated Environmental Concentrations (ppb) of NAA in Surface and Groundwater at Two Applications of 0.134 lb./acre-year.**

| Scenario | Peak (µg/L) | Long-Term Average (µg/L) | PCA |
|---|---|---|---|
| Surface water drinking water (FIRST) | 12.9 | 0.712 | 0.87 |
| Ambient surface water (GENEEC2) | 9.09 | Not Applicable | Not Applicable |
| Groundwater drinking water (SCIGROW2.3) | <0.006 | | Not Applicable |

## Introduction

1-Naphthaleneacetic acid (NAA) is a plant growth regulator that mimics auxin (indole-3-acetic acid) a naturally occurring plant growth hormone that is important in seed and root development. In this respect, NAA and related compounds are similar to 2,4-D, another auxin mimic, but distinct from 2,4,5-T, an anti-auxin (Cooke et al. 2002). This risk assessment covers NAA and five related compounds as specified below:

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| PC Code | CASN | Chemical |
|---|---|---|
| 056001 | 86-86-2 | 1-naphthaleneacetamide |
| 056002 | 86-87-3 | 1-naphthaleneacetic acid |
| 056003 | 15165-79-4 | potassium 1-naphthaleneacetate |
| 056004 | 25545-89-5 | ammonium 1-naphthaleneacetate |
| 056007 | 61-31-4 | sodium 1-naphthaleneacetate |
| 056008 | 2122-70-5 | ethyl 1-naphthaleneacetate |

A summary of the agricultural uses of NAA is presented in Figure 1 (USGS 2004a). These use statistics are for 1992, the most recent year for which data are available. As indicated in this figure, 13,665 lbs of NAA were applied, primarily to apples (80% of total) and pears (19.4%) of total, with a relatively small amount (about 0.6% of total) applied to olives. Most NAA is used in the northeast and west coast, with lesser amounts used in the central and southeast regions. The USGS (2004a) reports the use data only as NAA and does not specify which compounds of NAA were used.

Formulations containing sodium 1-naphthaleneacetate (STIK Clean Crop, Liqui-Stik 200, and Fruitone N), potassium 1-naphthaleneacetate (K-Salt Fruit Fix 200 and K-Salt Fruit Fix 800) or ammonium 1-naphthaleneacetate (Fruit Fix Concentrate 200, Fruit Fix Concentrate 800) may be used in ground broadcast or aerial applications on apple and pear trees as well as on some ornamental shrubs and shade trees to prevent preharvest fruit drop (apples and pears) and seed pod and nut formation (shrubs and shade trees). Broadcast applications of a formulation of sodium 1-naphthaleneacetate (STIK Clean Crop) are also used for thinning olive trees.

NAA itself, as well as 1-naphthaleneacetamide and ethyl 1-naphthaleneacetate, is not labeled for broadcast applications. 1-Naphthaleneacetic acid is used as a rooting compound – i.e., applied as a solution to roots of plants to stimulate grow – and is applied as a mixture with indole-3-butyric acid or Vitamin B-1. Only one formulation, Amcotone, contains 1-naphthaleneacetamide. This is a formulation of both 1-naphthaleneacetamide and 1-naphthaleneacetic acid that is used to induce fruit set and promote growth in apples and pears. Similarly, there is only one formulation of ethyl 1-naphthaleneacetate (Tre-Hold RTU) and this formulation is used as a sprout inhibitor in cut surface and basal bark applications to apple, pear, and olive trees as well as a number of other woody plants.

The distinction between the broadcast and non-broadcast applications of NAA and related compounds is important to this risk assessment in terms of exposure potential. The non-broadcast applications used to promote root growth (for transplantations or to boost established plants), occur primarily in a nursery environment and the potential for substantial unintended environmental contamination is limited. Similarly, the uses of the 1-naphthaleneacetamide formulations to induce fruit set and the ethyl 1-naphthaleneacetate formulation to inhibit sprouting are conducted on individual plants as needed and application rates in units of lb/acre are not a meaningful expression of potential exposure. The formulations that are used in broadcast applications, either aerial or ground, will entail a greater potential for environmental contamination and exposure to nontarget species and general exposures may be estimated based on application rates in units of lb/acre.

The environmental fate characteristics of the salts of NAA are expected to be similar to those of the acid. In the environment, the NAA salts will rapidly dissociate to naphthaleneacetic acid and the corresponding cation. Thus, for this risk assessment, all references to application rate will be in units of lb a.e. (acid equivalents) per acre (lb a.e./acre). Of the three NAA salts labeled for broadcast applications – i.e., the sodium, potassium, and ammonium salts – the product with the maximum use rate (STIK Clear Crop) can be applied at a rate of 0.134 lb a.e./acre per

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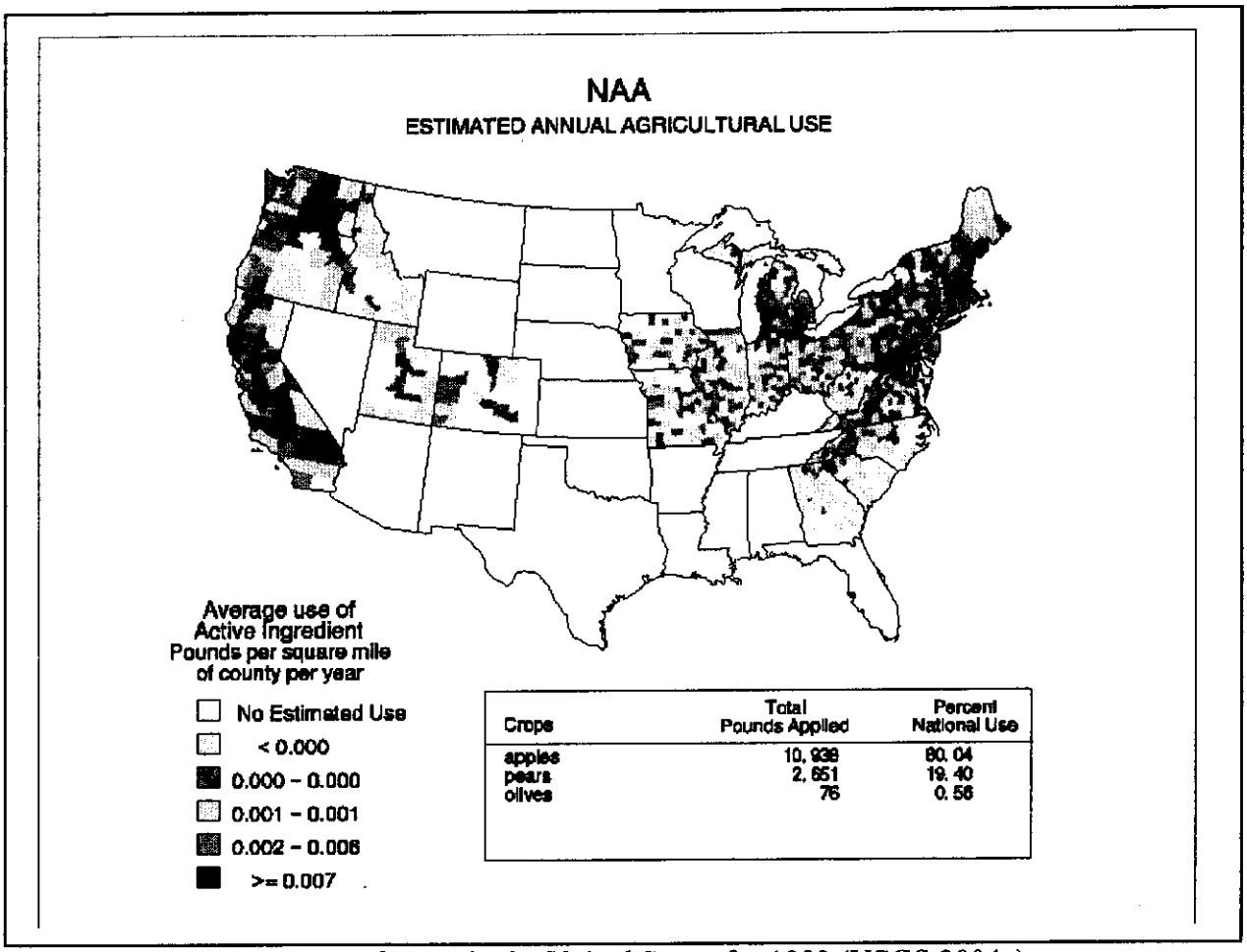


**Figure 1:**. Agricultural use of NAA in the United States for 1992 (USGS 2004a).

application. Two applications are allowed as close as 5 days apart. The maximum broadcast use rates for the other formulations range from 0.076 lb a.e./acre to 0.11 lb a.e./acre. Only the highest rate, 0.134 lb a.e./acre, is considered quantitatively in this Tier 1 risk assessment.

EFED reviewed the chemical specific files for available information to use in a "standard" pesticide active ingredient risk assessment (EPA, 2002). The database for NAA and related compounds dates back to the 1960's to mid 1980's, with some more recent study submissions in the 1990's. While some data on the toxicity of NAA have been published in the open literature, they are not applicable to a quantitative risk assessment (Appendix A). Nonetheless, the available studies contain an adequate subset of the Agency's ecotoxicity guideline studies to conduct a qualitative and, where appropriate, quantitative dose-response assessment for most groups of nontarget species.

Relatively little information is available on the environmental fate of NAA and related compounds. As noted above, the environmental fate characteristics of the salts of NAA are expected to be similar to those of the acid. To augment the limited data on the environmental fate of NAA, EFED conducted a structure activity relationship analysis (SAR) on NAA using the Agency's Estimation Program Interface program (EPI) (Meylan, 1998 and 2000) to further compare the potential similarities between these molecules using a structure-based approach.

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## Approach to Risk Assessment

The approach to this assessment first focused on the available compound-specific fate and ecotoxicity information submitted in support of registration. Information on environmental fate was taken, for the most part, from the report "*Tier I Estimated Drinking Water Concentrations of 1-Naphthaleneacetic Acid for use in Human Health Risk Assessment*" (Appendix E). This report was supplemented with information on the foliar half-life of NAA, naphthaleneacetamide, and naphthaleneacetic acid ethyl ester on apple leaves (Obrist1994), which is summarized in Appendix A and used in the ELL-FATE model. The fate database for NAA and related compounds is sparse and a SAR approach was conducted on NAA to fill gaps in knowledge using the Agency's EPI-Suite program.

The ecotoxicity database on terrestrial and aquatic organisms for NAA and related compounds was reviewed, including both EPA submissions and studies from the open literature. The database on terrestrial organisms and aquatic plants was adequate to estimate risks using the Agency's Level of Concern (LOC) approach. Because of the lack of chronic toxicity data for fish and aquatic invertebrates, SAR estimates were obtained, again using the Agency's EPI-Suite program. Based on the available experimental values on acute toxicity in aquatic species, the EPI-Suite program appeared to adequately predict the toxicity of naphthaleneacetic acid ethyl ester but consistently under-predicted the toxicity of NAA. Thus, for characterizing chronic risk to aquatic species, the SAR estimates of chronic toxicity values from EPI-Suite were adjusted downward based on observed to predicted ratios for acute toxicity.

Once a reasonable fate and ecotoxicity profile was compiled, a Tier I surface water assessment for aquatic and drinking water exposures was conducted using the the highest broadcast application rate for any NAA compound – i.e., STIK Clear Crop. The product, a formulation of sodium 1-naphthaleneacetate, can be applied at a rate of 0.134 lb a.e./acre per application. Two applications are allowed as close as 5 days apart. Aquatic risks were based on the Tier I aquatic exposure results and the available aquatic toxicity data as well as the chronic estimates for aquatic species based on corrected SAR approximations. Terrestrial risks were based on exposures from the terrestrial model ELL-FATE (ELL-FATE, Version 1.2, dated July 19, 2001) and available bird and mammal toxicity data. Risks to plants were quantified based on the TERR PLANT and AGDRIFT models and the available toxicity studies for seedling emergence and vegetative vigor. The available data on insects were not adequate for quantitative risk assessment and risks were only characterized qualitatively.

## Integrated Risk Characterization

### Risks to Aquatic Organisms

The results of this risk assessment suggest no concern for acute and chronic risks to non-endangered and endangered aquatic species. NAA is practically non-toxic to fish and invertebrates on an acute basis. Estimates of chronic toxicity based on SAR are uncertain because the SAR program consistently underestimated acute toxicity. Thus, estimates were adjusted to account for this factor. The corrected estimates resulted in calculated RQ's which are substantially below a level of concern for all representative organisms.

### Risks to Terrestrial Organisms

Based on the available toxicity data and the proposed application rates on the label, acute and chronic risks to wild mammals and acute risks to birds are unlikely. No chronic toxicity data are available for birds. Nonetheless, based on the use of the acute toxicity data for birds, RQ's are below unity by factors of about 300 to 5000. Given the apparent lack of a strong dose-duration relationship in mammals and these very low risk quotients, there is no basis for predicting adverse effects in birds following longer term exposures.

No toxicity data useful for quantitative risk assessment are available in insects – i.e., the standard honey bee toxicity assay has not been submitted. However, a Pacific Northwest Extension Publication (Mayer et al.) indicates that NAA "can be applied at any time with reasonable safety to bees." Also, based on a number of screening assays conducted in Europe (Appendix A), substantial adverse effects in insects from exposures to NAA do not seem likely.

There are a number of areas of uncertainty in the terrestrial risk assessment. This assessment accounts only for exposure of terrestrial organisms to NAA, but not to its degradates. Only dietary exposure is included in the exposure assessment, and it is assumed that 100% of the diet is relegated to single food types foraged only from treated fields. Vegetation half-life is one of the more sensitive parameters impacting the risk assessment for mammals and birds. The potential impacts of this uncertainty are outlined in the Terrestrial Risk Assessment section of this document.

Endangered Species Assessment

For endangered species the Agency adopts lower levels of concern (LOC's) for risks to some groups – i.e., 0.1 for mammals and birds and 0.05 for aquatic animals – relative to levels of concern for acute risks in non-endangered species – i.e., 0.5 for mammals and birds as well as aquatic animals (EFED 2001). The Agency's levels of concern for endangered and threatened species in these groups are not exceeded for the highest use rate scenarion (broadcast application of the salts of NAA on apples, pears, or olives). A somewhat different approach is taken for terrestrial and aquatic plants, in which the LOC = 1 for all plants, but the endpoint used to calculate the RQ for endangered species is based on a more sensitive toxicity endpoint – i.e., $EC_{05}$ or NOEC – than for non-endangered species – i.e., an $EC_{25}$ (EFED 2001). Based on these criteria, no risks to endangered aquatic plants is apparent (Table 9). The RQ for endangered terrestrial plants is equal to the LOC (value of 1), but does not exceed the LOC. There is also significant reduction of risk with distance from point of application (Appendix D), and siginificant degradation of the pesticide soon after application (Appendix G).

## Environmental Fate and Transport

Summary

Very little experimental data are available on the physical and chemical properties or the environmental fate of NAA and related compounds. Apart from a measured water solubility of 420 mg/L, a pKa of 4.2, and a measured Kow of about 174 (log Kow=2.24), all for NAA, and a water solubility of 39 mg/L for naphthaleneacetamide, no experimental information is available on chemical or physical properties. The only experimental data on environmental fate is a foliar dissipation study which measured half-life of 34.2 hours for naphthaleneacetic acid, 131.6 hours for naphthaleneacetamide, and 12.8 hours for naphthaleneacetic acid ethyl ester.

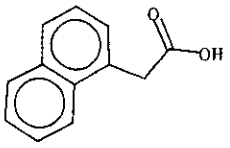
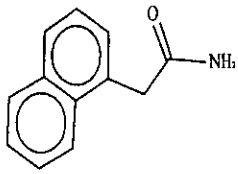
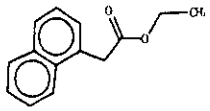
The ethyl-1-naphthaleneacetate and 1-naphthaleneacetamide are susceptible to hydrolysis, and the end product is 1-naphthaleneacetic acid (Acc. No. 129382). Based on the pKa of 4.2, a proportion of about 0.0015 of 1-naphthaleneacetic acid will be nonionized at pH 7. Based on the estimates of vapor pressure as well as differences in half-life on vegetation, volatility may be an important route of dissipation, particularly for ethyl 1-naphthaleneacetate and to a lesser extent for naphthaleneacetic acid. 1-Naphthaleneacetic acid and structurally similar compounds such as 1-methyl-naphthalene and ethyl-naphthalene are susceptible to biodegradation. No quantitative experimental data on degradation rates, however, are available. Thus, all estimates of biodegradation rates used for quantifying exposures must be based on SAR relationships.

Physical-Chemical Properties and Structure

The chemical structures of naphthaleneacetic acid, naphthaleneacetamide, and ethyl 1-naphthaleneacetate are given in Table 2 along with the corresponding molecular weights and

SMILES notation. SMILES notation is a method of specifying chemical structure that is used in the Agency's EPI Program (Meylan and Howard, 1998, 2000). The sodium, potassium, and ammonium salts of NAA are not shown. For these salts, the hydrogen on the hydroxyl group of NAA is simply replaced with the corresponding cation.

**Table 2: Naphthalene acetic acid (NAA) and Related Compounds [1]**

| Property | Compound | | |
|---|---|---|---|
| | Naphthalene acetic acid | Naphthaleneacetamide | Ethyl 1-naphthaleneacetate |
| Molecular weight [1] | 186.2098 | 185.225 | 214.2634 |
| Structure [2] |  |  |  |
| SMILES Notation [2] | O=C(O)Cc(c(c(ccc1)cc2)c1)c2 | O=C(N)Cc(c(c(ccc1)cc2)c1)c2 | O=C(OCC)Cc(c(c(ccc1)cc2)c1)c2 |

[1] Information from ChemFinder [http://chemfinder.cambridgesoft.com/]
[2] Information from EPI Suite, Version 3.11.

Table 3 lists measured and estimated physical-chemical properties of naphthaleneacetic acid, naphthaleneacetamide, and ethyl 1-naphthaleneacetate. Estimated values were derived from the Agency's EPI Program. As noted in the Tier I Estimated Drinking Water Assessment for NAA, very little specific information is available on the environmental fate of NAA. Under ambient conditions in an aqueous solution, the salts of NAA are expected to dissociate to NAA and the cation. The pKa value for NAA is 4.2 (USDA/ARS 1995) – i.e., at a pH of 4.2, half of the molecules are ionized and half are nonionized. At ambient pH (i.e., pH 7) in an aqueous solution, very little NAA will be nonionized – i.e, $1 \div (1 + 10^{pH-pKa}) \approx 0.0015$ using the Henderson-Hasselbalch equation (Keys et al., 1999).

Table 3: Measured and Estimated Properties of NAA and Related Compounds

| Property | Compound | | | | | |
|---|---|---|---|---|---|---|
| | Naphthalene acetic acid | | Naphthaleneacetamide | | Ethyl 1-naphthaleneacetate | |
| | Measured | Estimated | Measured | Estimated | Measured | Estimated |
| **Environmental Fate** | | | | | | |
| Water Solubility (mg/L) | 420 [2] | 1557 | 39 | 1758 | | 23.24 |
| Vapor Pressure (mm Hg) | | 9.57E-006 | | 5.41E-007 | | 1E-004 |
| Log $K_{ow}$ | 2.24 [3] | 2.60 | | 1.72 | | 3.75 |
| Henry's Law Coefficient (atm-$m^3$/mole) | | 1.506E-009 | | 7.500E-011 | | 1.213E-006 |
| $K_{oc}$ (mL/g) | | 297 | | 2585 | | 2929 |
| BCF (L/kg) | | 3.162 | | 1.72 | | 153.4 |
| Halftime in Air (hrs) | | 6.929 | | 4.553 | | 6.794 |
| Halftime in Water (hrs) | | 360 [Acid] 900 [Na] | | 900 | | 360 |
| Halftime in Soil (hrs) | | 360 [Acid] 900 [Na] | | 900 | | 360 |
| Aerobic soil metabolism halftime (days) [1] | | 3.9 [for SciGrow] 11.7 [for FIRST] | | | | |
| Aerobic aquatic metabolism halftime (days) [1] | | 23.4 | | | | |
| Halftime in Sediment (hrs) | | 1440 | | 3600 | | 1440 |
| Halftime on vegetation (hrs) [4] | 34.2 | | 131.6 | | 12.8 | |

[1] Estimates taken from the Tier I Estimated Drinking water Assessment
[2] MRID 00162239 and 40522903.
[3] EPI Suite
[4] Obrist 1994. See Appendix A for summary.

## Abiotic Degradation

Very little information is available on the abiotic degradation or dissipation of NAA and related compounds. Ethyl-1-naphthaleneacetate and 1-naphthaleneacetamide are probably susceptible to hydrolysis, and the end product is 1-naphthaleneacetic acid (Acc. No. 129382). Based on the estimates of vapor pressure, volatility may be an important route of dissipation from plant surfaces, particularly for ethyl 1-naphthaleneacetate and to a lesser extent for naphthaleneacetic acid. The vapor pressure of naphthaleneacetamide is much lower – i.e., about 20 times less than NAA and 200 times less than ethyl 1-naphthaleneacetate – and volatilization may be a much less important process. This speculation is consistent with the vegetation half-life study by Obrist (1994), in which the much shorter half-life for ethyl ester relative to naphthaleneacetamide – about a factor of 10 – was attributed to the more rapid volatilization of the ester. In this study, the dissipation of both naphthaleneacetic acid and naphthaleneacetamide followed first-order kinetics over the observation periods (72 hours for naphthaleneacetic acid and 166 hours for naphthaleneacetamide). The dissipation of naphthaleneacetic acid ethyl ester, however, followed first order kinetics up to hour 48 but was non-linear (biphasic) at 72 hours. The non-linear pattern is probably due to initial rapid volatilization of the ester but concurrent and slower hydrolysis of the ester to NAA. While volatilization from plant surfaces may be an

important route of dissipation, volatilization from water and soil is not likely to be substantial. 1-Naphthaleneacetic acid is expected to undergo rapid photolysis in water, on soil, and in air. Observed products in water and soil were 1-naphthoic acid and phthalic acid.

Biotic Degradation

Very little information is available on the biodegradation of NAA or related compounds. 1-naphthaleneacetic acid and structurally similar compounds such as 1-methyl-naphthalene and ethyl-naphthalene are susceptible to biodegradation. No quantitative experimental data, however, are available. Based on SAR analyses (Table 3), half-lives in soil and water are expected to be about 360 hours (15 days) for NAA and the NAA ester. Naphthaleneacetamide is expected to be more persistent in soil and water with a half-life of 900 hours (about 38 days) in both media. Much longer half-lives are estimated in sediment, 1440 hours (60 days) for NAA and the NAA ester and 3600 hours (about 150 days) for naphthaleneacetamide. The groundwater exposure assessment conducted by HED used an aerobic soil metabolism half-life of 3.9 days in the SCIGROW model, similar to the estimates for half-lives in soil and water from the EPI model (Table 3). In the surface water assessment using the FIRST model, current guidelines were followed, and estimated aerobic soil metabolism was 11.7 days (3 × 3.9 days) and anaerobic soil metabolism was 23.4 days (2 × estimated aerobic soil metabolism of 11.7 days).

Mobility

No studies on the mobility of NAA or related compounds have been encountered. Based on the estimated Koc values from EPI-Suite, NAA is likely to be more mobile in soil than either naphthaleneacetamide or the NAA ester. Based on the estimated $K_{o/c}$ values for NAA, this compound is expected to have medium to low mobility in soil. An estimated $K_{OC}$ range was provided was 160-610.[1]

## Water Resources

Drinking Water Assessment

Monitoring data were not available for surface or ground water. While the USGS does provide use data on NAA (USGS 2004a), NAA is not included in the list of pesticides monitored in streams, rivers, and ground water of the United States under NAWQA (USGS 2004b). Drinking water exposures were estimated using the Tier I surface water exposure model FQPA Index Reservoir Screening Tool (FIRST, Version 1.0, dated August 1, 2001) and Tier I ground water exposure model Screening Concentrations in Ground Water (SCI-GROW2, Version 2.2, dated November 1, 2001 ). Modeling inputs, using the above environmental fate data and available label information are presented in Table 4 and 5. Table 6 contains the modeled concentrations in surface (FIRST) and ground (SCI-GROW2) water. The input and output files for FIRST and SCI-GROW are provided in Appendix B.

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[1] Lyman, W.J., et. al.; Handbook of Chemical Property Estimation Methods, NY; McGraw-Hill, p. 4-9 (1982)

| Table 4. NAA Modeling Input Parameters for FIRST and GENEEC. | | |
|---|---|---|
| Parameter | Value | Source |
| Maximum single application rate (lb/acre) | 0.134 | STIK Clear Crop Label (Platte Chemical Co.) |
| Application Method | Aerial Spray [Fine to Medium Spray][1] | STIK Clear Crop Label (Platte Chemical Co.) |
| Number of Applications per Year | 2 | STIK Clear Crop Label (Platte Chemical Co.) |
| Application Interval (days) | 5 | STIK Clear Crop Label (Platte Chemical Co.) |
| PCA factor (decimal) | 0.87 | Effland et al. 2000 |
| Depth of Incorporation | 0 | Broadcast spray |
| Adsorption/Desorption Coefficient ($K_{oc}$) | 297 | Table 3 |
| Aerobic Soil met. $t_{1/2}$ (days) | 11.7 | Per input guidelines, available value (3.9 days × 3) (Meléndez 2003) |
| Aerobic aquatic met. $t_{1/2}$ (days) | 23.4 | Per input guidelines, twice the aerobic soil metabolism (11.7 days × 2) |
| Water Solubility (mg/L) | 420 | Table 3 |
| Hydrolysis (pH 7) $t_{1/2}$ (days) | 0 | Acc. No. 129382 |
| Aqueous photolysis $t_{1/2}$ (days) | 0 | Assume no photolysis as conservative approximation |
| [1] It is possible that coarser sprays would be used but the label does not specify this. Fine to medium spray is used as the EFED default. | | |

| Table 5. NAA Modeling Input Parameters for SCIGROW. | | |
|---|---|---|
| Parameter | Value | Source |
| Maximum single application rate (lb/acre) | 0.134 | STIK Clear Crop Label (Platte Chemical Co.) |
| Number of Applications per Year | 2 | STIK Clear Crop Label (Platte Chemical Co.) |
| Application Interval (days) | 5 | STIK Clear Crop Label (Platte Chemical Co.) |
| Koc (mL/g) | 297 | Table 3 |
| Aerobic Soil met. $t_{1/2}$ (days) | 3.9 | Biowin Output |

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| Table 6. Modeled NAA Surface Water and Ground Water Drinking Water Exposures | | |
|---|---|---|
| Drinking Water Source | Peak (µg/L) | Annual Average (µg/L) |
| Surface Water | 12.9 | 0.712 |
| Ground Water | <0.006 (0.0008) | N/A |

Surface Water Ecological Exposure

To determine ecological risks from NAA use, estimated environmental concentrations (EECs) were modeled using the Tier I model Generic Estimated Environmental Concentrations (GENEEC, Version 2.0, dated August 1, 2001) and based on input parameter data presented in Table 4. An additional input variable in GENEEC is the spray drift application method. Aerial application was selected as the application method. The product label does not specify or characterize recommended droplet sizes. Fine to medium spray is used as the EFED default although it is possible that coarser droplets would be used to ensure wetting of the leaves.

| Table 7. NAA Surface Water Exposures for Ecological Risk Based on GENEEC | | |
|---|---|---|
| Peak (µg/L) | 96 hour (µg/L) | 21-day (µg/L) |
| 9.09 | 8.88 | 7.71 |

Uncertainties

The FIRST model is designed to yield concentration values which exceed those predicted by the linked EPA PRZM and EXAMS models for all but the most vulnerable sites, application patterns and environmental fate properties. PRZM/EXAMS predictions may exceed FIRST predictions under the following circumstances:

Applications to crops in managed environments known to produce excessive runoff (e.g., crops grown over plastic mulch).

Applications at sites with hydrologic group D soils which also receive excessively high rainfall (e.g., EFED sweet potato scenario in southern Louisiana).

Multiple applications over a window of 30 days or longer in exceptionally high rainfall areas (e.g., far southeastern US).

Because few of these conditions are known to exist in the major apple growing regions of the U.S. (See Figure 1), EFED expects FIRST estimates to exceed the Tier 2 estimates in all but the most vulnerable sites.

The SCI-GROW model is used for estimating concentrations of pesticides in ground water under "maximum loading" conditions. SCI-GROW provides an estimate of likely ground water concentrations if the pesticide is used at the maximum allowed label rate in areas with ground water highly vulnerable to contamination due to specific site conditions, high sand content, and high water table. In most cases, a majority of the use area will have ground water that is less vulnerable to contamination than the areas used to derive the SCI-GROW estimate.

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## Ecological Toxicity and Risk Assessment

Ecological Toxicity

The following is a summary of the ecological toxicity data for NAA and related

compounds used in this risk assessment. A fuller summary of these studies as well as other studies submitted to the Agency and studies published in the open literature is given in Appendix A.

***Terrestrial Species***

Avian Acute Oral Toxicity

$LD_{50}$: >2150 mg/kg; NAA acid is practically non-toxic to Bobwhite Quail. (MRID 00065840, Core)

Dietary $LC_{50}$ Study with the Mallard Duck and Bobwhite Quail:

NAA Technical
$LC_{50}$ >10000 ppm (8-day Study). NAA technical is practically non-toxic to Mallard Duck and Bobwhite Quail. (MRID 00083052, 00085909, Supplemental)

NAA Ester
$LC_{50}$ >5620 ppm/NOEC 5620 ppm (8-day Study). NAA ester is practically non-toxic to Bobwhite Quail. (MRID 42584202, Core)

Chronic Study with Mallard Duck and Bobwhite Quail

No studies available.

Mammalian Toxicity Acute $LD_{50}$

NAA Technical: $LD_{50}$, 2520 mg/kg; Toxicity Category III (MRID 00103128)
NAA Amine: $LD_{50}$, >5000 mg/kg; Toxicity Category IV (MRID 43495901)
NAA Na Salt: $LD_{50}$, 933-1350 mg/kg; Toxicity Category III (MRID 00108829)
NAA Ester: $LD_{50}$, 2186 mg/kg; Toxicity Category III (MRID 43494101)

Mammalian Toxicity Acute NOAEL

NAA Technical
Acute NOAEL: 50 mg/kg/day from developmental study in rats (MRID 00042765).

Mammalian Toxicity Chronic NOAEL

NAA, , Sodium Salt
Dog Chronic NOAEL: 15 mg/kg/day from 1-year feeding study used for RfD (MRID 43744201).
Rat Chronic NOAEL: 44-56 mg/kg/day from 20.5-23 month feeding study (MRID 44157501).

Terrestrial Insects

No standard toxicity studies are available. Based on screening studies used in Europe involving several terrestrial insect species, NAA and NAA formulations have been classified as *harmless* (Hassan et al. 1991; Oomen et al. 1994; Samsoe-Petersen 1987, 1995; Thistlewood and Elfving, 1992). Also, a Pacific Northwest Extension Publication (Mayer et al.) indicates that NAA "can be applied at any time with reasonable safety to bees." See Appendix A for additional details.

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Non-Target Terrestrial Plants

Seedling Emergence:
Carrot: NOEC, 0.01 lb ai/A; $EC_{25}$ 0.06 lb ai/A; $EC_{50}$ 0.13 lb ai/A (MRID 43803201, Core)

Seed Germination:
Cucumber and Tomato: Radical Length NOEC, 0.01 lb ai/A; $EC_{25}$ 0.02 lb ai/A (MRID's 42584203 and 43803201, Core)

Vegetative Vigor:
Tomato: NOEC, 62.5 ppm (equivalent to 0.01 lb ae/A); $EC_{25}$ 261.5 ppm (0.043 lb ae/A); $EC_{50}$ >500 ppm (equivalent to > 0.083 lb ae/A) (MRID 43141101, Core)

***Aquatic Species***

96-Hour Static Acute Toxicity Test with the Rainbow Trout:

$LC_{50}$: 28 mg/L; NAA technical is slightly toxic to Rainbow Trout. (MRID 00082528, Core).

96-Hour Static Acute Toxicity Test with the Bluegill Sunfish:

NAA technical
$LC_{50}$: 41 mg/L; NAA technical is slightly toxic to Bluegill Sunfish. (MRID 00082527, Core)

NAA Ester
$LC_{50}$: 2.68 mg/L; NAA ester is moderately toxic to Bluegill Sunfish. (MRID 42498101, Core)

Early-Life Stage Toxicity Test in Fish

No studies were available. EPI-Suite estimates a chronic NOEC of 53.457 mg/L. Based on the corresponding estimates of acute toxicity, this is likely to underestimate toxicity and this concentration is adjusted downward by a factor of 0.074 to 4 mg/L. See discussion below.

48-Hour Static Acute Toxicity Test with the Cladoceran (*Daphnia magna*):

NAA Technical
$LC_{50}$: 180 mg/L (48-hour); NAA technical is practically non-toxic to *Daphnia*. (MRID 00082526, Core). This $LC_{50}$ is similar to the $LC_{50}$ for NAA of 137 (101 to 148) mg/L reported by Fargasova (1994). A somewhat lower 96-hour $LC_{50}$ value of 78.6 (71.6 to 97.3) was reported by Fargasova (1994) for *Tubifex tubifex*.

NAA Ester
$LC_{50}$: 5.68 mg/L (48-hour); NAA ester is moderately toxic to *Daphnia*. (MRID 42470801, Core)

Daphnid Reproduction

No studies were available. EPI-Suite estimates a chronic NOEC of 28.055 mg/L. Based on the corresponding estimates of acute toxicity, this is likely to underestimate toxicity and this concentration is adjusted downward by a factor of 0.43 to 12 mg/L. See discussion below. 15

Aquatic Algae

NAA formulation
$LC_{50}$ in *Selenastrum capricornutum*: 14.9 (11.2 to 19.2) mg/L (MRID 42582203, Core for formulated product)

Aquatic Macrophytes

NAA, potassium salt formulation
14-day NOEC in *Lemna gibba*: 0.46 mg a.i./L (MRID 42582202, Core for formulated product). LOEC of 1.76 mg a.i./L.

***Use of QSAR***

As noted above, experimental values were not available for chronic toxicity in fish or aquatic invertebrates. Estimates for these as well as other endpoints are available from EPI-Suite and these estimates as well as the available experimental data are summarized in Table 8.
As noted in Table 8, EPI-Suite provided reasonably accurate estimates (±30%) of the toxicity of ethyl 1-naphthaleneacetate for acute toxicity in both fish and daphnids. For ethyl 1-naphthaleneacetate, the estimated values are based on other organic esters. The predicted values for NAA are less concordant with the available measured values and the predicted values are uniformly less than the experimental values – i.e., the toxicity of NAA is consistently under-predicted for fish, invertebrates and algae. This may reflect that fact that NAA is a weak acid. As discussed in some detail by Clements et al. (1996), ECOSAR does not contain QSAR functions for weak acids and the QSAR relationships used by EPI Suite for the weak acids – i.e., all but the NAA ester – are based on and should be limited to neutral and non-ionizable organics (Clements et al. 1996).

In the absence of any experimental data on chronic effects in fish or invertebrates, however, the data on the estimated and experimental acute toxicity values in fish or invertebrates were used to adjust the chronic toxicity estimates from EPI-Suite. Thus, the adjustment factor for fish was 0.074 [28 mg/L observed ÷ 376.711 mg/L predicted] and the adjustment factor for *Daphnia* was 0.43 [180 mg/L observed ÷ 420.734 mg/L predicted].

As discussed in the introduction, the use patterns for naphthaleneacetamide and ethyl 1-naphthaleneacetate do not suggest any potential for significant environmental exposure and a quantitative risk assessment was not conducted. Thus, the values for these NAA compounds estimated from EPA-Suite are not used directly in this risk assessment. The estimated value for NAA in green algae is not used other than to note the underestimate in toxicity by EPI-Suite.

Table 8: Summary of QSAR on NAA and Related Compounds for Aquatic Toxicity

| Property | Compound | | | | | |
|---|---|---|---|---|---|---|
| | Naphthalene acetic acid | | Naphthaleneacetamide | | Ethyl 1-naphthaleneacetate | |
| | Measured | Estimated | Measured | Estimated | Measured | Estimated |
| Freshwater Fish Acute 96h $LC_{50}$ (mg/L) | 28 (Trout)<br>41 (Bluegill) | 376.711 | | 251.713 | 2.68 (Bluegill) | 3.756 |
| Freshwater Fish Chronic (mg/L) | | 53.457 | | 30.996 | | 0.444 |
| Marine/Estuarine Fish Acute 96h $LC_{50}$ (mg/L) | | 115.347 | | 50.362 | | N/A |
| *Daphnia magna* Acute 48h $EC_{50}$ (mg/L) | 180 | 420.734 | | 264.548 | 5.68 | 4.350 |

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| Table 8: Summary of QSAR on NAA and Related Compounds for Aquatic Toxicity | | | | | | |
|---|---|---|---|---|---|---|
| Property | Compound | | | | | |
| | Naphthalene acetic acid | | Naphthaleneacetamide | | Ethyl 1-naphthaleneacetate | |
| | Measured | Estimated | Measured | Estimated | Measured | Estimated |
| *Daphnia magna* Chronic (mg/L) | | 28.055 | | 12.003 | | N/A |
| Mysid Shrimp Acute 96h $LC_{50}$ (mg/L) | | 70.796 | | 88.655 | | N/A |
| Aq. Macrophyte 96h $EC_{50}$ (mg/L) | | N/A | | N/A | | N/A |
| Green Algae 96h $EC_{50}$ (mg/L) | 41 | 272.275 | | 162.744 | | 0.319 |

## Ecological Risk Assessment

The risks to terrestrial and aquatic organisms are determined based on Risk Quotient (RQ) and exceedance of Levels of Concern (LOC) method. This method provides an indication of a chemical's potential to cause an effect in the field from effects observed in laboratory studies, when used as directed. Risk quotients are a function of the EEC and the toxicity endpoints as:

$$RQ = \frac{\textit{Estimated Environmental Concentrations}}{\textit{Species Toxicity Value}}$$

The RQ is compared to the level of concern (LOC) to determine the potential for risks.

Terrestrial Organisms

The risk assessment for birds and mammals was based on ELL-FATE (Version 1.2, dated July 19, 2001). In addition to the toxicity data summarized in the previous section and discussed further below, ELL-FATE requires an estimate of half-lives on vegetation. The only available data on vegetation half-lives is a study by Obrist (1994, MRID 43482101), detailed at the end of Appendix A. For input into ELL-FATE, the half-life for NAA of 34.2 hours was converted to 1.425 days and used directly in the risk assessment (Appendix C). Naphthaleneacetamide has a somewhat longer halftime (131.6 hours or about 5.5 days) but, as discussed in the introduction, naphthaleneacetamide is not used in broadcast applications and the potential for substantial exposure is low. The use of this somewhat longer halftime would not impact the risk assessment for birds but would lead to a marginal chronic risk in mammals – i.e., 1 exceedence with an RQ of 1.12.

The toxicity data indicate that NAA and related compounds are practically non-toxic to birds on an acute basis. For the quantitative characterization of risk using ELL-FATE (Appendix C), only toxicity data on NAA technical are used – i.e., a dietary $LC_{50}$ value of >10,000 ppm. Nonetheless, both NAA technical and the NAA ester are classified as practically non-toxic to birds. No chronic studies are available on birds. As discussed below, there are no substantial differences between the acute and chronic NOEC values in mammals. Thus, the acute value of >10,000 ppm was used for the risk characterization of chronic exposures to birds. The highest risk quotient is 0.003, substantially below any level of concern for acute risk (RQ=0.5), restricted use (RQ=0.2), or endangered species (RQ=0.1). Therefore, risks to endangered and non-endangered birds are considered low.

Mammalian toxicity data from OPP's Health Effects Division is used as a surrogate for wild mammal toxicity. The lowest acute oral $LD_{50}$ for rats is 933 mg/kg – the sodium salt of

NAA from MRID 00108829. Thus, Na-NAA is classified as slightly toxic. The chronic toxicity value for mammals is taken as 44 mg/kg from a chronic toxicity/oncogenicity study (MRID 44157501) in which male and female rats were fed dietary concentrations of the sodium salt of NAA at concentrations of 0, 100, 1000, or 5000 ppm (corresponding to 0, 4.4, 43.8, and 224.5 mg/kg/day for males and 0, 5.6, 55.8, and 303.6 mg/kg/day for females). The LOAEL is 5000 ppm (224.5 mg/kg/day for males and 303.6 mg/kg/day for females), based on an increased incidence of stomach (mucosal gland dilation) and lung lesions (focal alveolar macrophages) in both sexes of rats, and on lowered body weight gain and food efficiency in females. The corresponding NOAEL is 1000 ppm (43.8 mg/kg/day for males and 55.8 mg/kg/day for females). As summarized in Appendix C, the highest acute RQ for mammals is 0.04 and the highest chronic RQ is 0.8 – both for a small mammal consuming short grass. Therefore, risks to endangered and non-endangered mammals are considered low.

As summarized in the previous section, standard toxicity studies are available in non-target plants for seedling emergence, seed germination, and vegetative vigor. All of these studies are classified as scientifically valid (Core, see Appendix A). The most sensitive endpoint is seedling emergence, with an NOEC of 0.01 lb ai/acre and an $EC_{25}$ of 0.06 lb ai/acre. In the broadcast application of the salts of NAA, offsite drift is the most plausible route of exposure. For this risk assessment, the TERR PLANT model was used to estimate an EEC, and the AgDRIFT model was used to estimate the proportion of off-site deposition as a fraction of the application rate. Calculations are provided in Appendix D. The level of concern for acute risk is not exceeded for non-endangered or endangered terrestrial plants. However, for endangered species, the RQ is equal to the level of concern. It should be noted that TERR PLANT is a very simple model that does not take into consideration the biodegradation of the compounds of interest. As an additional measurement of precaution, EFED used the model Oasis Catabol V. 4.55, to predict the biodegradation pathway of NAA. Background information about the model, results of the run, and figures of the predicted degradates appear in Appendix G. It is important to note that the first biodegradation pathway expected, according to the model is the loss of the acid moiety, to form 1-methyl-naphthalene, which causes the molecule to lose its herbicide activity. The predicted rate of biodegradation from EPISUITE was only 3.9 days. Furthermore, deposition curves generated using AgDRIFT (both for aerial applications and for airblast applications) indicate that at very short distances from the point of application (less than 25 feet), the level of deposition decreases substantially; RQ values would decrease proportionally, as well. Based on these calculations and modeling, it can be concluded that risks to nontarget terrestrial plants, including endangered species, would not be expected.

No quantitative data are available on the toxicity of NAA or related compounds to the honey bee. However, a Pacific Northwest Extension Publication (Mayer et al.) indicates that NAA "can be applied at any time with reasonable safety to bees." As summarized in Appendix A, all other studies from the open literature are essentially screening studies for ranking or classifying toxicity to terrestrial insects. The results of these studies cannot be readily expressed in units of application rate that would be directly applicable to this risk assessment. Nonetheless, all of the open literature studies classify NAA as "harmless" relative to a large number of other pesticides.

Aquatic Organisms

The toxicity data indicate NAA is practically non-toxic on an acute basis for all species tested. Acute and chronic risks to aquatic organisms – fish, invertebrates, and plants – are provided in Table 9. Based on the available data and calculated risk quotients, exposure to NAA applied to apples at 0.134 lbs a.e./acre does not approach the acute (LOC, 0.5), restricted use (LOC, 0.1) or endangered species (LOC, 0.05) levels of concern for freshwater fish or invertebrates. Based on limited data – chronic SAR estimates corrected for available acute toxicity data – chronic risks to invertebrates and fish are below the level of concern (LOC $\leq$1) by a factor of about 500. While these chronic estimates are highly uncertain, this margin of safety is substantial.

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| Table 9: Risk Quotients for Aquatic Species | | | |
|---|---|---|---|
| **Species** | **RQ** | **Toxicity Value (mg/L)** | **End-point** |
| Fish, Acute Exposures | | | |
| Bluegill sunfish | 2e-04 | 41 | $LC_{50}$ |
| Trout | 3e-04 | 28 | $LC_{50}$ |
| Fish, Chronic Exposures | | | |
| Estimated from EPI-Suite | 2e-03 | 4 | NOEC |
| | | | |
| Aquatic Invertebrates, Acute Exposures | | | |
| *Daphnia magna* | 5e-05 | 180 | $LC_{50}$ |
| *Tubifex tubifex* | 1e-04 | 78.6 | $LC_{50}$ |
| Aquatic Invertebrates, Chronic Exposures | | | |
| Estimated from EPI-Suite | 6e-04 | 12 | NOEC |
| | | | |
| Aquatic Plants, Acute exposures | | | |
| *Selenastrum capricornutum* | 2e-04 | 41 | $EC_{50}$ |
| *Lemna gibba* | 2e-02 | 0.46 | NOEC |
| Exposures (mg/L) | | | |
| Acute | 9.1e-03 | Peak exposure from GENEEC | |
| Longer-term | 7.7e-03 | 21-Day average exposure from GENEEC | |

Given the locations of the principle apple, pear, and olive growing regions (Figure 1) exposure to estuarine and marine environments is plausible. Toxicity data are not available from testing with estuarine/marine organisms. However, based on the toxicity data from freshwater organism testing, risks to estuarine and marine organisms (fish, aquatic invertebrates, and plants) are unlikely.

Uncertainties

Ecotoxicity data for terrestrial animals on an acute basis is limited by the number of species tested. Variability in toxicity to chemicals across species can, at times, be quite high. Using two birds and one mammal species to represent all terrestrial animals may result in the underestimation of risks for some particularly sensitive animal while overestimating the risks of others. In addition, use of laboratory rats as surrogates for wild mammals has inherent uncertainties because laboratory mammals are generally bred to minimize genetic variability and to be sensitive to chemical exposures – i.e, likely to exhibit responses at lower does. In these cases, toxicity may be overstated. Further, chronic risks to mammals may be overestimated because the effects seen in the two-year feeding study could require an analogous exposure in the field. Concentrations on apples or other vegetation from two applications in a year would likely decrease as plant biomass increases and not all of the field is treated, thus exposure will be reduced over time.

Most of these issues apply to the aquatic assessment, as well. Specific to this aquatic assessment, additional factors derive from the use of EPI-Suite (in the absence of actual data), and the use of data from freshwater organism tests to conclude low probability of risk to estuarine and marine species.

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Samsoe-Petersen L. 1987. Laboratory method for testing side effects of pesticides on the rove beetle *Aleochara-bilineata* adults. Entomophaga. 32(1): 73-82.

Samsoe-Petersen L. 1995. Effects of 67 herbicides and plant growth regulators on the rove beetle *Aleochara bilineata* (Col.: Staphylinidae) in the laboratory. Entomophaga. 40: 95-104.

SCI-GROW, 2001. Screening Ground Water Model, Version 2.2. November 1, 2001. Environmental Fate and Effects Division, Office of Pesticide Programs, U.S. Environmental Protection Agency, Washington, D.C.

Thistlewood H MA; Elfving DC. 1992. Laboratory and field effects of chemical fruit thinners on tetranychid and predatory mites (Acari) of apple. J Econ Entomol. 85(2): 477-485.

USDA/ARS (U.S. Department of Agriculture Agricultural Research Station). 1995. ARS Pesticide Properties Database. http://wizard.arsusda.gov/rsml/testfiles. NAA listing last updated May 1995.

USGS (U.S. Geological Survey). 2004a. National Water Quality Assessment Program (NAWQA) Pesticide National Synthesis Project. Annual Use Maps. http://ca.water.usgs.gov/pnsp/use92/

USGS (U.S. Geological Survey). 2004b. National Water Quality Assessment Program (NAWQA) Pesticide National Synthesis Project. National assessment of pesticides in the streams, rivers, and ground water of the United States. National statistical summaries updated to 1992-2001. http://ca.water.usgs.gov/pnsp/

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# APPENDIX A

## Summary of Toxicity Data

### Avian Acute Oral Toxicity

*Submissions:*

Fink R. 1976a. Final Report: Acute Oral LD 50^--Mallard Duck: Project No. 113-124.. (Unpublished study received Sep 19, 1979 under 264-336; prepared by Truslow Farms, Inc., submitted by Union Carbide Agricultural Products Co., Inc., Ambler, Pa.; CDL: 099029-B) MRID 00065839.

This study used NAA Acid, Technical Grade. The reported $LD_{50}$ is 1750 (1337-2289) mg/kg bw. The study is classified as scientifically sound, Supplemental (cannot be repaired to CORE) EFED used as somewhat different calculation method to estimate an $LC_{50}$ value of 1690 mg/kg.

Fink R; Beavers JB. 1979. Final Report: Acute Oral $LD_{50}$ -- Bobwhite Quail: Project No. 113-153. (Unpublished study received Sep 19, 1979 under 264-336; prepared by Wildlife International, Ltd. and Washington College, submitted by Union Carbide Agricultural Products Co., Inc., Ambler, Pa.; CDL:099029-C) MRID 00065840.

This study used NAA Acid, Technical grade and reports an $LD_{50}$ value >2150 mg/kg bw – i.e., no mortality noted over a 14 day observation period. The study is classified as scientifically sound, Core.

Fink R; Beavers JB; Grimes J; et al. 1979a. Final Report: Acute Oral $LD_{50}$ --Bobwhite Quail: Project No. 113-154. (Unpublished study received Sep 19, 1979 under 264-336; prepared by Wildlife International, Ltd. and Washington College, submitted by Union Carbide Agricultural Products Co., Ambler, Pa.; CDL: 099029-H) MRID 00042753.

This study reports an $LD_{50}$ = >2510 mg/kg. The study used a formulation and thus does not meet guideline requirements. The study is classified as Scientifically sound, Supplemental.

Fink R; Beavers JB; Grimes J; et al. 1979b. Final Report: Acute Oral $LD_{50}$ --Mallard Duck: Project No. 113-155.. (Unpublished study received Sep 19, 1979 under 264-336; prepared by Wildlife International, Ltd. and Washington College, submitted by Union Carbide Agricultural Products Co., Ambler, Pa.; CDL: 099029-I) MRID 00042754.

This study reports an $LD_{50}$ = >2510 mg/kg. At this dose, mortality was noted in only one animal. The study used a formulation and thus does not meet guideline requirements. The study is classified as Scientifically sound, Supplemental.

*Open Literature:* No studies encountered.

### Avian Dietary $LC_{50}$

*Submissions:*

Campbell S; Jaber M. 1992a. Technical 1-Naphthaleneacetamide: A dietary $LC_{50}$ Study with the Northern Bobwhite: Lab Project Number: 246-108. Unpublished study prepared by Wildlife International Ltd. 37 p. MRID 42584201.

This study tested 1-Naphthaleneacetamide and reports a dietary $LC_{50}$ value >5620 ppm and a NOEC of 1780 ppm based on decreased body weight at 3160 ppm and 5620 ppm. Based on these results technical grade 1-naphthaleneacetamide is classified as practically non-toxic to birds. The study meets guidelines and is classified as Core.

Campbell S; Jaber M. 1992b. Technical 1-Naphthalene Acetic Acid Ethyl Ester: A Dietary $LC_{50}$ Study with the Northern Bobwhite: Lab Project Number: 246-109R. Unpublished study prepared by Wildlife International Ltd. 37 p. MRID 42584202.

This study tested NAA ethyl ester and reports a dietary $LC_{50}$ value >5620 ppm. Based on these results technical grade NAA ethyl ester is classified as practically non-toxic to birds. The study meets guidelines and is classified as Core.

Fink R. 1976b. Final Report: Eight-Day Dietary $LC_{50}$--Bobwhite Quail: Project No. 113-118. (Unpublished study received Sep 19, 1979 under 264-336; prepared by Truslow Farms, Inc., submitted by Union Carbide Agricultural Products Co., Ambler, Pa.; CDL: 099029-G) MRID 00072749.

This study tested a formulation containing NAA and reported an dietary $LC_{50}$ value > 10000 ppm with no mortality in any animals. While the study is classified as scientifically sound, the use of a formulation does not fulfill guideline requirements
Category: Supplemental.

Fink R. 1976c. Final Report: Eight-Day Dietary $LC_{50}$ --Mallard Duck: Project No. 113-119. (Unpublished study received Sep 19, 1979 under 264-336; prepared by Truslow Farms, Inc., submitted by Union Carbide Agricultural Products Co., Ambler, Pa.; CDL: 099029-F) MRID 00083052.

This study tested a formulation containing NAA (different from Fink 1976b above) and reported an dietary $LC_{50}$ value > 10000 ppm with no mortality in any animals. While the study is classified as scientifically sound, the use of a formulation does not fulfill guideline requirements
Category: Supplemental.

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Fink R. 1976d. Final Report: Eight-day Dietary $LC_{50}$ --Bobwhite Quail: Project No. 113-122. (Unpublished study received Sep 19, 1979 under 264-336; prepared by Truslow Farms, Inc., submitted by Union Carbide Agricultural

Products Co., Inc., Ambler, Pa.; CDL:099029-D) MRID 00085909.
This study test technical grade NAA at a dietary concentration of 10,000 ppm. No mortality or overt signs of toxicity. This study is scientifically sound and meets guideline requirements. Category: Core. Classification: Practically non-toxic.

*Open Literature:* No studies encountered.

**Avian Reproduction**

*Submissions*: None

*Open Literature*
Bishop CA; Collins B; Mineau P; Burgess NM; Read WF; Risley C. 2000. Reproduction of Cavity-Nesting Birds in Pesticide-Sprayed Apple Orchards in Southern Ontario, Canada, 1988-1994.
This is a field study that specifically looks at reproduction in birds in apple orchards sprayed with various pesticides. There is no specific information on NAA or related compounds.

**96-Hour Static Acute Toxicity Test with Rainbow Trout**

*Submissions*:
LeBlanc GA; Sousa JV. 1981b. Acute Toxicity of NAA to Rainbow Trout (~Salmo gairdneri~): Report #BW-81-4-876.. (Unpublished study received Oct 14, 1981 under 264-336; prepared by EG & G, Bionomics, submitted by Union Carbide Agricultural Products Co., Inc., Ambler, Pa.; CDL: 246079-C) MRID 00082528.
This study used technical grade NAA and originally reported an $LC_{50}$ value of 57 (47-68) mg/L ai with an NOEC of 32 mg/L. After review by EFED, the study was resubmitted and classified as Core with a corrected 96-hour $LC_{50}$ value: 28 mg/L. THe compound is classified as Slightly Toxic to trout.

Morrissey AE. 1979. The Acute Toxicity of 72-A112 to the Rainbow Trout,~Salmo gairdneri~Richardson: UCES Project No. 11506-24-10.. (Unpublished study received Sep 19, 1979 under 264-336; submitted by Union Carbide Agricultural Products Co., Ambler, Pa.; CDL:099029-K) MRID 00042756.
This study used a formulation of NAA and reported an $LC_{50}$ value 14.1 mg/L (12.6-15.8 mg/L) and a NOEC <5.6 mg/L – i.e., the lowest dose tested. Sublethal effects included surfacing and sounding. The study is classified as scientifically sound but does not fulfill guideline because it used a NAA acid formulation. Category: Supplemental

Wessel RD. 1969. Letter sent to Harold G. Alford dated May 29, 1969 Fish toxicity on coho salmon for Kling-title : File No. 706.11.. (Unpublished study, including letter dated May 22, 1969 from H.G. Alford to R.D. Wessel, received Jun 23, 1969 under 239-2169; submitted by Chevron Chemical Co., Richmond, Calif.; CDL:001458-A) MRID 00082525.
This is a summary of a study in coho salmon that reports a 96 h $LC_{50}$ value of 75.7 mg/L.

*Open Literature:* None

**96-Hour Static Acute Toxicity Test with Bluegill Sunfish**

*Submissions*:
LeBlanc GA; Sousa JV. 1981a. Acute Toxicity of NAA to Bluegill (*Lepomis macrochirus*): Report #BW-81-4-867. (Unpublished study received Oct 14, 1981 under 264-336; prepared by EG & G, Bionomics, submitted by Union Carbide Agricultural Products Co., Inc., Ambler, Pa.; CDL:246079-B) MRID 00082527.
This study used technical grade NAA and originally reported an $LC_{50}$ value of 82 (68-100) mg a.i./L and an NOEC of 68 mg/L. As originally submitted, the study was classified as *not scientifically sound* because of reporting deficiencies. On re-submission, the study was classified as scientifically sound and core (fulfills guideline requirements. The 96h $LC_{50}$ value was corrected to 41 mg/L and the technical grade NAA is classified as slightly toxic.

Schneider C. 1979. The Acute Toxicity of 72-A112 to the Bluegill Sunfish, *Lepomis macrochirus* Rafinesque: UCES Project No. 11506- 24-09. (Unpublished study received Sep 19, 1979 under 264-336; submitted by Union Carbide Agricultural Products Co., Ambler, Pa.; CDL:099029-L) MRID 00042757.
This study used a formulation of NAA and reported an $LC_{50}$ value 23.7 mg/L and a NOEC 5.6 mg/L. The study is classified as scientifically sound but does not fulfill guideline because it used a NAA formulation. Category: Supplemental

Terrell Y. 1992b. Technical 1-Naphthaleneacetic Acid, Ethyl Ester: Acute Effects on the Bluegill Sunfish, *Lepomis macrochirus*: Lab Project Number: 92-700110-100-1: BR-1895B. Unpublished study prepared by Aqua Survey, Inc. 88 p. MRID 42498101.
This study used technical grade 1-Naphthaleneacetic Acid, Ethyl Ester and reports an $LC_{50}$ value 3.75 mg/L with an NOEC of 1.36 mg/L. On review by EFED, the $LC_{50}$ was recalculated as 2.68 mg/L and the NOEC was adjusted to 0.79 mg/L based on final mean measured concentrations. The study is classified as Core and the agent is classified as moderately toxic.

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*Open Literature:* No studies encountered.

**Early-Life Stage Static Toxicity Test with Fathead Minnow**

No studies available in submissions or open literature.

**48-Hour Static Acute Toxicity Test with the Cladoceran (*Daphnia magna*)**

LeBlanc GA; Surprenant DC. 1981. Acute Toxicity of Naphthaleneacetic Acid to the Water Flea (*Daphnia magna*): Report #BW-81-4-866.. (Unpublished study received Oct 14, 1981 under 264-336; prepared by EG & G, Bionomics, submitted by Union Carbide Agricultural Products Co., Inc., Ambler, Pa.; CDL:246079-A) MRID 00082526.

This study used technical grade NAA and reports an $LC_{50}$ value of 360 (220-590) mg/L and an NOEC of 220 mg/L. As originally submitted, the study was classified as not scientifically sound because of reporting deficiencies. The study was re-submitted and accepted as scientifically sound and classified as core. The 48h $LC_{50}$ value was corrected to 180 mg/L and NAA was classified as practically non-toxic.

Terrell Y. 1992a. Technical 1-Naphthaleneacetic Acid, Ethyl Ester Acute Effects on the Cladoceran, *Daphnia magna*: Lab Project Number: 92-330110-100-1: BR-1895A. Unpublished study prepared by Aqua Survey, Inc. 95 p. MRID 42470801.

This study used technical grade 1-Naphthaleneacetic Acid, Ethyl Ester and reported an 48h $LD_{50}$ of 5.68 mg/L and NOEC of less than 4.38 mg/L.

Union Carbide Corporation. 1979. The Acute Toxicity of 72-A112 to the Water Flea, *Daphnia magna* Straus: UCES Project No. 11506-24- 11. (Unpublished study received Sep 19, 1979 under 264-336; submitted by Union Carbide Agricultural Products Co., Ambler, Pa.; CDL:099029-J) MRID 00042755.

This study used as formulation of NAA and reports an LC50 value of 23.8 mg/L with an NOEC of 18 mg/L. No individual dose-response data are presented. Category: Supplemental.

*Open Literature*:

Fargasova A. 1997. Toxicity determination of plant growth regulators in selected aquitic organism Daphnia magna and Tubifex tubifex. Biologia, Bratislava. 52(3): 405-408.

This study used NAA obtained from Ciba Geigy, Basel, Switzerland (purity not reported). Bioassays followed ASTM protocols. The study reports a 48 h $LC_{50}$ of 137. (101.24-147.57) mg/L and an $LC_5$ of 36.6 (35.72-38.29) mg/L for *Daphnia magna*. The study also gives a 96 h $LC_{50}$ of 78.6 (71.6-97.31) mg/L and an $LC_5$ of 1.82 (1.78-2.03) mg/L for *Tubifex tubifex*. Statistical method for calculating the reports $LC_x$ values given only as moving average method.

**Daphnid Reproduction**

No studies encountered in submissions or open literature.

**Aquatic Macrophytes**

*Submissions*:

Hughes J; Alexander M. 1992b. The toxicity of K-Salt Fruit Fix 800 to Lemna gibba G3: Lab Project Number: B015-001-2. Unpublished study prepared by Malcolm Pirnie, Inc. 36 p.. MRID 42582202.

This study tested as potassium-salt formulation of NAA and reports an $EC_{50}$ = 5.09 (4.05-6.38) mg/L, an $EC_{25}$ of 1.67 (1.18-2.41) mg/L, and an NOEC of 0.459 mg/L. The study is classified as scientifically sound, meeting guideline for Tier 2 aquatic plant study with formulated product. Classification: CORE for formulated product.

Hughes J; Alexander M. 1992d. The Toxicity of Fruit Fix Super Concentrate 800 to Lemna gibba G3: Lab Project Number: B015-001-4. Unpublished study prepared by Malcolm Pirnie, Inc. 35 p.. MRID 42582204. [Set No. CBI01]

This study tested an ammonium-salt formulation of NAA and reports an $EC_{50}$ = 5.61 (4.29-7.35) mg/L, an $EC_{25}$ of 2.2 (1.46-3.32) mg/L, and an NOEC of 1.81 mg/L. The study is classified as scientifically sound, meeting guideline for Tier 2 aquatic plant study with formulated product. Classification: CORE for formulated product.

*Open Literature*: None

**Aquatic Algae**

*Submissions*

Hughes J; Alexander M. 1992c. The Toxicity of Fruit Fix Super Concentrate 800 to *Selenastrum capricornutum*: Lab Project Number: B015-001-3. Unpublished study prepared by Malcolm Pirnie, Inc. 37 p. MRID 42582203.

This study tested an ammonium-salt formulation of NAA and reports an $EC_{50}$ = 14.9 (11.2 - 19.2) mg/L, an $EC_{25}$ of 10.2 (6.77 to 15.4) mg/L, and an NOEC of 6.47 mg/L. The study is classified as scientifically sound, meeting guideline for aquatic algae study with formulated product. Classification: CORE for formulated product.

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*Open Literature*

Fargasova A. 1994. Toxicity determination of plant growth hormones on aquatic alga-*Scenedesmus quadricauda*.

Bull Environ Contam Toxicol. 52(5): 706-711.

This study used NAA acid (source and purity not reported). $EC_x$ values for growth reported for after 20 days. The study reports $EC_{50}$ of 66 (63.21-86.73) mg/L and an $LC_{95}$ of 78.4 mg/L. Statistical method for calculating the reports $LC_x$ values given as moving average method. Individual response points and concentration-time curves presented.

**Non-Target Terrestrial Plants**

*Submissions*

Harnish W. 1992a. Fruit Fix Super Concentrate 800. (NAA-Ammonium 21. 4%) Tier I Non-target Plant Hazard Evaluation-terrestrial Vegetative Vigor Study: Lab Project Number: 22925B002. Unpublished study prepared by Landis International, Inc. and AMVAC Chemical Corp. 87 p. MRID 42564201.

Ammonium salt formulation with several species. Scientifically sound accept for assay on peanuts. Cucumber only species affected at treatment rate of 0.1 lb a.e./acre, reported as the maximum application rate. Classification: CORE except for peanut (invalid).

Harnish W. 1992b. K-Salt Fruit Fix 800 (NAA-Potassium Salt 24.2%) Tier I Non-target Plant Hazard Evaluation-terrestrial Vegetative Vigor Study: Lab Project Number: 22925B004. Unpublished study prepared by Landis International, Inc. and AMVAC Chemical Corp. 92 p. MRID 42564202.

Formulation of potassium salt. Study classified as scientifically sound and meeting guideline requirements except for assay in peanut which was not considered scientifically sound because the seeds were treated with Captan. Based on the results of the study, Tier II is testing required. Classification: CORE except for peanut (invalid). Most sensitive species was the tomato based on both plant height (34% inhibition) and dry weight (20% inhibition but not statistically significant).

Harnish W. 1992c. K-Salt Fruit Fix 800 (NAA-Potassuim 24. 2%): Tier I and Tier II Non-Target Plant Hazard Evaluation: Terrestrial Seed Germination and Seedling Emergence Study: Lab Project Number: 22925B003. Unpublished study prepared by Landis International, Inc. 406 p. MRID 42584203.

Assayed seed germination, seedling emergence and vegetative vigor. No assays not scientifically sound for seed germination. Cucumber, radish and tomato are scientifically sound but do not meet guideline – NOEL for radicle length not determined. Other assays are acceptable. Most sensitive monocot was oat based on radicle length – NOEL, LOEL, $EC_{25}$, and $EC_{50}$ of 0.02, 0.03, and 0.05, and 0.12 lb ai/A. Only valid dicot assay was sunflower: NOEL, LOEL, $EC_{25}$ and $EC_{50}$ of 0.05, 0.1, 0.14 and 0.24 lb ai/A.

Harnish W. 1992d. Fruit Fix Super Concentrate 800: Tier I and II Non-target Plant Hazard Evaluation--Terrestrial Seed Germination and Seedling Emergence Study: Lab Project Number: 22925B001. Unpublished study prepared by Landis Int'l, Inc. 502 p.. MRID 42589901.

Seed Germination: Peanut not scientifically sound. Radish, cucumber, sunflower, corn, and wheat scientifically sound but not guideline – NOEL for radicle length not determined. Oats, onion, soybean, and tomato are scientifically sound and meet guideline. Most sensitive monocot: oat based on radicle length – NOEL, LOEL, $EC_{25}$, and $EC_{50}$ of 0.01, 0.02, 0.02, and 0.05 lb ai/A. Seedling emergence: invalid. Follow-up study submitted under MRID 43803201.

Harnish W. 1994a. K-Salt Fruit Fix 800 Tier II Non-Target Plant Hazard Evaluation-Terrestrial Vegetative Vigor: Final Report: Lab Project Number: 22925B006: 1231-93-229-02-25B-02. Unpublished study prepared by Landis International, Inc. 52 p.. MRID 43141101.

Tomato is most sensitive species. The study is scientifically sound and fulfills guideline requirements for Tier 2 Vegetative Vigor Assay. EFED calculated the following toxicity values: NOEC , $ED_{25}$ and $EC_{50}$ of 62.5, 261.5, and >500 ppm. Classification: Core.

Harnish W. 1994b. K-Salt Fruit Fix 800 (NAA-Potassium 24.2%): Tier I Non-Target Plant Hazard Evaluation-Terrestrial Vegetative Vigor Study on Carrot: Supplement: Lab Project Number: 22925B004: 21-92-229-02-25B-04. Unpublished study prepared by Landis International, Inc. 52 p. MRID 43168101.

The study is scientifically sound but does not meet guideline requirements because no raw height and weight data are reported. All responses were less than 25% inhibition at doses of up to 500 ppm (0.083 lb a.e./acre). Classification: Supplemental and Tier II testing is not required.

Harnish W. 1994c. Fruit Fix Super Concentrate 800. (NAA-Ammonium 21.4%): Tier I Non-Target Plant Hazard Evaluation-Terrestrial Vegetative Vigor Study on Carrot: Supplement: Lab Project Number: 22925B002: 21-92-229-01-25B-02. Unpublished study prepared by Landis International, Inc. 52 p. MRID 43168301. [Set No. CBI01]

This is a supplement to Harnish 1994b. See previous entry for comments.

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Harnish W. 1995a. NAA: Determination of the Effects of NAA Ammonium Salt. (800 g/Gallon End Use Formulation) on Seed Germination and Seedling Emergence: Final Report: Lab Project Number: 22925B007: 1231-94-229-01-25B-01. Unpublished study prepared by Landis International, Inc. 107 p. MRID 43803201.

This is follow-up study to Harnish (1992d, MRID 42589901) that had deficiencies in the seedling emergence assay, as discussed above. Partial DER is available for this study. Carrot is most sensitive species, with NOEC (dry weight) = 0.01 lb ai/A, EC25 = 0.06 lb ai/A, EC50 = 0.13 lb ai/A. Classification: Core

Harnish W. 1995b. NAA: Determination of the Effects of NAA Potassium Salt. (800 g/Gallon End Use Formulation) on Seed Germination and Seedling Emergence: Final Report: Lab Project Number: 22925B008: 1231-94-229-02-25B-02. Unpublished study prepared by Landis International, Inc. 105 p. MRID 43837401. [Set No. CBI01]

This study is scientifically sound but not guideline because only 5 and not 10 species tested. Nonetheless, this study was designed to get NOELS on 5 species not found in Harnish (1992c, MRID 42584203). The most sensitive dicots were the cucumber and tomato, both with $EC_{25}$ 0.02 lb/acre and an NOEC of 0.01 lb/acre for the most sensitive parameter, radicle length. No monocots were tested.

*Open Literature*

Borkowski J. 1998. The effect of growth regulators on the healthiness, growth and sproutig of inflorescense shoot of lettuce. ACTA Agrobotanica. 41: 275-284. (In Polish with English abstract).

Based on the abstract, this study used a solution of the potassium salt of NAA. When lettuce was sprayed at a concentration 25 mg/dm$^3$, tip burn was noted. Additional details are not provided in the abstract.

**Terrestrial Insects**

*Submissions*: None

*Open Literature*:

Hassan SA; Bigler K; Bogenschuetz H; Boller E; Brun J; Calis J NM; Chiverton P; Coremans-Pelseneer J; Duso C; et al. 1991. Results of the Fifth Joint Pesticide Testing Program carried out by the International Organization for Biological Control, West Plearctic Regional Section Working Group on pesticides and beneficial organisms. Entomophaga. 36(1): 55-68.

This is a summary of results of a series of screening studies used in Europe to assess effects of a variety of compounds on several non-target terrestrial invertebrates. Based on the criteria used in interpreting the screening studies, an NAA formulation is classified as harmless.

Mayer, DF; Johansen, CA; Baird, C.R. 19??. How to Reduce Bee Poisoning from Pesticides. A Pacific Northwest Extension Publication (PNW518). NAA is included in a list of pesticides which can be applied at any time with reasonable safety to bees. http://cru.cahe.wsu.edu/CEPublications/pnw0518/pnw0518.pdf

Oomen PA; Jobsen JA; Romeijn G; Wiegers GL. 1994. Side-effects of 107 pesticides on the whitefly parasitoid *Encarsia formosa*, studies and evaluated according to EPPO guideline no. 142. Bull OEPP. 24(1): 89-107.

NAA is classified as harmless.

Samsoe-Petersen L. 1987. Laboratory method for testing side effects of pesticides on the rove beetle *Aleochara-bilineata* adults. Entomophaga. 32(1): 73-82.

NAA is classified as harmless.

Samsoe-Petersen L. 1995. Effects of 67 herbicides and plant growth regulators on the rove beetle *Aleochara bilineata* (Col.: Staphylinidae) in the laboratory. Entomophaga. 40: 95-104.

NAA is classified as harmless.

Thistlewood H MA; Elfving DC. 1992. Laboratory and field effects of chemical fruit thinners on tetranychid and predatory mites (Acari) of apple. J Econ Entomol. 85(2): 477-485.

NAA is classified as harmless to Tetranychid and predatory mites.

*General Comment on Studies on Terrestrial Insects*: There is no standard toxicity test on honey bees. All studies from the open literature are essentially screening studies for crudely ranking or classifying toxicity to terrestrial insects. The results of these studies cannot be readily expressed in units of application rate that would be directly applicable to this risk assessment.

## Summary of Data on Foliar Half-lives

Obrist, J. (1994) NAA Bridging Study: Determination of the Half-life of Naphthaleneacetic Acid, (NAA), Naphthaleneacetamide, and Naphthaleneacetic Acid Ethyl Ester on Apple Leaves: Lab Project Number: 94399. Unpublished study prepared by Pan-Agricultural Labs, Inc. 136 p. MRID 43482101.

This study determined foliar halftimes from apple leaves of $^{14}$C-labeled naphthaleneacetic acid, naphthaleneacetamide, and naphthaleneacetic acid ethyl ester. The halftimes for these compounds were 34.2 hours, 131.6 hours, and 12.8 hours, respectively. The major mechanism of dissipation appeared to be volatilization. The dissipation of both naphthaleneacetic acid and naphthaleneacetamide followed first-order kinetics over the observation periods (72 hours for naphthaleneacetic acid and 166 hours for naphthaleneacetamide). The dissipation of naphthaleneacetic acid ethyl ester followed first order kinetics up to hour 48 but was non-linear (two compartment) at 72 hours. The 72 hour time point was not used in calculating the halftime. The non-linear pattern is probably due to initial rapid volatilization of the ester but concurrent and slower hydrolysis of the ester to NAA.

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# APPENDIX B

## Environmental Exposure Modeling Outputs

### Ambient Surface Water Concentrations for use in the Ecological Risk Assessment

***Drinking Water (FIRST)***

RUN No. 1 FOR NAA ON Apples * INPUT VALUES *

| RATE (#/AC) ONE (MULT) | No.APPS & INTERVAL | SOIL Koc | SOLUBIL (PPM ) | APPL TYPE (%DRIFT) | %CROPPED AREA | INCORP (IN) |
|---|---|---|---|---|---|---|
| .134 ( .234) | 2 5 | 297.0 | 420.0 | AERIAL(16.0) | 87.0 | .0 |

FIELD AND RESERVOIR HALFLIFE VALUES (DAYS)

| METABOLIC (FIELD) | DAYS UNTIL RAIN/RUNOFF | HYDROLYSIS (RESERVOIR) | PHOTOLYSIS (RES.-EFF) | METABOLIC (RESER.) | COMBINED (RESER.) |
|---|---|---|---|---|---|
| 11.70 | 2 | N/A | .00- .00 | 23.40 | 23.40 |

UNTREATED WATER CONC (MICROGRAMS/LITER (PPB)) Ver 1.0 AUG 1, 2001

| PEAK DAY (ACUTE) CONCENTRATION | ANNUAL AVERAGE (CHRONIC) CONCENTRATION |
|---|---|
| 12.923 | .712 |

**Ambient Surface Water Concentrations for use in the Drinking Water Assessment**

***Shallow Ground Water (SCI-GROW2)***

RUN No. 1 FOR NAA INPUT VALUES

| APPL (#/AC) RATE | APPL. NO. | URATE (#/AC/YR) | SOIL KOC | SOIL AEROBIC METABOLISM (DAYS) |
|---|---|---|---|---|
| .134 | 2 | .268 | 297.0 | 3.9 |

GROUND-WATER SCREENING CONCENTRATIONS IN PPB

.000802

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| A= | .650 | B= | 302.000 | C= | -.187 | D= | 2.480 |
| F= | -2.524 | G= | .003 | URATE= | .268 | GWSC= | .000802 |

RILP= -.464

***Surface Water (GENEEC2)***

RUN No. 1 FOR NAA ON Apples * INPUT VALUES *

| RATE (#/AC) ONE(MULT) | No.APPS & INTERVAL | SOIL Koc | SOLUBIL (PPM ) | APPL TYPE (%DRIFT) | NO-SPRAY (FT) | INCORP (IN) |
|---|---|---|---|---|---|---|
| .134( .234) | 2 5 | 297.0 | 420.0 | AERL_B( 13.0) | .0 | .0 |

FIELD AND STANDARD POND HALFLIFE VALUES (DAYS)

| METABOLIC (FIELD) | DAYS UNTIL RAIN/RUNOFF | HYDROLYSIS (POND) | PHOTOLYSIS (POND-EFF) | METABOLIC (POND) | COMBINED (POND) |
|---|---|---|---|---|---|
| 11.70 | 2 | N/A | .00- | .00 23.40 | 23.40 |

GENERIC EECs (IN MICROGRAMS/LITER (PPB)) Version 2.0 Aug 1, 2001

| PEAK GEEC | MAX 4 DAY AVG GEEC | MAX 21 DAY AVG GEEC | MAX 60 DAY AVG GEEC | MAX 90 DAY AVG GEEC |
|---|---|---|---|---|
| 9.09 | 8.88 | 7.71 | 5.71 | 4.66 |

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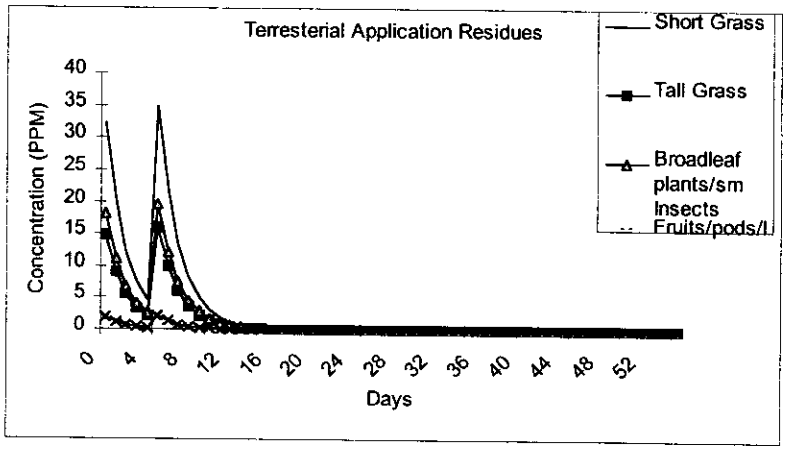
# APPENDIX C

## Output from ELL-FATE for NAA

ELL-FATE, Version 1.2, dated July 19, 2001

| | |
|---|---|
| **Chemical Name:** | **NAA** |
| Use | Herbicide |
| Formulation | STIK Clear Crop |




## Inputs

| | | |
|---|---|---|
| **Application Rate** | 0.134 | lbs a.i./acre |
| **Half-life** | 1.425 | days |
| **Frequency of Application** | 5 | days |
| **Maximum # Apps./Year** | 2 | |

Outputs

| | Maximum Concentration (PPM) | 56 day Average Concentration (PPM) | |
|---|---|---|---|
| **Short Grass** | 34.99 | 2.98 | |
| **Tall Grass** | 16.03 | 1.37 | # days |
| **Broadleaf plants/sm Insects** | 19.68 | 1.68 | Exceeded |
| **Fruits/pods/lg insects** | 2.19 | 0.19 | on short grass (in first 56) |

**Avian**

| | | |
|---|---|---|
| Acute LC50 (ppm) | 10000 | 0 |
| Chronic NOAEC (ppm) | 10000 | 0 |

| | Acute RQ | Chronic RQ (Max. res. mult. apps.) | |
|---|---|---|---|
| **Short Grass** | 3.E-03 | 3.E-03 | |
| **Tall Grass** | 2.E-03 | 2.E-03 | # days |
| **Broadleaf plants/sm Insects** | 2.E-03 | 2.E-03 | Exceeded |
| **Fruits/pods/lg insects** | 2.E-04 | 2.E-04 | on short grass (in first 56) |

Max Single Application which does NOT exceed

| | | |
|---|---|---|
| Avian Acute | 41.667 | (lb a.i.) |
| Avian Chronic | 41.667 | |
| Mammalian Acute | 25.92 | |
| Mammalian Chronic | 0.18 | |

**Mammalian**

| | | |
|---|---|---|
| ute LD50 (mg/kg bw/d) | 933 | 0 |
| ic NOAEL (mg/kg diet) | 44 | 0 |

Rat Calculated LD50 (ppm) 19680
Rat Calculated NOAEL (ppm) 880

| | 15 g mammal Acute RQ (mult. apps) | 35 g mammal Acute RQ (mult. apps) | 1000 g mammal Acute RQ (mult. apps) | Rat Acute Dietary RQ | Rat Chronic Dietary RQ |
|---|---|---|---|---|---|
| **Short Grass** | 0.04 | 0.02 | 0.01 | 2.E-03 | |
| **Tall Grass** | 0.02 | 0.01 | 3.E-03 | 9.E-04 | |
| **Broadleaf plants/sm Insects** | 0.02 | 0.01 | 3.E-03 | 1.E-03 | |
| **Fruits/pods/lg Insects** | 2.E-03 | 2.E-03 | 4.E-04 | 1.E-04 | |
| | 5.E-04 | 4.E-04 | 7.E-05 | 1.E-04 | |

APPENDIX D: Formulas for Calculating Nontarget Plant EECs and RQs

Table D-1. Terrestrial Plant Environmental Exposure Concentrations (EECs)

| | EEC Dry Area (lbs a.i./acre) | EEC Semi Aquatic Area (lbs a.i./acre) |
|---|---|---|
| **GROUND** | | |
| Unincorporated (Non granular) | Sheet Run Off Application Rate(lb a.i./acre)* Run Off Value[a] + Drift (Application Rate(lb a.i./acre)* 0.01 | Channelized Run Off Application Rate(lb a.i./acre)* Run Off Value[a] * Factor 10[b] + Drift (Application Rate(lb a.i./acre)* 0.01 |
| Unincorporated (Granular) | Sheet Run Off Application Rate(lb a.i./acre)* Run Off Value[a] | Channelized Run Off Application Rate(lb a.i./acre)* Run Off Value[a] * Factor 10[b] |
| Incorporated With Drift (Non Granular) | Sheet Run Off [Application Rate(lb a.i./acre)/Incorporation Depth in cm] * Run Off Value[a] + Drift (Application Rate (lb a.i./acre)* 0.01 | Channelized Run Off [Application Rate(lb a.i./acre)/Incorporation Depth in cm] * Run Off Value[a] * Factor 10[b] + Drift (Application Rate(lb a.i./acre)* 0.01 |
| Without Drift (Granular) | Sheet Run Off [Application Rate(lb a.i./acre)/Incorporation Depth in cm] * Run Off Value[a] | Channelized Run Off [Application Rate(lb a.i./acre)/Incorporation Depth in cm] * Run Off Value[a] * Factor 10[b] |
| AERIAL | Sheet Run Off Application Rate(lb a.i./acre) * Run Off Value[a] * Appl. Eff, 0.6 + Drift (Application Rate (lb a.i./acre)* 0.05 | Channelized Run Off Application Rate(lb a.i./acre) * Run Off Value[a] * Appl. Eff, 0.6 * Factor 10[b] + Drift (Application Rate(lb a.i./acre)* 0.05 |

[a] Run Off Value = 0.01 or .02 or 0.05 depending upon the solubility of the chemical, <10 ppm, 10-100 ppm, and >100 ppm, respectively.
[b] for 10 treated acres.

**For Seedling Emergence RQs: Use Runoff+ Drift values (except for granular pesticide RQs, runoff values alone used)**
**For Vegetative Vigor RQs: Use only Drift values**

**Calculation for aerial application and most sensitive endpoint:**

**Sheet runoff: 0.134 lb ai/acre X 0.05 (runoff value) X 0.6 (appl. efficiency)**
**plus Drift: 0.134 lb ai/acre X 0.05**
**= 0.01 lb ai/acre EEC**

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**Endpoint (seedling emergence NOEC, carrot) = 0.01 lb ai/acre**

**0.01/0.01 = 1.0 RQ value**

**RQ equals LOC for endangered species exposed to direct application. However, as illustrated in the following graphs, deposition decreases significantly within a short distance from the point of application.**

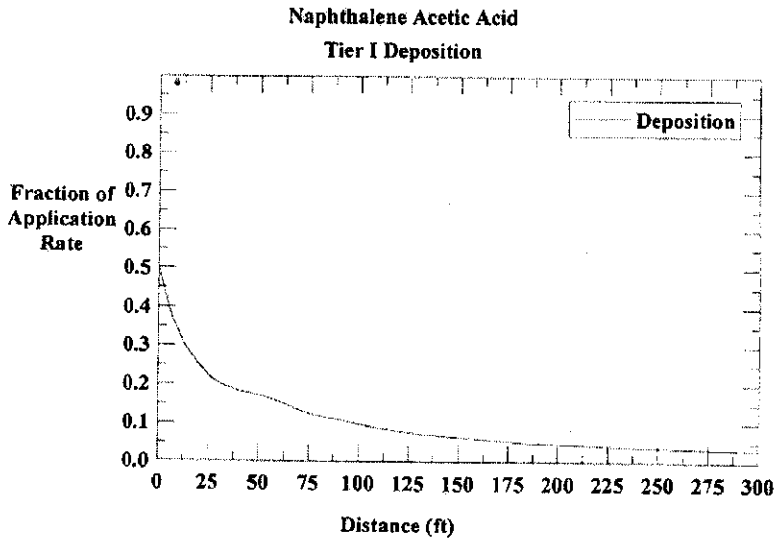
**Figure D.1. Standard Deposition Curve for Aerial Applications Obtained from AGDRIFT.**

AgDRIFT® Input Data Summary

--General--
Tier: I
Title: Naphthalene Acetic Acid
Notes:

Default values appear when they differ from the Current values.

| | ----------Current---------- | ----------Default---------- |
|---|---|---|
| Application Method | Aerial | |
| Application Selection | ASAE Fine to Medium | |




**At a distance of 25 ft, the deposition has decreased to a fraction of about 0.2 of the applied.**

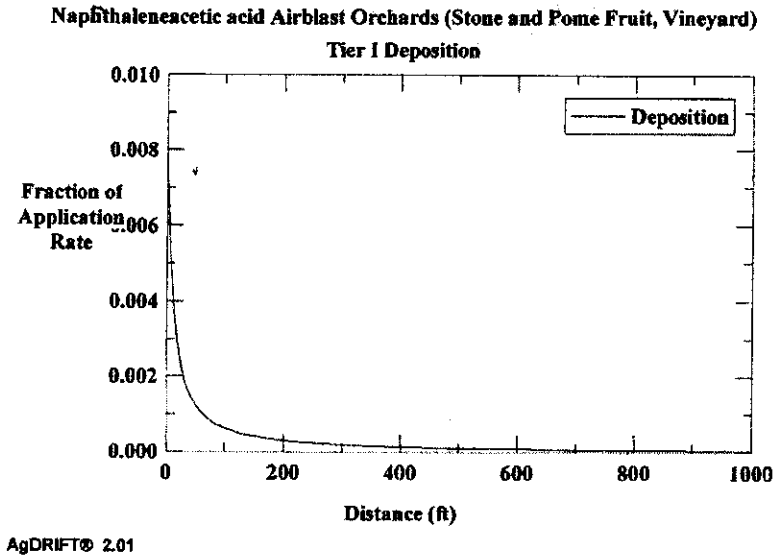
**Figure D.2. Standard Deposition Curve for Airblast Applications Obtained from AGDRIFT.**

AgDRIFT® Input Data Summary

--General--
Tier: I
Title: Naphthaleneacetic acid Airblast Orchards (Stone and Pome Fruit, Vineyard)
Notes:

Default values appear when they differ from the Current values.

| | Current | Default |
|---|---|---|
| Application Method | Orchard Airblast | Aerial |
| Application Selection | Normal (Stone and Pome Fr... | Aerosol to Very Fine |




**The level of deposition is much lower than that observed for aerial applications. Note the fraction of the application rate**

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# APPENDIX E: Portion of Drinking Water Memorandum

September 25, 2003

**MEMORANDUM**

**SUBJECT:** Tier I Estimated Drinking Water Concentrations of **1-Naphthaleneacetic Acid** for use in Human Health Risk Assessment (PC Code 056003; Case Number 0379; DPBarcode D293886)

**TO:** Michael Goodis, Acting Branch Chief
Mark Howard, Team Leader
Registration Division (7505C)

**and** Ray Kent, Branch Chief
Health Effects Division (7509C)

**FROM:** José Luis Meléndez, Chemist
Environmental Risk Branch V/EFED

**THROUGH:** Mah Shamim, Ph.D., Chief
Environmental Risk Branch V
Environmental Fate and Effects Division (7507C)

This memo presents the Tier I Estimated Drinking Water Concentrations (EDWCs) for 1-naphthaleneacetic acid, calculated using FIRST (surface water) and SCIGROW (ground water) for use in the human health risk assessment.

**Table 1. Tier I Estimated Drinking Water Concentrations of 1-Naphthaleneacetic acid[2]**

| Chemical | Acute (peak) Surface Water Concentration (ppb) | Annual Average Surface Water Concentration (ppb) | Ground Water Concentration (ppb) |
|---|---|---|---|
| NAA | 12.9 | 0.71 | 0.0008 |

These values generally represent upper-bound estimates of the concentrations of 1-naphthalene-acetic acid equivalents that might be found in surface and ground water due to the use of 1-naphthalenacetic acid (sodium salt) on apples, which represents the highest use rate scenario. Both models provide estimates suitable for screening purposes. Additional refinements may be developed should they be needed by HED.

***Introduction***

1-Naphthaleneacetic acid (NAA) is a plant growth regulator, with effects at low concentrations. It acts as a chemical messenger effecting natural plant functions and is the most widely used synthetic auxin. It also acts as a herbicide at high rates. Target crops include apples, pears, citrus, olives, prunes, cherries, pomegranates and ornamental woody plants.



[2] Results of 1-naphthaleneacetic acid, sodium salt, expressed as equivalents of 1-naphthalneacetic acid.

Applications of NAA are made at various periods of the year. NAA is used in the Spring to thin all varieties of apples, and a small percentage of pears. It is used during the Summer to enhance return bloom. In addition, NAA is used during the Fall on Red Delicious and Golden Supreme apple trees to prevent pre-harvest drop and as a sprout inhibitor applied after a pruning cut to prevent water sprouts from developing.

1-Naphthaleneacetic acid (NAA) belongs to a family of related products, which include, sodium 1-naphthaleneacetate, 1-naphthaleneacetamide, ethyl 1-naphthaleneacetate, potassium 1-naphthaleneacetate, ammonium 1-naphthaleneacetate, and ethyl-1-naphthaleneacetate.

Most products containing 1-naphthaleneacetic acid (NAA) are used to promote root growth (for transplantations or to boost established plants), primarily in a nursery environment. The use rate is lower than the one used to prevent fruit drop. One product contains a mixture of NAA (0.45%) and 1-naphthaleneacetamide (1.20%), which is used on apples and pears to induce fruit set (it is applied prior to flowering).

EFED used as representative high use rate scenario/product, the sodium salt of 1-naphthaleneacetic acid. The environmental fate characteristics of the sodium salt are expected to be similar to those of the acid. In the environment, both species occur in an equilibrium that depends on the pH. Three products are registered that contain exclusively sodium 1-naphthaleneacetate, that are also used aerially on apples and pears. The product with the maximum use rate can be applied at 0.134 lb a.i.(equivalents of NAA)/A per application. Two applications are allowed.

***Environmental Fate Database for 1-Naphthaleneacetic Acid***

The Division has very little environmental fate data about 1-naphthaleneacetic acid and its related products. One study (Acc. No. 129382) suggests that the ethyl-1-naphthaleneacetate and 1-naphthaleneacetamide are susceptible to hydrolysis, and the end product is 1-naphthaleneacetic acid. Literature information suggests that 1-naphthaleneacetic acid, and structurally similar compounds such as 1-methyl-naphthalene and ethyl-naphthalene, are susceptible to biodegradation, however, no quantitative results are available. A search of the TOXNET database provided additional qualitative information about the environmental fate of this chemical. 1-Naphthaleneacetic acid is expected to undergo rapid photolysis in water, on soil, and in air. The observed products in water and soil were 1-naphthoic acid and phthalic acid (refer to Appendix C).[3] An estimated $K_{OC}$ range was provided was 160-610.[4]

***Approach for Calculation of Naphthaleneacetic Acid***

In the absence of environmental fate data, EFED assumed a conservative approach.

A calculation of physicochemical properties of 1-naphthaleneacetic acid was performed using EPI Suite™ [5]. The EPI (Estimation Program Interface) Suite™ is a Windows® based suite of physical/chemical property and environmental fate estimation models developed by the EPA's

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[3] Crosby, D.G. Adv. Chem. Ser. 111:173-88(1972), and Crosby, D.G. Advances in Pest. Sci. III Geissbuhler H (ed) Oxford: Pergamon Press, pp. 568-76 (1979)

[4] Lyman, W.J., et. al.; Handbook of Chamical Property Estimation Methods, NY; McGraw-Hill, p. 4-9 (1982)

[5] The EPI Suite™ and the individual models included within the software are owned by the U.S. Environmental Protection Agency and are protected by copyright throughout the world.

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Office of Pollution Prevention Toxics and Syracuse Research Corporation. EPI Suite™ uses a single input to run various estimation models.

PCKOCWIN (refer to Appendix I for details) yielded a $K_{OC}$ of 297. This value lies well within the range reported by Lyman, et. al.. The value was considered suitable for calculations at the Tier I level.

BIOWIN (refer to Appendix I for details) yielded a biodegradation half-life of 3.9 days for 1-naphthaleneacetic acid. EFED believed that this value was reasonable in light of the literature data available for this and similar compounds. Since the guidelines for input parameters for FIRST call for the multiplication of the value by 3 (when there is only one value available), EFED considered that this constituted a reasonable conservative approach. The aerobic aquatic metabolism is twice the aerobic soil metabolism input value as per current guidelines.

For this Tier I level analysis, in the absence of any data about the photolysis on soil or in water for 1-naphthaleneacetic acid, EFED assumed persistance (despite the fact that they are expected to be important routes of degradation). This also constitutes a conservative approach.

The input parameters are presented in Tables 2 and 3. The modeling results are shown in the Table 1.

For background information about PCKOCWIN, and BIOWIN, models of the EPI Suite™ program, please refer to Appendix A.

For background information about FIRST, and SCIGROW, the models used to estimate surface and ground waters, respectively, refer also to Appendix A.

Appendix B shows the output files from FIRST and SCIGROW.

**Table 2. Environmental Fate and Other Input Parameters for the Estimation of Naphthaleneacetic Acid using FIRST**

| Parameter | Value | Source |
|---|---|---|
| Water Solubility (20°C) | 420 ppm | Herbicide Handbook, 5th Edition |
| Hydrolysis Half-Life (pH 7) | 0 | ACC# 129382 |
| Aerobic Soil Metabolism Half-Life (3X available value = 3 x 3.9 days = 11.7 days) | 11.7 days | BIOWIN v.4.00 |
| Aerobic Aquatic Metabolism Half-life (2X aerobic soil metabolism input) | 23.4 days | Per guidelines |
| Aqueous Photolysis Half-Life | 0 | No data available |
| Adsorption/Desorption Coefficient ($K_{OC}$) | 297 | PCKOCWIN v.1.66 |
| Pesticide is Wetted-In | No | Label |
| PCA (apples, highest use rate scenario) | 0.87 | Default value for other crops |
| Application Method | aerial | Label |
| Application Rate (lb a.i./A) | 0.134 | Label |
| Applications Permitted per Year | 2 | Label |

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**Table 2. Environmental Fate and Other Input Parameters for the Estimation of Naphthaleneacetic Acid using FIRST**

| Parameter | Value | Source |
|---|---|---|
| Application Interval (days) | 5 | Label |
| Depth of Incorporation (Broadcast) | 0.0 | Label |

**Table 3. Environmental Fate Input Parameters for the Estimation of Naphthaleneacetic Acid using SCIGROW.**

| Parameter | Value | Source |
|---|---|---|
| Organic Carbon Adsorption/Desorption Coefficient ($K_{OC}$)[2] | 297 | PCKOCWIN v.1.66 |
| Aerobic Soil Metabolism Half-Life | 3.9 days | BIOWIN v.4.00 |

## Background Information About PCKOCWIN, BIOWIN, FIRST, and SCIGROW

### *PCKOCWIN Overview*

The following overview of the PCKOCWIN program was obtained from the program manual. The Soil Adsorption Coefficient Program (PCKOCWIN) estimates the soil adsorption coeffiecient ($K_{OC}$) of organic compounds. $K_{OC}$ can be defined as "the ratio of the amount of chemical adsorbed per unit weight of organic carbon (OC) in the soil or sediment to the concentration of the chemical in solution at equilibrium" (Lyman, 1990); it is represented by the following equation (Lyman, 1990):

Koc = (ug adsorbed/g organic carbon) / (ug/mL solution)

$K_{OC}$ provides an indication of the extent to which a chemical partitions between solid and solution phases in soil, or between water and sediment in aquatic ecosystems. Estimated values of $K_{OC}$ are often used in environmental fate assessment because measurement of $K_{OC}$ is expensive. Traditional estimation methods rely upon the octanol/water partition coefficient or related parameters, but recently the first-order molecular connectivity index (1-MCI) has been used successfully to predict $K_{OC}$ values for hydrophobic organic compounds (Sabljic, 1984, 1987; Bahnick and Doucette, 1988). PCKOCWIN uses 1-MCI and a series of group contribution factors to predict Koc. The group contribution method outperforms traditional estimation methods based on octanol/water partition coefficients and water solubility.

PCKOCWIN requires only a chemical structure to make these predictions. Structures are entered into PCKOCWIN by SMILES (Simplified Molecular Input Line Entry System) notations.

The first-order molecular connectivity index (MCI) has been successfully used to predict soil sorption coefficients (Koc) for nonpolar organics. For polar compounds, a new estimation method based on MCI and series of statistically derived fragment contribution factors for polar compounds was developed. After developing an extensive database of measured $K_{OC}$ values, we divided the dataset into a training set of 189 chemicals and an independent validation set of 205 chemicals. Two linear regressions were then performed. First, measured log $K_{OC}$ values for nonpolar compounds in the training set were correlated with MCI. The second regression was developed by using the deviations between measured log $K_{OC}$ and the log $K_{OC}$ estimated with the nonpolar equation and the number of certain structural fragments in the polar compounds. The final equation for predicting log Koc accounts for 96% and 86% of the variation in the measured values for the training and validation sets, respectively. Results also show that the model outperforms and covers a wider range of chemical structures than do models based on octanol-water partition coefficients ($K_{OW}$) or water solubility.

### *BIOWIN Overview*

The following overview of the BIOWIN program was obtained from the program manual. The Biodegradation Probability Program (BIOWIN) estimates the probability for the rapid aerobic biodegradation of an organic chemical in the presence of mixed populations of environmental microorganisms. Estimates are based upon fragment constants that were developed using multiple linear and non-linear regression analyses.

BIOWIN requires only a chemical structure to make these predictions. Structures are entered into BIOWIN by SMILES notations. The BIOWIN program was developed at Syracuse Research Corporation. The prediction methodology was developed jointly by efforts of the Syracuse Research Corporation and the U.S. Environmental Protection Agency.

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Two independent training sets were used to develop four mathematical models for predicting aerobic biodegradability from chemical structure. All four of the models are based on multiple regressions against counts of 36 preselected chemical substructures plus molecular weight. Two of the models, based on linear and nonlinear regressions, calculate the probability of rapid biodegradation and can be used to classify chemicals as rapidly or not rapidly biodegradable. The training set for these models consisted of qualitative summary evalutions of all available experimental data on biodegradability for 295 chemicals. The other two models allow semi-quantitive prediction of primary and ultimate biodegradation rates using multiple linear regression. The training set for these models consisted of estimates of primary and ultimate biodegradation rates for 200 chemicals, gathered in a survey of 17 biodegradation experts. The two probability models correctly classified 90% of the chemicals in their training set, wheras the two survey models calculated biodegradation rates for the survey chemicals with $R^2 = 0.7$. These four models are intended for use in chemical screening and in setting priorities for further review.

***Background Information on FIRST:***

FIRST is a screening model designed to estimate the pesticide concentrations found in surface water for use in drinking water assessments. It provides high-end values on the concentrations that might be found in a small drinking water reservoir due to the use of pesticide. Like GENEEC, the model previously used for Tier I screening level, FIRST is a single-event model (one run-off event), but can account for spray drift from multiple applications. FIRST takes into consideration the so called Index Drinking Water Reservoir by representing a larger field and pond than the standard GENEEC scenario. The FIRST scenario includes a 427 acres field immediately adjacent to a 13 acres reservoir, 9 feet deep, with continuous flow (two turnovers per year). The pond receives a spray drift event from each application plus one runoff event. The runoff event moves a maximum of 8% of the applied pesticide into the pond. This amount can be reduced due to degradation on field and the effect of binding to soil. Spray drift is equal to 6.4% of the applied concentration from the ground spray application and 16% for aerial applications.

FIRST also makes adjustments for the percent crop area. While FIRST assumes that the entire watershed would not be treated, the use of a PCA is still a screen because it represents the highest percentage of crop cover of any large watershed in the US, and it assumes that the entire crop is being treated. Various other conservative assumptions of FIRST include the use of a small drinking water reservoir surrounded by a runoff-prone watershed, the use of the maximum use rate, no buffer zone, and a single large rainfall.

***Background Information on SCIGROW:***

SCIGROW provides a groundwater screening exposure value to be used in determining the potential risk to human health from drinking water contaminated with the pesticide. Since the SCIGROW concentrations are likely to be approached in only a very small percentage of drinking water sources, i.e., highly vulnerable aquifers, it is not appropriate to use SCIGROW for national or regional exposure estimates.

SCIGROW estimates likely groundwater concentrations if the pesticide is used at the maximum allowable rate in areas where groundwater is exceptionally vulnerable to contamination. In most cases, a large majority of the use area will have groundwater that is less vulnerable to contamination than the areas used to derive the SCIGROW estimate.

# SURFACE WATERS (FIRST) and GROUND WATERS OUTPUT RUNS

RUN No. 1 FOR NAA ON Apples * INPUT VALUES *

| RATE (#/AC) ONE(MULT) | No.APPS & INTERVAL | SOIL Koc | SOLUBIL (PPM ) | APPL TYPE (%DRIFT) | %CROPPED AREA | INCORP (IN) |
|---|---|---|---|---|---|---|
| .134( .234) | 2 5 | 297.0 | 420.0 | AERIAL(16.0) | 87.0 | .0 |

FIELD AND RESERVOIR HALFLIFE VALUES (DAYS)

| METABOLIC (FIELD) | DAYS UNTIL RAIN/RUNOFF | HYDROLYSIS (RESERVOIR) | PHOTOLYSIS (RES.-EFF) | METABOLIC (RESER.) | COMBINED (RESER.) |
|---|---|---|---|---|---|
| 11.70 | 2 | N/A | .00- .00 | 23.40 | 23.40 |

UNTREATED WATER CONC (MICROGRAMS/LITER (PPB)) Ver 1.0 AUG 1, 2001

| PEAK DAY (ACUTE) CONCENTRATION | ANNUAL AVERAGE (CHRONIC) CONCENTRATION |
|---|---|
| 12.923 | .712 |

SCIGROW
VERSION 2.3
ENVIRONMENTAL FATE AND EFFECTS DIVISION
OFFICE OF PESTICIDE PROGRAMS
U.S. ENVIRONMENTAL PROTECTION AGENCY
SCREENING MODEL
FOR AQUATIC PESTICIDE EXPOSURE

SciGrow version 2.3
chemical:Naphthaleneacetic acid
time is 9/23/2003 10:32:23

| Application rate (lb/acre) | Number of applications | Total Use (lb/acre/yr) | Koc (ml/g) | Soil Aerobic metabolism (days) |
|---|---|---|---|---|
| 0.134 | 2.0 | 0.268 | 2.97E+02 | 3.9 |

groundwater screening cond (ppb) = 8.02E-04
**********

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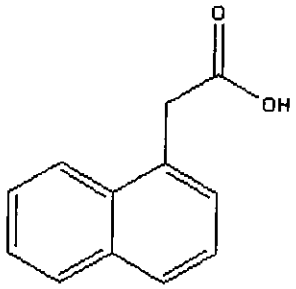
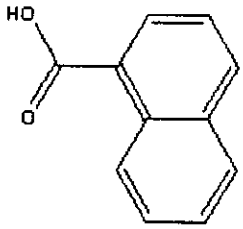
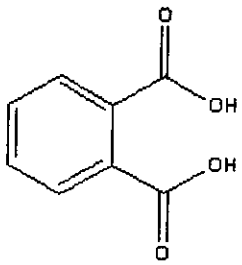
## Appendix F.
Chemical Structures of NAA and Photolysis Products




1-naphthaleneacetic acid




1-naphthoic acid




phthalic acid

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## Appendix G.

Background Data About Oasis Catabol V. 4.55

Metabolism (the breakdown of the molecule by bacteria) stops before the compound is fully degraded, leaving a partially degraded compound called a metabolite. Due to the importance of biodegradation for pesticide products and the need to understand the formation of metabolites, a QSAR program called CATABOL was developed. CATABOL predicts the biodegradation pathway and predicts the possibility that degradation may stop at one or more metabolites.

CATABOL is a mechanistic modeling approach for quantitative assessment of biodegradability in biodegradation pathways of chemicals. The system generates most plausible biodegradation products and provides quantitative assessment for their solubility and toxic endpoints. The core of CATABOL is the biodegradability simulator including a library of hierarchically ordered individual transformations (catabolic steps) and matching substructure engine providing their subsequent performance. The catabolic steps are derived from a set of most plausible metabolic pathways predicted by experts for each chemical from the training set.

The hierarchy of implementation of individual transformations in the simulator is set according to the descending order of their probabilities. For deriving these probabilities, a frequency matrix is constructed where observed BOD (or ThCO2) for training set chemicals are used as dependent variables and probabilities of individual transformations — as independent variables. The matrix is solved for probabilities of individual transformations by nonlinear least squares Marquart''s method.

The data in the training set agreed well with the calculated BODs ($r^2 = 0.90$) in the entire range (i.e. a good fit was observed for readily, intermediate and difficult to degrade chemicals). After introducing 60% ThOD as a cut off value the model predicted correctly 98 % ready biodegradable structures and 96 % not ready biodegradable structures. Crossvalidation by 4 times leaving 25% of data resulted in Q2=0.88 between observed and predicted values. To make biodegradability predictions the model only needs the structure of a chemical. For structure input we have also provided a structure editor. The output is given as % of theoretical BOD. The model allows for identifying potentially persistent catabolic intermediates, their molar amounts, solubility (log Kow, BCF) and toxic properties (acute toxicity, phototoxicity, mutagenicity, ER/AR binding affinity). Presently, the system simulates the biodegradability in MITI-I OECD 301 C and Ready Sturm OECD 301 B tests. Other simulators will be available in the program upgrades.

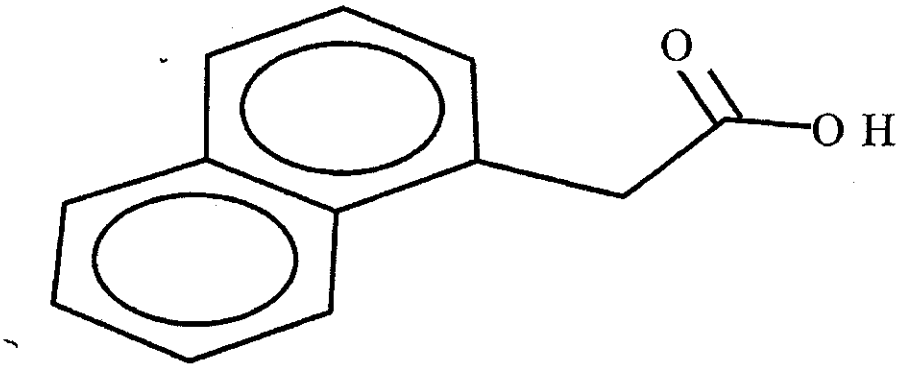
In order to improve the reliability of the CATABOL predictions a new training set of documented multiple biodegradation routes for 260 chemicals was collected. The new training set was used to train the CATABOL to simulate multiple metabolic pathways. The performance of the multiple pathways based microbial simulator to reproduce biodegradation of chemicals and their stable metabolites was reported and analyzed.

The new version of CATABOL allows evaluating the performance of the simulator and the degree of belonging of chemicals into the domain of the biodegradation simulator.

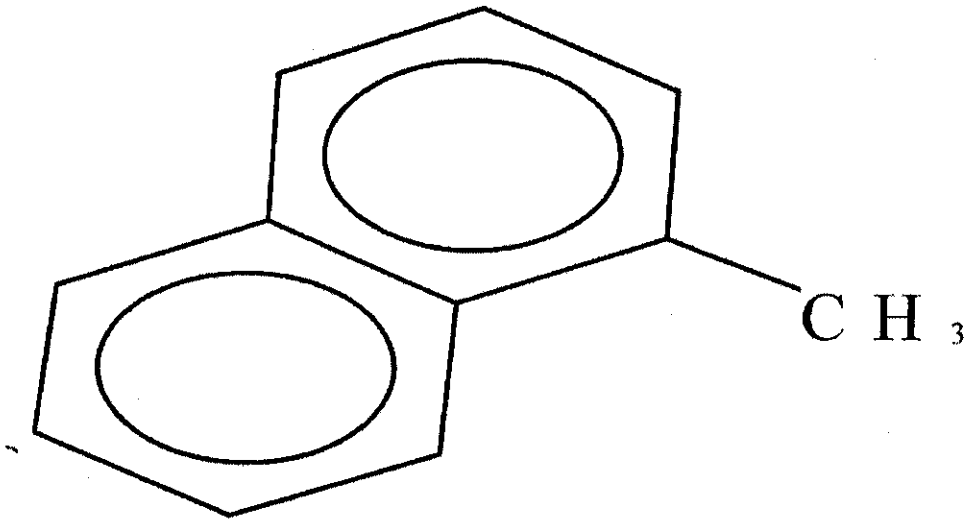
Output from Oasis Catabol:

| | Trans | Level | Quantity | P_obtain | P_stable | LogKOW | Smiles |
|---|---|---|---|---|---|---|---|
| 1 | 391 | 1 | 0.999 | 1 | 0.999 | 2.6044 | c1(CC(=O)O)c2c(cccc2)ccc1 |
| 2 | 363 | 2 | 0.000776 | 0.001 | 0.000776 | 3.7163 | c1(C)c2c(cccc2)ccc1 |
| 3 | 78 | 3 | 0 | 0.000224 | 0 | 2.2515 | c1(CO)c2c(cccc2)ccc1 |
| 4 | 54 | 4 | 0 | 0.000224 | 0 | 2.8862 | c12c(c(C=O)ccc1)cccc2 |
| 5 | 272 | 5 | 0.000031 | 0.000224 | 0.000031 | 3.0504 | C(=O)(O)c1c2c(cccc2)ccc1 |
| 6 | 120 | 6 | 0 | 0.000193 | 0 | 2.2086 | c1(O)c(O)c2c(cccc2)cc1 |
| 7 | 105 | 7 | 0 | 0.000193 | 0 | 1.0405 | C(=O)(O)C(=O)C=Cc1c(O)cccc1 |
| 8 | 54 | 8 | 0 | 0.000193 | 0 | 2.007 | c1(O)c(C=O)cccc1 |
| 9 | 205 | 9 | 0.000018 | 0.000193 | 0.000018 | 2.2447 | C(=O)(O)c1c(O)cccc1 |
| 10 | 129 | 10 | 0 | 0.000175 | 0 | 1.0326 | c1(O)c(O)cccc1 |
| 11 | 49 | 11 | 0 | 0.000175 | 0 | -0.4424 | C(=O)(O)C(O)=CC=CC=O |
| 12 | 54 | 12 | 0 | 0.000175 | 0 | 0.35 | C=O |
| 13 | 7 | 13 | 0 | 0.000175 | 0 | -0.4605 | C(=O)O |
| 14 | 60 | 12 | 0 | 0.000175 | 0 | 0.6346 | C(=O)(O)C(O)=CC=C |
| 15 | 46 | 13 | 0 | 0.000175 | 0 | -0.3974 | C(=O)(O)C(=O)CC=C |
| 16 | 101 | 14 | 0 | 0.000175 | 0 | -1.7993 | C(=O)(O)C(=O)CC(C)O |
| 17 | 54 | 15 | 0 | 0.000175 | 0 | -0.1659 | C(C)=O |
| 18 | 10 | 16 | 0 | 0.000175 | 0 | 0.0868 | C(C)(=O)O |
| 19 | 13 | 15 | 0 | 0.000193 | 0 | -1.2432 | C(=O)(O)C(C)=O |

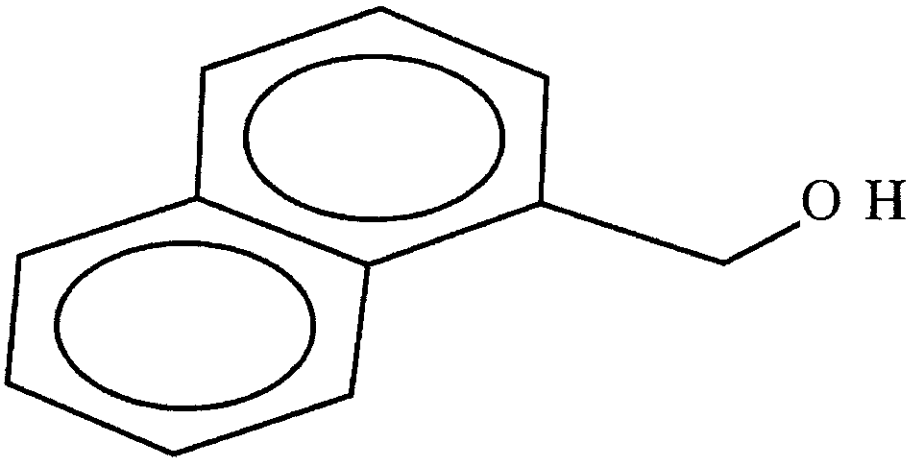
The Smiles codes were converted into structures and the names of such structures were located. These appear in the next page.



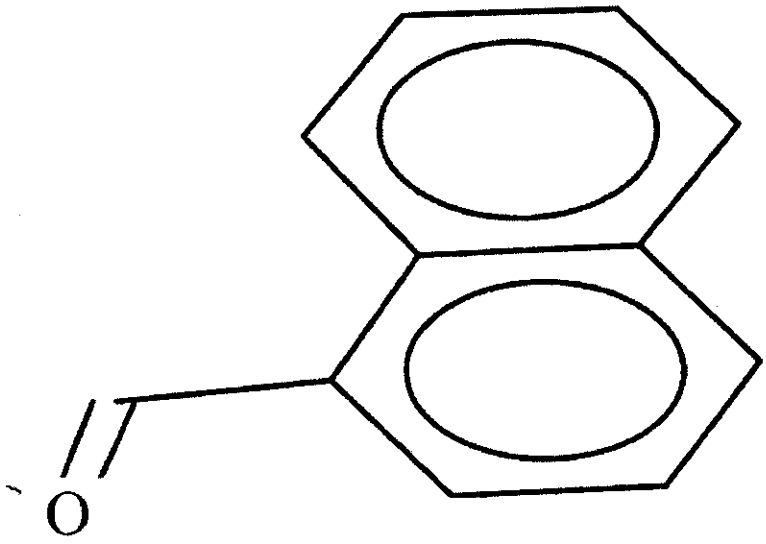

Naphthaleneacetic acid



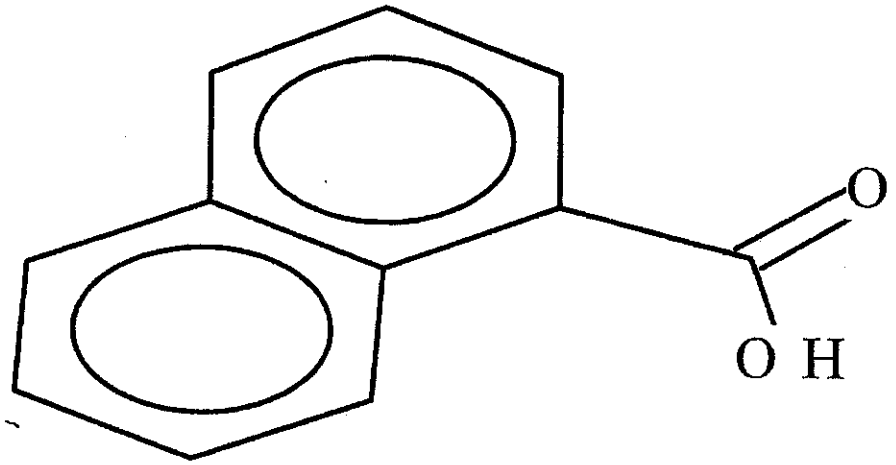

1-methyl-naphthalene



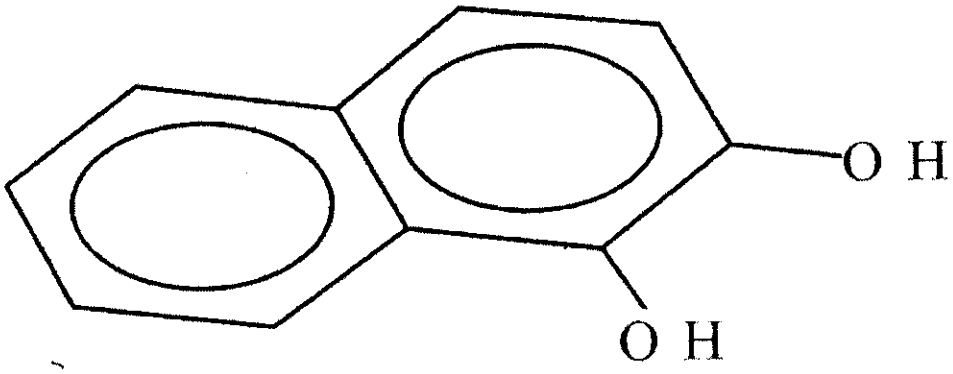

2-naphthylmethanol



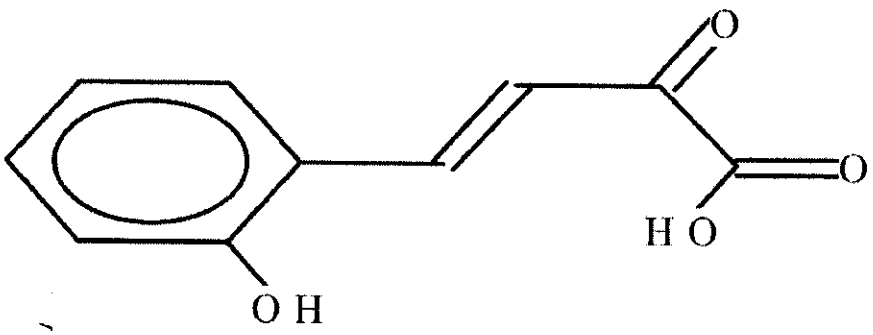

2-naphthaldehyde



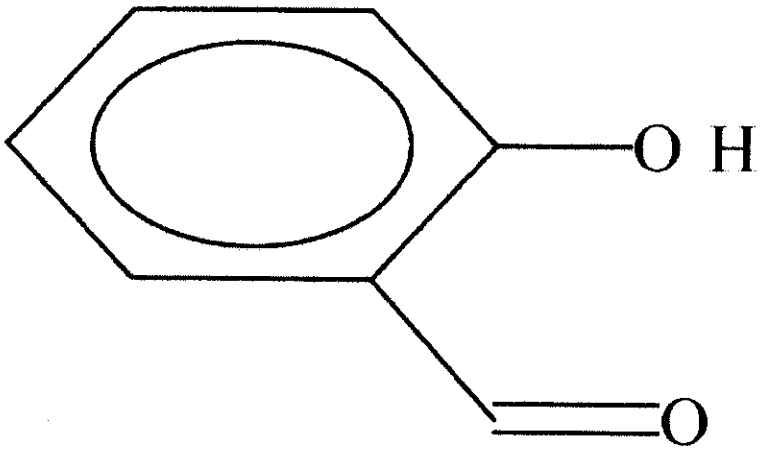

2-naphthoic acid



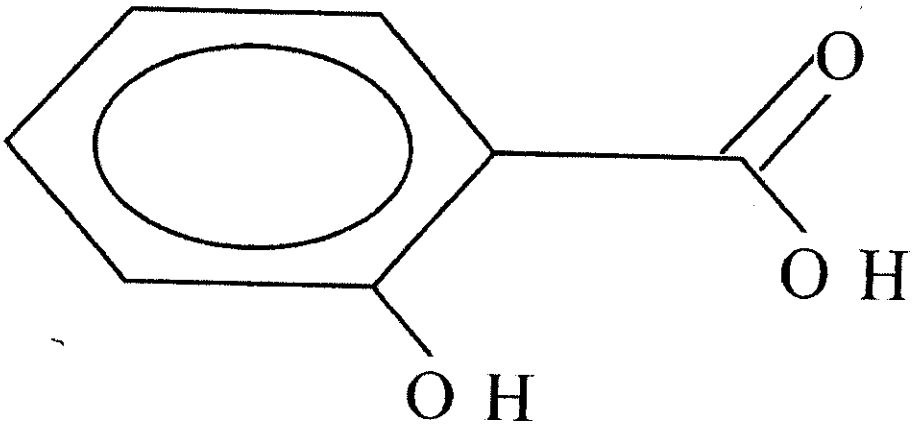

naphthalene-1,2-diol




(3E)-4-(2-hydroxyphenyl)-2-oxobut-3-enoic acid



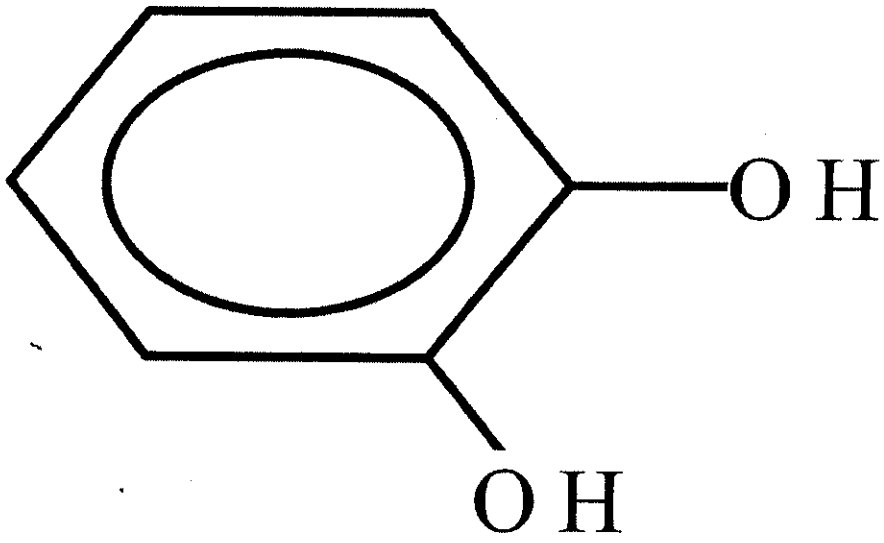

salicylaldehyde



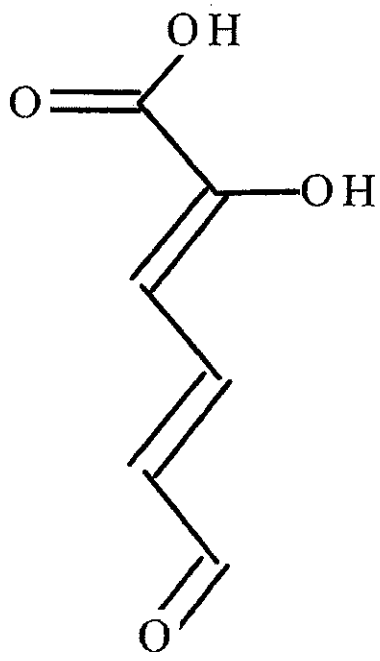

salicylic acid



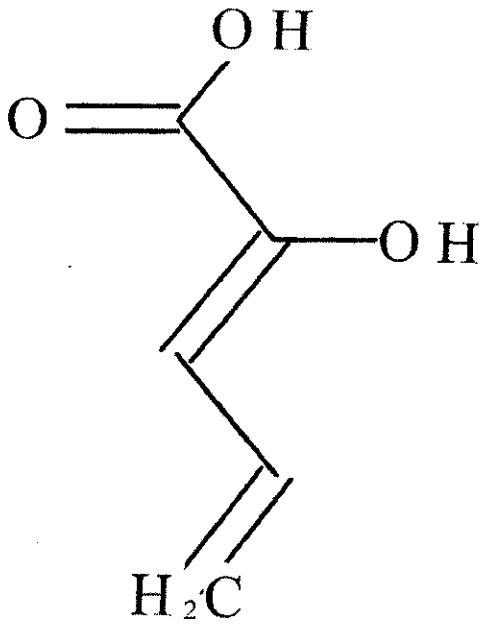
Appendix G-6



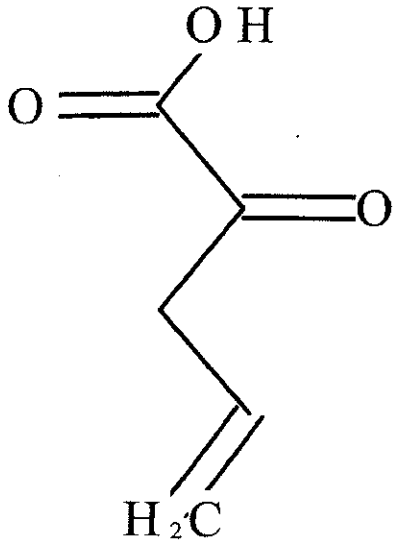

pyrocatechol



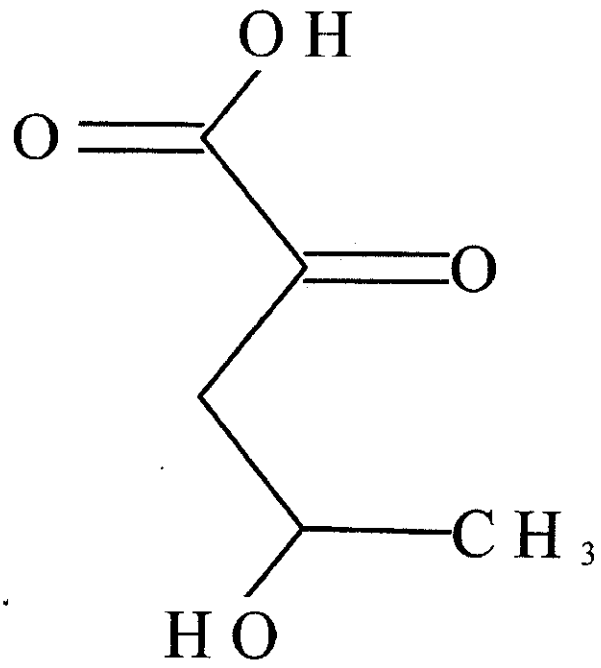

(2Z,4E)-2-hydroxy-6-oxohexa-2,4-dienoic acid



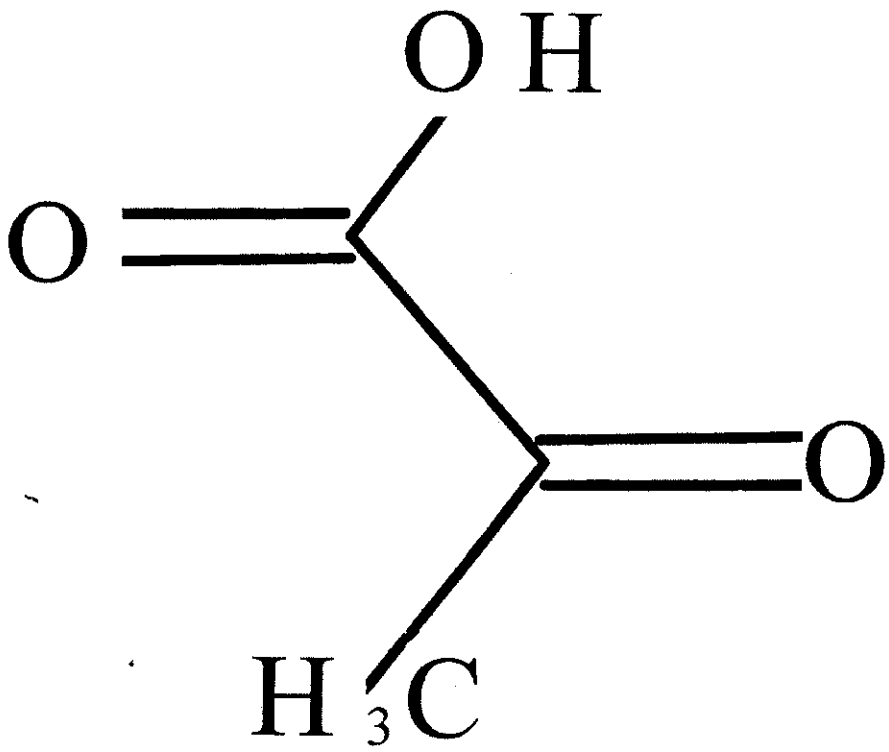

(2Z)-2-hydroxypenta-2,4-dienoic acid




2-oxopent-4-enoic acid




4-hydroxy-2-oxopentanoic acid




2-oxopropanoic acid

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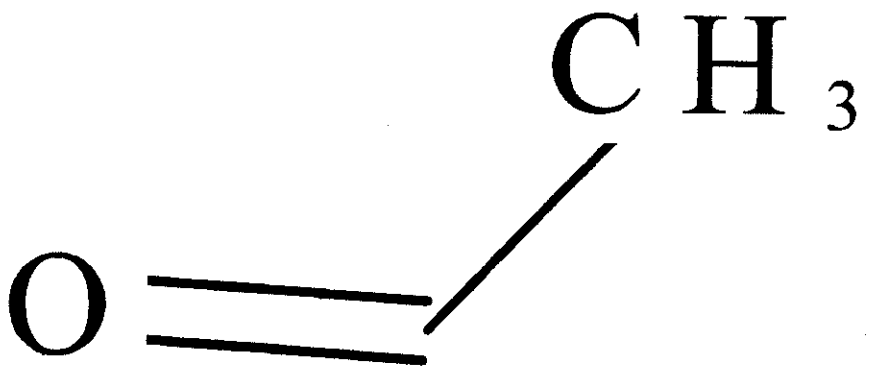
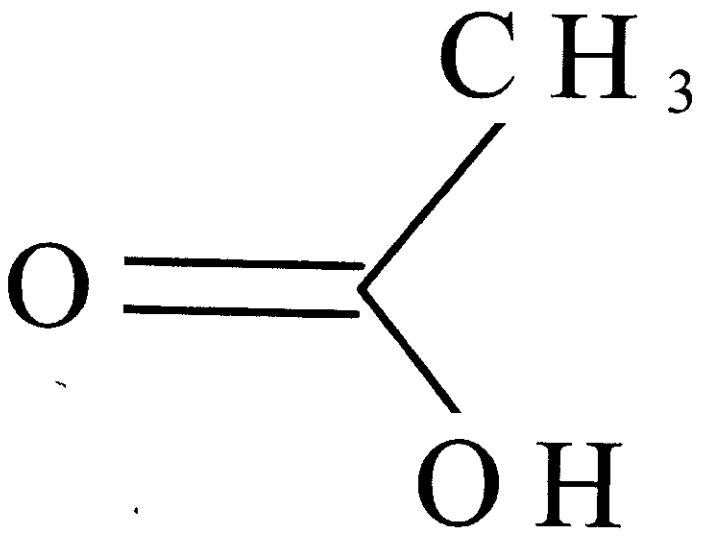
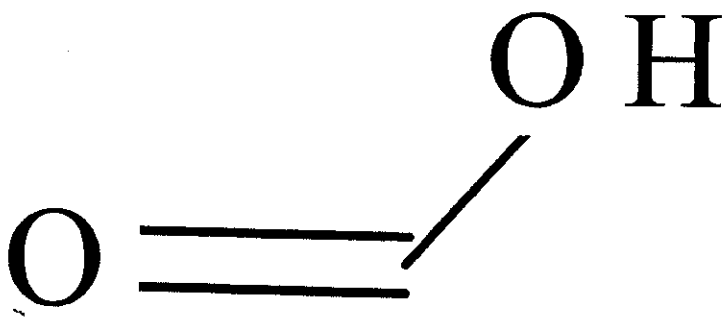



acetaldehyde




acetic acid


formaldehyde




formic acid