

ENVIRONMENTAL CONTAMINANTS ENCYCLOPEDIA

2,3,5-TRIMETHYLNAPHTHALENE ENTRY

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This document was put together by human beings, mostly by compiling or summarizing what other human beings have written. Therefore, it most likely contains some mistakes and/or potential misinterpretations and should be used primarily as a way to search quickly for basic information and information sources. It should not be viewed as an exhaustive, "last-word" source for critical applications (such as those requiring legally defensible information). For critical applications (such as litigation applications), it is best to use this document to find sources, and then to obtain the original documents and/or talk to the authors before depending too heavily on a particular piece of information.

Like a library or many large databases (such as EPA's national STORET water quality database), this document contains information of variable quality from very diverse sources. In compiling this document, mistakes were found in peer reviewed journal articles, as well as in databases with relatively elaborate quality control mechanisms [366,649,940]. A few of these were caught and marked with a "[sic]" notation, but undoubtedly others slipped through. The [sic] notation was inserted by the editors to indicate information or spelling that seemed wrong or misleading, but which was nevertheless cited verbatim rather than arbitrarily changing what the author said.

Most likely additional transcription errors and typos have been added in some of our efforts. Furthermore, with such complex subject matter, it is not always easy to determine what is correct and what is incorrect, especially with the "experts" often disagreeing. It is not uncommon in scientific research for two different researchers to come up with different results which lead them to different conclusions. In compiling the Encyclopedia, the editors did not try to resolve such conflicts, but rather simply reported it all.

It should be kept in mind that data comparability is a major problem in environmental toxicology since laboratory and field methods are constantly changing and since there are so many different "standard methods" published by EPA, other federal agencies, state agencies, and various private groups. What some laboratory and field investigators actually do for standard operating practice is often a unique combination of various standard protocols and impromptu "improvements." In fact, the interagency task force on water methods concluded that [1014]:

It is the exception rather than the rule that water-quality monitoring data from different programs or time periods can be compared on a scientifically sound basis, and that...

No nationally accepted standard definitions exist for water quality parameters. The different organizations may collect data using identical or standard methods, but identify them by different names, or use the same names for data collected by different methods [1014].

Differences in field and laboratory methods are also major issues related to (the lack of) data comparability from media other than water: soil, sediments, tissues, and air.

In spite of numerous problems and complexities, knowledge is often power in decisions related to chemical contamination. It is therefore often helpful to be aware of a broad universe of conflicting results or conflicting expert opinions rather than having a portion of this information arbitrarily censored by someone else. Frequently one wants to know of the existence of information, even if one later decides not to use it for a particular application. Many would like to see a high percentage of the information available and decide for themselves what to throw out, partly because they don't want to seem uninformed or be caught by surprise by potentially important information. They are in a better position if they can say: "I knew about that data, assessed it based on the following quality assurance criteria, and decided not to use it for this application." This is especially true for users near the end of long decision processes, such as hazardous site cleanups, lengthy ecological risk assessments, or complex natural resource damage assessments.

For some categories, the editors found no information and inserted the phrase "no information found." This does not necessarily mean that no information exists; it

simply means that during our efforts, the editors found none. For many topics, there is probably information "out there" that is not in the Encyclopedia. The more time that passes without encyclopedia updates (none are planned at the moment), the more true this statement will become. Still, the Encyclopedia is unique in that it contains broad ecotoxicology information from more sources than many other reference documents. No updates of this document are currently planned. However, it is hoped that most of the information in the encyclopedia will be useful for some time to come even without updates, just as one can still find information in the 1972 EPA Blue Book [12] that does not seem well summarized anywhere else.

Although the editors of this document have done their best in the limited time available to insure accuracy of quotes or summaries as being "what the original author said," the proposed interagency funding of a bigger project with more elaborate peer review and quality control steps never materialized.

The bottom line: The editors hope users find this document useful, but don't expect or depend on perfection herein. Neither the U.S. Government nor the National Park Service make any claims that this document is free of mistakes.

The following is one chemical topic entry (one file among 118). Before utilizing this entry, the reader is strongly encouraged to read the README file (in this subdirectory) for an introduction, an explanation of how to use this document in general, an explanation of how to search for power key section headings, an explanation of the organization of each entry, an information quality discussion, a discussion of copyright issues, and a listing of other entries (other topics) covered.

See the separate file entitled REFERENC for the identity of numbered references in brackets.

HOW TO CITE THIS DOCUMENT: As mentioned above, for critical applications it is better to obtain and cite the original publication after first verifying various data quality assurance concerns. For more routine applications, this document may be cited as:

**Irwin, R.J., M. VanMouwerik, L. Stevens, M.D. Seese, and W. Basham.** 1997. Environmental Contaminants Encyclopedia. National Park Service, Water Resources Division, Fort Collins, Colorado. Distributed within the Federal Government as an Electronic Document (Projected public availability

on the internet or NTIS: 1998).

Naphthalene, 2,3,5-Trimethyl- (2,3,5-Trimethylnaphthalene, 2,3,5-Methyl naphthalene)

NOTE: Currently there is relatively little information available on specific alkyl homologs of naphthalene. Thus many of the sections listed below contain the phrase "no information found." In such cases, until more information is available, the following data interpretation procedures are recommended:

To interpret concentrations of this particular grouping of alkyl PAHs, the reader may first total naphthalene concentrations and then compare the total to naphthalene benchmarks (see naphthalene entry). The concentration of total naphthalenes is the sum of the following concentrations: total C1 naphthalenes (including all methyl naphthalenes) + total C2 naphthalenes (including dimethylnaphthalenes) + total C3 naphthalenes (including trimethyl naphthalenes) + total C4 naphthalenes + C0 (naphthalene parent compound concentration). Such tentative comparisons are justified on the basis that alkyl PAHs often (there may be exceptions) tend to be equally or more toxic, be equally phototoxic, and be equally or more carcinogenic than the parent compound PAH (see "PAHs as a group" entry).

In the case of text discussion sections where little or no information is available on this particular grouping of alkyl PAHs, the reader is encouraged to also read the "parent" entry (in this case, the Naphthalene entry), but to keep in mind the generalizations (there may be exceptions) that alkyl PAHs often tend to be more persistent, have higher KOWs, be less volatile, be less soluble, be less mobile, bioaccumulate more, have different chemical/physical characteristics, be equally or more toxic, be equally phototoxic, and be equally or more carcinogenic than the parent compound PAH.

**Brief Introduction:**

**Br.Class:** General Introduction and Classification Information:

2,3,5-Trimethylnaphthalene is an alkyl (alkylated) naphthalene; naphthalenes are low molecular weight, 2-ring polyaromatic hydrocarbons (PAHs, also called polycyclic aromatic hydrocarbons) [697]. This compound is one of the alkyl PAHs.

2,3,5-Trimethylnaphthalene is a C3 alkyl homolog of the naphthalene parent compound, for risk assessment best analyzed by a GC/MS/SIM expanded scan for PAHs and alkyl PAHs (such as the NOAA Protocol expanded scan [828]). The C3-naphthalene reported quantity includes all

naphthalenes with three carbon groups attached (for example, the reported concentration would include 2,3,5-Trimethylnaphthalene as well as any other naphthalene with three carbon groups attached). The concentration of just 2,3,5-Trimethylnaphthalene is also sometimes reported separately on expanded scan lists [680].

**Br.Haz:** General Hazard/Toxicity Summary:

Potential Hazards to Fish, Wildlife, and other Non-human Biota:

Probably the most important target analytes in natural resource damage assessments for oil spill are PAHs and the homologous series (alkylated) PAHs [468]. In the aquatic environment, naphthalenes are especially hazardous PAHs due to their particular combination of mobility, toxicity, and general environmental hazard (summary of details presented below). In fact, some studies have concluded that the toxicity of an oil appears to be a function of its di-aromatic hydrocarbon (that is, two-ring hydrocarbons such as naphthalene) content [770,854].

The "relatively" soluble aromatics of an oil (such as benzene, toluene, ethylbenzene, and xylenes, as well as naphthalenes) produce the majority of its toxic effects in the marine environment [770,853].

Alkyl naphthalenes are usually found in the same petroleum products as naphthalenes, often in higher concentration than the parent compound naphthalene [796]. Since alkyl PAHs are often more abundant in fresh petroleum products than their parent compounds, and the proportion of alkyl PAHs to parent compound PAHs increases as the oil ages, it is very important to analyze oil samples for alkyl PAHs any time that biological effects are a concern.

In general, alkyl naphthalenes pose similar hazards or worse hazards than naphthalene [851]. Within an aromatic series, acute aquatic toxicity increases with increasing alkyl substitution on the aromatic nucleus [851]. Naphthalenes are no exception to this overall generalization for PAHs, as there is an increase in toxicity as alkylation of the naphthalene structure increases [853]. For example, the order of most toxic to least in a study using grass shrimp (*Palaemonetes pugio*) and brown shrimp (*Penaeus aztecus*) was dimethylnaphthalenes > methylnaphthalenes >

naphthalenes [853].

There is also an increase in toxicity to marine planktonic algae as alkylation of the naphthalene structure increases [366, Jensen K et al; Limnol 15 (2): 581-4 (1984)]. Comparing several parent compound PAHs (including naphthalene) to alkyl PAH counterparts, the methylated compounds were most toxic [366, Jensen K et al; Limnol 15 (2): 581-4 (1984)].

Although there is less toxicity information available for most of the alkyl PAHs than for their parent compounds, most alkyl PAHs appear to be at least as toxic or hazardous as the parent compound. As can be seen from the preceding paragraph, some have been documented to be more toxic.

One study indicated that pure naphthalene and alkylnaphthalenes are from 3 to 10 times more toxic to test animals than are benzene and alkylbenzene [770]. However, another source states that naphthalene and its homologous series are less acutely toxic than benzene, but prevalent for a longer period during oil spills [773].

At the initial stages of the release of naphthalene- and benzene-derived compounds, when these compounds are present at their highest concentrations, acute toxic effects are most common. Noncarcinogenic effects include subtle changes in detoxifying enzymes and liver damage [773].

Total naphthalenes (Total NPHs): Until more complete information on the effects of all the alkyl naphthalenes is available, risk assessment experts suggest adding all alkyl naphthalene concentrations plus the parent compound concentration and comparing the sum to known toxicological effects benchmarks and criteria for the respective parent compound (Bill Stubblefield, ENSR, personal communication, 1995). In this method, naphthalenes are the sum of C0-C4 naphthalenes (Total NPHs) [521]. In other words, the concentration of total naphthalenes is the sum of the following concentrations: total C1 naphthalenes (including all methyl naphthalenes) + total C2 naphthalenes (including dimethylnaphthalenes) + total C3 naphthalenes (including trimethyl naphthalenes) + total C4 naphthalenes + C0 (naphthalene parent compound concentration). C0-C4 naphthalenes are typically



identified in expanded scans [828].

The heavier (4-, 5-, and 6-ring) PAHs are more persistent than the lighter (2- and 3-ring) PAHs, such as all naphthalenes, and tend to have greater carcinogenic and other chronic impact potential [796].

Acute toxicity is rarely reported in humans, fish, or wildlife, as a result of exposure to low levels of a single PAH compound such as this one. PAHs in general are more frequently associated with chronic risks. These risks include cancer and often are the result of exposures to complex mixtures of chronic-risk aromatics (such as PAHs, alkyl PAHs, benzenes, and alkyl benzenes), rather than exposures to low levels of a single compound (Roy Irwin, National Park Service, Personal Communication, 1996, based on an overview of literature on hand). See also "PAHs as a group" entry.

This compound often occurs together with other aromatics (sometimes including other alkyl PAHs), and a typical complex mixture of aromatics may be more toxic or hazardous in general than just this compound would be alone (see "PAHs as a group" entry).

#### Potential Hazards to Humans:

Most available information is about naphthalene rather than trimethylnaphthalenes [867]. Until more information is available, little can be said about potential effects, although some effects may be similar to other individual alkyl naphthalenes (see separate alkyl naphthalene entries).

Additional human health issues related to the naphthalene parent compound as well as two alkyl naphthalenes (2-methylnaphthalene and 1-methylnaphthalene) have been summarized by ATSDR [867].

#### **Br.Car:** Brief Summary of Carcinogenicity/Cancer Information:

Most of the information available is about the parent compound naphthalene itself rather than trimethylnaphthalenes. Alkyl substitution often confers or enhances carcinogenic potential of PAHs. A few examples:

Very few alkyl PAHs have been broadly tested for

carcinogenicity, but it is known that both dimethylbenzo(a)anthracene and its parent compound benzo(a)anthracene are carcinogenic [40,793,788,881]. Methylbenzo(a)anthracene is actually more carcinogenic than its parent compound benzo(a)anthracene, and dimethylbenzo(a)anthracene is still more carcinogenic [40].

Both cholanthrene and its 3 methyl alkyl cholanthrene counterpart are carcinogenic [40,793]. It is also known that alkylation does not significantly change phototoxicity [888] and that there are some relationships between phototoxicity and potential carcinogenicity (see discussion above). Thus it would not be surprising to discover that a notable number of alkyl PAHs are carcinogenic although they are not now typically added to the list of "carcinogenic PAHs" considered in risk assessments.

These PAH often occurs together with other PAHs, in complex mixtures possibly more carcinogenic than the individual components (see "PAHs as a group" entry). The debates on exactly how to perform both ecological and human risk assessments on the complex mixtures of PAHs typically found at contaminated sites, are likely to continue. There are some clearly wrong ways to go about it, but defining clearly right ways is more difficult. PAHs such as these usually occur in complex mixtures rather than alone. One of the few things that seems clear is that complex PAH mixtures in water, sediments, and organism internal tissues may be carcinogenic and/or phototoxic (Roy Irwin, National Park Service, personal communication, 1996; see also "PAHs as a group" entry and Arfsten et al [911]).

One way to approach site specific risk assessments is to collect the complex mixture of PAHs and other lipophilic organic contaminants in a semipermeable membrane device (SPMD, also known as a fat bag) [894,895,896], retrieve the organic contaminant mixture from the SPMD, then test the mixture for carcinogenicity, toxicity, and phototoxicity (James Huckins, National Biological Survey, and Roy Irwin, National Park Service, personal communication, 1996).

Since alkyl PAHs may be equally or more carcinogenic than the parent compound PAH (see "PAHs as a group" entry), the following information about the naphthalene is presented:

EPA 1996 IRIS Database [893]:

Evidence for classification as to human

carcinogenicity; weight-of-evidence classification:

Classification: D; not classifiable as to human carcinogenicity

BASIS: Based on no human data and inadequate data from animal bioassays.

HUMAN CARCINOGENICITY DATA: None.

ANIMAL CARCINOGENICITY DATA: Inadequate.

However, according to information in IRIS [893], naphthalene may soon be upgraded to "possible carcinogen." status (confirmed by Robert McGaughy, EPA, personal communication, 1996). Further details:

EPA IRIS Note ADDED IN JULY 1995 [893]: Subsequent to the verification of this cancer assessment in 1990, the National Toxicology Program completed a two-year cancer bioassay (1991); its results suggest that naphthalene may be more appropriately classified as a possible human carcinogen (Group C under current EPA guidelines) [893]. The NTP concluded, "Under the conditions of these 2-year studies, there was no evidence of carcinogenic activity of naphthalene in male B6C3F1 mice exposed by inhalation to concentrations of 10 or 30 ppm for 6 hours daily, 5 days per week, for 103 weeks [893]. There was some evidence of carcinogenic activity of naphthalene in female B6C3F1 mice, as indicated by the increased incidences of pulmonary alveolar/bronchiolar adenomas [893]."

The IARC and EPA carcinogenic classifications for naphthalene are group 3 and group D, respectively (both stand for "not classifiable as to its carcinogenicity to humans") [766,893]. This rating was given by EPA in 1990 and may change [893] (see below discussions for details):

Formerly, naphthalene has not been considered carcinogenic [773]. This compound has not been treated as a carcinogen for model calculation purposes in some EPA risk-based (RBC and PRG) models [868,903], but this tentative distinction was made for the purpose of choosing a modeling scenario based on current (often inadequate) knowledge rather than for the purpose of strongly stating that this compound is definitely not a carcinogen; the non-carcinogenic benchmarks are sometimes nearly as low as the carcinogenic benchmarks

(Stan Smucker, personal communication, EPA, 1996).

EPA Historical (modeling purposes only) Classification:  
Not a Carcinogen [302,446].

There is some (mixed) evidence of naphthalene carcinogenicity to mice exposed by inhalation [867,893] as well as some indications that naphthalene may act as a promoter for lung tumors started by other carcinogens [766]. Since naphthalenes often occur in petroleum hydrocarbon mixtures which contain strong carcinogens, a carcinogenic promoter role may prove environmentally significant.

Data available from animal studies do not agree regarding the carcinogenic effects resulting from naphthalene exposure. There is some evidence that naphthalene causes lung cancer in female mice but not in male mice, or rats of either sex [867]. The EPA has determined that naphthalene is not classifiable as to its human carcinogenicity based on the absence of animal data [766].

The observations of Adkins et al. (1986) that there was an increased incidence of tumors in each tumor-bearing mouse, but not in the numbers of mice with tumors, supports classifying naphthalene as a promoter for lung tumors rather than a carcinogen. If this hypothesis is correct, naphthalene may be of greatest environmental concern when exposure to naphthalene is accompanied by exposure to pulmonary carcinogens [766]. This is of interest because naphthalene occurs in various petroleum fuel mixtures which also contain known carcinogens such as benzene, 1,3 butadiene, and various carcinogenic PAHs.

Naphthalene was predicted not to be phototoxic using QSAR estimates [891].

Some interactions are known for certain naphthalenes. For example, when either naphthalene, 1-methylnaphthalene, or 2-methylnaphthalene was applied dermally in combination with benzo(a)pyrene (BaP), there was an inhibitory effect on the induction of skin tumors in female mice. The authors suggested that it is likely that certain naphthalenes compete with BaP for the same enzyme site, resulting in alteration of the BaP metabolic pathway and decreased production of the active BaP metabolite [766].

**Br.Dev:** Brief Summary of Developmental, Reproductive, Endocrine, and Genotoxicity Information:

The little information available is about naphthalene itself rather than trimethylnaphthalenes [867]:

Naphthalene is an endocrine disrupter; when elevated to 10 ppm in water, naphthalene caused crawfish ovaries to shrink, resulting in fewer eggs and smaller offspring [883,884] (Naphthalene confirmed as an endocrine disrupter by Milton Fingerman, Tulane University, personal communication, 1996).

Noncarcinogenic effects of naphthalene exposure include interference with reproductive behavior [773].

One study results suggested that naphthalene metabolites are responsible for its embryotoxicity and support the hypothesis that a medium that decreased naphthalene bioavailability would also reduce its toxicity during the early stages of reproduction [766].

**Br.Fate:** Brief Summary of Key Bioconcentration, Fate, Transport, Persistence, Pathway, and Chemical/Physical Information:

The heavier (4-, 5-, and 6-ring) PAHs are more persistent than the lighter (2- and 3-ring) PAHs, such as all naphthalenes [796].

Most of the fate information available is about naphthalene itself rather than methylnaphthalenes [867].

Naphthalene does not have a strong tendency to accumulate in the flesh of animals that humans eat [867]. However, methyl and other alkyl naphthalenes accumulate to a greater degree in fish than naphthalene [366] (see bio.detail section below for more detail).

Introduction or extension of an alkyl group increases persistence and lipophilicity; increased lipophilicity is often associated with increased absorption [856].

In some media, methylnaphthalenes are suspected to act somewhat like naphthalene [867]. However, several differences have been documented since:

- 1) Alkyl naphthalenes tend to be less volatile (lower vapor pressure and Henry's Law Constant), less soluble, and have a higher log KOW and bioconcentration factors than naphthalene [867], and

2) Alkylated PAHs are more abundant, persist for a longer time than the parent PAHs [468]. Alkyl naphthalenes are no exception, as they tend to persist longer in sediments or amphipod tissues [885] and to bioaccumulate faster in tissues [851] than naphthalene.

3) Naphthalene does not have a strong tendency to accumulate in the flesh of animals that humans eat [867]. However, methyl and other alkyl naphthalenes accumulate to a greater degree in fish than naphthalene [366].

4) Naphthalene is a solid, while 1-methylnaphthalene is a liquid [867].

Low molecular weight PAHs (naphthalenes through phenanthrenes) are removed from the water column primarily by evaporation, microbial oxidation, and sedimentation [851]. Naphthalene and methylnaphthalenes are degraded in water by photolysis and biological processes [766].

PAH Alkyl naphthalenes were more persistent in sediments [521,885] and amphipod tissues [885] than naphthalene. Persistence increases with increasing alkyl substitution, with methyl naphthalene being more persistent than naphthalene and dimethyl naphthalene being still more persistent in sediments and amphipod tissues [885]. Alkyl naphthalenes tend to bioaccumulate faster in tissues [851] than naphthalene.

The crude oil aromatic compounds that are most resistant to weathering, include highly alkylated naphthalenes, phenanthrenes, and dibenzothiophenes [521,523]. In one study, the proportions of the C0-C2 naphthalenes are much smaller and proportions of the highly alkylated (C3-C4) naphthalenes, phenanthrenes, and dibenzothiophenes are larger in weathered Prudhoe Bay Crude Oil than in fresh Prudhoe Bay Crude Oil [521].

Naphthalene and methylnaphthalenes are degraded in water by photolysis and biological processes [766].

Alkyl substitution usually decreases water solubility of PAHs [754]. Alkyl PAHs tend to bioaccumulate to a greater degree than parent compound PAHs [347,885]. Comparing PAHs and alkyl PAHs, the parent compound is typically the first to degrade. Thus, as mixed composition petroleum products age, the percentage of alkyl PAHs vs. PAHs increases, yet most standard EPA scans (even 8270) do not pick up alkyl PAHs [796]. This, coupled with the need for lower detection limits, is one reason the NOAA protocol expanded scan [828] is often

recommended rather than the standard EPA scans.

**Synonyms/Substance Identification:**

2,3,5-Trimethylnaphthalene  
2,3,5-Methyl naphthalene

**Associated Chemicals or Topics (Includes Transformation Products):**

See also individual entries:

Naphthalene  
Naphthalene, C3-  
PAHs as a group  
PAH, Alkyl Homologs of

**Water Data Interpretation, Concentrations and Toxicity (All Water Data Subsections Start with "W."):**

**W.Low** (Water Concentrations Considered Low):

No information found. Compare total naphthalenes to concentrations in the naphthalene entry.

**W.High** (Water Concentrations Considered High):

No information was found for this 2,3,5 isomer, but the water solubility of another (1,4,5) trimethyl naphthalene does not exceed 5.77 mg/L at 25 degrees C, so concentrations near 5 mg/L may be close to the maximum that water can ordinarily hold at that temperature [848].

**W.Typical** (Water Concentrations Considered Typical):

No information found. Compare total naphthalenes to concentrations in the naphthalene entry.

**W.Concern Levels, Water Quality Criteria, LC50 Values, Water Quality Standards, Screening Levels, Dose/Response Data, and Other Water Benchmarks:**

**W.General** (General Water Quality Standards, Criteria, and Benchmarks Related to Protection of Aquatic Biota in General; Includes Water Concentrations Versus Mixed or General Aquatic Biota):

No information found. Until more information is available, compare total naphthalenes concentration to naphthalene entry concentration. Total naphthalenes = total concentrations of C1 naphthalenes (including methyl naphthalenes) + total C2 naphthalenes (including dimethylnaphthalenes) + total C3 naphthalenes

(including this compound, 2,3,5-Trimethylnaphthalene and all other C3 naphthalenes) + total C4 naphthalenes + naphthalene itself (C0, also known as naphthalene parent compound).

**W.Plants** (Water Concentrations vs. Plants):

No information found; compare total naphthalene concentration to naphthalene entry concentrations.

**W.Invertebrates** (Water Concentrations vs. Invertebrates):

LC50 Values [851,998]:  
Eurytemora affinis  
(estuarine Calanoid copepod) - 0.32 ppm, 24 h

Most other available information seems to be about naphthalene itself rather than alkyl naphthalenes.

**W.Fish** (Water Concentrations vs. Fish):

No information found; compare total naphthalene concentration to naphthalene entry concentrations.

**W.Wildlife** (Water Concentrations vs. Wildlife or Domestic Animals):

No information found; compare total naphthalene concentration to naphthalene entry concentrations.

**W.Human** (Drinking Water and Other Human Concern Levels):

No information found; compare total naphthalene concentration to naphthalene entry concentrations.

**W.Misc.** (Other Non-concentration Water Information):

Naphthalene was predicted not to be phototoxic using QSAR estimates [891]. Alkyl PAHs often (there may be exceptions) tend to be equally phototoxic to the parent compound PAH (see "PAHs as a group" entry).

**Sediment Data Interpretation, Concentrations and Toxicity** (All Sediment Data Subsections Start with "Sed."):

**Sed.Low** (Sediment Concentrations Considered Low):

No information found. Compare total naphthalenes to concentrations in the naphthalene entry.

**Sed.High** (Sediment Concentrations Considered High):

No information found. Compare total naphthalenes to



concentrations in the naphthalene entry.

**Sed. Typical** (Sediment Concentrations Considered Typical):

No information found. Compare total naphthalenes to concentrations in the naphthalene entry.

**Sed. Concern Levels, Sediment Quality Criteria, LC50 Values, Sediment Quality Standards, Screening Levels, Dose/Response Data and Other Sediment Benchmarks:**

**Sed. General** (General Sediment Quality Standards, Criteria, and Benchmarks Related to Protection of Aquatic Biota in General; Includes Sediment Concentrations Versus Mixed or General Aquatic Biota):

No information found; compare total naphthalene concentration to naphthalene entry concentrations.

**Sed. Plants** (Sediment Concentrations vs. Plants):

No information found; compare total naphthalene concentration to naphthalene entry concentrations.

**Sed. Invertebrates** (Sediment Concentrations vs. Invertebrates):

No information found; compare total naphthalene concentration to naphthalene entry concentrations.

**Sed. Fish** (Sediment Concentrations vs. Fish):

No information found; compare total naphthalene concentration to naphthalene entry concentrations.

**Sed. Wildlife** (Sediment Concentrations vs. Wildlife or Domestic Animals):

No information found; compare total naphthalene concentration to naphthalene entry concentrations.

**Sed. Human** (Sediment Concentrations vs. Human):

No information found; compare total naphthalene concentration to naphthalene entry concentrations.

**Sed. Misc.** (Other Non-concentration Sediment Information):

No information found.

**Soil** Data Interpretation, Concentrations and Toxicity (All Soil Data Subsections Start with "Soil."):

**Soil.Low** (Soil Concentrations Considered Low):

No information found. Compare total naphthalenes to concentrations in the naphthalene entry.

**Soil.High** (Soil Concentrations Considered High):

No information found. Compare total naphthalenes to concentrations in the naphthalene entry.

**Soil.Typical** (Soil Concentrations Considered Typical):

No information found. Compare total naphthalenes to concentrations in the naphthalene entry.

**Soil.Concern Levels, Soil Quality Criteria, LC50 Values, Soil Quality Standards, Screening Levels, Dose/Response Data and Other Soil Benchmarks:**

**Soil.General** (General Soil Quality Standards, Criteria, and Benchmarks Related to Protection of Soil-dwelling Biota in General; Includes Soil Concentrations Versus Mixed or General Soil-dwelling Biota):

No information found; compare total naphthalene concentration to naphthalene entry concentrations.

**Soil.Plants** (Soil Concentrations vs. Plants):

No information found; compare total naphthalene concentration to naphthalene entry concentrations.

**Soil.Invertebrates** (Soil Concentrations vs. Invertebrates):

No information found; compare total naphthalene concentration to naphthalene entry concentrations.

**Soil.Wildlife** (Soil Concentrations vs. Wildlife or Domestic Animals):

No information found; compare total naphthalene concentration to naphthalene entry concentrations.

**Soil.Human** (Soil Concentrations vs. Human):

No information found; compare total naphthalene concentration to naphthalene entry concentrations.

**Soil.Misc.** (Other Non-concentration Soil Information):

No information found.

**Tissue and Food Concentrations (All Tissue Data Interpretation Subsections Start with "Tis."):**

**Tis.Plants:**

A) As Food: Concentrations or Doses of Concern to Living Things Which Eat Plants:

No information found; compare total naphthalene concentration to naphthalene entry concentrations.

B) Body Burden Residues in Plants: Typical, Elevated, or of Concern Related to the Well-being of the Organism Itself:

No information found; compare total naphthalene concentration to naphthalene entry concentrations.

**Tis.Invertebrates:**

A) As Food: Concentrations or Doses of Concern to Living Things Which Eat Invertebrates:

No information found; compare total naphthalene concentration to naphthalene entry concentrations.

B) Concentrations or Doses of Concern in Food Items Eaten by Invertebrates:

No information found; compare total naphthalene concentration to naphthalene entry concentrations.

C) Body Burden Residues in Invertebrates: Typical, Elevated, or of Concern Related to the Well-being of the Organism Itself:

No information found; compare total naphthalene concentration to naphthalene entry concentrations.

**Tis.Fish:**

A) As Food: Concentrations or Doses of Concern to Living Things Which Eat Fish (Includes FDA Action Levels for Fish and Similar Benchmark Levels From Other Countries):

No information found; compare total naphthalene concentration to naphthalene entry concentrations.

B) Concentrations or Doses of Concern in Food Items Eaten by Fish:

No information found; compare total naphthalene concentration to naphthalene entry concentrations.

C) Body Burden Residues in Fish: Typical, Elevated, or of Concern Related to the Well-being of the Organism Itself:

No information found; compare total naphthalene concentration to naphthalene entry concentrations.

**Tis.Wildlife:** Terrestrial and Aquatic Wildlife, Domestic Animals and all Birds Whether Aquatic or not:

A) As Food: Concentrations or Doses of Concern to Living Things Which Eat Wildlife, Domestic Animals, or Birds:

No information found; compare total naphthalene concentration to naphthalene entry concentrations.

B) Concentrations or Doses of Concern in Food Items Eaten by Wildlife, Birds, or Domestic Animals (Includes LD50 Values Which do not Fit Well into Other Categories, Includes Oral Doses Administered in Laboratory Experiments):

No information found; compare total naphthalene concentration to naphthalene entry concentrations.

C) Body Burden Residues in Wildlife, Birds, or Domestic Animals: Typical, Elevated, or of Concern Related to the Well-being of the Organism Itself:

No information found; compare total naphthalene concentration to naphthalene entry concentrations.

**Tis.Human:**

A) Typical Concentrations in Human Food Survey Items:

No information found. Compare total naphthalenes to concentrations in the naphthalene entry.

B) Concentrations or Doses of Concern in Food Items Eaten by Humans (Includes Allowable Tolerances in Human Food, FDA, State and Standards of Other Countries):

No information found; compare total naphthalene concentration to naphthalene entry concentrations.

C) Body Burden Residues in Humans: Typical, Elevated, or of Concern Related to the Well-being of Humans:

No information found; compare total naphthalene concentration to naphthalene entry concentrations.

**Tis.Misc.** (Other Tissue Information):

Naphthalene was predicted not to be phototoxic using QSAR estimates [891]. Alkyl PAHs often (there may be exceptions) tend to be equally phototoxic to the parent compound PAH (see "PAHs as a group" entry).

**Bio.Detail:** Detailed Information on Bioconcentration, Biomagnification, or Bioavailability:

Alkyl PAHs tend to bioaccumulate to a greater degree than parent compound PAHs [347,885]. Introduction or extension of an alkyl group increases lipophilicity, which often appears as increased absorption [856].

Alkyl naphthalenes tend to persist longer in amphipod tissues [885] and to bioaccumulate faster in tissues [851] than naphthalene. Bioconcentration of naphthalenes by amphipods was greatest (about 1000 times) in flow through systems. In the sediment exposure system, no naphthalene was present in amphipod tissues after four days and by the 18th day only dimethyl naphthalenes were present [885].

Log Kow values for alkyl naphthalenes [971]:

Naphthalene:	3.37
C1-Naphthalene:	3.87
C2-Naphthalene:	4.37
C3-Naphthalene:	5.0
C4-Naphthalene:	5.55

During the Exxon Valdez spill, bioconcentration explained the buildup of PAHs in tissues better than biomagnification; most accumulation was of an equilibrium partitioning nature across the gills rather than from the food chain [971]. Immature fish seem have higher bioconcentration of PAHs than adults, perhaps because their PAH breakdown systems are not fully developed and at times perhaps because of a higher percentage of lipid tissues (yolk tissues, etc) [971] (confirmed by Jerry Neff, Battelle Ocean Sciences, Duxbury, MA, personal communication 1996).

Coho salmon were exposed to a dilute water soluble fraction (WSF) of Prudhoe Bay crude oil for five weeks. They accumulated the more highly alkylated naphthalenes in muscle tissue faster than the less-substituted aromatics [851]:

HYDROCARBON	CONCENTRATION (PPB)		BIOACCUMULATION FACTOR
	Water	Muscle Tissue	
Naphthalene	4	240	60
C3-Naphthalenes	6	680	113.3

**Interactions:**

No information found.

**Uses/Sources:**

Trimethyl naphthalenes are found in various crude oils, No. 2 fuel oil oils, and Bunker C [177,770]. 2,3,5-Trimethylnaphthalene is found in Prudhoe Bay crude [854]. This compound is a C3 alkyl homolog of naphthalene, and various C3 alkyl homologs of naphthalene are found in many petroleum products (see individual product entries, such as entry for Fuel Oil 5).

**Forms/Preparations/Formulations:**

No information found.

**Chem.Detail:** Detailed Information on Chemical/Physical Properties:

Alkylation of PAHs tends to increase Kow and significantly or drastically change other physical/chemical parameters (for more detailed discussions, see Chem.detail section of "PAHs as a group" entry). Gasolines, including unleaded gasolines [746], contain a small but significant amount of PAHs including naphthalene and alkyl naphthalenes [797]. Naphthalenes make up from 0.09 to 0.49 weight percent of gasoline and from 0.08 to 0.5 volume percent of various gasolines [796]. Methyl naphthalenes constituted the single largest class of chemicals in soils contaminated by no. 6 fuel oil [814].

Details of naphthalene content (mg/kg or ppm) in one fresh sample of Exxon Valdez Crude Oil [971]:

Note: these values are wet weight (Jerry Neff, Battelle Ocean Sciences, Duxbury, MA, personal communication 1996):

Naphthalene:	622 mg/kg = ppm
C1-Naphthalene:	1400 mg/kg = ppm
C2-Naphthalene:	1780 mg/kg = ppm
C3-Naphthalene:	1410 mg/kg = ppm
C4-Naphthalene:	696 mg/kg = ppm

Details of naphthalene content (mg/kg or ppm) in salmon carcass (fatty viscera removed, so the concentrations may have been higher from whole body samples) from Snug Harbor, Alaska, an area heavily oiled by the Exxon Valdez Crude Oil, 4/15/89 [971]:

Note: Concurrent measurements of water quality, as well as equilibrium partitioning estimates of water quality based on concentrations in fish and mussels, both confirm that PAH concentrations did not exceed water quality criteria at the time these concentrations were measured in fish tissues [971]. These values are wet weight (Jerry Neff, Battelle Ocean Sciences, Duxbury, MA, personal communication 1996):

Naphthalene:	7.15 ug/kg = ppb
C1-Naphthalene:	65.11 ug/kg = ppb
C2-Naphthalene:	29.75 ug/kg = ppb

C3-Naphthalene: 93.95 ug/kg = ppb  
 C4-Naphthalene: 36.63 ug/kg = ppb

Details of naphthalene content (ug/kg or ppb) in whole body samples of mussels) from Snug Harbor, Alaska, an area heavily oiled by the Exxon Valdez Crude Oil, 4/15/89 [971]:

Note: Concurrent measurements of water quality, as well as equilibrium partitioning estimates of water quality based on concentrations in fish and mussels, both confirm that PAH concentrations did not exceed water quality criteria at the time these concentrations were measured in mussel tissues [971]. These values are wet weight (Jerry Neff, Battelle Ocean Sciences, Duxbury, MA, personal communication 1996):

Naphthalene: 12.9 ug/kg = ppb  
 C1-Naphthalene: 17.3 ug/kg = ppb  
 C2-Naphthalene: 247 ug/kg = ppb  
 C3-Naphthalene: 905 ug/kg = ppb  
 C4-Naphthalene: 850 ug/kg = ppb

Concentrations of trimethylnaphthalenes in South Louisiana crude, Kuwait crude, No. 2 fuel oil, and Bunker C residual were 2400, 1900, 18400, and 8800 mg/kg (ppm), respectively [177].

For comparison, the following table lists some of the specific naphthalene contents (ppm) of water soluble fraction (WSF) from 10% oil-in-water solution of four test oils (measured by gas chromatography) [770]:

COMPOUNDS	SOUTH LA CRUDE	KUWAIT CRUDE	NO. 2 FUEL OIL	BUNKER C RESIDUAL
Di-aromatics				
Naphthalene	0.12	0.02	0.84	0.21
Trimethylnaphthalene	0.008	0.003	0.03	0.10

Aromatic hydrocarbons concentrations (ug/g, ppb) measured in a study using Prudhoe Bay Crude oil [854]:

COMPOUNDS	CONCENTRATION (ppb)
Naphthalene	777
2,3,5-Trimethylnaphthalene	466

No information was summarized on the 2,3,5 isomer, but a similar compound (1,4,5 trimethylnaphthalene) has reported water solubilities ranging from 2.1 to 5.77 mg/L at 25 degrees C, a vapor pressure of 0.681 Pa at 25 degrees C, a Henry's law constant of 23.5 Pa M<sup>3</sup>/mol, and a Log Kow of 4.87 to 4.89 [848].

**Fate.Detail:** Detailed Information on Fate, Transport, Persistence, and/or Pathways:

See Br.Fate section above. No other information found.

**Laboratory and/or Field Analyses:**

In the past, many methods have been used to analyze for PAHs [861,1010,1013] but most do not cover alkyl PAHs such as this one. Parent compound semi-volatile PAHs have often been analyzed using routine monitoring methods EPA 8270 for solid waste/RCRA purposes [1013] or by EPA NPDES method 610 as specified in 40 CFR Part 136 [1010]. However, the standard EPA methods 8270, 610, and 625 are all inadequate for generating scientifically defensible information for Natural Resource Damage Assessments [468].

For risk, or damage assessment, or biological impact studies, or drinking water purposes, or to determine if biodegradation has occurred, the NOAA expanded scan for PAHs and alkyl PAHs [828], or equivalent improvements, should be used since such scans generally give more rigorous and comprehensive results than the unmodified EPA scans. The NOAA scan also covers C3 naphthalenes such as this one.

Most of the historically used methods for PAHs, including EPA standard semi-volatile scan numbers 8270 and 610, do not cover important alkyl PAHs and do not utilize low-enough detection limits.

Recommended detection limits: 10 ppt for water, 0.3 to 1 ppb for tissues, sediments, and soil.

Note: Utilizing up to date techniques, many of the better labs can use detection limits of 0.3 to 1 ppb for tissues, sediments, and soils, and these lower detection limits are far better for risk or hazard assessment, but in all cases detection limits for these media should not be above 10 ppb.

Recent (1991) studies have indicated that EPA approved methods used for oil spill assessments (including total petroleum hydrocarbons method 418.1, semivolatile priority pollutant organics methods 625 and 8270, and volatile organic priority pollutant methods 602, 1624, and 8240) are all inadequate for generating scientifically defensible information for Natural Resource Damage Assessments [468]. These general organic chemical methods are deficient in chemical selectivity (types of constituents analyzed) and sensitivity (detection limits); the deficiencies in these two areas lead to an inability to interpret the environmental significance of the data in a scientifically defensible manner [468].

If a Park Service groundwater investigation at Colonial National Historical Park performed in response to contamination by Fuel Oil 5 had utilized EPA semi-volatile scan 8270 or any of the other typical EPA scans (625, etc.) all of which only include parent compounds and typically utilize detection limits in the 170-600 ppb range, the false conclusion reached would have been that no PAHs were present in significant (detection limit) amounts. This



false negative conclusion would have been made because the parent compound PAHs present constituted only 7.6% of the PAHs detected in groundwater by the expanded scan [828], and the highest concentration found for any parent compound was 8.4 ppb, far below the detection limits used on the older standard EPA scans. Utilizing the NOAA protocol expanded scan [828], it was determined that 92.4% of the total concentration values of the PAHs detected in groundwater were alkyl PAHs, and that all 39 PAHs and alkyl PAHs were present. Of course, all 39 PAHs were also present in the fresh product, in much higher concentrations, and also having alkyl compounds with the highest percentage of higher values compared to parent compounds (see Chem.Detail section in separate PAHs entry for more details).

In a similar vein, if the Park Service sediment investigation at Petersburg National Historical Battlefield (see Chem.Detail section in separate PAHs entry, this study was performed in response to contamination by Diesel) had utilized EPA semi-volatile scan 8270 or any of the other typical EPA scans (625, etc.), all of which only include parent compounds and often utilize detection limits no lower than the 170-600 ppb range, the false conclusion reached would have been that only one PAH was present in significant (detection limit) amounts. This false negative conclusion would have been made because the parent compound PAHs present constituted only 2.4% of the PAHs detected in sediments, and the highest concentration found for any parent compound except pyrene was 85.5 ppb, far below the detection limits used on the older standard EPA scans. Pyrene was 185 ppb, which would have been non-detected on many of the EPA scans, but not all. However, utilizing the NOAA protocol expanded scan [828], it was determined that 97.6% of total quantity of PAHs detected in sediments were alkyl PAHs, and that all 39 PAHs and alkyl PAHs were present in these sediments.

Some labs use screening HPLC fluorescence methods to screen for alkylated naphthalenes and dibenzothiophenes that fluoresce at naphthalene wavelengths and the alkylated phenanthrenes that fluoresce at phenanthrene wavelengths [521]. Other HPLC/fluorescence scans are used to examine fish bile directly for the presence of metabolites of PAHs such as naphthalene [523].

Some labs use screening HPLC fluorescence methods to screen for alkylated naphthalenes and dibenzothiophenes that fluoresce at naphthalene wavelengths and the alkylated phenanthrenes that fluoresce at phenanthrene wavelengths [521]. Other HPLC/fluorescence scans are used to examine fish bile directly for the presence of metabolites of PAHs such as naphthalene [523].

It should be kept in mind that quality control field and lab blanks and duplicates will not help in the data quality assurance goal as well as intended if one is using a method prone to false negatives. Methods may be prone to false negatives due to the use of detection limits that are too high, the loss of contaminants through inappropriate handling, or the use of an inappropriate methods such as many of the EPA standard scans. This is one reason for using the NOAA expanded scan for PAHs [828]; or method 8270 [1013] modified for SIM detection limits (10 ppt for water, 0.3 to 1 ppb for solids) and additional alkyl PAH analytes; or alternative

rigorous scans; rather than many of the standard EPA parent compound PAH scans which are prone to false negatives (Roy Irwin, National Park Service, Personal Communication, 1997).

For a much more detailed discussion of lab methods for naphthalenes, see the naphthalene entry. In the lab section of the naphthalene (general) entry, the reader will find much more detailed discussions of lab methods, holding times, containers, comparability of data from different methods, field methods, quality assurance procedures, the relationship of various methods to each other, the various EPA standard methods for various EPA programs, and why many standard EPA methods are inadequate for certain applications. A decision tree key for selecting the most appropriate methods for oil or oil products spills is also provided in the lab section of the naphthalene entry. Pros and cons of various lab and field methods are detailed in the separate PAHs entry. Due to the length of these discussions, they are not repeated here (see naphthalene and PAHs entries).