Comments Of The
Alkylphenols & Ethoxylates Research Council
On The
Oregon Department of Environmental Quality
Draft Development Of A Priority Persistent Pollutant List (P^3L) for Oregon
(March 2, 2009)

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Introduction

The Alkylphenols & Ethoxylates Research Council (APERC) submits these comments on the Oregon Department of Environmental Quality (DEQ) draft Technical Document "Development of a Priority Persistent Pollutants List (P^3L) for Oregon (March 2, 2009)." APERC is comprised of major North American producers of alkylphenols (APs) including nonylphenol (CAS RN 25154-52-3), 4-nonylphenol (CAS RN 104-40-5), 4-tert-octylphenol (CAS RN 140-66-9), p-tert-butylphenol (CAS RN 98-54-4) and 2,6-di-tert-butylphenol (CAS RN 128-39-2), which DEQ proposed to add to the P^3L. For more than twenty years APERC, its predecessor the American Chemistry Council's Alkylphenols and Ethoxylates Panel, and its member companies have been actively engaged in toxicological and environmental fate and effects research on APs and their derivative compounds.[1] Consequently, APERC can contribute considerable information and expertise relevant to the environmental and toxicological assessment of these substances.

Oregon Senate Bill 737 was enacted under the premise that "persistent, bioaccumulative and toxic pollutants can pose a threat to the health and well-being of humans, fish and wildlife, especially aquatic species."[2] When enacted on June 22, 2007, this bill directed DEQ to conduct "a study of persistent pollutants discharged in the State of Oregon and report the results of that study to an appropriate interim committee of the Legislative Assembly related to the environment by June 1, 2010." 'Persistent pollutant' is defined in the Act as "a substance that is toxic and either persists in the environment or accumulates in the tissues of humans, fish, wildlife or plants."[3] In the draft Technical Document, DEQ recognizes that this definition of persistent is inconsistent with other nationally and internationally recognized definitions of persistent and bioaccumulative and toxics (PBTs) and persistent organic pollutants (POPs). In fact, DEQ broadened the scope of chemicals for consideration to be listed on the P^3L even further to include "pesticides, herbicides, suspected endocrine disruptors, industrial chemicals, pharmaceutical and personal care products, as well as others not previously recognized as potentially problematic (e.g., "emerging" contaminants)."[4]

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[1] Members of the Alkylphenols & Ethoxylates Research Council include: Dover Chemical Corporation; SI Group; Texas Petrochemicals, Inc. and The Dow Chemical Company.
[2] 74th Oregon Legislative Assembly. (2007). Senate Bill 737. http://www.leg.state.or.us/07reg/measures/sb0700.dir/sb0737.en.html
[3] 74th Oregon Legislative Assembly. (2007).
[4] Oregon Department of Environmental Quality (DEQ), Water Quality Division. (2009, March 2). Draft Development of a Priority Persistent Pollutant List (P^3L) for Oregon. http://www.deq.state.or.us/wq/SB737/docs/DraftTechnicalReport.pdf

These comments present APERC's concerns regarding the lack of transparency and opportunity for public comment in the P^3L development process as well as concerns regarding the superficial methodology and arbitrary criteria used to prioritize the persistence, bioaccumulation and aquatic and mammalian toxicity of compounds in the draft Technical Report, which does not take into account the availability of more robust data. APERC also presents specific comments to explain why the P^3L prioritization assessment scores of the alkylphenols referenced above should be reduced and these substances should be removed from the P^3L.

I. APERC CONCERNS WITH THE LACK OF TRANSPARENCY AND LACK OF OPPORTUNITY FOR PUBLIC COMMENT ON THE ACTIVITIES OF THE DEQ AND THE PRIORITY PERSISTENT POLLUTANT SCIENCE WORKGROUP DURING THE PROCESS OF DEVELOPING THE P^3L

DEQ convened a Priority Persistent Pollutant Science Workgroup (PPSWG) to function solely as an advisory and technical body to the P^3L process rather than as a committee designed to reflect stakeholder views. Its members will have served from August 2008 to June 2009, during the P^3L development process. During this time they will have held eight meetings divided between locations in Portland and Salem that were presumably publicly accessible. The draft Technical Document states that "the direction and details of list development were discussed at each meeting; agendas and notes for each meeting are available on the SB 737/PPSWG website." A review of that website finds that there are no notes available for any of the three meetings that occurred in 2009 during which the PPSWG and DEQ discussed and agreed on the draft P^3L. A review of the meeting notes that are available for the meetings that occurred in 2008 finds, with the exception of a representative from the ACWA and the League of Oregon Cities at one meeting, no stakeholders representing industry or other groups were in attendance at any of the meetings to either observe or provide comment.

The only public comment period provided by DEQ is the four week period between March 2 and March 27, 2009. While public information sessions were held in four locations throughout the state of Oregon between March 3 and March 17 these sessions provided only "the opportunity for stakeholders and interested members of the public, to learn, and ask questions, about the list development process and the draft final P^3L". Since these were not public hearings, no transcripts or recordings will be made available.

Of great concern regarding the process is the notable absence of industry stakeholders who are most knowledgeable in the properties of chemical and their uses in products. The draft Technical Report highlights the fact that the PPSWG was not intended to reflect stakeholder views. Unfortunately this did not provide the group with an industry expert that could direct the group to relevant data and information on the chemicals they were considering (and perhaps even those that they excluded). Considering the implications of the resulting P^3L and subsequent regulatory actions that will likely be related to these activities, it is APERC's view that there was insufficient transparency and opportunity for public comment during this process.

II. APERC CONCERNS WITH THE APPROACH TAKEN IN THE DEQ DRAFT TECHNICAL DOCUMENT TO DEVELOP THE P^3L

A. DEQ should have conducted thorough assessments that consider the highest quality data available utilizing a scientifically-based approach before listing compounds on a "Priority Persistent Pollutants List" (P^3L).

The market implications for a compound listed as "persistent" by any regulatory authority are grave even if that compound is subsequently removed from the list. In forums that address persistent, bioaccumulative and toxic chemicals, a PBT designation generally infers a need to severely restrict or even essentially eliminate the use of a compound. While it may not have been the intention of Oregon Senate Bill 737 to cause confusion with its new definition of "persistent" this will not be recognized by other regulatory authorities or the businesses and consumers that use products containing compounds incorrectly designated persistent. Considering the likelihood that the Oregon legislature's intention regarding a P^3L listing could be misperceived and result in unnecessary market disruption and economic impact to affected businesses, consideration should be given to changing the name of the list to more accurately reflect the status of the listed compounds (e.g., Screening Priority List). In the event that the P^3L designation remains, DEQ has an obligation to conduct thorough and scientifically-based assessments prior to listing any compound on the final P^3L.

B. The approach taken by DEQ and the PPSWG to identify P^3L chemicals is not scientifically defensible and expanded the scope of chemicals and criteria beyond that intended in the Act through the use of inappropriate source lists.

The draft Technical Document states the first step in the process of developing the P^3L was to identify chemicals on "existing lists of PBTs, POPs, endocrine disruptors, "emerging" contaminants, and pesticides developed by a variety of other state, federal, and international agencies"; whereas the Act directing these activities stipulates that there should be a focus first on persistent pollutants discharged in the State (SB 737 Section 3(1)), then a narrower focus on those that pose a threat to the waters of the State (SB 737 Section 3(2)(a)).

There were no underlying principles provided in the draft Technical Report as to what organizations were appropriate sources and why the source lists were selected; therefore, the first step in the P^3L process appears arbitrary. A more scientifically defensible approach would be to work from lists generated from authoritative bodies and from consensus-based groups with broad stakeholder inclusion. In fact, some of the list sources cited in the draft Technical Document are not appropriate to identify persistent and/or bioaccumulative and toxic compounds. For example, while the US Geological Survey (USGS) is a Department of the federal government it is not a regulatory authority, nor does it conduct chemical risk assessments or establish policy about chemical priorities. Therefore the detection of a compound in a USGS environmental monitoring

study does not justify inclusion of that compound on the P^3L as a persistent compound that is a threat to the waters of Oregon.

Perhaps of greater concern is the expansion of scope in the development of the P^3L to include lists of compounds suspected of having some endocrine activity despite the fact that this specific mode of action is not called out in the Senate Bill 737. There is no need for special focus on endocrine activity since higher-level chronic effects, which are based on dose-response and adverse ecotoxicity effects, account for effects resulting from all modes of action (including endocrine) and should be considered in the assessments of chemicals for listing on the P^3L. Even if the mode of action of a substance is not completely established or understood, these more traditional studies provide a better measure of the hazard and/or risk of any compound – including alkylphenols –toward the health of an organism or population. In fact, in the case of nonylphenol, governmental assessments have found that traditional apical endpoints are more sensitive than endocrine-mediated endpoints.[5,6,7]

The use by the PPSWG of lists such as the Institute for Environment and Health's list of "Chemicals Purported to be Endocrine Disruptors: A Compilation of Published Lists" is unnecessary and inappropriate in light of the charge put forth by Senate Bill 737. In fact, this specific list includes a prominent disclaimer that "inclusion of a particular substance in this report should not be taken to constitute any endorsement of its status as a proven or potential endocrine disrupting or modifying agent by either IEH or DEFRA."[8] In addition, it does not address the characteristics of persistence and bioaccumulation as called out by Senate Bill 737.[9] The deficiencies in the development of the P^3L seriously flaw the identification and prioritization process.

C. DEQ should conduct P^3L assessments that are consistent with those generally accepted in the regulatory and scientific community; utilizing a preferred hierarchy of data sources where the weight-of-evidence is preferred over single measured values, which are in turn preferred over estimated, calculated or modeled values.

DEQ should adopt a policy and screening mechanism that requires consideration of a hierarchy of data sources that is consistent with other regulatory authorities and the scientific community in general. Governmental authorities such as the US Environmental Protection Agency (EPA) and the Organisation for Economic Co-operation and

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[5] US Environmental Protection Agency (EPA). (2005). Aquatic Life Ambient Water Quality Criteria - Nonylphenol. Report 822-R-05-005. US Environmental Protection Agency, Washington, DC, USA.

[6] Environment Canada and Health Canada (EC and HC). (2001). Priority Substances List Assessment Report: Nonylphenol and its Ethoxylates. www.ec.gc.ca/ccebl/eng/final/index_e.html.

[7] European Union (EU). (2002). European Union Risk Assessment Report: 4-Nonylphenol (branched) and Nonylphenol. http://ecb.jrc.it/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT/4-nonylphenol_nonylphenolreport017.pdf.

[8] Institute for Environmental and Health (IEH). (2005). Chemicals Purported to be Endocrine Disrupters: A Compilation of Published Lists. Web Report W20. Medical Research Council Institute for Environment and Health, Leicester, UK. http://www.cranfield.ac.uk/health/researchareas/environmenthealth/ieh/ieh%20publications/w20.pdf

[9] Institute for Environmental and Health (IEH). (2005).

Development (OECD) routinely require characterization of data quality in risk assessments and data submissions such as those conducted under the High Production Volume (HPV) Challenge Program.[10] In order to be consistent with the hierarchy of data sources approach that is generally accepted in the scientific and regulatory communities, DEQ should assign the greatest weight to studies that are the most reliable, relevant and adequate.

DEQ should more diligently pursue the collection of chemical specific data and should leverage numerous available data sources. Methods or models, such as the PBT Profiler, that do not meet these criteria should be considered only as supplementary information.

1. Decisions regarding the listing of chemicals on the P^3L should not rely on the screening results from models such as EPA's PBT Profiler, which is not intended for making regulatory decisions, especially when higher quality data and/or weight-of-evidence assessments are available.

EPA's PBT Profiler was designed to help interested parties voluntarily screen chemicals on the basis of their estimated persistence, bioaccumulation and aquatic toxicity characteristics when no experimental data are available. DEQ selected this tool to make "an initial consistent evaluation of the PBT characteristics of each chemical" that it identified as a candidate for the P^3L. This premise that consistent application of a model such PBT Profiler to all of the candidate compounds - regardless of whether there are existing high quality data available for some - in some way enhances the screening process is misconceived. DEQ and the PPSWG appear to have taken this approach because they assume the "overwhelming majority of known chemical substances do not have experimental persistence, bioaccumulation, and toxicity data available."[11] This is not the case for the many of the compounds, including alkylphenols, listed on the P^3L. A discussion of the data available for the alkylphenol compounds is presented later in these comments.

Of greater concern is the fact that categorizing the persistence, bioaccumulation and toxicity of the P^3L candidate compounds based solely on the output of the EPA PBT Profiler violates a number of important principles explicitly stated in the purpose of the PBT Profiler model itself. First, the PBT Profiler was never intended to be used for making regulatory decisions; however, the categorization of compounds on the P^3L is clearly being done for regulatory purposes. The purpose of the PBT Profiler states that the model is a screening tool - not a regulatory tool. Its purpose is to assist in identifying chemicals that may need further evaluation when no additional data are available. The PBT Profiler cautions, "It is important to stress that the PBT Profiler is a screening level predictive tool and cannot be used for all chemical substances… the PBT Profiler is a tool that, like all tools, has strengths, weaknesses, and limitations. These limitations should be considered before using this model. For example, predicted data should never

[10] US Environmental Protection Agency (EPA). (2004). High Production Volume Challenge Program. Guidance for Meeting SIDS Requirements. http://www.epa.gov/opptintr/chemrtk/sidsappb.htm.
[11] Oregon Department of Environmental Quality (DEQ), Water Quality Division. (2009, March 2).

be used in place of experimental data." Additional model limitations are described on the PBT Profiler website including the fact that since the PBT Profiler "is not a definitive tool, estimates rendered may overestimate or underestimate persistence, bioaccumulation, or toxicity characteristics." The PBT Profiler also cautions that "results should be evaluated with care, this evaluation may take several forms including, but not limited to, detailed technical evaluation by subject matter experts experienced in the evaluation of chemicals for PBT characteristics." In addition, there is specific guidance that "chemicals with experimental data from a well conducted laboratory study should not be run through the PBT Profiler. Experimental data should always be used in preference to estimations."[12]

However, perhaps more troubling is the second prioritization step in which output from the PBT Profiler was put into the Canadian Risk Assessment IDentification And Ranking (RAIDAR) Model. It appears DEQ and the PPSWG have ignored some fundamental principles of simulating data in using these models; the use of data generated from one model (PBT Profiler) as input for a second model (RAIDAR) will not generate any meaningful output and certainly should not be used for regulatory prioritization decisions.

2. If DEQ relies on the PBT Profiler for screening chemicals with little available data the most updated models and guidance from EPA should apply.

The PBT Profiler was developed for use by EPA's Office of Pollution Prevention and Toxics and uses models developed by EPA that are also packaged as EPISuite models. The EPISuite models have been updated (v4.00) and are more advanced in terms of incorporating the most recent scientific information than the versions used in the PBT Profiler.[13,14] Also, according to PBT Profiler guidelines, persistence should be determined for the environmental compartment in which the highest percentage of a test substance would be found using Mackay Level III multi-media modeling. Relying on outdated models and guidance leads to erroneous conclusions. Application of these updated models and guidance to some of the alkylphenols listed in the current draft of the P^3L changes the conclusions regarding their persistence and/or bioaccumulation and supports their removal from this list.

3. The P3L process did not adequately research mammalian and/or human health effects data during the list prioritization process and errantly assigned human health rankings of 0.5 to compounds, including alkylphenols, on the list.

[12] US Environmental Protection Agency (EPA) PBT Profiler. http://www.epa.gov/oppt/sf/tools/pbtprofiler.htm.
[13] US Environmental Protection Agency (EPA) EpiSuite 4.0. (2009). http://www.epa.gov/oppt/exposure/pubs/episuitedl.htm.
[14] Environmental Science Center under contract to the Office of Pollution Prevention and Toxics , US Environmental Protection Agency (EPA). (2006). Purpose of the PBT Profiler: Identifying materials that may need additional technical evaluation for Persistence, Bioaccumulation and Toxicity characteristics. http://www.pbtprofiler.net/notice.asp.

Under Section 4.3.3 (1) of the draft Technical Document there is a description of the general basis for the health rankings; however, there is no discussion of the process by which DEQ and PPSWG researched and assessed either the mammalian or human health effects of the chemicals on the P^3L. Other than a search for Human Reference Doses for drinking water and a review of the EPA Integrated Risk Information System (IRIS) there appears to have been no effort during the development of the P^3L to identify relevant mammalian or human health effects data or risk assessments. The draft Technical Document states "those chemicals without human health information were assigned a default rank of 0.5 (the mid-point between non-hazardous and very hazardous), so that any unknown hazard they might pose to humans would not be completely overlooked."

In the case of the alkylphenols listed on the P^3L not only are there numerous high quality mammalian toxicity data available in the published literature but governmental health assessments have concluded that they do not represent a risk to human health.[15] DEQ and the PPSWG would have found this to be true for many of the compounds assigned a default health categorization of 0.5 had there been even minimal efforts to search the literature or contact informed stakeholders during the P^3L development process.

D. The criteria to score and prioritize candidate compounds for inclusion on the P^3L were developed independently and arbitrarily by DEQ without stakeholder input.

The draft Technical Document describes the first step in the prioritization process as summing the separate scores (0, 1, or 2) for overall persistence and bioaccumulation generated by the PBT Profiler, then adding that "aquatic" value to the "human" toxicity score obtained as described in Section 3.2 of the same document. This provided a "total PBT score" (with a minimum value of 0 and a maximum of 6) for each chemical. The draft Technical Document states "DEQ made an independent policy choice to establish a total PBT score of "3" as a prioritization cut-off point to focus the P^3L on those chemicals likely to be of greater persistence, accumulative ability, or toxicity. The PPSW discussed and concurred with this choice." This decision resulted in the exclusion of 534 chemicals that scored a total of "2" or lower from the P^3L. In any case, DEQ should revisit the question of cut off thresholds after providing for adequate stakeholder input.

E. The mandate in Senate Bill 737 to consider feasibility to achieve reductions in developing the P^3L does not preclude consideration of natural sources of endocrine active compounds as P^3L candidates since wastewater treatment is a feasible discharge reduction option.

Senate Bill 737 directs DEQ to develop "a priority listing of persistent pollutants that pose a threat to the waters of this state, as defined in ORS 196.800, and have documented harmful effects on the health and well-being of humans, fish or wildlife, especially aquatic species, based on factors including… the feasibility of reduction options."

[15] Environment Canada and Health Canada (EC and HC). (2001).

The draft Technical Document states "with respect to feasibility, DEQ believes it may be more feasible to achieve reductions in persistent pollutants that come primarily from local (in-state) anthropogenic sources (ones over which local toxic reduction plans may exert control)."[16] This is particularly relevant since DEQ chose to include substances listed on "suspected endocrine lists" on the P^3L. If there is a concern for the endocrine mediated impact of pollutants on the aquatic environment then DEQ should expand the list of substances to include natural phytoestrogens and the highly potent residual natural human hormones that also contribute to the endocrine activity of receiving waters, with greater potency than trace levels of weakly endocrine active substances present in the environment due to their use in commerce. It is entirely feasible to control the discharge of human hormones and other persistent components in wastewater effluent through adequate wastewater treatment. Failing to recognize this may result in a lower health standard for ecosystems and the environment in Oregon while presenting a burden to industry.

III. THE DEQ AND PPSWG CATEGORIZATIONS OF ALKYLPHENOLS ARE INCONSISTENT WITH OTHER GOVERNMENTAL ASSESSMENTS AND DO NOT CONSIDER ALL AVAILABLE INFORMATION AND DATA ABOUT THESE COMPOUNDS THAT SUPPORT THEIR REMOVAL FROM THE P^3L

As described above, APERC is concerned with the process and approach taken to prioritize all compounds, including alkylphenols, for the P^3L. More specifically, the lack of rigor in the research and assessment of the alkylphenols currently listed on the P^3L also raises concern and has resulted in categorizations of these compounds that are inconsistent with other more robust governmental assessments. The following discussion addresses issues with the assessment of individual alkylphenol compounds and CAS RNs and provides additional information to justify removal of these compounds from the P^3L.

A. Comprehensive and scientifically defensible assessments by various governmental authorities have concluded that nonylphenol (CAS RNs 84852-15-3 and 25154-52-3), 4-tert-octylphenol (CAS RN 140-66-9), and 2,6-di-tert-butylphenol (CAS RN 128-39-2) are <u>not</u> persistent and <u>not</u> bioaccumulative; categorization of these compounds otherwise by DEQ is inconsistent with their status at the international and national levels as well in other states. Review of the data available in these assessments support reduction in the P^3L scores for NP and OP as well as their removal from the P^3L.

Several governmental assessments have already evaluated some of the alkylphenols listed on the P^3L and concluded that they do not meet various criteria for classification as a persistent or bioaccumulative compound.[17,18,19,20,21,22 23] The European Commission (EC)

[16] Oregon Department of Environmental Quality (DEQ), Water Quality Division. (2009, March 2).
[17] Environment Canada and Health Canada (EC and HC). (2001).
[18] Rodier, D. (1996). EPA RM-1 Document for *Para*-Nonylphenol.

Joint Research Center Institute for Health and Consumer Protection conducted assessments for 2,6-di-tert-butylphenol, nonylphenol, and 4-tert-octylphenol and concluded they do not fulfill the EC criteria to be classified as persistent or bioaccumulative.[24] More recently, Environment Canada completed a review of NP and OP as part of a categorization assessment under the Canadian Environmental Protection Act (CEPA), which requires an assessment of all substances on the Canadian Domestic Substances List (DSL) with respect to persistence, bioaccumulation and inherent toxicity (PBiT) characteristics. Attached is a document that summarizes the basis behind Environment Canada's conclusion that neither nonylphenol nor octylphenol is persistent or bioaccumulative according to the CEPA criteria.[25]

In addition, the Washington State Department of Ecology removed nonylphenol (CAS RNs 84852-15-3 and 25154-52-3) from its list of PBT chemicals in a final rule on persistent bioaccumulative toxic (PBT) substances (Chapter 173-333 WAC) that was effective on February 13, 2006. Washington concluded that nonylphenol does not meet that state's criteria to be classified as persistent (half-life in water, soil or sediment > 60 days) or bioaccumulative (BCF or BAF >1000) after reviewing a weight-of-evidence summary of the available data. Classifying nonylphenol as a Priority Persistent Pollutant in Oregon will be distinctly out of step with international and federal programs as well as with Oregon's neighboring state Washington, which will be particularly confusing since Washington has criteria that are similar to those proposed in the P^3L.

Numerous laboratory and field studies on the persistence and bioaccumulative properties of nonylphenol and 4-tert-octylphenol are referenced in governmental assessments and are available to DEQ. In addition, a pair of companion manuscripts by Staples et al. (2008) and Klecka et al. (2008) summarize and provide references to the available data on the persistence and bioaccumulative properties of nonylphenol and octylphenol.[26,27] As such, numerous studies on these two compounds are available to DEQ that consider the highest quality data in order to conduct more robust assessments in the development of the P^3L. A review of the environmental half-lives for nonylphenol and octylphenol

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[19] European Union (EU). (2001). Risk Assessment Report: 4-Nonylphenol (branched) and Nonylphenol: Final Report. http://ecb.jrc.it/DOCUMENTS/Existing-Chemicals/RISK_ASSESSMENT/REPORT.

[20] European Chemicals Bureau (ECB). (2003). PBT Working Group Substance Information Sheets for Nonylphenol (CAS 25154-52-3) and Phenol, 4-Nonyl, branched (CAS 84852-15-3).

[21] Environment Canada (EC). (2007). Ecological categorization of substances on the Domestic Substance List; Categorization Decisions. (Completed in September 2006). http://www.ec.gc.ca/substances/ese/eng/dsl/cat_index.cfm.

[22] US Environmental Protection Agency (EPA). (2005). Aquatic Life Ambient Water Quality Criteria - Nonylphenol. Report 822-R-05-005. US Environmental Protection Agency, Washington, DC, USA.

[23] UK Environment Agency. (2005). Environmental Risk Evaluation Report: 4-tert-Octylphenol.

[24] European Commission Joint Research Centre Institute for Health and Consumer Protection http://ecb.jrc.ec.europa.eu/esis/index.php?PGM=pbt

[25] Environment Canada (EC). (2005, November 21). Response to APERC's Proposal Regarding Environment Canada's Preliminary Categorization of Nonylphenol, Octylphenol and their Ethoxylates.

[26] Staples, C.A., Klecka, G.M., Naylor, C.G., and Losey, B.S. (2008). C8- and C9-Alkylphenols and Ethoxylates: I. Identity Physical Characterization, and Biodegradation Pathways Analysis Human and Ecological Risk Assessment, 14: 1007–1024.

[27] Klecka, G.M., Staples, C.A., Naylor, C.G., Woodburn, K.B., and Losey, B.S. (2008). C8- and C9-Alkylphenols and Ethoxylates: II. Assessment of Environmental Persistence and Bioaccumulation Potential Human and Ecological Risk Assessment, 14: 1025–1055.

shows that the majority fall below 60 days supporting a reduction in their persistence score in the P^3L from 1 to 0. A review of the bioconcentration factors and bioaccumulation factors for octylphenol shows that the majority fall below 1000 supporting a reduction in its bioaccumulation score in the P^3L from 1 to 0. These changes will reduce the aggregate P^3L aquatic scores for these compounds to less than 2, which should result in their removal from the P^3L list.

B. Commercially available nonylphenol (available under CAS RNs 84852-15-3 and 25154-52-3) is a mixture of isomers with branched nonyl groups. Since the PBT Profiler cannot reliably be used to predict the persistence, bioaccumulative and/or toxic properties of a mixture, CAS RN 25154-52-3 should be removed from the P^3L in accordance with DEQ's previous decision to remove CAS RN 84852-15-3.

A review of the P^3L Chemical Disposition log, which includes the rationale for removing chemicals during the prioritization process, indicates that nonylphenol, 4-(branched) (CAS RN 84852-15-3) was removed at R2 because it represents a chemical mixture that could not be evaluated by the PBT Profiler. As discussed previously, the use of models (e.g., EPA PBT Profiler) to predict persistence and bioaccumulative properties of compounds is always less reliable than experimental data and actual measured half-lives; in addition, the complexity of the mixture of isomers in commercially available NP makes results from model estimations even less reliable and is not recommended by the PBT profiler guidelines. DEQ and the PPSWG already recognized this limitation of the PBT Profiler and removed nonylphenol (CAS RN 84852-15-3) from the P^3L on this basis; therefore, the same decision should be taken for nonylphenol (CAS RN 25154-52-3).

DEQ should be aware that all commercially relevant nonylphenol is a mixture of isomers with various levels of branching in the nonyl group. This mixture of branched structures is best described by CAS RN 84852-15-3; however, the CAS RN 25154-52-3 is also recognized as a more generic description of essentially the same substance. The EPISuite modeling programs incorrectly present this CAS RN as representing only a linear compound. Following is an explanation of why the manufacture of nonylphenol precludes production of anything but a complex mixture of branched nonylphenol isomers.

Nonylphenol is produced through the Friedel-Crafts alkylation of phenol with propylene trimer in the presence of an acid catalyst, which preferentially alkylates at the *para* position of phenol. Commercial propylene trimer does not contain linear C_9H_{18} *alpha*-olefin; rather it is a complex mixture of highly branched, predominantly nine-carbon olefins. Therefore, any nonylphenol formed by the alkylation of phenol with propylene trimer is also a very complex mixture of branched isomers with the following approximate composition: *ortho*-NP (3-6%), *para*-NP (90-93%) and decylphenol (2-5%). Since the *para* isomer predominates, the product is most accurately described as *para*-

nonylphenol, branched (*p*-NP or PNP).[28] Table 1 lists the results of high-resolution gas chromatography analyses of *p*-NP and identifies 22 branched *para*-isomers, within five distinct groups. Group designations are presented based on the substitution of the *alpha*-carbon on the alkyl chain.[29]

Table 1. *Para* Isomers of Nonylphenol

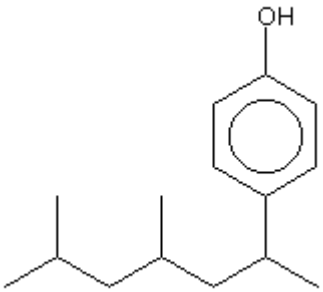
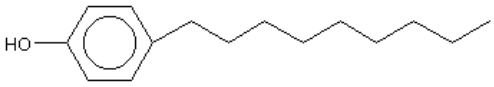
Group #	Isomer Type	Number of Isomers	Para Isomers %
1	Alpha-dimethyl	10	48.6%
2	Alpha-methyl, alpha- ethyl, beta-primary	3	8.9%
3	Alpha-methyl, beta-methyl	4	24.7%
4	Alpha-methyl	2	6.6%
5	Alpha-methyl, alpha- propyl	3	11.2%
	Total Isomers	22	100%

The complexity of the isomers represented in commercial nonylphenol as described by CAS RNs 84852-15-3 and 25154-52-3 has been recognized in US EPA's Aquatic Life Ambient Water Quality Criteria (WQC) and Risk Management 1 (RM1) documents for nonylphenol as well as in both Environment/Health Canada's Priority Substance List Assessment for nonylphenol and nonylphenol ethoxylate and their categorization of nonylphenol.[30,31,32,33] The European Union (EU) also recognized that commercial nonylphenol is a complex mixture in the EU Risk Assessment on nonylphenol and its ethoxylates.[34] Table 2 summarizes CAS RNs for nonylphenol, their nomenclature and related governmental assessments.

Table 2. Nonylphenol Descriptions, Structures and Governmental Assessments

CAS RN	Description	Governmental Assessments	Structure (Sources: CAS, NIST, APERC)[35,36,37]
84852-15-3	Phenol, 4-nonyl-, branched **Other** Nonylphenol; 4-Nonylphenol; p-Nonylphenol, branched; Branched 4-nonylphenol (mixed isomers)	US EPA (1996) EC CEPA (2001) EU (2001) ECB (2003) US EPA (2005) EC (2007)	Unspecified, mixed isomers

[28] Bhatt, B.D., Prasad, J.V., and Ali, S. (1992). Separation and characterization of isomers of *p*-nonylphenols by capillary GC/GC-MS/GC-FTIR techniques. J. Chromatographic Sci., 30, 203-210.
[29] Wheeler, T.F., Heim, J.R., LaTorre, M.R., and Janes, A.B. (1997). Mass Spectral Characterization of *p*-Nonylphenol Isomers using High-Resolution Capillary GC-MS. Journal of Chromatographic Science, 35(1).
[30] US Environmental Protection Agency (EPA). (2005).
[31] Rodier, D. (1996).
[32] Environment Canada and Health Canada (EC and HC). (2001).
[33] Environment Canada (EC). (2007).
[34] European Union (EU). (2001).
[35] Chemical Abstract Services. http://www.cas.org.
[36] National Institute of Standards and Technology Standard Reference Database. http://webbook.nist.gov/chemistry.
[37] Alkylphenols & Ethoxylates Research Council. www.aperc.org.

25154-52-3 **Other** 84852-15-3 **Former** 1300-16-9; 56459-00-4	Phenol, nonyl **Other** Phenol, nonyl-; x-Nonylphenol; Nonylphenol (mixed isomers); Nonylphenol (mixture)	US EPA (1996) EC CEPA (2001) EU (2001) ECB (2003) US EPA (2005) EC (2007)	
104-40-5	p-Nonylphenol **Other** 4-Nonylphenol; Phenol, p-nonyl-; 4-n-Nonyl phenol; Phenol, 4-n-nonyl	US EPA (1996) EC (2007)	

C. A large body of data on mammalian toxicity effects are available for some of the alkylphenols and support changing their P^3L health prioritization rank scores to zero.

The draft Technical Document states those "chemicals without human health information were assigned a default rank of 0.5 (the mid-point between non-hazardous and very hazardous), so that any unknown hazard they might pose to humans would not be completely overlooked." All of the alkylphenols on the P^3L are assigned health rank values of 0.5 presumably because DEQ thought there were no available data. The draft Technical Document states "prior to use of the PBT Profiler, each of the 1,196 chemicals identified at Step 3 was screened against the following criteria:

> (1) An oral reference dose (RfD) of ≤ 0.003 mg/kg/day (for non-carcinogens), or
> (2) Identification (for non-carcinogens) as a developmental toxin by the California Environmental Protection Agency (CalEPA) per California's Proposition 65, or
> (3) A U.S. EPA IRIS carcinogenic weight-of-evidence classification of A, B1, or B2 (USEPA, 1986) [or *Carcinogenic to Humans*, *Likely to Be Carcinogenic to Humans*, or *Suggestive Evidence of Carcinogenic Potential* per the 2005 guidelines (USEPA, 2005)], or
> (4) An International Agency for Research on Cancer (IARC) carcinogenic weight-of-evidence classification of 1, 2A, or 2B"

None of the alkylphenols meet any of the above health criteria. In addition, numerous mammalian toxicity studies are available and have been reviewed in governmental assessments of nonylphenol and 4-tert-octylphenol that concluded no concern for human risk.[38,39,40] These are available for DEQ's review in order to revise the human health rank of these compounds in the P^3L prioritization tables. The lowest No Observable Adverse

[38] UK Environment Agency. (2005).
[39] Environment Canada and Health Canada (EC and HC). (2001).
[40] European Union (EU). (2001).

Effect Level (NOAEL) for nonylphenol is 12 mg/kg/day[41] and the lowest NOAEL for 4-tert-octylphenol is 15mg/kg/day.[42] Both of these results were determined in multi-generation rat studies. Since these compounds are relatively nontoxic to mammals, their human health rank in the P^3L tables should be changed to zero.

D. Several of the alkylphenols listed on the P^3L should be removed from the list because they are unlikely to be used or discharged in significant amounts - if at all - in Oregon water.

The draft Technical Report notes that DEQ deleted 200 chemicals from the draft P^3L during its development based on the fact that they are "obscure industrial or process intermediary chemicals unlikely to be used or discharged in any significant amounts, if at all, in Oregon."[43] This rationale also supports the removal of 4-nonylphenol (CAS RN 104-40-5), p-tert-butylphenol (CAS RN 98-54-4) and 2,6-di-tert-butylphenol (CAS RN 128-39-2) from the P^3L.

1. 4-nonylphenol (CAS RN 104-40-5), which represents a chemical structure with a linear nonyl group, is not commercially relevant and only available in research quantities; therefore this compound and CAS RN should be removed from the P^3L.

Based on APERC's understanding of the manufacture and availability of alkylphenols there are in principle only two forms of NP: one has a linear nonylphenol group and the other is a mixture of isomers with branched nonylphenol groups. Linear NP, which is best described by CAS RN 104-40-5, is not available other than in small research quantities and is unlikely to be used or discharged in any significant amounts in Oregon. Therefore, this compound should be removed from the P^3L.

2. Two compounds, p-tert-butylphenol (CAS RN 98-54-4) and 2,6-di-tert-butylphenol (CAS RN 128-39-2) are used as process intermediary chemicals that are unlikely to be used or discharged in any significant amounts - if at all - in Oregon; therefore they should be removed from the P^3L.

The compound p-tert-butylphenol is used exclusively as a contained process intermediate in the chemical synthesis of other compounds, primarily phenolic resins. In the United States the percentage of 2,6-di-tert-butylphenol used as a synthetic intermediate for the production of higher molecular weight phenolic antioxidants is reported to be greater than 90%. The remaining percentage of the production is used as an oxidation inhibitor and stabilizer mainly for fuel, oil and gasoline. The substance, however, is not volatile (vapor

[41] Tyl, R., Myers, C.B., Marr, M.C., Castillo, N.P., Seely, J.C., Sloan, C.S., Veselica, M.M., Joiner, R.J., Van Miller, J.P., and Simon, G.S. (2006). Three-Generation Evaluation of Dietary *para*-nonylphenol in CD (Sprague-Dawley) Rats. Toxicological Sciences, 92, 295-310.

[42] Tyl, R., Myers, C.B., Marr, M.C., Brine, D.R., Fail, P.A., Seely, J.C., and Van Miller, J.P. (1999). Two-Generation Reproduction Study with *para*-tert-Octylphenol in Rats. Regulatory Toxicology and Pharmacology 30, 81-95.

[43] Oregon Department of Environmental Quality (DEQ), Water Quality Division. (2009, March 2).

pressure at 25C = 1 Pa) and it is expected that most will be incinerated directly, when used as an additive in gasoline and fuel or oil. APERC and its member companies are not aware of any companies in Oregon that are purchasing either of these compounds for processing; therefore it is highly unlikely that they will be used or discharged in any significant amounts - if at all - in Oregon. Both p-tert-butylphenol (CAS RN 98-54-4) and 2,6-di-tert-butylphenol (CAS RN 128-39-2) should be removed from the P^3L.