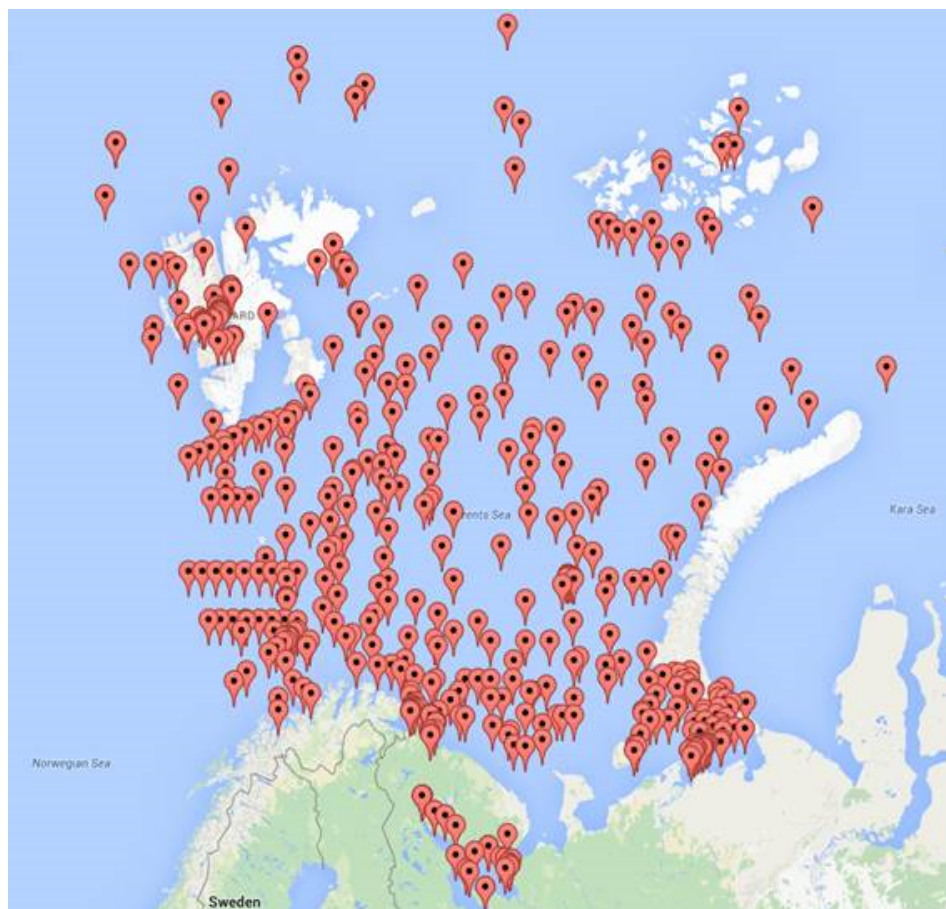


PAH in sediments from the Barents and White Seas. Metadata and database



Rapporttittel / Report title

**PAH in sediments from the Barents and White Seas.
Metadata and database**

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The report presents the data and metadata for polycyclic aromatic hydrocarbons (PAH) in bottom sediments from 510 stations in the Barents and White Seas.

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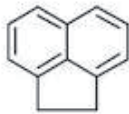
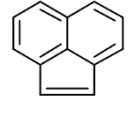
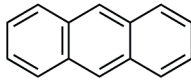
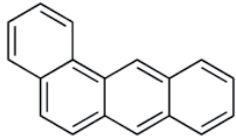
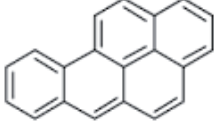
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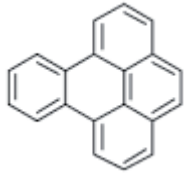
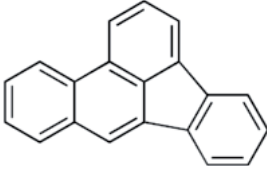
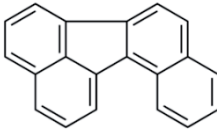
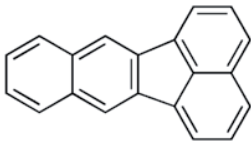

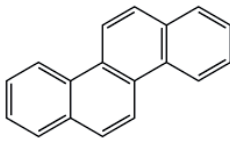
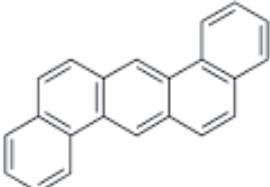
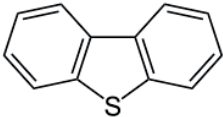
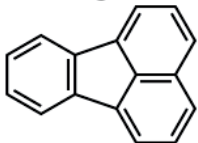
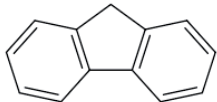
1 Introduction

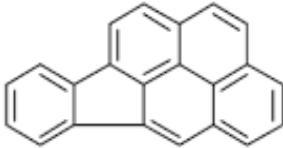
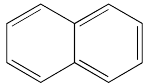
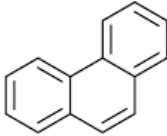
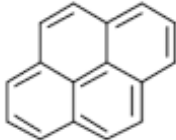
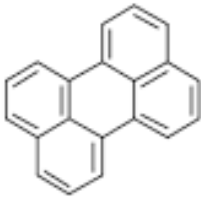
Polycyclic aromatic hydrocarbons (PAHs) are common environmental contaminants which can be derived from anthropogenic sources, such as combustion and discharges from extraction and transport, and natural processes, including leakage and erosion of fossil carbon. Natural PAH sources contribute, along with biological activities and terrestrial run-off, to the organic carbon content in sediments. Spatial distribution of PAHs dependent on the genesis of sedimentary material and transport mechanisms within the environment. In addition, locations of hydrocarbon extraction, transport, and burning further determine the distribution, relative contribution, and composition of PAHs in sedimentary organic material.

There are three major types of PAHs: petrogenic, pyrogenic, and biogenic. PAHs of pyrogenic origin are formed as a result of both natural (volcanism, hydrothermal or catagenetic transformation of organic matter) and anthropogenic (combustion of fossil fuels and recent organic material e.g. wood) processes. PAHs from combustion sources are mainly parent (non-alkylated) PAHs. (Table 1) The relative amounts of the less stable kinetic PAH isomers (e.g., anthracene) compared to the more stable thermodynamic isomers of the same molecular mass (e.g., phenanthrene) can indicate combustion or anthropogenic inputs. (Alberty & Rei 1988; Gschwend & Hites 1981; Colombo et al. 1989; Budzinski et al. 1997).

Table 1. Chemical identity of parent polycyclic aromatic hydrocarbons (PAH) of interest for environmental studies included into database

Compounds: name and acronyms	Chemical structure	Chemical formula	Molecular mass $\text{g} \cdot \text{mol}^{-1}$
Acenaphthene ACN		$\text{C}_{12}\text{H}_{10}$	154.21
Acenaphthylene ACL		C_{12}H_8	152.20
Anthracene ANT		$\text{C}_{14}\text{H}_{10}$	178.2
Benzo[a]anthracene BAA		$\text{C}_{18}\text{H}_{12}$	228.29
Benzo[a]pyrene BAP		$\text{C}_{20}\text{H}_{12}$	252.3

Compounds: name and acronyms	Chemical structure	Chemical formula	Molecular mass $\text{g}\cdot\text{mol}^{-1}$
Benzo[e]pyrene BEP		$\text{C}_{20}\text{H}_{12}$	252.3
Benzo[b]fluoranthene BBF		$\text{C}_{20}\text{H}_{12}$	252.3
Benzo[j]fluoranthene BJF		$\text{C}_{20}\text{H}_{12}$	252.32
Benzo[k]fluoranthene BKF		$\text{C}_{20}\text{H}_{12}$	252.3
Benzo[g,h,i]perylene BP		$\text{C}_{22}\text{H}_{12}$	276.34
Chrysene CHR		$\text{C}_{18}\text{H}_{12}$	228.3
Dibenz[a,h]anthracene DBA		$\text{C}_{22}\text{H}_{14}$	278.35
Dibenzothiophene DBT		$\text{C}_{12}\text{H}_8\text{S}$	184.26
Fluoranthene FLT		$\text{C}_{16}\text{H}_{10}$	202.26
Fluorene FLN		$\text{C}_{13}\text{H}_{10}$	166.2

Compounds: name and acronyms	Chemical structure	Chemical formula	Molecular mass $\text{g}\cdot\text{mol}^{-1}$
Indeno[1,2,3-c,d]pyrene IND		$\text{C}_{22}\text{H}_{12}$	276.3
Naphthalene NAP		C_{10}H_8	128.17
Phenanthrene PHE		$\text{C}_{14}\text{H}_{10}$	178.2
Pyrene PYR		$\text{C}_{16}\text{H}_{10}$	202.3
Perylene PER		$\text{C}_{20}\text{H}_{12}$	252.31

PAHs of petrogenic origin, including a wide range of alkylated PAHs, form during diagenetic processes of sedimentary organic matter to fossil fuels (Table 2).

Table 2. Alkylated PAHs of interest for environmental studies included into data base

Compound: name and acronyms	Molecular mass	Compound: name and acronyms	Molecular mass
C1-Naphthalenes (C1N)	142	C1-Dibenzothiophenes (C1D)	198
C2-Naphthalenes (C2N)	156	C2-Dibenzothiophenes (C2D)	212
C3-Naphthalenes (C3N)	170	C3-Dibenzothiophenes (C3D)	226
C1-Phenanthrene/Anthracenes (C1P)	192		
C2-Phenanthrene/Anthracenes (C2P)	206		
C3-Phenanthrene/Anthracenes (C3P)	220		

Phenanthrene and its alkylated homologues can be petrogenic, pyrogenic, or diagenic. The presence of the more highly alkyl homologues usually indicates a petroleum source. Dibenzothiophene and its C1 to C3 alkylated homologues are distinct components of many fresh crude oils. Therefore, data on the alkylated PAHs along with parent PAHs are used to determine the approximate percentage of fossil PAHs relative to total PAHs (Boehm & Farrington 1984).

PAHs of biogenic origin are generated either by biological processes, or in the early stages of diagenesis in marine sediments (e.g. perylene) (Venkatesan 1988) (Table 1).

Although the health effects of individual PAHs are not exactly alike, following 17 PAHs are considered to be potentially dangerous: acenaphthene, acenaphthylene, anthracene, benz[a]anthracene, benzo[a]pyrene, benzo[e]pyrene, benzo[b]fluoranthene, benzo[g,h,i]perylene, benzo[j]fluoranthene, benzo[k]fluoranthene, chrysene, dibenz[a,h]anthracene, fluoranthene, fluorene, indeno[1,2,3-c,d]pyrene, phenanthrene and pyrene. These PAHs were chosen because (1) more information is available on these than on the others; (2) they are suspected to be more harmful than some of the others, and they exhibit harmful effects that are representative of the PAHs; (3) there is a greater chance that you will be exposed to these PAHs than to the others; and (4) of all the PAHs analyzed, these were the PAHs identified at the highest concentrations at hazardous waste sites (Mumtaz, George, 1995).

Less is known about the toxicity of alkylated PAHs, although one study has demonstrated that alkylated PAHs may have greater toxicity than the parent compound (Marvanova et al., 2008).

2 Materials and Methods

Sediment samples were collected from 520 stations in the Barents and White Seas (*Figure 1*) between 1991 and 2009 by Akvaplan-niva AS, Tromsø, Norway (APN), Institute of Marine Research, Bergen, Norway (IMR), All-Russian Scientific Research Institute for Geology & Mineral Resources of the Ocean "VNIIOkeangeologia", St. Petersburg, Russia (VNIIO) and Polar Research Institute of Marine Fisheries and Oceanography, Murmansk, Russia, (PINRO) (Alexeeva et al., 2003; 2004; Boitsov et al., 2009a; Christensen, 2007; Cochrane et al., 2001; Dahle et al., 2006; 2009; dos Santos et al., 1992; Evenset et al., 2006; 2009; Evenset, Killie, 1997; Killie et al., 1997a; 1997b; Killie, Dahle, 1995; Loring et al., 1995; Ollsson et al., 1997; Savinov et al., 1999; 2000; 2006; 2008; 2010; 2011; Savinova et al. 2007a; 2007b; 2009; Stange, Klungsøyr, 1997; Velvin, Evenset, 2008).

Sediment samples were retrieved using either a 0.1 m² van Veen grab or a gravity corer with a plastic liner. All samples were frozen onboard ship at -20°C and stored frozen until analysis.

The chemical analysis were performed at Unilab Analyse AS, Tromsø, Norway (Unilab), Marine Chemistry Group of IMR (MCG IMR), Norwegian Institute of Water Research, Oslo, Norway (NIVA), Laboratory of Organic Geochemistry of VNIIO (LabOG VNIIO), Centre of Environmental Chemistry of Research and Production Association "Typhoon", Obninsk, Russia (CEC RPA Typhoon), Laboratory of Applied Ecology, Toxicology of PINRO (Labeco-PINRO) and the Geochemical and Environmental Research Group, Texas A&M University, USA (GERG-TAMU).

2.1. Unilab

(from Savinov et al., 2000)

PAH analyses

The procedure used for the analysis of PAHs is based on the International Oceanographic Commission (UNESCO) guidelines (IOC, 1982) with minor modifications. Individual sediment samples (25-110 g) were homogenized, treated with methanol and KOH, and refluxed for 1.5 h.

together with a 1.0 ml solution of seven deuterated PAHs. This solution included the following PAHs: naphthalene-d8 (CIL, DLM-365), biphenyl-d10 (CIL, DLM-494), anthracene-d10 (CIL, DLM-102), phenanthrene -d10 (CIL, DLM-371), pyrene -d10 (CIL, DLM-155), chrysene-d12 (CIL, DLM-261) and perylene -d12 (CIL, DLM-366). The solid fraction was removed by filtration and the elute containing PAHs was extracted with pentane. The extracts were purified by column chromatography using Varian Bond Elute solid phase extraction cartridges containing 500 mg silica (Varian LRC, A1211-3036), and eluted with pentane and dichloromethane. The final extract was analyzed by capillary column gas chromatography with mass spectrometric detection (Hewlett-Packard MS 5971, HP 5890 Gas Chromatograph equipped with a split/splitless injector and a 25 m × 0.20 mm i.d. HP Ultra 1 column, and HP G 1034 B software for MS ChemStation). Detection limits for naphthalene, phenanthrene, anthracene, dibenzothiophene and their alkyl homologues were on the order of 1 ng/g dry sediment. Detection limits for other PAH compounds were approximately 0.1 ng/g dry sediment.

Unilab laboratory is accredited for hydrocarbon analyses according to the European standards of NS-EN 45001 and ISO/IEC Guide 25. Since 1996, the laboratory has participated in the European Commission sponsored intercomparison exercise, QUASIMEME (Quality Assurance of Information for Marine Environmental Monitoring in Europe). Quality assurance and control protocols are described in (Cochrane et al., 2009). Laboratory quality control procedures include analyses of sample blanks, reference material and spiked samples. The reference material used for quality control was supplied by the National Research Council of Canada (HS4 reference material). Instrument stability and response is checked using NIST-solutions.

Grain Size, Total Organic Carbon (TOC) and Total Nitrogen (TN) Determinations

Grain size distribution was determined for each sample gravimetrically after wet sieving. Sediment water content was determined after drying a sample to constant weight (for 4 days at 50°C).

Samples analyzed for TOC content were pre-treated with HCL to remove inorganic carbon, followed by catalytic (Fe, Cu) combustion at 480°C. The content of CO₂ gas formed was quantified by IR detection using a LECO IR 212 carbon analyzer. The TN-levels were determined according to a modified Kjeldahl method. Samples were pre-digested with H₂SO₄, K₂SO₄ and Se (catalyst), followed by spectrophotometric detection of the NH₄ complex formed using a ChemLab autoanalyser.

2.2. MCG IMR – 90s (for samples collected in the period 1991-1993)

(from Stange, Klungsøyr, 1997)

PAH analyses

Two separate grab samples from each location were analysed for PAHs. Wet samples (ca. 50 g) were saponified in methanolic KOH (0.5 M) for 1.5 h followed by liquid/liquid extraction with pentane. Extracts were reduced in volume and cleaned on silica columns prior to injection on a Hewlett Packard 5987A GC/MS in SIM mode (Klungsøyr et al., 1988). The instrument was equipped with a 50 m×0.22 mm×0.11 µm HP Ultra 2 fused silica capillary column. GC/MS analysis was performed using four fully deuterated internal standards (biphenyl, anthracene, pyrene, perylene) added to the samples prior to extraction. Sediment particle size distribution was determined by wet sieving of the silt and clay fractions and dry sieving of the sand fraction using stainless steel sieves (Retsch GmbH & CO, Germany). Total organic carbon in the sediments was

determined with a LECO SC-444 elemental analyser. The PAH components included in the analytical protocol represent both natural sources, and anthropogenic sources resulting from the use of oil, and the incomplete combustion of fossil fuels: Naphthalene and C1-, C2- and C3-alkyl derivatives, anthracene, phenanthrene and C1- and C2-alkyl derivatives, Dibenzothiophene and C1-, C2- and C3-alkyl derivatives, fluoranthene, pyrene, benz[a]anthracene, chrysene, benzo[fluoranthenes], benzo[e]pyrene, benzo[a]pyrene, perylene, benzo[g,h,i]perylene, indeno[1,2,3-cd]pyrene, and dibenzo[a,c+a,h]anthracenes.

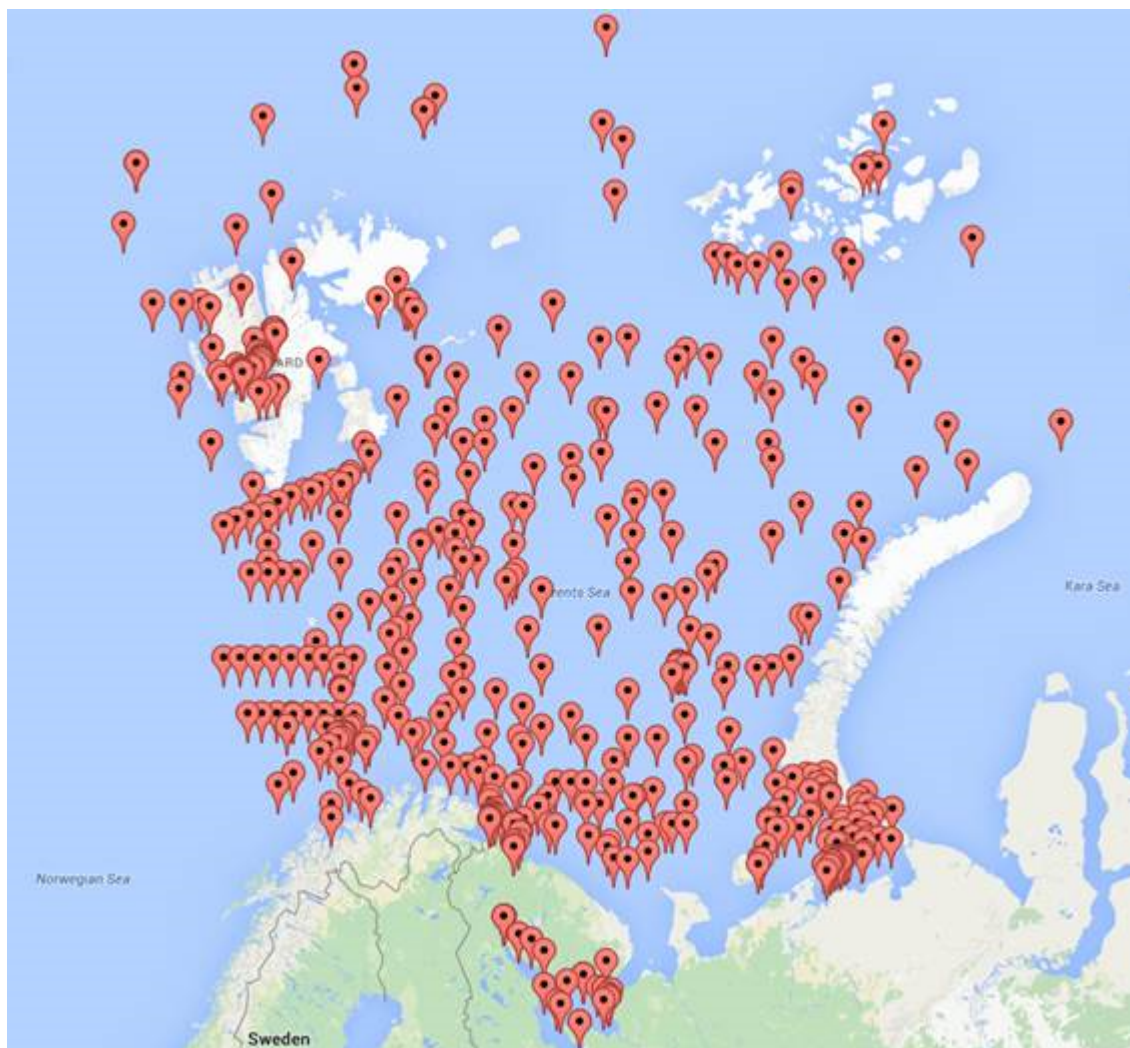


Figure 1. Sampling site locations

2.3. MCG IMR – 2000s (for samples collected in the period 2003-2004)

(from Boitsov et al., 2009b)

PAH analyses

The chemical analysis of PAH in sediments was carried out according to a method routinely used at IMR and accredited by the official Norwegian accreditation body, Norsk Akkreditering. Sediment samples were dried in open air at room temperature until complete dryness. The samples were then

ground in a mortar, and sample of known size was extracted by saponification in methanolic KOH followed by extraction by hexane, removal of sulphur by active copper, clean-up on silica Bond-Elute column and the hydrocarbon fraction then analysed by gas chromatography-mass spectrometry (GC-MS), with gas chromatograph HP-6890 coupled to Micromass Autospec Ultima mass spectrometer, in Selected Ion Recording (SIR) mode. GC-column was HP-5MS, fused silica, 30 m × 0.25 mm, 0.25 µm. The carrier gas was Helium, with a constant flow rate of 1.5 ml min⁻¹. Injection was done in splitless mode, injection volume 1 µl, injector temperature 280°C. Purge-off time was 1 min. Oven program was 60°C initial temperature held for 1 min, then increased to 100°C by 15°C min⁻¹, and then increased to 280°C by 6°C min⁻¹ and held at this temperature for 9 min. The mass spectrometer was used in electron impact (EI) mode and the spectrum was scanned for molecular masses of analytes: naphthalene, 2-methylnaphthalene, 1-methylnaphthalene, C2-naphthalenes, C3-naphthalenes, acenaphthene, fluorene, anthracene, phenanthrene, C1-phenanthrenes, C2-phenanthrenes, C3-phenanthrenes, dibenzothiophene, C1-dibenzothiophenes, C2-dibenzothiophenes, C3-dibenzothiophenes, fluoranthene, pyrene, benz[*a*]anthracene, chrysene, benzo[*b,j,k*]fluoranthenes, benzo[*e*]pyrene, benzo[*a*]pyrene, perylene, indeno[*1,2,3-cd*]pyrene, dibenz[*a,h*]anthracene and benzo[*g,h,i*]perylene and the deuterated internal standards, biphenyl-d₁₀, anthracene-d₁₀, pyrene-d₁₀ and perylene-d₁₂, used for quantification, as well as phenanthrene-d₁₀, used as recovery internal standard. The results were quantified with Opus Quan software package. Limits of quantification (LOQ) were 0.5 ng g⁻¹ dry weight for individual PAH. Analytical precision varies from compound to compound but is set to 30% for individual PAH compounds.

TOC and grain size determination

One set of sediment sub-samples was analysed for weight percentages (wt.%) of total organic carbon (TOC) using a LECO CS 244 analyser. For the TOC analyses, aliquots (200 mg) of the samples were treated with 10% (volume) hydrochloric acid (HCl) at 60°C to remove carbonate, and then washed with distilled water to remove HCl. The samples were dried overnight (50°C) and then analysed.

Grain size analyses of total sediment were obtained from laser diffraction techniques (Coulter LS 2000) and wet sieving. The Coulter LS 2000 measured the fractions from 0.4 µm to 2 mm while particles larger than 2 mm were determined by wet sieving. Prior to each analysis, the samples were freeze-dried.

2.4. NIVA

(from Loring et al., 1995)

PAH analyses

PAH concentration were determined by GC VSD equipped with a split/splitless injector and a 12 m × 0.2 mm i.d. HP-1 column after Soxhlet extraction of freeze-dried sediment (0.1-2 g) with cyclohexane. The extracts were purified as described by Grimmer and Böhnke (1975).

The relative analytical accuracies for PAH determinations were within 1 standard deviation (σ) for the reference material (SRM) 1941 from NIST, and within 2 σ for phenanthrene and benzo(b)fluoranthene.

TOC and TN analyses Total organic carbon and TN were determined on a dry weight basis with a CHN-element analyser after acid treatment (HCl) to remove inorganic carbon.

2.5. **LabOG VNIIO**

(from Boitsov *et al.*, 2011 with additions)

PAH analyses

Sample preparation: Individual samples of freeze-dried sediments (50-100 g) were extracted with chloroform using Soxhlet for 20 hours. The extract was cleaned from elemental sulfur using an activate-copper column and then the asphaltenic fraction was precipitated. The solution was filtered or centrifuged and the volume reduced at temperature less than 30°C and low pressure. The hydrocarbon extract was separated using the preparative chromatography (on Silica gel Column 3% deact.) into aliphatic (Fraction I, hexane elution) and aromatic (Fraction II, DCM:hexane 4:1 elution) fractions.

Hydrocarbon fraction II was analysed by GC-MS on a quadrupole Hewlett Packard 6850/5973 system. The analytical method described below has been certified in 2001 and 2005 by Russian State Standardization Service (Gosstandart), №POCC RU.0001.512785 of 18.07.2001.

Polycyclic aromatic hydrocarbons (PAH) were analysed on the following system: GC capillary column HP DB 30 m×0.25 mm×0.25 µm, stationary phase 5% phenyl-95% methylpolysiloxane. Carrier gas helium, flow rate 1.2 ml/min; injector temperature 290°C; oven temperature gradient from 60° C to 200° C at 20° C/min, to 300° at 10° C/min and 5 min at 300° C; full scan detection at 50e500 m/z, 70 eV. Parent PAH were analysed in selected ion monitoring mode (SIM) by ion masses m/z 128, 152, 154, 178, 192, 202, 206, 228, 252, 276 and 278. Alkylated PAH were analysed by selective ion masses m/z 142, 156, 192, 206, 220, 216, 234 and 242.

Calibration of the instrument was carried out using a standard mixture of PAHs Supelco 47930-U. The instrument linearity was monitored by calibration by 5 points in the concentration range from 40 to 2000 ng/ml. After running a batch of samples, calibration was monitored by analysis of a mid-level standard solution.

2.6. **CEC RPA Typhoon**

(for details see Alexeeva *et al.*, 2003).

PAH analyses

PAHs were extracted a sample with dichloromethane/acetone in an ultrasonic bath, and crude extracts were purified using activated copper (to remove sulfur) and then on silica gel and alumina (5% deactivated H₂O) columns. Identification and quantification of individual PAHs were performed using GC/MS. The determination ranges were from 0.5 to 5000 ng/g. For quality control, deuterated surrogate standards and recovery internal standards were added at different stages of analysis and recovery was assessed.

The analysis was performed using a GC/MS HP 5890/5972A. GC/MS Conditions: injector type-split/splitless; injector purge delay -1 min; solvent disposal time - 3 min; column type - DB-5M: 30m×0.25mm×0.25µm.

Detection limit determined statistically with the probability 99% using a batch of blank replicates was estimated to be 0.5-5.0 ng/g for different PAHs for soil and bottom sediments. This detection limit was verified in the analysis of the prepared control samples.

Quality Assurance/ Quality Control. The analysis was based on running batches of samples. The batch included 8 field samples, the certified reference material EC-5 of National Water Research Institute of Canada and a procedural blank. The surrogate standard was the mixture PP-HC8 Lot

¹119-14A Chem.Service US containing naphthalene-d₈, acenaphthene-d₁₀, phenanthrene-d₁₀, chrysene-d₁₀ and perylene-d₁₂. The recovery internal standard was 1-bromoadamantane.

TOC, TN and grain size determination

The moisture of sediment samples was determined before mechanical analysis. Coarser sediment fractions (2, 1, 0.5, 0.25 mm) were assessed by sieving, and the finer fractions were assayed by gravimetric sedimentation determination. All fractions were dried at 105°C. TOC was analyzed by spectrophotometric method after oxidation of organic carbon by KCrO₇ in accordance with GOST 26213-91 "Soil. Methods of Analysis of Organic Substance". TN analysis in sediment samples was carried out in accordance with Kjeldahl method.

2.7. Labeco-PINRO

(for details see Savinov *et al.*, 2006).

PAH analyses

A weighed part of dry bottom sediment was placed in an Erlenmeyer flask. Known amounts of the appropriate surrogate standards (a mixture of deuterated PAHs) are added at this stage. The sample extracted by two 100 ml portions of chloroform using an ultrasonic bath during 25 min. Chloroform extracts were combined and dried over anhydrous sodium sulphate. The extract was cleaned up with activated copper. Clean-up of the extract was carried out using column chromatography on silica gel. The sample was allowed just soak into the silica gel and then the aliphatic hydrocarbons (1 x 6 ml aliquots of the hexane) and PAH (1 x 2 ml aliquots of the hexane and 1 x 8 ml aliquots of the eluent [50% n-hexane in benzene]) were eluted. The cleaned PAH extracts were reduced to 500 µl volume prior to analysis by GC/MS and transferred to crimp-top auto sampler vials. Gas chromatographic analyses for PAHs were conducted on an Agilent 6890 GC Series N equipped with an Agilent 7683 auto sampler (Agilent Technologies, Inc. USA). In all analyses, 1.0 µl sample extract was injected in splitless mode with helium as the carrier gas (1.2 ml/min). An HP-5MS (30 m × 0.25 mm i.d. × 0.25 µm film thickness) capillary column (Agilent Technologies, Inc. USA) was used with the following temperature program: injection at 50 °C, held for 2 min, then ramped at 25 °C/min to 130 °C, held for 1 min, followed by 6 °C/min to 310 °C and held at 310 °C for 5 min. Detection was performed with a 5973 mass selective detector (Agilent Technologies, Inc. USA) in the selected ion mode (SIM). Detector zone temperatures were set at 310 °C for the MSD transfer line, 150 °C at the quadrupole, at 230 °C at the source. The instrument calibration was based on using the standard solution of PAHs Standard Reference Material (SRM) 2260 Certified Conc. of National Institute of Standards and Technology, USA. Data were collected with HP MS ChemStation Data Acquisition Software. The quality assurance was based on running batches of samples. The batch included the Standard Reference Material (SRM) 1941a of National Institute of Standards and Technology, USA and a procedural blank. The surrogate standard was the mixture containing biphenyl-d₁₀, anthracene-d₁₀, pyrene-d₁₀ and perylene-d₁₂.

TOC, TN and grain size determination

Contents of various grain-size fractions of the bottom sediment samples were determined gravimetrically after wet sieving. TOC and TN contents were determined with a CHN element analyser on a dry weight basis after acid (HCl) treatment to remove inorganic carbon.

2.8. GERG-TAMU

(for details see Wade *et al.*, 1993)

PAH analyses

Freeze-dried sediments were extracted in a Soxhlet apparatus. An aliquot of 10 g dry weight of the sediment sample was placed in an extraction thimble and attached to an extraction flask containing 150 mL of CH₂Cl₂. An internal standard (IS) consisting of naphthalene-d₈, acenaphthene-d₁₀, phenanthrene-d₁₀, chrysene-d₁₂, and perylene-d₁₂ was added to the sediment in the thimble. at a concentration of 40 ng/mL of the extract. The sample was extracted for 4-8 hrs. When necessary, the extract was filtered through glass wool and dried with Na₂SO₄.

Quality control samples were processed in a manner identical to actual samples. A minimum of one method blank was processed with every 20 samples. Blank levels were no more than 3 times the method detection limit (MDL). If blank levels for any component were above 3 times the MDL, samples analyzed in that sample set were re-extracted and reanalyzed. Sediment reference materials were analyzed with each sample set for aromatic hydrocarbons.

A 30-m long x 0.32-mm ID fused silica capillary column with DB-5 bonded phase was used. The autosampler was capable of making 1-4 µL injections. Instrument description and conditions for PAH analyses:

Injector Temp: 300°C;
Transfer Line Temp: 280°C;
Initial Oven Temp: 40°C;
Initial Hold Time: 0 min.
Ramp Rate: 10°C/min
Final Temperature: 300°C
Final Ran Time: 4 min.

3 Structure of the Database

The PAH database for sediments from the Barents and White Sea is a document in Excel format ("PAH Metadatabase Barents&White.xlsx") which includes four worksheets: *PAH data*; *Header row and Acronyms*; *Contact persons*; *References*

3.1. PAH data

This worksheet is a matrix of size 42 × 590, which includes information about the sampling site locations and data for a specific PAH concentration in sediments from this site and also some additional information.

3.2. Header row and Acronyms

The header row of the matrix and the necessary explanations are presented in *Table 3*. Acronyms of the Institutes are presented in *Table 4*. Acronyms of the analytical laboratories and reference to the description of the methods are presented in *Table 5*.

Table 3. Header row of matrix of PAH data in sediments from the Barents and White Seas (transposed).

<i>Name of the column</i>	<i>Explanation</i>
Reference	Reference to the source of the first data publication
Area	Area of studies (Barents Sea or White Sea)
Location	Sub-area of sampling station location
Institute	Acronym of the Institute, where you can get more information through the contact person

<i>Name of the column</i>	<i>Explanation</i>
Analytical lab	Acronym of the analytical lab where analyses were performed
Station	Original station number
Sampler	Type of the sediment sampler
Layer, cm	Sediment slice collected for analyses
Year	Year of sediment sampling
Latitude, N	Latitude of the sampling site location (North, decimal)
Longitude, E	Longitude of the sampling station location (East, decimal)
Depth, m	Depth in the station location (m)
TOC, mg/g dw	Total organic carbon, mg/g dry weight
TN, mg/g dw	Total nitrogen
Pelites, %<63µm	Percentage of sediment particles less than 63µm
NAP, ng/g dw	Naphthalene, ng/g dry weight
PHE, ng/g dw	Phenanthrene
ANT, ng/g dw	Anthracene
ACL, ng/g dw	Acenaphthylene
ACN, ng/g dw	Acenaphthene
FLN, ng/g dw	Fluorene
FLT, ng/g dw	Fluoranthene
PYR, ng/g dw	Pyrene
BAA, ng/g dw	Benzo(a)anthracene
CHR, ng/g dw	Chrysene
BBKF, ng/g dw	Benzo(b,k)fluoranthene = Benzo(b)fluoranthene + Benzo(k)fluoranthene
BAP, ng/g dw	Benzo(a)pyrene
BP, ng/g dw	Benzo(ghi)perylene
IND, ng/g dw	Indeno(1,2,3-cd)pyrene
DBA, ng/g dw	Dibenzo(a,h)anthracene
C1N, ng/g dw	C1-naphthalenes
C2N, ng/g dw	C2-naphthalenes
C3N, ng/g dw	C3-naphthalenes
C1P, ng/g dw	C1-phenantrenes/anthracenes
C2P, ng/g dw'	C2-phenantrenes/anthracenes
C3P, ng/g dw	C3-phenantrenes/anthracenes
DBT, ng/g dw	Dibenzothiophene
C1D, ng/g dw	C1-dibenzothiophenes
C2D, ng/g dw	C2-dibenzothiophenes
C3D, ng/g dw	C3-dibenzothiophenes
BEP, ng/g dw	Benzo(e)pyrene
PER, ng/g dw	Perylene

Table 4. Name and acronyms of the Institutes

<i>Acronym</i>	<i>Name</i>	<i>Website</i>
APN	Akvaplan-niva AS, Tromsø, Norway	http://www.akvaplan.niva.no/en/
IMR	Institute of Marine Research, Bergen, Norway	http://www.imr.no/en
VNIIO	All-Russian Scientific Research Institute for Geology & Mineral Resources of the Ocean "VNIIOkeangeologia" named after I.S.Gramberg	http://en.vniio.ru/

Table 5. Names and acronyms of the analytical laboratories and reference to the description of the method

<i>Acronym</i>	<i>Name</i>	<i>Reference to the description of the method</i>
Unilab	Unilab Analyse AS, Tromsø, Norway	Savinov et al., 2000; Cochrane et al., 2009
MCG IMR 90s	Marine Chemistry Group of IMR	Stange,Klungsoyr, 1997

<i>Acronym</i>	<i>Name</i>	<i>Reference to the description of the method</i>
	(Methods 90s)	
MCG IMR 2000s	Marine Chemistry Group of IMR (Methods 2000s)	Boitsov et al., 2009b
Labeco-PINRO	Laboratory of Applied Ecology and Toxicology of Knipovich Polar Research Institute of Marine Fisheries and Oceanography, Murmansk, Russia	Savinov et al., 2006
LabOG VNIIO	Laboratory of organic geochemistry of VNIIO	Boitsov et al., 2011
TAMU-GERG	Geochemical and Environmental Research Group Texas A&M University, USA	Wade et al., 1993
CEC RPA Typhoon	Centre of Environmental Chemistry of Research and Production Association "Typhoon", Obninsk, Russia	Alexeeva et al., 2003
NIVA	Norwegian Institute of Water Research, Oslo, Norway	Loring et al., 1995

3.3. Contact persons

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3.4. References

This worksheet contains list of references to the sources of the first data publication and references to the description of the method (*Table 6*).

Table 6. References to the sources of the first data publication and to the description of the methods

<i>References</i>	<i>Sources</i>
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Carrol, M., et al. (unpublished.)	Carroll, M., et al. Carbon flux and ecosystem feedback in the northern Barents Sea in an era of climate change (CABANERA). APN2603.
Christensen, 2007	Christensen, G. 2007. Feltrapport – innsamling av innsjø- og marine sedimenter i Nord-Norge og Svalbard 2005-2006. APN51.3432
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Evenset et al., 2006	Evenset, A., Christensen, G.N., Palerud, R. 2006. Miljøgifter i marine sedimenter, Isfjorden, Svalbard 2005. APN414.3341.
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5 Appendix

CD-disk attached to this report. This disc contains:

- Electronic version of the report.
- Excel file "PAH Metadatabase Barents&WhiteSeas.xlsx".
- Refereed sources (as pdf files) which describe the analytical methods (*Table 5*).