

Supplementary data

Characterization of the organic contamination pattern of a hyper-saline ecosystem by rapid screening using gas chromatography coupled to high-resolution time-of-flight mass spectrometry

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Material and Methods

Reagents

Reference standards of pesticides, octyl/nonyl phenols, PCBs (Mix 3, 100 µg/mL in cyclohexane; Mix 41, 10 µg/mL in cyclohexane) and PAHs (Mix 9, 100 µg/mL) were purchased from Dr. Ehrenstorfer (Augsburg, Germany). PBDE standard mixture “Lake Michigan Study”, containing BDE 28, 47, 66, 85, 99, 100, 138, 153 and 154 (50 µg/mL in isooctane) and two individual standards of BDE 71 and 183 (50 µg/mL in isooctane) were purchased from Chiron (Trondheim, Norway). When the solid reference standard was available, stock solutions (around 500 µg/mL) were prepared by dissolving the reference standard in acetone and stored in a freezer at –20°C. Working solutions were prepared by diluting stock solutions in acetone for sample fortification or in hexane for injection in the chromatographic system.

Acetone (residue analysis), ethyl acetate, dichloromethane and hexane (ultra-trace quality) were purchased from Scharlab (Barcelona, Spain). HPLC-grade water was obtained by purifying demineralized water in a Milli-Q Gradient A10 (Millipore, Bedford, MA, USA). 500 mg Bond Elut cartridges C₁₈ (Varian, Harbor City, CA, USA) were used for solid-phase extraction.

Table I. List of target compounds

Compound	Compound	Compound	Compound
4-n-nonylphenol	Diflufenican	<i>p,p'</i> -DDT	Trifluraline
4-n-Octylphenol	Dimethoate	Parathion ethyl	α -endosulfan
4-t-Octylphenol	Diphenylamine	Parathion methyl	β -endosulfan
Acenaphthene	Endosulfan ether	PCB 101	λ -cyhalothrin
Acenaphthylene	Endosulfan sulfate	PCB 105	
Alachlor	Ethion	PCB 114	
Aldrin	Etrimfos	PCB 118	
Anthracene	Fenarimol	PCB 123	
Atrazine	Fenchlorfos	PCB 126	
Atrazine desethyl	Fenitrothion	PCB 138	
Atrazine desisopropyl	Fenoxycarb	PCB 153	
BDE 100	Fenthion	PCB 156	
BDE 138	Fenvalerate I	PCB 157	
BDE 153	Fenvalerate II	PCB 167	
BDE 154	Fluoranthene	PCB 169	
BDE 183	Fluorene	PCB 180	
BDE 28	Fonofos	PCB 189	
BDE 47	Forate	PCB 28	
BDE 66	Fosalone	PCB 52	
BDE 71	Fosfamidon	PCB 77	
BDE 85	Heptachlor	PCB 81	
BDE 99	Heptachlor epoxide A	Penconazole	
Benzo(a)anthracene	Heptachlor epoxide B	Pentachlorobenzene	
Benzo(a)pyrene	Heptenofos	Permethrin I	
Benzo(b)fluoranthene	Hexachlorobenzene	Permethrin II	
Benzo(g,h,l)perylene	Hexythiazox	Phenanthrene	
Benzo(k)fluoranthene	Imazalil	Phosmet	
Bifentrin	Indeno(1,2,3,cd)pyrene	Pirimicarb	
Bupimirate	Iprodione	Pirimiphos ethyl	
Buprofezin	Isodrin	Pirimiphos methyl	
Carbaryl	Isofenfos	Procymidone	
Chlorfenvinphos	Lindane	Profenofos	
Chlorpropham	Malathion	Propyzamide	
Chlorpyrifos	Metalaxyl	Pyrazofos	
Chlorpyrifos methyl	Methacrifos	Pyrene	
Chlozolate	Methamidophos	Quinalfos	
Chrysene	Methidathion	Simazine	
Coumaphos	Methiocarb	Tau-fluvalinate I	
Cypermethrin I	Methiocarb sulfone	Tau-fluvalinate II	
Cypermethrin II	Metolachlor	Tebuconazole	
Cypermethrin III	Metoxychlor	Tecnazene	
Cypermethrin IV	Mevinfos	Terbacil	
Cyprodinil	Mirex	Terbumeton	
Deltamethrin	Molinate	Terbumeton desethyl	
Diazinon	Naphthalene	Terbutylazine	
Dibenzo(a,h)anthracene	Omethoate	Terbutylazine desethyl	
Dichlofluanide	Oxadixyl	Terbutryn	
Diclorvos	<i>p,p'</i> -DDD	Tetradifon	
Dieldrin	<i>p,p'</i> -DDE	Thiabendazole	