

1 **SUPPORTING INFORMATION**

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3 **Non-targeted screening of halogenated organic compounds in bottlenose**
4 **dolphins (*Tursiops truncatus*) from Rio de Janeiro, Brazil.**

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23 **Supporting Information Summary**

24 Glossary of acronyms and four supplemental figures are included in SI. A separate supporting
25 information, a mass spectral library report for the 158 halogenated organic compounds is
26 provided in PDF format. These materials are available free of charge via the Internet at
27 <http://pubs.acs.org/>.

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29 **Glossary of Acronyms**

- 30 B/CDE: brominated chlorinated diphenyl ether
- 31 BDE: brominated diphenyl ether
- 32 BDE-77: 3,3',4,4'-tetrabromodiphenyl ether
- 33 BDE-166: 2,3,4,4',5,6-hexabromodiphenyl ether -
- 34 octa-BDE: octabrominated diphenyl ether
- 35 penta-BDE: pentabrominated diphenyl ether
- 36 Bromophenol-M: bromophenol mixed source
- 37 Bromophenol-U: bromophenol unknown source
- 38 Chlorophenol-M: chlorophenol mixed source
- 39 Chlorophenol-U: chlorophenol unknown source
- 40 *o,p'*-DDD: *o,p'*-dichlorodiphenyldichloroethane
- 41 *p,p'*-DDD: *p,p'*-dichlorodiphenyldichloroethane
- 42 *p-p'*-DDE: *p-p'*-dichlorobis(chlorophenyl)ethene
- 43 DDT: dichlorodiphenyltrichloroethane
- 44 Dec 602: dechlorane 602
- 45 Dec 603: dechlorane 603
- 46 di-MeO-PBB-80: 2,2'-dimethoxy-3,3',5,5'-tetrabromobiphenyl
- 47 di-MeOBB-Br3Cl: dimethoxy tribromo chloro biphenyl
- 48 2MeO-Biphenyl-N: dimethoxy biphenyl natural source
- 49 2MeO-Biphenyl-U: dimethoxy biphenyl unknown source
- 50 1D: first-dimension column
- 51 2D: second dimension column
- 52 DMBP: 1,1'-dimethyl-2,2'-bipyrrroles
- 53 EI: electron ionization

- 54 eV: electron volts
- 55 4-FBDE-69: 4-fluoro-2,3',4,6-tetrabromodiphenyl ether
- 56 6-FBDE-47: 6-fluoro-2,2',4,4'-tetrabromodiphenyl ether
- 57 GC×GC: comprehensive two-dimensional gas chromatography
- 58 GPC: gel permeation chromatography
- 59 HCB: hexachlorobenzene
- 60 α -HCH: α -hexachlorocyclohexane
- 61 β -HCH: β - hexachlorocyclohexane
- 62 γ -HCH: γ - hexachlorocyclohexane
- 63 HOC: halogenated organic compound
- 64 MBP: 1'-methyl-1,2'-bipyrrole
- 65 MeO-B/CDE: methoxy brominated chlorinated diphenyl ether
- 66 MeO-BDE: methoxy brominated diphenyl ether
- 67 MeO-CDE: methoxy chlorinated diphenyl ether
- 68 MS: mass spectra
- 69 MeSO₂-PCB: methyl sulfonyl polychlorinated biphenyl
- 70 m/z: mass-to-charge ratio
- 71 Na₂SO₄: sodium sulfate
- 72 NE Pacific: North Eastern Pacific Ocean
- 73 NIST: National Institute of Standards and Technology
- 74 NTA: non-targeted analysis
- 75 NW Atlantic: North Western Atlantic Ocean
- 76 OH-PCB: hydroxy polychlorinated biphenyl
- 77 PBB: polybrominated biphenyl
- 78 PBDE: polybrominated diphenyl ether

79 PBHD: polybrominated hexahydroxanthene derivative
80 PCA: principal component analysis
81 PCB: polychlorinated biphenyl
82 PCDE: polychlorinated diphenyl ether
83 PCS: polychlorinated styrene
84 PCT: polychlorinated terphenyl
85 PDF: portable document format
86 PFAS: perfluoroalkyl substances
87 POP: persistent organic pollutant
88 RT: retention time
89 SI: supporting information
90 S/N: signal-to-noise ratio
91 SpecLibDolphin2014: Southern California Dolphin Blubber Contaminant Library
92 SpecLibDolphin2011: Massachusetts Dolphin Blubber Contaminant Library
93 SpecLibBrazilDolphin2016: Rio de Janeiro Dolphin Blubber Contaminant Library
94 SW Atlantic: South Western Atlantic Ocean
95 TCPM: tris(chlorophenyl)methane
96 TCPMOH: tris(chlorophenyl)methanol
97 TOF-MS: time-of-flight mass spectrometry
98 T. truncatus: *Tursiops truncatus*
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105 **Figure S1.** Map of Brazil and the sampling areas in the Rio de Janeiro coastal area (dolphin silhouettes
106 with arrows), South Western Atlantic Ocean. Map data: Imagery©2015TerraMetrics, Map data ©2015
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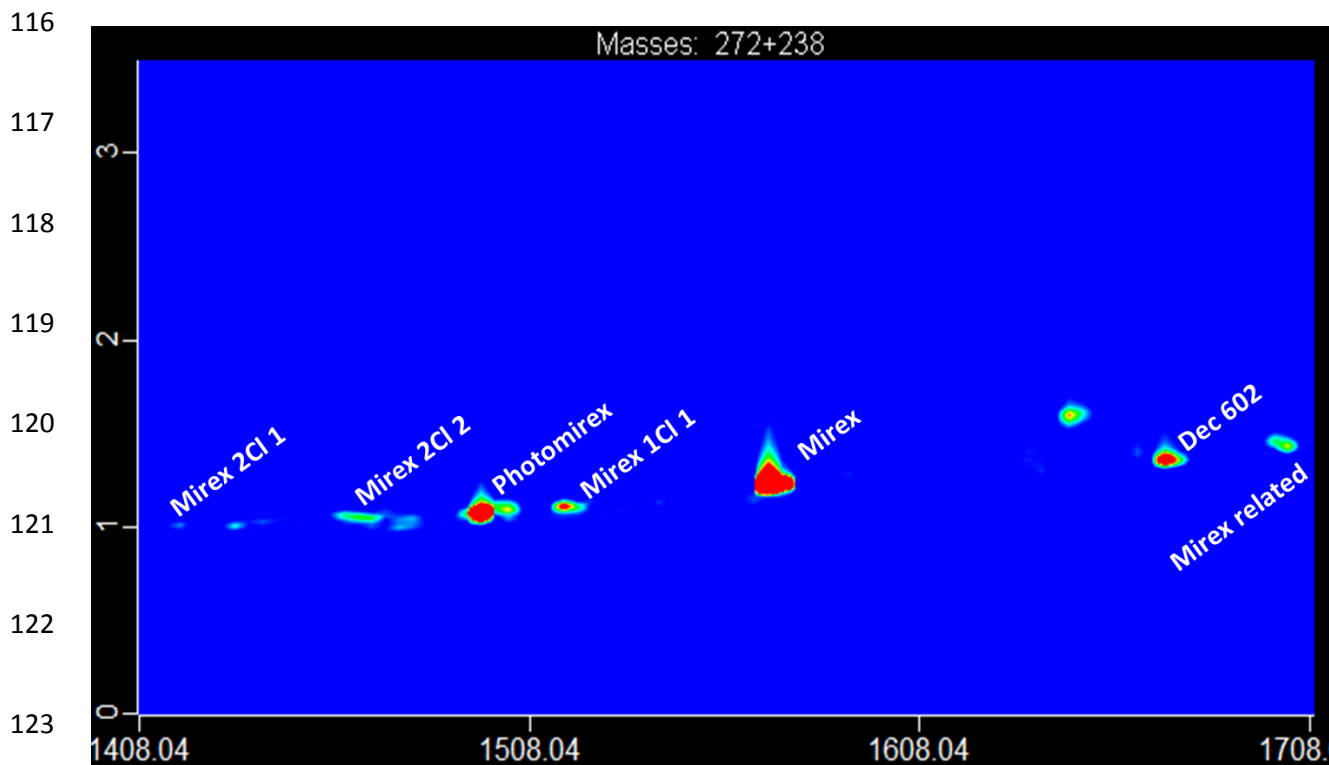
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124 **Figure S2.** GC×GC/TOF-MS contour map of m/z 272 and 238 from mirex/dechlorane related compounds
 125 detected in adult male bottlenose dolphins (*T. truncatus*) from Rio de Janeiro, Brazil. The x-axis is the 1st
 126 GC retention time (s) and the y-axis the 2nd GC retention time (s). Software: *ChromaTOF*.

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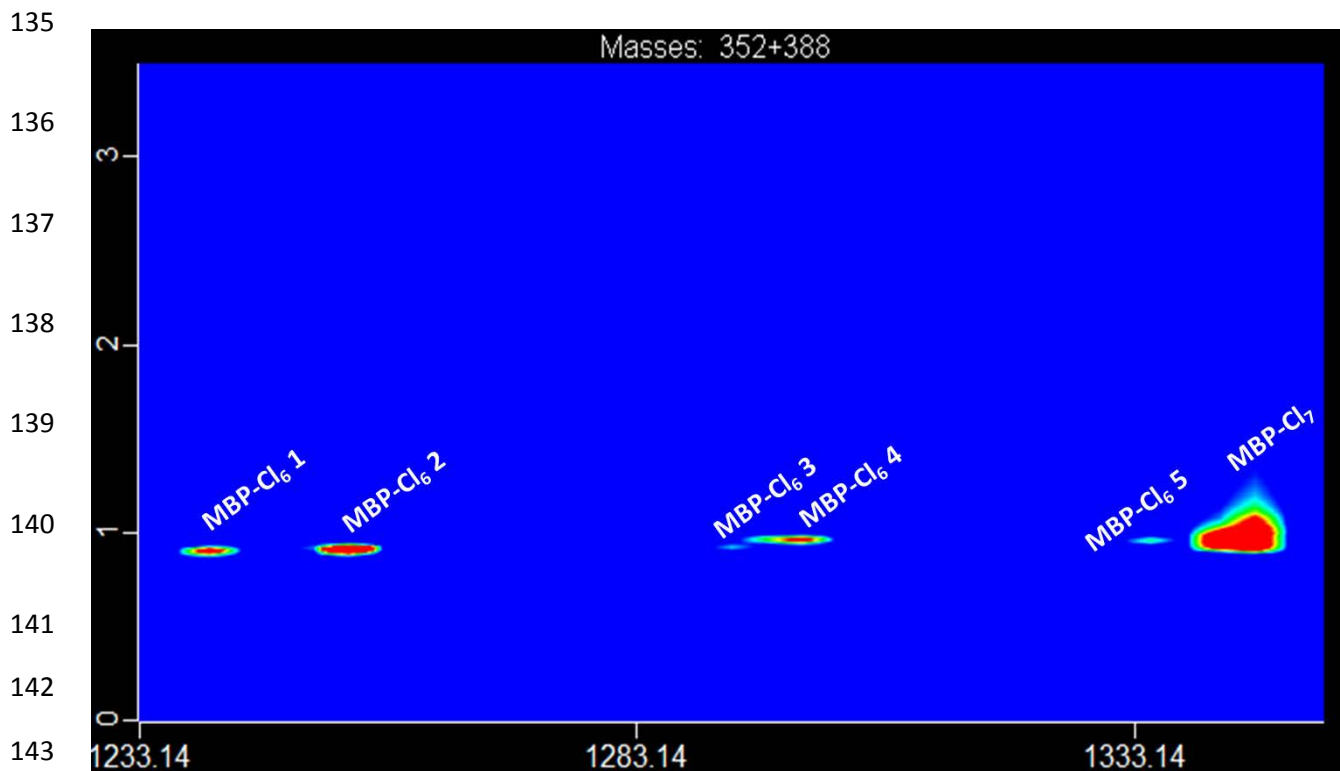
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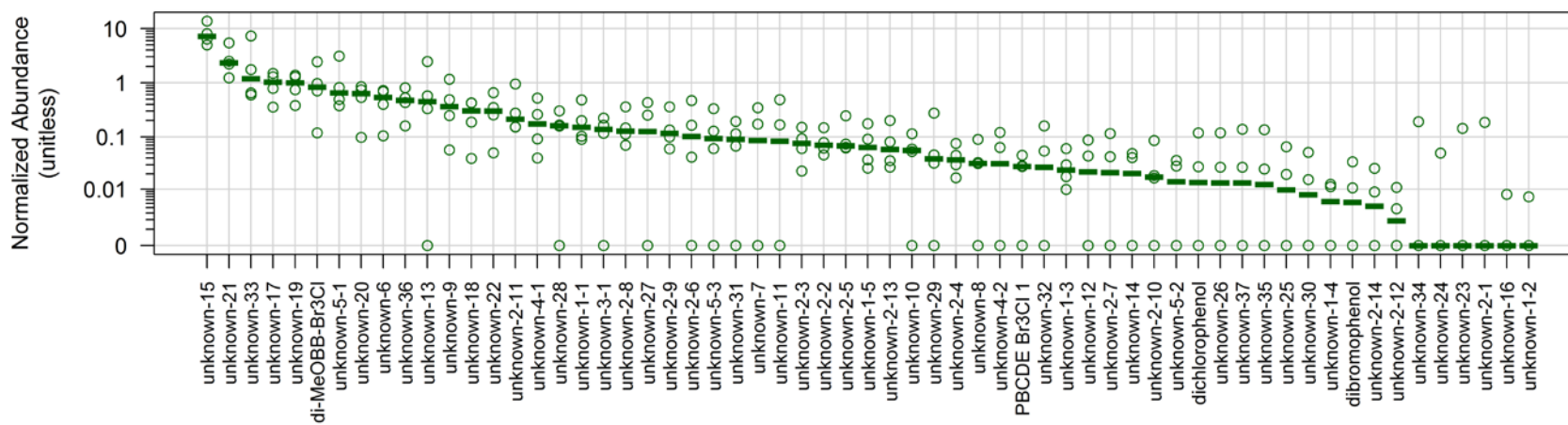


145 **Figure S3.** GC×GC/TOF-MS contour map of m/z 352 and 388 from chlorinated methyl bipyroles
 146 (MBPs) detected in adult male bottlenose dolphins (*T. truncatus*) from Rio de Janeiro, Brazil. The x-axis
 147 is the 1st GC retention time (s) and the y-axis is the 2nd GC retention time (s). Software: ChromaTOF.

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153 **Figure S4.** Relative abundance of HOCs at unknown origin detected in the blubber of adult male bottlenose dolphins (*T. truncatus*)
 154 from the Rio de Janeiro coast, Brazil. The acronyms are listed in the SI.