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APPLICATION NOTE 10644

Overcoming analytical challenges for polybrominated diphenyl ethers (PBDEs) analysis in environmental samples using gas chromatography – Orbitrap mass spectrometry

Authors

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Keywords

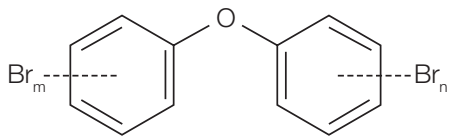
Polybrominated diphenyl ethers, PBDE, high-resolution GC-MS, accurate mass, quantification, GC Orbitrap, environmental, sediment, filter dust, sludge, air

Goal

To demonstrate the quantitative performance of the Thermo Scientific™ Exactive™ GC Orbitrap™ GC-MS mass spectrometer for the analysis of polybrominated diphenyl ethers (PBDEs) in environmental samples.

Introduction

Polybrominated diphenyl ethers (Figure 1) are a group of organobromine chemicals that inhibit or suppress combustion in organic material. They have been widely used since the 1970s as flame retardants in a broad range of commercial and household products including textiles, building materials, electronics, furnishings, motor vehicles, and plastics.[1]



where m + n = 1 to 10

Figure 1. Structure of polybrominated diphenyl ethers (PBDEs)

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Most PBDEs resist degradation, persist and bioaccumulate in both the environment and food chains, and can be transported through air and water over long distances. They have been identified, in some cases far from their place of use, in a wide range of samples including air, water, sediment, fish, birds, marine mammals, and humans.[2] Many PBDEs are toxic, with links to cancer and endocrine disruption.[3] As a consequence, the use of certain PBDEs (including penta-, tetra-, and deca-BDE) have been prohibited in many countries and are currently listed in the Stockholm Convention inventory of persistent organic pollutants.[4]

Due to their chemico-physical properties, gas chromatography (GC) is the standard analytical technique used to analyze PBDEs, with detection using either an electron capture detector (ECD), or a mass spectrometer (MS). However, there are many analytical challenges to consider when using gas chromatography-mass spectrometry (GC-MS) for the analysis of PBDEs. The active nature of high molecular mass PBDEs (e.g. BDE-209), the large number of compounds, and the potential chromatographic interferences from matrix (e.g. chromatographic separation of BDE-49 and BDE-71 can be challenging in complex environmental samples).

This work demonstrates the applicability of high-resolution, accurate-mass GC-Orbitrap technology for the targeted analysis of 27 PBDE congeners in environmental samples with variable complexity using a sensitive, fast, robust method. This approach takes into account the selectivity, sensitivity, linearity, reproducibility of the results, method robustness, and analysis time.

Experimental conditions

Sample preparation

The following environmental samples were provided by the Dioxins Laboratory, IDAEA-CSIC, Barcelona, Spain: three sediment samples (including two samples previously used in an inter-laboratory study, and one sample previously used in a QA/QC study), three sludge samples (from a waste water treatment plant), three filter dust samples (previously used in a QA/QC study), and one air sample (previously used in an inter-laboratory study).

Samples (2 g), were Soxhlet extracted with toluene for 24 hours, followed by a basic alumina purification stage (6 g), activated overnight at 300 °C, and elution with 50 mL n-hexane/DCM (80:20). The extracts were then blown to dryness and reconstituted with 20 µL nonane prior to GC-MS analysis. A mass-labelled (^{13}C) PBDE surrogate standard was added prior to extraction and a mass-labelled (^{13}C) PBDE recovery standard was added prior to injection, as illustrated in the PBDE analytical workflow (Figure 2).

Instrument and method setup

An Exactive GC Orbitrap GC-MS mass spectrometer coupled with a Thermo Scientific™ TRACE™ 1310 Gas Chromatograph was used in all experiments.

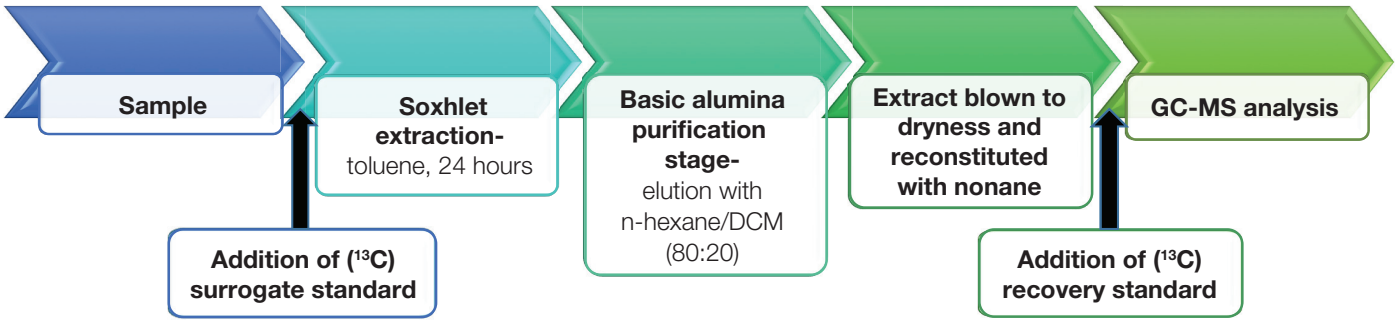


Figure 2. PBDE analytical workflow, including sample extraction, extract purification, and concentration stages required prior to GC-MS analysis

Liquid sample injections were performed with a Thermo Scientific™ TriPlus™ RSH™ autosampler, using the Thermo Scientific™ Instant Connect Programmed Temperature Vaporizing (PTV) injector for the TRACE 1300 GC system. Compound separation was achieved on a Thermo Scientific™ TraceGOLD™ TG-PBDE 15 m × 0.25 mm I.D. × 0.10 µm film capillary column (P/N 26061-0350). The mass spectrometer was tuned and calibrated in <1.5 min using FC43 (CAS 311-89-7) to achieve mass accuracy of <0.5 ppm. The system was operated in electron ionization mode (EI) using full-scan, and 60,000 mass resolution (full width at half maxima, measured at *m/z* 200). Additional details of instrument parameters are shown in Table 1 and Table 2.

Table 1. GC and injector conditions

TRACE 1310 GC system parameters

Injection volume:	1.0 µL
Liner:	PTV baffled liner (Siltek™) (P/N: 453T2120)
Inlet:	40 °C
Carrier gas, (mL/min):	He, 1.5 mL/min
Inlet module and mode:	PTV, Large Volume mode
Column:	TraceGOLD TG-PBDE 15 m × 0.25 mm I.D. × 0.10 µm film capillary column (P/N 26061-0350)
Transfer delay:	0.2 min
Injection time:	0.1 min

PTV Parameters:	Rate (°C/s)	Temperature (°C)	Time (min)	Flow (mL/min)
Injection	—	40	0.10	—
Transfer	2.5	330	5.00	—
Cleaning	14.5	330	5.00	50

Oven Temperature Program:	RT (min)	Rate (°C/min)	Target Temperature (°C)	Hold Time (min)
Initial	0	—	100	2.00
Final	2.00	30	340	3.00
Run time	13.00	—	—	—

Table 2. Mass spectrometer conditions

Exactive GC mass spectrometer parameters

Transfer line temperature:	300 °C
Ionization type:	EI
Ion source:	250 °C
Electron energy:	35 eV
Acquisition modes:	Targeted SIM/full-scan
Mass range:	68–1000 Da
Isolation window:	25 Da
Mass resolution:	60,000 FWHM at *m/z* 200

Calibration standards (BDE-CSV-G), containing 27 native PBDE congeners at five concentration levels (Appendix A), and 16 (^{13}C labelled) PBDE internal standards (Appendix B), were acquired from Wellington Laboratories, Inc. (Ontario, Canada).

Targeted screening experiments were developed for the PBDE congeners considered. The targeted-SIM inclusion list, start and end times, and PBDEs included within each entry are given in Appendix C.

Data processing

Data were acquired and processed using Thermo Scientific™ Chromeleon™ Chromatography Data System (CDS), version 7.2. Chromeleon CDS allows the analyst to build acquisition, processing, and reporting methods for high-throughput analysis, with easy data reviewing and data reporting.

Results and discussion

The objective of this study was to evaluate the utility of Orbitrap-based GC-MS technology for the quantification of PBDEs to increase sample throughput and laboratory productivity. Various analytical parameters, including chromatographic resolution, instrument sensitivity, and linearity, were assessed and the results of these experiments are described below.

Chromatography

Good chromatographic separation, in <11 minutes, was obtained using the GC conditions described in Table 1. Extracted ion chromatograms (EICs) for 27 native PBDE congeners in a mixed solvent standard are shown in Figure 3a, with the excellent chromatographic resolution of the critical pair (BDE-49 and BDE-71) highlighted (Figure 3b).

Quantification

The quantitative performance of the Exactive GC Orbitrap GC-MS system was tested for all 27 PBDEs. System sensitivity, linearity, and peak area repeatability were evaluated. Additionally, mass accuracy of the target compounds was assessed across the concentration ranges. Linearity was assessed using five calibration levels (1 to 400 pg on column for mono- to penta-BDEs, 2 to 800 pg on column for hexa- to octa-BDEs, and 5 to 2000 pg on column for nona- to deca-BDEs).

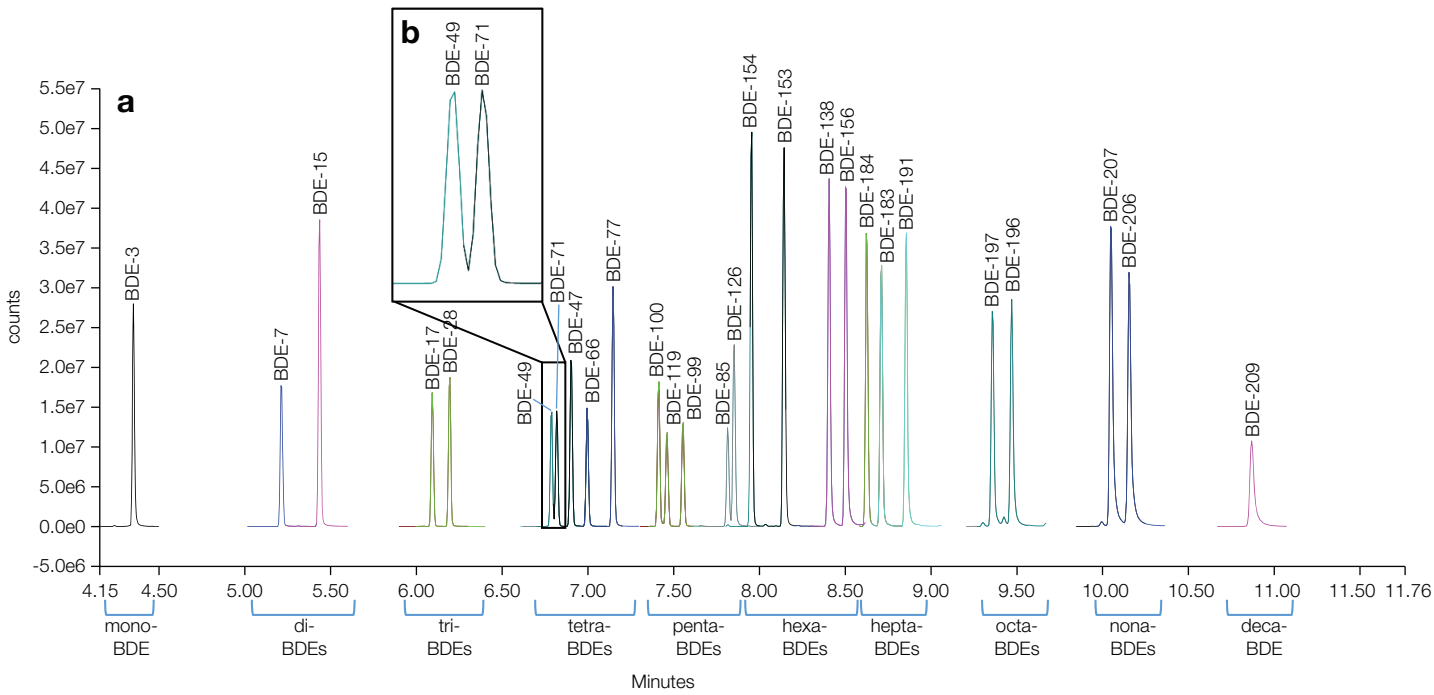


Figure 3. (a) Overlaid extracted ion chromatograms (EICs ±5 ppm extraction window) for the 27 native PBDE congeners in a solvent standard at 400 pg on column for mono- to penta-BDEs, 800 pg on column for hexa- to octa-BDEs, and 2000 pg on column for nona- to deca-BDEs and (b) separation of critical pair (BDE-49 and BDE-71)

Data was acquired using targeted-SIM, with compound detection, and identification based on retention time (±0.1 min window), accurate mass (±5 ppm window), and ion ratio of quantification vs. confirming ion (±15% window). Details of the calibration range, retention times, quantification and confirming ions, and ion ratio average values and acceptable ranges are shown in Appendix D.

Sensitivity

All PBDEs were detected in the lowest calibration standard, 1.0 ng/mL for mono- to penta-BDEs, 2.0 ng/mL for hexa- to octa-BDEs, and 5 ng/mL for nona- to deca-BDEs.

Estimation of instrument detection limit (IDL)

System sensitivity, defined as instrument detection limit (IDL) were determined experimentally for each compound by performing n=14 replicate injections of the lowest serially diluted solvent standard (with PBDE concentrations ranging from 50 to 100 fg on column). Calculations of IDLs were made using a one-tailed student *t*-test at the 99% confidence interval for the corresponding degrees of freedom and taking into account the concentration on column for each PBDE congener and absolute peak area %RSD (Figure 4).

Mass accuracy

Maintaining mass accuracy and spectral fidelity is critical for correct compound identification in complex environmental samples. Figure 5 illustrates the mass accuracy and the isotopic pattern match achieved for BDE-209 with mass accuracy of <2 ppm consistently achieved for each ion in the isotopic cluster.

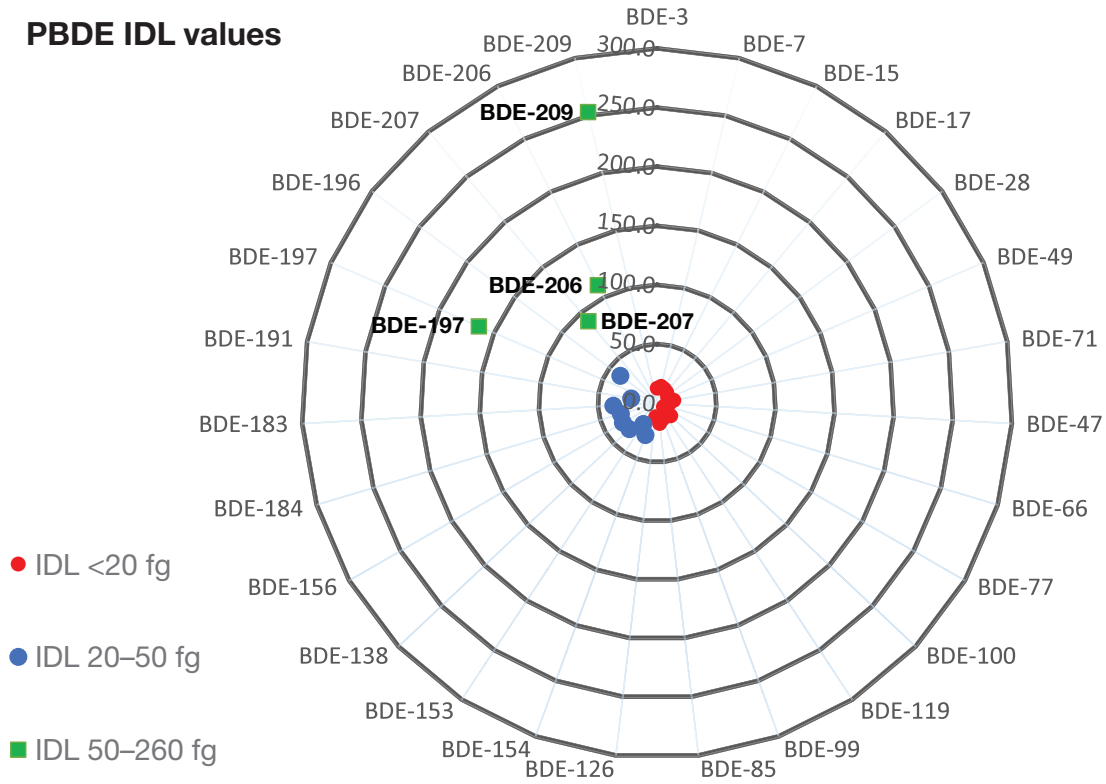


Figure 4. Calculated IDL values for 27 native PBDE congeners, statistically calculated from the results of n=14 replicate injections of the lowest serial diluted solvent standard

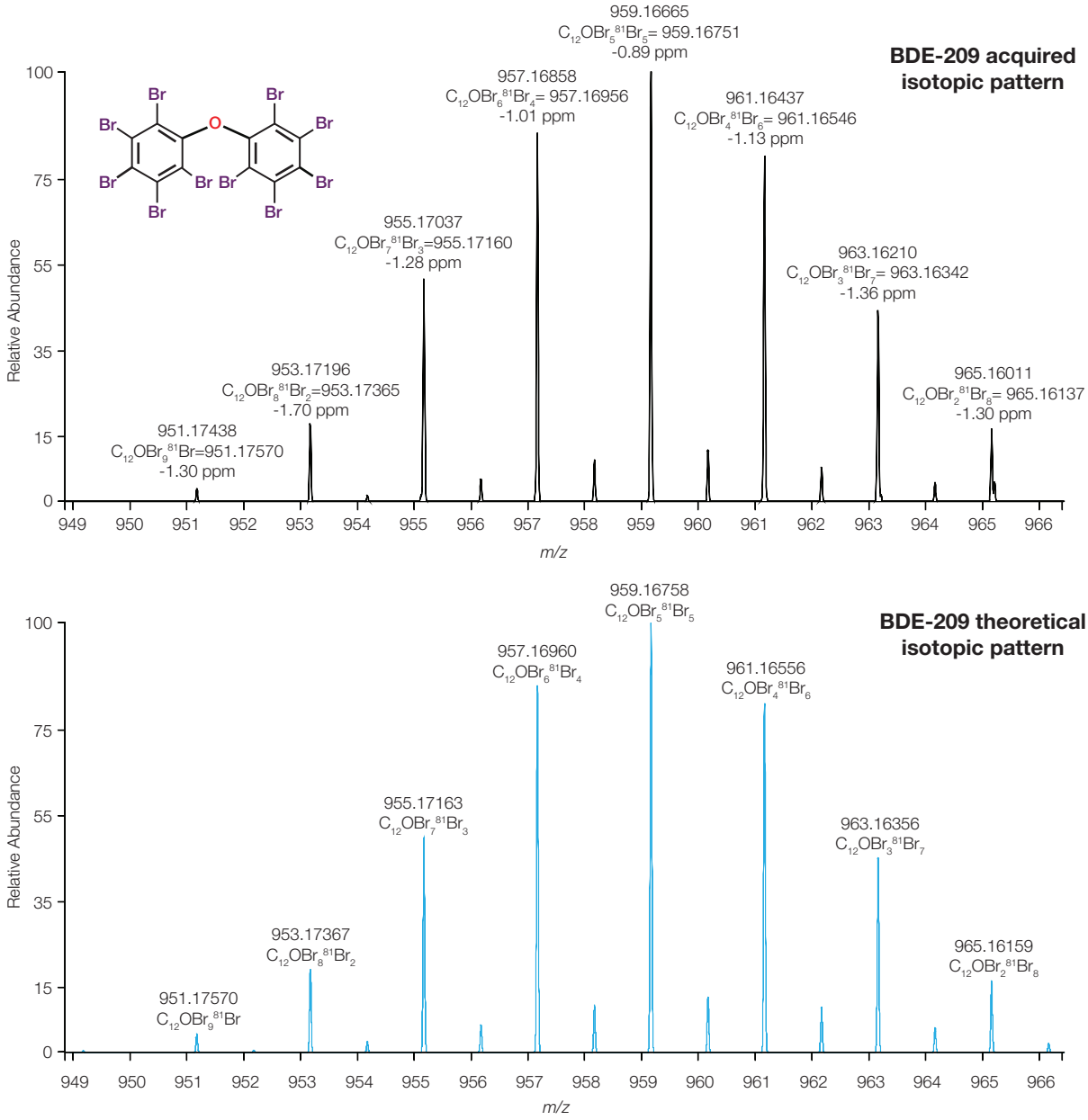
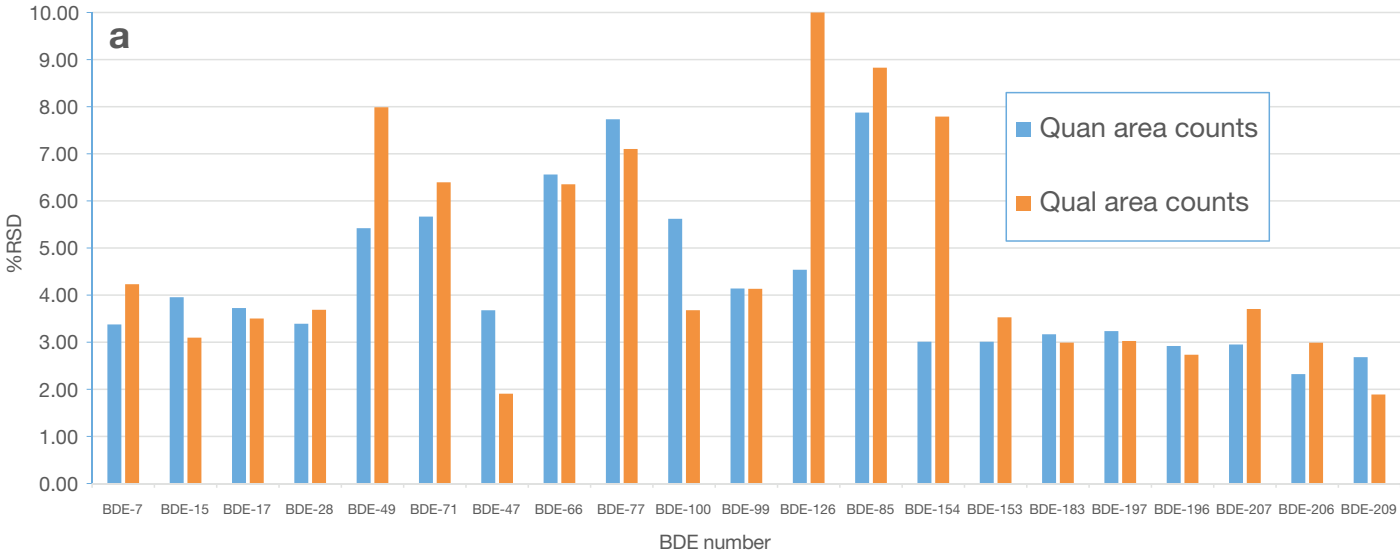


Figure 5. Comparison of mass spectra for BDE-209, acquired isotopic pattern (upper) versus the theoretical isotopic pattern (lower). Consistent <2 ppm mass accuracy obtained for each of the ion in the cluster. Annotated are the measured mass, the elemental composition, and the theoretical mass as well as the mass accuracy (ppm).

Peak area repeatability in matrix

In order to have confidence in routine PBDE quantitation results achieved, stability of responses in matrix is critical. Repeatability of PBDE responses in matrix were accessed by carrying out n=12 repeat injections of a filter dust sample extract. Excellent repeatability was obtained as shown in Figure 6a, with %RSD for quantification and qualifier peak area counts between 2% and 10% for all identified congeners, and Figure 6b, overlaid EICs (*m/z* 799.33995) for BDE-209.



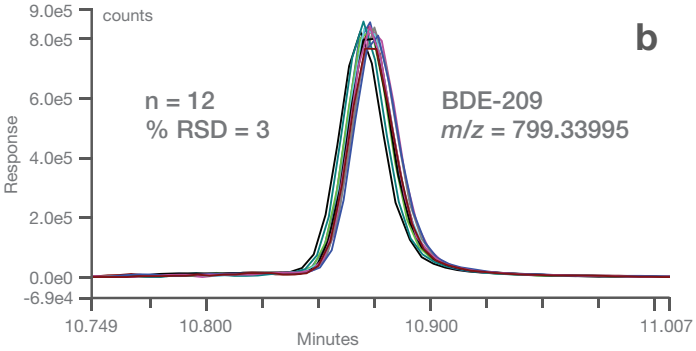


Figure 6. Replicate injections (n=12) of a filter dust sample, a) quantification and qualification area counts %RSD values for identified congeners, b) overlaid EICs (*m/z* 799.33995) for BDE-209

Linearity of response

To assess compound linearity, five calibration levels (pg on column 1 to 400 for mono- to penta-BDEs, 2 to 800 for hexa- to octa-BDEs, and 5 to 2000 for nona- to deca-BDEs) were quantified using isotopic dilution for all the congeners considered. For all PBDEs excellent linearity was obtained with R^2 values >0.995 and residual values %RSD <13% (Figure 7). Example calibration curves for BDE-209 and BDE-71 are shown in Figure 8 where both the coefficient of determination (R^2) and the residual %RSD are annotated.

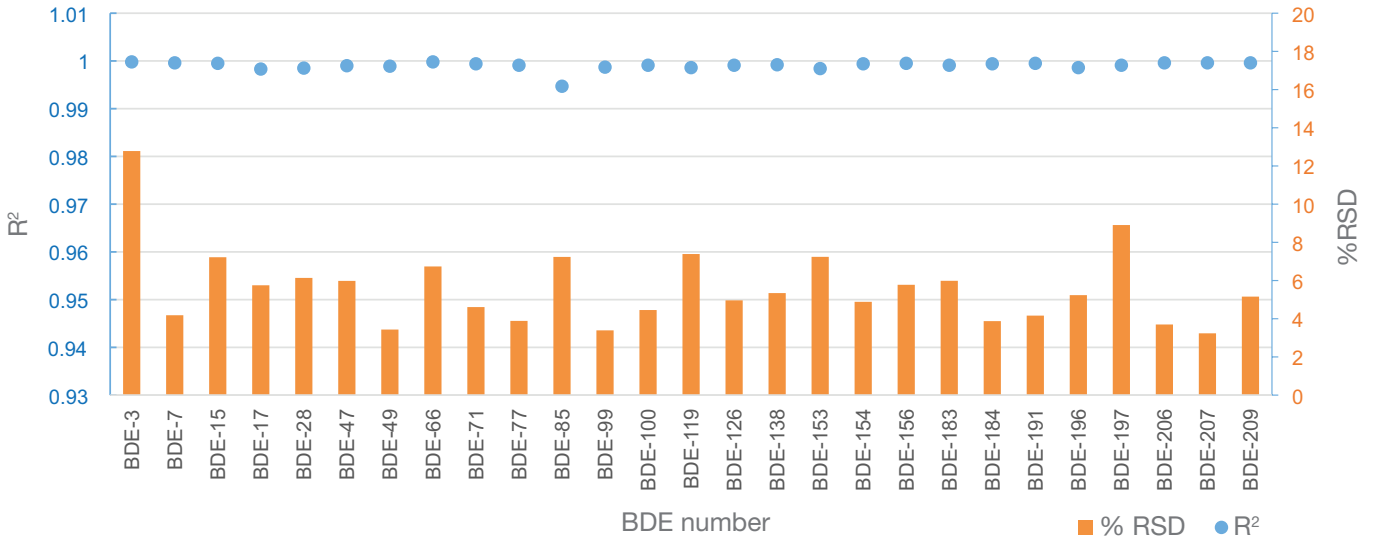


Figure 7. Coefficient of determination (left) and residuals values (%RSD) for 27 native PBDE congeners (right)

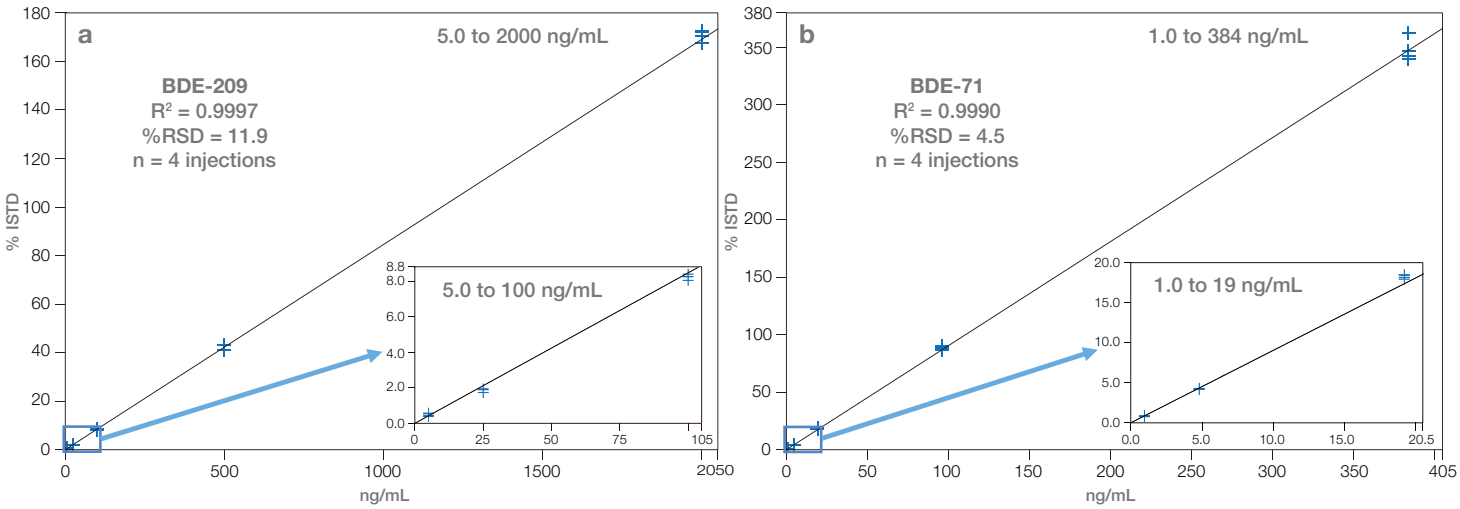


Figure 8. Example calibration curves (a) BDE-209 and (b) BDE-71, illustrating the linearity obtained. The inset calibration curves exemplify the maintained linearity for the lowest 3 calibration levels.

Sample analysis

Samples of sludge, sediment, filter dust, and air were prepared and analyzed as detailed; concentrations of the PBDEs identified are illustrated in Figure 9. The samples analyzed were extracted and quantified using isotopic dilution, using the mass-labelled PBDE surrogate standards, added to the sample prior to extraction as internal standards, and the mass-labelled PBDE recovery standard added to the extract prior to analysis as a syringe recovery standard.

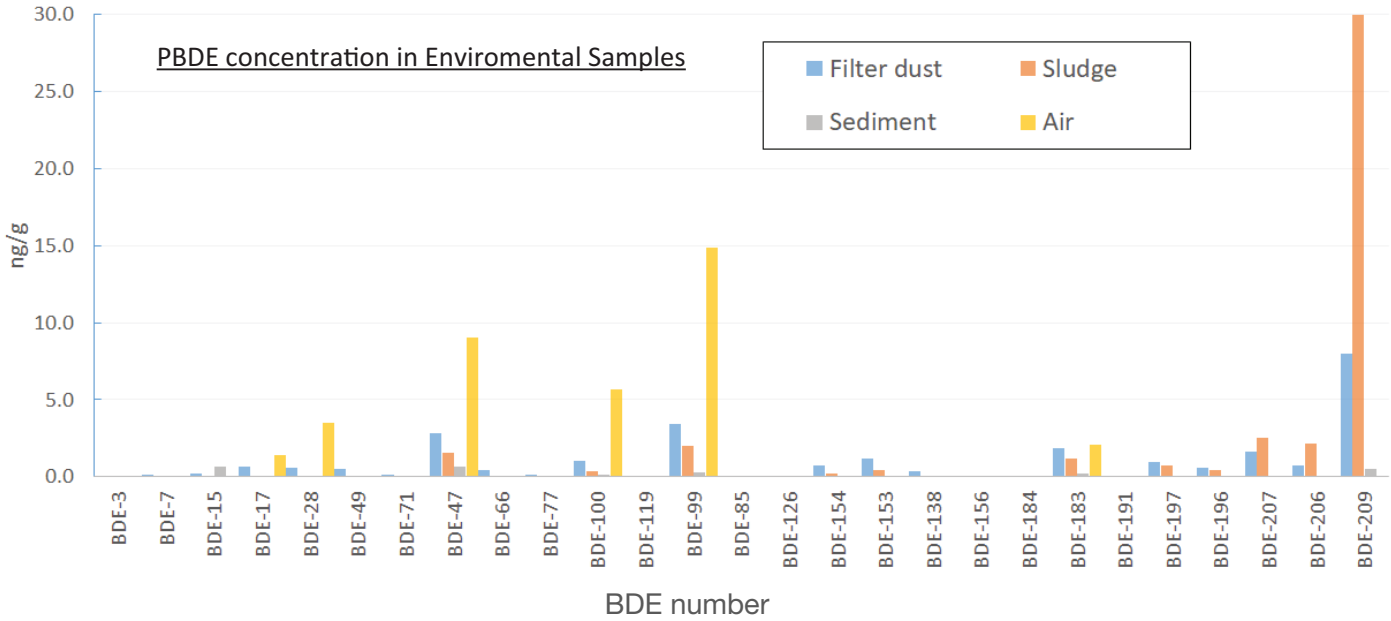


Figure 9. Calculated concentration of PBDEs, extracted and quantified from filter dust, sludge, sediment and air samples, thus illustrating the predominant PBDE congeners identified in the analyzed sludge samples as BDE-209, 206, 207, and 99, filter dust samples as BDE-209, 47, and 99, air samples as BDE-99, 47, and 100, and sediment samples as BDE-15, 47, and 99

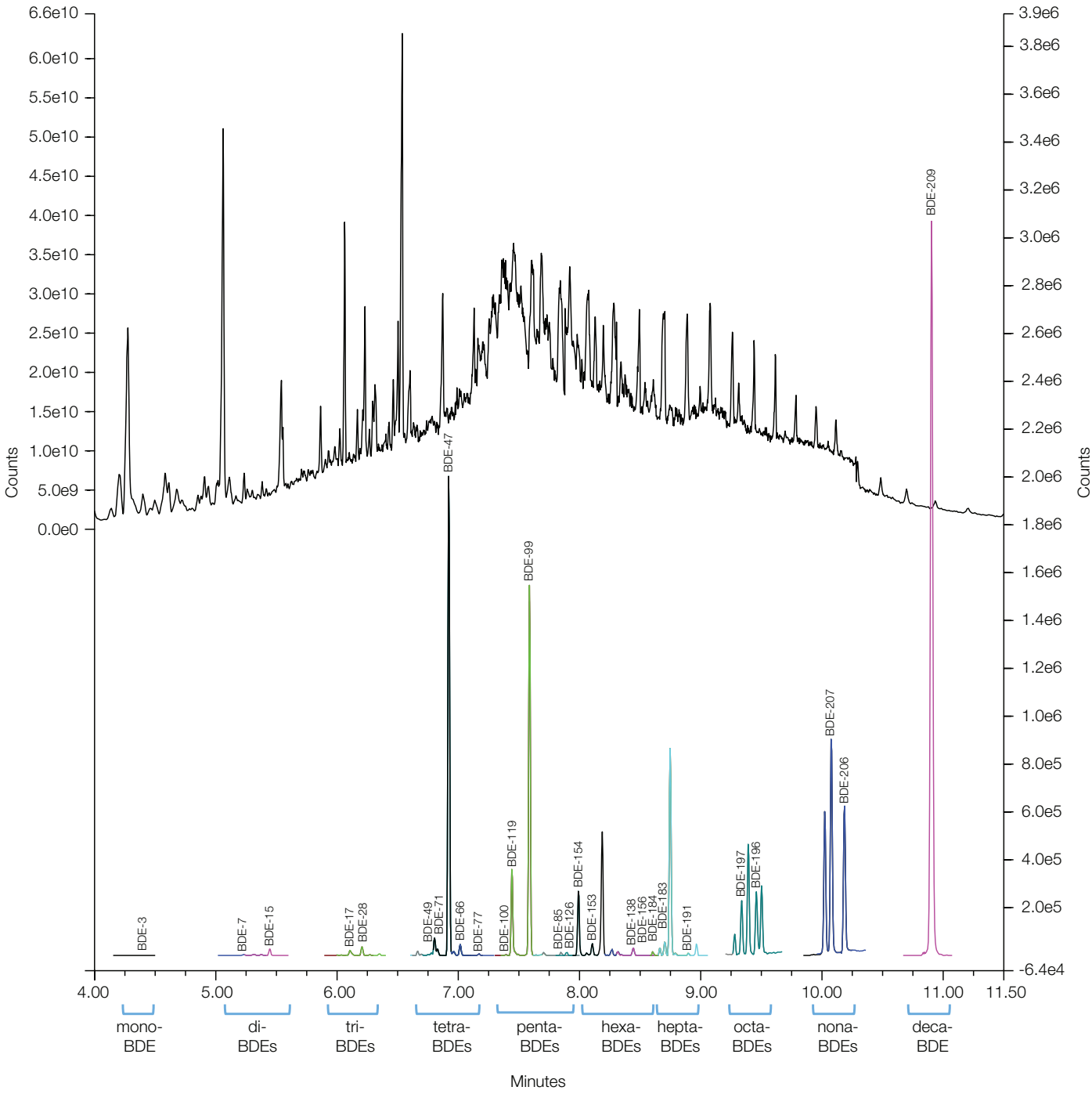


Figure 10. Sludge sample chromatograms: (upper) TIC full scan; (lower) EICs for the native PBDE congeners identified in the sample

An example of the complexity of extracted samples is shown as a total ion chromatogram (TIC) versus overlaid PBDEs EICs for a sludge sample (Figure 10), where the predominant PBDE congeners detected were BDE-209, 207, 206, 99, 47, and 183. TIC and PBDE EICs signal intensities (Y-axis) were normalized to simplify the visual comparison.

These results achieved demonstrate excellent selectivity and sensitivity for the analysis of PBDEs even in the most complex samples. Moreover, the routine high resolution of the Exactive GC offers excellent selectivity in difficult matrices, and the mass accuracy obtained allows for unambiguous identification and elemental composition confirmation of chemical contaminants.

Selectivity in matrix

The selectivity of the established method can be illustrated considering the lowest level standards, for BDE-28 and 17 (1 ng/mL, 1 pg on column), identified in a sludge sample at a similar level (Figure 11).

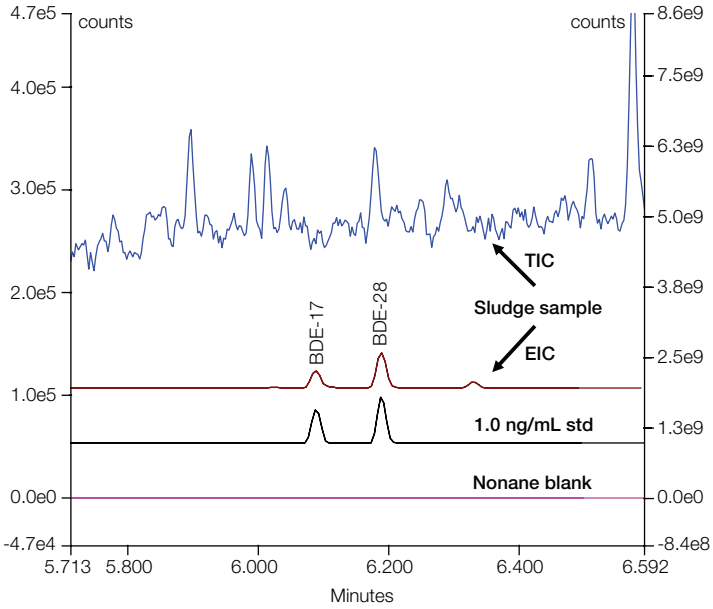


Figure 11. Overlaid EICs for BDE-17 and BDE-28 (left), in 1.0 ng/mL standard, an extracted sludge sample at a similar level, and a nonane blank. In addition, the TIC for the extracted sludge sample (right).

Conclusions

- The results of this study demonstrate that the Exactive GC Orbitrap GC-MS coupled with a TRACE 1310 GC system provides an excellent solution for routine quantification of PBDEs in complex environmental samples.
- The predominant PBDE congeners identified, confirmed, and quantified in the samples were BDE-209, 206, 207, and 99 in sludge, BDE-209, 47, and 99 in filter dust, BDE-99, 47, and 100 in air, and BDE-15, 47, and 99 in sediment.
- Using a TraceGOLD TG-PBDE 15 m capillary column, good chromatographic separation in <11 minutes for all the PBDE congeners was achieved, with excellent chromatographic resolution of the critical pair (BDE-49 and BDE-71).
- Outstanding peak area repeatability of PBDE responses in matrix with RSD% for quantification and qualifier peak area counts between 2% and 10% for all identified congeners, an important analytical parameter for routine GC-MS workflows.
- Compound linearity was demonstrated with R^2 >0.995 and residual values RSD% <13%, over five calibration levels.
- All PBDEs were detected in the lowest calibration standard, 1.0 ng/mL for mono- to penta-BDEs, 2.0 ng/mL for hexa- to octa-BDEs, and 5 ng/mL for nona- to deca-BDEs. Instrumental detection limits between 6 and 250 fg on column were achieved for the PBDEs targeted.
- Chromeleon CDS software offers an ideal solution for the targeted isotopic dilution quantification of PBDEs in environmental samples with user-friendly data processing and reporting features.

Acknowledgment

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References

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Appendices

Appendix A. Details of 27 native PBDE congeners analyzed, including BDE number, chemical formula, CAS number, and calibration range

BDE number	Native BDEs	Chemical formula	CAS number	Calibration range (ng/mL)
3	4-Bromodiphenyl ether	$C_{12}H_9BrO$	101-55-3	1.0 to 400
7	2,4-Dibromodiphenyl ether	$C_{12}H_8Br_2O$	171977-44-9	1.0 to 400
15	4,4'-Dibromodiphenyl ether	$C_{12}H_8Br_2O$	2050-47-7	1.0 to 400
17	2,2',4-Tribromodiphenyl ether	$C_{12}H_7Br_3O$	147217-75-2	0.96 to 384
28	2,4,4'-Tribromodiphenyl ether	$C_{12}H_7Br_3O$	41318-75-6	1.0 to 400
47	2,2',4,4'-Tetrabromodiphenyl ether	$C_{12}H_6Br_4O$	5436-43-1	1.0 to 400
49	2,2',4,5'-Tetrabromodiphenyl ether	$C_{12}H_6Br_4O$	243982-82-3	1.0 to 400
66	2,3',4,4'-Tetrabromodiphenyl ether	$C_{12}H_6Br_4O$	189084-61-5	1.0 to 400
71	2,3',4',6-Tetrabromodiphenyl ether	$C_{12}H_6Br_4O$	189084-62-6	1.0 to 400
77	3,3',4,4'-Tetrabromodiphenyl ether	$C_{12}H_6Br_4O$	93703-48-1	1.0 to 400
85	2,2',3,4,4'-Pentabromodiphenyl ether	$C_{12}H_5Br_5O$	182346-21-0	1.0 to 400
99	2,2',4,4',5-Pentabromodiphenyl ether	$C_{12}H_5Br_5O$	32534-81-9	1.0 to 400
100	2,2',4,4',6-Pentabromodiphenyl ether	$C_{12}H_5Br_5O$	189084-64-8	1.0 to 400
119	2,3',4,4',6-Pentabromodiphenyl ether	$C_{12}H_5Br_5O$	189084-66-0	1.0 to 400
126	3,3',4,4',5-Pentabromodiphenyl ether	$C_{12}H_5Br_5O$	366791-32-4	1.0 to 400
138	2,2',3,4,4',5-Hexabromodiphenyl ether	$C_{12}H_4Br_6O$	446254-95-1	2.0 to 800
153	2,2',4,4',5,5'-Hexabromodiphenyl ether	$C_{12}H_4Br_6O$	68631-49-2	2.0 to 800
154	2,2',4,4',5,6'-Hexabromodiphenyl ether	$C_{12}H_4Br_6O$	207122-15-4	2.0 to 800
156	2,3,3',4,4',5-Hexabromodiphenyl ether	$C_{12}H_4Br_6O$	405237-85-6	2.0 to 800
183	2,2',3,4,4',5',6-Heptabromodiphenyl ether	$C_{12}H_3Br_7O$	207122-16-5	2.0 to 800
184	2,2',3,4,4',6,6'-Heptabromodiphenyl ether	$C_{12}H_3Br_7O$	117948-63-7	2.0 to 800
191	2,3,3',4,4',5',6-Heptabromodiphenyl ether	$C_{12}H_3Br_7O$	446255-30-7	2.0 to 800
196	2,2',3,3',4,4',5,6'-Octabromodiphenyl ether	$C_{12}H_2Br_8O$	446255-39-6	2.0 to 800
197	2,2',3,3',4,4',6,6'-Octabromodiphenyl ether	$C_{12}H_2Br_8O$	117964-21-3	2.0 to 800
206	2,2',3,3',4,4',5,5',6-Nonabromodiphenyl ether	$C_{12}HBr_9O$	63936-56-1	5.0 to 2000
207	2,2',3,3',4,4',5,6,6'-Nonabromodiphenyl ether	$C_{12}HBr_9O$	437701-79-6	5.0 to 2000
209	Decabromodiphenyl ether	$C_{12}Br_{10}O$	1163-19-5	5.0 to 2000

Appendix B. Details of 16 ^{13}C-labelled PBDEs internal standards, including BDE isomer number, chemical formula, CAS number, and concentration (suffix "L" indicates mass-labelled)

BDE isomer number	^{13}C labelled PBDEs	Chemical formula	Concentration (ng/mL)
3L	4-Bromo[$^{13}C_{12}$]diphenyl ether	$^{13}C_{12}H_9BrO$	100
15L	4,4'-Dibromo[$^{13}C_{12}$]diphenyl ether	$^{13}C1_2H_8Br_2O$	100
28L	2,4,4'-Tribromo[$^{13}C_{12}$]diphenyl ether	$^{13}C_{12}H_7Br_3O$	100
47L	2,2',4,4'-Tetrabromo[$^{13}C_{12}$]diphenyl ether	$^{13}C_{12}H_6Br_4O$	100
79L	3,3',4,5'-Tetrabromo[$^{13}C_{12}$]diphenyl ether	$^{13}C_{12}H_6Br_4O$	100
99L	2,2',4,4',5-Pentabromo[$^{13}C_{12}$]diphenyl ether	$^{13}C_{12}H_5Br_5O$	100
100L	2,2',4,4',6-Pentabromo[$^{13}C_{12}$]diphenyl ether	$^{13}C_{12}H_5Br_5O$	100
126L	3,3',4,4',5-Pentabromo[$^{13}C_{12}$]diphenyl ether	$^{13}C_{12}H_5Br_5O$	100
138L	2,2',3,4,4',5-Hexabromo[$^{13}C_{12}$]diphenyl ether	$^{13}C_{12}H_4Br_6O$	200
153L	2,2',4,4',5,5'-Hexabromo[$^{13}C_{12}$]diphenyl ether	$^{13}C_{12}H_4Br_6O$	200
154L	2,2',4,4',5,6'-Hexabromo[$^{13}C_{12}$]diphenyl ether	$^{13}C_{12}H_4Br_6O$	200
183L	2,2',3,4,4',5',6-Heptabromo[$^{13}C_{12}$]diphenyl ether	$^{13}C_{12}H_3Br_7O$	200
197L	2,2',3,3',4,4',6,6'-Octabromo[$^{13}C_{12}$]diphenyl ether	$^{13}C_{12}H_2Br_8O$	200
206L	2,2',3,3',4,4',5,5',6-Nonabromo[$^{13}C_{12}$]diphenyl ether	$^{13}C_{12}HBr_9O$	500
207L	2,2',3,3',4,4',5,6,6'-Nonabromo[$^{13}C_{12}$]diphenyl ether	$^{13}C_{12}HBr_9O$	500
209L	Decabromo[$^{13}C_{12}$]diphenyl ether	$^{13}C_{12}Br_{10}O$	500

Appendix C. Details of the targeted-SIM inclusion list, listing for each entry the mass (*m/z*), start and end times, and PBDEs

Mass (*m/z*)	Start time (min)	End time (min)	BDE number
260.02339	4.00	4.50	3L, 3
327.89164	4.50	5.60	7, 15
339.93186	4.50	5.60	15L
405.80214	5.60	6.60	17, 28
417.84237	5.60	6.60	28L
485.71063	6.60	7.30	47, 49, 66, 71, 77
497.75084	6.60	7.30	47L, 79L
563.62113	7.30	8.00	85, 99, 100, 119, 126
575.66135	7.30	8.00	99L, 100L, 126L
483.69498	7.80	8.62	138, 153, 154, 156
495.73518	7.80	8.62	153L, 154L, 138L
561.60525	8.58	9.20	183. 184, 191
573.64569	8.58	9.20	183L
641.51390	9.20	9.70	196, 197
653.55416	9.20	9.70	197L
719.42446	9.70	10.40	206, 207
731.46467	9.70	10.40	207L, 206L
799.30000	10.40	12.50	209
811.30000	10.40	12.50	209L

Appendix D. PBDE retention times, quantification and confirming ions, and ion ratio averages and ranges

BDE number	RT (min)	Quantification ion	Confirming ion	Ion ratio average	Ion ratio range (±15%)	
BDE-3	4.35	249.98108	247.98313	60	51	69
BDE-7	5.21	327.89164	325.89364	50	43	58
BDE-15	5.43	327.89164	325.89364	49	42	56
BDE-17	6.09	405.80214	407.80014	74	63	85
BDE-28	6.19	405.80214	407.80014	95	81	109
BDE-47	6.92	485.71063	783.71264	68	58	78
BDE-49	6.78	485.71063	783.71264	68	58	78
BDE-66	7.00	485.71063	783.71264	68	58	78
BDE-71	6.84	485.71063	783.71264	66	56	76
BDE-77	7.14	485.71063	783.71264	67	57	77
BDE-85	7.81	563.62113	565.61912	99	84	114
BDE-99	7.54	563.62113	565.61912	100	85	115
BDE-100	7.40	563.62113	565.61912	96	81	110
BDE-119	7.45	563.62113	565.61912	98	83	112
BDE-126	7.84	563.62113	565.61912	99	84	114
BDE-138	8.40	483.69498	481.69699	66	56	75
BDE-153	8.14	483.69498	481.69699	67	57	77
BDE-154	7.95	483.69498	481.69699	67	57	77
BDE-156	8.50	483.69498	481.69699	68	58	78
BDE-183	8.71	561.60525	563.60321	102	87	118
BDE-184	8.62	563.60315	565.60120	48	41	55
BDE-191	8.85	561.60525	563.60321	100	84	116
BDE-196	9.46	641.51390	639.51595	75	64	86
BDE-197	9.35	641.51390	639.51595	73	62	84
BDE-206	10.15	719.42446	721.42000	96	82	111
BDE-207	10.04	719.42446	721.42280	99	84	113
BDE-209	10.86	799.33295	797.33497	80	68	91

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