

Electronic Supplementary Information (ESI†)

Determination of benzophenone and related compounds in plastic-packaged baby food by ultra-high-performance liquid chromatography coupled to tandem mass spectrometry

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Supplementary Tables

Table S1: MS/MS working conditions.

Analyte	Precursor ion (<i>m/z</i>)	Quantitation		Confirmation		Tube lens (V)	Ion ratio	SD (%)
		Product ion (<i>m/z</i>)	NCE (%)	Product ion (<i>m/z</i>)	NCE (%)			
44DHBP	215	121	18	93	31	83	4.7	0.2
THBP	245	135	17	109	23	73	1.4	0.01
TrHBP	229	151	23	123	29	75	1.6	0.01
HBP	197	92	36	120	27	90	6.5	0.1
MBB	241	209	21	152	35	73	1.6	0.03
24DHBP	213	135	22	91	29	84	1.4	0.02
DiOBP	245	121	17	151	19	80	2.3	0.1
BP	183	105	15	77	34	80	2.1	0.1
DHMBP	275	151	18	95	35	80	6.6	0.2
4-MBP	197	105	16	77	34	75	2.2	0.1
HMBP	229	151	20	105	19	80	3.8	0.1
CIHBP	231	121	24	77	32	84	3.3	0.1
AHBP	255	105	18	177	16	74	1.6	0.1
5CIHBP	245	121	25	77	31	84	3.1	0.1
PBZ	259	105	18	77	36	75	1.9	0.1
DEAB	325	176	25	281	30	92	1.6	0.1
HOBP	327	137	27	215	19	95	1.6	0.05

Table S2: Matrix effect, extraction efficiency of BPs obtained in the dSPE UHPLC–MS/MS analysis of different matrices (yogurt, homemade custards and chocolate product).

Analyte	YOGURT		HOMEMADE CUSTARDS		PRODUCT CHOCOLATE	
	Matrix effect	Extraction efficiency	Matrix effect	Extraction efficiency	Matrix effect	Extraction efficiency
	% (SD, %)	% (SD, %)	% (SD, %)	% (SD, %)	% (SD, %)	% (SD, %)
44DHBP	6 (5)	83 (4)	7 (2)	80 (8)	6 (2)	90 (9)
THBP	16 (5)	86 (9)	6 (6)	72 (4)	21 (9)	84 (10)
TrHBP	12 (3)	82 (3)	15 (5)	86 (3)	24 (3)	95 (4)
HBP	29 (4)	88 (2)	9 (4)	86 (3)	6 (1)	96 (5)
MBB	16 (5)	81 (10)	5 (2)	80 (4)	7 (5)	107 (7)
24DHBP	5 (5)	88 (2)	7 (5)	86 (3)	5 (4)	95 (7)
DiOBP	6 (5)	81 (8)	23 (6)	83 (12)	17 (8)	104 (11)
BP	10 (5)	75 (4)	8 (3)	78 (8)	26 (8)	105 (10)
DHMBP	9 (5)	87 (2)	16 (8)	94 (13)	28 (6)	100 (9)
4-MBP	14 (7)	81 (1)	20 (9)	79 (8)	30 (8)	92 (9)
HMBP	15 (7)	85 (3)	19 (5)	85 (12)	42 (1)	102 (11)
CIHBP	27 (8)	79 (9)	15 (5)	80 (10)	54 (4)	107 (9)
AHBP	29 (6)	89 (3)	13 (4)	80 (4)	55 (3)	90 (3)
5CIHBP	39 (8)	80 (6)	13 (7)	80 (10)	59 (3)	92 (10)
PBZ	38 (6)	85 (4)	13 (12)	79 (4)	54 (5)	95 (6)
DEAB	15 (7)	88 (1)	4 (3)	78 (7)	52 (2)	100 (10)
HOBP	89 (3)	49 (1)	43 (7)	37 (5)	98 (4)	65 (3)

Table S3: dSPE UHPLC–MS/MS quality parameters for the analysis of BPs in homemade custard and chocolate product matrices.

Analyte	HOMEMADE CUSTARD					CHOCOLATE PRODUCT				
	MLOQ ($\mu\text{g kg}^{-1}$)	Run-to-run precision (RSD, %)		Trueness (Rel. Error, %)		MLOQ ($\mu\text{g kg}^{-1}$)	Run-to-run precision (RSD, %)		Trueness (Rel. Error, %)	
		Low level ^a	Medium level ^b	Low level ^a	Medium level ^b		Low level ^a	Medium level ^b	Low level ^a	Medium level ^b
44DHBP	19	-	3	-	4	98	-	4	-	1
THBP	1.3	9	9	2	8	1.2	20	9	8	7
TrHBP	1.8	2	8	14	8	1.5	16	6	14	1
HBP	4.6	4	3	10	20	1.1	5	4	1	6
24DHBP	1.2	3	2	1	10	1.2	7	3	4	6
MBB	4.5	5	2	20	7	1.3	3	2	5	5
DiOBP	8.6	3	3	4	5	4.1	9	7	5	1
BP	250	-	2	-	4	92	-	4	-	1
DHMBP	3.9	2	1	14	2	6.6	5	7	18	14
4-MBP	34	5	2	7	4	24	7	3	1	6
HMBP	48	3	2	1	4	9.4	9	4	2	3
CIHBP	3.6	2	4	4	10	48	13	4	1	2
AHBP	9.5	1	3	5	6	8.8	6	3	9	13
5CIHBP	42	12	4	5	7	31	11	3	1	3
PBZ	9.3	5	3	3	1	48	6	6	15	10
DEAB	21	2	1	11	9	2.3	5	1	10	11
HOBP	59	-	1	-	1	247	-	5	-	12

(-) Below its MLOD

^a Trueness at low level concentration ($50 \mu\text{g kg}^{-1}$)

^b Trueness at medium level concentration ($500 \mu\text{g kg}^{-1}$)

Supplementary Figures

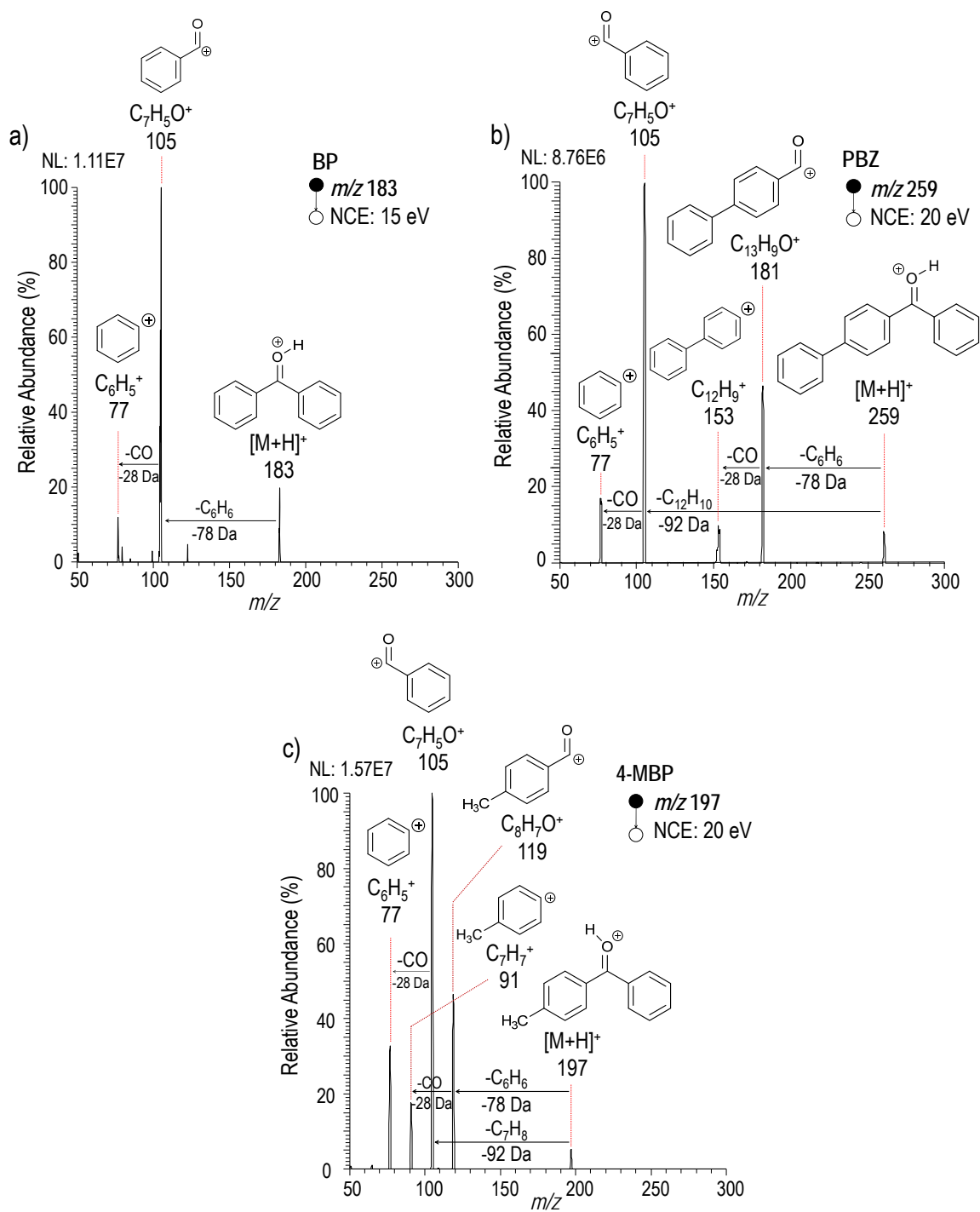


Figure S1: Product ion scan spectrum of a) BP b) PBZ and c) 4-MBP acquired in positive ion mode.

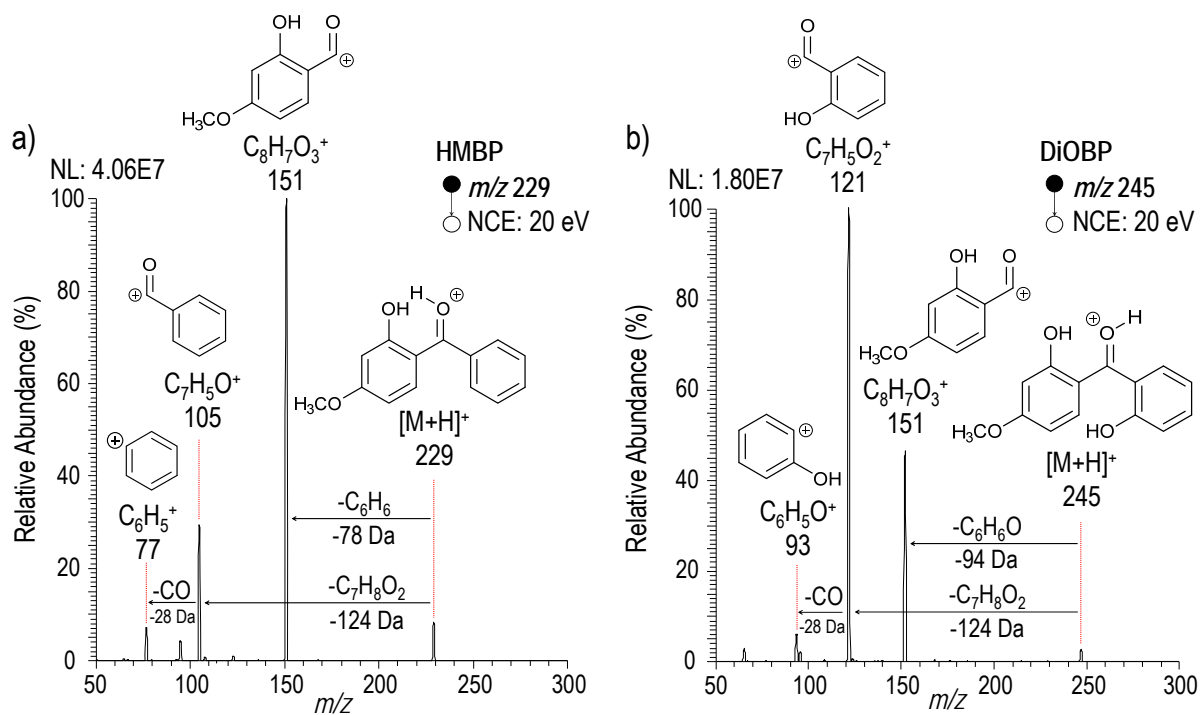


Figure S2: Product ion scan spectrum of a) HMBP and b) DiOBP acquired in positive ion mode.

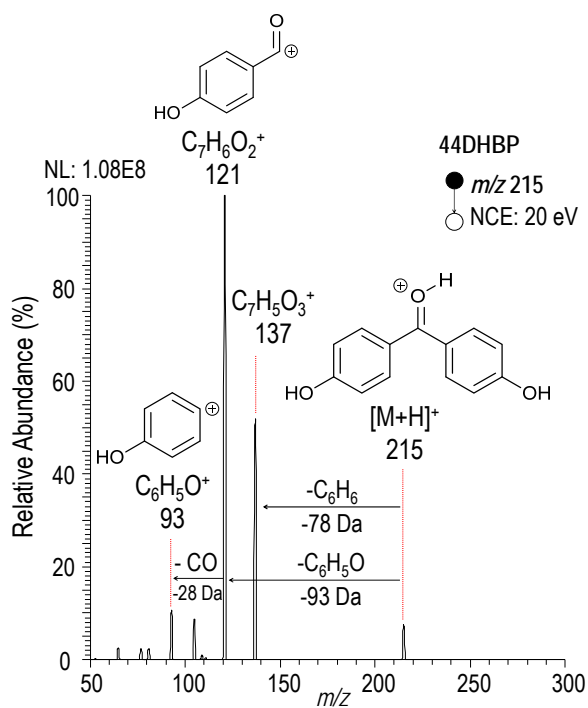


Figure S3: Product ion scan spectrum of 44DHBP acquired in positive ion mode.

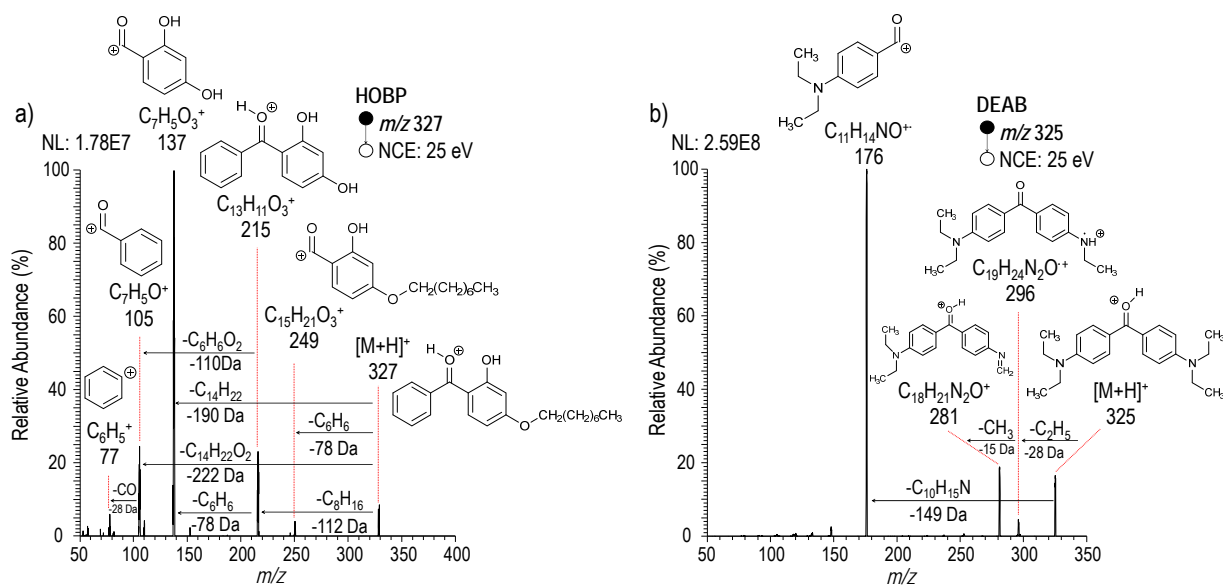


Figure S4: Product ion scan spectrum of a) HOBP and b) DEAB acquired in positive ion mode.

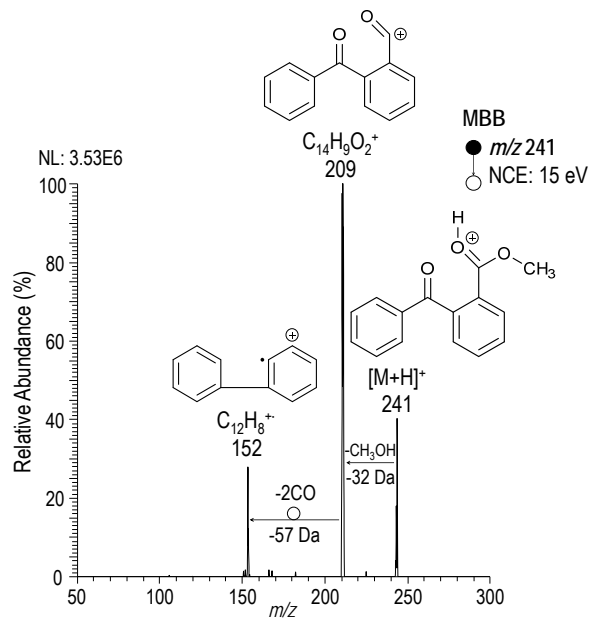


Figure S5: Product ion scan spectrum of MBB acquired in positive ion mode.

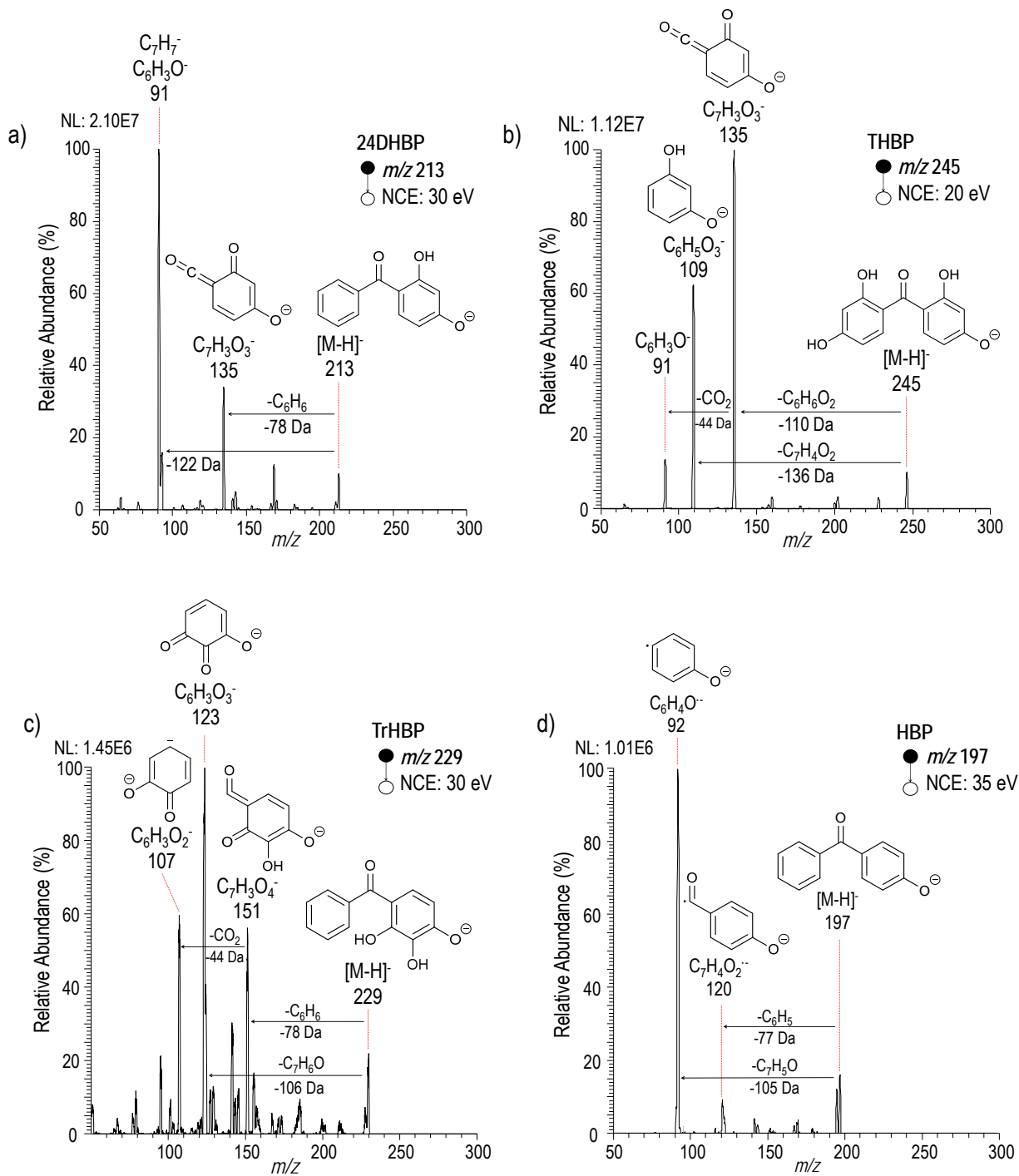


Figure S6: Product ion scan spectrum of a) 24DHBP, b) THBP, c) TrHBP and d) HBP acquired in positive ion mode.

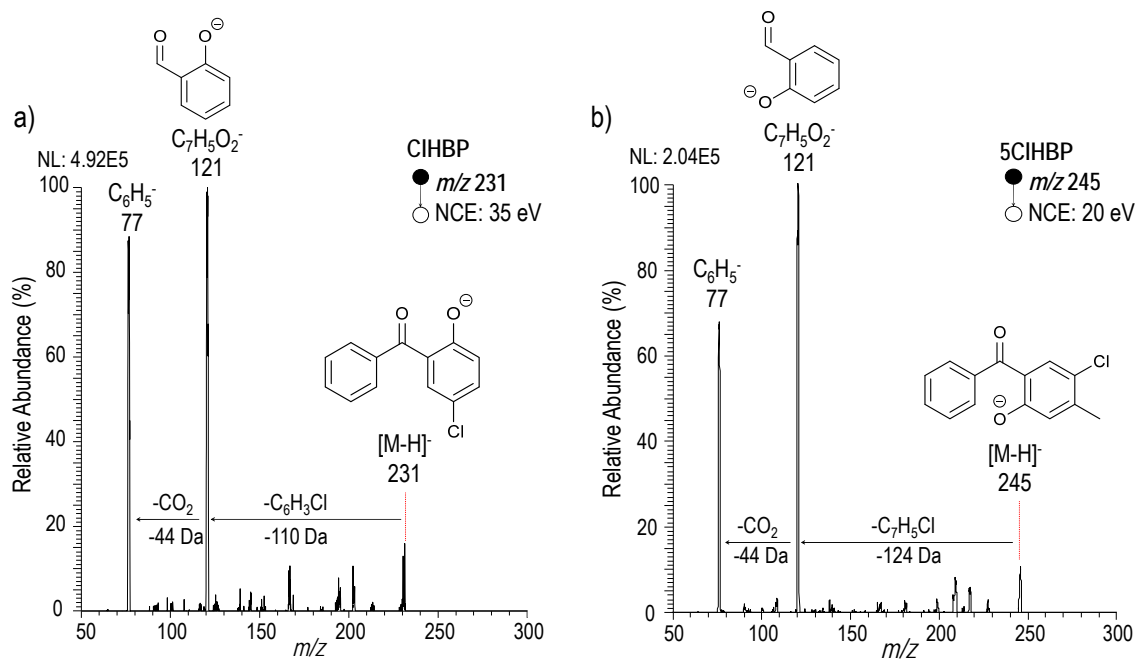


Figure S7: Product ion scan spectrum of a) CIHBP and b) 5CIHBP acquired in positive ion mode.

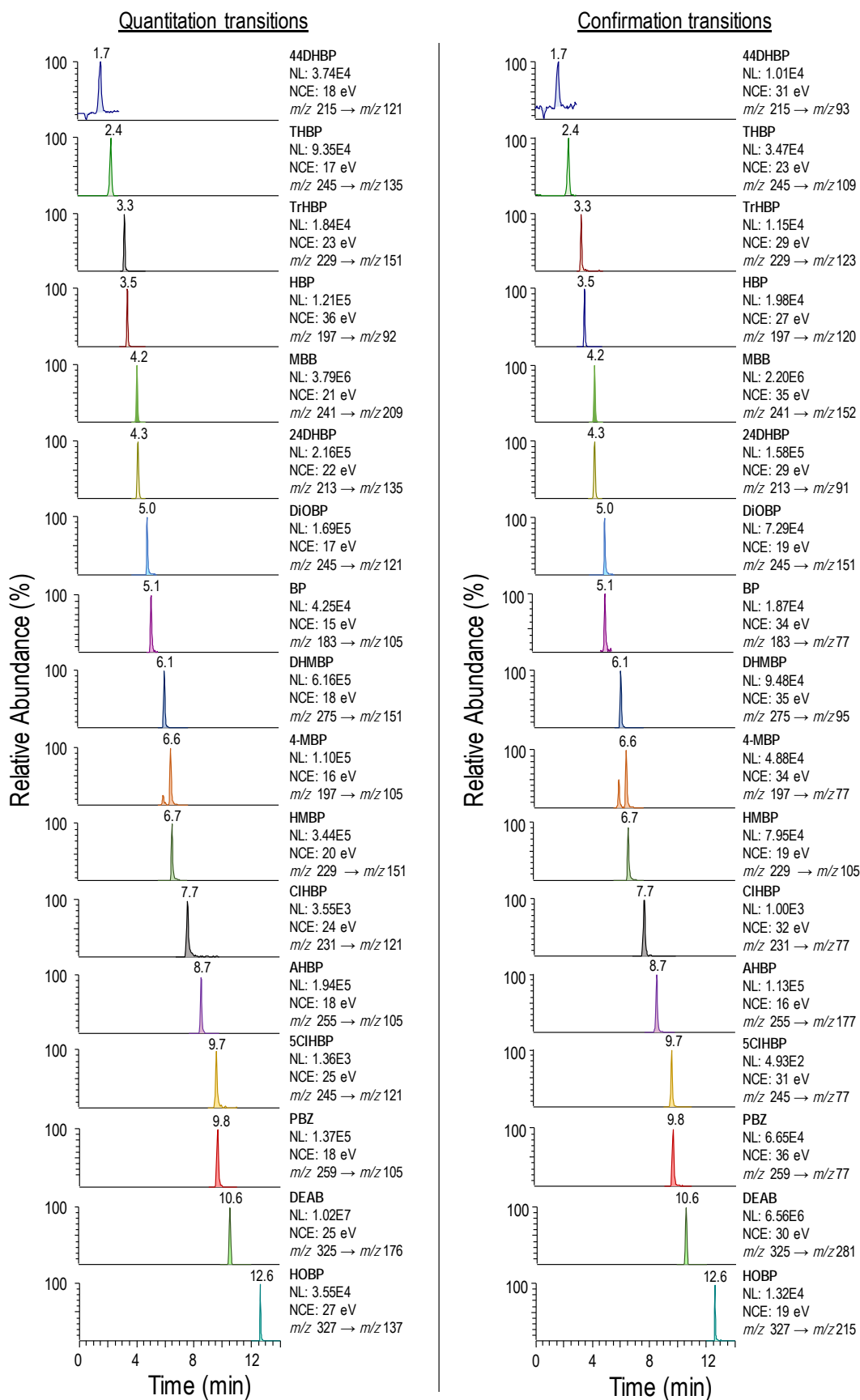


Figure S8: MRM chromatogram with quantitation and confirmation transitions of the yogurt spiked sample at $50 \mu\text{g kg}^{-1}$ level.

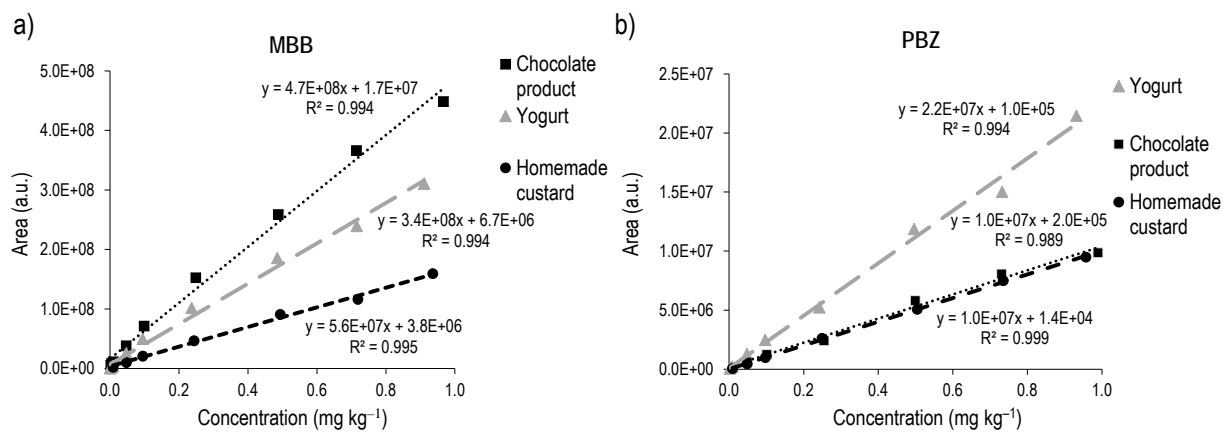


Figure S9: Matrix matched calibration curves for a) MBB and b) PBZ in different matrices.