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## Data Article

# Dataset of liver proteins changed in eu- and hypothyroid female rats upon in vivo exposure to hexabromocyclododecane (HBCD)

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## ABSTRACT

Female Wistar rats with different thyroid status (eu-, hypothyroid) were exposed to 0, 3 or 30 mg/kg body weight of the flame retardant HBCD for 7 days. Changes in protein patterns obtained by 2D-DIGE were evaluated, and different animal groups compared taking into account their exposure and thyroid status. Proteins significantly altered in abundance in any of these comparisons were identified by mass spectrometry. These data, together with hormone data of the animals, are discussed in “Hexabromocyclododecane (HBCD) induced changes in the liver proteome of eu- and hypothyroid female rats” (Miller et al., 2016) [1].

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## Specifications Table

Subject area	<i>Biology</i>
More specific subject area	<i>Environmental Toxicology</i>
Type of data	<i>Tables, image (annotated gel image)</i>
How data was acquired	<i>2D Fluorescence Difference Gel Electrophoresis (2D-DIGE) and mass spectrometry</i>
Data format	<i>Analyzed and filtered data</i>
Experimental factors	<i>Liver lysates of eu- and hypothyroid female rats differently exposed to HBCD</i>
Experimental features	<i>Comparative proteomic analysis of rat liver lysates using 2D-DIGE. Proteins present in differentially abundant protein spots (regarding HBCD exposure, amount, and thyroid status) were identified using MALDI TOF/TOF analysis.</i>
Data source location	<i>Origin of samples: Wageningen University, Wageningen, The Netherlands Data collection: Luxembourg Institute of Science and Technology, Esch-sur-Alzette, Luxembourg</i>
Data accessibility	<i>MS- and regulation data is with this article as Supplementary material</i>

## Value of the data

- Identification of liver proteins from female rats altered due to HBCD exposure.
- Identification of liver proteins from female rats changed in hypothyroid status.
- Data showing single and combined effects (HBCD exposure, hypothyroidism).
- Identified liver proteins form the basis for further studies to achieve a more detailed understanding of involved mechanism.

## 1. Data

Two-dimensional electrophoresis of liver protein lysates showed complex patterns of about 3000 spots per gel. Patterns of 24 gels from different exposures of eu- and hypothyroid rats were evaluated quantitatively. The data from different animals groups were compared, taking different aspects into account (HBCD exposure, thyroid status). Statistically significant fold-changes of at least 30% between groups ( $P < 0.05$  within group) were considered to be relevant.

The master gel is presented in [Fig. 1](#), and all spots with significant abundance changes in any of the performed comparisons are labelled. Spot numbers refer to the protein identifications listed in [Table 1](#) (peptide list in [Supplemental Table 1](#)), and to abundance changes in the various animal groups ([Supplemental Table 2](#)).

## 2. Experimental design, materials and methods

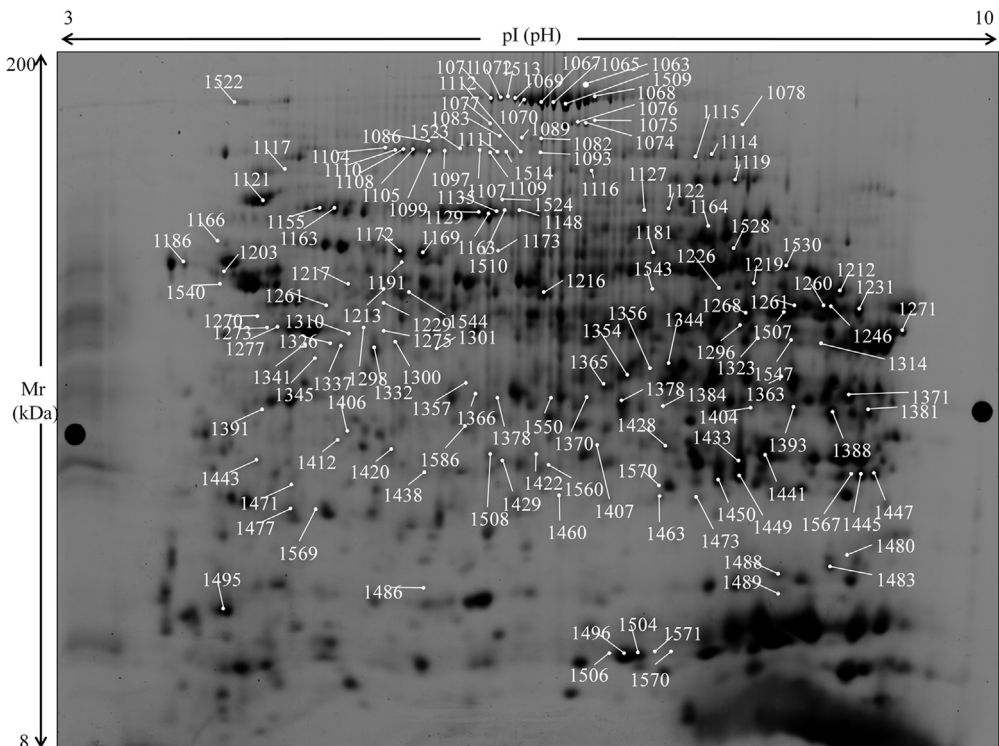
### 2.1. Animals, treatment and experimental protocol

The animal experiment was detailed in [\[1\]](#) and was approved under number 2007-041 by the Animal Welfare Committee of Wageningen University. In brief, female Wistar WU (HsdCpbWU) rats with normal or reduced thyroid function (hypothyroid) were orally exposed to 0, 3 or 30 mg/kg bw/d HBCD, respectively, for 7 consecutive days. Four liver samples per group were analyzed by proteomic methods.

## 2.2. Proteomic analysis

Two-dimensional fluorescence difference gel electrophoresis (2D-DIGE) was performed as previously described, with minor modifications [2,3]. Rat livers were homogenized using the GE sample grinding kit in lysis buffer (urea 7 M; thiourea 2 M; CHAPS 2% w/w; tris 30 mM) containing protease inhibitor Complete Mini (Roche, Brussels, Belgium). Supernatants obtained after centrifugation (15 min at 30,000 g) were collected and stored at  $-20^{\circ}\text{C}$  until use. Protein concentration was determined according to Bradford [4]. Fifty  $\mu\text{g}$  per sample were labelled with CyDyes according to the manufacturer's instructions and separated on IPGs of a non-linear 3–10 pH-range. The second dimensional SDS-PAGE was performed in 12.5% precast gels (SERVA Electrophoresis GmbH, Heidelberg, Germany). Gel images (acquired on a Typhoon 9400) were analyzed with the DeCyder 7.0 software package (both GE Healthcare, Diegem, Belgium). Gels were matched and subjected to univariate and multivariate analysis in order to highlight differentially regulated spots (fold change at least 1.3) with a  $P$ -value in the respective univariate ANOVA or two way ANOVA  $< 0.05$ .

Differentially abundant spots were automatically picked, tryptically digested and spotted on the MALDI target by the use of the Ettan Spot Handling Workstation (GE Healthcare, Diegem, Belgium). Protein identification was carried out on the Applied Biosystems MALDI-ToF-ToF 4800 Proteomics Analyser (Applied Biosystem, Gent, Belgium) as previously described [2]. Protein identification was performed by searching protein mass fingerprints (PMF) and MS/MS spectra against the SwissProt database with "*Rattus norvegicus*" as taxonomy. Searches were performed using the ProteinPilot software (Sciex, Nieuwerkerk aan den IJssel, The Netherlands) and the searching algorithm MASCOT (Matrix Science, [www.matrixscience.com](http://www.matrixscience.com), London, UK). For each spot one protein mass fingerprint and up to 8 MS/MS spectra were generated. Parameters for the search were set as follow: up to two



**Fig. 1.** Image of a rat liver 2D-DIGE gel (master gel, grey level image). All spots with statistically significant abundance changes are labelled; spot numbers refer to identifications in Table 1. For details on protein identification see Supplemental Table 1, for data on protein abundance, see Supplemental Table 2.

**Table 1**  
Proteins of the present dataset, identified by MALDI-TOF/TOF analysis.

Spot number	Protein name	Species	Swiss-Prot Acc. N°
<b>1063, 1065, 1067–1071, 1074–1076, 1078</b>	Carbamoyl-phosphate synthase[ammonia], mitochondrial	Rattus norvegicus	CPSM_RAT
<b>1072</b>	Murinoglobulin-2	Rattus norvegicus	MUG2_RAT
<b>1077, 1082, 1083</b>	Pyruvate carboxylase, mitochondrial	Rattus norvegicus	PYC_RAT
<b>1086</b>	ATP-citrate synthase	Rattus norvegicus	ACLY_RAT
<b>1089</b>	C-1-tetrahydrofolate synthase, cytoplasmic	Rattus norvegicus	C1TC_RAT
<b>1093</b>	Alpha-aminoadipic semialdehyde synthase, mitochondrial	Rattus norvegicus	AASS_RAT
<b>1094, 1100</b>	2-oxoglutarate dehydrogenase, mitochondrial	Rattus norvegicus	ODO1_RAT
<b>1099, 1105, 1107–1110, 1114</b>	Aldehyde dehydrogenase family1 member L1	Rattus norvegicus	AL1L1_RAT
<b>1111</b>	Aldehyde dehydrogenase1 family, member L2	Mus musculus	gil21961590
<b>1112, 1115–1117, 1119</b>	Sarcosine dehydrogenase, mitochondrial	Rattus norvegicus	SARDH_RAT
<b>1121, 1122</b>	Elongation factor2	Rattus norvegicus	EF2_RAT
<b>1123</b>	Cytoplasmic aconitate hydratase	Rattus norvegicus	ACOC_RAT
<b>1129</b>	Dimethylglycine dehydrogenase, mitochondrial	Rattus norvegicus	M2GD_RAT
<b>1135</b>	Serotransferrin	Rattus norvegicus	TRFE_RAT
<b>1148</b>	Propionyl-CoA carboxylase alpha chain, mitochondrial	Rattus norvegicus	PCCA_RAT
<b>1155</b>	78kDa glucose-regulated protein	Rattus norvegicus	GRP78_RAT
<b>1161, 1165</b>	Heat shock cognate 71 kDa protein	Rattus norvegicus	HSP7C_RAT
<b>1163, 1164</b>	rCG56002	Rattus norvegicus	gil149036727
<b>1169, 1172, 1173, 1181, 1186</b>	Serum albumin	Rattus norvegicus	ALBU_RAT
<b>1191</b>	Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial	Cricetulus griseus	gil344249754
<b>1203</b>	UV excision repair protein RAD23 homolog B	Rattus norvegicus	RD23B_RAT
<b>1212</b>	PREDICTED: aldehyde dehydrogenase 8 family, member A1-like isoform 2	Rattus norvegicus	gil109460389
<b>1213</b>	Pyruvatekinase isozymes R/L	Rattus norvegicus	KPYR_RAT
<b>1216, 1219</b>	Protein disulfide-isomerase A3	Rattus norvegicus	PDIA3_RAT
<b>1217</b>	Liver carboxylesterase 4	Rattus norvegicus	EST4_RAT
<b>1226</b>	Formimidoyl transferase-cyclodeaminase	Rattus norvegicus	FTCD_RAT
<b>1229</b>	Calreticulin	Rattus norvegicus	CALR_RAT
<b>1231</b>	Methylmalonate-semialdehyde dehydrogenase[acylating], mitochondrial	Rattus norvegicus	MMSA_RAT
<b>1246</b>	Alpha-1-antiproteainase	Rattus norvegicus	A1AT_RAT
<b>1260, 1268</b>	Alanine-glyoxylate aminotransferase 2, mitochondrial	Rattus norvegicus	AGT2_RAT

Table 1 (continued)

Spot number	Protein name	Species	Swiss-Prot Acc. N°
1261	Glutathione synthetase	Rattus norvegicus	GSHB_RAT
1262	4-trimethylaminobutyraldehyde dehydrogenase	Rattus norvegicus	AL9A1_RAT
1270, 1277	Phenylalanine-4-hydroxylase	Rattus norvegicus	PH4H_RAT
1271	Succinate-semialdehyde dehydrogenase, mitochondrial	Rattus norvegicus	SSDH_RAT
1273	Hydroxymethylglutaryl-CoA synthase, mitochondrial	Rattus norvegicus	HMCS2_RAT
1275	Alpha-enolase	Rattus norvegicus	ENOA_RAT
1296	Ifl47 protein	Rattus norvegicus	gjl44890246
1298, 1301, 1310	Betaine-homocysteine S-methyltransferase 1	Rattus norvegicus	BHMT1_RAT
1300	Eukaryotic initiation factor 4A-II	Rattus norvegicus	IF4A2_RAT
1314	3-ketoacyl-CoA thiolase, mitochondrial	Rattus norvegicus	THIM_RAT
1323, 1326	Argininosuccinate synthase	Rattus norvegicus	ASSY_RAT
1332	Keratin, type I cytoskeletal 18	Rattus norvegicus	K1C18_RAT
1337	Aspartate aminotransferase, cytoplasmic	Rattus norvegicus	AATC_RAT
1341, 1345, 1354	Actin, cytoplasmic 1	Rattus norvegicus	ACTB_RAT
1344	Creatinekinase B-type	Rattus norvegicus	KCRB_RAT
1356	Aspartate aminotransferase, mitochondrial	Rattus norvegicus	AATM_RAT
1357	Serum paraoxonase/arylesterase2	Rattus norvegicus	PON2_RAT
1363, 1365	Fructose-bisphosphate aldolase B	Rattus norvegicus	ALDOB_RAT
1366	Serum paraoxonase/lactonase 3	Rattus norvegicus	PON3_RAT
1370, 1371, 1374, 1378, 1384	Fructose-1,6-bisphosphatase 1	Rattus norvegicus	F16P1_RAT
1381	Adipocyte plasmamembrane-associated protein	Rattus norvegicus	APMAP_RAT
1388	Farnesyl pyrophosphate synthase	Rattus norvegicus	FPPS_RAT
1391, 1393	Arginase-1	Rattus norvegicus	ARG11_RAT
1404, 1417	3-oxo-5-beta-steroid 4-dehydrogenase	Rattus norvegicus	AK1D1_RAT
1406	Glyceraldehyde-3-phosphate dehydrogenase	Rattus norvegicus	G3P_RAT
1412	3-alpha-hydroxy steroid dehydrogenase	Rattus norvegicus	DIDH_RAT
1420, 1429	Glycerol-3-phosphate dehydrogenase[NAD+], cytoplasmic	Rattus norvegicus	GPDA_RAT
1422	L-lactate dehydrogenase A chain	Rattus norvegicus	LDHA_RAT
1428	Beta-lactamase-like protein 2	Rattus norvegicus	LACB2_RAT

Table 1 (continued)

Spot number	Protein name	Species	Swiss-Prot Acc. N°
1433	Ester hydrolase C11 orf 54 homolog	Rattus norvegicus	CK054_RAT
1438	Sulfotransferase 1A1	Rattus norvegicus	ST1A1_RAT
1441, 1443	Thiosulfate sulfurtransferase	Rattus norvegicus	THTR_RAT
1445	Guanine nucleotide-binding protein subunit beta-2-like1	Rattus norvegicus	GBLP_RAT
1447	Regucalcin	Rattus norvegicus	RGN_RAT
1449	D-beta-hydroxybutyrate dehydrogenase, mitochondrial	Rattus norvegicus	BDH_RAT
1450	Hydroxyacyl-coenzyme A dehydrogenase, mitochondrial	Rattus norvegicus	HCDH_RAT
1460	Nitrilase homolog 1	Rattus norvegicus	NIT1_RAT
1463	Proteasome activator complex subunit1	Rattus norvegicus	PSME1_RAT
1471	Nicotinate-nucleotide pyrophosphorylase [carboxylating]	Rattus norvegicus	NADC_RAT
1473	Thiopurine S-methyltransferase	Rattus norvegicus	TPMT_RAT
1477, 1483	Electron transfer flavoprotein subunit beta	Rattus norvegicus	ETFB_RAT
1480	Isoamyl acetate-hydrolyzing esterase 1 homolog	Rattus norvegicus	IAH1_RAT
1486	Glutathione S-transferase Mu2	Rattus norvegicus	GSTM2_RAT
1488	Glutathione S-transferase alpha-5	Rattus norvegicus	GSTA5_RAT
1489	Peroxiredoxin-4	Rattus norvegicus	PRDX4_RAT
1495	protein ETHE1, mitochondrial	Rattus norvegicus	gil157819563
1496, 1509, 1510	Carbonic anhydrase 3	Rattus norvegicus	CAH3_RAT
1504	Endoplasmic reticulum resident protein 29	Rattus norvegicus	ERP29_RAT
1506	Glutathione S-transferase alpha-1	Rattus norvegicus	GSTA1_RAT
1507	Glutathione S-transferase alpha-2	Rattus norvegicus	GSTA2_RAT
1508	Glutathione S-transferase alpha-3	Rattus norvegicus	GSTA3_RAT
1512	Glutathione S-transferase alpha-4	Rattus norvegicus	GSTA4_RAT
1514	NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial	Rattus norvegicus	NDUV2_RAT
1522	Glutathione S-transferase P	Rattus norvegicus	GSTP1_RAT
1523	biliverdin reductase B (flavinreductase(NADPH)) (predicted), isoform CRA_c	Rattus norvegicus	gil149056527
1524	Peroxiredoxin-1	Rattus norvegicus	PRDX1_RAT
1528, 1530	Abhydrolase domain-containing protein 14B	Rattus norvegicus	ABHEB_RAT
1540	Peptidyl-prolyl cis-trans isomerase F, mitochondrial	Rattus norvegicus	PPIF_RAT
1543	Cofilin-1	Rattus norvegicus	COF1_RAT

**Table 1** (continued)

Spot number	Protein name	Species	Swiss-Prot Acc. N°
1544	Peptidyl-prolyl cis-trans isomerase A	Rattus norvegicus	PPIA_RAT
1547	Low molecular weight phosphotyryne protein phosphatase	Rattus norvegicus	PPAC_RAT
1550	Ubiquitin-conjugating enzyme E2D2	Rattus norvegicus	UB2D2_RAT
1560	Cytochrome b5	Rattus norvegicus	CYB5_RAT
1567–1569	Hemoglobin subunit alpha-1/2	Rattus norvegicus	HBA_RAT
1570, 1571	Fatty acid-binding protein, liver	Rattus norvegicus	FABPL_RAT
1586	Enoyl-CoA hydratase, mitochondrial	Rattus norvegicus	ECHM_RAT

missed cleavages allowed, 100 ppm tolerance in PMF, 0.75 Da mass tolerance for precursor ion mass, carbamidomethyl cysteine as fixed modification, oxidation of methionine and oxidation of tryptophan (single oxidation, double oxidation and kynurenin) as variable modifications. Identifications were considered to be significant when the combined MOWSE score had  $P < 0.05$ .

Statistics, including univariate analysis (ANOVA and *t*-test) and multivariate analysis (two way ANOVA), was performed using the Extended Data Analysis (EDA) module, which is present inside the Decyder 7.0 software package.

## Appendix A. Supplementary material

Supplementary data associated with this paper can be found in the online version at <http://dx.doi.org/10.1016/j.dib.2016.02.047>.

## References

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