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Supplemental Material

Linking Bisphenol S to Adverse Outcome Pathways Using a Combined Text Mining and Systems Biology Approach

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Table S1: List of the synonyms and identifiers for BPS

4,4'-Sulfonyldiphenol	ChemDiv3_000253	AK112768
Bisphenol S	EC 201-250-5	AN-24012
80-09-1	4,4'-Sulfonylbis[phenol]	CJ-00421
Phenol, 4,4'-sulfonylbis-	AC1L1MY1	SC-74946
Bis(4-hydroxyphenyl) sulfone	AC1Q78SH	SMR000554491
4,4'-Dihydroxydiphenyl sulfone	Cambridge id 5137133	ZB001898
4-Hydroxyphenyl sulfone	di-(4-Hydroxyphenyl)sulfone	AB0007499
Bis(p-hydroxyphenyl) sulfone	Oprea1_709121	KB-105037
4,4'-Sulfonylbisphenol	SCHEMBL18838	LS-105122
Diphone C	4-06-00-05809 (Beilstein Handbook Reference)	ST2410869
Bis(4-hydroxyphenyl)sulfone	KSC448A6N	TR-025385
4-(4-hydroxyphenyl)sulfonylphenol	MLS001195068	B0495
4,4'-Bisphenol S	4,4;-Dihydroxydiphenylsulfone	EU-0066997
Bis(p-hydroxyphenyl)sulfone	BIDD:ER0209	FT-0623040
BPS 1	bis(4-hydroxylphenyl) sulfone	ST50308058
1,1'-Sulfonylbis(4-hydroxybenzene)	Bis(4-hydroxyphenyl) sulphone	T8193
4,4-Sulfonyldiphenol	4,4'-Dihydroxydiphenylsulphone	4,4'-DIHYDROXYDIPHENYL SULFONE, TECH
P,P'-Dihydroxydiphenyl sulfone	ACMC-20977e	C14216
4,4'-Sulphonyldiphenol	4,4'-dihydroxy diphenylsulfone	4,4'-Dihydroxydiphenyl sulfone (4,4'-DHDPS)
NSC 8712	CHEMBL384441	4,4'-Dihydroxydiphenyl sulphone (4,4'-DHDPS)
PHENOL, 4,4'-SULFONYLDI-	4,4'-Sulfonyldiphenol, 98%	AB00275288-05
UNII-3OX4RR782R	DTXSID3022409	A839834
NSC 683541	CTK3E8066	I01-1512
CCRIS 2647	ZINC56964	W-104249
4-(4-hydroxybenzenesulfonyl)phenol	Bisphenol??S, analytical standard	Z57158549
EINECS 201-250-5	MolPort-000-279-673	F0266-0794
4-[(4-hydroxyphenyl)sulfonyl]phenol	HMS2866C04	4,4-Dihydroxydiphenyl Sulfone; Bis(4-hydroxyphenyl) Sulfone
BRN 2052954	4,4'-Sulfonyldiphenol, 99.7%	280144-23-2
4,4'-dihydroxydiphenylsulfone	PHENOL,3,3'-SULFONYLBIS-	98388-00-2
AI3-08667	KS-00000JP2	
3OX4RR782R	NSC-8712	
4,4'-Dihydroxydiphenyl sulphone	Tox21_201743	
CHEBI:34372	Tox21_302843	
NSC8712	ANW-13608	
4-(4-hydroxyphenylsulfonyl)phenol	BBL004108	
VPWNQTHUCYMVMZ-UHFFFAOYSA-N	SBB056786	
1,1'-Sulfonylbis[4-hydroxybenzene]	STK267009	

MFCD00002350	AKOS000119535	
NSC683541	DS-5781	
DSSTox_CID_2409	MCULE-1599233293	
DSSTox_RID_76579	NSC-683541	
DSSTox_GSID_22409	RP28900	
4,4'-Sulfonyldiphenol (4,4'-Dihydroxydiphenylsulfone)	RTR-025385	
CAS-80-09-1	IDI1_019571	
bisphenols	NCGC00164029-01	
HSDB 8087	NCGC00164029-02	
DHDPhS	NCGC00256437-01	
Phenol,4'-sulfonylbis-	NCGC00259292-01	
4,4\'-sulfonyldiphenol	AC-11720	
WLN: QR DSWR DQ	AJ-09513	

Table S2: List of the 109 publications mentioning BPS, and used to run the *AOP-helpFinder* tool to identify links between BPS and KE/MIE/AO.

Data source of information	RE*	AO**	MIE-KE**
biofax industrial bio-test laboratories (RTECS database)	1		
national technical information service (RTECS database)	2		necrosis
Naderi M, Wong MYL, Gholami F. 2014. Developmental exposure of zebrafish (Danio rerio) to bisphenol-S impairs subsequent reproduction potential and hormonal balance in adults. Aquat Toxicol 148:195–203; doi:10.1016/j.aquatox.2014.01.009.	3		decreased body length - decrease fertility - skewed sex ratio - decreased body weight
Crump D, Chiu S, Williams KL. 2016. Bisphenol S alters embryonic viability, development, gallbladder size, and messenger RNA expression in chicken embryos exposed via egg injection: Effects of BPS in chicken embryos. Environ Toxicol Chem 35:1541–1549;	4		decrease thyroid hormone synthesis - increased lethality
Ivry Del Moral L, Le Corre L, Poirier H, Niot I, Truntzer T, Merlin J-F, et al. 2016. Obesogen effects after perinatal exposure of 4,4′-sulfonyldiphenol (Bisphenol S) in C57BL/6 mice. Toxicology 357–358:11–20; doi:10.1016/j.tox.2016.05.023	5		hippocampal gene expression altered - increased triglyceride - altered gene expression - obesity - chronic high fat diet
Ullah H, Jahan S, Ain QU, Shaheen G, Ahsan N. 2016. Effect of bisphenol S exposure on male reproductive system of rats: A histological and biochemical study. Chemosphere 152:383–391; doi:10.1016/j.chemosphere.2016.02.125.	6		oxidative stress - production reactive oxygen species - increase reactive oxygen species production - increased reactive oxygen species - increase lipid peroxidation
Eladak S, Grisin T, Moison D, Guerquin M-J, N'Tumba-Byn T, Pozzi-Gaudin S, et al. 2015. A new chapter in the bisphenol A story: bisphenol S and bisphenol F are not safe alternatives to this compound. Fertil Steril 103:11–21; doi:10.1016/j.fertnstert.2014.11.005.	7		decreased testosterone
Catanese MC, Vandenberg LN. 2016. Bisphenol S (BPS) alters maternal behavior and brain in mice exposed during pregnancy/lactation and their daughters. Endocrinology en.2016-1723; doi:10.1210/en.2016-1723.	8		

Chen Y, Shu L, Qiu Z, Lee DY, Settle SJ, Que Hee S, et al. 2016. Exposure to the BPA-Substitute Bisphenol S Causes Unique Alterations of Germline Function. P.E. Cohen, ed PLOS Genet 12:e1006223; doi:10.1371/journal.pgen.1006223.	9		apoptosis
Kinch CD, Ibhazehiebo K, Jeong J-H, Habibi HR, Kurrasch DM. 2015. Low-dose exposure to bisphenol A and replacement bisphenol S induces precocious hypothalamic neurogenesis in embryonic zebrafish. Proc Natl Acad Sci 112:1475–1480; doi:10.1073/pnas.1417731112.	10	cancer	obesity
Ji K, Hong S, Kho Y, Choi K. 2013. Effects of Bisphenol S Exposure on Endocrine Functions and Reproduction of Zebrafish. Environ Sci Technol 47:8793–8800; doi:10.1021/es400329t.	11		increase plasma vitellogenin concentrations - impaired development - decreased testosterone
Wenhui Qiu, Zhao Y, Yang M, Farajzadeh M, Pan C, Wayne NL. 2016. Actions of Bisphenol A and Bisphenol S on the Reproductive Neuroendocrine System During Early Development in Zebrafish. Endocrinology 157:636–647; doi:10.1210/en.2015-1785.	12		increased neuronal synaptic inhibition
Liu J, Li J, Wu Y, Zhao Y, Luo F, Li S, et al. 2017. Bisphenol A Metabolites and Bisphenol S in Paired Maternal and Cord Serum. Environ Sci Technol 51:2456–2463; doi:10.1021/acs.est.6b05718.	13		
Mersha MD, Patel BM, Patel D, Richardson BN, Dhillon HS. 2015. Effects of BPA and BPS exposure limited to early embryogenesis persist to impair non-associative learning in adults. Behav Brain Funct 11; doi:10.1186/s12993-015-0071-y.	14	cancer	
Roelofs MJE, Berg M van den, Bovee TFH, Piersma AH, Duursen MBM va. 2015. Structural bisphenol analogues differentially target steroidogenesis in murine MA-10 Leydig cells as well as the glucocorticoid receptor. Toxicology 329:10–20; doi:10.1016/j.tox.2015.01.003.	15		activation glucocorticoid receptor - glucocorticoid receptor agonist activation - decreased androgen receptor activity - activation androgen receptor - increased glucocorticoid receptor activity
Schöpel M, Herrmann C, Scherkenbeck J, Stoll R. 2016. The Bisphenol A analogue Bisphenol S binds to K-Ras4B - implications for 'BPA-free' plastics. C. Griesinger, ed FEBS Lett 590:369–375; doi:10.1002/1873-3468.12056.	16	cancer	

Rochester JR, Bolden AL. 2015. Bisphenol S and F: A Systematic Review and Comparison of the Hormonal Activity of Bisphenol A Substitutes. Environ Health Perspect 123:643–650; doi:10.1289/ehp.1408989.	17		
Zhao C, Tang Z, Yan J, Fang J, Wang H, Cai Z. 2017. Bisphenol S exposure modulate macrophage phenotype as defined by cytokines profiling, global metabolomics and lipidomics analysis. Sci Total Environ 592:357–365; doi:10.1016/j.scitotenv.2017.03.035.	18		
Zhang R, Liu R, Zong W. 2016a. Bisphenol S Interacts with Catalase and Induces Oxidative Stress in Mouse Liver and Renal Cells. J Agric Food Chem 64:6630–6640; doi:10.1021/acs.jafc.6b02656.	19		oxidative stress - activation oxidative stress pathway - oxidative stress - apoptosis
Grignard E, Lapenna S, Bremer S. 2012. Weak estrogenic transcriptional activities of Bisphenol A and Bisphenol S. Toxicol In Vitro 26:727–731; doi:10.1016/j.tiv.2012.03.013.	20		
Thayer KA, Taylor KW, Garantziotis S, Schurman SH, Kissling GE, Hunt D, et al. 2016. Bisphenol A, Bisphenol S, and 4-Hydroxyphenyl 4-Isoprooxyphenylsulfone (BPSIP) in Urine and Blood of Cashiers. Environ Health Perspect 124:437–444; doi:10.1289/ehp.1409427.	21		
Ma M, Crump D, Farmahin R, Kennedy SW. 2015. Comparing the effects of tetrabromobisphenol-A, bisphenol A, and their potential replacement alternatives, TBBPA-bis(2,3-dibromopropyl ether) and bisphenol S, on cell viability and messenger ribonucleic acid expression in chicken embryonic hepatocytes: Effects of BPA-like chemicals on avian mRNA expression. Environmental Toxicology and Chemistry 34:391–401; doi:10.1002/etc.2814.	22		
Molina-Molina J-M, Amaya E, Grimaldi M, Sáenz J-M, Real M, Fernández MF, et al. 2013. In vitro study on the agonistic and antagonistic activities of bisphenol-S and other bisphenol-A congeners and derivatives via nuclear receptors. Toxicol Appl Pharmacol 272:127–136; doi:10.1016/j.taap.2013.05.015.	23		activation estrogen receptor alpha

Skledar DG, Schmidt J, Fic A, Klopčič I, Trontelj J, Dolenc MS, et al. 2016. Influence of metabolism on endocrine activities of bisphenol S. Chemosphere 157:152–159; doi:10.1016/j.chemosphere.2016.05.027.	24		
Peyre L, Rouimi P, de Sousa G, Héliès-Toussaint C, Carré B, Barcellini S, et al. 2014. Comparative study of bisphenol A and its analogue bisphenol S on human hepatic cells: A focus on their potential involvement in nonalcoholic fatty liver disease. Food Chem Toxicol 70:9–18; doi:10.1016/j.fct.2014.04.011.	25		
Viñas R, Watson CS. 2013b. Mixtures of xenoestrogens disrupt estradiol-induced non-genomic signaling and downstream functions in pituitary cells. Environ Health 12; doi:10.1186/1476-069X-12-26.	26		
Danzl E, Sei K, Soda S, Ike M, Fujita M. 2009a. Biodegradation of Bisphenol A, Bisphenol F and Bisphenol S in Seawater. Int J Environ Res Public Health 6:1472–1484; doi:10.3390/ijerph6041472.	27		
Guo H, Li H, Liang N, Chen F, Liao S, Zhang D, et al. 2016. Structural benefits of bisphenol S and its analogs resulting in their high sorption on carbon nanotubes and graphite. Environ Sci Pollut Res 23:8976–8984; doi:10.1007/s11356-016-6040-7.	28		
Le Fol V, Aït-Aïssa S, Cabaton N, Dolo L, Grimaldi M, Balaguer P, et al. 2015. Cell-Specific Biotransformation of Benzophenone-2 and Bisphenol-S in Zebrafish and Human in Vitro Models Used for Toxicity and Estrogenicity Screening. Environ Sci Technol 49:3860–3868; doi:10.1021/es505302c.	29		
Kang J, Choi J-S, Kim W-K, Lee Y-J, Park J-W. 2014. Estrogenic potency of bisphenol S, polyethersulfone and their metabolites generated by the rat liver S9 fractions on a MVLN cell using a luciferase reporter gene assay. Reprod Biol Endocrinol 12:102; doi:10.1186/1477-7827-12-102.	30		
Liao C, Liu F, Kannan K. 2012b. Bisphenol S, a New Bisphenol Analogue, in Paper Products and Currency Bills and Its Association with Bisphenol A Residues. Environ Sci Technol 46:6515–6522; doi:10.1021/es300876n.	31		

Wang X, Ma J, Wang Z, Guo R, Hu X. 2014. Aqueous phototransformation of bisphenol S: the competitive radical-attack pathway to p-hydroxybenzenesulfonic acid. Water Sci Technol 70:540–547; doi:10.2166/wst.2014.257.	32		production reactive oxygen species - increased reactive oxygen species
Boucher JG, Ahmed S, Atlas E. 2016a. Bisphenol S Induces Adipogenesis in Primary Human Preadipocytes From Female Donors. Endocrinology 157:1397–1407; doi:10.1210/en.2015-1872.	33	adipogenesis	
Vela-Soria F, Ballesteros O, Zafra-Gómez A, Ballesteros L, Navalón A. 2014b. UHPLC–MS/MS method for the determination of bisphenol A and its chlorinated derivatives, bisphenol S, parabens, and benzophenones in human urine samples. Anal Bioanal Chem 406:3773–3785; doi:10.1007/s00216-014-7785-9.	34		
Björnsdotter MK, Jonker W, Legradi J, Kool J, Ballesteros-Gómez A. 2017b. Bisphenol A alternatives in thermal paper from the Netherlands, Spain, Sweden and Norway. Screening and potential toxicity. Sci Total Environ 601–602:210–221; doi:10.1016/j.scitotenv.2017.05.171.	35		
Bruyere A, Hubert C, Le Vee M, Chedik L, Sayyed K, Stieger B, et al. 2017. Inhibition of SLC drug transporter activities by environmental bisphenols. Toxicol In Vitro 40:34–44; doi:10.1016/j.tiv.2016.12.009.	36		
Héliès-Toussaint C, Peyre L, Costanzo C, Chagnon M-C, Rahmani R. 2014. Is bisphenol S a safe substitute for bisphenol A in terms of metabolic function? An in vitro study. Toxicol Appl Pharmacol 280:224–235; doi:10.1016/j.taap.2014.07.025.	37	hepatic steatosis - steatosis	obesity
Castro B, Sánchez P, Torres JM, Ortega E. 2015. Bisphenol A, bisphenol F and bisphenol S affect differently 5α-reductase expression and dopamine–serotonin systems in the prefrontal cortex of juvenile female rats. Environ Res 142:281–287; doi:10.1016/j.envres.2015.07.001.	38		
Maćczak A, Cyrkler M, Bukowska B, Michałowicz J. 2017. Bisphenol A, bisphenol S, bisphenol F and bisphenol AF induce different oxidative stress and damage in human red blood cells (in vitro study). Toxicol In Vitro 41:143–149;	39		depletion gsh - production reactive oxygen species - increased reactive oxygen species - ros formation - increase lipid peroxidation

doi:10.1016/j.tiv.2017.02.018.			
Le Fol V, Brion F, Hillenweck A, Perdu E, Bruel S, Aït-Aïssa S, et al. 2017b. Comparison of the In Vivo Biotransformation of Two Emerging Estrogenic Contaminants, BP2 and BPS, in Zebrafish Embryos and Adults. Int J Mol Sci 18:704; doi:10.3390/ijms18040704.	40		
Viñas R, Watson CS. 2013a. Bisphenol S Disrupts Estradiol-Induced Nongenomic Signaling in a Rat Pituitary Cell Line: Effects on Cell Functions. Environ Health Perspect 121:352–358; doi:10.1289/ehp.1205826.	41		
Liao C, Liu F, Alomirah H, Loi VD, Mohd MA, Moon H-B, et al. 2012a. Bisphenol S in Urine from the United States and Seven Asian Countries: Occurrence and Human Exposures. Environ Sci Technol 46:6860–6866; doi:10.1021/es301334j.	42		
Kuruto-Niwa R, Nozawa R, Miyakoshi T, Shiozawa T, Terao Y. 2005. Estrogenic activity of alkylphenols, bisphenol S, and their chlorinated derivatives using a GFP expression system. Environ Toxicol Pharmacol 19:121–130; doi:10.1016/j.etap.2004.05.009.	43		
Cao G, Lu J, Wang G. 2012. Photolysis kinetics and influencing factors of bisphenol S in aqueous solutions. J Environ Sci China 24: 846–851.	44		
Gao X, Ma J, Chen Y, Wang H-S. 2015. Rapid Responses and Mechanism of Action for Low-Dose Bisphenol S on *ex Vivo* Rat Hearts and Isolated Myocytes: Evidence of Female-Specific Proarrhythmic Effects. Environ Health Perspect 123:571–578; doi:10.1289/ehp.1408679.	45		
Boucher JG, Gagné R, Rowan-Carroll A, Boudreau A, Yauk CL, Atlas E. 2016b. Bisphenol A and Bisphenol S Induce Distinct Transcriptional Profiles in Differentiating Human Primary Preadipocytes. H. Guillou, ed PLOS ONE 11:e0163318; doi:10.1371/journal.pone.0163318.	46	adipogenesis	activation lxr - liver fibrosis - hippocampal gene expression altered - alteration lipid metabolism - activation hepatic nuclear receptor(s) - altered gene expression - activated lxr

Asati A, Satyanarayana GNV, Panchal S, Thakur RS, Ansari NG, Patel DK. 2017. Ionic liquid based vortex assisted liquid–liquid microextraction combined with liquid chromatography mass spectrometry for the determination of bisphenols in thermal papers with the aid of response surface methodology. J Chromatogr A 1509:35–42; doi:10.1016/j.chroma.2017.06.040.	47		
Liang S, Yin L, Shengyang Yu K, Hofmann M-C, Yu X. 2017. High-Content Analysis Provides Mechanistic Insights into the Testicular Toxicity of Bisphenol A and Selected Analogues in Mouse Spermatogonial Cells. Toxicol Sci 155:43–60; doi:10.1093/toxsci/kfw178.	48		
Yang H, Hou G, Zhang L, Ju L, Liu C. 2017. Exploring the effect of bisphenol S on sludge hydrolysis and mechanism of the interaction between bisphenol S and α-Amylase through spectrophotometric methods. J Photochem Photobiol B 167:128–135; doi:10.1016/j.jphotobiol.2016.12.020.	49		
Chen S, Chang Q, Yin K, He Q, Deng Y, Chen B, et al. 2017. Rapid Analysis of Bisphenol A and Its Analogues in Food Packaging Products by Paper Spray Ionization Mass Spectrometry. J Agric Food Chem 65:4859–4865; doi:10.1021/acs.jafc.7b02061.	50		
Pivnenko K, Pedersen GA, Eriksson E, Astrup TF. 2015. Bisphenol A and its structural analogues in household waste paper. Waste Manag 44:39–47; doi:10.1016/j.wasman.2015.07.017.	51		
Rocha BA, Azevedo LF, Gallimberti M, Campiglia AD, Barbosa F. 2015. High Levels of Bisphenol A and Bisphenol S in Brazilian Thermal Paper Receipts and Estimation of Daily Exposure. J Toxicol Environ Health A 78:1181–1188; doi:10.1080/15287394.2015.1083519.	52		
Zhang T, Xue J, Gao C, Qiu R, Li Y, Li X, et al. 2016b. Urinary Concentrations of Bisphenols and Their Association with Biomarkers of Oxidative Stress in People Living Near E-Waste Recycling Facilities in China. Environ Sci Technol 50:4045–4053; doi:10.1021/acs.est.6b00032.	53		oxidative stress

Vela-Soria F, Ballesteros O, Zafra-Gómez A, Ballesteros L, Navalón A. 2014a. A multiclass method for the analysis of endocrine disrupting chemicals in human urine samples. Sample treatment by dispersive liquid–liquid microextraction. Talanta 129:209–218; doi:10.1016/j.talanta.2014.05.016.	54		
Xue J, Wan Y, Kannan K. 2016. Occurrence of bisphenols, bisphenol A diglycidyl ethers (BADGEs), and novolac glycidyl ethers (NOGEs) in indoor air from Albany, New York, USA, and its implications for inhalation exposure. Chemosphere 151:1–8; doi:10.1016/j.chemosphere.2016.02.038.	55		
Rajasärkkä J, Koponen J, Airaksinen R, Kiviranta H, Virta M. 2014. Monitoring bisphenol A and estrogenic chemicals in thermal paper with yeast-based bioreporter assay. Anal Bioanal Chem 406:5695–5702; doi:10.1007/s00216-014-7812-x.	56		
Maćczak A, Cyrkler M, Bukowska B, Michałowicz J. 2016. Eryptosis-inducing activity of bisphenol A and its analogs in human red blood cells (in vitro study). J Hazard Mater 307:328–335; doi:10.1016/j.jhazmat.2015.12.057.	57		
Wilkinson JL, Swinden J, Hooda PS, Barker J, Barton S. 2016. Markers of anthropogenic contamination: A validated method for quantification of pharmaceuticals, illicit drug metabolites, perfluorinated compounds, and plasticisers in sewage treatment effluent and rain runoff. Chemosphere 159:638–646; doi:10.1016/j.chemosphere.2016.06.039.	58		
Feng Y, Jiao Z, Shi J, Li M, Guo Q, Shao B. 2016. Effects of bisphenol analogues on steroidogenic gene expression and hormone synthesis in H295R cells. Chemosphere 147:9–19; doi:10.1016/j.chemosphere.2015.12.081.	59		reduction testosterone level
Liao C, Kannan K. 2014a. A Survey of Alkylphenols, Bisphenols, and Triclosan in Personal Care Products from China and the United States. Arch Environ Contam Toxicol 67:50–59; doi:10.1007/s00244-014-0016-8.	60		

Mokra K, Kuźmińska-Surowaniec A, Woźniak K, Michałowicz J. 2017. Evaluation of DNA-damaging potential of bisphenol A and its selected analogs in human peripheral blood mononuclear cells (in vitro study). Food Chem Toxicol 100:62–69; doi:10.1016/j.fct.2016.12.003.	61		increase dna damage - increased dna damage repair
Lu L, Yang Y, Zhang J, Shao B. 2014. Determination of seven bisphenol analogues in reed and Callitrichaceae by ultra performance liquid chromatography–tandem mass spectrometry. J Chromatogr B 953–954:80–85; doi:10.1016/j.jchromb.2014.02.003.	62		
Yang Y, Lu L, Zhang J, Yang Y, Wu Y, Shao B. 2014b. Simultaneous determination of seven bisphenols in environmental water and solid samples by liquid chromatography–electrospray tandem mass spectrometry. J Chromatogr A 1328:26–34; doi:10.1016/j.chroma.2013.12.074.	63		
Usman A, Ahmad M. 2016. From BPA to its analogues: Is it a safe journey? Chemosphere 158:131–142; doi:10.1016/j.chemosphere.2016.05.070.	64		
Rocha BA, da Costa BRB, de Albuquerque NCP, de Oliveira ARM, Souza JMO, Al-Tameemi M, et al. 2016. A fast method for bisphenol A and six analogues (S, F, Z, P, AF, AP) determination in urine samples based on dispersive liquid-liquid microextraction and liquid chromatography-tandem mass spectrometry. Talanta 154:511–519; doi:10.1016/j.talanta.2016.03.098.	65		
Lin X, Cheng C, Terry P, Chen J, Cui H, Wu J. 2017. Rapid and sensitive detection of bisphenol a from serum matrix. Biosens Bioelectron 91:104–109; doi:10.1016/j.bios.2016.12.024.	66		
Li N, Mruk DD, Lee WM, Wong CKC, Cheng CY. 2016. Is toxicant-induced Sertoli cell injury in vitro a useful model to study molecular mechanisms in spermatogenesis? Semin Cell Dev Biol 59:141–156; doi:10.1016/j.semcdb.2016.01.003.	67		
Toyama T, Ojima T, Tanaka Y, Mori K, Morikawa M. 2013. Sustainable biodegradation of phenolic endocrine-disrupting chemicals by Phragmites australis–rhizosphere bacteria association.	68		

Water Sci Technol 68:522–529; doi:10.2166/wst.2013.234.			
Choi YJ, Lee LS. 2017. Partitioning Behavior of Bisphenol Alternatives BPS and BPAF Compared to BPA. Environ Sci Technol 51:3725–3732; doi:10.1021/acs.est.6b05902.	69		
Lee S, Liu X, Takeda S, Choi K. 2013. Genotoxic potentials and related mechanisms of bisphenol A and other bisphenol compounds: A comparison study employing chicken DT40 cells. Chemosphere 93:434–440; doi:10.1016/j.chemosphere.2013.05.029.	70		
Yang Y, Guan J, Yin J, Shao B, Li H. 2014a. Urinary levels of bisphenol analogues in residents living near a manufacturing plant in south China. Chemosphere 112:481–486; doi:10.1016/j.chemosphere.2014.05.004.	71		
Liao C, Kannan K. 2013. Concentrations and Profiles of Bisphenol A and Other Bisphenol Analogues in Foodstuffs from the United States and Their Implications for Human Exposure. J Agric Food Chem 61:4655–4662; doi:10.1021/jf400445n.	72		
Andra SS, Charisiadis P, Arora M, van Vliet-Ostaptchouk JV, Makris KC. 2015. Biomonitoring of human exposures to chlorinated derivatives and structural analogs of bisphenol A. Environ Int 85:352–379; doi:10.1016/j.envint.2015.09.011.	73		obesity
Sun X, Wang J, Li Y, Jin J, Zhang B, Shah SM, et al. 2014. Highly selective dummy molecularly imprinted polymer as a solid-phase extraction sorbent for five bisphenols in tap and river water. J Chromatogr A 1343:33–41; doi:10.1016/j.chroma.2014.03.063.	74		
Desdoits-Lethimonier C, Lesné L, Gaudriault P, Zalko D, Antignac JP, Deceuninck Y, et al. 2017. Parallel assessment of the effects of bisphenol A and several of its analogs on the adult human testis. Hum Reprod 32:1465–1473; doi:10.1093/humrep/dex093.	75		

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* RE are the reference identifiers from the in-house database that are included in figure 3 for clarity of the figure.
**empty cells correspond to no or not relevant associations (e.g. 'increase' term observed alone) between BPS and an AO or MIE/KE term, identified with the *AOPhelp-Finder tool*.
*** the reference 104 has been removed, as it was a duplicate of RE 103

Table S3. List of the diseases (based on the MESH terms) associated to bisphenol S (BPS).

Disease	Score (*pS*)*	MESH ID
body weight	0.73	D001835
carcinogenesis	0.11	D063646
cholestasis	0.46	D002779
chromosome aberrations	0.79	D002869
death	0.27	D003643
dermatitis	0.36	D003872
diabetes mellitus	0.84	D003920
dyspnea	1	D004417
fibrosis	0.46	D005355
hemolysis	0.53	D006461
hepatic fibrosis	0.45	D008103
hepatitis	0.63	D006505
infertility	0.39	D007246
insulin receptor	0.82	D056731
lipid metabolism	0.90	D052439
obesity	0.93	D009765
osteosarcoma	0.16	D012516
overweight	0.56	D050177
poisoning	0.98	D011041
seizures	1	D012640
thyroiditis	0.92	D013966

* MESH: Medical Subject Headings. The position score (*pS*) reflects the position of the AO term in the abstract. A value close to 1 corresponds to a position at the end, which means that the association BPS-AO is more likely to be a finding.