

Supplementary Material S4

List of Potential Xenoestrogens according to literature

Naturally occurring					
Compound	Chemical Formula	M.Wt	CAS #	Occurrence and use	
1	20S-Protopanaxadiol	C ₃₀ H ₅₂ O ₃	460.7	30636-90-9	Gastrointestinal metabolic product of ginsenosides Metabolite of zearalenone, used as growth promoter in beef cattle in certain non-European Union countries
2	Alpha-zearalenol	C ₁₈ H ₂₄ O ₅	320.4	36455-71-7	Flavonoid
3	Apigenin	C ₁₅ H ₁₀ O ₅	270.24	520-36-5	phytoestrogen
4	Ferutinine	C ₂₂ H ₃₀ O ₄	358.5	41743-44-6	Sesquiterpenoid, Umbelliferae family
5	Formononetin	C ₁₆ H ₁₂ O ₄	268.26	485-72-3	Isoflavonoid, in red clover and soy extracts
6	Genistein	C ₁₅ H ₁₀ O ₅	270.24	446-72-0	Isoflavonoid, in red clover and soy extracts
7	Kaempferol	C ₁₅ H ₁₀ O ₆	286.24	520-18-3	Flavonoid phytoestrogen
8	1,5-Dibromo-2-(2,4-dibromophenoxy)-3-methoxybenzene	C ₁₃ H ₈ Br ₄ O ₂	515.8	102739-99-1	Occur naturally in marine organisms
9	Zearalenone	C ₁₈ H ₂₂ O ₅	318.4	17924-92-4	Mycotoxin, food contaminant
Industrial products and pollutants including organohalogens, plastic components, detergents					
1	3,9-Dihydroxy-benz[a]anthracene	C ₁₈ H ₁₂ O ₂	260.3	56614-97-2	Potential metabolite of benz[a]anthracene
2	3-Methylcholanthrene	C ₂₁ H ₁₆	268.4	56-49-5	PAH, mainly incomplete combustion
3	4-n-Octylphenol	C ₁₄ H ₂₂ O	206.32	1806-26-4	Intermediate in production of and degradation product of octylphenol ethoxylates used to in rubber, in pesticides and paints

4	4-Nonylphenol	C ₁₅ H ₂₄ O	220.35	104-40-5	Precursor to and degradation product of commercially important detergents
5	4-n-Propylphenol	C ₉ H ₁₂ O	136.19	645-56-7	Degradation product of surfactants
6	4-Tert-butyl 2-methylphenol	C ₁₁ H ₁₆ O	164.24	98-27-1	Industrial product and environmental contaminant
7	4-Tert-octylphenol	C ₁₄ H ₂₂ O	206.32	140-66-9	Used in the manufacture of nonionic surfactants
8	7,12-Dimethyl-benz(a)anthracene	C ₂₀ H ₁₅ F	274.3	737-22-4	PAH, mainly < incomplete combustion
9	Benzotriazole	C ₆ H ₅ N ₃	119.12	95-14-7	Anticorrosive agent used in aircraft de-icing, antifreeze fluids, and dishwasher detergents
10	Benzyl butyl phthalate	C ₁₉ H ₂₀ O ₄	312.4	85-68-7	Plasticizer for polyvinyl chloride in vinyl floor tiles, vinyl foam, and carpet backing, in cellulosic resins
11	Bisphenol A	C ₁₅ H ₁₆ O ₂	228.29	80-05-7	Used in the production of polycarbonate plastic and epoxy resins used as coatings on the inside of food and beverage cans
12	Dibutylphthalate	C ₁₆ H ₂₂ O ₄	278.34	84-74-2	Mainly used as plasticiser, also in paints, inks, and cosmetics
13	Dichlorostyrene	C ₈ H ₆ Cl ₂	173.04	50852-77-2	Intermediate in chemical industry
14	Dodecylphenol	C ₁₈ H ₃₀ O	262.4	27193-86-8	Used in phenol resins in adhesives and paints
15	Nonylphenols	C ₁₅ H ₂₄ O	220.35	25154-52-3	Precursor to and degradation product of commercially important detergents
16	Polybrominated diphenyl ether	C ₁₂ H ₄ Br ₆ O ₃	675.6	80246-27-1	Flame retardants used in plastics, foams, building materials, electronics,

					furnishings, motor vehicles
	Polychlorinated biphenyl	C12H4Cl6	360.9	32774-16-6	Industrial products, used as dielectric and coolant fluids
Substances used in personal care products					
				15087-24-8	UV filters, used in sunscreens and cosmetics
1	3-Benzylidene camphor	C17H20O	240.34		
	4,4-Dihydroxy-benzophenone	C13H10O3	214.22	611-99-4	UV filter, used in sunscreens and cosmetics
	4-Hydroxybenzoic acid n-butyl ester	C11H14O4	210.23	123910-88-3	Preservatives in foods, drugs, and personal products
	4-hydroxybenzoic acid ethyl ester	C9H10O3	166.17	120-47-8	UV filter, used in sunscreens and cosmetics
	4-hydroxybenzoic acid propyl ester	C10H12O3	180.2	94-13-3	UV filter, used in sunscreens and cosmetics
	4-Hydroxybenzophenone	C13H10O2	198.22	1137-42-4	Metabolite of UV filter, used in sunscreens and cosmetics
	4-Methylbenzylidene camphor	C18H22O	254.4	36861-47-9	UV filters, used in sunscreens and cosmetics
	Benzophenone-1	C13H10O3	214.22	131-56-6	UV filter, used in sunscreens and cosmetics
	Benzophenone-2	C13H10O5	246.21	131-55-5	UV filter, used in sunscreens and cosmetics
	Benzophenone-3	C14H12O3	228.24	131-57-7	UV filter, used in sunscreens and cosmetics
	Benzophenone-4	C14H12O6S	308.31	4065-45-6	UV filter, used in sunscreens and cosmetics
	Benzyl salicylate	C14H12O3	228.24	118-58-1	UV filter, used in sunscreens and cosmetics
13	Ethoxylated ethyl 4-amino benzoate				UV filter, used in sunscreens and cosmetics

14	Ethyl-4-aminobenzoate	C9H11NO2	165.19	94-09-7	UV filter, used in sunscreens and cosmetics
15	Eusolex 2292,	C18H26O3	290.4	5466-77-3	UV filter, used in sunscreens and cosmetics
16	Eusolex 6300,	C18H22O	254.4	36861-47-9	UV filter, used in sunscreens and cosmetics
17	Eusolex 6007,	C17H27NO2	277.4	21245-02-3	UV filter, used in sunscreens and cosmetics
18	Eusolex HMS				UV filter, used in sunscreens and cosmetics
19	Galaxolide (HHCB)	C18H26O	258.4	1222-05-5	Fragrance, used in sunscreens and cosmetics
20	Homosalate	C16H22O3	262.34	118-56-9	UV filter, used in sunscreens and cosmetics
21	Isopentyl-4-methoxycinnamate	C15H20O3	248.32	71617-10-2	UV filter, used in sunscreens and cosmetics
22	Octocrylene	C24H27NO2	361.5	6197-30-4	UV filter, used in sunscreens and cosmetics
23	Octyl dimethyl para amino benzoate	C17H27NO2	277.4	58817-05-3	UV filter, used in sunscreens and cosmetics
24	Octyl salicylate	C15H22O3	250.33	6969-49-9	UV filter, used in sunscreens and cosmetics
25	Octyl-methoxycinnamate	C18H26O3	290.4	83834-59-7	UV filter, used in sunscreens and cosmetics
26	Para amino-benzoic acid	C7H7NO2	137.14	150-13-0	UV filter, used in sunscreens and cosmetics
27	Phenyl salicylate	C13H10O3	214.22	118-55-8	UV filter, used in sunscreens and cosmetics
28	Tonalide (AHTN)	C18H26O	258.4	21145-77-7	UV filter, used in sunscreens and cosmetics

	Pesticides				
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1	2,4,5-Trichloro- phenoxyacetic acid 3-(2,2-Dichlorovinyl)- 2,2- dimethylcyclopropene carboxylic acid	C8H5Cl3O3	255.5	93-76-5	Herbicide, defoliant used in Agent Orange in Vietnam
2				55701- 05-8	Pyrethroid insecticide metabolite
3	3-Phenoxybenzoic acid	C13H10O3	214.22	3739- 38-6	Pyrethroid insecticide metabolite
4	Alachlor	C14H20ClNO2	269.77	15972- 60-8	Acid amide herbicide against grasses and broadleaf weeds. Use as herbicide banned in European Union (2006)
5	Aldrin	C12H8Cl6	364.9	309-00- 2	Organochlorine insecticide, widely used until 1970s
6	Atrazine	C8H14ClN5	215.68	1912- 24-9	Still widely used triazine herbicide, banned in the European Union
7	Azinphos-methyl	C10H12N3O3PS2	317.3	86-50-0	Organophosphate insecticide, banned in the European Union (2006)
8	Benomyl	C14H18N4O3	290.32	17804- 35-2	Carbamate fungicide has been used on fruits
9	Bromopropylate	C17H16Br2O3	428.1	18181- 80-1	Carbinol acaricide, used on fruits and legumes, in viticulture
10	Carbaryl	C12H11NO2	201.22	63-25-2	Carbamate insecticide, widely used in gardens, agriculture, and forestry
11	Chlomethoxyfen	C13H9Cl2NO4	314.12	32861- 85-1	Diphenyl ether herbicide, used on rice
12	Chlordane	C10H6Cl8	409.8	12789- 03-6	Organochlorine pesticide, banned in USA in 1988
13	Chlordecone	C10Cl10O	490.6	143-50- 0	Organochlorine insecticide and fungicide, banned by the Stockholm Convention on persistent organic pollutants
14	Chlornitrofen	C12H6Cl3NO3	318.5	1836- 77-7	Diphenyl ether herbicide

15	Chlorpropham	C10H12ClNO2	213.66	101-21-3	Carbamate herbicide and plant growth regulator
16	Chlorpyrifos	C9H11Cl3NO3PS	350.6	2921-88-2	Organophosphorus insecticide, highly used on corn and fruit trees, still frequently used in Danish greenhouses in 2001
17	Cycloprothrin	C26H21Cl2NO4	482.4	63935-38-6	Pyrethroid insecticide used in agriculture
18	Cyfluthrin	C22H18Cl2FNO3	434.3	68359-37-5	Pyrethroid insecticide, agriculture, home, garden
19	Cyhalothrin	C23H19ClF3NO3	449.8	68085-85-8	pyrethroid insecticide, agriculture, home, garden
20	Cypermethrin	C22H19Cl2NO3	416.3	52315-07-8	Pyrethroid insecticide, in agriculture, home, garden
21	Cyprodinil	C14H15N3	225.29	121552-61-2	Fungicide used in agriculture and on fruit
22	DDE	C14H8Cl4	318	72-55-9	DDT metabolite
23	DDT,	C14H9Cl5	354.5	50-29-3	Organochlorine pesticide. Banned
24	Deltamethrin	C22H19Br2NO3	505.2	52918-63-5	Pyrethroid insecticide, widely used, still frequently used in Danish greenhouses in 2001
25	Dichlorvos	C4H7Cl2O4P	220.97	62-73-7	Organophosphate insecticide widely used to control household pests, also on outdoor fruit, and vegetable crops. Frequently used in Danish greenhouses in 2001
26	Dicofol	C14H9Cl5O	370.5	115-32-2	Organochlorine pesticide for mite control on agricultural crops, ornamentals, and around buildings
27	Dieldrin	C12H8Cl6O	380.9	60-57-1	Organochlorine pesticide, now banned in many countries

28	Dimethomorph	C ₂₁ H ₂₂ ClNO ₄	387.9	110488-70-5	Cinnamic acid fungicide, used in agriculture (potatoes)
29	Endosulfan,	C ₉ H ₆ Cl ₆ O ₃ S	406.9	959-98-8	Organochlorine insecticide, banned by the Stockholm Convention (2011)
30	Endrin	C ₁₂ H ₈ Cl ₆ O	380.9	72-20-8	Organochlorine pesticide, used in agriculture. Now banned in many countries
31	Ethoxyquin	C ₁₄ H ₁₉ NO	217.31	91-53-2	Quinoline-based antioxidant used as a food preservative (E324) and a pesticide
32	Etofenprox	C ₂₅ H ₂₈ O ₃	376.5	80844-07-1	Pyrethroid insecticide used in homes (pet and foggers)
33	Fenarimol	C ₁₇ H ₁₂ Cl ₂ N ₂ O	331.2	60168-88-9	Heterocyclic organochlorine fungicide, used on ornamentals, trees, horticulture (frequently used in Danish greenhouses in 2001)
34	Fenbuconazole	C ₁₉ H ₁₇ ClN ₄	336.8	114369-43-6	Triazole fungicide used in agriculture, fruit
35	Fenhexamid	C ₁₄ H ₁₇ Cl ₂ NO ₂	302.2	126833-17-8	Fungicide, used on fruit, ornamentals, trees
36	Fenitrothion	C ₉ H ₁₂ NO ₅ PS	277.24	122-14-5	Organophosphorus insecticide, agriculture, grain storage
37	Fenthion	C ₁₀ H ₁₅ O ₃ PS ₂	278.3	55-38-9	Organothiophosphate insecticide, avicide, and acaricide, widely used in sugar cane, rice, field corn, beets, pome and stone fruit, citrus fruits, pistachio, cotton, olives, coffee, cocoa, vegetables, and vines
38	Fenvalerate	C ₂₅ H ₂₂ ClNO ₃	419.9	51630-58-1	Pyrethroid pesticide, agriculture, home, garden

39	Fludioxonil	C ₁₂ H ₆ F ₂ N ₂ O ₂	248.18	131341-86-1	Fungicide used on sowing-seed,vegetables, fruits, and ornamentals
40	Imazalil	C ₁₄ H ₁₄ Cl ₂ N ₂ O	297.2	35554-44-0	Imidazole fungicide: sowing seed, potatoes, and fruits after harvesting
41	Lindane	C ₆ H ₆ Cl ₆	290.8	319-84-6	Organochlorine insecticide, used to treat lice and scabies
42	Linuron	C ₉ H ₁₀ Cl ₂ N ₂ O ₂	249.09	330-55-2	Phenylureum herbicide: horticulture
43	Methiocarb	C ₁₁ H ₁₅ NO ₂ S	225.31	2032-65-7	Carbamate insecticide, still frequently used in Danish greenhouses in 2001
44	Methoxychlor	C ₁₆ H ₁₅ Cl ₃ O ₂	345.6	72-43-5	Organochlorine pesticide, used on crops, ornamentals, livestock, and pets against insects. Banned in the USA (2003) and European Union (2002)
45	Metolachlor	C ₁₅ H ₂₂ ClNO ₂	283.79	51218-45-2	Chloroacetanilide herbicide, grass and broadleaf weed control in agriculture
46	O-Phenylphenol	C ₁₂ H ₁₀ O	170.21	90-43-7	Fungicide, generally applied after harvest; used for waxing citrus fruits. As a food additive, it has E number E231
47	Pentachlorophenol	C ₆ Cl ₅ OH	266.3	87-86-5	Organochlorine pesticide: herbicide, insecticide, fungicide, antifouling paint, preservation of wood. Use now restricted
48	Permethrin	C ₂₁ H ₂₀ Cl ₂ O ₃	391.3	52645-53-1	Pyrethroid insecticide, agriculture, home, garden
49	Pirimicarb	C ₁₁ H ₁₈ N ₄ O ₂	238.29	23103-98-2	Carbamate insecticide: vegetable, cereal, and orchard crops

					Phosphorothioate insecticide: postharvest insecticide used on stored corn and sorghum grain and seed
50	Pirimiphos-methyl	C11H20N3O3PS	305.34	29232-93-7	Imidazole-type foliar fungicide: gardening and agriculture, still frequently used in Danish greenhouses in 2001.
51	Prochloraz	C15H16Cl3N3O2	376.7	67747-09-5	Dicarboximide fungicide: preharvest spray or postharvest dip of lupins, grapes, stone fruit, strawberries
52	Procymidone	C13H11Cl2NO2	284.13	32809-16-8	Carbamate fungicide: horticulture, ornamentals, agriculture
53	Propamocarb	C9H20N2O2	188.27	24579-73-5	Benzoylpyrazole herbicide
54	Pyrazoxyfen	C20H16Cl2N2O3	403.3	71561-11-0	Fungicide: fruit, vineyards
55	Pyrimethanil	C12H13N3	199.25	53112-28-0	Fungicide: cereals, beets, strawberries, some berries
56	Quinoxifen	C15H8Cl2FNO	308.1	124495-18-7	Triazole fungicide: agriculture. Assessed by the Swedish Chemicals Agency as potentially toxic;
57	Tebuconazole	C16H22ClN3O	307.82	107534-96-3	Pyrethroid insecticide: Primarily pressurized aerosols in household, industrial, commercial, and institutional settings
58	Tetramethrin	C19H25NO4	331.4	7696-12-0	Organophosphorous fungicide, still frequently used in Danish greenhouses in 2001
59	Tolclofos-methyl	C9H11Cl2O3PS	301.13	57018-04-9	Organochlorine insecticide (banned in many countries)
60	Toxaphene	C10H8Cl8	411.8	8001-35-2	Organochlorine insecticide: agriculture
61	Trans-nonachlor	C10H5Cl9	444.2	5103-73-1	

62	tribenuron-methyl	C ₁₅ H ₁₇ N ₅ O ₆ S	395.4	101200-48-0	Herbicide: grains; still frequently used in Danish greenhouses in 2001
63	Triflumizole	C ₁₅ H ₁₅ ClF ₃ N ₃ O	345.75	68694-11-1	Conazole fungicide: plant protection
64	Vinclozolin	C ₁₂ H ₉ Cl ₂ NO ₃	286.11	50471-44-8	Dicarboximide fungicide, used on fruits and vegetables, still frequently used in Danish greenhouses in 2001. Use now strictly regulated