

Supplementary Materials for

Ecotoxicological Evaluation of Bisphenol A and alternatives: A Comprehensive in silico Modelling Approach

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Table S1. Dataset of bisphenol alternatives utilized in the study.

| ID | EC/List No | CAS | Chemical Name | Common name |
|----|------------|-------------|---|---|
| 1 | 201-240-0 | 79-97-0 | 4,4'-isopropylidenedi-o-cresol | 3,3'-Dimethylbisphenol A; Dicresylolpropane, BPC |
| 2 | 201-245-8 | 80-05-7 | 4,4'-isopropylidenediphenol | BPA, bisphenol A |
| 3 | 204-137-9 | 116-37-0 | 1,1'-isopropylidenebis(p-phenyleneoxy)dipropyl-2-ol | Bisphenol A bis(2-hydroxypropyl) ether; BPA 2 PO |
| 4 | 212-985-6 | 901-44-0 | 2,2'-isopropylidenebis(p-phenyleneoxy)diethanol | Bisphenol A bis(2-hydroxyethyl) ether; BPA 2 EO |
| 5 | 214-590-4 | 1156-51-0 | 4,4'-isopropylidenediphenyl dicyanate | Bisphenol A cyanate ester; BADCy |
| 6 | 216-823-5 | 1675-54-3 | 2,2'-[(1-methylethylidene)bis(4,1-phenyleneoxymethylene)]bisoxirane | BISPHENOL A DIGLYCIDYL ETHER; BADGE |
| 7 | 217-121-1 | 1745-89-7 | 4,4'-isopropylidenebis[2-allylphenol] | Allyl bisphenol A; DAB |
| 8 | 227-033-5 | 5613-46-7 | 4,4'-isopropylidenedi-2,6-xylol | Tetramethylbisphenol A; TMBPA |
| 9 | 235-985-8 | 13080-86-9 | 4,4'-[isopropylidenebis(4,1-phenyleneoxy)]dianiline | BAPP |
| 10 | 242-895-2 | 19224-29-4 | 2,2'-[(1-methylethylidene)bis(4,1-phenyleneoxy)]bisethyl diacetate | SCHEMBL11889494, EINECS 242-895-2 |
| 11 | 248-607-1 | 27689-12-9 | (1-methylethylidene)bis(4,1-phenyleneoxy-3,1-propanediyl) bis-methacrylate | 2,2-bis-(4-(3-methacryloxypropoxy)phenyl)propane; BIS-PMA |
| 12 | 253-781-7 | 38103-06-9 | 4,4'-[(isopropylidene)bis(p-phenyleneoxy)]diphthalic dianhydride | 4,4'-Bisphenol A dianhydride; BPA-DA |
| 13 | 425-220-8 | 5945-33-5 | (1-methylethylidene)di-4,1-phenylene tetraphenyl diphosphate | Bisphenol A bis(diphenyl phosphate); BPA-DP |
| 14 | 432-380-2 | 147504-92-5 | 4,6-bis[2-(4-hydroxyphenyl)isopropylidene]resorcinol | HBPX-1 |
| 15 | 434-000-0 | n/a | 3-{2-[2,4-dihydroxy-5-(2-phenylpropan-2-yl)phenyl]propan-2-yl}phenyl 6-(-lambda5-diazynylidene)-5-methylidene-4a,5,6,8a-tetrahydronaphthalene-1-sulfonate | PURAM |

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| 16 | 216-367-7 | 1565-94-2 | (1-methylethylidene)bis[4,1-phenyleneoxy(2-hydroxy-3,1-propanediyl)] bismethacrylate | Silux; Bisphenol A glycidylmethacrylate |
| 17 | 223-123-3 | 3739-67-1 | 4,4'-isopropylidenebis[(allyloxy)benzene] | Bisphenol A bisallyl ether; 2,2-Bis(4-allyloxyphenyl)propane |
| 18 | 225-144-3 | 4687-94-9 | (1-methylethylidene)bis[4,1-phenyleneoxy(2-hydroxy-3,1-propanediyl)] diacrylate | Bisphenol a diglycidyl ether diacrylate |
| 19 | 246-263-7 | 24448-20-2 | (1-methylethylidene)bis(4,1-phenyleneoxy-2,1-ethanediyl) bismethacrylate | Bisphenol A bis(2-hydroxyethyl ether) dimethacrylate |
| 20 | 605-281-9 | 16224-36-5 | 4,4'-(1-Methylethyliden)-bis-[2,6-bis-(dimethylaminomethyl)-phenol] | Tetrakis(dimethylaminomethyl)bisphenol A |
| 21 | 605-913-3 | 181028-79-5 | [4-[2-(4-phosphonooxyphenyl)propan-2-yl]phenyl] dihydrogen phosphate | Bisphenol A diphosphate |
| 22 | 613-584-2 | 64401-02-1 | 2,2-Bis[4-(2-Acryloxyethoxy)phenyl]propane | Ethoxylated (2) bisphenol A diacrylate |
| 23 | 678-196-8 | 127-54-8 | 2,2-Bis(4-hydroxy-3-isopropylphenyl)propane | Bisphenol G; BPG |
| 24 | 678-197-3 | 24038-68-4 | 2,2-Bis(2-hydroxy-5-biphenyl)propane | Bisphenol PH; BPPH |
| 25 | 201-250-5 | 80-09-1 | 4,4'-sulphonyldiphenol | BPS |
| 26 | 235-986-3 | 13080-89-2 | 4,4'-[sulphonylbis(4,1-phenyleneoxy)]dianiline | n/a |
| 27 | 263-920-3 | 63134-33-8 | p-[p-benzyloxyphenyl]sulphonylphenol | BPS-MPE |
| 28 | 405-520-5 | 95235-30-6 | 4-(4-isopropoxyphenyl)sulphonylphenol | D8 (D88); D8(HPS); BPS-monoP |
| 29 | 411-570-9 | 41481-66-7 | 2,2'-diallyl-4,4'-sulfonyldiphenol | TG-SB, TG-SH, TG-SH(H) |
| 30 | 479-880-7 | 97042-18-7 | 4-(4-Allyloxy-benzenesulfonyl)phenol | BPS-MAE |
| 31 | 204-279-1 | 118-82-1 | 2,2',6,6'-tetra-tert-butyl-4,4'-methylenediphenol | TBMD; 4,4'-Methylenebis(2,6-DI-tert-butylphenol) |
| 32 | 210-658-2 | 620-92-8 | 4,4'-methylenediphenol | BPF |
| 33 | 218-257-4 | 2095-03-6 | 2,2'-[methylenebis(p-phenyleneoxymethylene)]bisoxirane | Bisphenol F diglycidyl ether; Bis(4-glycidyoxyphenyl)methane |
| 34 | 226-378-9 | 5384-21-4 | 4,4'-methylenedi-2,6-xyleneol | Tetramethyl Bisphenol F |
| 35 | 405-790-4 | 101657-77-6 | 4,4'-methylenebis(2,6-dimethylphenylcyanate) | n/a |

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| 36 | 439-910-1 | 93705-66-9 | 2-[[4-[[3,5-dimethyl-4-(oxiran-2-ylmethoxy)phenyl]methyl]-2,6-dimethylphenoxy]methyl]oxirane | YSLV-80XY |
| 37 | 908-912-9 | 1333-16-0 | 2-[(2-hydroxyphenyl)methyl]phenol | 2,2'-Bisphenol F |
| 38 | 433-130-5 | 1571-75-1 | 4-[1-(4-hydroxyphenyl)-1-phenylethyl]phenol | Bisphenol AP; BPAP |
| 39 | 811-683-7 | 1799707-26-8 | 4,4'-(1-phenylethane-1,1-diyl)bis(heptyloxybenzene) | n/a |
| 40 | 201-025-1 | 77-40-7 | 4-[2-(4-hydroxyphenyl)butan-2-yl]phenol | Bisphenol B; BPB |
| 41 | 679-999-6 | 1844-01-5 | 4,4'-Dihydroxytetraphenylmethane | BPBP |
| 42 | 238-940-0 | 14868-03-2 | 4-[2,2-dichloro-1-(4-hydroxyphenyl)ethenyl]phenol | Bisphenol C; BPC2 (BPC12) |
| 43* | 945-909-1 | 69415-01-6 | bis(2-[[4-(2,2-dichloro-1-{4-[(oxiran-2-yl)methoxy]phenyl]ethylphenoxy]methyl]oxirane) | 1,1-Bis(p-hydroxyphenyl)-2,2-dichloroethylene diglycidyl ether |
| 44 | 627-637-2 | 2081-08-5 | 4-[1-(4-hydroxyphenyl)ethyl]phenol | Bisphenol E; BPE |
| 45 | 405-740-1 | 47073-92-7 | 4,4'-ethylidenediphenyl dicyanate | 1,1-Bis(4-cyanatophenyl)ethane |
| 46 | 404-470-1 | n/a | 2-[[4-(9-{4-[(oxiran-2-yl)methoxy]phenyl}-9H-fluoren-9-yl)phenoxy]methyl]oxirane | EPIKOTE 1079 |
| 47 | 406-950-6 | 3236-71-3 | 9,9-bis(4-hydroxyphenyl)fluorene | BPFL; Fluorene-9-bisphenol |
| 48 | 428-970-4 | 13595-25-0 | 4,4'-(1,3-phenylene-bis(1-methylethylidene))bis-pheno | Bisphenol M; BPM |
| 49 | 606-820-0 | 2167-51-3 | 4,4'-(1,4-Phenylenediisopropylidene)bisphenol | Bisphenol P; BPP |
| 50 | 404-140-7 | 129188-99-4 | 1,1-Bis(4-hydroxyphenyl)-3,3,5-trimethylcyclohexane | BISPHENOL TMC; BP-TMC |
| 51 | 212-677-1 | 843-55-0 | 4,4'-cyclohexylidenebisphenol | Bisphenol Z; BPZ |
| 52 | 219-110-7 | 2362-14-3 | Phenol, 4,4'-cyclohexylidenebis[2-methyl- | 4,4'-cyclohexylidenedi-o-cremol |
| 53 | 810-464-3 | 13446-84-9 | 2,2'-[cyclohexane-1,1-diylbis(4,1-phenyleneoxymethylene)]dioxirane | 1,1-Bis[4-(glycidyloxy)phenyl]cyclohexane |
| 54 | 216-036-7 | 1478-61-1 | 4,4'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]diphenol | Bisphenol AF; BPAF |
| 55* | 278-305-5 | 75768-65-9 | benzyltriphenylphosphonium,salt with 4,4'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis[phenol] (1:1) | BPAF-salt |
| 56 | 425-060-9 | n/a | disodium 4-[1,1,1,3,3,3-hexafluoro-2-(4-oxidophenyl)propan-2-yl]benzen-1-olate | T-6627 |

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| 57* | 468-740-0 | n/a | Tributyl-2-methoxypropylphosphonium salt with 4,4'-[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]bis[phenol] | BPAF-salt |
| 58 | 469-080-6 | 1478-61-1 | 4-[1,1,1,3,3,3-hexafluoro-2-(4-hydroxyphenyl)propan-2-yl]phenol | BPAF-salt |
| 59* | 479-100-5 | 577705-90-9 | benzyl(diethylamino)diphenylphosphonium 4-[1,1,1,3,3,3-hexafluoro-2-(4-hydroxyphenyl)propan-2-yl]phenolate | BPAF-salt |
| 60 | 201-618-5 | 85-60-9 | 6,6'-di-tert-butyl-4,4'-butylidenedi-m-cresol | Santowhite |
| 61 | 210-039-7 | 603-41-8 | p,p'-(2-pyridylmethylene)bisphenol | DDPM |
| 62 | 217-420-7 | 1843-03-4 | 4,4',4''-(1-methylpropanyl-3-ylidene)tris[6-tert-butyl-m-cresol] | Topanol CA |
| 63 | 255-002-6 | 40615-36-9 | 1,1'-(chlorophenylmethylene)bis[4-methoxybenzene] | DMT-Cl |
| 64 | 255-003-1 | 40615-39-2 | 5'-O-(p,p'-dimethoxytrityl)thymidine | DMT-T |
| 65 | 401-720-1 | n/a | 2,2-bis(4'-hydroxyphenyl)-4-methylpentane | n/a |
| 66 | 405-800-7 | 27955-94-8 | 4,4',4''-(ethan-1,1,1-triyl)triphenol | n/a |
| 67 | 433-980-7 | n/a | 4-[1,3,5-tris(4-hydroxyphenyl)pentan-3-yl]phenol | CHEMICAL CODE NO 1592 |
| 68 | 610-104-3 | 43100-47-6 | 3-phenyl-5-(1,1,1-trifluoro-2-{6-hydroxy-5-phenyl-[1,1'-biphenyl]-3-yl}propan-2-yl)-[1,1'-biphenyl]-2-ol | n/a |
| 69 | 680-046-1 | 74462-02-5 | 4,4'-(2-ethylhexane-1,1-diyl)diphenol | BisP-IOTD |
| 70 | 201-236-9 | 79-94-7 | 2,6-dibromo-4-[2-(3,5-dibromo-4-hydroxyphenyl)propan-2-yl]phenol | Tetrabromobisphenol A; TBBPA |
| 71 | 221-346-0 | 3072-84-2 | 2-[[2,6-dibromo-4-[2-[3,5-dibromo-4-(oxiran-2-ylmethoxy)phenyl]propan-2-yl]phenoxy]methyl]oxirane | Tetrabromobisphenol A diglycidyl ether; TBBPA-bGE |
| 72 | 244-617-5 | 21850-44-2 | 1,3-dibromo-5-[2-[3,5-dibromo-4-(2,3-dibromopropoxy)phenyl]propan-2-yl]-2-(2,3-dibromopropoxy)benzene | Tetrabromobisphenol A bis(dibromopropyl ether); TBBPA-bDiBPrE |

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| 73 | 246-850-8 | 25327-89-3 | 1,3-dibromo-5-[2-(3,5-dibromo-4-prop-2-enoxyphenyl)propan-2-yl]-2-prop-2-enoxybenzene | Tetrabromobisphenol A diallyl ether; TBBPA-bAE |
| 74 | 253-693-9 | 37853-61-5 | 1,3-dibromo-5-[2-(3,5-dibromo-4-methoxyphenyl)propan-2-yl]-2-methoxybenzene | Tetrabromobisphenol A dimethyl ether; TBBPA-bME |
| 75 | 306-832-3 | 97416-84-7 | 1,1'-(Isopropylidene)bis(3,5-dibromo-4-(2,3-dibromo-2-methylpropoxy)benzene) | n/a |
| 76 | 436-220-2 | n/a | 2,2-bis(3,5-dibromo-4-(3-acryloyloxy-2-hydroxypropoxy)phenyl)propane | n/a |

* Compounds with disconnected structure.