## SI 2: Structural alerts

**Supplemental information** to:

Screening for potential endocrine disruptors in fish: evidence from structural alerts and *in vitro* and *in vivo* toxicological assays

Monika Nendza (nendza@al-luhnstedt.de), Analytical Laboratory, Bahnhofstr. 1, 24816 Luhnstedt, Germany \*

Andrea Wenzel (andrea.wenzel@ime.fraunhofer.de) and Martin Müller (martin.mueller@ime.fraunhofer.de), Fraunhofer Institute for Molecular Biology and Applied Ecology IME, Auf dem Aberg 1, 57392 Schmallenberg, Germany

Geertje Lewin (g.lewin@web.de) and Nelly Simetska (nelly.simetska@item.fraunhofer.de), Fraunhofer Institute for Toxicology and Experimental Medicine ITEM, Nikolai-Fuchs-Str. 1, 30625 Hannover, Germany

Frauke Stock (frauke.stock@uba.de) and Jürgen Arning (Juergen.Arning@uba.de), German Environment Agency UBA, Wörlitzer Platz 1, 06844 Dessau-Roßlau, Germany

The following tables provide a collection of structural alerts from the literature to detect potential endocrine disruptors (EDs) (Table SI 2A: Chemical structures related to interactions with estrogen receptors, Table SI 2B: Chemical structures related to interactions with androgen receptors). Most currently known EDs operate via sexual endocrine pathways and estrogenic and androgenic EDs (EA-EDs) are thus an important group of possible SVHC candidates under REACH. The experimental data that were analysed to derive the structural alerts, cover sexual endocrine activities of substances, the effects of which are mediated by competitive interactions with EA receptors. Accordingly, the structural alerts derived with these data are limited to the identification of potential EA-EDs.

Notably, many chemicals are potential ligands of both, the estrogen and androgen receptors. Substantial similarity of EA receptors regarding their binding sites can thus be assumed. Only a few chemical classes interact only with one of these receptor families, such as phthalates [1].

**Table SI 2A: Chemical structures related to interactions with estrogen receptors. MP: Structure of the pharmacophore, MS: Substructure.**

| **Chemical structure** | **MP** | **MS** | **Structural alert (SA)** | **Description** | **Endpoint** | **Binding affinity** | **Data set**  | **Comments** | **References** |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Steroids** |  |  |  |  |  |  |  |  |  |
|  | ⮟ |  | SA 01 steroid backbone with any pattern of double bonds | Steroid backbone (with aromatic A Ring) | ER binding | strong | Training set: n=232(NCTR) | Steroid backbone of 17ß-estradiol | DSSTox [2] |
|  | ⮟ |  | SA 01 steroid backbone with any pattern of double bonds | Steroid backbone | ER binding | --- | Training set: n=232(NCTR) | any pattern of bonds | Hong et al. [3] |
|  | ⮟ |  | SA 02partial steroid structure without restrictions (see comments), conservative approach | Partial steroid structure | ER binding | --- | Diverse literature dataStatistics: r²=0.96sensitivity:100%specificity: NA | C1, C2: aromaticC3: aromatic, aliphaticC4: aliphatic | Klopman & Chakravati [4] |
|  | ⮟ |  | SA 03partial steroid structure without restrictions (see comments), conservative approach | Partial steroid backbone | ER binding | --- | Diverse literature data | C1, C2: aromaticC3: aromatic, aliphaticC4: aliphatic | Klopman & Chakravati [5] |
| **DES** |  |  |  |  |  |  |  |  |  |
|  | ⮟ |  | SA 04 without restrictions (see comments), conservative approach | DES backbone | ER binding | strong | Training set: N=232(NCTR) | DES has p-OH on both ringsR is not definedEthyl substitution of the ethenyl bridge allowed  | DSSTox [2] |
|  | ⮟ |  | SA 05 without restrictions (see comments), conservative approach | DES backbone (hexestrol derivative) | ER binding | strong | Training set: N=232(NCTR) | p-OH or p-OR on one ringR is not definedMethyl, ethyl substitution of the ethenyl bridge allowed | DSSTox [2] |
|  | ⮟ |  | SA 06 | DES backbone (including mostphytoestrogens [6]) | ER binding | --- | Training set: N=232(NCTR) | Any binding of substituents, bridge | Hong et al. [3] |
|  | ⮟ |  |  | 2 aromatic rings, connected by 2 C atomsexamples: steroids, biogenic estrogens, diphenylethanes | ER RBA % | log RBA %: +2,60 to -3,671 of 5 inactive | 188 diverse structures (100 binding, 88 non-binding)  | Stronger activity than compounds with only 1 ring or 2 rings connected by 1 C atom Binding of agonists as well as antagonists | Blair et al. [1] |
|  | ⮟ |  | SA 07 without restrictions (see comments), conservative approach | DES backbone (triphenylethylen derivative) | ER binding | strong | Training set: N=232(NCTR) | Antiestrogenes Ethyl and alkoxyamine substitution allowed 4-OH substitution allowed | DSSTox [2] |
| **Phytoestrogenes** |  |  |  |  |  |  |  |  |  |
|  | ⮟ |  | SA 08 without restrictions (see comments), conservative approach | PhytoestrogenesFlavones | ER binding | weak | Training set: N=232(NCTR) | Includes DES backbone, OH substituents on one or more rings allowed | DSSTox [2] |
|  | ⮟ |  | SA 09 without restrictions (see comments), conservative approach | PhytoestrogenesFlavones | ER binding | weak | Training set: N=232(NCTR) | Includes DES backbone, OH substituents on one or more rings allowed | DSSTox [2] |
|  | ⮟ |  | SA 10 without restrictions (see comments), conservative approach | PhytoestrogenesIsoflavones | ER binding | weak | Training set: N=232(NCTR) | Includes DES backbone, one or more OH or OR substituents on one or more rings allowed  | DSSTox [2] |
|  | ⮟ |  | SA 11 without restrictions (see comments), conservative approach | PhytoestrogenesCoumestanes | ER binding | weak to moderate | Training set: N=232(NCTR) | Includes DES backbone, at C4: ethyl substitution or O-bridge to C2’ allowedat C4’: OH and OCH3 substitution allowed | DSSTox [2] |
|  | ⮟ |  | SA 12 without restrictions (see comments), conservative approach | PhytoestrogenesChalcanoides | ER binding | weak | Training set: N=232(NCTR) | Very similar to flavanonesp-OH substitution at one or both rings allowed | DSSTox [2] |
|  | ⮟ |  | SA 13 without restrictions (see comments), conservative approach, double bond C11=C12 considered | Mycoestrogenes | ER binding | weak to moderate | Training set: N=232(NCTR) | Double bond C11=C12 allowedOH or Oxo substitution at C7 allowed | DSSTox [2] |
|  |  |  |  | Flavonoides | estrogenic gene expressionEC50 [mol/l] | 8 of 15 inactive | 120 aromatic compounds | --- | Schultz et al. [7] |
| **Diphenylmethanes** |  |  |  |  |  |  |  |  |  |
|  | ⮟ |  | SA 14 | 2 aromatic rings separated by 1 C atom Examples: Bisphenol A derivatives, benzophenones | ER RBA % | log RBA %: +2,60 to -3,672 of 8 inactive | 188 diverse structures (100 binding, 88 non-binding) | Less active than 2 aromatic rings separated by 2 C atoms Binding of agonists as well as antagonists | Blair et al. [1] |
|  | ⮟ |  | SA 14 (conservative version) | DiphenylmethanesDiphenolalkanes | ER binding | weak | Training set: N=232(NCTR) | 3. ring at C bridge alloweddiverse substituents at C bridge and phenol rings allowed4-OH required for binding2,6-bulk reduces binding affinity  | DSSTox [2] |
|  | ⮟ |  | SA 15 benzophenone with any substitution | Diphenylmethanes Benzophenones | ER binding | weak | Training set: N=232(NCTR) | min. 1 phenolic ringCarbonyl or sulfonyl bridgediverse OH and OCH3 substitution allowed | DSSTox [2] |
|  | ⮟ |  |  | Benzophenones | ER RBA % | 3 of 5 inactive | 188 diverse structures | --- | Blair et al. [1] |
|  | ⮟ |  |  | Benzophenones | estrogenic gene expressionEC50 [mol/l] | 8 of 15 inactive | 120 aromatic compounds | --- | Schultz et al. [7] |
|  | ⮟ |  | SA 16 without restrictions (see comments), conservative approach | DiphenylmethanesDDTs | ER binding | weak | Training set: N=232(NCTR) | CClx (x=2 or 3) with single or double bond to C bridgediverse OH, OCH3 and Cl substitution allowed | DSSTox [2] |
|  | ⮟ |  | SA 17 any substitution allowed, conservative approach | Methoxychlor analoga | ER RBA % | 2 of 7 inactive | 188 diverse structures | -X: =CCl2, -CCl3R1, R2: H, OH, OMe | Blair et al. [1] |
|  | ⮟ |  | SA 17 | DDT analogs and bisphenols | ER binding | --- | Training set: N=232(NCTR) | OH, Cl substitution at aromatic rings allowedAlkyl, Cl substitution at bridge allowed | Shi et al. [6] |
| **Biphenyls** |  |  |  |  |  |  |  |  |  |
|  | ⮟ |  | SA 18 | PCBs | Antiestrogenic in MCF-7 cells | --- | Cl6, Cl5 and Cl4 PCBs, div. Aroclors | koplanar PCBs are more active, mono-ortho-koplanar PCBs are active only at high concentrationsAroclors are inactive  | Krishnan & Safe [8] |
|  | ⮟ |  |  | PCBs | competitive ER binding | --- | 4 OH PCBs | non-koplanar PCBs (= ortho substitution) are estrogenic | Waller et al. [9] |
|  | ⮟ |  |  | PCBs | competitive ER binding | --- | 4 OH PCBs | ↑ binding affinity with: ↑ size and ↓ branching↑ HOMO-LUMO-Gap | Bradbury et al. [10] |
|  | ⮟ |  |  | PBBs | DR-CALUX | --- | 2 PCBs1 PBB | polybrominated biphenyls can bind to AhR, probably in non-coplanar conformation | Navas et al. [11] |
|  | ⮟ |  |  | PBBs | ER RBA % | 3 of 9 inactive | 188 diverse structures | --- | Blair et al. [1] |
|  | ⮟ |  |  | Biphenyls | ER RBA % | 1 of 3 inactive | 188 diverse structures | Active: 4-phenylphenol, 3-phenylphenolInactive: 2-phenylphenol | Blair et al. [1] |
|  | ⮟ |  |  | Biphenyls | estrogenic gene expressionEC50 [mol/l] | 3 of 21 inactive | 120 aromatic compounds | --- | Schultz et al. [7] |
|  | ⮟ |  | SA 19 with or without OH substitution (conservative approach) | Biphenyls (polychlorinated) | ER binding | weak | Training set: N=232(NCTR) | ≥1 Cl substituentOH substitution allowed | DSSTox [2] |
|  | ⮟ |  | SA 20 | Biphenyls (not chlorinated) | ER binding | weak | Training set: N=232(NCTR) | min. 1 phenolic ring | DSSTox [2] |
| **Dioxins, Furans** |  |  |  |  |  |  |  |  |  |
|  | ⮟ |  | SA 21 | Dibenzodioxins | Antiestrogenic in MCF-7 cells | --- | Cl5 dibenzodioxins | Most activity with 4 lateral Cl (position 2,3,7,8) | Krishnan & Safe [8] |
|  | ⮟ |  | SA 22 | Dibenzofurans | Antiestrogenic in MCF-7 cells | --- | Cl4 and Cl5 dibenzofurans | Most activity with 4 lateral Cl (position 2,3,7,8) | Krishnan & Safe [8] |
| **Phthalates** |  |  |  |  |  |  |  |  |  |
|  | ⮟ |  | SA 23 | Phthalates | ER RBA % | 8 of 8 inactive | 188 diverse structures | Phthalates bind to AR, but not to ER! | Blair et al. [1] |
| **Phenols** |  |  |  |  |  |  |  |  |  |
|  | ⮟ | ⮟ | all phenols are covered by SA 26  | Alkylphenols | ER binding | very weak | Training set: N=232(NCTR) | diverse Cl or alkyl substitution allowed↑ binding affinity with ↑ log *K*OW (para-substituted), maximum at C9 | DSSTox [2] |
|  | ⮟ | ⮟ |  | Alkylphenols | ER RBA % | 3 of 21 inactive | 188 diverse structures | diverse Cl or alkyl substitutioninactive: 2-ethylphenol, eugenol, isoeugenol | Blair et al. [1] |
|  | ⮟ | ⮟ | SA 24 | Parabens | ER binding | very weak | Training set: N=232(NCTR) | para-substitution required↑ binding affinity with ↑ log *K*OW | DSSTox [2] |
|  | ⮟ | ⮟ |  | Parabens | ER RBA % | 0 von 7inactive | 188 diverse structures | --- | Blair et al. [1] |
|  | ⮟ | ⮟ | SA 25 | Alkoxyphenols | ER binding | very weak | Training set: N=232(NCTR) | diverse alkoxy substitution  | DSSTox [2] |
|  |  | ⮟ |  | Phenols | --- | --- | --- | No ortho substitution, meta- para-: bulky, hydrophobic substitution | Katzenellenbogen [12] |
|  |  | ⮟ |  | Phenols | ER binding | --- | Training set: N=232(NCTR) | Not specified | Hong et al. [3] |
|  |  | ⮟ |  | Phenols | ER RBA % | --- | 188 diverse structures | ↑ binding affinity with ↑ chain length (maximum at ~ C8) | Blair et al. [1] |
|  |  | ⮟ |  | Phenols | estrogenic gene expressionEC50 [mol/l] | --- | 29 Alkylphenols | ↑ binding affinity with: ↑ chain length (≥3, max. 8)↑ branching ↑ ortho → meta → para  | Routledge & Sumpter [13] |
|  |  | ⮟ |  | Phenols | estrogenic gene expressionEC50 [mol/l] | --- | 29 Alkylphenols from [13] | Decision trees:Lmax (~chain length)Distance O\_C(sp³) (~branching)LUMO (~preferred para-substitution) | Schmieder et al. [14] |
|  |  | ⮟ |  | Phenols | estrogenic gene expressionEC50 [mol/l] | --- | 120 aromatic compounds | p-substitution: hydrophobic, >3 atoms | Schultz et al. [7] |
|  |  | ⮟ |  | Phenols | ER binding | --- | Diverse literature data Statistics:r²=0,90Sensitivity 99%Specificity 77% | No ortho-substitution, max. 1 meta-substituent, para-substituent allowedalternative: 1 or 2 OH or Cl in ortho positionModulators: ↑ binding affinity with: ↑ *K*OW, 2. OH at 12,8 Å distance  | Klopman & Chakravati [4] |
|  |  | ⮟ |  | Phenols | ER binding | --- | Diverse literature data | No ortho-substitution, max. 1 meta-substituent, para-substituent allowedalternative: 2 meta substituents and/or 1 para-substituent  | Klopman & Chakravati [5] |
|  |  | ⮟ |  | Phenols | Diverse | --- | Diverse literature data | No ortho-Alkyl substitution | Jordan et al. [15] |
| **Diverse structures** |  |  |  |  |  |  |  |  |  |
| --- |  |  |  | Pesticides | ER RBA % | 18 von 19inactive | 188 diverse structures | Active: keponeInactive: 2,4,5-T, 2,4-D, α-chlordane, alachlor, aldrin, atrazin, carbaryl, carbofuran, dieldrin, endosulfan, heptachlor, hexachlorbenzene, lindane, metolachlor, mirex, prometon, simazin, vinclozolin | Blair et al. [1] |
|  |  |  |  | “miscellaneous compounds“ | ER RBA % | --- | 188 diverse structures | Inactive:All tested - acids (N=4)- alcohols (N=4)- aldehydes (N=3)- amines (N=5)- hydrocarbons (N=6)Active:- 2 of 5 ethers/esters(4-heptyloxyphenol, 4-benzyloxyphenol)- 4 of 11 “others“(aurin, nordihydroguaiaretic acid, phenol red, phenolphthalein) | Blair et al. [1] |
| **Other substructures** |  |  |  |  |  |  |  |  |  |
|  |  |  | SA 27 | Ketonic carbonyl | ER binding | --- | Diverse literature data | No ortho-substitution, max. 1 meta substituent, para-substitution allowed | Klopman & Chakravati [4] |
|  |  | ⮟ | NOT used as structural alert, see comment | Single aromatic ring | ER RBA % | log RBA %: +2,60 to -3,67 | 188 diverse structures (100 binding, 88 non-binding) | Less active than 2 aromatic rings separated by 2 C atomsExamples: alkylphenols, phthalates, parabensBinding of agonists as well as antagonists | Blair et al. [1] |
|  |  | ⮟ |  | Ring structure | estrogenic gene expressionEC50 [mol/l] | --- | 120 aromatic compounds | Rings without OH are inactive | Schultz et al. [7] |

**Table SI 2B: Chemical structures related to interactions with androgen receptors. MP: Structure of the pharmacophore, MS: Substructure.**

| **Chemical structure** | **MP** | **MS** | **Structural alert (SA)** | **Description** | **Endpoint** | **Binding affinity** | **Data set**  | **Comments** | **References** |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Steroids** |  |  |  |  |  |  |  |  |  |
|  | ⮟ |  | SA 01 | Steroid backbone | AR binding | --- | 202 diverse structures | Androgenic and estrogenic steroids bind to AR and ERdifference:3-Keto at A ring: more likely AR binding3-OH at A ring: more likely ER binding | Fang et al. [16] |
| **DES** |  |  |  |  |  |  |  |  |  |
|  | ⮟ |  | SA 05 | DES backbone | AR binding | --- | 202 diverse structures  | DES analogues bind to AR and ERdifference:3-Keto at A ring: more likely AR binding3-OH at A ring: more likely ER binding | Fang et al. [16] |
| **Phytoestrogens** |  |  |  |  |  |  |  |  |  |
| Structures see Table SI1A | ⮟ |  |  | FlavonesFlavanonesIsoflavonesCoumestanesChalcanoidesMycoestrogenes | AR binding | 3 of 17inactive | 202 diverse structures  | ↑ Binding affinity with ↑ log *K*OWNon-binder have very low log *K*OW Inactive: coumestrol, 7-hydroxyflavone, naringin | Fang et al. [16] |
| **Diphenylmethanes** |  |  |  |  |  |  |  |  |  |
|  | ⮟ |  | SA 17 | Methoxychlor analoga | AR binding | 0 of 5inactive | 202 diverse structures  | -X: =CCl2, -CCl3R1, R2: OH, OMe | Fang et al. [16] |
|  | ⮟ |  | SA 15 | Benzophenones | AR binding | 0 of 4inactive | 202 diverse structures  | R: H, OH | Fang et al. [16] |
|  | ⮟ |  | SA 15 | Benzophenones | AR binding | 0 of 4inactive 2 of 4:agonists | N=66 (SPEED 98) | X: O, CH2R1: H, Cl, OH | Tamura et al. [17] |
|  | ⮟ |  | SA 17 | DDT analoga | AR binding | 0 of 6inactive | 202 diverse structures  | X: =CCl2, -CHCl2, -CCl32. ring: Cl in o- or p- | Fang et al. [16] |
|  | ⮟ |  | SA 17 | Bisphenols | AR binding | 0 of 3inactive | 202 diverse structures  | R1: methyl or ethylR2: H, OH | Fang et al. [16] |
|  | ⮟ |  | SA 17 | DDT analoga and Bisphenols | AR binding | 0 of 11inactive | N=66 (SPEED 98) | R1: H, OH, CH3R2: CCl2, CCl3, C(O)O-alkyl, 3-pyrimidine, CH3R3: Cl, Br, OCH3, OHR4: H, Cl, Br, OCH3, OHR5: H, Cl | Tamura et al. [17] |
|  | ⮟ |  | SA 16 | DDE analoga  | AR binding | 0 of 2inactive | N=66 (SPEED 98) | R1: H, ClR2: H, Cl | Tamura et al. [17] |
|  |  | ⮟ | SA 28 | Triphenylmethanes | AR binding | 2 of 3inactive | 202 diverse structures  | Active: aurinInactive: phenol red, phenolphthalein | Fang et al. [16] |
|  | ⮟ |  | SA 29 | Sulfonyldiphenols | AR binding | 0 of 1inactive | 202 diverse structures  |  | Fang et al. [16] |
| **Diphenylether** |  |  |  |  |  |  |  |  |  |
|  | ⮟ |  | SA 30 | Diphenylether | AR binding | 0 of 5inactive 3 of 5:agonists | N=66 (SPEED 98) | R1: Cl, NO2R2: H, CH3O, C(O)OCH3R3: H, ClR4: H, Cl | Tamura et al. [17] |
| **Biphenyls** |  |  |  |  |  |  |  |  |  |
|  | ⮟ |  | SA 18 | PCBs | AR binding | 1 of 6inactive | 202 diverse structures  | Substituents : H, OH, Cl | Fang et al. [16] |
| **Isoindoles** |  |  |  |  |  |  |  |  |  |
|  | ⮟ |  | SA 31 | Isoindoles | AR binding | 0 of 3inactive | 202 diverse structures  | R: H, NO2, OH | Fang et al. [16] |
| **Hydrocarbons (aromatic)** |  |  |  |  |  |  |  |  |  |
| --- | ⮟ |  |  | Aromatic hydrocarbons | AR binding | 6 of 7inactive | 202 diverse structures  | Active: triphenylethyleneInactive: sec-butylbenzene, n-butylbenzene, 1,6-dimethylnaphthalene, diphenylbutadiene, chrysene, triphenylpropane | Fang et al. [16] |
| --- | ⮟ |  |  | PAK | AR binding | 1 of 7inactive 4 of 6:agonists | N=66 (SPEED 98) | Active (agonist): benz[a]pyrene, perylene, chrysene, phenanthreneActive (antagonist): pyrene, antraceneInactive: naphtalene | Tamura et al. [17] |
| **Phthalates** |  |  |  |  |  |  |  |  |  |
|  | ⮟ |  | SA 23 | Phthalate ester | AR binding | 1 of 7inactive | 202 diverse structures  | R1, R2: alkylInactive: bis(2-ethylhexyl)-phthalate | Fang et al. [16] |
|  | ⮟ |  |  | Phthalate ester | AR binding | 0 of 5 inactive | N=66 (SPEED 98) | AR antagonistsR1, R2: alkyl | Tamura et al. [17] |
| **Phenols** |  |  |  |  |  |  |  |  |  |
|  | ⮟ |  | SA 26 | Alkylphenols, Parabens, Alkoxyphenols | AR binding | 5 of 19inactive | 202 diverse structures  | ↑ Binding affinity with ↑ log *K*OW Non-binder have very low log *K*OWInactive: vanillin, phenol, methylparaben, 2-chlorophenol, 4-ethylphenol | Fang et al. [16] |
|  | ⮟ |  | SA 26 | Alkylphenols | AR binding | 1 of 7inactive | N=66 (SPEED 98) | p-Alkylphenols (pentyl- to nonyl); 2,4-Cl2-phenol: very low binding affinity | Tamura et al. [17] |
|  |  | ⮟ | SA 26 | Phenol analoga | AR binding | 2 of 6inactive | 202 diverse structures  | Active: 1-methoxy-4-[1-propylphenyl] benzene, carbaryl, nordihydroguaiaretic acid, 4-(3,5-diphenylcyclohexyl)phenol,Inactive: 2,6-dihydroxyanthrachinone, 2-naphthol | Fang et al. [16] |
|  |  | ⮟ |  | Aromatic phosphoric acid ester | AR binding | 0 of 3inactive | 202 diverse structures  | Active: methylparathion, ethylparathion, triphenylphosphate | Fang et al. [16] |
| **Flutamides** |  |  |  |  |  |  |  |  |  |
|  | ⮟ |  | SA 36 | Flutamides | AR binding | 1 of 9inactive | 202 diverse structures  | ↑ Binding affinity with ↑ e-affinity of substituents at ring Non-binder have e-donating substituents at ringInactive: p-lactophenetid | Fang et al. [16] |
|  |  | ⮟ | SA 36 | “miscellaneous compounds“ | AR binding | 1 of 8inactive 2 of 7:agonists | N=66 (SPEED 98) | 7 of the 8 compounds have a common substructure (with X1: N, O, C, X2=X3: C=O, P=S, at ring: 1 to 2 m-, p-substituents): flutamide, linuron, fenitrothion, ethyl-parathion, vinclozoline, procymidon, iprodion (inactive), Exception with a different structure: octachlorostylene (active) | Tamura et al. [17] |
| **Aromatic acids** |  |  |  |  |  |  |  |  |  |
|  |  | ⮟ |  | Aromatic acids, amides, esters | AR binding | 4 of 6inactive | 202 diverse structures  | X: O, NRing substituents: NH2, OH, O-alkylActive: 4-aminobutylbenzoate, 4-heptyloxybenzoic acid | Fang et al. [16] |
| **Triazines** |  |  |  |  |  |  |  |  |  |
|  |  | ⮟ | SA 33 | Triazines | AR binding | 3 of 3inactive | 202 diverse structures  | Inactive: simazine, atrazine, prometone | Fang et al. [16] |
| **Diverse structures**  |  |  |  |  |  |  |  |  |  |
| --- |  |  |  | Organochlorines | AR binding | 3 of 10inactive | 202 diverse structures  | Active: 2,4,5-T, γ-hexachlorocyclohexane, aldrine, endosulfane, heptachlor, kepone, chlordaneInactive: 2,4-D, hexachlorobenzene, mirex | Fang et al. [16] |
| --- |  |  |  | Organochlorines | AR binding | 11 of 17inactive | N=66 (SPEED 98) | Active: dieldrine, endrine, aldrine, toxaphene, γ-hexachlorocyclohexane, trans-heptachlorepoxidInactive: heptachlor, trans-nonachlor, chlordane, trans-chlordane, cis-chlordane, oxychlordane, chlordecone, mirex, ß-hexachlorocyclohexane, hexachlorbenzene, cis-heptachlorepoxid | Tamura et al. [17] |
| --- |  |  |  | Non-cyclic compounds | AR binding | 8 of 10inactive | 202 diverse structures  | Active: diisobutyladipate, dibutyladipate | Fang et al. [16] |
| --- |  |  |  | Siloxanes | AR binding | 1 of 3inactive | 202 diverse structures  | Active: 1,3-diphenyltetramethyldisiloxane, triphenylsilanoleInactive: 1,3-dibenzyltetramethyldisiloxane | Fang et al. [16] |

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