

AI4NAMS - Deliverable 5

Draft case study report – Supplementary data

Case study 2

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1. Initial Data Collection, Unstructured Data Sources

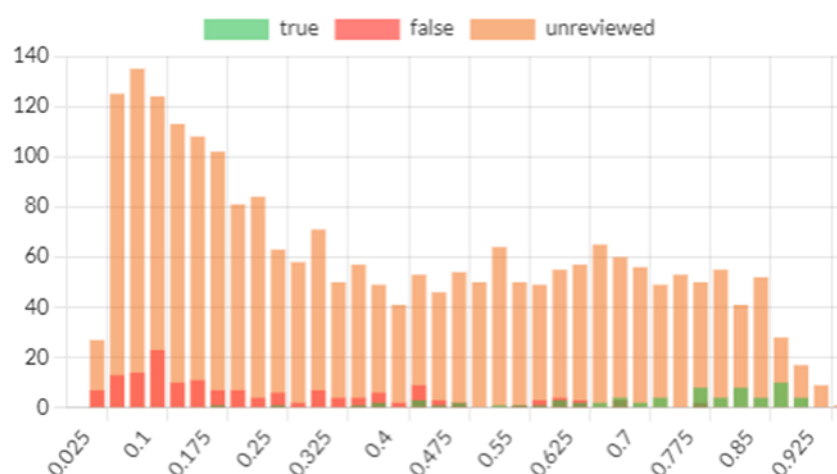
Full search string for PubMed used in Initial Data Collection workflow step.

((in vitro) OR (in chemico) OR (in silico) OR (QSAR) OR (zebrafish) OR (danio rerio) OR (c. elegans) OR (transcriptom) OR (cell culture) OR (organ chip) OR (ex vivo) OR (cell line) OR (organoid) OR (drosophila melanogaster)) AND ("dibutyl phthalate"[Title/Abstract] OR "84-74-2"[Title/Abstract] OR "Di-n-butyl phthalate"[Title/Abstract] OR "n-Butyl phthalate"[Title/Abstract] OR "Butyl phthalate"[Title/Abstract] OR "DBP"[Title/Abstract] OR "mono-n-butyl phthalate"[Title/Abstract] OR "Monobutyl phthalate"[Title/Abstract] OR "131-70-4"[Title/Abstract] OR "Benzyl butyl phthalate"[Title/Abstract] OR "85-68-7"[Title/Abstract] OR "Butylbenzyl phthalate"[Title/Abstract] OR "n-Butyl benzyl phthalate"[Title/Abstract] OR "butyl benzyl phthalate"[Title/Abstract] OR "BBP"[Title/Abstract] OR "Monobenzyl phthalate"[Title/Abstract] OR "MBzP"[Title/Abstract] OR "Bis(2-ethylhexyl)phthalate"[Title/Abstract] OR "DEHP"[Title/Abstract] OR "Di 2 Ethylhexylphthalate"[Title/Abstract] OR "Di(2-ethylhexyl)phthalate"[Title/Abstract] OR "Di-2-Ethylhexylphthalate"[Title/Abstract] OR "Diethylhexyl Phthalate"[Title/Abstract] OR "117-81-7"[Title/Abstract] OR "Diocetyl Phthalate"[Title/Abstract] OR "Mono(2-ethylhexyl)-phthalate "[Title/Abstract] OR "Mono(2-ethyl-5-oxohexyl)-phthalate "[Title/Abstract] OR "Mono(2-ethyl-5-hydroxyhexyl)-phthalate "[Title/Abstract] OR "Mono(2-ethyl-6-hydroxyhexyl)-phthalate "[Title/Abstract] OR "Mono(2-hydroxyethylhexyl)-phthalate "[Title/Abstract] OR "Mono(2-carboxymethylhexyl)-phthalate "[Title/Abstract] OR "Mono(2-ethyl-5-carboxypentyl)-phthalate "[Title/Abstract] OR "MEHP"[Title/Abstract] OR "MEOHP"[Title/Abstract] OR "MEHHP"[Title/Abstract] OR "MHEHP"[Title/Abstract] OR "MCMHP"[Title/Abstract] OR "MECPP"[Title/Abstract] OR "5oxo-MEHP"[Title/Abstract] OR "5OH-MEHP"[Title/Abstract] OR "2cx-MMHP"[Title/Abstract] OR "6OH-MEHP"[Title/Abstract] OR "5cx-MEPP"[Title/Abstract] OR "Diisononyl phthalate"[Title/Abstract] OR "di-isononylphthalate"[Title/Abstract] OR "28553-12-0"[Title/Abstract] OR "DINP"[Title/Abstract] OR "Di-isononylphthalate"[Title/Abstract] OR "Monoisononyl-phthalate"[Title/Abstract] OR "Mono(carboxyisooctyl)-phthalate"[Title/Abstract] OR "Mono(hydroxyisononyl)-phthalate"[Title/Abstract] OR "Mono(oxoisononyl)-phthalate"[Title/Abstract] OR "MINP"[Title/Abstract] OR "MCIOP"[Title/Abstract] OR "MHINP"[Title/Abstract] OR "MOINP"[Title/Abstract] OR "oxo-MINP"[Title/Abstract] OR "OH-MINP"[Title/Abstract] OR "cx-MINP"[Title/Abstract] OR "di-isodecyl phthalate"[Title/Abstract] OR "diisodecyl phthalate"[Title/Abstract] OR "89-16-7"[Title/Abstract] OR "Monoisodecyl-phthalate"[Title/Abstract] OR "Mono(carboxyisononyl)-phthalate"[Title/Abstract] OR "Mono(hydroxyisodecyl)-phthalate"[Title/Abstract] OR "Mono(oxoisodecyl)-phthalate"[Title/Abstract] OR "MIDP"[Title/Abstract] OR "MCINP"[Title/Abstract] OR "cx-MIDP"[Title/Abstract] OR "MHIDP"[Title/Abstract] OR "oxo-MIDP"[Title/Abstract] OR "MOIDP"[Title/Abstract] OR "OH-MIDP"[Title/Abstract])

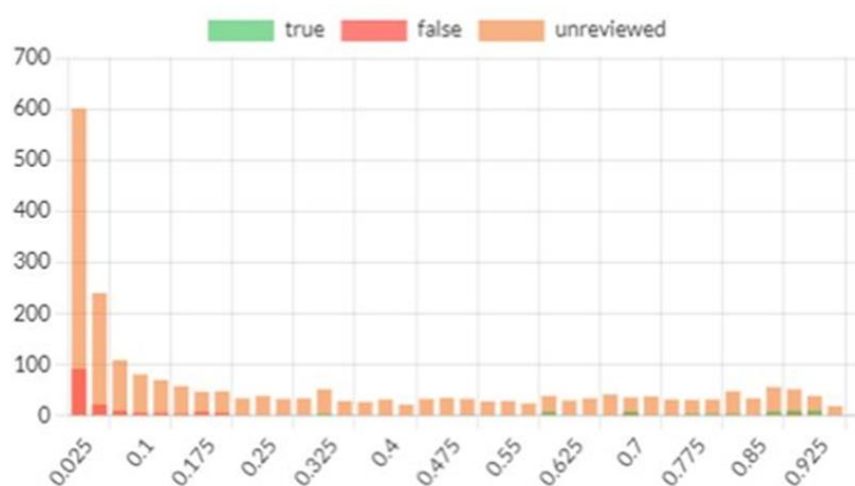
2. Initial Review, Unstructured Data Sources

Prediction histograms created by Sysrev after A) Evaluation run 1, B) Evaluation run 2 and C) Evaluation run 3. D) Prediction histogram after Evaluation run 3.1, which was generated after only model updates of evaluation run 3, without additional manual reviewing. The y-axis refers to the number of publications, the x-axis includes the prediction scores.

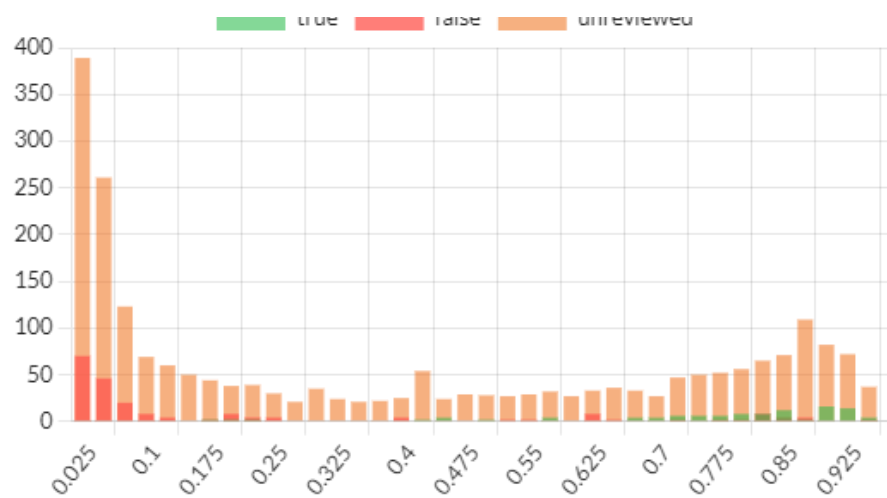
A



B



C



D

