



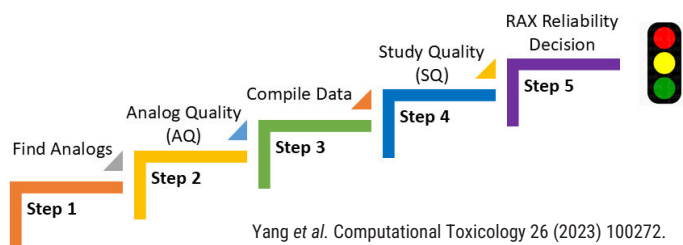
ToxGPS® Read-Across

Relevant, Reliable, Reproducible

ToxGPS® Read-Across is an easy-to-use and interactive workflow for read-across analysis. The workflow enables inclusion of various types of experimental and in silico information, including structural, physicochemical, biological and toxicity data. After lining up all available information, the user can select which evidence sources to combine to obtain a Weight-of-Evidence outcome with associated estimate of uncertainty. The workflow supports consistent, reproducible, and transparent decision making steps involved in read-across.

Workflows Strategy

Five steps to complete a quantitative read-across assessment



	Target	Analog	Analog	Analog
Compound Information				
Summary	CMS-7321 	CMS-4400 	CMS-2194 	CMS-6748
Chemical Similarity				
Tanimoto				
<input checked="" type="checkbox"/> ToxPrint		0.53	0.47	0.44
Skyline Plots				
sky-propld				
Skyline				
<input checked="" type="checkbox"/> Pearson similarity (0-1)		0.90	0.88	0.86
Analog Quality	1.00 automatic	0.69 automatic	0.64 automatic	0.61 automatic
Skin Sensitization Data				
<input checked="" type="checkbox"/> Skin Sens		<input checked="" type="checkbox"/> LLNA	<input checked="" type="checkbox"/> LLNA	<input checked="" type="checkbox"/> LLNA
Study Type	No data			
Study Description		SCCS 2011; weak positive	GHS 1B	BASF; GHS 1B
Study Quality [High, Med-High, Med, Med-Low, Low]		Med	High	High
Study Quality (SQ) [Numeric 1-0]		0.9	0.95	0.95
Study Call [Positive or Negative]	none	none	none	none
Study Result [Numeric 1 or 0]				
Study Result - EC3 (wt/vol %)	20	4.9	6.3	
RAX Reliability WOE				
Reliability per Analog		0.62	0.61	0.58
Reliability All Analogs	0.94	The read-across approach to skin sensitization based on the selected analogs is justified by the high overall RAX reliability (94%). This value is obtained by a combination of AQ and SQ using Dempster-Shafer theory (DST).		
RAX Outcome				
SS Hazard				
Experiment only	POSITIVE [pNEG=0.00, uncertainty=0.06]	Based on the selected assay data, the target is deemed positive with 6% uncertainty.		
EC3 Bounds				
95% CI from the selected analogues (averaging)	1 ≤ EC3 ≤ 55			

Interactive templates for assessment of skin sensitization, carcinogenicity, genetic, and target organ toxicity as well as Analog Quality and user-defined Weight of Evidence combination

- Five steps to complete the quantitative read-across assessment for skin sensitization
- Quantitative results for hazard (probability) and EC3
- RAX reliability was high (0.94); the LLNA outcome is positive: EC3 95% CI is between 1 and 55