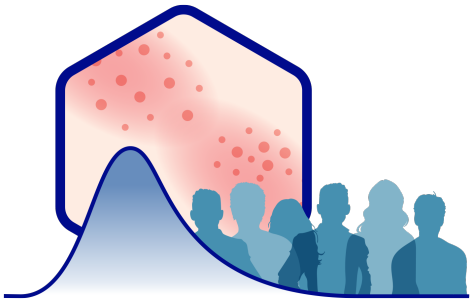


SARA-ICE Summary Report

Model Run:
OECD TG 497 Defined Approach (version 1.0)
March 16, 2026

Contents

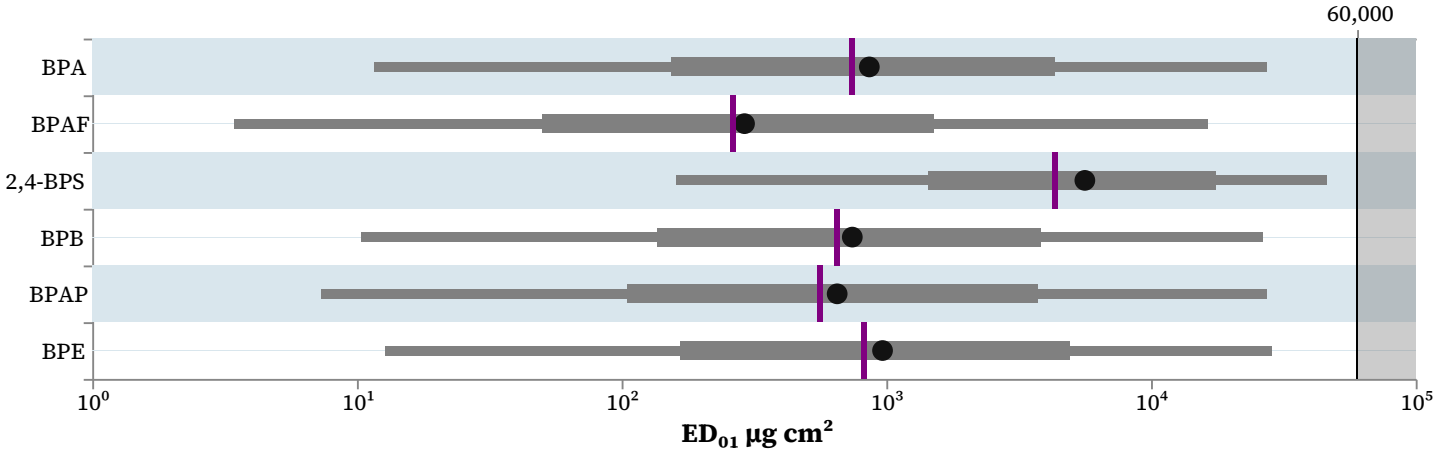
1 Introduction

This report includes chemical summaries for SARA-ICE estimates generated on March 16, 2026 with SARA-ICE OECD TG 497 Defined Approach (version 1.0).

1.1 Outputs Key

Field	Description
Substance	Name of Chemical Substance
CASRN	Chemical Abstracts Service Registry Number (CAS RN or CAS Number)
POD	(Point of Departure) geometric mean of the ED_{01} predicated on being a sensitizer
ED_{01} 5th	5th Percentile of the ED_{01} distribution ($\mu g/cm^2$)
ED_{01} 50th	50th Percentile of the ED_{01} distribution ($\mu g/cm^2$)
ED_{01} 95th	95th Percentile of the ED_{01} distribution ($\mu g/cm^2$)

2 Summary



2.1 Summary Key

Mark	Description
Thin Gray Line	Centered 90% credible intervals of ED_{01}
Thick Gray Line	Centered 50% credible intervals of ED_{01}
Black Bullet	Median of ED_{01}
Vertical Purple Line	Point of Departure

3 Individual Chemicals

3.1 BPA (80-05-7)

3.1.1 SARA-ICE Inputs

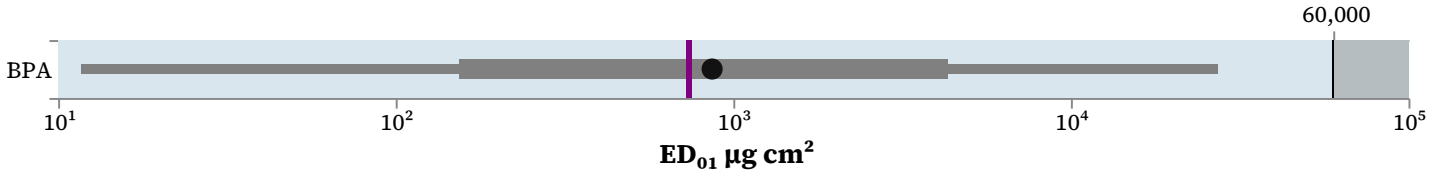
DPRA		
Depletion Lys (%)	Depletion Cys (%)	Reference
0.9	0.5	BRT-NIEHS unpublished

KeratinoSens		
IC50 (μM)	EC1.5 (μM)	Reference
14.7710487977	1.8349666103	BRT-NIEHS unpublished

h-CLAT			
CD54, EC200 (μg/ml)	CD86, EC150 (μg/ml)	CV75 (μg/ml)	Reference
14.2838143927	>43	35.85	BRT-NIEHS unpublished
25.7179574047	>43	35.85	BRT-NIEHS unpublished

3.1.2 SARA-ICE OECD TG 497 Defined Approach (version 1.0) Outputs

POD	ED_{01} 5th	ED_{01} 50th	ED_{01} 95th
740	12	870	27,000



3.2 BPAF (1478-61-1)

3.2.1 SARA-ICE Inputs

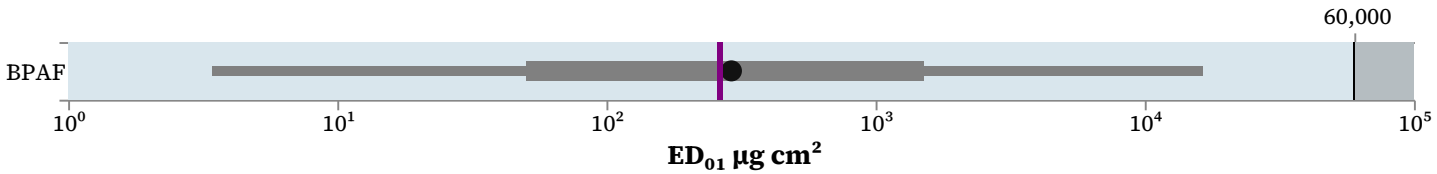
DPRA		
Depletion Lys (%)	Depletion Cys (%)	Reference
1.1	0	BRT-NIEHS unpublished

KeratinoSens		
IC50 (μM)	EC1.5 (μM)	Reference
1.2464185196	0.5032811065	BRT-NIEHS unpublished

h-CLAT			
CD54, EC200 (μg/ml)	CD86, EC150 (μg/ml)	CV75 (μg/ml)	Reference
10.68856359	9.4360271079	18.85	BRT-NIEHS unpublished
16.0444525665	15.488678092	18.85	BRT-NIEHS unpublished

3.2.2 SARA-ICE OECD TG 497 Defined Approach (version 1.0) Outputs

POD	ED_{01} 5th	ED_{01} 50th	ED_{01} 95th
260	3.4	290	16,000



3.3 2,4-BPS (5397-34-2)

3.3.1 SARA-ICE Inputs

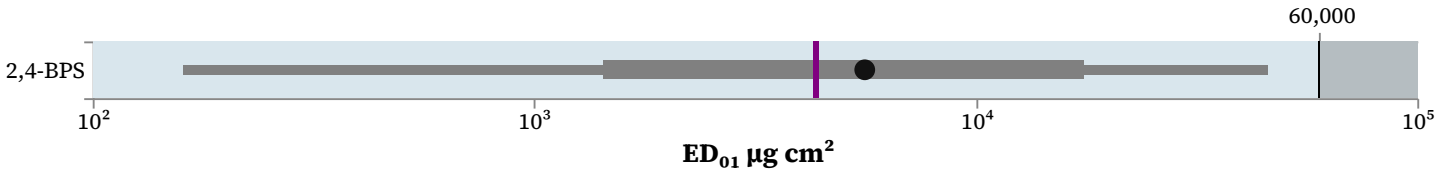
DPRA		
Depletion Lys (%)	Depletion Cys (%)	Reference
6.4	0	BRT-NIEHS unpublished

KeratinoSens		
IC50 (µM)	EC1.5 (µM)	Reference
1410.3532372344	499.4781801582	BRT-NIEHS unpublished

h-CLAT			
CD54, EC200 (µg/ml)	CD86, EC150 (µg/ml)	CV75 (µg/ml)	Reference
82.9765880507	>205	170.4	BRT-NIEHS unpublished
101.1381733514	>205	170.4	BRT-NIEHS unpublished

3.3.2 SARA-ICE OECD TG 497 Defined Approach (version 1.0) Outputs

POD	ED_{01} 5th	ED_{01} 50th	ED_{01} 95th
4,300	160	5,600	46,000



3.4 BPB (77-40-7)

3.4.1 SARA-ICE Inputs

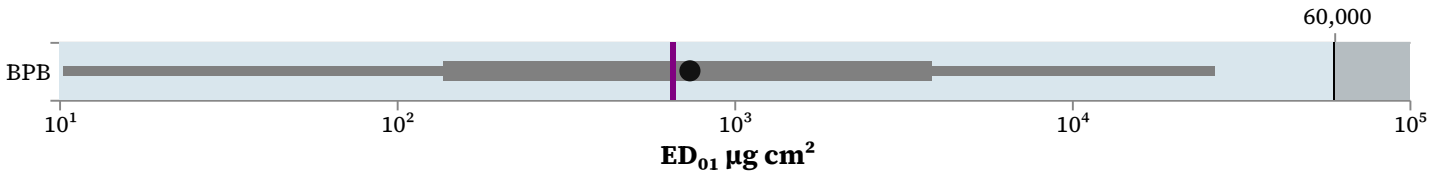
DPRA		
Depletion Lys (%)	Depletion Cys (%)	Reference
0	0	BRT-NIEHS unpublished

KeratinoSens		
IC50 (µM)	EC1.5 (µM)	Reference
6.1581790193	2.5498550413	BRT-NIEHS unpublished

h-CLAT			
CD54, EC200 (µg/ml)	CD86, EC150 (µg/ml)	CV75 (µg/ml)	Reference
12.2337341063	10.9645972704	32.4	BRT-NIEHS unpublished
25.0317023965	>38.9	32.4	BRT-NIEHS unpublished

3.4.2 SARA-ICE OECD TG 497 Defined Approach (version 1.0) Outputs

POD	ED_{01} 5th	ED_{01} 50th	ED_{01} 95th
650	10	740	27,000



3.5 BPAP (1571-75-1)

3.5.1 SARA-ICE Inputs

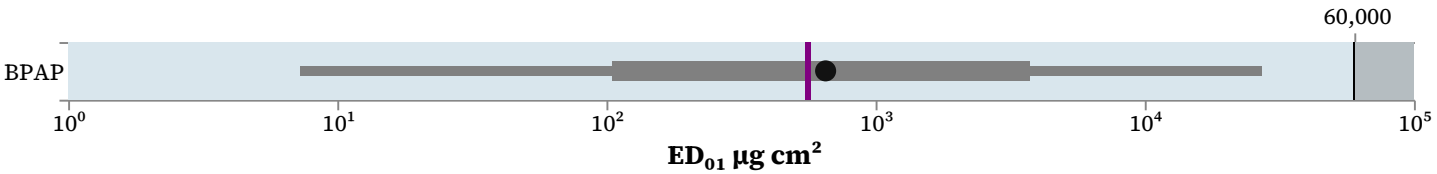
DPRA		
Depletion Lys (%)	Depletion Cys (%)	Reference
0.2	0	BRT-NIEHS unpublished

KeratinoSens		
IC50 (µM)	EC1.5 (µM)	Reference
1.931170344	0.653528118	BRT-NIEHS unpublished

h-CLAT			
CD54, EC200 (µg/ml)	CD86, EC150 (µg/ml)	CV75 (µg/ml)	Reference
14.602920864	15.2027123553	20.5	BRT-NIEHS unpublished
17.6282528853	>24.6	20.5	BRT-NIEHS unpublished

3.5.2 SARA-ICE OECD TG 497 Defined Approach (version 1.0) Outputs

POD	ED_{01} 5th	ED_{01} 50th	ED_{01} 95th
570	7.3	650	27,000



3.6 BPE (2081-08-5)

3.6.1 SARA-ICE Inputs

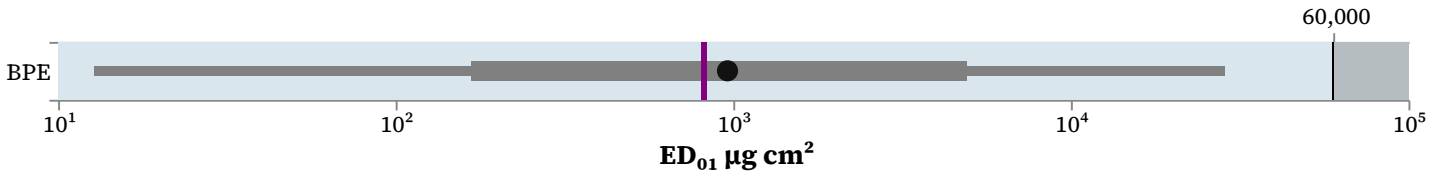
DPRA		
Depletion Lys (%)	Depletion Cys (%)	Reference
0	0	BRT-NIEHS unpublished

KeratinoSens		
IC50 (μM)	EC1.5 (μM)	Reference
17.9318837101	0.9612960219	BRT-NIEHS unpublished

h-CLAT			
CD54, EC200 (μg/ml)	CD86, EC150 (μg/ml)	CV75 (μg/ml)	Reference
22.591742094	>79.7	66.45	BRT-NIEHS unpublished
45.8339400864	>79.7	66.45	BRT-NIEHS unpublished

3.6.2 SARA-ICE OECD TG 497 Defined Approach (version 1.0) Outputs

POD	ED_{01} 5th	ED_{01} 50th	ED_{01} 95th
820	13	960	29,000



4 Appendix

4.1 Inputs Key

Field	Description
Substance Name	Full substance name that will appear in reports containing results.
Abbreviated Substance Name	Abbreviated substance name that is used in tables and figures.
CASRN	CASRN for the substance. This must be included alongside each datapoint on assay-specific sheets. This is used to link datapoints to the correct substance on the "Substances" sheet.
MW (g/mol)	Molecular weight of the substance. Necessary when including data on the kDPRA and KeratinoSens sheets to enable appropriate unit conversion.
Dose per Skin Area (µg/cm^2)	Dermal induction dose of the HPPT study
Number of Test Subjects	The number of test subjects in the HPPT study
Number of Positive Responses	The number of test subjects judged to be sensitised after the elicitation phase of the HPPT study
EC3 (%)	Estimated EC3 from the LLNA study. Negative studies should be entered as >X where X is the maximum concentration tested. LLNA studies with SI > 3 at the lowest tested concentration can be entered as <X where X is the lowest concentration tested.
Depletion Cys (%)	Percentage depletion of the cysteine peptide in a DPRA study
Depletion Lys (%)	Percentage depletion of the lysine peptide in a DPRA study
log Kmax (M-1 s-1)	Log Kmax value estimated from a kinetic DPRA study. When reactivity rate is too low to measure, input as <X where X is the lowest possible measurable reactivity rate. Typically X=-3.5 M-1 s-1
EC1.5 (µM)	Concentration in the KeratinoSens study resulting in a 1.5-fold increase in luciferase activity
IC50 (µM)	Concentration resulting in 50% cell death in the KeratinoSens study
CD54, EC200 (µg/ml)	Concentration resulting in a 200% increase in expression of the CD54 biomarker in the h-CLAT study
CD86, EC150 (µg/ml)	Concentration resulting in a 150% increase in expression of the CD86 biomarker in the h-CLAT study
CV75 (µg/ml)	Concentration at which there is 75% cell viability in the h-CLAT study

Field	Description
CD86, EC150 (µg/ml)	Concentration resulting in a 150% increase in expression of the CD86 biomarker in the U-Sens study
CV70 (µg/ml)	Concentration at which there is 70% cell viability in the U-Sens study
Reference	Source of input values. Not used within the model but will be included in output reports.