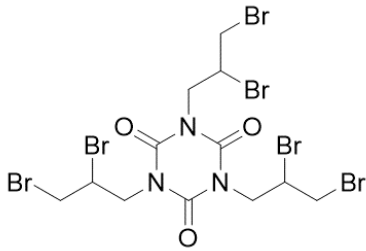


1	<b>Substance</b>  
1.1.	<b>CAS number:</b> 52434-90-9
1.2	<b>EC number:</b> EINECS 257-913-4
1.3.	<b>Chemical name:</b> 1,3,5-tris(2,3-dibromopropyl)-1,3,5-triazinane-2,4,6-trione (IUPAC) Tris(2,3-dibromopropyl) isocyanurate (CAS)
1.4.	<b>Structural formula:</b> C <sub>12</sub> H <sub>15</sub> Br <sub>6</sub> N <sub>3</sub> O <sub>3</sub>
1.5.	<b>Structure codes:</b> <b>a. SMILES:</b> C(C(CBr)Br)N1C(=O)N(C(=O)N(C1=O)CC(CBr)Br)CC(CBr)Br (canonical, input) <b>b. InChI:</b> InChI= 1S/C12H15Br6N3O3/c13-1-7(16)4-19-10(22)20(5-8(17)2-14)12(24)21(11(19)23)6-9(18)3-15/h7-9H,1-6H2 <b>c. Other structural representation:</b> <b>d. Stereochemical features:</b> There are three chiral carbons. However, the prediction model itself does not take chirality into account.
2	<b>General information</b>
2.1.	<b>Date of QPRF:</b> 2022/Jul/6
2.2.	<b>QPRF author and contact details:</b> NIHS
3	<b>Prediction</b>
3.1.	<b>Endpoint (OECD Principle 1)</b> <b>a. Endpoint:</b> Bacterial Mutagenicity by OECD 471 test guidance <b>b. Dependent variable:</b> in vitro Ames positive, in vitro Ames negative
3.2.	<b>Algorithm (OECD Principle 2)</b> <b>a. Model or submodel name:</b> CASE Ultra Model: GT1_BMUT (Statistical-based Model for Bacterial Mutagenicity by OECD 471 test guidance)) <b>b. Model version:</b> 1.8.0.1.11479.500 Tested by CASE Ultra Version: 1.8.0.5 <b>c. Reference to QMRF:</b> The corresponding QMRF is included in the purchased software. <b>d. Predicted value (model result):</b> <i>Positive</i> <b>e. Predicted value (comments):</b> The QSAR calculated probability is 93.8%. The calculated probability is HIGHER than the model's current classification threshold (50.0%) and not within the gray zone. The gray zone for this model is between 40.0% to 60.0%.

	<p><b>f. Input for prediction:</b> canonical SMILES</p> <p><b>g. Descriptor values:</b> -</p>
	<p><b>Applicability domain (OECD principle 3)</b></p> <p>a. <b>Domains:</b></p> <p>i. <i>descriptor domain</i> : -</p> <p>ii. <i>structural fragment domain</i>: No unknown structural fragment.</p> <p>iii. <i>mechanism domain</i>: not applicable (statistical model)</p> <p>iv. <i>metabolic domain, if relevant</i>: not applicable.</p> <p>b. <b>Structural analogues:</b></p> <p>3.3. - 1,2-dibromopropane: CAS RN 78-75-1, Formula C3H6Br2, SMILES CC(CBr)Br, other source.</p> <p>- cyanuric acid: CAS RN 108-80-5, Formula C3H3N3O3, SMILES C1(=O)NC(=O)NC(=O)N1, other source</p> <p>c. <b>Considerations on structural analogues:</b></p> <p>The prediction results of 1,2-dibromopropane (CAS RN 78-75-1) and cyanuric acid (CAS RN 108-80-5) are consistent with the experimental data. The prediction of test substance by other models (TIMES kinetic, TIMES nonkinetic, DEREK nexus) are consistent (all "positive").</p>
3.4.	<p><b>The uncertainty of the prediction (OECD principle 4)</b></p> <p>No analogue for whole molecule structure was found. However, the uncertainty is expected to be relatively low from consideration of Applicable Domains and analogues.</p>
3.5.	<p><b>The chemical and biological mechanisms according to the model underpinning the predicted result (OECD principle 5).</b></p> <p>not applicable (statistical model)</p>
4	<p><b>Adequacy (optional)[2]</b></p>
4.1.	<p><b>Regulatory purpose:</b> screening level assessment of the substance for mutagenicity.</p>
4.2.	<p><b>Approach for regulatory interpretation of the model result:</b></p> <p>The model is compliant with the OECD TG471 which is specified by the regulation. The endpoint "bacterial mutagenicity in vitro" is consistent with the specification of the</p>
4.3.	<p><b>Outcome:</b> Predicted as positive.</p>
4.4.	<p><b>Conclusion:</b></p> <p>Adequate. This result will be discussed with other assessment results for further conclusion under the FSCJ guidance.</p>

[\[1\] Various software tools \(e.g. the OECD \(Q\)SAR Toolbox\) could be used to support the search for analogues.](#)

[\[2\] In any case, adequate and reliable documentation is required \(section 1.3 of REACH Annex XI\). The format provides guidance on which elements are needed.](#)