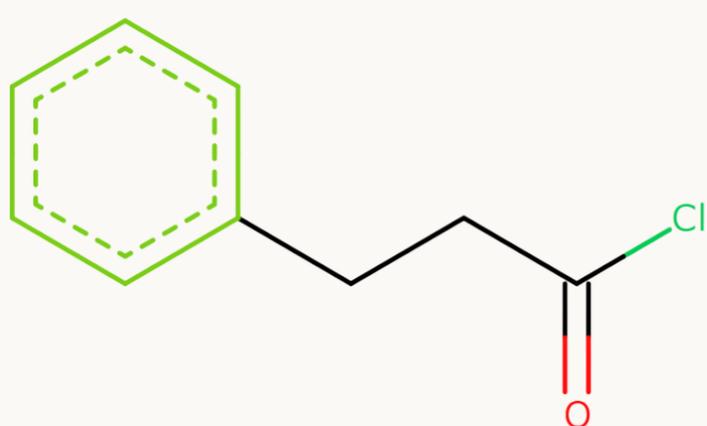


# How carboxylic and sulfonic acid halides are represented within Derek Nexus and Sarah Nexus



## 3-Phenylpropanoyl Chloride

	Derek	Mutagenicity in vitro	bacterium	EQUIVOCAL
	Sarah	Mutagenicity in vitro	bacterium	NEGATIVE (100%)

Source: Acid Halide Mutagenicity Dataset  
Dataset Call: Negative  
Source activity call: Negative  
Structure ID: CAS RN® 645-45-4

[Reference\(s\)](#)

Source: Vitic Summary Call Table  
Dataset Call: Negative  
Source activity call: Positive  
Structure ID: CAS RN® 645-45-4

[Reference\(s\)](#)

Source: ISSSTY Mutagenicity Dataset  
Dataset Call: Negative  
Source activity call: Positive  
Structure ID: CAS RN® 645-45-4

[Reference\(s\)](#)

3-Phenylpropanoyl chloride is predicted to be equivocal in Derek Nexus.



**Equivocal predictions** made by Derek should be considered a **positive prediction** that warrants expert review.

This acid halide alert discusses the **inconsistency** of Ames test results for this chemical class **depending on the solvent used**.

**Positive Ames test results** may be due to the presence of **halodimethyl sulfides**, formed by reaction of acyl halides with DMSO, whereas **negative results** may be due to the **relative stability of acyl halides in water**.

- This paper discusses the concept in more detail: ['Do carboxylic/sulfonic acid halides really present a mutagenic and carcinogenic risk as impurities in final drug products?'](#)



3-Phenylpropanoyl chloride is predicted to be negative in Sarah Nexus.

A Sarah prediction depends on the **activity of the nearest neighbours** used to support the prediction.

- 3-Phenylpropanoyl chloride is a **known non-mutagen** with 100% confidence, as there is a compound in the Sarah training set which **exactly matches** the query structure.
- Conflicting data has been resolved to a **negative call** based on the **acid halide mutagenicity dataset**. This dataset is taken from the paper linked above and includes the results of **acid halides tested in multiple solvents**, where **positive results** are generally observed **only** when **DMSO** is used as a solvent.

The Sarah Nexus training set incorporates data from the acid halide mutagenicity dataset and **a range of other trusted sources**.

Where data is conflicted for a compound, the overall call depends on data source priority listed below:

1. Member data
2. **Acid halide mutagenicity dataset**
3. Derek Nexus example compounds
4. Data points with strain information
5. Other sources



To summarise, as highlighted by Derek Nexus, for these chemical classes it is important to consider the solvent used.

[Find out how conflicting data sources are resolved to a single call in this infographic](#)