

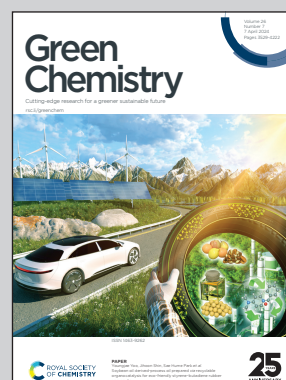


**Showcasing work from the Chemistry Development  
Unit from Suzhou Novartis Pharmaceutical Technology  
Research and Development Co., Ltd.**

An automated carcinogenic potency categorization  
approach for nitrosamine drug substance-related impurities

In compliance with guidelines from health authorities that  
providing acceptable intake limits for various *N*-nitrosamine,  
a web-based digital tool is developed that can autonomously  
analyze the *N*-nitrosamine risk category of compounds from  
their SMILES notation, providing instant screening to identify  
high-risk formations of *N*-nitrosamines. The accuracy of  
the tool was validated using an FDA dataset of compounds  
with known *N*-nitrosamine risks, indicating it can quickly and  
reliably analyze large datasets.

**As featured in:**



See Jiazhou Zhu, Yang Qu, Ning Ye,  
*Green Chem.*, 2024, **26**, 3717.