

## Licensing Opportunity

### Nitration of arenes with controllable source of nitronium ions



#### Summary

An inexpensive and bench-stable nitrating reagent enables access to nitro(hetero)arenes under very mild reaction conditions. There are minimal side-products and the core of the reagent is recyclable.

#### Background

The large scale preparation of nitroarenes suffers from a number of drawbacks such as the use of excess corrosive superacids or toxic and high cost reagents, difficulties in work-up procedures to isolate desired products and generation of superstoichiometric amounts of acidic or metal waste.

#### Invention

N-Nitrosaccharins act as mild and highly efficient nitration agents. They demonstrate a high tolerance towards acid-sensitive functional groups and show nitration yields in the 64 - 100 % range. Steroids, vanillin, ibuprofen and other biologically active molecules have been nitrated with high chemical efficiency. Charges of 30-50 g were handled easily in the research laboratory. The proposed methodology for the synthesis of the reagent has great potential for upscaling to industrial production volumes.

#### Features & Benefits

- Easy-to-handle, safe and bench-stable solid chemicals
- Inexpensive and scalable one-step synthesis
- Environmentally benign nitration process
- High nitration yields

#### Fields of Application

- Late stage functionalization of complex molecules
- Pharmaceuticals, dyes, explosives, agrochemicals

#### Patent Status

- Patent pending

#### Publication

- Calvo R., Zhang K., Passera A., Katayev D., "Facile success to nitroarenes and nitroheteroarenes using N-nitrosaccharin", *nature communications*, 2019 <https://doi.org/10.1038/s41467-019-11419-y>

#### Technology Readiness Level



#### ETH transfer

transfer@sl.ethz.ch  
www.transfer.ethz.ch  
+41 44 632 23 82

Reference: 2018-136  
Developed by: Laboratory of Inorganic Chemistry  
Dmitry Katayev, Kun Zhang, Roxan Calvo