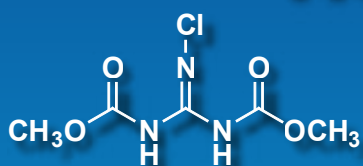


New

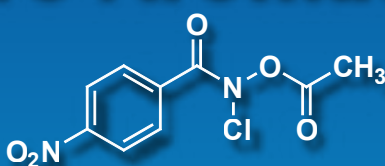
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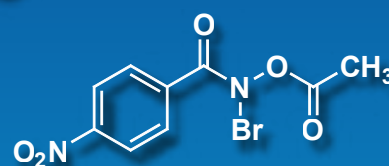
# High-Performance Chlorinating Agents and Brominating Agent for Regioselective Halogenation of Hetero Aromatics



**2-Chloro-1,3-bis(methoxycarbonyl)guanidine**  
1g / 5g / 25g [C4028]



**N-Acetoxy-N-chloro-4-nitrobenzamide**  
1g / 5g [A3694]

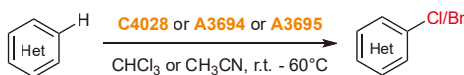


**N-Acetoxy-N-bromo-4-nitrobenzamide**  
1g / 5g [A3695]

## Advantages

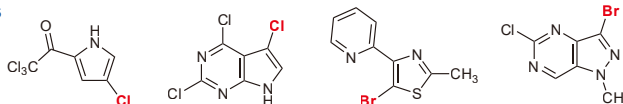
- Easy-to-handle solid
- Enables the regioselective halogenation of drug-like complicated hetero aromatics in mild conditions
- Applicable to multi-gram scale synthesis and continuous flow technique
- Suitable for late-stage functionalization in drug discovery research

## Application

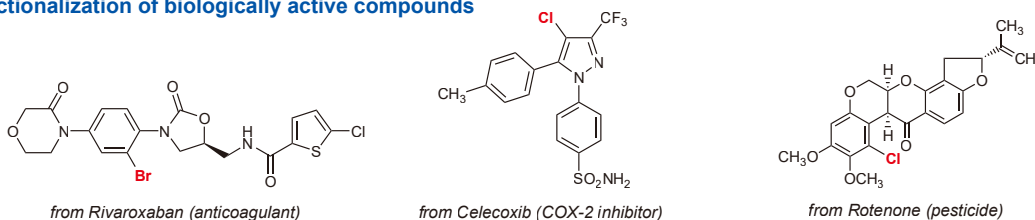


C4028,<sup>1)</sup> A3694 and A3695,<sup>2)</sup> are applicable to less reactive substrates, which are challenging with traditional reagents such as Cl<sub>2</sub>, Br<sub>2</sub>, NBS, NCS, TCCA and so on. Especially, A3694 shows even higher reactivity than C4028, owing to its anomeric amide moiety.<sup>2)</sup> For chlorination, if C4028 does not work, A3694 is recommended.

### Synthesis of halogenated building blocks



### Late-stage functionalization of biologically active compounds



The impact of chloro group introduced to target compounds are reported as "magic chloro effect".<sup>3)</sup> Chloro group effect on potency, clearance, ADMET etc. In addition to "block effect" and "mimic effect" of fluoro group and "magic methyl effect" of methyl group, "magic chloro effect" is gathering more and more attentions.

- References 1) R. A. Rodriguez, P. S. Baran, *et al.*, *J. Am. Chem. Soc.* **2014**, *136*, 6908. <https://doi.org/10.1021/ja5031744>  
2) Y. Wang, P. S. Baran, *et al.*, *Nat. Chem.* **2024**, *16*, 1539. <https://doi.org/10.1038/s41557-024-01539-4>  
3) D. Chiodi, Y. Ishihara, *J. Med. Chem.* **2023**, *66*, 5305. <https://doi.org/10.1021/acs.jmedchem.2c02015>

## Related Products

**N-Chlorosuccinimide (= NCS)**  
**N-Bromosuccinimide (= NBS)**

25g / 100g / 500g [C0291]  
25g / 100g / 500g [B0656]

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