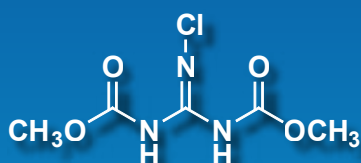


New

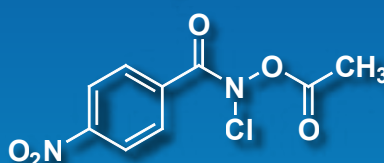
CHEMISTRY

TCI®

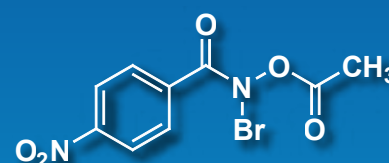
# High-Performance Chlorinating Agents and Brominating Agent for Regioselective Halogenation of (Hetero)arenes



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



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

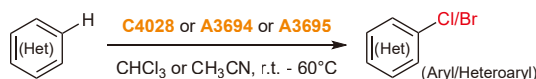


**N-Acetoxy-N-bromo-4-nitrobenzamide**  
1g / 5g [A3695]

## Advantages

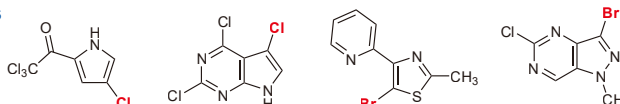
- Easy-to-handle solid
- Enables the regioselective halogenation of drug-like complicated hetero aromatics in mild conditions
- Applicable to multi-gram scale synthesis and continuous flow technique
- Suitable for late-stage functionalization in drug discovery research

## Application

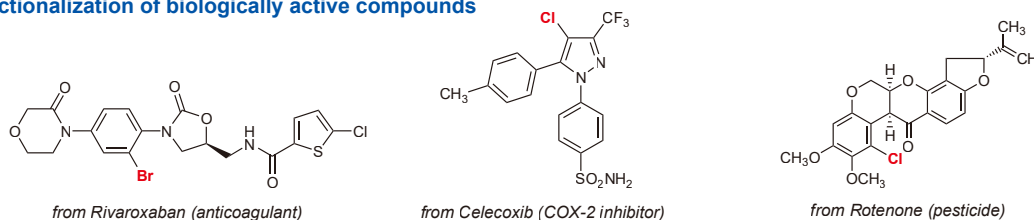


C4028,<sup>1)</sup> A3694 and A3695,<sup>2)</sup> are applicable to less reactive substrates, which are challenging with traditional reagents such as Cl<sub>2</sub>, Br<sub>2</sub>, NBS, NCS, TCCA and so on. Especially, A3694 shows even higher reactivity than C4028, owing to its anomeric amide moiety.<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]

## Ordering and Customer Service

### TCI AMERICA

Tel : 800-423-8616 / 503-283-1681  
Fax : 888-520-1075 / 503-283-1987  
E-mail : Sales-US@TCIchemicals.com

### TCI EUROPE N.V.

Tel : +32 (0)3 735 07 00  
Fax : +32 (0)3 735 07 01  
E-mail : Sales-EU@TCIchemicals.com

### TCI Deutschland GmbH

Tel : +49 (0)6196 64053-00  
Fax : +49 (0)6196 64053-01  
E-mail : Sales-DE@TCIchemicals.com

### Tokyo Chemical Industry UK Ltd.

Tel : +44 (0)1865 78 45 60  
E-mail : Sales-UK@TCIchemicals.com

### 梯希爱(上海)化成工业发展有限公司

Tel : 800-988-0390 / 021-67121386  
Fax : 021-6712-1385  
E-mail : Sales-CN@TCIchemicals.com

### Tokyo Chemical Industry (India) Pvt. Ltd.

Tel : 1800 425 7889 / 044-2262 0909  
E-mail : Sales-IN@TCIchemicals.com

### TOKYO CHEMICAL INDUSTRY CO., LTD.

Tel : +81 (0)3-5640-8878  
E-mail : globalbusiness@TCIchemicals.com

• Chemicals itemized in this brochure are for research and testing use only. Please avoid use other than by chemically knowledgeable professionals. • Information such as listed products and its specifications and so on are subject to change without prior notice. • The contents may not be reproduced or duplicated in whole or in part without permission of Tokyo Chemical Industry Co., Ltd.