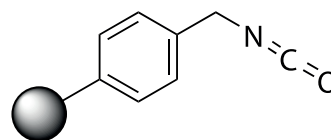


# Biotage® MP-Isocyanate

## Macroporous Nucleophile Scavenger

(Also see PS-Isocyanate)



### Key Facts



Shelf Life



Capacity  
(mmol/g)



BSE/TSE



Scalable



Particle Size  
(μm)



Thermally &  
Mechanically  
Stable



Good  
Laboratory  
Practice



Bulk Density  
(g/L)

### Specifications

<b>Chemical Name:</b>	Polystyrene methyl isocyanate
<b>Resin Type:</b>	Highly cross-linked macroporous poly(styrene-co-divinylbenzene)
<b>Application:</b>	Scavenging nucleophiles, including amines and alkoxides
<b>Scavenging Conditions:</b>	2–3 equivalents relative to nucleophile, 1–16 h, 20 °C
<b>Compatible Solvents:</b>	Non-acidic organic solvents and water
<b>Storage:</b>	Cool, dry location

MP-Isocyanate is a macroporous polystyrene-bound scavenger, for nucleophiles such as amines and alkoxides. Resin-bound scavengers are added after a reaction is complete in order to quench and react selectively with excess reactants and/or reaction by-products. The resulting resin-bound adducts are removed by simple filtration.

Biotage supplies two isocyanate scavenger resins: PS-Isocyanate and MP-Isocyanate. The resin backbone in PS-Isocyanate consists of 1% cross-linked polystyrene-co-divinylbenzene. Nucleophiles to be scavenged gain access to the isocyanate sites by diffusion through the polystyrene gel. The MP-base copolymer is a highly cross-linked a robust and low-swelling material, which makes it ideal for restricted volume environments (e.g. microwave vials and 96-well plates etc.). Its unique pore structure provides greater access to the reactive sites without the need for solvent swelling, resulting in

faster reactions and higher recoveries. The abrasion-resistant matrix has better handling characteristics and reduced transfer losses. Both these scavengers can be applied to similar chemistries; the main criteria for differentiation is the intended solvent choice and the format preference.

### Representative Procedures

#### Scavenging Amines using MP-Isocyanate and PS-Isocyanate in 1,2-Dichloroethane

This study compares the ability of PS-Isocyanate and MP-Isocyanate to scavenge four amines from solution in DCE. Three equivalents of scavenger were used relative to the amine.

At ambient temperature, the scavenging rates correlated directly with amine nucleophilicity (Table 1). Both resins were able to scavenge piperidine and benzylamine from solution within 1 h. Scavenging of aniline took place more slowly, reaching only 60–63% completion within 1 h. At 60 °C, PS-Isocyanate scavenged aniline to 92% completion, while MP-Isocyanate removed it completely from solution within 1 h. Scavenging of the highly hindered 2-aminobenzophenone was slow with both scavengers, even at 60 °C.

#### The Effect of Different Solvents on Scavenging by MP-Isocyanate and PS-Isocyanate

Scavenging in THF, which swells 1% cross-linked polystyrene, was compared with scavenging in acetonitrile and methyl tert-butyl ether (MTBE). Acetonitrile and MTBE are poor solvents for swelling 1% cross-linked polystyrene. MTBE was chosen as a method for other ethereal solvents commonly employed in organic synthesis.

Scavenging rates for both scavengers followed the order THF > Acetonitrile > MeOH > MTBE (Table 2). Benzyl amine was scavenged rapidly in THF reaching 93% and 98% completion within 2 h with PS-Isocyanate and MP-Isocyanate, respectively. MP-Isocyanate scavenged more rapidly and more completely in the three other solvents, demonstrating it to be the scavenger of choice in solvents that do not swell 1% cross linked polystyrene.

Reducing the amount of scavenger from 3.5 equivalents to 2 equivalents reduced the amount of benzyl amine scavenged within the given time. We recommend the use of 3.5 equivalents for complete scavenging, but there is much scope for further optimization, depending on the application.

Electrophile	Temp (°C)	Resin	% Scavenged in 1h	% Scavenged in 3.3 h	% Scavenged in 18 h
<b>Piperidine</b>	RT	PS-Isocyanate	100	100	-
		MP-Isocyanate	100	100	-
<b>Benzylamine</b>	RT	PS-Isocyanate	100	100	-
		MP-Isocyanate	100	100	-
<b>Aniline</b>	RT	PS-Isocyanate	60	91	91
		MP-Isocyanate	63	85	100
<b>Aniline</b>	60 °C	PS-Isocyanate	92	-	100
		MP-Isocyanate	100	-	100
<b>2-Aminobenzophenone</b>	RT	PS-Isocyanate	13	30	83
		MP-Isocyanate	34	57	90
<b>2-Aminobenzophenone</b>	60 °C	PS-Isocyanate	13	-	77
		MP-Isocyanate	39	-	90

**Table 1.** Comparative scavenging of amines by PS-Isocyanate and MP-Isocyanate in 1,2-dichloroethane.

Solvent	Time (h)	PS-Isocyanate % Scavenged	MP-Isocyanate % Scavenged
<b>THF</b>	2	93	98
	5.5	96	100
	20	97	100
<b>Acetonitrile</b>	1	69	100
	4	91	-
<b>MTBE</b>	1	0	84
	4	0	100
	20	0	-
<b>MeOH</b>	2	0	66
	5.5	8	75
	20	20	78

**Table 2.** Scavenging benzylamine by 3.5 equivalents of PS-Isocyanate or MP-Isocyanate in various solvents at ambient temperature in different solvents at room temperature. 2.0 equivalent of resin was used in these reactions.

## Summary

In comparison with PS-Isocyanate, MP-Isocyanate offers the following benefits:

- » Scavenges effectively in solvents that do not swell 1% cross-linked polystyrene
- » Limited swelling, so can be used where volume is restricted (e.g. 96 well plates, microwave vials)
- » Faster scavenging than PS-Isocyanate
- » For certain substrates MP-Isocyanate offers more complete scavenging than PS-Isocyanate

## Ordering Information

Part Number	Quantity
<b>801504</b>	3 g
<b>801409</b>	10 g
<b>801410</b>	25 g
<b>801411</b>	100 g
<b>801412</b>	1000 g

## References

- Booth, R. J., Hodges, J. C. *J. Am. Chem. Soc.* 1997, 119, 4882.
- Gooding, O., Labadie, J.; Porco, J. *J. Comb. Chem.* 1999, 1, 420–422.



Biotage holds certification for both  
ISO9001 Quality Management and  
ISO14001 Environmental Management.

### EUROPE

Main Office: +46 18 565900  
Toll Free: +800 18 565710  
Fax: +46 18 591922  
Order Tel: +46 18 565710  
Order Fax: +46 18 565705  
order@biotage.com  
Support Tel: +46 18 56 59 11  
Support Fax: + 46 18 56 57 11  
eu-1-pointsupport@biotage.com

### NORTH & LATIN AMERICA

Main Office: +1 704 654 4900  
Toll Free: +1 800 446 4752  
Fax: +1 704 654 4917  
Order Tel: +1 704 654 4900  
Order Fax: +1 434 296 8217  
ordermailbox@biotage.com  
Support Tel: +1 800 446 4752  
Outside US: +1 704 654 4900  
us-1-pointsupport@biotage.com

### JAPAN

Tel: +81 3 5627 3123  
Fax: +81 3 5627 3121  
jp\_order@biotage.com  
jp-1-pointsupport@biotage.com

### CHINA

Tel: +86 21 2898 6655  
Fax: +86 21 2898 6153  
cn\_order@biotage.com  
cn-1-pointsupport@biotage.com

To locate a distributor,  
please visit our website  
[www.biotage.com](http://www.biotage.com)

Part Number: PPS399.V.1

© 2016 Biotage. All rights reserved. No material may be reproduced or published without the written permission of Biotage. Information in this document is subject to change without notice and does not represent any commitment from Biotage. E&OE. A list of all trademarks owned by Biotage AB is available at [www.biotage.com/legal](http://www.biotage.com/legal). Other product and company names mentioned herein may be trademarks or registered trademarks and/or service marks of their respective owners, and are used only for explanation and to the owners' benefit, without intent to infringe.