

Reactive cyclodextrins for

Click chemistry and single isomer cyclodextrin synthesis



Reactive cyclodextrins

CycloLaboffersawidevarietyof cyclodextrins (CDs)which bear functional groups atwell-definedpositionsandthesegroupsparticipateeasily in chemical reactions.These versatilederivativesare milestonesfor cyclodextrin chemistry:

- Primary-side halogenated/tosylated cyclodextrins are ideal substrates for further modification as they can be efficiently substituted by any nucleophile.
- Azido-bearing CDs are extremely versatile intermediates. They can be reduced to the corresponding amino CDs or can be promptly used in azide-alkyne cycloaddition.
- CD derivatives modified with amino or thiol groups are able to react, in suitable conditions, with a large variety of electrophiles.



αCD

 $[N_3]_7$

ÓCH₃]₄

 $\left[N_3\right]_6$

Reactive cyclodextrins for click chemistry

 N_3

Azido-modified CDs are among the most versatile intermediates. They are stable and convenient precursor of the corresponding amino-CD derivatives. They can be efficiently reacted with the alkyne counterpart to generate multifunctional systems able to interact through cooperative forces with the selected biological target.

G. Cravotto: Alkyne-azide click reaction catalyzed by metallic copper under ultrasound

 $\left[N_3\right]_7$

A. Vargas-Berenguel: Ferrocene–β-cyclodextrin conjugates: synthesis, supramolecular behavior and use as electrochemical sensors

H. Ritter: Pseudopolyanions based on poly(NIPAAM-co-β-Cyclodextrin methacrylate) and ionic liquids

 $[N_3]_8$



Reactive cyclodextrins bearing -NH₂ functions



agents. Cationic, amphiphilic CDs can assemble into supramolecular system able to effectively deliver nucleic acids. Amino-CDs can be applied as effective chiral catalyst.

J.F. Stoddart: Amino acid derivatives of β-cyclodextrin
V.A. Karginov: β-cyclodextrin derivatives that inhibit anthrax lethal toxin
K. Fujita: Heptakis(6-deoxy-6-guanidino)-b-cyclodextrin: an artificial model for mitochondrial ADP/ATP carrier



Reactive cyclodextrins bearing -SH functions



CDs modified with thiol groups have a large variety of applications. They can be used to coat surfaces, for building-up gene delivery system and for forming hydrogels to carry hydrophobic drugs. They have been used as well as chelating agent and electrochemical sensors.

J.F. Stoddart: Supported monolayers containing preformed binding sites. Synthesis and interfacial binding properties of a thiolated β -cyclodextrin derivative

G. Wenz: Supported monolayers containing preformed binding sites. Synthesis and interfacial binding properties of a thiolated β-cyclodextrin derivative

D. Klockow: Investigation of the adsorption of gaseous aromatic compounds at surfaces coated with heptakis(6-thio-6-deoxy)-β-cyclodextrin by surface-enhanced Raman scattering



Reactive cyclodextrins bearing leaving groups

OTs

Halogenation and tosylation are the reactions that allow the selective modification of the CD's primary rim.

 $\left[\mathsf{C}\mathsf{I}\right]_{8}$

vCD

Br]a $V \subset D$ $V \subset D$ $V \subset$

The class of per-6-halo-CDs represents the fundamental starting point for any modification based on nucleophilic substitution.

6-monotosyl- and 6-monohalogenated CDs are the most widely utilized derivative for single modification of the upper rim.

A. Gadelle: Selective halogenation at primary positions of cyclomaltooligosaccharides and a synthesis of per-3,6-anhydro cyclomaltooligosaccharides
 R. Darcy: 6^A-O-p-Toluenesulfonyl-β-cyclodextrin



Reactive cyclodextrins for selective bifunctionalization

This unique derivative was *adhoc* developed for heterobifunctionalization of the CD on the primary side.



This interesting compound is the optimal starting point for the design of sophisticated architectures.

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Compound available as mixture of three pairs of positional isomer or as single pair of pseudo enantiomer (AB-BA or AC-CA or AD-DA).



Reactive cyclodextrins List of available Betacyclodextrin products at CycloLab

Product code	Product name	Product code	Product name	
CY-2024	6-Monodeoxy-6-monoamino-BCD	CY-2021	6-Monotosyl-BCD	
CY-2050	<mark>6-Monodeoxy-6-monoazido</mark> -BCD	CY-2051	6-Monodeoxy-6-monoiodo-BCD	
CY-2055 CY-2056	6-Monodeoxy-6-monoamino-per- methyl-BCD 6-Monodeoxy-6-monoamino-random- methyl-BCD	CY-2053	6-Monodeoxy-6-monobromo-BCD	
		CY-2061	Heptakis(6-deoxy-6-bromo)-BCD	
		CY-2062	Heptakis(6-deoxy-6-iodo)-BCD	
CY-2059	6-Monodeoxy-6-monothio-BCD	CY-2204	Heptakis(6-deoxy-6-chloro)-BCD	
CY-2065	Heptakis(6-deoxy-6-amino)-BCD	CY-2217	6-Monodeoxy-6-monoazido-6- monotosyl-BCD	
CY-2066	Heptakis(2,3-di- <i>O</i> -methyl-6-deoxy-6- amino)-BCD	Alpha and commo		
CY-2075	Heptakis(6-deoxy-6-azido)-BCD		Alpha- and gamma-	
CY-2076	Heptakis(2,3-di- <i>O</i> -methyl-6-deoxy-6- azido)-BCD	cyclodextrin derivatives are also available of the		

For any other specific derivative to be designed, please reach out to us for discussion at info@cyclolab.hu

listed products!



Reactive cyclodextrins

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