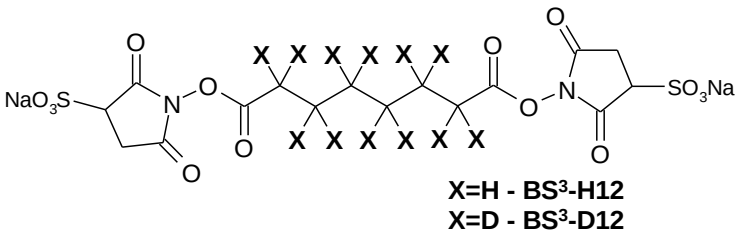
BS^3-H12/D12

Product Information



BS^3-H12/D12
BisSulfoSuccinimidylSuberate
12 x 1 mg of 1:1 molar ratio mixture of BS^3-H12 and BS^3-D12
Cat. Number: 001SS
$C_{16}H_{18}N_2Na_2O_{14}S_2$ / $C_{16}D_{12}H_6N_2Na_2O_{14}S_2$
MW 572 / 584

Features:
Isotopically-coded.
Water-soluble.
240/252 immonium ion for dead-end crosslinks.

BS^3-H12/D12 is a water-soluble, homobifunctional, isotopically-coded crosslinker BisSulfoSuccinimidylSuberate. Light (H12) and heavy (D12) forms of the reagent differ by 12 deuterium atoms in heavy form instead of 12 hydrogen atoms of light form, and otherwise are chemically identical. Isotopic coding enables univocal detection of the crosslinked products in mass spectra. Reaction products of BS^3-H12/D12 will manifest in mass spectra as doublets of peaks of equal intensity corresponding to light (H12) and heavy (D12) forms of the reagent separated by 12.07573 Da divided by charge state (12.07 for +1, 6.04 for +2, 4.03 for +3 etc.).

N-HydroxySulfoSuccinimide (NHSS) esters react mainly with primary amino groups ($-NH_2$) in pH 7-9 buffers to form stable amide bonds. Therefore, amine-containing buffers (Tris, Glycine, ammonium salts, etc.) should be avoided for crosslinking reaction. BS3 is water-soluble and stock solutions can be prepared in water. To make 50 mM stock solution of the BS^3-H12/D12, add 35 μl water to the pre-weigh tube containing 1 mg of the reagent.

To calculate masses of peptide crosslinks use following formulas:
$[M_{12}+H]^+ = [M_1+H]^+ + [M_2+H]^+ + 137.06025$
$[M_1OH+H]^+ = [M_1+H]^+ + 156.07864$
$[M_1i+H]^+ = [M_1+H]^+ + 138.06808$
$[M_1NH_2+H]^+ = [M_1+H]^+ + 155.09462$
, where M_1, M_2 - masses of free peptides; M_{12} – mass of inter-peptide crosslink; M_1OH – mass of dead-end crosslink; M_1i – mass of intra-peptide crosslink; M_1NH_2 – mass of dead-end amide (if reaction was quenched with ammonium salts).
MS-Bridge (http://prospector.ucsf.edu) bridge elemental composition: C8 H10 O2; modification elemental composition for –OH dead-ends: C8 H12 O3; modification elemental composition for $–NH_2$ dead-ends: C8 H13 O2 N.

Typical MALDI mass spectrum of the test reaction with FLAG (DYKDDDDK) peptide is shown in Figure 1. Masses of the reaction products for the light (H12) form of the reagent are: 1013 – free FLAG peptide; 1151 – intra-peptide crosslink; 1169 – dead-end crosslink; 2163 – inter-peptide crosslink.
240/252 doublet of signals in the MSMS spectrum corresponding to the modified with the reagent lysine immonium ion is indicative of the –OH dead-end crosslink (Ref. 1, 2), (Figure 2).

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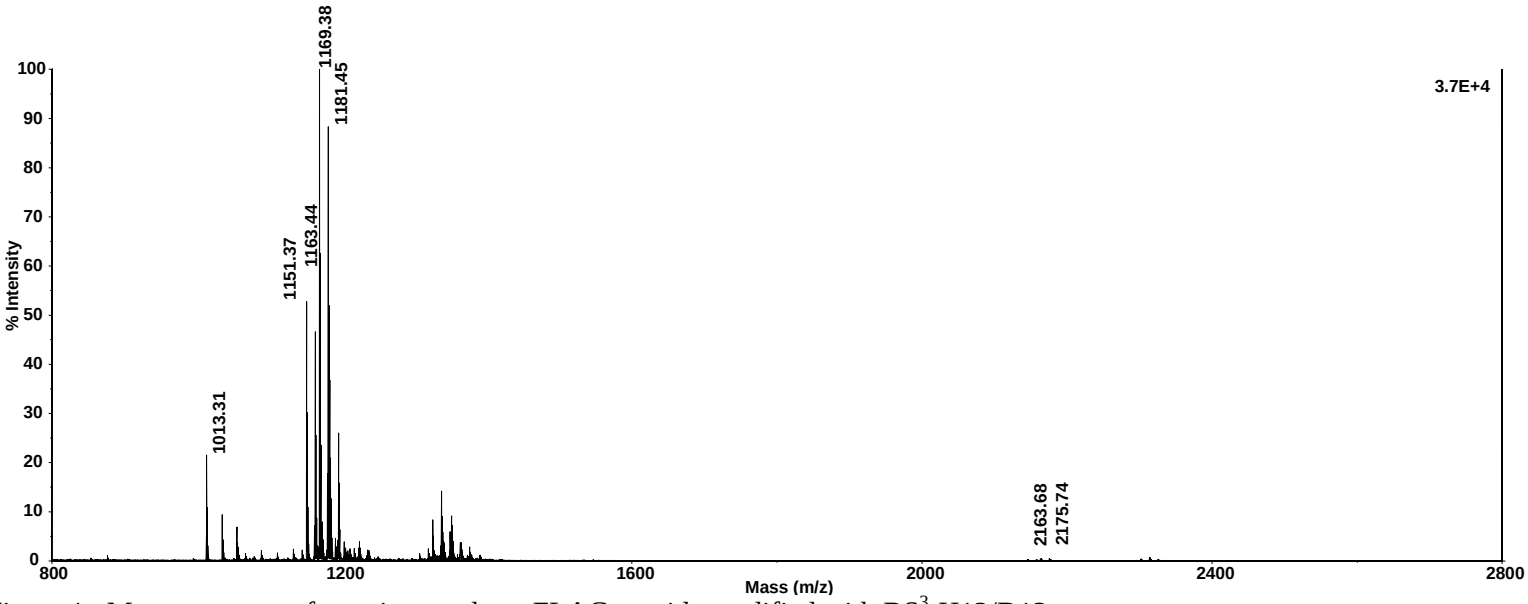

Figure 1. Mass spectrum of reaction products FLAG peptide modified with BS^3-H12/D12.

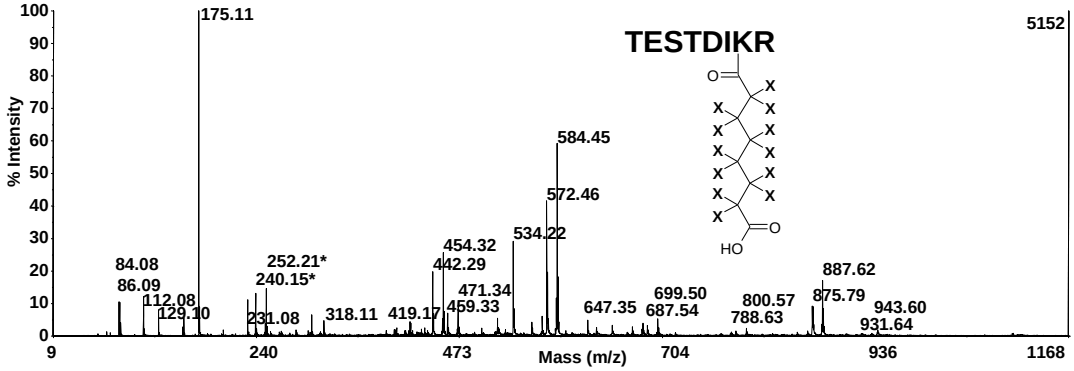

Figure 2. MSMS spectrum of dead-end BS^3-H12/D12 peptide crosslink. Characteristic for dead-end crosslinks immonium 240/252 Da ion doublet is marked by asterisks.

Material Safety Data information: substance is not fully tested yet.

References:

1. Schilling B, Row RH, Gibson BW, Guo X, Young MM.
MS2Assign, automated assignment and nomenclature of tandem mass spectra of chemically crosslinked peptides.
J Am Soc Mass Spectrom. 2003 Aug;14(8):834-50.

2. Seebacher J, Mallick P, Zhang N, Eddes JS, Aebersold R, Gelb MH.
Protein cross-linking analysis using mass spectrometry, isotope-coded cross-linkers, and integrated computational data processing.
J Proteome Res. 2006 Sep;5(9):2270-82.

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