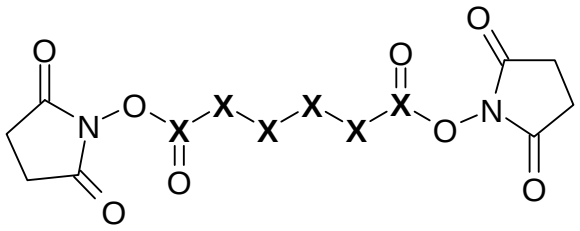
DSA-^{12}C6/^{13}C6

Product Information



X=^{12}C - DSA-^{12}C6
X=^{13}C - DSA-^{13}C6

DSA-^{12}C6/^{13}C6
DiSuccinimidylAdipate
12 x 0.34 mg of 1:1 molar ratio mixture of DSA-^{12}C6 and DSA-^{13}C6
Cat. Number: 013SC
Formula: C14H16N2O8 /^{12}C8^{13}C6H16N2O8
Molecular Weight: 340 / 346

Features:
Isotopically-coded.
Membrane-permeable.
212/218 immonium ion for dead-end crosslinks.
HPLC co-eluting light and heavy isotopic forms.

DSA-^{12}C6/^{13}C6 is a membrane-permeable, homobifunctional, isotopically-coded crosslinker DiSuccinimidylGlutarate. Light (^{12}C6) and heavy (^{13}C6) forms of the reagent differ by 6 ^{13}C atoms in heavy form instead of ^{12}C atoms of light form, and otherwise are chemically identical. Isotopic coding enables univocal detection of the crosslinked products in mass spectra. Reaction products of DSA-^{12}C6/^{13}C6 will manifest in mass spectra as doublets of peaks of equal intensity corresponding to light (^{12}C6) and heavy (^{13}C6) forms of the reagent separated by 6.02016 Da divided by charge state (6.02 for +1, 3.01 for +2, 2.00 for +3 etc.).

N-HydroxySuccinimide (NHS) 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. DSA is water-insoluble and stock solutions should be prepared in an organic solvent such as DMSO or DMF and then added to the aqueous reaction mixture. To make 10 mM stock solution of the DSA-^{12}C6/^{13}C6, add 100 µl DMSO to the pre-weigh tube containing 0.34 mg of the reagent.

To calculate masses of peptide crosslinks use following formulas:
$[M_{12}+H]^+ = [M_1+H]^+ + [M_2+H]^+ + 109.02841$
$[M_1OH+H]^+ = [M_1+H]^+ + 128.04680$
$[M_1i+H]^+ = [M_1+H]^+ + 110.03624$
$[M_1NH_2+H]^+ = [M_1+H]^+ + 127.06278$
, 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: C6 H6 O2; modification elemental composition for –OH dead-ends: C6 H8 O3; modification elemental composition for –NH_2 dead-ends: C6 H9 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 (H6) form of the reagent are: 1013 – free FLAG peptide; 1123 – intra-peptide crosslink; 1141 – dead-end crosslink; 2135 – inter-peptide crosslink.
212/218 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).

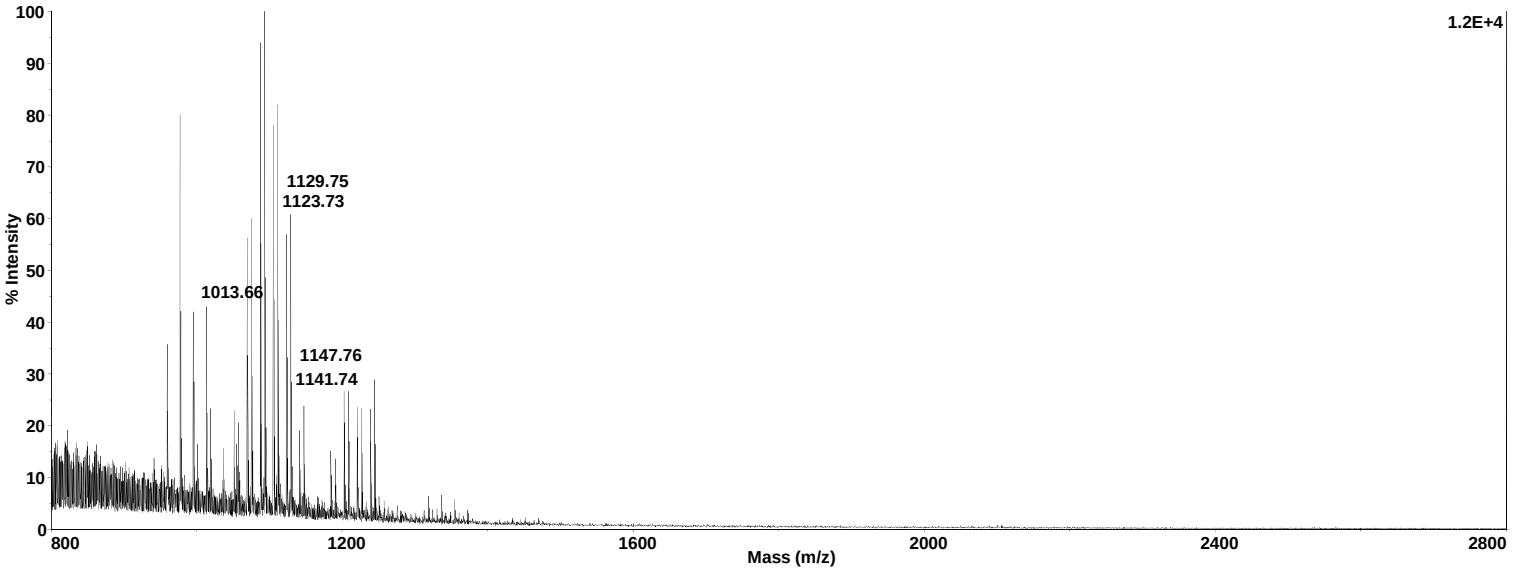


Figure 1. Mass spectrum of reaction products FLAG peptide modified with DSA-^{12}C6/^{13}C6.

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.

