

DSG-H6/D6**Product Information**

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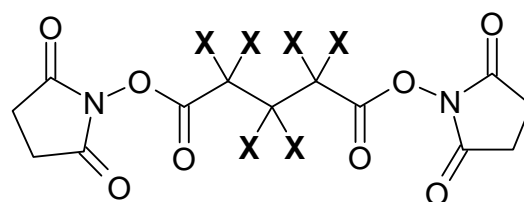
DiSuccinimidylGlutarate

12 x 1 mg of 1:1 molar ratio mixture of DSG-H6 and DSG-D6

Cat. Number: 010S

Formula: C₁₃H₁₄N₂O₈ / C₁₃D₆H₈N₂O₈

Molecular Weight: 326 / 332

**X=H - DSG-H6****X=D - DSG-D6****Features:**

Isotopically-coded.

Membrane-permeable.

198/204 immonium ion for dead-end crosslinks.

DSG-H6/D6 is a membrane-permeable, homobifunctional, isotopically-coded crosslinker DiSuccinimidylGlutarate. Light (H6) and heavy (D6) forms of the reagent differ by 6 deuterium atoms in heavy form instead of 6 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 DSG-H6/D6 will manifest in mass spectra as doublets of peaks of equal intensity corresponding to light (H6) and heavy (D6) forms of the reagent separated by 6.04368 Da divided by charge state (6.04 for +1, 3.02 for +2, 2.01 for +3 etc.).

N-HydroxySuccinimide (NHS) esters react mainly with primary amino groups (-NH₂) 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. DSS 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 50 mM stock solution of the DSG-H6/D6, add 61 µl DMSO to the pre-weigh tube containing 1 mg of the reagent.

To calculate masses of peptide crosslinks use following formulas:

$$[M_{12}+H]^+ = [M_1+H]^+ + [M_2+H]^+ + 95.01276$$

$$[M_1OH+H]^+ = [M_1+H]^+ + 114.03115$$

$$[M_{1i}+H]^+ = [M_1+H]^+ + 96.02059$$

$$[M_1NH_2+H]^+ = [M_1+H]^+ + 113.04713$$

, where M₁, M₂ - masses of free peptides; M₁₂ – mass of inter-peptide crosslink; M₁OH – mass of dead-end crosslink; M₁i – mass of intra-peptide crosslink; M₁NH₂ – mass of dead-end amide (if reaction was quenched with ammonium salts).

MS-Bridge (<http://prospector.ucsf.edu>) bridge elemental composition: C₅ H₄ O₂; modification elemental composition for –OH dead-ends: C₅ H₆ O₃; modification elemental composition for –NH₂ dead-ends: C₅ H₇ 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; 1109 – intra-peptide crosslink; 1127 – dead-end crosslink; 2121 – inter-peptide crosslink.

198/204 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).

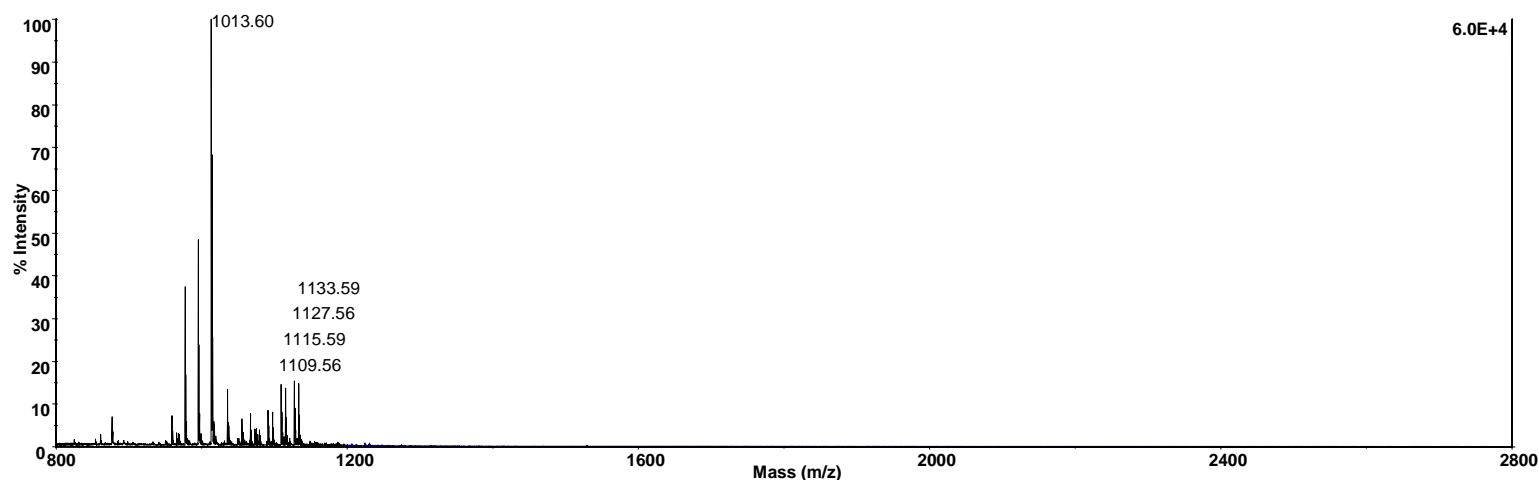


Figure 1. Mass spectrum of reaction products FLAG peptide modified with DSG-H6/D6.

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.