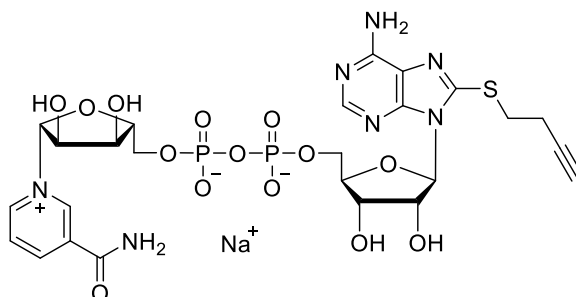


Technical Information about 8-Bu(3-yne)T-NAD⁺

Update: March 13, 2024 ss



Abbreviation: 8-Bu(3-yne)T-NAD⁺

Formula	CAS No.	Molecular Weight	UV	BIOLOG Cat. No.
C ₂₅ H ₃₁ N ₇ O ₁₄ P ₂ S (free acid)	[2022926-15-2]	747.6 (free acid)	λ _{max} 276 nm / ε 21400 / pH 7	N 055

Name: β- Nicotinamide- 8- (3- butynylthio)adenine dinucleotide

Description: 8-Bu(3-yne)T-NAD⁺ is an analogue of the natural signal molecule β-NAD⁺, in which the hydrogen in position 8 of the heterocyclic nucleobase is replaced by the lipophilic 3-butynylthio moiety.

Properties: The alkyne-containing 8-Bu(3-yne)T-NAD⁺ is an analogue of NAD⁺ and a suitable molecular tool for the copper-catalysed Huisgen azide-alkyne [3+2] cycloaddition (CuAAC), which has attracted particular interest for the introduction of reporter groups and for the labelling of NAD⁺-binding proteins like substrate proteins of poly(ADP-ribose) polymerases (PARPs) by the so-called click-chemistry technique.

Specification: Lyophilized or crystallized sodium salt. Other salt forms are available upon request. Equal concentrations of 8-Bu(3-yne)T-NAD⁺ can appear very different in volume due to sensitivity of the lyophilized form to humidity. The compound can even contract to small volume droplets. Normally the product is located in the conical bottom of the tube. Micromolar quantities are determined by UV at λ_{max}.

Purity: Typical analysis is better than 95% (HPLC / UV / 276 nm). The product is not sterile and has not been tested for endotoxins.

Solubility: 8-Bu(3-yne)T-NAD⁺ is soluble in water (≥ 5 mM, limits have not been determined). Please rinse tube walls carefully and preferably use ultrasonic or vortex to achieve total and uniform mixing. When opening the tube please make sure that no substance is lost within the cap.

Stability and Storage: 8-Bu(3-yne)T-NAD⁺ has limited stability at ambient temperature. We recommend that the compound should be stored in the freezer (-20° Celsius necessary, -80° recommended), for longer storage periods preferably in freeze-dried form.

Toxicity and Safety: Since β-NAD⁺ has multiple tasks in every organism, it is very likely that its analogues will interfere with many cell regulation processes *in vivo*. However, due to the rather small quantities to work with, no health hazards have been reported. Nevertheless please keep in mind, that the *in vivo* properties of this compound are not sufficiently characterized up to now. Avoid skin contact or ingestion and allow only trained personnel to handle the product.

Our products are designed, developed and sold for research purposes only! They are intended for *in vitro* and nonhuman *in vivo* laboratory applications. Any other use requires approval of health authorities.

Not for drug, household or related uses!

Selected References for 8-Bu(3-yne)T-NAD⁺:

Rogge, R.A.; Gibson, B.A.; Kraus, W.L., *Methods Mol. Biol.*, **1813**, 371-387 (2018): "Identifying Genomic Sites of ADP-Ribosylation Mediated by Specific Nuclear PARP Enzymes Using Click-ChIP"

Gibson, B.A.; Zhang, Y.; Jiang, H.; Hussey, K.M.; Shrimp, J.H.; Lin, H.; Schwede, F.; Yu, Y.; Kraus, W.L., *Science*, **353**, 45 - 50 (2016): "Chemical Genetic Discovery of PARP Targets Reveals a Role for PARP-1 in Transcription Elongation"