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## Product Data Sheet

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Product Name: 4'-bromo-Resveratrol

Cat. No.: GC17922

### Chemical Properties

Cas. No. 1224713-90-9

Chemical Name 5-[(1E)-2-(4-bromophenyl)ethenyl]-1,3-benzenediol

SMILES OC1=CC(O)=CC(/C=C/C2=CC=C(Br)C=C2)=C1

Formula  $C_{14}H_{11}BrO_2$

M.Wt 291.1

Solubility  $\leq 50\text{mg/ml}$  in ethanol;  $50\text{mg/ml}$  in DMSO;  $100\text{mg/ml}$  in dimethyl formamide

Storage Store at  $-20^{\circ}\text{C}$

General tips For obtaining a higher solubility, please warm the tube at  $37^{\circ}\text{C}$  and shake it in the ultrasonic bath for a while. Stock solution can be stored below  $-20^{\circ}\text{C}$  for several months.

Shipping Condition Evaluation sample solution: ship with blue ice. All other available size: ship with RT, or blue ice upon request.

Structure

### Background

4'-bromo-Resveratrol is a Sirt1 and Sirt3 inhibitor.

Sirtuins are protein deacetylases regulating aging processes and many physiological functions. Resveratrol activates human Sirt1 and inhibits Sirt3, and can mimic calorie restriction effects including lifespan extension in lower organisms.

In vitro: Sirtuin modulation was studied by using 4'-bromo-resveratrol in a previous study. 4'-bromo-Resveratrol inhibited Sirt3 with much higher potency than resveratrol, and it also inhibited rather than activated Sirt1. Crystal structures of human Sirt3/peptide complexes of 4'-bromo-resveratrol identified two binding sites. An internal site caused the potent inhibitory effect. 4'-bromo-Resveratrol interfered with  $\text{NAD}^+$  and substrate peptide binding, and it extended its bromo-phenyl group in a unrecognized site pocket. The second binding site for 4'-bromo-resveratrol was found to be located on the surface of Sirt3 and connected via two helices to peptide-binding active site loops. In

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Sirt1, this site appeared to comprise a residue that was essential for its activation by small molecules and 4'-bromo-resveratrol therefore constituted a candidate for the long-sought allosteric Sirt1 activator binding site [1].

In vivo: So far, there is no animal in vivo data for 4'-bromo-resveratrol.

Clinical trial: Up to now, 4'-bromo-resveratrol is still in the preclinical development stage.

Reference:

[1] Nguyen GT, Gertz M, Steegborn C. Crystal structures of Sirt3 complexes with 4'-bromo-resveratrol reveal binding sites and inhibition mechanism. Chem Biol. 2013 Nov 21;20(11):1375-85.

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