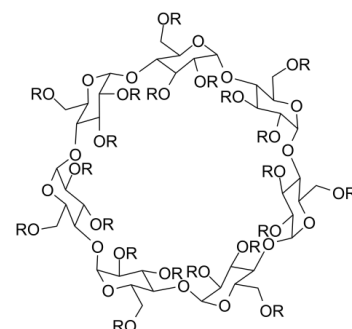


## Data Sheet

<b>Product Name:</b>	SBE-β-CD
<b>Cat. No.:</b>	CS-0731
<b>CAS No.:</b>	182410-00-0
<b>Molecular Formula:</b>	N/A
<b>Molecular Weight:</b>	N/A
<b>Target:</b>	Others
<b>Pathway:</b>	Others
<b>Solubility:</b>	DMSO : 5.625 mg/mL (Need ultrasonic and warming); H <sub>2</sub> O : 250 mg/mL (Need ultrasonic)



### BIOLOGICAL ACTIVITY:

SBE-β-CD is a sulfobutylether β-cyclodextrin derivative used as an excipient or a formulating agent to increase the solubility of poorly soluble drugs. **In Vitro:** SBE-β-CD is a chemically modified β-CD that is a cyclic hydrophilic oligosaccharide which is negatively charged in aqueous media. β-CD functioned as a solubilizer only at low concentrations, whereas SBE-β-CD exhibits strong solubilizing effects over a wide concentration range<sup>[1]</sup>. **In Vivo:** SBE-β-CD is a derivatized form of β-cyclodextrin that has been developed as a safe and effective solubilizing agent for drugs being administered by parenteral and other routes (including oral). SBE-β-CD is a cyclic carbohydrate comprised of seven glucose molecules; the resulting truncated cone-like structure being further derivatized with an average of seven sulfobutyl ether groups<sup>[2]</sup>. The calorimetric data for the Compound 1/SBE-β-CD complex indicates an extremely strong interaction, with an association constant of  $2.3 \pm (0.2) \times 10^6 M^{-1}$  at 25°C and  $1.6 \pm (0.2) \times 10^6 M^{-1}$  at 37°C<sup>[3]</sup>. SBE-β-CD alone evokes a mild cardio-depressant effect independent of cocaine treatment ( $p = 0.0001$  compared to baseline) but attenuates further cocaine-induced decreases in RPP, dP/dtmax, and dP/dtmax<sub>abs</sub> at high cocaine concentrations. No significant effect is seen on line pressure. SBE-β-CD alleviates the most pronounced cardiac depression for RPP, dP/dtmax, and dP/dtmax<sub>abs</sub>. This differential effect of SBE-β-CD at low and high concentrations produces an interaction effect in the two-way ANOVA for RPP ( $p < 0.0001$ ), dP/dtmax ( $p = 0.0001$ ), and dP/dtmax<sub>abs</sub> ( $p = 0.0015$ ), and prevents any overall treatment effect. Infusing SBE-β-CD also attenuates the cardiac depression associated with cocaethylene toxicity for RPP and dP/dtmax. No differences are observed between ethanol-treated controls and cocaethylene plus SBE-β-CD groups<sup>[4]</sup>.

### PROTOCOL (Extracted from published papers and Only for reference)

**Animal Administration:** SBE-β-CD is prepared in saline<sup>[3]</sup>.<sup>[3]</sup>Rats<sup>[3]</sup>

A 300 g rat is administered with 1 mL of a 0.1 M SBE-β-CD solution containing 5.64 mg of Compound 1, and assuming an extracellular volume of 90 mL, less than 0.1% of the complex would rapidly dissociate due to the initial effects of dilution. This calculation, combined with the changing blood to plasma ratio in the presence of SBE-β-CD, provides a reasonable explanation for the observed differences in the blood and plasma profiles of Compound 1 after intravenous administration in either the cyclodextrin or cyclodextrin-free formulations. After IV administration of the cyclodextrin formulation, Compound 1 would initially be prevented from distributing into erythrocytes thereby resulting in a whole blood to plasma ratio of less than one. Subsequently, clearance of SBE-β-CD from the circulation would lead to changes in the complexation equilibrium such that the unbound fraction of Compound 1 would increase, thereby reestablishing normal blood to plasma partitioning (i.e. in favour of whole blood) and clearance.

### References:

[1]. Fukuda M, et al. Influence of sulfobutyl ether beta-cyclodextrin (Captisol) on the dissolution properties of a poorly soluble drug from extrudates prepared

by hot-melt extrusion. Int J Pharm. 2008 Feb 28;350(1-2):188-196

[2]. Lockwood SF, et al. Improved aqueous solubility of crystalline astaxanthin (3,3'-dihydroxy-beta, beta-carotene-4,4'-dione) by Captisol (sulfobutyl ether beta-cyclodextrin). J Pharm Sci. 2003 Apr;92(4):922-926.

[3]. Charman SA, et al. Alteration of the intravenous pharmacokinetics of a synthetic ozonide antimalarial in the presence of a modified cyclodextrin. J Pharm Sci. 2006 Feb;95(2):256-67

[4]. Fettiplace MR, et al. Cardiac depression induced by cocaine or cocaethylene is alleviated by lipid emulsion more effectively than by sulfobutylether- $\beta$ -cyclodextrin. Acad Emerg Med. 2015 May;22(5):508-17

### CAIndexNames:

$\beta$ -Cyclodextrin, sulfobutyl ethers, sodium salts

### SMILES:

[R]O[C@@H]1[C@H](O[R])[C@H](O[C@@H]2[C@H](O[R])C(O[R])[C@H](O3[C@@H](CO[R])O2)[C@@H](CO[R])O[C@@H]1O[C@H]4[C@H](O[R])[C@@H](O[R])[C@@H](O[C@H]5[C@H](O[R])[C@@H](O[R])[C@@H](O[C@H]6C(O[R])[C@H](O[R])[C@H](O[C@@H]7[C@@H](O[R])[C@H](O[R])[C@H](O[C@@H]8[C@@H](O[R])[C@H](O[R])[C@H]3O[C@H]8CO[R])O[C@H]7CO[R])O[C@H]6CO[R])O[C@@H]5CO[R])O[C@@H]4CO[R].[R= H 21-m or C4H8SO3-Na+ m , m= 6.0-7.1]

**Caution: Product has not been fully validated for medical applications. For research use only.**

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