

## Product Data Sheet

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Product Name: Pracinostat (SB939)

Cat. No.: GC16734

### Chemical Properties

Cas. No. 929016-96-6

Chemical Name (E)-3-[2-butyl-1-[2-(diethylamino)ethyl]benzimidazol-5-yl]-N-hydroxyprop-2-enamide

SMILES CCCCC1=NC2=C(N1CCN(CC)CC)C=CC(=C2)C=CC(=O)NO

Formula  $C_{20}H_{30}N_4O_2$  M.Wt 358.48

Solubility  $\geq 11.4$  mg/mL in DMSO,  $\geq 24.8$  mg/mL in EtOH with ultrasonic 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.

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

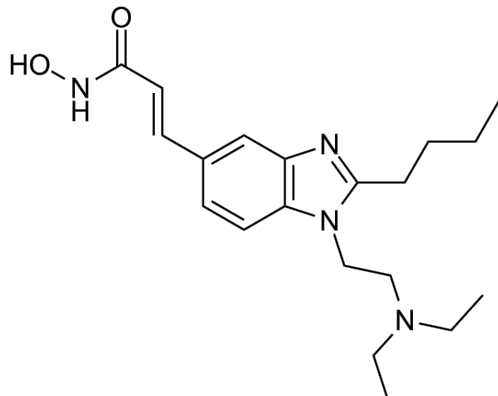
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### Structure



### Protocol

#### Cell experiment:

Cell lines                      Ovarian (A2780) , colon (HCT-116), and prostate (PC-3) cell lines

Preparation method                      The solubility of this compound in DMSO is >10 mM. General tips for obtaining a higher concentration: Please warm the tube at 37 °C for 10 minutes and/or shake it in the ultrasonic bath for a while. Stock solution can be stored below -20°C for several months.

Reaction Conditions                      96 h; IC<sub>50</sub>=0.48±0.21 μM (A2780), 0.48±0.27 μM (HCT-116), 0.34±0.06 μM (PC-3)

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**Applications** SB939 showed broad anti-proliferative activity against representative tumor cells from ovarian (A2780) , colon (HCT-116), and prostate (PC-3) with cellular IC50 values of  $0.48 \pm 0.21$ ,  $0.48 \pm 0.27$  and  $0.34 \pm 0.06$   $\mu$ M, respectively.

### Animal experiment:

**Animal models** Athymic nude mice

**Dosage form** 200 mg/kg, 100 mg/kg, 50 mg/kg; oral taken.

**Applications** SB939 was clearly toxic at the highest dose tested (200 mg/kg); however, at the MTD dose of 100 mg/kg and at 50mg/kg, it demonstrated very significant antitumor effects on day 21 with TGI = 90% ( $p < 0.001$ ) and 66% ( $p < 0.001$ ), respectively, with acceptable body weight loss.

**Other notes** Please test the solubility of all compounds indoor, and the actual solubility may slightly differ with the theoretical value. This is caused by an experimental system error and it is normal.

### References:

[1] Wang H, Yu N, Chen D, et al. Discovery of (2 E)-3-{2-butyl-1-[2-(diethylamino) ethyl]-1 H-benzimidazol-5-yl}-N-hydroxyacrylamide (SB939), an orally active histone deacetylase inhibitor with a superior preclinical profile[J]. Journal of medicinal chemistry, 2011, 54(13): 4694-4720.

### Background

Pracinostat, also known as SB939, is a potent and orally available inhibitor of histone deacetylase (HDAC) with a relatively stronger selectivity (more than 1000-fold) for class I, class II and class IV HDACs rather than class III HDACs. Pracinostat potently suppresses proliferation in a wide range of cancer cell lines, including colon cancer, ovarian cancer, prostate carcinomas, acute myeloid

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leukaemia (AML) and B cell lymphoma. Recent study results have shown that SB939 induces the accumulation of acetylated histone H3 (AcH3) and acetylated  $\alpha$ -tubulin and increases the expression of the cyclin dependent kinase inhibitor p21 in cancer cells.

### Reference

[1].Razak AR, Hotte SJ, Siu LL, Chen EX, Hirte HW, Powers J, Walsh W, Stayner LA, Laughlin A, Novotny-Diermayr V, Zhu J, Eisenhauer EA. Phase I clinical, pharmacokinetic and pharmacodynamic study of SB939, an oral histone deacetylase (HDAC) inhibitor, in patients with advanced solid tumours. Br J Cancer. 2011;104(5):756-762.

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