



## Alogliptin (SYR-322) benzoate

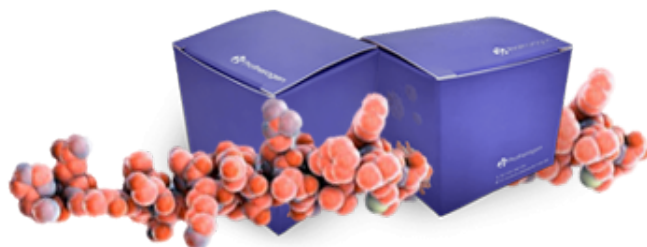
|                    |                             |
|--------------------|-----------------------------|
| <b>Cat. No.:</b>   | OB0225WX-2531               |
| <b>Appearance:</b> | Solid                       |
| <b>Purity:</b>     | ≥99%                        |
| <b>Identity:</b>   | Confirmed by NMR, and HPLC. |
| <b>Size:</b>       | 5 mg; 10 mg; 50 mg; 100 mg  |

This product is for research use only and is not intended for diagnostic use.

### Product Overview

#### Description

Alogliptin (SYR-322) benzoate is a potent DPP-4 inhibitor with an IC<sub>50</sub> of less than 10 nM, displaying a massive 10,000-fold selectivity over related enzymes DPP-8 and DPP-9.



|                       |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
|-----------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Synonym</b>        | SYR-322; 850649-62-6; Alogliptin benzoate; Nesina; SYR-322; SYR 322; Alogliptin (Benzoate); Alogliptin (as benzoate); (R)-2-((6-(3-aminopiperidin-1-yl)-3-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl)benzonitrile benzoate; 2-[[6-[(3R)-3-aminopiperidin-1-yl]-3-methyl-2,4-dioxopyrimidin-1-yl]methyl] benzonitrile; benzoic acid; 6-((3R)-3-aminopiperidin-1-yl)-1-(2-cyanobenzyl)-3-methylpyrimidin-2,4(1H,3H)-dione monobenzoate; Benzonitrile, 2-((6-((3R)-3-amino-1-piperidinyl)-3,4-dihydro-3-methyl-2,4-dioxo-1(2H)-pyrimidinyl)methyl)-, monobenzoate; Benzonitrile, 2-[[6-[(3R)-3-amino-1-piperidinyl]-3,4-dihydro-3-methyl-2,4-dioxo-1(2H)-pyrimidinyl]methyl]-, monobenzoate; MFCD0983319 5; 2-((6-((3R)-3-amino-1-piperidinyl)-3,4-dihydro-3-methyl-2,4-dioxo-1(2H)-pyrimidinyl)methyl)benzonitrile monobenzoate; (3R)-1-(3-(2-cyanobenzyl)-1-methyl-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)piperidin-3-aminium benzoate; (3R)-1-[3-(2-cyanobenzyl)-1-methyl-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl]piperidin-3-aminium benzoate; 2-((6-((3R)-3-aminopiperidin-1-yl)-3-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl)benzonitrile benzoate; 2-((6-((3R)-3-aminopiperidin-1-yl)-3-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)methyl)benzonitrile monobenzoate |
| <b>CAS No.</b>        | 850649-62-6                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| <b>Compound CID</b>   | 16088021                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| <b>Formula</b>        | C <sub>18</sub> H <sub>21</sub> N <sub>5</sub> O <sub>2</sub> ·C <sub>7</sub> H <sub>6</sub> O <sub>2</sub>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| <b>Formula Weight</b> | 461.51                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |

## Specification

|                      |                                                                                                                                                                                                               |
|----------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>IUPAC Name</b>    | 2-[[6-[(3R)-3-Aminopiperidin-1-yl]-3-methyl-2,4-dioxopyrimidin-1-yl]methyl]benzonitrile; benzoic acid                                                                                                         |
| <b>InChI</b>         | InChI=1S/C18H21N5O2.C7H6O2/c1-21-17(24)9-16(22-8-4-7-15(20)12-22)23(18(21)25)11-14-6-3-2-5-13(14)10-19;8-7(9)6-4-2-1-3-5-6/h2-3,5-6,9,15H,4,7-8,11-12,20H2,1H3;1-5H,(H,8,9)/t15-;/m1./s1                      |
| <b>InChI Key</b>     | KEJICXJTRHYAK-XFULWGLBSA-N                                                                                                                                                                                    |
| <b>SMILES string</b> | CN1C(=O)C=C(N(C(=O)CC2=CC=CC=C2C#N)N3CCC[C@H](C3)N.C1=CC=C(C=C1)C(=O)O                                                                                                                                        |
| <b>Stability</b>     | 3 years in powder form.                                                                                                                                                                                       |
| <b>Storage</b>       | Storage at -20°C.                                                                                                                                                                                             |
| <b>Applications</b>  | Alogliptin (SYR-322) benzoate is utilized in metabolic research as a selective DPP-4 inhibitor to investigate the enhancement of incretin hormone activity and the regulation of postprandial glucose levels. |

## Library Information

|                             |                     |
|-----------------------------|---------------------|
| <b>Target</b>               | DPP                 |
| <b>Receptor</b>             | DPP4                |
| <b>Pathways</b>             | Proteases           |
| <b>Plate Number</b>         | L6700-05            |
| <b>Empty Location</b>       | a1-h1; a12-h12      |
| <b>Container</b>            | 96-well plate       |
| <b>Formulation</b>          | 10mM DMSO           |
| <b>DMSO Max Solubility</b>  | 68 mg/mL; 147.34 mM |
| <b>Water Max Solubility</b> | 2 mg/mL; 4.33 mM    |
| <b>ALogP</b>                | 1.271               |
| <b>HBA_Count</b>            | 2                   |
| <b>HBD_Count</b>            | 1                   |
| <b>Rotatable Bond</b>       | 3                   |