# SAMPLE CHARACTERIZATION

NAME(CHEMICAL, MINERAL) (S)-N-[[3-(3-fluoro-4-morpholinylphenyl)- 2-oxo-5-oxazolidinyl] methyl] acetamide (Linezolid)

EMPIRICAL FORMULA C16H20FN3O4

CHEMICAL ANALYSIS NO YES ×

SOURCE/PREPRATION **Synthetic/ Supplied by Zhejiang Huadong Pharmaceutical Co.,LTD.**

CHEMICAL ABSTRACT REGISTRY NO. 165800-03-3 PEARSON PHASE DESIGNATION aP88 OTHER

# **TECHNIQUE**

**RADIATION TYPE, SOURCE X-ray, Cu λ VALUE USED 1.54056Å, Kα1**

**λDISCRIM.(Filters Mono, Etc) Incident beam, Vertical-Type Muti-Layer-Film Mirror Mono.**

**λdetector(Film, Scint, Position Sensitive etc.) Scint.**

**INSTRUMENT DESCRIPTION(Type, Slits, etc.) 285mm Vertical Diffractometer DIV 1° REC 0.3mm**

**SOLLER Yes No. 2 Position Inc., Diffract Aperture q=1.0**

**INSTRUMENTAL PROFILE BREADTH 0.069 °2θ TEMP(℃) 23±1**

**SPECIMEN FORM/PARTICLE SIZE Prepared on glass sample carrier/ <10µm particle size**

**RANGE OF 2θ FROM 3 °2θ to 40 °2θ SPECIMEN MOTION**

**INTERNAL/EXTERNAL 2θSTD (if any) Fluorophlogopite＋Silicon(external) LATTICE PARAMETER OF 2θSTD 9.98104Å, 5.43094Å**

**2θERROR CORRECTION PROCEDURE Parabolic fitting, -0.003+6.473×10-42θ- 3.725×10-62θ2**

**INTENSITY MEAS. TECHNIQUE peak height ERROR(～) 5% PEAK × INTEGERTED**

MINIMUM INTENSITY THRESHOLD(IN RELATIVE INTENSITY UNITS) 0.3

INTENSITY STD USED hkl’s OF INTENSITY STD

INTENSITY RATIO I/Ic CONVERSION FACTOR IF CORUNDUM NOT USED

RESOLUTION (FWHM) FOR THIS MATERIAL: ? °2θ AT ? °2θ

2θREPRODUCIBILITY FOR THIS MATERIAL: ? °2θ AT ? °2θ

# **UNIT CELL DATA**

METHOD OF CELL DETD. Cell and structure known from single crystal diffraction data

CELL REFINEMENT METHOD Least-squares, See Ref. 1

a= 6.5817 (29)Å; b= 10.9698 (29)Å; c= 12.9165 (20 )Å;

α= 69.3049°(13 )°; β= 88.1476°(60 )°; γ= 74.1953°( 21)°

Z= 2 ; Dm= g cm-3; Dx= 1.3380 g cm-3 ; V= 837.31 Å3;Formula Wt.= 337.35

CRYSTAL SYS. Triclinic SPACE GROUP P1 CRYSTAL DATA INDEX NO. ?

FIGURE OF MERIT TYPE ? VALUE ?

REFERENCES

[1]. Tanaka R., Hirayama N. (2008). Crystal Structure of Linezolid, Analytical Sciences 24:x43-44.

POWDER DATA

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| ESSENTIAL | | DESIRED | | |
| 2θ EXP  (DEGREES) | I/I0 | dEXP  (Å) | hkl | Δ2θ\*  (DEGREES) |
| 7.338  8.980  9.337  13.480  14.200  14.699  15.102  15.341  16.281  16.801  17.998  18.440  18.721  19.640  19.821  20.999  21.599  22.161  22.720  25.400  25.780  26.763  27.156  27.661  28.321  28.639  29.622  30.177  30.641  32.379  33.140  33.600  34.841  39.442 | 14.5  2.6  12.0  53.5  0.4  5.9  3.9  4.9  2.7  9.1  37.7  17.6  11.5  2.5  4.8  49.9  5.1  100.0  4.5  26.5  4.8  1.5  0.8  6.6  8.0  1.8  3.0  0.5  1.2  1.4  3.9  1.8  0.6  2.6 | 12.0367  9.8393  9.4644  6.5631  6.2319  6.0214  5.8618  5.7712  5.4398  5.2725  4.9245  4.8075  4.7361  4.5165  4.4757  4.2270  4.1110  4.0080  3.9107  3.5038  3.4530  3.3284  3.2811  3.2224  3.1487  3.1144  3.0134  2.9592  2.9154  2.7627  2.7011  2.6651  2.5730  2.2827 | ( 0 0 1)  ( 0 1 0)  ( 0 1 1)  ( 0-1 1)  ( 0 1 2)  ( 0 0 2)  ( 1 1 1)  (-1 0 1)  ( 1 0 1)  ( 0 2 1)  ( 0 2 0)  (-1 1 1)  ( 0 2 2)  (-1 0 2)  ( 0-1 2)  (-1 1 2)  ( 1-1 1)  (-1-1 2)  (-1-2 1)  ( 0 3 1)  (-1 2 2)  ( 0-1 3)  ( 0-2 2)  ( 0 1 4)  (-1-1 3)  ( 0 2 4)  ( 0 0 4)  (-1-3 1)  ( 1 2 4)  (-1 3 1)  ( 1 4 2)  (-1-2 3)  (-2 0 3)  (-2 2 3) | -0.010  -0.014  -0.007  0.000  0.005  -0.012  0.001  0.014  0.004  0.009  -0.009  0.009  0.002  -0.032  -0.004  0.018  -0.012  0.003  0.003  0.001  -0.002  0.013  -0.004  0.000  -0.002  -0.004  0.002  -0.032  0.000  0.069  -0.014  0.011  -0.006  -0.005 |

\* 2θEXP -2θCACL