# 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 oP176 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= 6.5266 (8)Å; b= 9.9584 (7)Å; c= 24.8315 (2 )Å;

α= °( )°; β= °( )°; γ= °( )°

Z= 4 ; Dm= g cm-3; Dx= 1.3883 g cm-3 ; V= 1613.93 Å3;Formula Wt.= 337.35

CRYSTAL SYS. Orthorhombic SPACE GROUP P212121 CRYSTAL DATA INDEX NO. ?

FIGURE OF MERIT TYPE ? VALUE ?

REFERENCES

[1]. Maccaroni E., Alberti E., Malpezzi L., Masciocchi N., Vladiskovic C.(**2008**). Polymorphism of linezolid: A combined single-crystal, powder diffraction and NMR study, Int. J. Pharm. **351** (1-2), 144-151.

POWDER DATA

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| ESSENTIAL | | DESIRED | | |
| 2θ EXP  (DEGREES) | I/I0 | dEXP  (Å) | hkl | Δ2θ\*  (DEGREES) |
| 7.118  9.562  11.382  13.903  14.261  16.221  16.821  17.739  19.461  19.722  19.963  20.802  21.467  21.661  22.441  22.724  22.882  23.578  24.219  25.319  26.698  27.079  27.801  28.240  28.623  28.822  28.960  29.397  30.520  30.925  31.037  31.240  32.101  32.405 | 1.9  11.3  0.5  5.6  22.6  3.5  100.0  3.3  5.2  2.4  5.8  0.9  6.9  21.3  34.8  3.2  5.3  11.2  2.2  15.1  1.6  6.0  1.8  0.4  1.6  2.4  3.0  0.7  1.2  1.7  1.7  1.7  2.5  0.9 | 12.4080  9.2425  7.7680  6.3646  6.2057  5.4599  5.2665  4.9959  4.5575  4.4978  4.4441  4.2666  4.1360  4.0995  3.9587  3.9101  3.8834  3.7702  3.6720  3.5148  3.3363  3.2902  3.2064  3.1576  3.1162  3.0951  3.0807  3.0359  2.9266  2.8893  2.8790  2.8609  2.7860  2.7606 | ( 0 0 2)  ( 0 1 1)  ( 0 1 2)  ( 0 1 3)  ( 0 0 4)  ( 1 1 0)  ( 0 1 4)  ( 1 1 2)  ( 1 1 3)  ( 1 0 4)  ( 0 1 5)  ( 0 2 3)  ( 0 0 6)  ( 1 1 4)  ( 1 2 0)  ( 1 2 1)  ( 0 2 4)  ( 1 2 2)  ( 1 1 5)  ( 0 2 5)  ( 1 2 4)  ( 0 3 1)  ( 0 3 2)  ( 2 0 2)  ( 1 0 7)  ( 1 2 5)  ( 0 3 3)  ( 2 0 3)  ( 0 3 4)  ( 0 2 7)  ( 1 3 2)  ( 1 2 6)  ( 1 3 3)  ( 0 3 5) | -0.004  0.000  0.000  -0.002  -0.005  0.004  -0.005  -0.004  0.002  -0.001  -0.001  0.000  -0.014  0.001  0.000  0.004  -0.005  -0.009  -0.010  -0.011  -0.012  0.000  -0.004  0.013  -0.005  -0.005  -0.002  0.000  -0.007  0.002  0.010  0.002  -0.001  0.010 |

\* 2θEXP -2θCACL

POWDER DATA

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| ESSENTIAL | | DESIRED | | |
| 2θ EXP  (DEGREES) | I/I0 | dEXP  (Å) | hkl | Δ2θ\*  (DEGREES) |
| 33.181  33.543  33.902  34.004  34.604  35.281  36.143  36.785  37.063  37.320  38.841  39.783 | 1.1  1.9  1.4  0.6  1.0  2.8  1.1  0.6  3.5  1.7  0.9  0.8 | 2.6978  2.6695  2.6420  2.6344  2.5900  2.5419  2.4832  2.4413  2.4236  2.4075  2.3167  2.2640 | ( 1 1 8)  ( 1 3 4)  ( 1 2 7)  ( 0 2 8)  ( 0 3 6)  ( 1 3 5)  (0,0,10)  ( 0 4 2)  ( 0 3 7)  ( 1 3 6)  ( 2 3 1)  ( 1 2 9) | -0.006  -0.019  0.002  0.004  0.008  0.000  0.001  0.005  -0.003  0.010  -0.005  0.008 |

\* 2θEXP -2θCACL