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## SigmaPlot 2000, Version 6.00, SPSS Inc.

Computer Software Project Management, Requirements, and Design Document

Prepared for the U.S. Department of Energy Assistant Secretary for Environmental Management

Project Hanford Management Contractor for the U.S. Department of Energy under Contract DE-AC06-96RL13200

P.O. Box 1000 Richland, Washington

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#### Fluor Hanford

P.O. Box 1000 Richland, Washington

What Approval Date

SEP 18 2000

DATE: HANFORD RELEASE ID:

Release Stamp

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#### PLUTONIUM FINISHING PLANT ANALYTICAL LABORATORY

SigmaPlot 2000, Version 6.00, SPSS, Inc. Computer Software Project Management, Requirements, and Design Document

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#### SigmaPlot

HNF-6994 09/12/2000 Revision 0

#### TABLE OF CONTENTS

1.	PRO	DIECT MANAGEMENT	I
	1.1	Project Overview	1
	1.2	Product Perspective	1
	1.3	Configuration Management	1
	1.3.1	·	
	1.3.2		
	1.3.3	Records Management	1
2.	SYS	TEM REQUIREMENTS AND DESIGN	2
	2.1	User characteristics	2
	2.2	Constraints	
	2.3	Functional Requirements	2
	2.4	Interface Requirements.	2
	2.5	Reliability and Recovery	2
	2.6	Standards Compliance	2
	2.7	Transferability	2
3	REE	FRENCES	- 1

#### 1. PROJECT MANAGEMENT

#### 1.1 Project Overview

SigmaPlot is a vendor software product that will be used to convert the area under an absorbance curve generated by a Fourier transform infrared spectrometer (FTIR) to a relative area. SigmaPlot will be used in conjunction with procedure ZA-565-301, "Determination of Moisture by Supercritical Fluid Extraction and Infrared Detection."

#### 1.2 Product Perspective

SigmaPlot is a proprietary program provided by the SPSS, Inc. SigmaPlot performs a wide variety of functions; however this test only concerns its ability to convert spectral data to relative areas using the following equation, known as the trapezoidal rule. This function calculates the area of a rectangle and adds the area of a triangle stacked on top of it.

$$\sum_{n=1}^{0} \{ (y_i)(x_{i+1} - x_i) + (1/2)(y_{i+1} - y_i)(x_{i+1} - x_i) \}$$

#### 1.3 Configuration Management

#### 1.3.1 Change Control

SigmaPlot is provided by the vendor as a finished product on compact disc (CD) and may not be changed in the field.

#### 1.3.2 Documentation

Documentation in the form of a User's Guide is provided by SPSS, Inc.

#### 1.3.3 Records Management

The CD and User's Guide will be maintained in the control of the cognizant scientist for the supercritical fluid extraction (SFE) system.

#### 2. SYSTEM REQUIREMENTS AND DESIGN

#### 2.1 User characteristics

The software will be used by Plutonium Finishing Plant Analytical Laboratory (PFPAL) personnel who have a need to use it and are trained on the associated analytical procedure.

#### 2.2 Constraints

This software will only be tested in regards to its applicability to water determination per ZA-565-301, "Determination of Moisture by Supercritical Fluid Extraction and Infrared Detection."

#### 2.3 Functional Requirements

SigmaPlot must install on the computer designated for operation of and interfaced with the FTIR. All functions pertaining to converting a text file containing infrared spectral data to a numeric area must operate in such a fashion that water can be measured in accordance with ZA-565-301, "Determination of Moisture by Supercritical Fluid Extraction and Infrared Detection."

#### 2.4 Interface Requirements

SigmaPlot must be able to import and operate on a text file containing spectrophotometric absorbance data and time data in a reproducible manner.

#### 2.5 Reliability and Recovery

There are no system impacts should the hard disk of the computer running this program become inoperable, as this software is not used to store data on the computer.

#### 2.6 Standards Compliance

There are no standards or regulations that impose constraints on this program.

#### 2.7 Transferability

The software license controls the number of copies that may be made.

#### 3. REFERENCES

SigmaPlot User's Guide, SPSS, Inc., Chicago, IL

ZA-565-301, Determination of Moisture by Supercritical Fluid Extraction and Infrared Detection, Fluor Hanford, Inc., Richland, WA

HNF-PRO-052, Corrective Action Management, Fluor Hanford, Inc., Richland, WA

HNF-PRO-1748, OCRWM Corrective Action and Stop Work, Fluor Hanford, Richland, WA

HNF-PRO-210, Records Management Program Standard, Fluor Hanford, Richland, WA