ACTRIS In Situ Aerosol:
Guidelines for Manual QC of MPSS Data[MF1]

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Due to the variety of MPSS systems and the complexity of the inversion algorithm for MPSS data, the main manual QC is to be performed on the level 1 data (inverted data). Raw data for level 0 (the raw data output from the instrument) are only augmented with essential information (e.g. from entries in the instrument/station log) and metadata recorded by the instrument and brought to a standardized data format. Level 0 shall be flagged for operation parameter deviations larger than described in Wiedensohler et al. 2018.[MF2]

When performing manual QC for a given time period of data, e.g. a year for an annual submission of data, the parameters contained in the level 0 data listed below are to be plotted as time series, and visually inspected. Data sequences exhibiting issues are to be flagged with an appropriate flag contained in this list below.

For manual QC of level 1 and level 2 data time series plots of individual parameters are not sufficient to identify all possible issues in a data set. Contour plots of the PNSD are helpful to identify major issues in the data (like arcing, possible local pollution or lack of CPC working fluid), which may not be visible in time series plots (see appendix A for examples). Frequency distributions may help to identify small negative values and uneven distributions of the measured values along with the time series plots that are not visible in countourplots (appendix B). Data with issues identified by these tools shall be flagged according to the list below.

Any non-invalidating flag (559, 640, 110) is to be propagated to the average if it occurs during the averaging period.

Group 0: Valid data

Flag	Validity	Description
000	V	Valid measurement

Group 1: Exception flags for accepted, irregular data

Flag	Validity	Description
110	V	Episode data checked and accepted by data originator. Valid measurement

Group 3: Flags for aggregated datasets (used for level 1.5 & 2 only)

Flag	Validity	Description
390	V	Data completeness less than 50%
392	V	Data completeness less than 75%
394	V	Data completeness less than 90%

Group 5: Chemical problem

Flag	Validity	Description
559	V	Unspecified contamination or local influence, but considered valid

Group 6: Mechanical or instrumental problem

Flag	Validity	Description
640	V	Instrument internal relative humidity above 40%
683	I	Invalid due to calibration. Used for Level 0.
686	I	Invalid due to zero check. Used for Level 0

Group 9: Missing flags

Flag	Validity	Description
999	M	Missing measurement, unspecified reason

Regardless in which data level the issue is found, the flags are added to the initial level 0 data version, thereby producing level 0a (manually QCed level 0) as output of the QC process. Some flags are used for level 0 only. The corresponding data lines are marked as missing in level 1, and are excluded from calculating hourly averages in levels 1.5 and 2.

The flags for aggregated datasets in group 3 apply only to levels 1.5 and 2. They indicate which fraction of the averaging period is covered by active sample time of the instrument.

The following parameters are to be inspected for the issues:

Level 0:

1. **Periods of zero and span checks**
   If not done automatically by the data acquisition software, periods of zero checks and calibrationscks are to be flagged with flags 686 and 683, respectively.
2. **Sample pressure, sample inlet temperature**
   Sample pressure varies with ambient pressure. Other types of variations should not occur, e.g. variations with fluctuating sample flow. Sample temperature at inlet and outlet normally varies only with lab temperature, and during zero and sizing checks. Other variations and spikes need to be inspected, the reason determined, and flagged according to the issue if needed.
3. **Sample relative humidity at inlet and outlet**
   Sample relative humidity varies with ambient relative humidity and the temperature difference between ambient and lab. The sample should be dried so that the sample has rH < 40% already at the instrument inlet. If rH is higher, apply flag 640. Spikes of rH can occur during zero and sizing checks. These periods need to be flagged 999. Other variations and spikes need to be inspected, the reason determined, and flagged according to issue if needed.
4. **Sample flow and sheath air flow**
   Sample flow and sheath air flow should be constant, with small variations caused by wind gusts. Sample flow under normal operation should typically be at least 1 l/min, with variations smaller than 5%. Sheath air flow should be stable as well. Variations and

spikes exceeding 5% need to be inspected, the reason determined, and flagged according to issue if needed.

5. **CPC operation parameters**
   Recorded CPC operation parameters need to be within manufacturer specifications. Time periods with deviations from these specifications must be inspected for data validity as such deviations might only be due to a faulty sensors in the CPC. A good indicator for the validity of data during such periods is the comparison of the integral particle number concentration determined by the MPSS with the number concentration reported by an extra total CPC.

Level 1:

1. Visually inspect contour plots of the PNSD on a daily or maximal biweekly basis and identify possible local pollution, arcing DMA or periods like zero checks or lack of CPC working fluid. See appendix A for examples. Flag data accordingly.
2. It is helpful to create histograms of the frequency distributions of all measured parameters. Typically these frequency plots are log normally distributed. Histograms can therefore easily help to identify unusual measurements, which cannot be identified in contour plots. Flag data where necessary.
3. Compare MPSS derived integral particle number concentration with total CPC (see level 0)

Level 2:

1. **Particle number size distribution**
   Create monthly contourplots of the PNSD to verify data integrity of the hourly average data check time series for flags.

Reference: A. Wiedensohler, A. Wiesner, K. Weinhold, W. Birmili, M. Hermann, M. Merkel,T. Müller, S. Pfeifer, A. Schmidt, T. Tuch, F. Velarde, P. Quincey, S. Seeger & A. Nowak (2018) Mobility particle size spectrometers: Calibration procedures and measurement uncertainties, Aerosol Science and Technology, 52:2, 146-164, DOI: 10.1080/02786826.2017.1387229

Appendix A: Problems identified by contour plots:

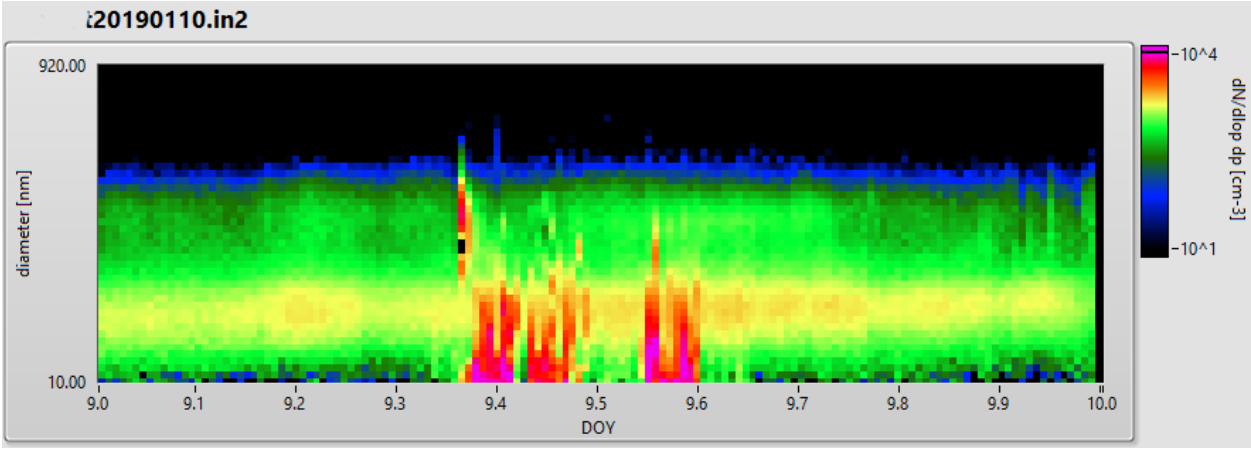

Fig 1: Possible local pollution

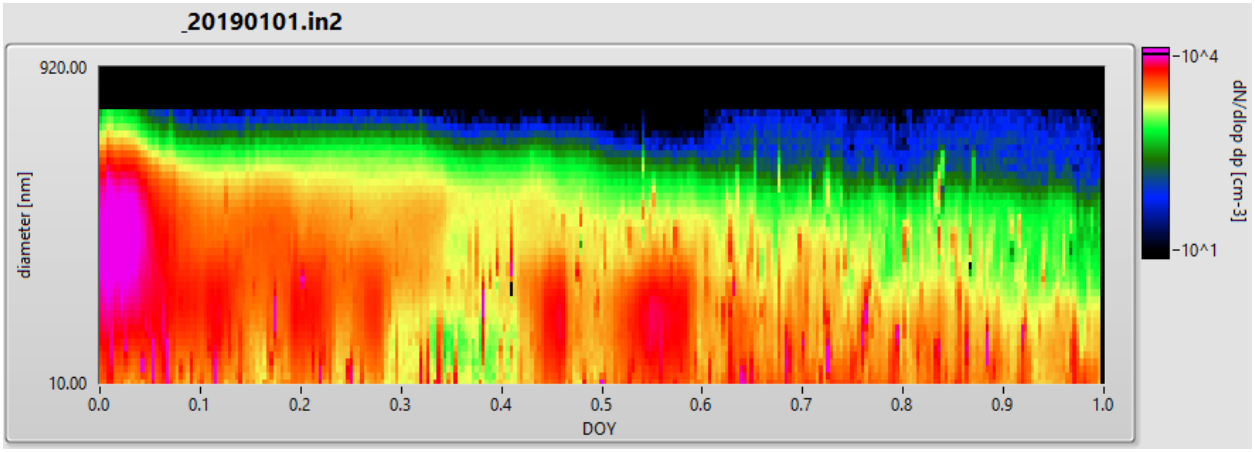

Fig 2: Local pollution (new years eve fireworks)

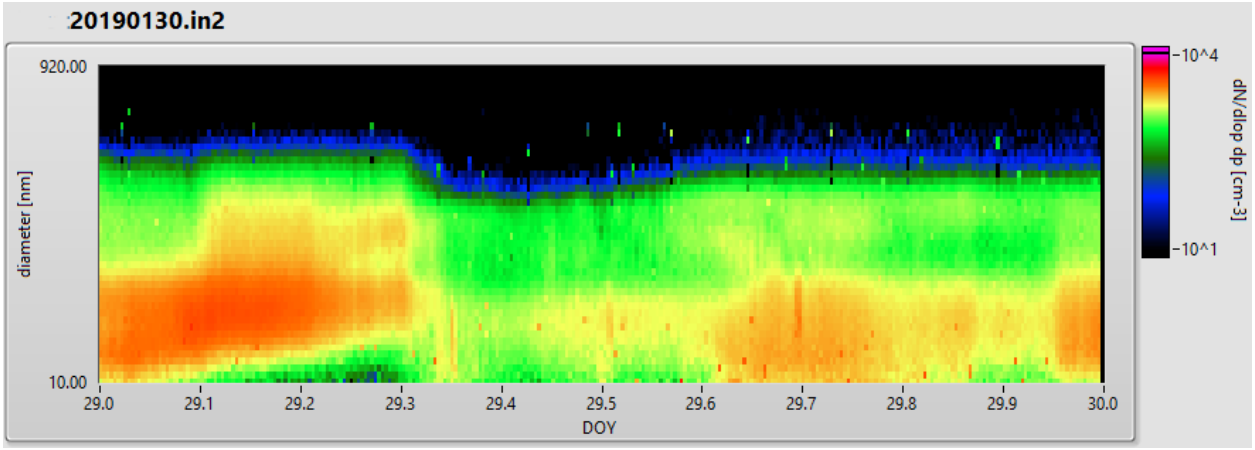

Fig.3: DMA is arcing

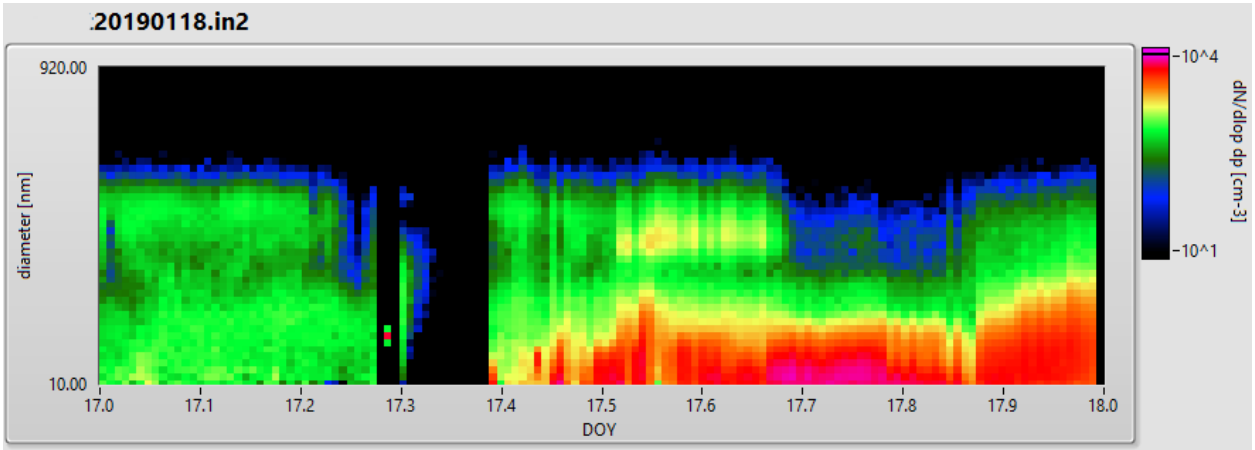

Fig 4: Zero check

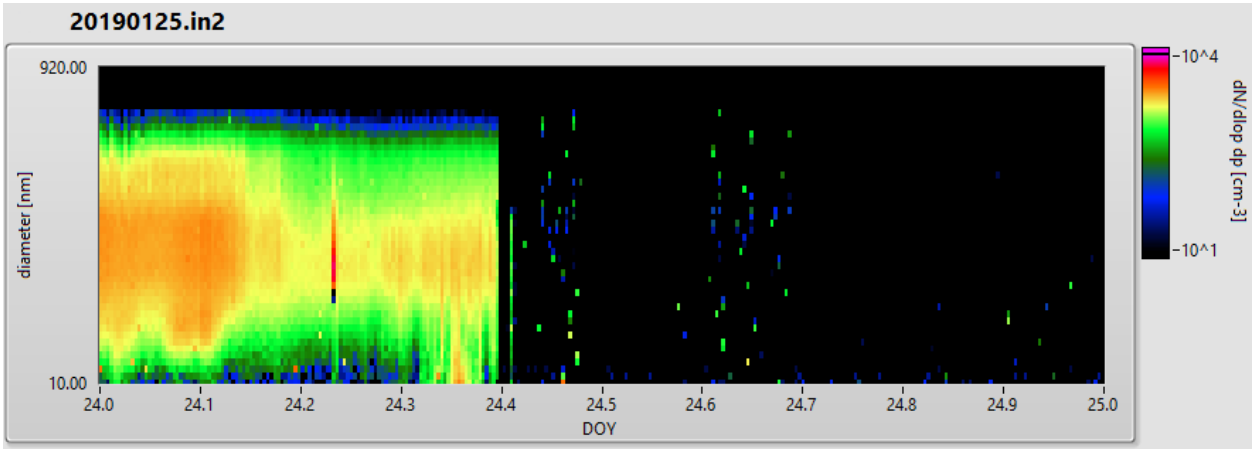

Fig 5: Lack of CPC working fluid

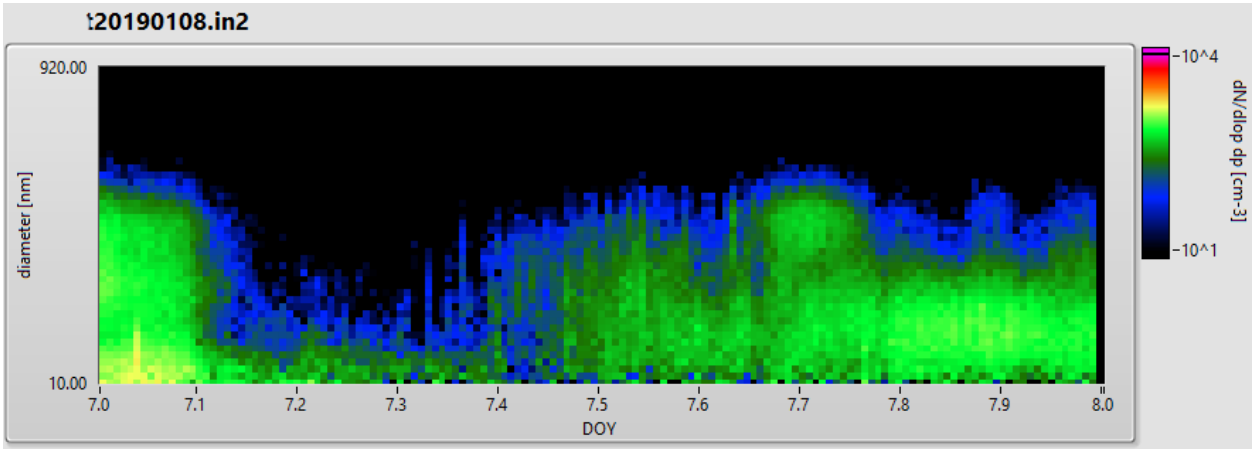

Fig 6: This is not a faulty measurement, just a period of clean air!

Appendix B: Problems identified by frequency plots/time series plot

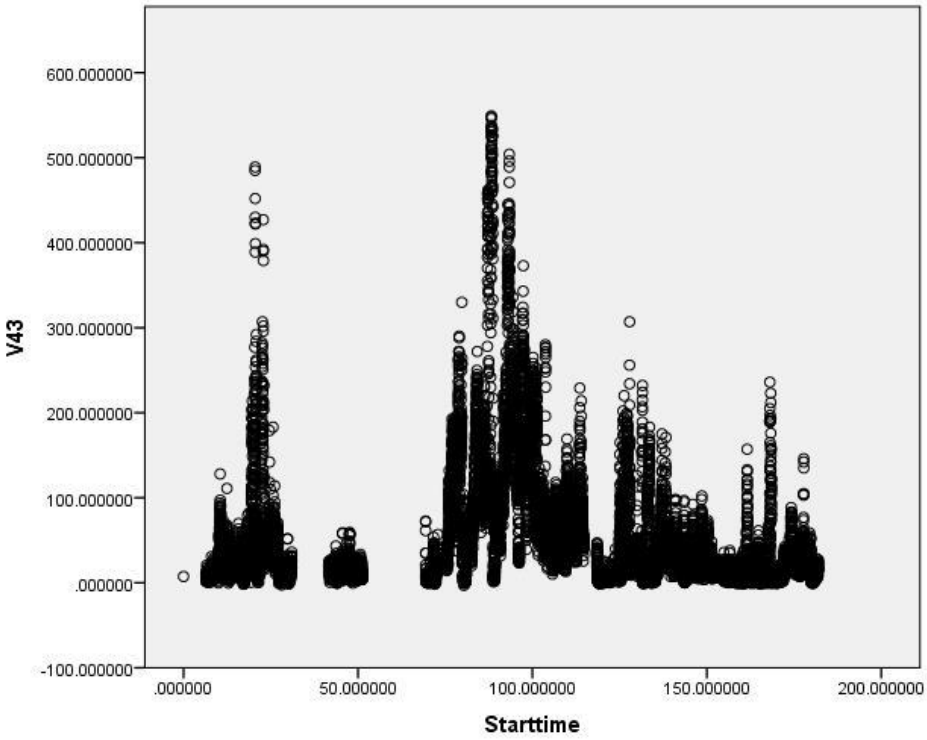

Fig 7: Time series plot bin 35 looks ok

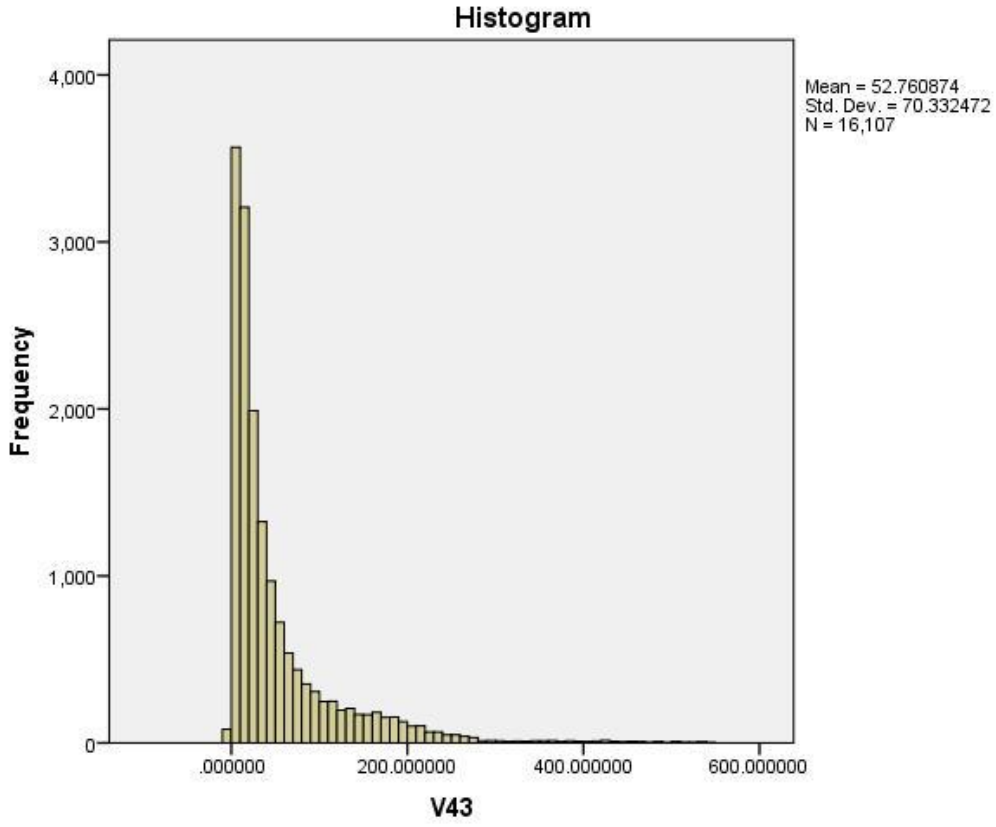

Fig. 8: But the histogram reveals almost 100 values less than zero due to inversion artefacts

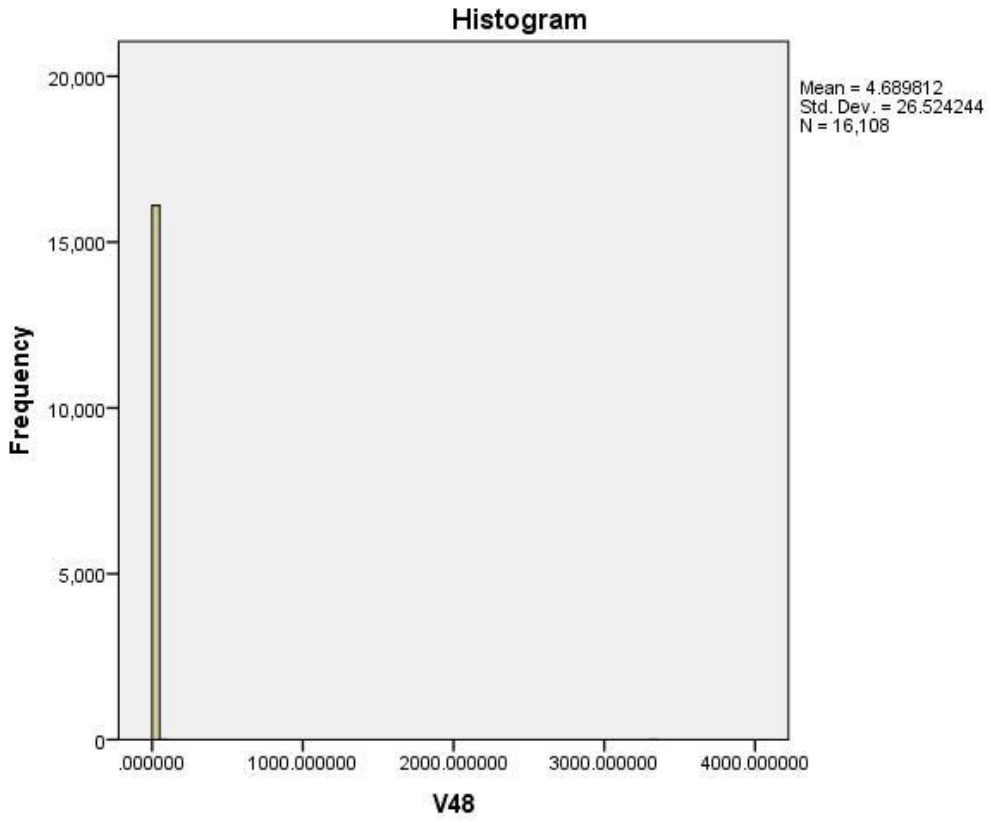

Fig 9: The histogram of bin 48 has maximum of 4000 at a mean value of 4.7

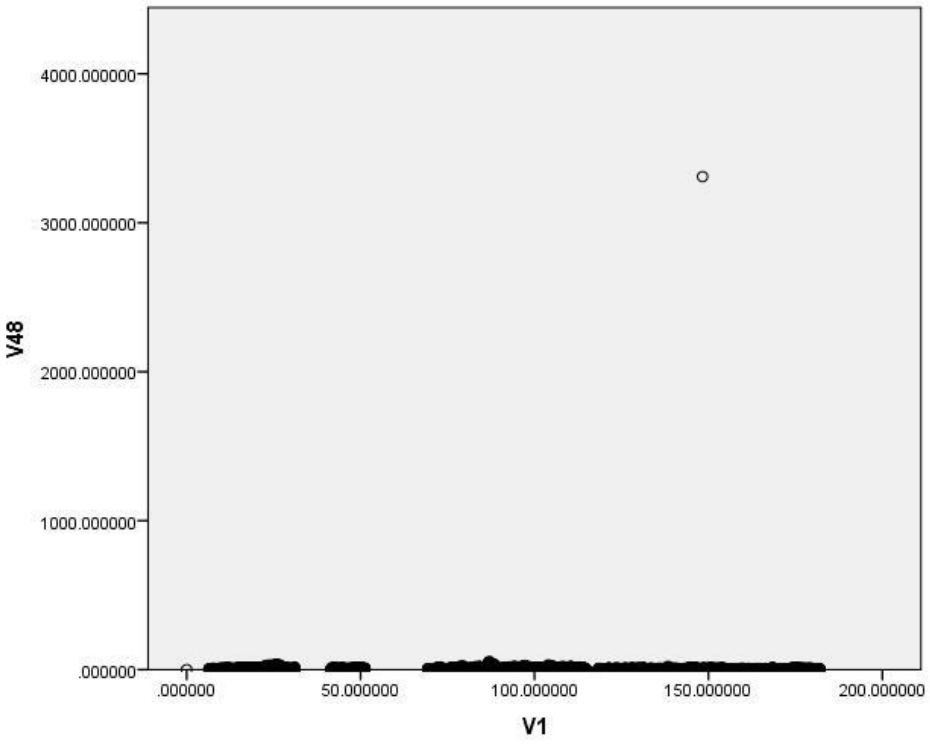

Fig 10: Due to one single outlier

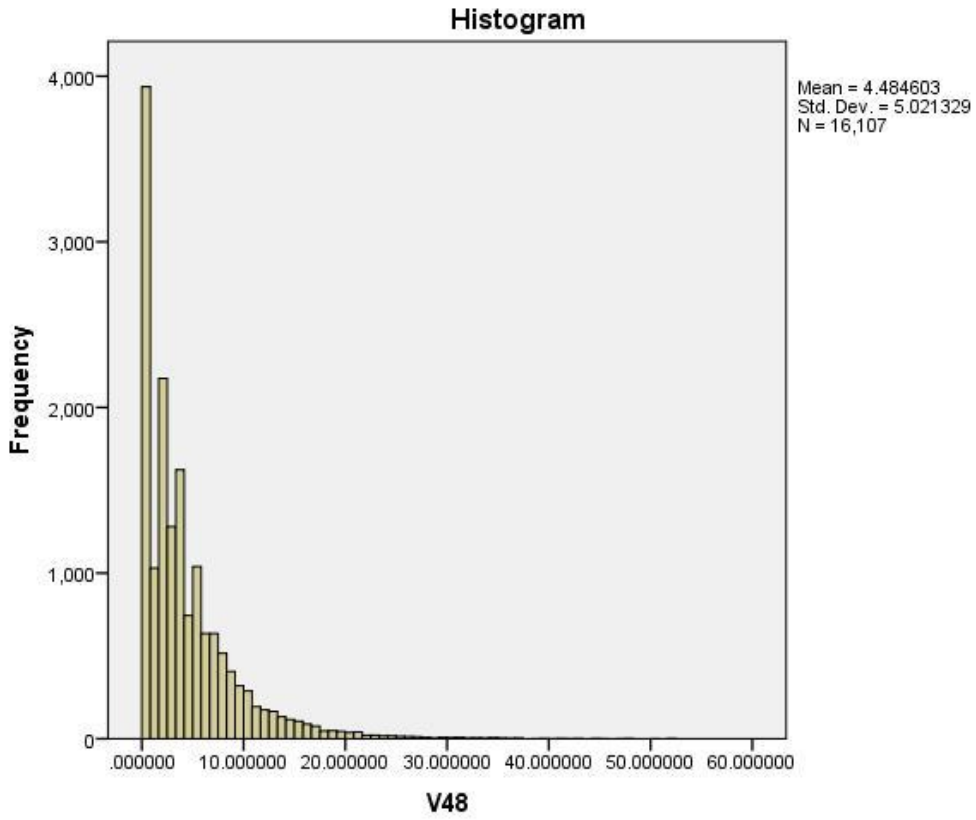

Fig 11: With this outlier removed the histogram looks good

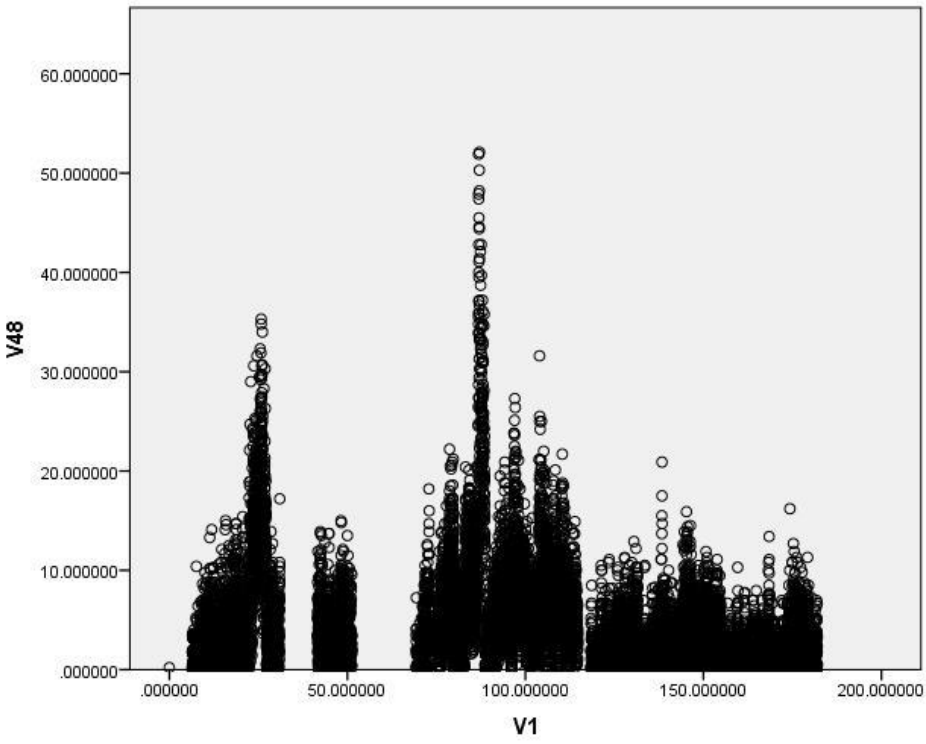

Fig 12: And so does the time series