1. **NMR SPECTROMETER**

Data are collected on 5mm Cryo Probe TXI, 600 MHz Avance II NMR spectrometer (Bruker Biospin Ltd.).

The instrument is equipped with SampleJet with refrigerated sample storage. Automated experiments are acquired using ICON-NMR running with Topspin 3.2 .5 software (Bruker Biospin Ltd.).

1. **PULSE SEQUENCE**

Nuclear overhauser effect spectroscopy sequence with presaturation (NOESYPR1d) is used to collect spectra from urine samples.

* 1. **GENERAL PARAMETERS FOR NOESYPR1d**

The experimental parameters are optimized on a representative sample for each sample set.

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| Acqusition Time | 2.726 sec |
| NMR Experiment type\* | 1D NOESY Presat |
| NMR Comments | parameters are different for blanks |
| Field Frequency Lock | 2H |
| NMR Solvent\* | D2O |
| NMR Tube Size | 5mm |
| Shimming Method | Topshim gradient shimming |
| Pulse Sequence | NOESYPR1D |
| Water Suppression | Presaturation |
| Chemical Shift Reference Compound | DSS |
| Temperature | 300 K |
| Number of Scans (Transients) | 128 |
| Dummy Scans | 4 |
| Dwell time | 41.6 μs |
| Acquisition Time | 2.726 sec |
| Relaxation Delay | 4 sec |
| Spectral Width | 20.0243 ppm |
| Number of Data Points (TD) Acquired | 65536 |

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| Created By: | Fariba Tayyari | Date: 12/17/2014 |
| Reviewed By: |  | Date:  |
| Approved By: |  | Date:  |

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| Revision Number | Name | Reason for Revision | Effective Date |
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