Appendix E
Performance Specifications

Note: For the purpose of the following specifications, signal-to-noise is calculated as the ratio of the chromatographic peak height to twice the standard deviation of the noise.

E.1 Electrospray Positive Ion

The measured signal-to-noise ratio obtained from the chromatogram monitoring the transition m/z 609 to m/z 195 on injection of 5 pg of reserpine is ≥500:1. This is based on a 5-μL injection of a 1 pg/μL reserpine solution in 70:30 acetonitrile/water (no additives) at a flow rate of 200 μL/min in MRM mode, 0.5 second dwell, span 0 Da.

The resolution of the precursor and product ions is <1 Da peak width at half-height.

E.2 Electrospray Negative Ion

The measured signal-to-noise ratio obtained from the chromatogram monitoring the transition m/z 503 to m/z 179 on injection of 25 pg of raffinose is ≥50:1. This is based on a 5-μL injection of a 5 pg/μL raffinose solution in 70:30 acetonitrile/water (no additives) at a flow rate of 200 μL/min in MRM mode, 0.5 second dwell, span 0 Da.

The resolution of the precursor and product ions is <1 Da peak width at half-height.

E.3 MS Resolution

The resolution is demonstrated using a 1 μg/μL solution of PPG 2000 in 50:50 acetonitrile/water containing 1 mM ammonium acetate. The peaks at m/z 2009.5 and 2010.5 should be resolved with a valley between them of no more than 15% of the height of the 2010.5 peak. It is recommended that fifteen 1-second scans are summed and the resulting spectrum smoothed (two passes, 0.5 Da SG).

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E.4 Mass Measurement Accuracy

The mass measurement accuracy is measured from the mean of five repeat analyses of the [M+NH₄]⁺ peak at m/z 1004.622 from 1 μg/μL PEG 1000 in 50:50 acetonitrile/water containing 2 mM ammonium acetate. The mean measured mass will be 1004.622 ±0.05 Da. The standard deviation of the mean will be ≤0.05 Da.

A mass calibration will be performed using the [M+H]⁺ peaks from a separate analysis over the mass range m/z 700 to 1300 and the resolution on the [M+H]⁺ peak at m/z 1031.62 must be between 0.3 and 0.4 Da wide at half height after smoothing.

E.5 APCI Positive Ion

Measured signal-to-noise ratio obtained from the chromatogram monitoring the transition m/z 331.2 to m/z 109.1 on injection of 50 pg of 17-α-hydroxyprogesterone will be ≥70:1, using a 5 μl injection of a 10 pg/μl 17-α-hydroxyprogesterone solution in 70:30 acetonitrile/water (no additives) at a flow rate of 1 mL/min in MRM mode, 0.2 second dwell, span 0 Da.

The resolution of the precursor and product ions will be <1 Da peak width at half height.