

### **Data Quality Control Protocol**

Before final reporting, all data must adhere to the following guidelines to maintain best practices throughout Raynell Labs. *Failure to maintain these guidelines could result in termination and breach of contract with the customer.*

#### **HPLC**

- All chromatographic peaks must be baseline separated for accurate quantification
- Retention times must be reported along with chromatographic conditions
- Peak resolution and separation efficiency (plate height) must be reported for any baseline separated peak, even if other peaks in the chromatogram are not fully separated in order to assess changes in instrument performance.
- Report % area for all peaks even if not fully separated
- Notes on general observations should be recorded carefully for future audits
- Requests for changes to the separation method must be accompanied by a scientific justification
- A calibration curve should be generated on Microsoft Excel for each baseline separated peak based on the varying injected quantities reported and the total area count for the peak
- Slope and  $r^2$  values (minimum value of 0.999) must be reported for all standard curves. Any  $r^2$  value less than 0.999 must be noted and discussed in any analytical reports.
- A final quantity of each compound in the sample should be clearly described

#### **MS**

- All mass spectra should be annotated with m/z ratio values for all major peaks
- Denote the presence of a molecular ion signal if observed
- Positive structural identification of a compound using electron ionization MS must be accompanied by at least three fragment ions; relative abundance for each fragment ion must be reported.