The Raman Barcode for Counterfeit Drug Product

Detection (Supplemental Information)

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I.) Figure S-1: Results from medicines quality database (MQDB) search of counterfeit and non-counterfeit pharmaceuticals that failed screening.

II.) Description of “Parameters used For Peak Finding Function”
Figure S-1: Counterfeit Data obtained from Medicines Quality Database (MQDB) search. The results span from 2003 to 2015 and include data obtained from South America, Africa, and Asia. The top panel corresponds to counterfeit samples that failed screening. In the top panel, the total number of counterfeits identified is 90. The bottom pie chart corresponds to both counterfeit and non-counterfeit samples that failed screening. In the bottom panel, the total number of counterfeit and non-counterfeit failures is 538.
A medicines quality database (MQDB) search produced the results in Figure S-1. The data is from South America, Africa, and Asia and spans from 2003 to 2015. Only data that failed screening is reported in Figure S-1. The top chart reflects counterfeit medications that failed screening. Ninety total counterfeit medications are represented on the top chart. Of the 90 cases from the search, 38 (42%) products did not have the API, 3 (3%) had the wrong API, and 7 (8%) had results that indicate either no API or the wrong API. Therefore 53% of the total counterfeits that failed screening in the MQDB are from pharmaceuticals with no API or the wrong API. The bottom panel is the MQDB search of both counterfeits and non-counterfeits that failed screening. A total of 583 cases were identified, and of those 38 (6%) did not have any API, 73 (13%) had the wrong API, and 7 (1%) had results that indicate either no API or the wrong API. Thus, a total of 20% of cases in the MQDB that failed screening were due to products having no API or the wrong API.

**Parameters used For Peak Find Function**

The Lieber method utilizes an iterative polynomial fit to automate background subtraction. A total of 100 iterations with a 9th order polynomial was used to subtract the background from each Raman spectrum. Following background subtraction, each API reference spectrum was smoothed (Savitzky-Golay 0th order, 14 point window) and a peak search algorithm was used to identify the peak frequencies in each API spectrum. This was performed by using the “Peakfind” function from the PLS Toolbox Version 7 (Eigenvector Research Inc., Manson, WA) to find the peak frequencies in the API spectra. The “Peakfind” function’s parameters were adjusted so that at least 95% of the peaks in each API spectrum were identified. The Peakfind function has the following form:

\[[i0,iw]=\text{peakfind}(x,\text{width},\text{tolfac},w,\text{options})\]
The width was set to 14, the tolfac was set to .05, ‘w’ was set to .003, and the options was set to option.algorythm = ‘d2’. The algorithm (‘d2’) applies a second derivative Savitzky-Golay filter with a second order polynomial and a width specified by the user to the Raman data. The ‘tolfac’ command is used to identify peaks. Peak heights are estimated to be greater than the product of ‘tolfac’ and the residuals. The value ‘w’ is a scalar window used for determining the local maxima.