Appendix A

Explanations of the Appendix A Table

**Column A**. Formulation number

A number assigned to each formulation analyzed. A letter designation indicated that multiple data sets were collected for this formulation. Overall 65 formulations were analyzed with 80 data sets being analyzed including several on the instrument control sample, Centrum Performance.

**Column B**. Year of data collection

Specimens were prepared from tablets and capsules at different times by different analysts. This column denotes the year of data collection.

**Column C**. Packaging name

This includes tradenames, registered names and generic names that were listed on the packing. Several generics were labelled by their API names. Specific tradenames and registered names are denoted in Table I.

**Column D**. Manufacturer

This is the manufacturer listed on the label. In some cases this name will be a distributor or marketing group associated with the manufacturer. With prescription drugs, sometimes this information was not recorded as in a few select cases tablets were supplied for analysis without the associated packaging. Note: Photographs were taken of some of these tablets and later identified by tablet labels. Sometime dosage, tablet shape and color, is specific to a manufacturer.

**Column E.** Purpose

The biological function of the API, usually identified through the packaging, PubMed or Wikipedia.

**Columns G, H, I**. Experimental details

These columns include the instrument type, maximum count intensity and unusual samples. In column I a black would denote a finely ground powder that passed through a 200 mesh sieve. Several tablet shells were isolated and analyzed and these are denoted.

**Columns J, K, L and M**. Phase identification

This includes all phases identified through the diffraction analyses. Column J denotes the highest intensity phase, column K the excipients and column L the active pharmaceutical ingredient(s) (API). Column M notes the PDF reference number, publication or patent that was used as a source of reference identification of the API. In gel caps the API was either solubilized or in very low concentration so an experimental API was not identified. In some cases, available references did not match the observed diffraction pattern (i.e. Nexium)

All identifications using the PDF were made using PDF-4/Organics 2018. This included a modern analysis of all older data sets.

**Columns N and O.** Top selling prescriptions and OTC drugs

Top selling drugs are noted. For prescription drugs the 2016 rank is also noted.

**Columns P, Q and R**. Weights and concentration

In the 2018 samples, a tablet or capsule weight was experimentally determined and recorded in column P. In column Q, we recorded the API tablet/capsule weight as found on the labelling. In column R is a calculated estimate of the API in the sample measured. If the capsule contents were isolated from the capsule itself, then capsule was weighed (not shown), and the API concentration % was adjusted.

**Column T**. Additional listed ingredients

For some formulations there was a very extensive list of ingredients either on the packaging or with associated documents on the manufacturer’s website. In many cases the list of ingredients covered several dosage formulations and not all ingredients were present in all dosage forms. We also found that for several generics there were changes in excipients between different generic manufacturers. Some ingredients, particularly PEG, anatase, Fe2O3, talc, were used in low concentrations in the tablet coating and the coating would need to be isolated for a positive identification by XRD. This column was used as reference and not an indication that these ingredients were in the bulk formulation.