SUPPLEMENTAL INFORMATION

Stability testing

Two QC pools, QCL and QCH were frozen and thawed three times at -70 ºC (3 freeze-thaw cycles). Three individual samples at each level were prepared and analyzed by single injection. Relative differences were calculated by comparing the average of the three samples to an average of the three replicate samples with just an initial freeze-thaw cycle for total-A (**Table S1**) and for PA83 only (**Table S2**).Compared to the once-thawed controls, the QCL mean value for total-PA was 11.9% lower and QCH was 0.8% lower after 3 freeze-thaws.

Processed sample stability was also evaluated after 48 hours in the LC autosampler at 6 ºC and means were 0.53% and 0.60% lower than freshly analyzed samples for total PA, for QCL and QCH respectively (**Table S3**). Long-term stability was also assessed by comparing current results for samples stored at -70 ºC for 3 years to initial results for samples analyzed 3 years prior. All findings were within FDA guidelines[44].

PA QCL and QCH	FREEZE THAW measurements		QC Levels
Total-PA	**Initial measurement**	**Three freeze-thaw cycles**	**Target concentration**
QC Low Replicate 1	2.813	2.502	**2.75**
QC Low Replicate 2	2.881	2.518	**2.75**
QC Low Replicate 3	2.892	2.544	**2.75**
MEAN	**2.862**	**2.521**	**2.75**
QC High Replicate 1	61.43	63.56	**60**
QC High Replicate 2	60.21	62.55	**60**
QC High Replicate 3	60.47	54.56	**60**
MEAN	**60.70**	**60.22**	**60**
% differences from initial measurements	**QC Low**	**11.91%**	–
	QC High	**0.79%**	–

Table S1. Results of freeze-thaw analyses on two representative QC pools, for total-PA.

PA QCL and QCH	FREEZE THAW measurements		QC Levels
PA83	**Initial measurement**	**Three freeze-thaw cycles**	**Target concentration**
QC Low Replicate 1	2.758	2.404	**2.75**
QC Low Replicate 2	2.892	2.443	**2.75**
QC Low Replicate 3	2.967	2.542	**2.75**
MEAN	**2.872**	**2.463**	**2.75**
QC High Replicate 1	59.41	61.53	**60**
QC High Replicate 2	59.39	58.98	**60**
QC High Replicate 3	57.77	54.02	**60**
MEAN	**58.86**	**58.18**	**60**
% differences from initial measurements	**QC Low**	**14.24%**	–
	QC High	**1.16%**	–

Table S2. Results of freeze-thaw analyses on two representative QC pools, for PA83.

PA QCL and QCH	48 hours sample stability		QC Level
Total-PA	**Initial measurement**	**Three freeze-thaw cycles**	**Target concentration**
QC Low Replicate 1	2.758	2.482	**2.75**
QC Low Replicate 2	2.867	2.483	**2.75**
QC Low Replicate 3	2.912	2.511	**2.75**
MEAN	**2.846**	**2.492**	**2.75**
QC High Replicate 1	58.19	62.57	**60**
QC High Replicate 2	58.64	59.44	**60**
QC High Replicate 3	59.11	53.61	**60**
MEAN	**58.65**	**58.54**	**60**
% differences from initial	**QC Low**	**12.44%**	–
Measurements	**QC High**	**0.19%**	–
% differences after 48 hours	**QC Low**	**0.53%**	–
from freshly analyzed samples	**QC High**	**0.60%**	–

Table S3. Results of 48-hour stability testing on two representative QC pools, for total-PA.