Supplementary Data

Quantitation of the ATR inhibitor elimusertib (BAY-1895344) in human plasma by LC-MS/MS

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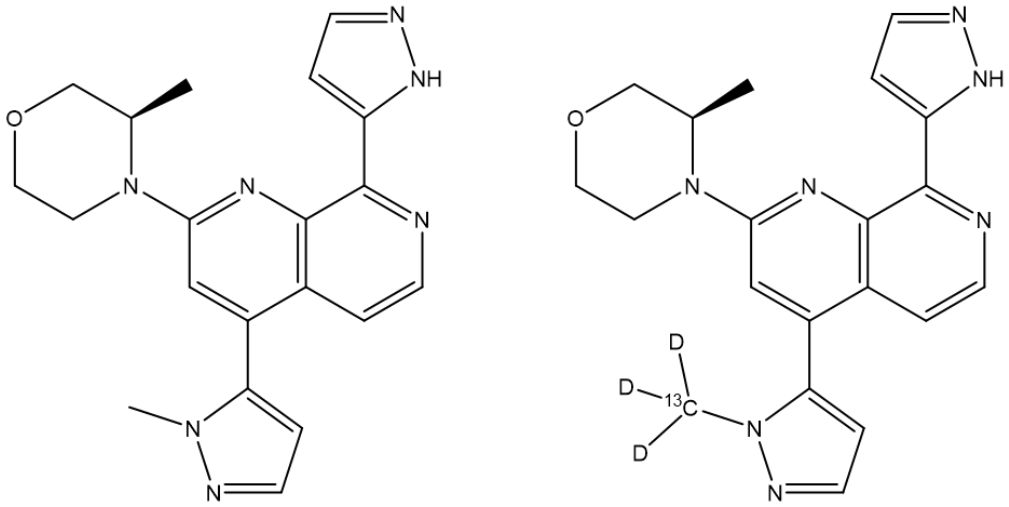
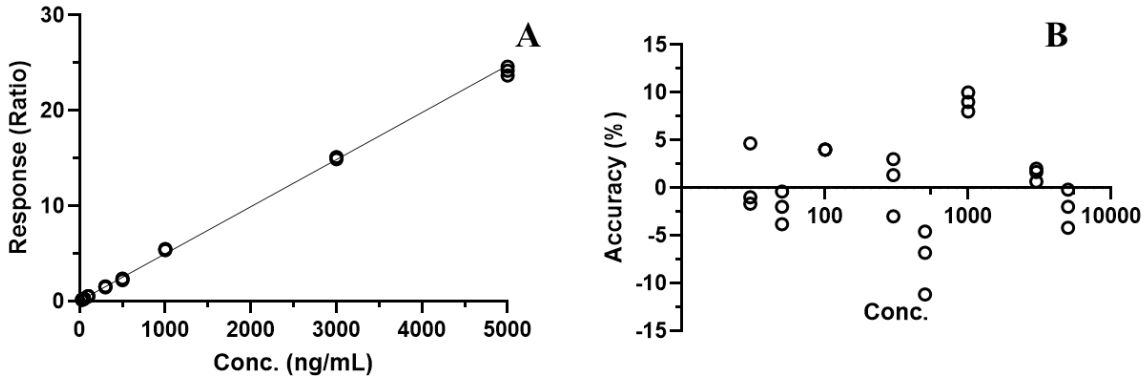
Suppl.Table 1. Assay performance data of the calibration samples for elimusertib in human plasma.

Conc. (ng/mL)	Intra-assay Accuracy (%)	Inter-assay Accuracy (%)	Intra-assay precision (%)	Inter-assay precision (%)
30	95.7-100.7	98.3	4.7	*
50	97.9-103.2	100.2	5.2	*
100	104.0-114.3	108.2	5.1	4.1
300	98.7-104.8	101.3	3.0	2.6
500	92.5-105.5	99.2	3.5	6.3
1000	103.7-111	107.9	2.9	3.1
3000	96.0-101.4	99.4	3.7	2.1
5000	91.0-97.9	93.5	2.2	3.9

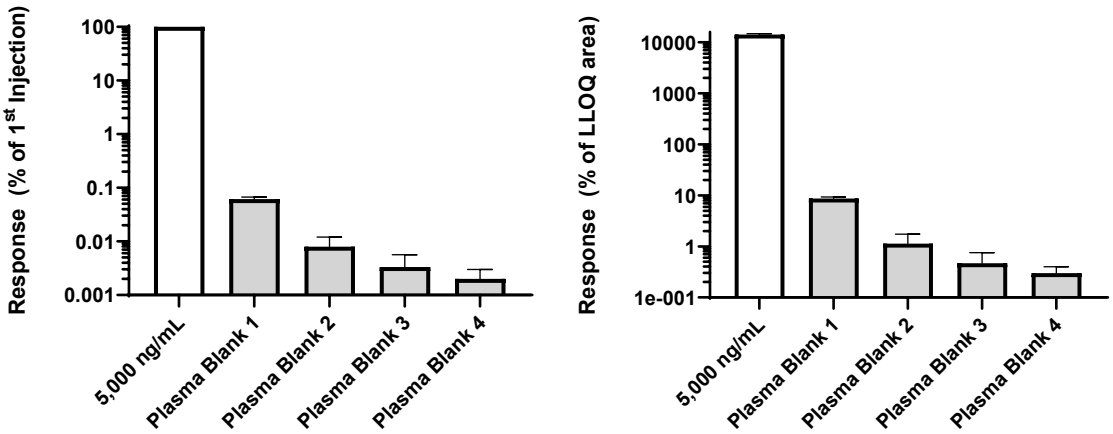
n=9; triplicate results, each in 3 separate runs, for each concentration. *The mean square of the within runs was greater than the mean square of the between runs, indicating that there was no significant additional variation due to the performance of the assay in different runs (Rosing, et al. 2000).



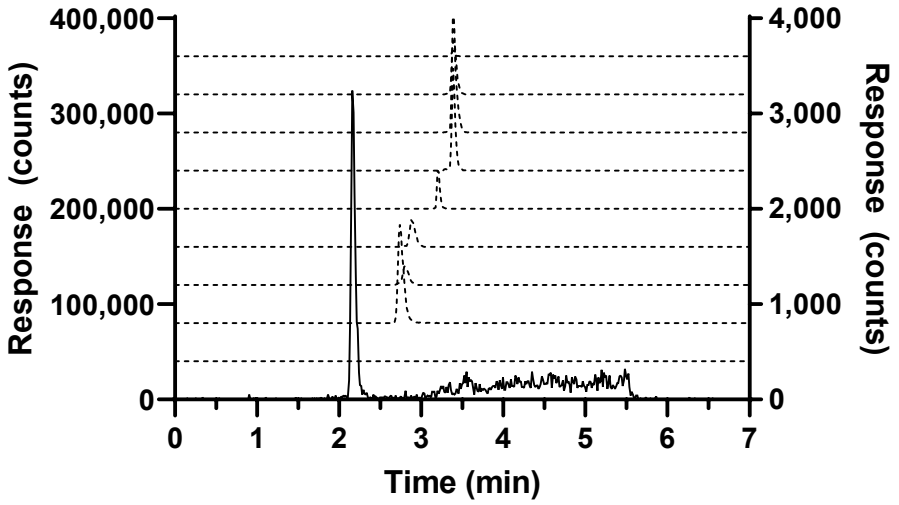
Suppl.Fig. 1. Chemical structures of A) elimusertib and B) [^{13}C,^{2}H$_3$]-elimusertib.



Suppl.Fig. 2. Representative calibration curve (N=3 for each concentration) of elimusertib in human plasma (response elimusertib= 0.00494•conc + .0284; R^2=0.9984). A) Calibration curve is depicted as response ratio versus nominal concentration; B) as residuals (%) of the back-calculated relative to the nominal concentrations versus the log transformed concentration.



Suppl.Fig. 3. Analytical carry-over of elimusertib described in serial blank human plasma sample injections following a 5,000 ng/mL spiked plasma sample represented as the mean percent analyte response relative to the 5,000 ng/mL response (error bars represent ± 1 SD), and the same data expressed as % of the LLOQ area.



Suppl.Fig. 4. Chromatogram of elimusertib HQC (bottom trace corresponding with right y-axis) with selected phospholipid MRM channels (left y-axis). For visual purposes phospholipid MRM channels were offset from baseline response in increments of 40,000 response counts and, from top trace, MRM channels were as follows: 806>184, 784>184, 760>184, 758>184, 704>184, 524>184, 522>184, 496>184, 184>184.