

Quantitative Analysis of Urea in Human Urine and Serum by ^1H Nuclear Magnetic Resonance

Lingyan Liu^a, Huaping Mo^b, Siwei Wei^c, and Daniel Raftery^{c*}

^aWeldon School of Biomedical Engineering, Purdue University, 206 S. Martin Jischke Dr.,
West Lafayette, IN 47907

^bPurdue Interdepartmental NMR Facility, Purdue University, West Lafayette, IN 47907

^cDepartment of Chemistry, Purdue University, 560 Oval Dr., West Lafayette, IN 47907

*Corresponding author:

Email: raftery@purdue.edu

Tel: (765) 494-6070

Fax: (765) 494-0239

Supplementary Information

Table S1: Preparation and composition information for the set of urea aqueous solutions.

sample label	urea stock solution weight (mg)	4 M PBS buffer (ml)	D ₂ O (ml)
1*	49.4	2.50	0.50
2*	251.8	2.50	0.50
3*	488.3	2.50	0.50
4*	994.8	2.50	0.50
5*	2484.5	2.50	0.50
6*	4895.7	2.50	0.50
7**	1011.4	1.25	0.25
8**	2411.5	1.25	0.25

* uses 0.206 M urea as the stock solution, and prepared in a 10.00 ml volumetric flask.

** uses 1.15 M urea as the stock solution, and prepared in 5.00 ml volumetric flask.

Table S2: Preparation details for the set of urine standard addition samples.

urine sample no.	bulk urine weight(g)	stock urea solution weight (g)/volume (ml)*	5 M PBS buffer (ml)	D ₂ O (ml)	total volume (ml)**
1	2.4899	0	1.0	0.25	5.00
2	2.4961	0.0502	1.0	0.25	5.00
3	2.4814	0.2513	1.0	0.25	5.00
4	2.4803	0.4942	1.0	0.25	5.00
5	2.4720	0.7448	1.0	0.25	5.00
6	2.5052	0.9894	1.0	0.25	5.00

*uses 2.07M urea as the stock solution, and 1.0304 g/ml as its density.

** H₂O was added to end sample to make 5.00 ml total volume.

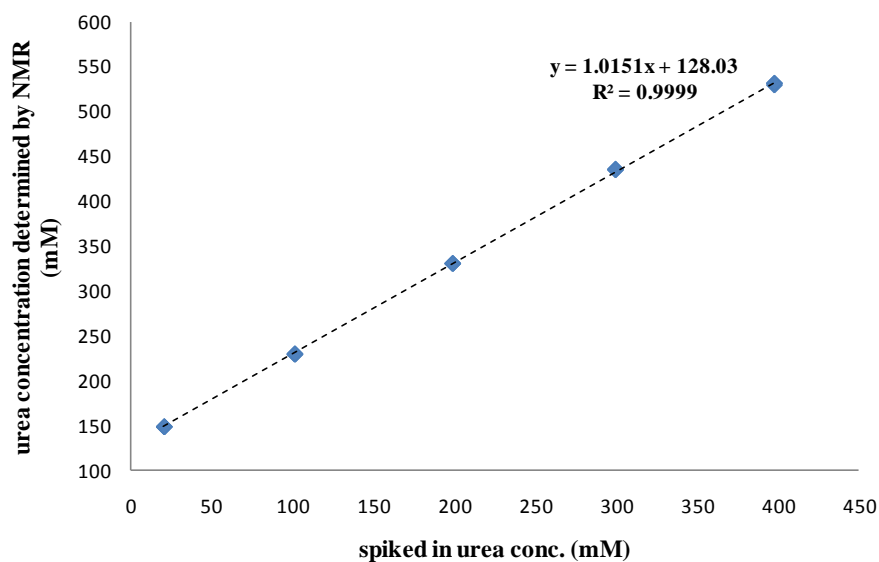


Figure S1: Determination of urea concentration in bulk urine by the standard addition method. The dashed line shows the linear trendline across all measurements. The fitted equation and R-squared value are shown.

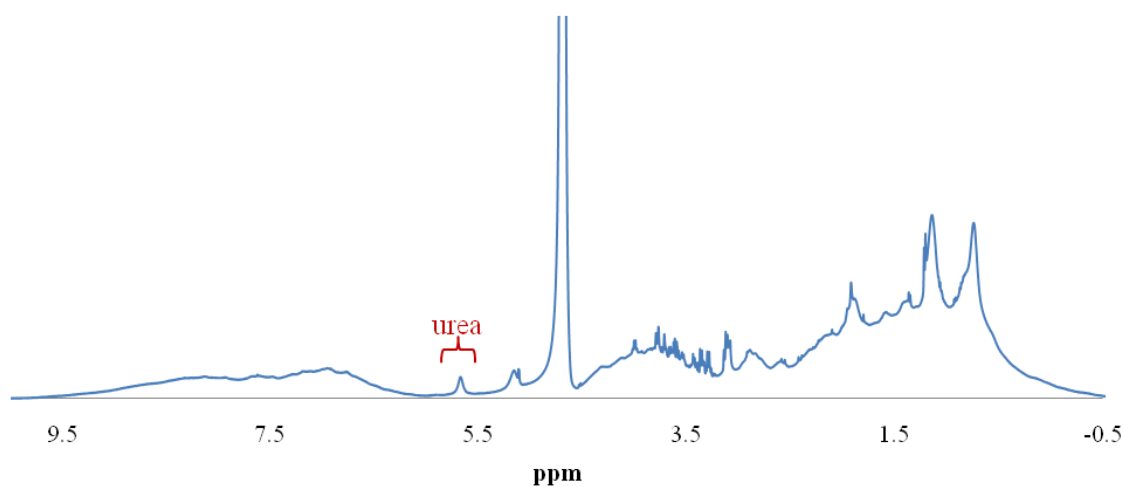


Figure S2: ^1H NMR spectrum of urea in human serum.