Electronic Supplementary Material (ESI) for Analyst.

Supporting Information

for

Lithium-7 qNMR as a Method to Quantify Lithium Content in Brine Pools Using Benchtop NMR

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Table S1. T_1 values for several lithium samples prepared in the lab and samples from brine pools. LiCl solutions are reported in w/w% LiCl.

Sample	**T_1 time (s)**
0.25%	23.25
0.50%	23.59
1.00%	22.64
3.00%	22.03
7.50%	19.25
15.00%	12.17
30.00%	3.66
4	12.86
2	13.91
3	14.63
6	0.013

Table S2. Intra- and inter-day precision experiments.

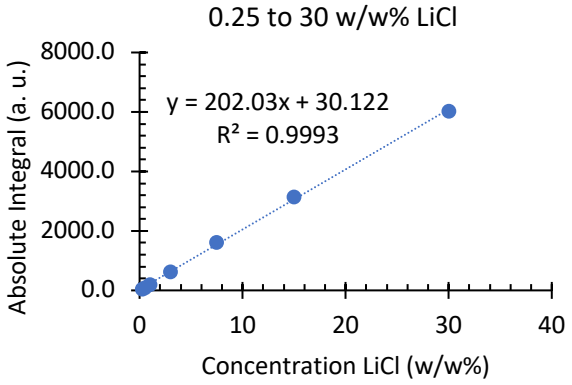
	Integral1	Integral2	Integral3	STDV	RSD
Day1	3198.51	3196.14	3181.02	9.49	0.30
Day2	3233.31	3240.22	3227.74	6.25	0.19
Day3	3212.55	3222.06	3209.39	6.59	0.21
Day4	3184.47	3183.9	3186.25	1.23	0.04
Day5	3216.91	3215.37	3215.03	1.00	0.03
Day6	3182.89	3174.18	3178.15	4.36	0.14

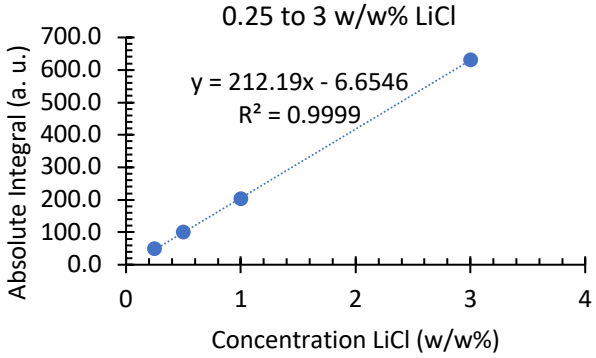
Table S3. Precision and bias by NMR using certified 1000ppm standard for ICP (1002 +/- 8 mg/L)

Run	Results (mg/L)	Difference (-1002)	Squared difference
1	1033.410	31.410	986.603
2	1019.944	17.944	321.994
3	985.563	-16.437	270.182
4	1009.312	7.312	53.460
5	981.230	-20.770	431.403
6	999.559	-2.441	5.958
7	978.673	-23.327	544.126
8	1008.934	6.934	48.080
9	1012.158	10.158	103.188
10	981.090	-20.910	437.218
	sum	-10.127	3202.211
	bias	-1.013	
	precision		18.863

Table S4. Calibration curves

% Li	% LiCl	Integration 1	Integration 2	Integration 3	Avg. Integration	sd	rsd
4.92	30	6011.89	6033.01	6044.9	6029.93	16.719	0.28
2.46	15	3154.84	3157.7	3151.94	3154.83	2.880	0.09
1.23	7.5	1620.28	1613.49	1600.12	1611.30	10.257	0.64
0.49	3	630.621	630.509	631.882	631.00	0.762	0.12
0.16	1	200.774	204.052	199.812	201.55	2.223	1.10
0.08	0.5	98.8305	101.767	98.0829	99.56	1.947	1.96
0.04	0.25	49.427	49.4711	48.6729	49.19	0.449	0.91





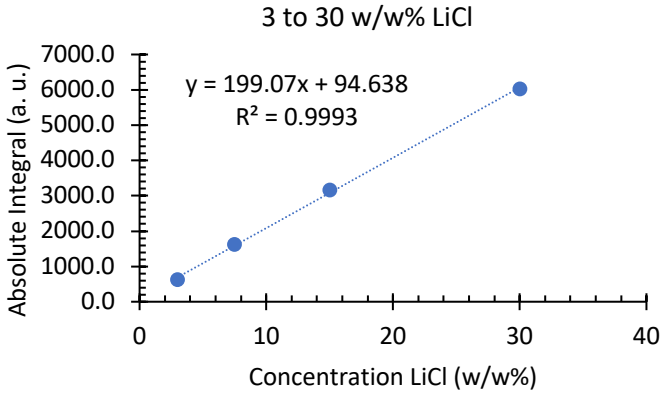


Table S5. Residual output calibration curves

RESIDUAL OUTPUT (0.25-30 w/w% LiCl)

Observation	*Predicted Avg. Integration*	*Residuals*
1	6091.170	-61.237
2	3060.646	94.180
3	1545.384	65.912
4	636.227	-5.223
5	232.157	-30.611
6	131.140	-31.580
7	80.631	-31.441

RESIDUAL OUTPUT (0.25-3 w/w% LiCl)

Observation	*Predicted Avg. Integration*	*Residuals*
1	629.926	1.078
2	205.539	-3.993
3	99.442	0.118
4	46.394	2.797

RESIDUAL OUTPUT (3-30 w/w% LiCl)

Observation	*Predicted Avg. Integration*	*Residuals*
1	6066.805	-36.872
2	3080.721	74.105
3	1587.680	23.617
4	691.854	-60.850

Regression analysis comparing results from NMR and AA

The intercept obtained is 0.0065 (b_0) and the slope of the graph is 1.0405 (b_1). Both values were obtained within the 95% confidence interval. The interval for the intercept is -0.0236 and 0.0366, and it was obtained using the following expression:

$$b_0 \pm t_{\alpha/2} \frac{s}{\sqrt{n\sum_{i=1}^{n}(x-\bar{x})^2}} \sqrt{\sum_{i=1}^{n} x_i^2}$$

Where $t_{\alpha/2}$ is the critical value tabulated to obtain the 95% confidence with 14 degrees of freedom and s is the standard error. The interval of the slope is 1.029 and 1.052 and it was calculated using the following expression:

$$b_1 \pm t_{\alpha/2} \, {}^{s}\Big/_{\sqrt{\sum_{i=1}^{n}(x-\bar{x})^2}}$$