U.S. DEPARTMENT OF COMMERCE
NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
PHYSICAL MEASUREMENT
LABORATORY
Boulder, Colorado 80305

Report of Measurement

Magnetic Resonance Measurements for MRI Biomarkers: Proton Spin Relaxation Times

Submitted for

NIST/ISMRM System Phantoms
SN: 130-0133; 130-0134

Certificate information		Sample information	
Certificate number	80100S-20200610-C1	**Sample set name**	System phantom solutions for NIST Phantom Lending Library
Sample receipt date	6/24/2019	**Sample type/photo** 	$NiCl_2$ (x14) $MnCl_2$ (x14) Proton density (x14) $CuSO_4$ fiducial (x1)
Total number of pages	16	**NIST reference number**	800100S_CaliberMRI_20200610

Requested measurements		Special instructions	
Number of samples	53	**Sample preparation**	25 µl sealed in Teflon capillary
Requested temperatures (C)	16.0, 18.0, 20.0, 22.0, 24.0, 26.0	**Measurement setup**	Nominal NMR setup, Doty Probe
Requested fields (T)	3T	**Comment**	

Service ID: 80100S-20200610-C1
Folder Number:
Date of Calibration: JUN 26-Oct 1, 2019
Date of Report: JUN 10, 2020
Reference: 800100S_CaliberMRI_20200610

System Calibration

System Calibration	Date	Calibration	target	Calibration file/ Comments
NMR time base frequency (MHz)	6/25/2019	**10.000 003**	10.000 000	20190624_NMR_time_base_Cal.pdf Measured values (MHz): 10.000 003 453 6 10.000 003 453 9 10.000 003 453 8 10.000 003 454 2
Optical fiber sample thermometer*	6/24/2019	< ±0.1C over 15C to 30C		FO calibration Opsens Tq-L014-0067-01.xlsx

*Fiber optic thermometer calibration is only one component of the temperature uncertainty, which also includes temperature transfer and fluctuation uncertainties.

NIST Reference Samples**	Date	Magnetic Field (T)	Temp (C)	T_1 reported (ms)	T_1 historical target (ms)	T_2 reported (ms)	T_2 historical target (ms)	CPMG refocusing time (ms)
NIST-$NiCl_2$-12	6/21/2019	3.00672	20.0±0.2	44.67	**44.53**	31.97	**31.86**	2.028
NIST Ni SRM-Ni-S25-C4	6/17/2019	3.00672	20.0±0.2	44.01	**44.37**	36.49	**36.70**	2.028
NIST Ni SRM-Ni-S25-C4* **	8/20/2020	3.00672	20.0±0.2	44.25	**44.37**	36.50	**36.70**	2.028

**All measured deviations of NIST reference samples from historical target values are within reported uncertainties.

***Recalibration after probe repair and replacement of $MnCl_2$-1 and $MnCl_2$-5 solutions

Customer data:

$NiCl_2$ array

Customer Sample ID/ Lot #	$NiCl_2$ Concen-tration (mM)*	Magnetic Field (T)	Temp (C)**	T_1 reported (ms)	T_1 uncertainty (ms)***	T_2 reported (ms)	T_2 uncertainty (ms)***	CPMG refocusing time (ms)
NiCl2-14 SHBH6185	65.3	3.00672	16	21.94	0.31	15.80	0.19	2.028
NiCl2-14 SHBH6185	65.3	3.00672	18	21.62	0.31	15.47	0.19	2.028
NiCl2-14 SHBH6185	65.3	3.00672	20	21.44	0.31	15.30	0.19	2.028
NiCl2-14 SHBH6185	65.3	3.00672	22	21.28	0.31	15.22	0.19	2.028
NiCl2-14 SHBH6185	65.3	3.00672	24	21.26	0.31	15.33	0.19	2.028
NiCl2-14 SHBH6185	65.3	3.00672	26	21.31	0.31	15.49	0.19	2.028
NiCl2-13 SHBH6184	46.0	3.00672	16	31.05	0.62	22.37	0.38	2.028
NiCl2-13 SHBH6184	46.0	3.00672	18	30.65	0.62	21.99	0.38	2.028
NiCl2-13 SHBH6184	46.0	3.00672	20	30.40	0.62	21.76	0.38	2.028
NiCl2-13 SHBH6184	46.0	3.00672	22	30.27	0.62	21.74	0.38	2.028
NiCl2-13 SHBH6184	46.0	3.00672	24	30.25	0.62	21.84	0.38	2.028
NiCl2-13 SHBH6184	46.0	3.00672	26	30.31	0.62	22.09	0.38	2.028
NiCl2-12 SHBH6183	32.7	3.00672	16	43.79	0.44	31.55	0.27	2.028
NiCl2-12 SHBH6183	32.7	3.00672	18	43.24	0.44	30.97	0.27	2.028
NiCl2-12 SHBH6183	32.7	3.00672	20	42.89	0.44	30.66	0.27	2.028
NiCl2-12 SHBH6183	32.7	3.00672	22	42.72	0.44	30.63	0.27	2.028
NiCl2-12 SHBH6183	32.7	3.00672	24	42.70	0.44	30.83	0.27	2.028
NiCl2-12 SHBH6183	32.7	3.00672	26	42.80	0.44	30.71	0.27	2.028

NiCl2-11 SHBH6182	23.3	3.00672	16	61.49	0.88	43.57	0.54	2.028
NiCl2-11 SHBH6182	23.3	3.00672	18	60.70	0.87	42.91	0.54	2.028
NiCl2-11 SHBH6182	23.3	3.00672	20	60.21	0.87	42.44	0.54	2.028
NiCl2-11 SHBH6182	23.3	3.00672	22	59.97	0.88	42.42	0.54	2.028
NiCl2-11 SHBH6182	23.3	3.00672	24	60.00	0.87	42.67	0.54	2.028
NiCl2-11 SHBH6182	23.3	3.00672	26	60.17	0.87	43.22	0.54	2.028
NiCl2-10 SHBH6181	16.5	3.00672	16	87.47	1.24	62.36	0.76	2.028
NiCl2-10 SHBH6181	16.5	3.00672	18	86.41	1.24	61.60	0.76	2.028
NiCl2-10 SHBH6181	16.5	3.00672	20	85.75	1.24	60.86	0.77	2.028
NiCl2-10 SHBH6181	16.5	3.00672	22	85.03	1.24	60.96	0.76	2.028
NiCl2-10 SHBH6181	16.5	3.00672	24	85.01	1.24	61.27	0.76	2.028
NiCl2-10 SHBH6181	16.5	3.00672	26	85.28	1.24	62.12	0.77	2.028
NiCl2-9 SHBH6179	11.3	3.00672	16	122.99	1.75	89.01	1.08	2.028
NiCl2-9 SHBH6179	11.3	3.00672	18	121.79	1.75	87.65	1.08	2.028
NiCl2-9 SHBH6179	11.3	3.00672	20	121.08	1.75	86.91	1.09	2.028
NiCl2-9 SHBH6179	11.3	3.00672	22	120.80	1.75	86.85	1.08	2.028
NiCl2-9 SHBH6179	11.3	3.00672	24	120.90	1.75	87.27	1.08	2.028
NiCl2-9 SHBH6179	11.3	3.00672	26	121.34	1.75	88.37	1.09	2.028
NiCl2-8 SHBH6178	7.74	3.00672	16	177.68	2.47	129.78	1.54	2.028
NiCl2-8 SHBH6178	7.74	3.00672	18	175.94	2.47	127.33	1.54	2.028
NiCl2-8 SHBH6178	7.74	3.00672	20	174.95	2.48	126.33	1.55	2.028
NiCl2-8 SHBH6178	7.74	3.00672	22	174.59	2.47	126.49	1.54	2.028

NiCl2-8 SHBH6178	7.74	3.00672	24	174.78	2.47	126.91	1.54	2.028
NiCl2-8 SHBH6178	7.74	3.00672	26	175.48	2.48	128.28	1.55	2.028
NiCl2-7 SHBH6177	5.43	3.00672	16	243.77	3.49	178.68	2.18	2.028
NiCl2-7 SHBH6177	5.43	3.00672	18	241.84	3.49	176.11	2.18	2.028
NiCl2-7 SHBH6177	5.43	3.00672	20	240.86	3.51	174.99	2.20	2.028
NiCl2-7 SHBH6177	5.43	3.00672	22	240.75	3.49	175.07	2.18	2.028
NiCl2-7 SHBH6177	5.43	3.00672	24	241.31	3.49	176.15	2.18	2.028
NiCl2-7 SHBH6177	5.43	3.00672	26	242.45	3.51	178.08	2.20	2.028
NiCl2-6 SHBH6176	3.68	3.00672	16	343.00	4.93	252.21	3.10	2.028
NiCl2-6 SHBH6176	3.68	3.00672	18	341.53	4.94	249.23	3.11	2.028
NiCl2-6 SHBH6176	3.68	3.00672	20	341.58	4.97	248.03	3.14	2.028
NiCl2-6 SHBH6176	3.68	3.00672	22	342.58	4.93	248.15	3.10	2.028
NiCl2-6 SHBH6176	3.68	3.00672	24	344.23	4.94	250.05	3.11	2.028
NiCl2-6 SHBH6176	3.68	3.00672	26	346.67	4.97	253.80	3.14	2.028
NiCl2-5 SHBH6175	2.52	3.00672	16	483.91	6.95	358.92	4.43	2.028
NiCl2-5 SHBH6175	2.52	3.00672	18	482.91	7.01	355.15	4.46	2.028
NiCl2-5 SHBH6175	2.52	3.00672	20	484.97	7.06	354.38	4.51	2.028
NiCl2-5 SHBH6175	2.52	3.00672	22	486.92	6.95	356.14	4.43	2.028
NiCl2-5 SHBH6175	2.52	3.00672	24	490.24	7.01	359.80	4.46	2.028
NiCl2-5 SHBH6175	2.52	3.00672	26	494.55	7.06	365.21	4.51	2.028
NiCl2-4 SHBH6174	1.64	3.00672	16	675.07	9.94	519.26	6.45	2.028
NiCl2-4 SHBH6174	1.64	3.00672	18	686.88	10.02	520.94	6.49	2.028

NiCl2-4 SHBH6174	1.64	3.00672	20	690.08	10.12	521.27	6.57	2.028
NiCl2-4 SHBH6174	1.64	3.00672	22	695.01	9.94	523.08	6.45	2.028
NiCl2-4 SHBH6174	1.64	3.00672	24	701.06	10.02	528.55	6.49	2.028
NiCl2-4 SHBH6174	1.64	3.00672	26	709.48	10.12	538.22	6.57	2.028
NiCl2-3 SHBH6173	1.04	3.00672	16	950.71	13.82	731.70	9.09	2.028
NiCl2-3 SHBH6173	1.04	3.00672	18	963.56	14.02	735.31	9.19	2.028
NiCl2-3 SHBH6173	1.04	3.00672	20	987.27	14.22	736.97	9.32	2.028
NiCl2-3 SHBH6173	1.04	3.00672	22	1000.81	13.82	744.39	9.09	2.028
NiCl2-3 SHBH6173	1.04	3.00672	24	1015.70	14.02	755.94	9.19	2.028
NiCl2-3 SHBH6173	1.04	3.00672	26	1030.78	14.22	768.69	9.32	2.028
NiCl2-2 SHBH6172	0.60	3.00672	16	1274.07	19.44	990.77	12.88	2.028
NiCl2-2 SHBH6172	0.60	3.00672	18	1317.71	19.97	1010.28	12.99	2.028
NiCl2-2 SHBH6172	0.60	3.00672	20	1330.16	20.41	1026.78	13.03	2.028
NiCl2-2 SHBH6172	0.60	3.00672	22	1355.29	19.44	1040.25	12.88	2.028
NiCl2-2 SHBH6172	0.60	3.00672	24	1367.79	19.97	1048.13	12.99	2.028
NiCl2-2 SHBH6172	0.60	3.00672	26	1395.94	20.41	1067.14	13.03	2.028
NiCl2-1 SHBH6171	0.29	3.00672	16	1766.68	28.54	1348.91	18.96	2.028
NiCl2-1 SHBH6171	0.29	3.00672	18	1830.34	29.44	1455.09	19.72	2.028
NiCl2-1 SHBH6171	0.29	3.00672	20	1883.97	30.32	1489.41	20.41	2.028
NiCl2-1 SHBH6171	0.29	3.00672	22	1937.34	28.54	1520.77	18.96	2.028
NiCl2-1 SHBH6171	0.29	3.00672	24	1987.50	29.44	1532.32	19.72	2.028
NiCl2-1 SHBH6171	0.29	3.00672	26	2066.95	30.32	1578.57	20.41	2.028

* Concentrations provided by CaliberMRI, based on Certificates of Analysis from Sigma-Aldrich.

** The temperatures listed are prescribed values. The uncertainty in the temperature measurement is included in the T1, T2 uncertainty values.

*** The uncertainties, *u*, are calculated using a Monte Carlo- Bloch simulator as described in NIST SP250-97. The uncertainty is given by *u* =3*SD where SD is the maximum observed T1, T2 standard deviation given by the Monte Carlo Bloch simulations. There is 99.7% probability that the real values fall within the reported values ± *u*. The full uncertainty analysis is available on request.

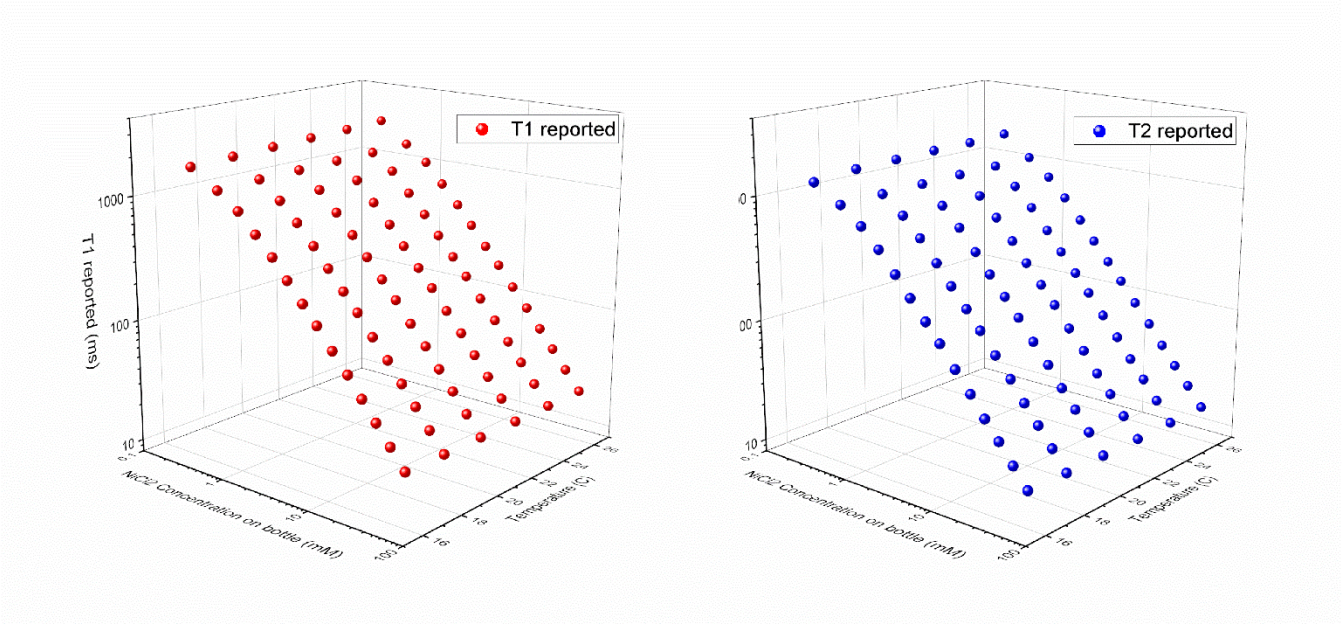

Figure 1. Proton spin relaxation times, T1 and T2, at 3 T for the $NiCl_2$ array as a function of temperature and customer-supplied Ni concentration.

$MnCl_2$ array

Customer Sample ID/ lot number	$MnCl_2$ Concentration (mM)*	Magnetic Field (T)	Temp (C)**	T_1 reported (ms)	T_1 uncertainty (ms)***	T_2 reported (ms)	T_2 uncertainty (ms)***	CPMG refocusing time (ms)
MnCl2-14 SHBH6109	1.5996	3.00672	16	73.65	1.84	4.79	0.05	2.028
MnCl2-14 SHBH6109	1.5996	3.00672	18	77.93	1.95	4.93	0.05	2.028
MnCl2-14 SHBH6109	1.5996	3.00672	20	82.46	2.06	5.10	0.05	2.028
MnCl2-14 SHBH6109	1.5996	3.00672	22	87.08	2.18	5.28	0.05	2.028

MnCl2-14 SHBH6109	1.5996	3.00672	24	91.82	2.30	5.48	0.05	2.028
MnCl2-14 SHBH6109	1.5996	3.00672	26	96.54	2.41	5.69	0.05	2.028
MnCl2-13 SHBH5402	1.1274	3.00672	16	104.57	2.61	6.83	0.06	2.028
MnCl2-13 SHBH5402	1.1274	3.00672	18	110.49	2.76	7.04	0.07	2.028
MnCl2-13 SHBH5402	1.1274	3.00672	20	116.70	2.92	7.27	0.07	2.028
MnCl2-13 SHBH5402	1.1274	3.00672	22	123.22	3.08	7.49	0.07	2.028
MnCl2-13 SHBH5402	1.1274	3.00672	24	129.67	3.24	7.76	0.07	2.028
MnCl2-13 SHBH5402	1.1274	3.00672	26	136.34	3.41	8.06	0.08	2.028
MnCl2-12 SHBH5401	0.7902	3.00672	16	141.21	3.53	9.88	0.09	2.028
MnCl2-12 SHBH5401	0.7902	3.00672	18	149.28	3.73	10.17	0.10	2.028
MnCl2-12 SHBH5401	0.7902	3.00672	20	158.17	3.95	10.52	0.10	2.028
MnCl2-12 SHBH5401	0.7902	3.00672	22	166.64	4.17	10.88	0.10	2.028
MnCl2-12 SHBH5401	0.7902	3.00672	24	175.31	4.38	11.25	0.11	2.028
MnCl2-12 SHBH5401	0.7902	3.00672	26	184.07	4.60	11.67	0.11	2.028
MnCl2-11 SHBH5400	0.5555	3.00672	16	203.53	5.09	13.94	0.13	2.028
MnCl2-11 SHBH5400	0.5555	3.00672	18	214.80	5.37	14.28	0.13	2.028
MnCl2-11 SHBH5400	0.5555	3.00672	20	226.53	5.66	14.74	0.14	2.028
MnCl2-11 SHBH5400	0.5555	3.00672	22	238.33	5.96	15.24	0.14	2.028
MnCl2-11 SHBH5400	0.5555	3.00672	24	250.61	6.27	15.80	0.15	2.028
MnCl2-11 SHBH5400	0.5555	3.00672	26	263.09	6.58	16.39	0.15	2.028
MnCl2-10 SHBH5399	0.4276	3.00672	16	262.14	6.55	18.22	0.17	2.028
MnCl2-10 SHBH5399	0.4276	3.00672	18	277.38	6.93	18.78	0.18	2.028

MnCl2-10 SHBH5399	0.4276	3.00672	20	292.87	7.32	19.40	0.18	2.028
MnCl2-10 SHBH5399	0.4276	3.00672	22	308.92	7.72	20.07	0.19	2.028
MnCl2-10 SHBH5399	0.4276	3.00672	24	325.23	8.13	20.78	0.20	2.028
MnCl2-10 SHBH5399	0.4276	3.00672	26	341.74	8.54	21.56	0.20	2.028
MnCl2-9 SHBH5398	0.2768	3.00672	16	384.99	9.62	28.04	0.26	2.028
MnCl2-9 SHBH5398	0.2768	3.00672	18	408.05	10.20	28.93	0.27	2.028
MnCl2-9 SHBH5398	0.2768	3.00672	20	431.22	10.78	29.88	0.28	2.028
MnCl2-9 SHBH5398	0.2768	3.00672	22	454.82	11.37	30.92	0.29	2.028
MnCl2-9 SHBH5398	0.2768	3.00672	24	478.81	11.97	32.06	0.30	2.028
MnCl2-9 SHBH5398	0.2768	3.00672	26	503.30	12.58	33.25	0.31	2.028
MnCl2-8 SHBH5397	0.193	3.00672	16	531.60	13.29	41.53	0.39	2.028
MnCl2-8 SHBH5397	0.193	3.00672	18	563.86	14.10	42.63	0.40	2.028
MnCl2-8 SHBH5397	0.193	3.00672	20	599.96	15.00	44.24	0.42	2.028
MnCl2-8 SHBH5397	0.193	3.00672	22	634.59	15.86	45.86	0.43	2.028
MnCl2-8 SHBH5397	0.193	3.00672	24	669.56	16.74	47.66	0.45	2.028
MnCl2-8 SHBH5397	0.193	3.00672	26	703.51	17.59	49.26	0.46	2.028
MnCl2-7 SHBH6119	0.1353	3.00672	16	711.11	17.78	59.45	0.56	2.028
MnCl2-7 SHBH6119	0.1353	3.00672	18	757.34	18.93	61.31	0.58	2.028
MnCl2-7 SHBH6119	0.1353	3.00672	20	805.10	20.13	63.42	0.60	2.028
MnCl2-7 SHBH6119	0.1353	3.00672	22	848.64	21.22	65.65	0.62	2.028
MnCl2-7 SHBH6119	0.1353	3.00672	24	892.41	22.31	67.82	0.64	2.028
MnCl2-7 SHBH6119	0.1353	3.00672	26	937.12	23.43	70.57	0.66	2.028

MnCl2-6 SHBH5396	0.0934	3.00672	16	892.29	22.31	81.86	0.77	2.028
MnCl2-6 SHBH5396	0.0934	3.00672	18	972.48	24.31	85.92	0.81	2.028
MnCl2-6 SHBH5396	0.0934	3.00672	20	1026.43	25.66	88.89	0.84	2.028
MnCl2-6 SHBH5396	0.0934	3.00672	22	1083.42	27.09	92.30	0.87	2.028
MnCl2-6 SHBH5396	0.0934	3.00672	24	1141.50	28.54	95.97	0.90	2.028
MnCl2-6 SHBH5396	0.0934	3.00672	26	1202.40	30.06	99.89	0.94	2.028
MnCl2-5 SHBM3477	0.0673	3.00672	16	1056.33	32.70	105.31	1.45	2.028
MnCl2-5 SHBM3477	0.0673	3.00672	18	1125.81	35.44	108.76	1.50	2.028
MnCl2-5 SHBM3477	0.0673	3.00672	20	1197.57	37.77	112.66	1.57	2.028
MnCl2-5 SHBM3477	0.0673	3.00672	22	1267.08	39.75	116.82	1.62	2.028
MnCl2-5 SHBM3477	0.0673	3.00672	24	1340.89	42.18	121.21	1.70	2.028
MnCl2-5 SHBM3477	0.0673	3.00672	26	1410.82	44.36	126.30	1.77	2.028
MnCl2-4 SHBH5394	0.0434	3.00672	16	1341.07	33.53	161.07	1.51	2.028
MnCl2-4 SHBH5394	0.0434	3.00672	18	1466.78	36.67	169.02	1.59	2.028
MnCl2-4 SHBH5394	0.0434	3.00672	20	1549.98	38.75	175.05	1.65	2.028
MnCl2-4 SHBH5394	0.0434	3.00672	22	1626.53	40.66	181.48	1.71	2.028
MnCl2-4 SHBH5394	0.0434	3.00672	24	1715.06	42.88	187.21	1.76	2.028
MnCl2-4 SHBH5394	0.0434	3.00672	26	1801.61	45.04	192.23	1.81	2.028
MnCl2-3 SHBH5393	0.0282	3.00672	16	1657.68	41.44	247.93	2.33	2.028
MnCl2-3 SHBH5393	0.0282	3.00672	18	1783.21	44.58	257.47	2.42	2.028
MnCl2-3 SHBH5393	0.0282	3.00672	20	1901.28	47.53	267.29	2.51	2.028
MnCl2-3 SHBH5393	0.0282	3.00672	22	2009.05	50.23	276.98	2.60	2.028

MnCl2-3 SHBH5393	0.0282	3.00672	24	2119.34	52.98	287.48	2.70	2.028
MnCl2-3 SHBH5393	0.0282	3.00672	26	2232.44	55.81	299.08	2.81	2.028
MnCl2-2 SHBH5392	0.0181	3.00672	16	1874.96	46.87	357.40	3.36	2.028
MnCl2-2 SHBH5392	0.0181	3.00672	18	2073.94	51.85	370.54	3.48	2.028
MnCl2-2 SHBH5392	0.0181	3.00672	20	2185.54	54.64	379.48	3.57	2.028
MnCl2-2 SHBH5392	0.0181	3.00672	22	2302.78	57.57	392.49	3.69	2.028
MnCl2-2 SHBH5392	0.0181	3.00672	24	2424.62	60.62	406.02	3.82	2.028
MnCl2-2 SHBH5392	0.0181	3.00672	26	2546.04	63.65	420.75	3.96	2.028
MnCl2-1 SHBM3478_	0.0113	3.00672	16	2127.95	66.75	506.65	16.03	2.028
MnCl2-1 SHBM3478_	0.0113	3.00672	18	2322.54	71.56	526.24	17.14	2.028
MnCl2-1 SHBM3478_	0.0113	3.00672	20	2478.19	75.63	552.73	18.13	2.028
MnCl2-1 SHBM3478_	0.0113	3.00672	22	2623.59	79.79	578.48	19.02	2.028
MnCl2-1 SHBM3478_	0.0113	3.00672	24	2775.52	84.13	610.51	20.11	2.028
MnCl2-1 SHBM3478_	0.0113	3.00672	26	2917.74	88.42	636.24	20.73	2.028

* Concentrations provided by CaliberMRI, based on Certificates of Analysis from Sigma-Aldrich.

** The temperatures listed are prescribed values. The uncertainty in the temperature measurement is included in the T1, T2 uncertainty values.

*** The uncertainties, *u*, are calculated using a Monte Carlo- Bloch simulator as described in NIST SP250-97. The uncertainty is given by $u = 3*SD$ where SD is the maximum observed T1, T2 standard deviation given by the Monte Carlo Bloch simulations. There is 99.7% probability that the real values fall within the reported values ± *u*. The full uncertainty analysis is available on request.

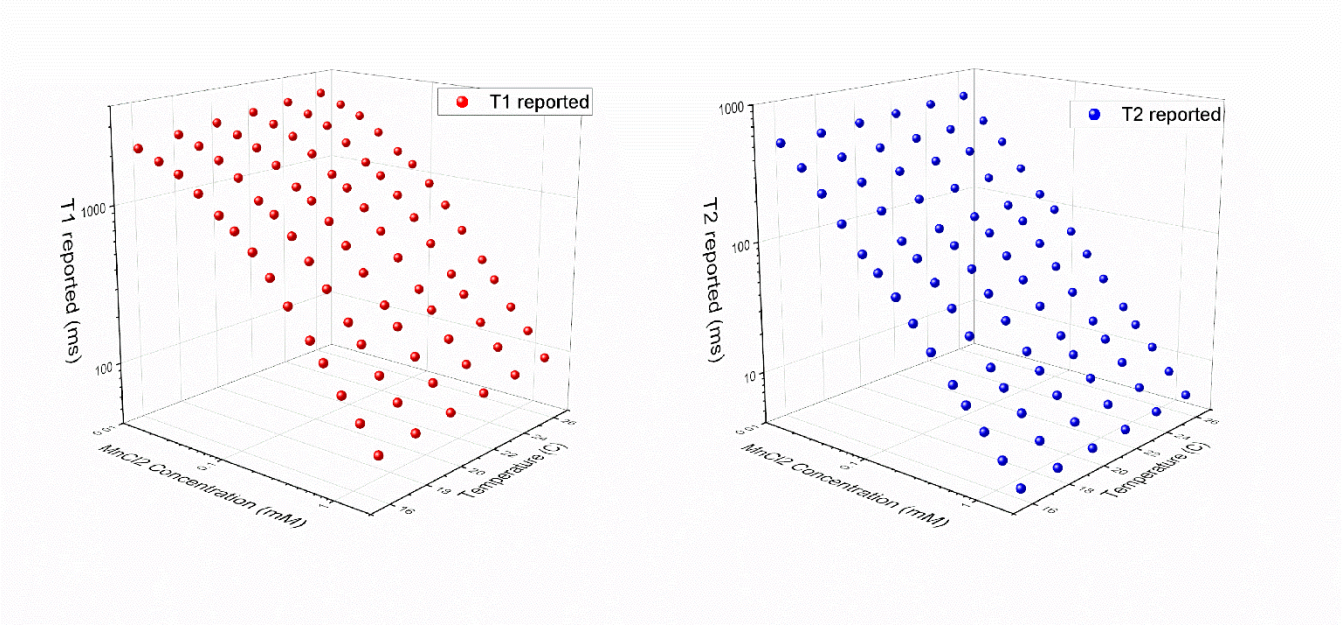

Figure 2. Proton spin relaxation times, T1 and T2, at 3 T for the $MnCl_2$ array as a function of temperature and customer-supplied concentration.

$CuSO_4$ Fiducial Solution

Customer Sample ID	$CuSO_4$ concentration (mM)*	Magnetic Field (T)	Temp (C)**	T_1 reported (ms)	T_1 uncertainty (ms)***	T_2 reported (ms)	T_2 uncertainty (ms)***	CPMG refocusing time (ms)
CuSO4 SHBH5566V	2.90	3.00672	16	350.23	7.71	300.27	6.61	2.028
CuSO4 SHBH5566V	2.90	3.00672	18	370.96	8.16	317.88	6.99	2.028
CuSO4 SHBH5566V	2.90	3.00672	20	391.51	8.61	335.56	7.38	2.028
CuSO4 SHBH5566V	2.90	3.00672	22	412.02	9.06	352.51	7.76	2.028
CuSO4 SHBH5566V	2.90	3.00672	24	432.78	9.52	370.62	8.15	2.028
CuSO4 SHBH5566V	2.90	3.00672	26	453.81	9.98	388.91	8.56	2.028

* Concentrations provided by CaliberMRI, based on Certificates of Analysis from Sigma-Aldrich.

** The temperatures listed are prescribed values. The uncertainty in the temperature measurement is included in the T1, T2 uncertainty values.

*** The uncertainties, *u*, are calculated using a Monte Carlo- Bloch simulator as described in NIST SP250-97. The uncertainty is given by *u* =3*SD where SD is the maximum observed T1, T2 standard deviation given by the Monte Carlo Bloch simulations. There is 99.7% probability that the real values fall within the reported values ± *u*. The full uncertainty analysis is available on request.

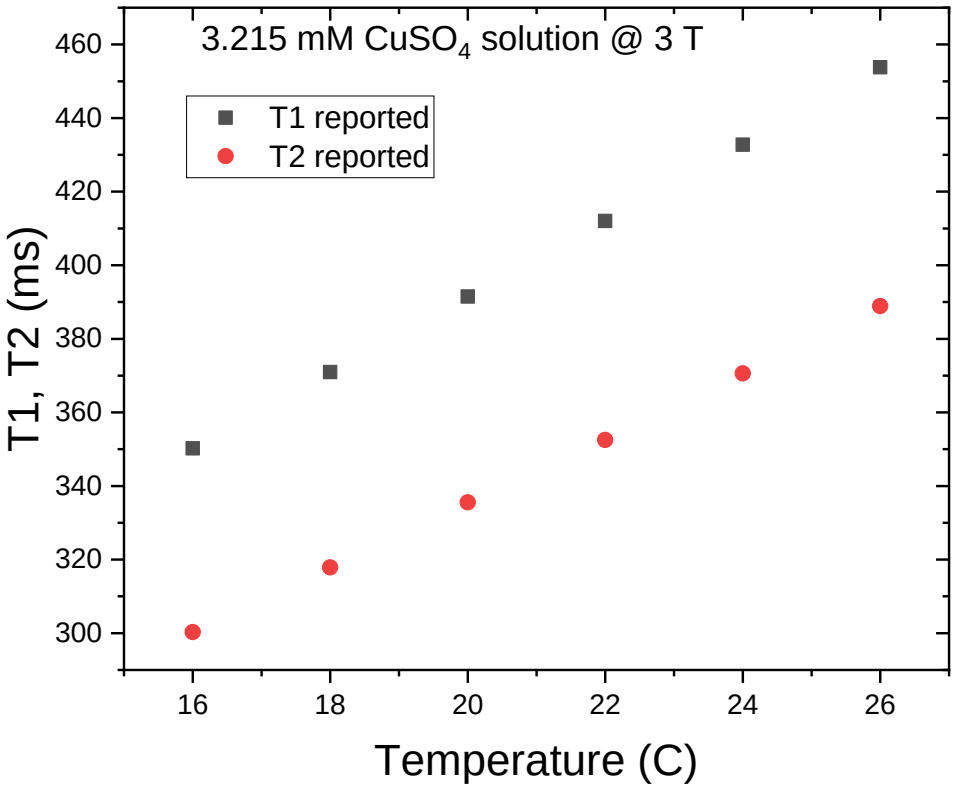

Figure 3. T1, T2 at 3T for $CuSO_4$ solution as a function of temperature.

Proton Density Array

Sample	Gravimetric proton density (%)*	Magnetic Field (T)	Temperature (C)**	sample mass (g)	PD: ratio of NMR signal to pure water (%)***	Normalized water reference	PD Uncertainty (%)****
PD1 PDTK190101	5	3.00672	20	2.5908	5.07	0.999	0.183
PD2 PDTK190101	10	3.00672	20	2.5864	10.23	0.994	0.370
PD3 PDTK190101	15	3.00672	20	2.529	15.01	1.006	0.542
PD4 PDTK190101	20	3.00672	20	2.5813	20.68	0.989	0.747
PD5 PDTK190101	25	3.00672	20	2.5222	25.47	0.990	0.920
PD6 PDTK190101	30	3.00672	20	2.5097	29.983	1.003	1.083
PD7 PDTK190101	35	3.00672	20	2.4865	34.887	0.998	1.260
PD8 PDTK190101	40	3.00672	20	2.4907	39.76	1.003	1.436
PD9 PDTK190101	50	3.00672	20	2.4911	48.42	1.000	1.749
PD10 PDTK190101	60	3.00672	20	2.4243	59.13	1.008	2.135
PD11 PDTK190101	70	3.00672	20	2.3792	68.55	1.006	2.476
PD12 PDTK190101	80	3.00672	20	2.3607	78.35	1.006	2.830
PD13 PDTK190101	90	3.00672	20	2.3712	90.59	0.996	3.272
PD14 PDTK190101	100	3.00672	20	2.2981	99.55	1.000	3.595

*Gravimetric proton density supplied by CaliberMRI. Gravimetric measurements of proton density will, in general, have less uncertainty then NMR-based measurements.

** The temperature uncertainty is ±0.2 C. The relative proton density is weakly dependent on temperature.

*** the reported NMR proton density (PD) is the ratio of the NMR signal of the provided sample to an identical sample of pure water.

**** The reported uncertainty is $u = 6\sigma PD$, where σ is the standard deviation of the normalized NMR signal of identical, but independently measured, water samples. The uncertainty is the sum of the relative uncertainty in the sample measurement and the water reference measurement, each taken to be 3σ. There is > 99.7% probability that the real values fall within the reported values ± u.

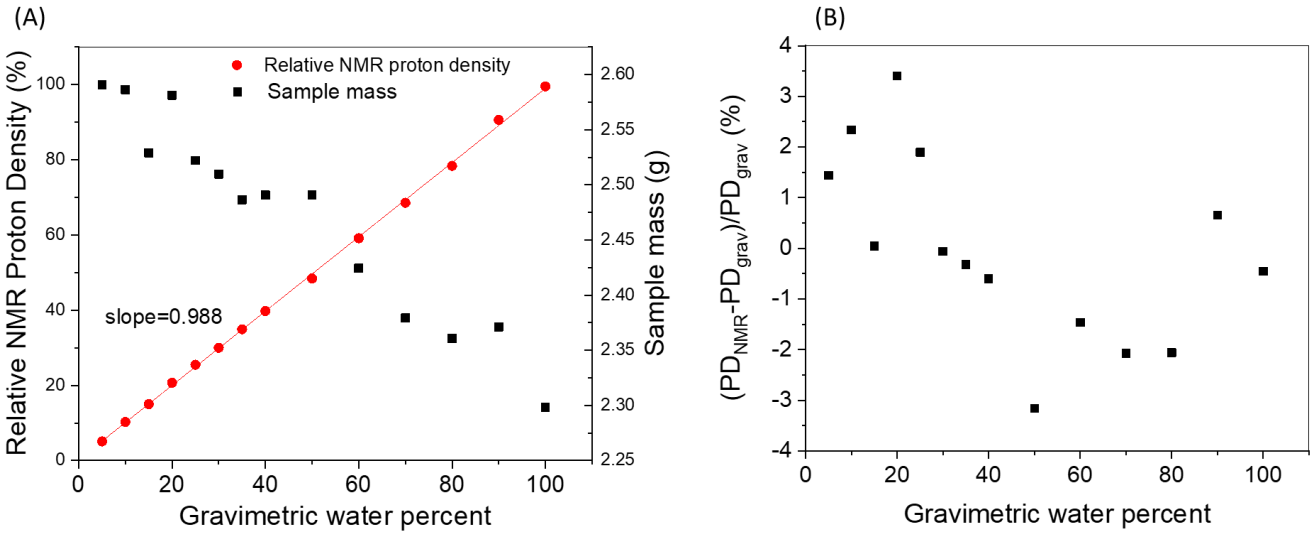

Figure 4. (A) Relative proton density (PD) measured by NMR along with sample mass plotted vs. gravimetric proton density. (B) Difference between NMR and gravimetric measurements of proton density.

Uncertainty and traceability: NIST certifies that the measurements of the proton relaxation times are done in accordance with the NIST internal publication SP250-97 "MRI Biomarker Calibration Service: Proton Relaxation Times," which details the traceability to the System International system of units and provides the computational framework for determining the reported uncertainties. The reported uncertainty is determined through a Monte Carlo simulation of the measurement that includes all known uncertainties. The true relaxation time values, T_1 and T_2, have > 99.7% probability of being within the range $T_{1reported} \pm T_{1uncertainty}$, $T_{2reported} \pm T_{2uncertainty}$, respectively, as determined by the Monte Carlo simulation. The quality control protocols are published in MRI Biomarker Calibration Service QMIII. A key quality control protocol is to measure three internal NIST reference standards, based on the Ni SRM 3136, before each customer measurement. SP250-97 is available online at www.nist.gov/calibrations and the QMIII document is available upon request.

Measurement overview: This calibration service provides traceable measurements of the proton spin relaxation times, T_1 and T_2, of materials used in magnetic resonance imaging (MRI) phantoms (calibration artifacts) at a specified field strength and temperature. T_1 is the longitudinal relaxation time, the exponential time constant required for the nuclear magnetization to relax back to its equilibrium value along the static magnetic field direction. T_2 is the transverse relaxation time, the exponential time constant required for the precessional component of the nuclear magnetization, transverse to the static field, to relax back to zero. Precise definitions of T_1, T_2 are given in SP250-97 Sec. 3. *We restrict measurements to water-proton magnetic moment relaxation in aqueous solutions.* The measurements are based on a variable-field, variable-temperature, nuclear magnetic resonance (NMR) system. NMR and MRI systems are qualitatively similar, however, given the smaller sample volumes in NMR systems, key parameters such as radio frequency (RF) field intensity, magnetic field distortions, and the timing of RF pulses can be better controlled and made more precise. Hence, NMR is a better system for primary measurements of key MRI biomarkers.

T_1 is measured using an inversion recovery sequence where the proton spins, starting in their equilibrium configuration, are rotated 180º by a composite on-resonance radio frequency pulse sequence and then detecting the longitudinal magnetization at a time TI later. The longitudinal magnetization is detected by rotating the magnetization into the transverse plane and recording the free induction decay. A set of 20 TI times are selected to logarithmically sample the magnetization relaxation. The signal, proportional to the magnitude of the magnetization at time TI, is plotted as a function of TI and then fit with a standard three-parameter exponential recovery model to obtain T_1. The reported T_1 is the average of 3 identical measurements.

T_2 is measured using a Carr-Purcell-Meiboom-Gill (CPMG) pulse sequence in which the equilibrium magnetization is tipped into the transverse plane with a 90° RF pulse and then refocused with n 180° RF pulses of duration t_{180}. The transverse magnetization free induction decay is sampled after the last refocusing pulse at an acquisition time $t_a(n) = n(2\tau_{cp} + t_{180})$. The refocusing pulses reverse the dephasing of the transverse proton magnetization due to extrinsic field variations and the observed magnetization decay is governed by intrinsic dephasing processes. The distinction between extrinsic and intrinsic dephasing processes is not unique and T_2 is uniquely determined by reporting the associated CPMG refocusing time $2\tau_{cp} + t_{180}$. A set of 20 even n-values are chosen to sample the magnetization decay over at least 3 orders of magnitude. The signal verses the acquisition time is fit with a simple exponential decay model to determine T_2. The reported T_2 is the average of 3 identical measurements.