

HMDB ID:HMDB00190

Compound name: L-Lactic acid

Spectrum type: ¹H NMR Spectrum

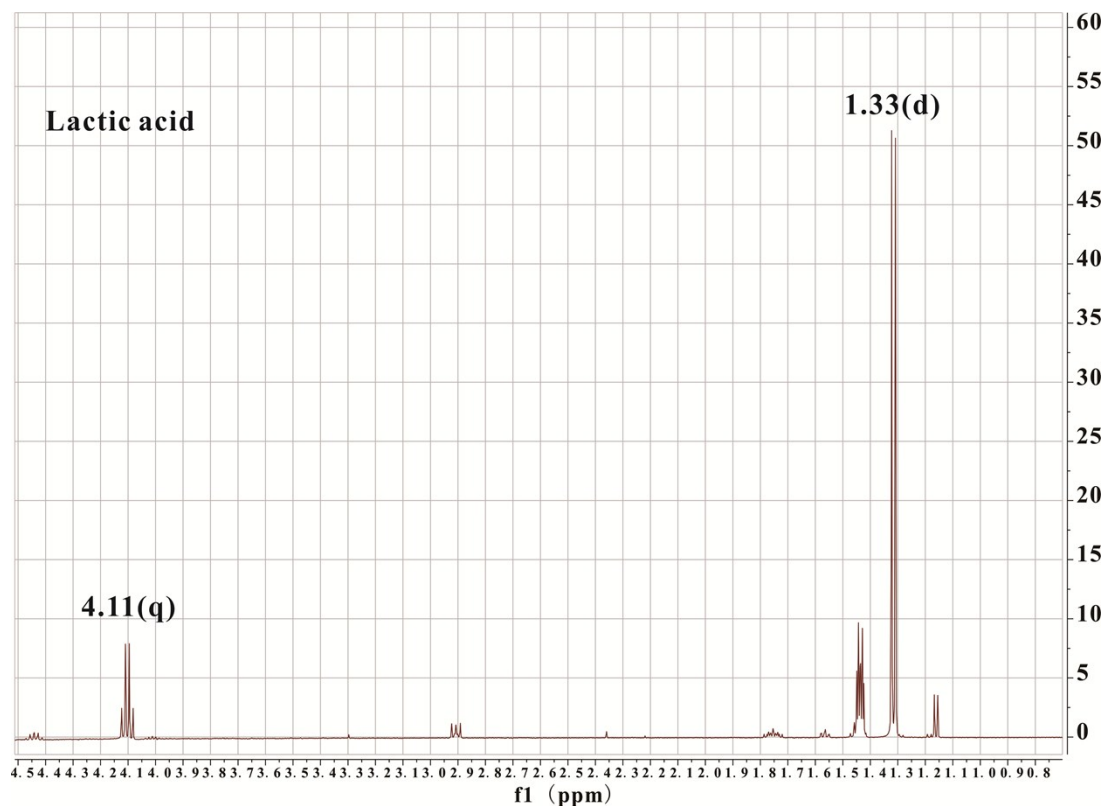


Table of Peaks

No.	(ppm)	(Hz)	Height
1	1.310	654.7	0.9981
2	1.324	661.7	1.0000
3	4.084	2041.1	0.0903
4	4.098	2048.1	0.2701
5	4.111	2055.0	0.2663
6	4.125	2061.9	0.0860

Table of Multiplets

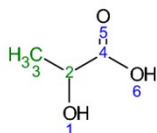
No.	Shift1 (ppm)	H's	Type	J (Hz)	Atom1	Connected Atoms	Multiplet1	Connections	(ppm)
1	1.32	4	d	6.96	3	2	M01	M02	1.30 .. 1.33
2	4.10	2	q	6.93	2	3	M02	M01	4.08 .. 4.13

Table of Assignments

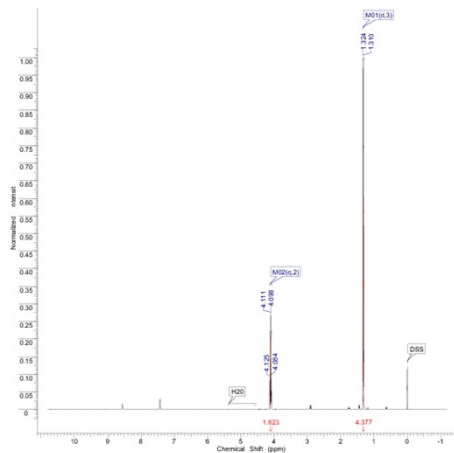
No.	Atom	Exp. Shift (ppm)	Multiplet
1	3	1.32	M01
2	2	4.10	M02

Spectra image with peak assignments

Lactic acid
 HMDB00190
¹H NMR Spectrum: 500 Mhz_0n H
 Sample: 50 mM at pH 7.0
 Referenced to DSS



Full ¹H NMR spectrum



Lactic acid
 HMDB00190
¹H NMR Spectrum: 500 Mhz_0n H
 Sample: 50 mM at pH 7.0
 Referenced to DSS

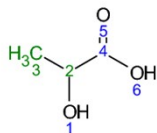


Table of Peaks

No.	ppm	Height
1	1.32	0.9681
2	1.324	1.0000
3	4.084	0.0903
4	4.098	0.2701
5	4.111	0.2693
6	4.125	0.0899

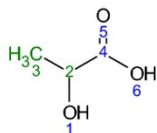
Table of Multiplets

No.	Shift (ppm)	H _s	Type	J (Hz)	Absor/Corrected A	Multiplet	Connections	(ppm)
1	1.32	4	d	6.90	3	M01	M02	[1.30 - 1.35]
2	4.10	2	q	6.55, 6.61	2	M02	5, M01	[4.08 - 4.13]

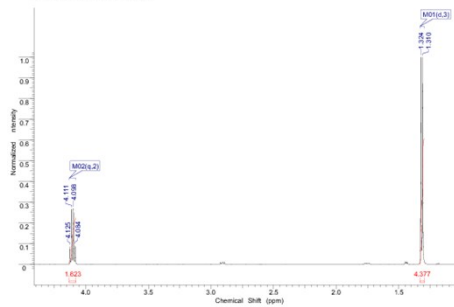
Table of Assignments

No.	Atom	Exp. Shift (ppm)	Multiplet
1	3	1.32	M01
2	2	4.10	M02

Lactic acid
 HMDB00190
¹H NMR Spectrum: 500 Mhz_0n H
 Sample: 50 mM at pH 7.0
 Referenced to DSS



Zoomed ¹H NMR spectrum



HMDB ID:HMDB00883

Compound name:L-Valine

Spectrum type:1H NMR Spectrum

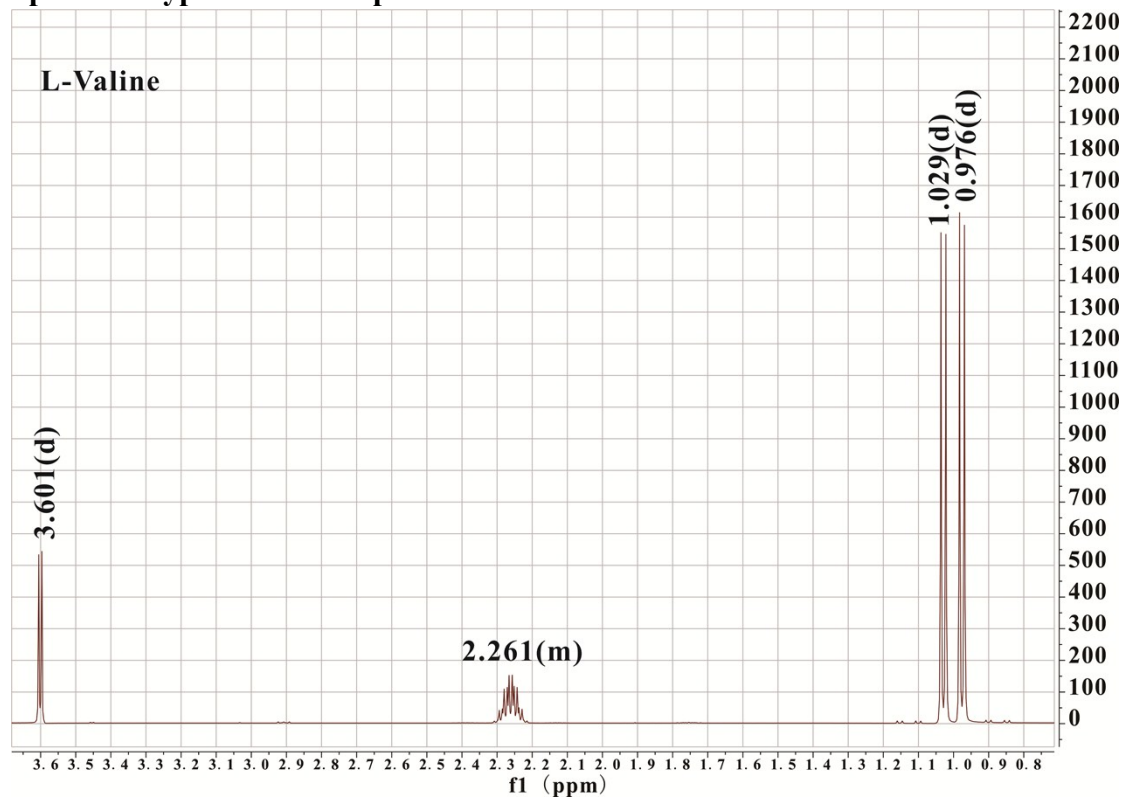


Table of Peaks

No.	(ppm)	(Hz)	Height
1	0.969	484.35	0.9681
2	0.983	491.35	1.0000
3	1.022	510.70	0.9530
4	1.036	517.75	0.9614
5	2.229	1114.12	0.0278
6	2.238	1118.51	0.0304
7	2.243	1121.14	0.0702
8	2.252	1125.49	0.0726
9	2.257	1128.15	0.0941
10	2.266	1132.52	0.0934
11	2.271	1135.16	0.0700
12	2.280	1139.55	0.0669
13	2.285	1142.16	0.0280
14	2.294	1146.58	0.0252
15	3.597	1797.66	0.3374
16	3.605	1801.99	0.3305

Table of Multiplets

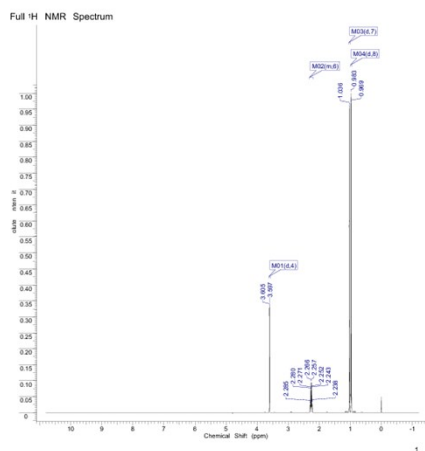
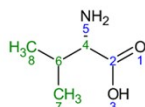
No.	Shift1 (ppm)	H's	Type	J (Hz)	Atom1	Multiplet1	(ppm)
1	0.976	3	d	7.01	8	M04	0.963 .. 0.990
2	1.029	3	d	7.05	7	M03	1.012 .. 1.045
3	2.261	1	m	14.03 7.01 4.41	6	M02	2.207 .. 2.314
4	3.601	1	d	4.33	4	M01	3.585 .. 3.618

Table of Assignments

No.	Atom	Exp. Shift (ppm)	Multiplet
1	8	0.978	M04
2	7	1.029	M03
3	6	2.261	M02
4	4	3.601	M01

Spectra image with peak assignments

L-Valine
 HMDB00883
¹H NMR Spectrum: 500 MHz in H₂O
 Sample: 50 mM at pH 7.0
 Referenced to DSS



L-Valine
 HMDB00883
¹H NMR Spectrum: 500 MHz in H₂O
 Sample: 50 mM at pH 7.0
 Referenced to DSS

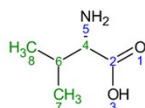


Table of Peaks

No.	Chem	Chem	Height
1	0.969	484.35	0.9691
2	0.983	491.35	1.9692
3	1.032	515.79	0.9630
4	1.038	521.79	0.9644
5	2.229	1114.12	0.0276
6	2.298	1151.51	0.0304
7	2.343	1171.14	0.0210
8	2.298	1151.51	0.0289
9	2.257	1128.15	0.0441
10	2.298	1151.51	0.0304
11	2.271	1134.16	0.0200
12	2.280	1139.15	0.0089
13	2.285	1142.16	0.0080
14	2.294	1148.18	0.0212
15	3.007	1501.66	0.2374
16	3.005	1501.69	0.2305

Table of Multiplets

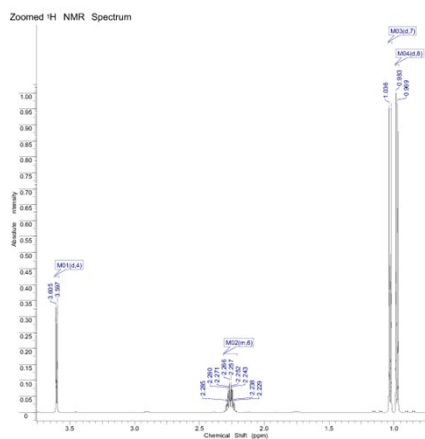
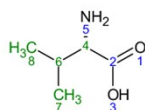
No.	Shift	Split	F ₁	Type	J (Hz)	Atom1	Multiplet	(ppm)
1	0.976	3	4	7.15	6	M4	[0.969 - 0.992]	
2	1.039	3	4	7.15	7	M3	[1.012 - 1.045]	
3	2.281	1	6	16.01	6	M2	[2.267 - 2.314]	
4	3.007	1	6	4.33	4	M1	[0.985 - 3.818]	

Table of Assignments

No.	Atom	Chem	Shift (ppm)	Multiplet
1	6	0.976	M4	
2	7	1.039	M3	
3	6	2.281	M2	
4	4	3.001	M1	

2

L-Valine
 HMDB00883
¹H NMR Spectrum: 500 MHz in H₂O
 Sample: 50 mM at pH 7.0
 Referenced to DSS



3

HMDB ID:HMDB00161

Compound name: L-Alanine

Spectrum type:1H NMR Spectrum

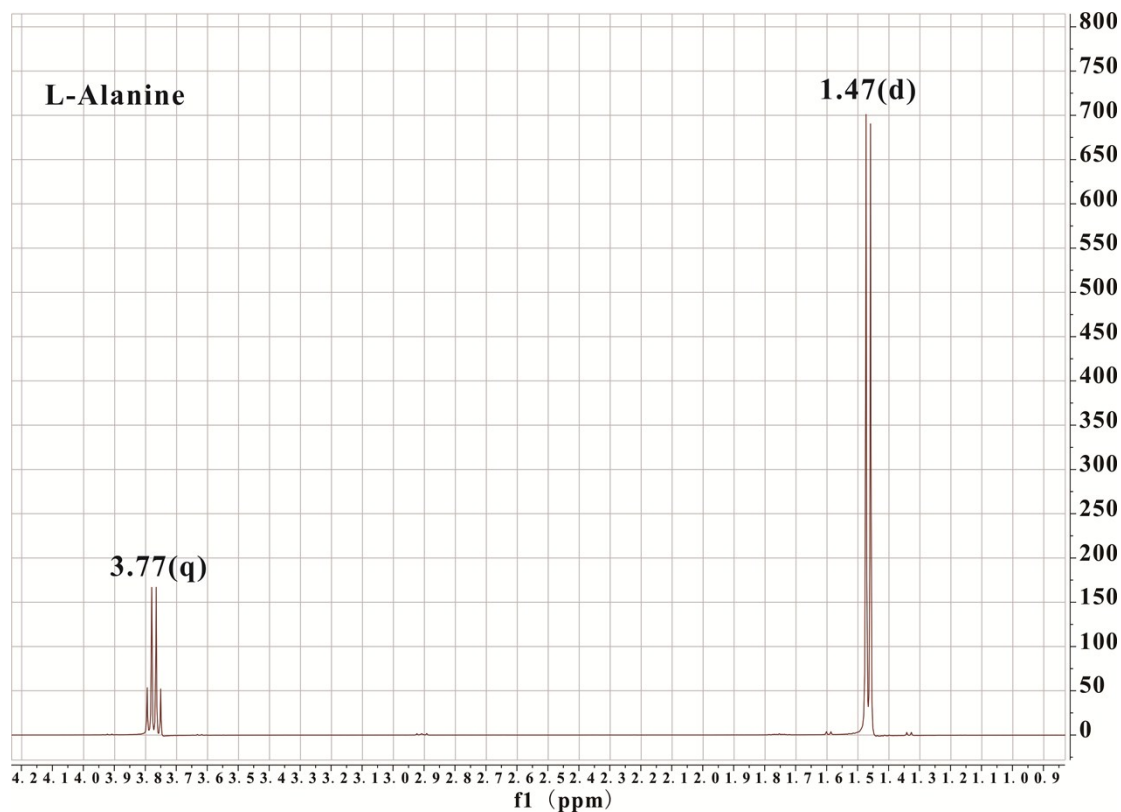


Table of Peaks

No.	(ppm)	(Hz)	Height
1	1.459	729.3	0.9806
2	1.474	736.5	1.0000
3	3.751	1874.9	0.0631
4	3.766	1882.2	0.2025
5	3.780	1889.4	0.2030
6	3.795	1896.6	0.0649

Table of Multiplets

No.	Shift1 (ppm)	H's	Type	J (Hz)	Atom1	Multiplet1	(ppm)
1	1.47	5	d	7.28	6	M02	1.41 .. 1.52
2	3.77	1	q	7.23	4	M01	3.73 .. 3.83

Table of Assignments

No.	Atom	Exp. Shift (ppm)	Multiplet
1	6	1.47	M02
2	4	3.77	M01

Spectra image with peak assignments

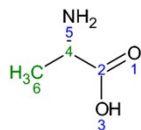
L-Alanine

HMDB00161

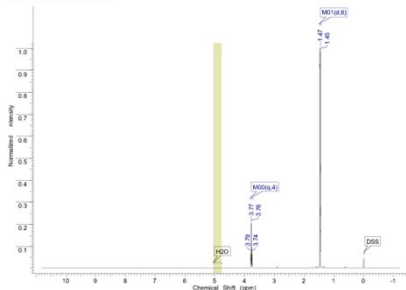
¹H NMR spectrum: 500 MHz in H₂O

Sample: 50 mM at pH 7.0

Referenced to DSS



Full ¹H NMR Spectrum



1

L-Alanine

HMDB00161

¹H NMR spectrum: 500 MHz in H₂O

Sample: 50 mM at pH 7.0

Referenced to DSS

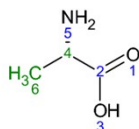


Table of Peaks

No.	Chem	Int	Height
1	3.73	1832.8	0.2673
2	3.77	1833.4	0.2678
3	3.76	1838.1	0.2684
4	3.75	1837.9	0.2683
5	4.7	725.3	0.9952
6	1.45	725.3	0.9952

Table of Multiplets

No.	Start	Stop	Type	F (Hz)	Atom1	Multiplet	Int
1	4.6	4.8	7.20	0	300	1372	3.60
2	3.70	3.8	7.20	0	300	1372	3.60

Table of Assignments

No.	Atom	Exp. Shift (ppm)	Multiplet
1	4	3.76	MQQ
2	4	3.76	MQQ

2

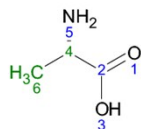
L-Alanine

HMDB00161

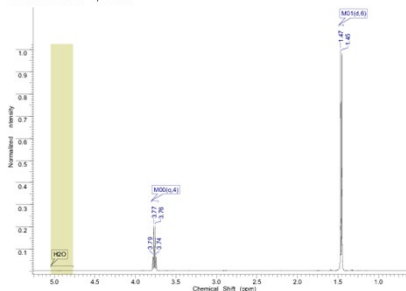
¹H NMR spectrum: 500 MHz in H₂O

Sample: 50 mM at pH 7.0

Referenced to DSS



Zoomed ¹H NMR Spectrum



HMDB ID:HMDB00042

Compound name: Acetic acid

Spectrum type: ^1H NMR Spectrum

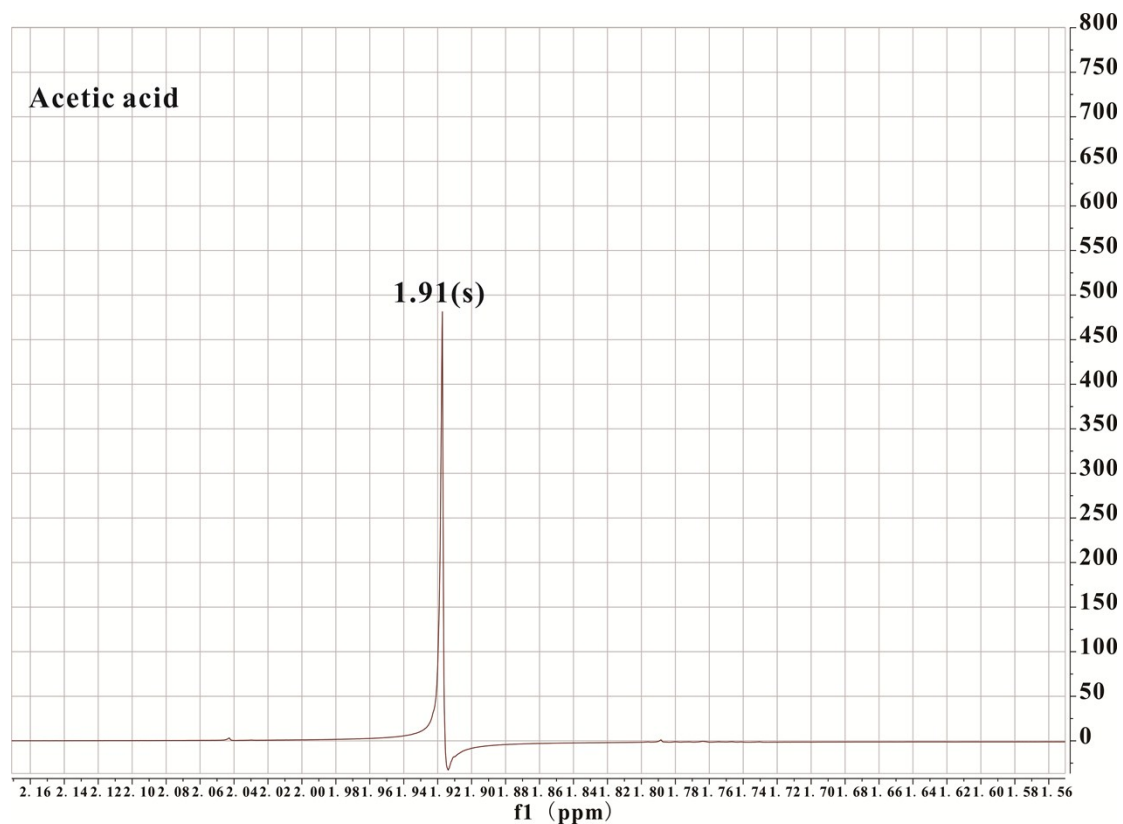


Table of Peaks

No.	(ppm)	(Hz)	Height
1	1.91	953.8	1.0000

Table of Multiplets

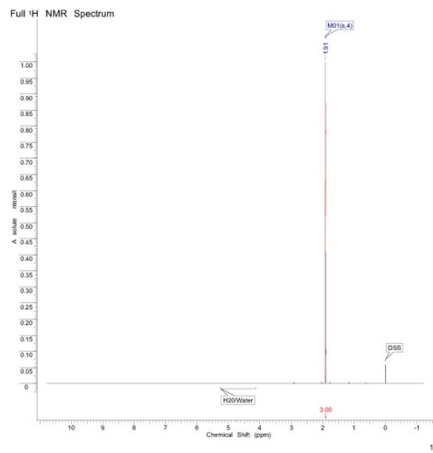
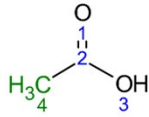
No.	Shift1 (ppm)	H's	Type	Atom1	Multiplet1	(ppm)
1	1.91	3	s	4	M01	1.89 .. 1.93

Table of Assignments

No.	Atom	Exp. Shift (ppm)	Multiplet
1	4	1.91	M01

Spectra image with peak assignments

Acetic acid
 HMDB00042
¹H NMR spectrum: 500 MHz in H₂O
 Sample: 23 mM at pH 7.0
 Referenced to DSS



Acetic acid
 HMDB00042
¹H NMR spectrum: 500 MHz in H₂O
 Sample: 23 mM at pH 7.0
 Referenced to DSS

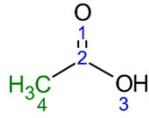


Table of Peaks

No.	Chem. Shift (ppm)	Height
1	1.91	953.8

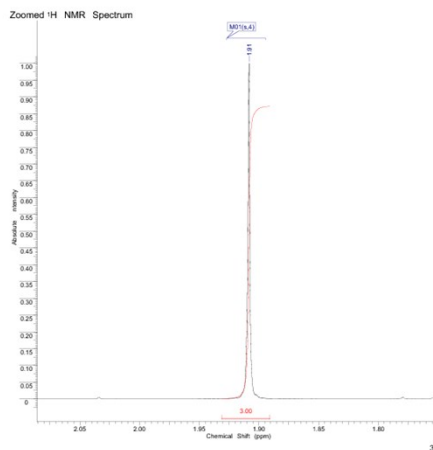
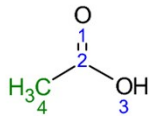
Table of Multiplets

No.	Chem. Shift (ppm)	Type	Atom	Multiplet	(ppm)
1	1.91	s	4	MS1	(1.89 - 1.93)

Table of Assignments

No.	Atom	Exp. Shift (ppm)	Multiplet
1	4	1.91	MS1

Acetic acid
 HMDB00042
¹H NMR spectrum: 500 MHz in H₂O
 Sample: 23 mM at pH 7.0
 Referenced to DSS



HMDB ID:HMDB00696

Compound name: L-Methionine

Spectrum type:1H NMR Spectrum

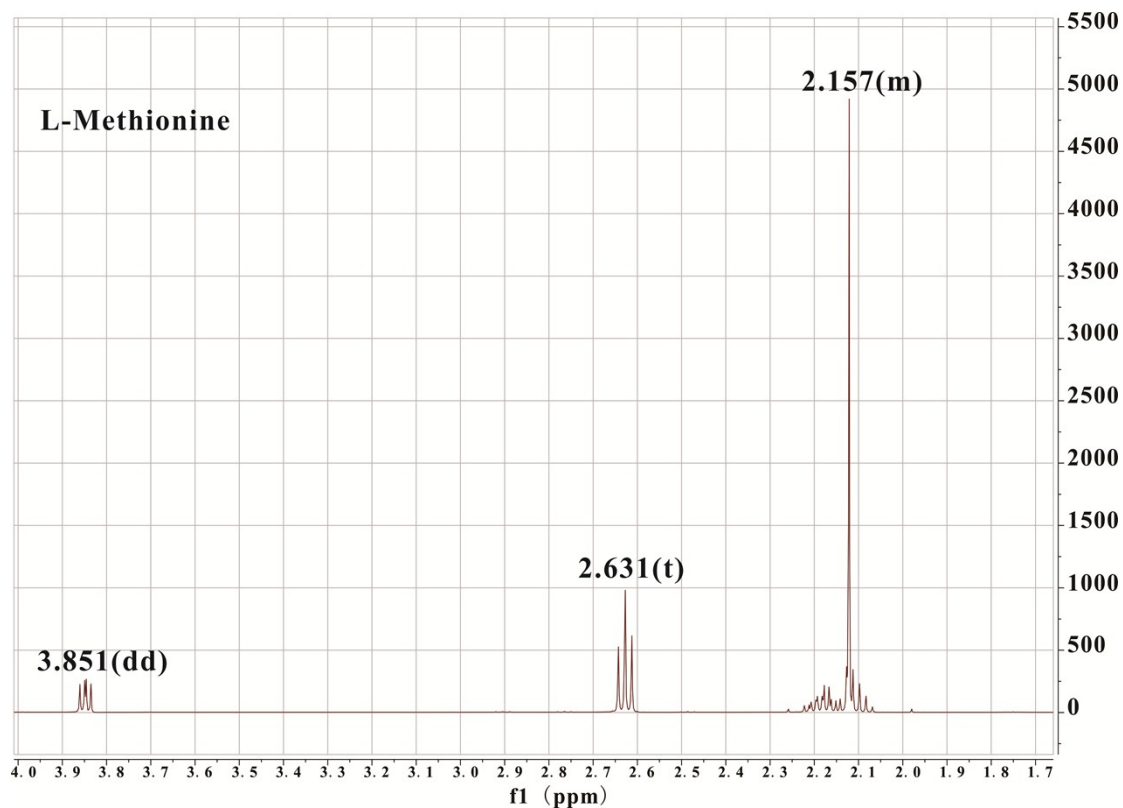


Table of Peaks

No.	(ppm)	(Hz)	Height
1	2.072	1035.7	0.0504
2	2.087	1042.9	0.1393
3	2.101	1050.3	0.2369
4	2.116	1057.6	0.3919
5	2.125	1062.1	4.0000
6	2.145	1072.2	0.1229
7	2.155	1077.0	0.1032
8	2.166	1082.4	0.1158
9	2.170	1084.8	0.2087
10	2.181	1090.2	0.2200
11	2.186	1092.5	0.1513
12	2.197	1098.0	0.1490
13	2.211	1105.1	0.0915
14	2.215	1107.3	0.0671
15	2.226	1112.7	0.0553
16	2.616	1307.6	0.6028
17	2.631	1315.1	1.0261
21	3.853	1925.8	0.3290
22	3.864	1931.2	0.2721

Table of Multiplets

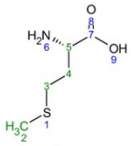
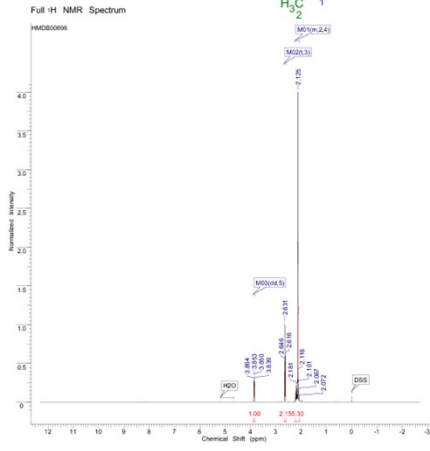
No.	Shift1 (ppm)	H's	Type	J (Hz)	Atom1	Multiplet1	(ppm)
1	2.157	31	m	-	2 4	M01	2.055 .. 2.241
2	2.631	13	t	7.587	3	M02	2.593 .. 2.673
3	3.851	6	d	7.100 5.382	5	M03	3.818 .. 3.888

Table of Assignments

No.	Atom	Exp. Shift (ppm)	Multiplet
1	2	2.157	M01
2	4	2.157	M01
3	3	2.631	M02
4	5	3.851	M03

Spectra image with peak assignments

L-Methionine
HMDB00696
¹H NMR Spectrum: 500 MHz in H₂O
Sample: 50 mM at pH 7.0
Referenced to DSS



L-Methionine
HMDB00696
¹H NMR Spectrum: 500 MHz in H₂O
Sample: 50 mM at pH 7.0
Referenced to DSS

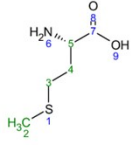


Table of Peaks

No.	(ppm)	(Hz)	Height
1	2.072	1036.7	0.0504
2	2.087	1042.9	0.1393
3	2.101	1050.3	0.3288
4	2.116	1057.6	0.3819
5	2.131	1065.1	0.4000
6	2.145	1072.2	0.1229
7	2.160	1079.0	0.1024
8	2.166	1082.4	0.1158
9	2.170	1084.8	0.2087
10	2.181	1092.2	0.2250
11	2.186	1092.5	0.1513
12	2.197	1098.0	0.1480
13	2.211	1105.1	0.0915
14	2.235	1120.3	0.0671
15	2.228	1112.7	0.0553
16	2.616	1307.6	0.0020
17	2.631	1315.1	1.0281
18	2.668	1322.7	0.0276
19	3.829	1916.7	0.2778
20	3.850	1924.1	0.3262
21	3.853	1925.8	0.3290
22	3.864	1931.2	0.2721

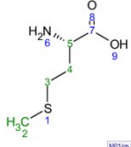
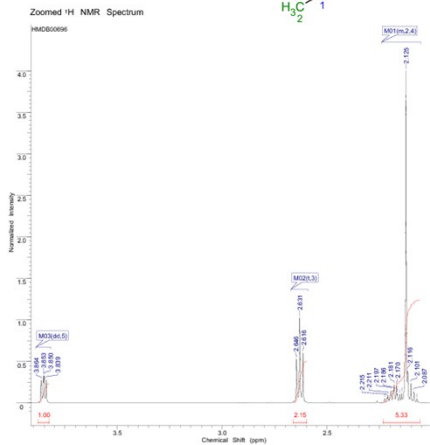
Table of Assignments

No.	Atom	Exp.	Shift (ppm)	Multiplet
1	2	2.157	M3(1)	
2	4	2.157	M3(1)	
3	3	2.851	M3(2)	
4	5	3.851	M3(3)	

Table of Multiplets

No.	Shift (ppm)	Int.	Type	J (Hz)	Abert	Multiplet	(ppm)
1	2.157	31	m	-	2, 4	M3(1)	(2.055 - 2.241)
2	2.851	13	l	7.587	3	M3(2)	(2.859 - 2.878)
3	3.851	6	bc	7.100, 5.3M	5	M3(3)	(3.818 - 3.886)

L-Methionine
HMDB00696
¹H NMR Spectrum: 500 MHz in H₂O
Sample: 50 mM at pH 7.0
Referenced to DSS



HMDB ID:HMDB00357

Compound name: 3-Hydroxybutyric acid

Spectrum type: ¹H NMR Spectrum

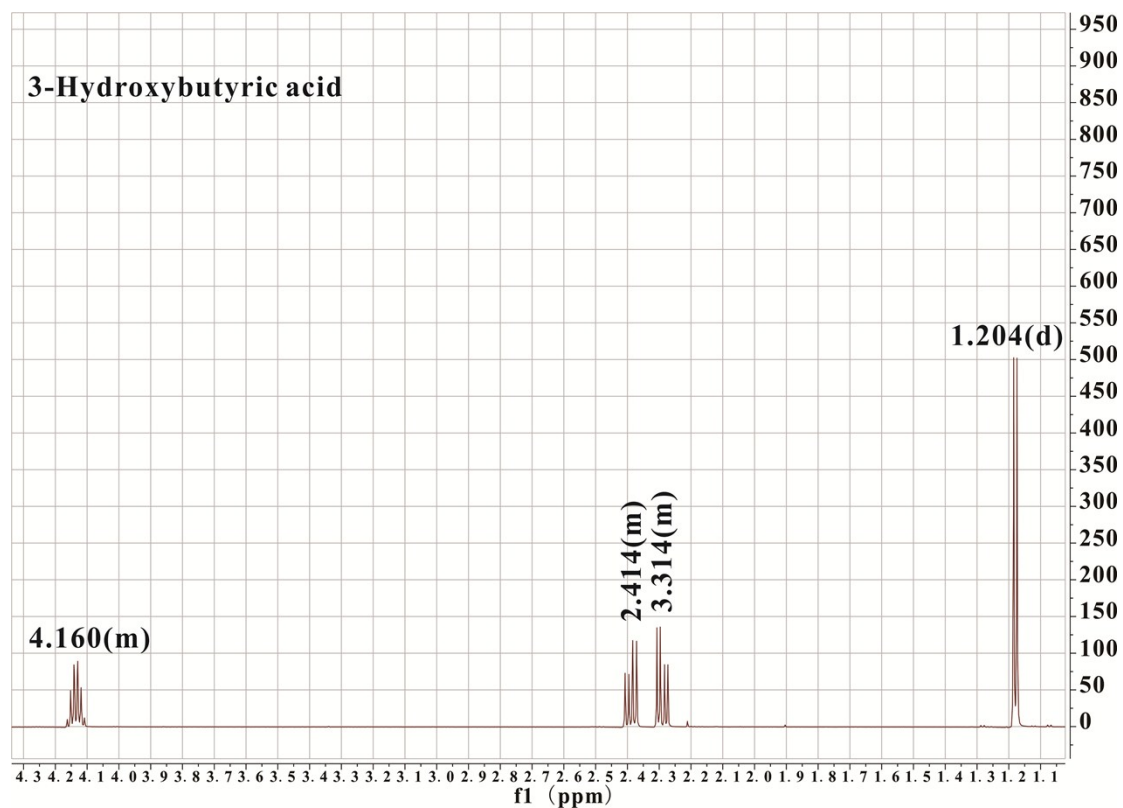


Table of Peaks

No.	(ppm)	(Hz)	Height
1	1.199	718.5	3.9858
2	1.209	724.7	4.0000
3	2.297	1376.9	0.5522
4	2.308	1383.3	0.5618
5	2.321	1391.3	0.8961
6	2.332	1397.6	0.8974
7	2.396	1436.0	0.8380
8	2.408	1443.3	0.8469
9	2.420	1450.4	0.5232
10	2.432	1457.7	0.5283
11	4.133	2477.4	0.0808
12	4.144	2483.7	0.3505
13	4.154	2490.0	0.6180
14	4.166	2497.1	0.6064
15	4.177	2503.4	0.3419
16	4.187	2509.7	0.0792

Table of Multiplets

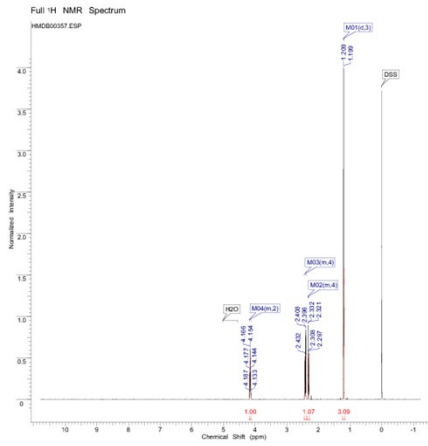
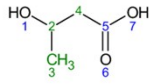
No.	Shift1 (ppm)	H's	Type	J (Hz)	Atom1	Multiplet1	(ppm)
1	1.204	39	d	6.262	3	M01	1.188 .. 1.220
2	2.314	14	m	-	4	M02	2.289 .. 2.342
3	2.414	14	m	-	4	M03	2.387 .. 2.440
4	4.160	13	m	-	2	M04	4.127 .. 4.192

Table of Assignments

No.	Atom	Exp. Shift (ppm)	Multiplet
1	3	1.204	M01
2	4	2.314	M02
3	4	2.414	M03
4	2	4.160	M04

Spectra image with peak assignments

3-Hydroxybutyric acid
 HMDB00357
 1H NMR Spectrum: 500 MHz in H2O
 Sample: 50 mM AT pH 7.0
 Referenced to DSS



3-Hydroxybutyric acid
 HMDB00357
 1H NMR Spectrum: 500 MHz in H2O
 Sample: 50 mM AT pH 7.0
 Referenced to DSS

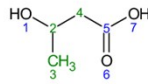


Table of Peaks

No.	(ppm)	(Hz)	Height
1	1.199	718.5	3.9658
2	1.209	724.7	4.0000
3	2.297	1376.0	0.9552
4	2.306	1383.3	0.9618
5	2.321	1391.3	0.8991
6	2.332	1397.6	0.9074
7	2.356	1434.0	0.8380
8	2.408	1443.3	0.8493
9	2.420	1450.4	0.8232
10	2.432	1457.7	0.8083
11	4.133	2477.4	0.0808
12	4.144	2483.7	0.3055
13	4.156	2490.0	0.1930
14	4.166	2497.1	0.8064
15	4.177	2503.4	0.3479
16	4.187	2509.7	0.0792

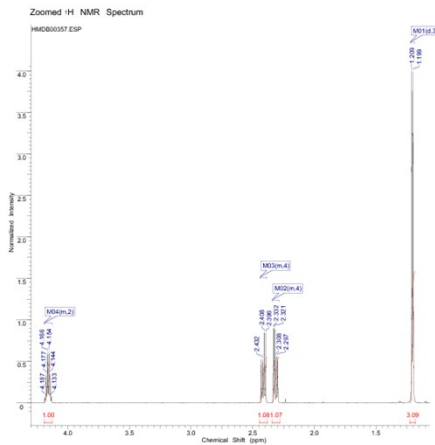
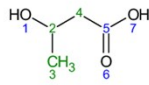
Table of Multiplets

No.	Start (ppm)	End (ppm)	Integ.	J (Hz)	AbnInt	Multiplet	(ppm)
1	1.204	39	d	6.262	3	M01	[1.188 - 1.220]
2	2.314	16	m	-	4	M02	[2.289 - 2.342]
3	2.414	14	m	-	4	M03	[2.387 - 2.440]
4	4.160	13	m	-	2	M04	[4.127 - 4.192]

Table of Assignments

No.	Atom	Exp. Shift (ppm)	Multiplet
1	3	1.204	M01
2	4	2.314	M02
3	4	2.414	M03
4	2	4.160	M04

3-Hydroxybutyric acid
 HMDB00357
 1H NMR Spectrum: 500 MHz in H2O
 Sample: 50 mM AT pH 7.0
 Referenced to DSS



HMDB ID:HMDB00254

Compound name:Succinic acid

Spectrum type:1H NMR Spectrum

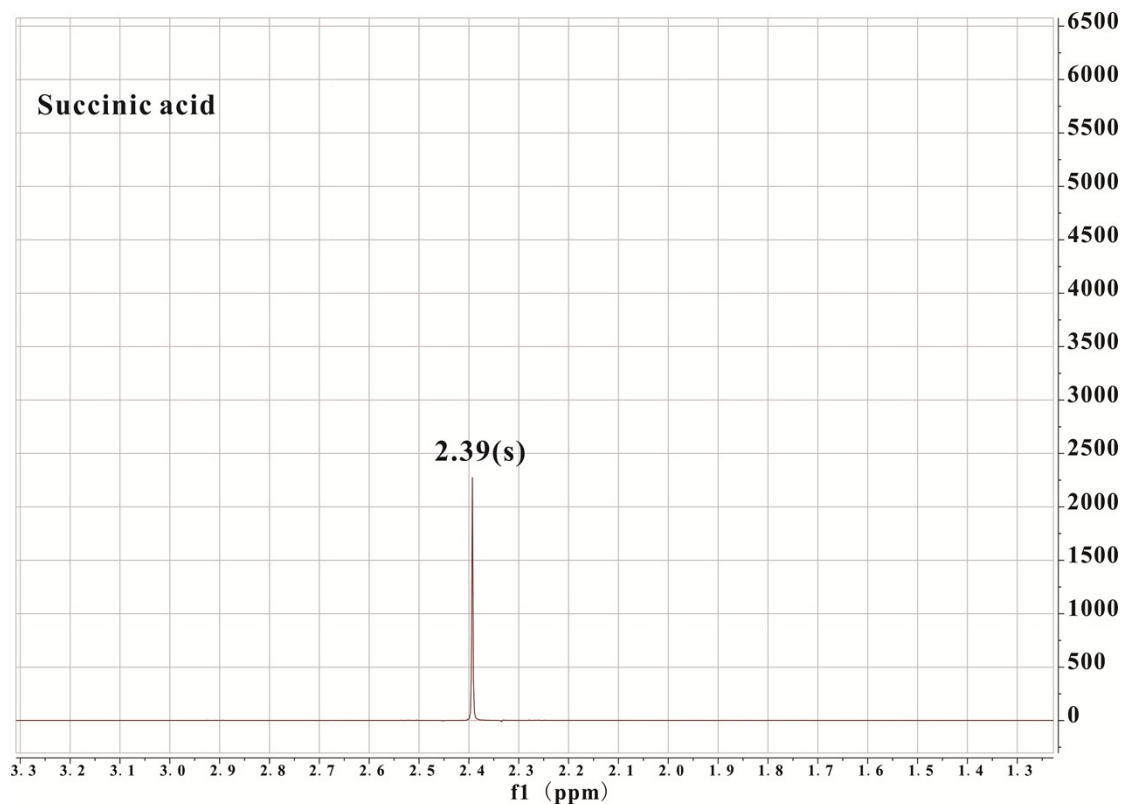


Table of Peaks

No.	(ppm)	(Hz)	Height
1	2.393	1196.3	1.0000

Table of Multiplets

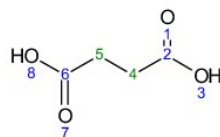
No.	Shift1 (ppm)	H's	Type	Atom1	Multiplet1	(ppm)
1	2.39	93	s	5 4	M01	2.38 .. 2.41

Table of Assignments

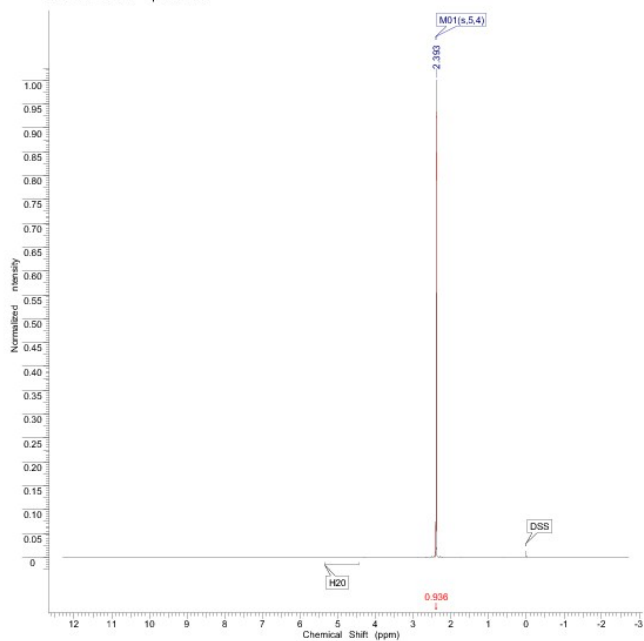
No.	Atom	Exp. Shift (ppm)	Multiplet
1	5	2.39	M01
2	4	2.39	M01

Spectra image with peak assignments

Succinic acid
 HMDB00254
¹H NMR spectrum: 500 MHz, Qn H
 Sample: 50mM at pH 7.0
 Referenced to DSS



Full ¹H NMR spectrum



Succinic acid
 HMDB00254
¹H NMR spectrum: 500 MHz, Qn H
 Sample: 50mM at pH 7.0
 Referenced to DSS

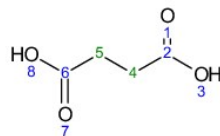


Table of Peaks

No.	Shift1 (ppm)	H's	Type	Atom1	Multiplet1	(ppm)
1	2.39	93	s	5, 4	M01	[2.38 .. 2.41]

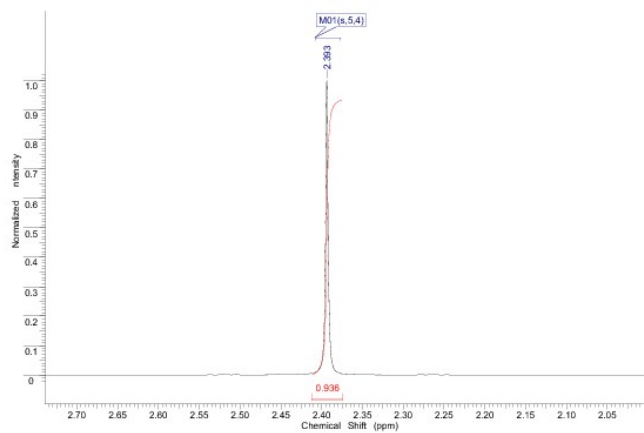
Table of Multiplets

No.	(ppm)	Height
1	2.393	1.0000

Table of Assignments

No.	Atom	Exp.	Shift (ppm)	Multiplet
1	5	2.39		M01
2	4	2.39		M01

Zoomed ¹H NMR spectrum



HMDB ID:HMDB00641

Compound name: L-Glutamine

Spectrum type:1H NMR Spectrum

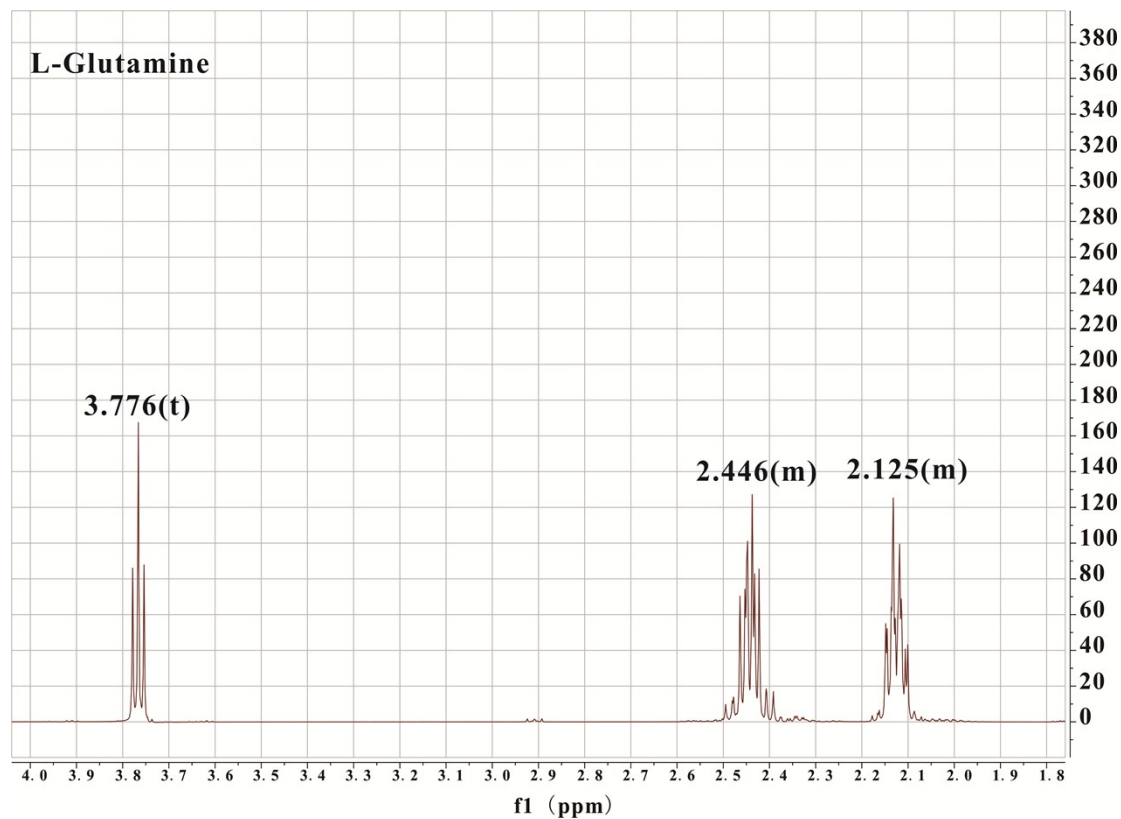


Table of Peaks

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	2.086	1042.87	0.0438	15	2.407	1203.22	0.1308
2	2.101	1049.97	0.3039	16	2.422	1210.82	0.6081
3	2.106	1052.58	0.2769	17	2.432	1215.58	0.5646
4	2.115	1057.07	0.4611	18	2.438	1218.38	0.8876
5	2.118	1058.76	0.6724	19	2.447	1223.18	0.6860
6	2.120	1059.49	0.5773	20	2.449	1224.19	0.6285
7	2.122	1060.64	0.4401	21	2.453	1226.07	0.5102
8	2.128	1063.52	0.3889	22	2.464	1231.47	0.4812
9	2.132	1065.67	0.8706	23	2.478	1238.48	0.0929
10	2.136	1067.83	0.4371	24	2.480	1239.81	0.0780
11	2.145	1072.22	0.3668	25	2.495	1246.95	0.0684
12	2.148	1073.82	0.3791	26	3.754	1876.22	0.5095
13	2.162	1080.78	0.0404	27	3.766	1882.40	1.0000
14	2.392	1195.39	0.1213	28	3.778	1888.58	0.5318

Table of Multiplets

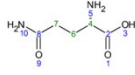
No.	Shift1 (ppm)	H's	Type	J (Hz)	Atom1	Multiplet1	(ppm)
1	2.125	2	m	-	6	M03	2.062 .. 2.188
2	2.446	2	m	-	7	M02	2.375 .. 2.511
3	3.776	1	t	6.18	4	M01	3.726 .. 3.810

Table of Assignments

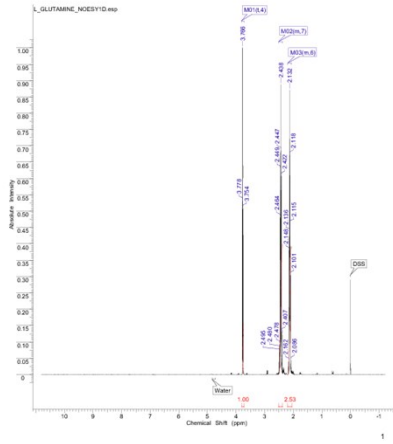
No.	Atom	Exp. Shift (ppm)	Multiplet
1	6	2.125	M03
2	7	2.446	M02
3	4	3.776	M01

Spectra image with peak assignments

L-Glutamine
 HMDB00641
¹H NMR Spectrum: 500MHz in H₂O
 Sample: 50 mM at pH 7.00
 Referenced to DSS



Full ¹H NMR Spectrum



L-Glutamine
 HMDB00641
¹H NMR Spectrum: 500MHz in H₂O
 Sample: 50 mM at pH 7.00
 Referenced to DSS

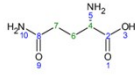


Table of Peaks

No.	ppm	Int	Height	No.	ppm	Int	Height
1	2.586	1042.87	0.5438	16	2.422	1215.82	0.8051
2	2.531	1048.97	0.2029	17	2.452	1215.58	0.5661
3	2.536	1052.58	0.2789	18	2.438	1218.38	0.8876
4	2.515	1057.67	0.4871	19	2.467	1223.18	0.8986
5	2.518	1058.76	0.8724	20	2.489	1228.19	0.8295
6	2.539	1059.48	0.9773	21	2.463	1228.37	0.9162
7	2.522	1060.64	0.4421	22	2.484	1231.47	0.4812
8	2.538	1063.51	0.3889	23	2.478	1238.48	0.5269
9	2.532	1065.87	0.8706	24	2.480	1239.81	0.5780
10	2.538	1067.63	0.4371	25	2.491	1248.95	0.6084
11	2.545	1072.22	0.3668	26	3.754	1878.22	0.5085
12	2.548	1073.62	0.3781	27	3.768	1882.42	0.6060
13	2.542	1080.78	0.6464	28	3.778	1888.58	0.5318
14	2.552	1185.28	0.1253				
15	2.497	1093.22	0.1308				

Table of Multiplets

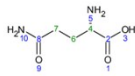
No.	Start	End	Type	J (Hz)	Align	Multiplet	ppm
1	2.525	2	m	-	6	M03	[2.502 - 2.538]
2	2.488	2	m	-	7	M02	[2.470 - 2.518]
3	3.766	1	t	6.18	4	M01	[3.748 - 3.810]

Table of Assignments

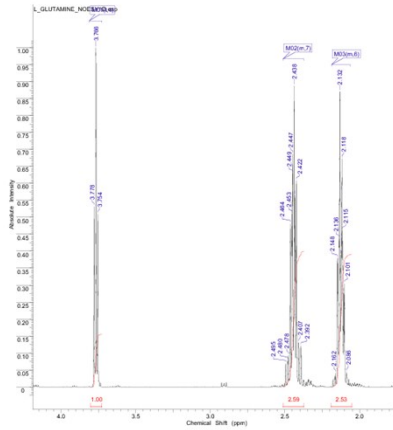
No.	Atom	Exp. Shift (ppm)	Multiplet
1	6	2.525	M03
2	7	2.488	M02
3	4	3.766	M01

2

L-Glutamine
 HMDB00641
¹H NMR Spectrum: 500MHz in H₂O
 Sample: 50 mM at pH 7.00
 Referenced to DSS



Zoomed ¹H NMR Spectrum



3

HMDB ID:HMDB00064

Compound name: Creatine

Spectrum type: ¹H NMR Spectrum

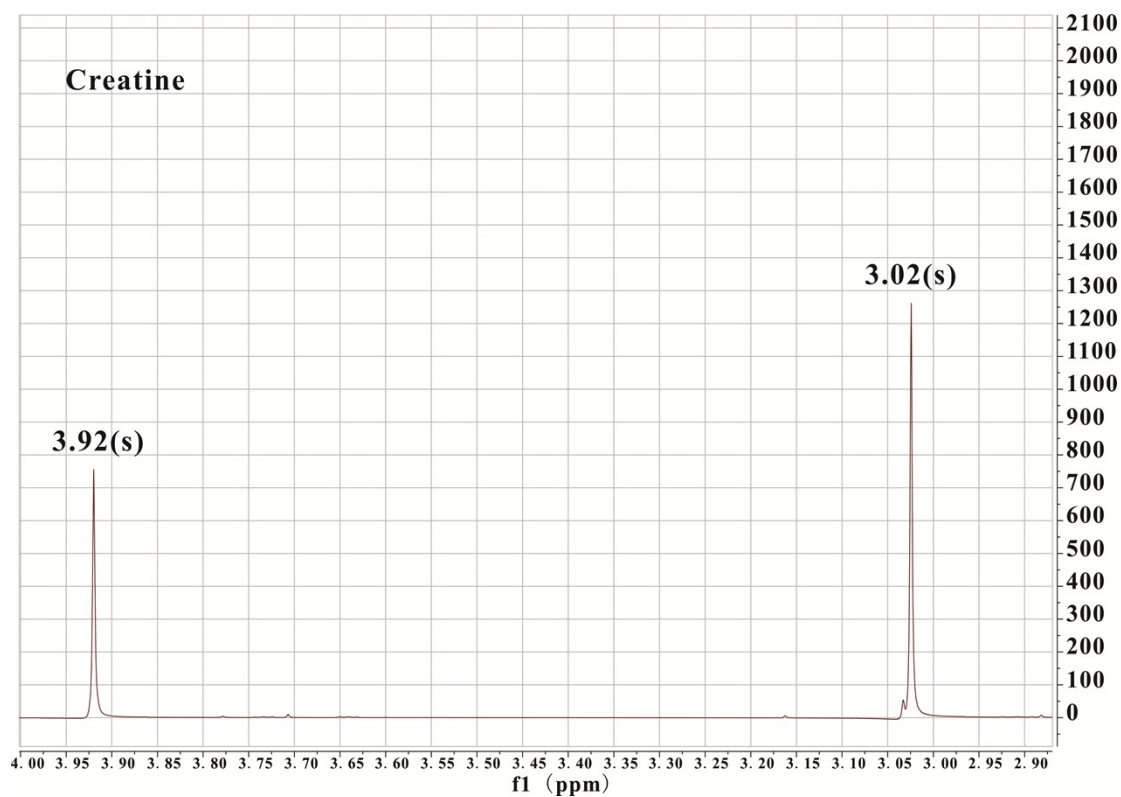


Table of Peaks

No.	(ppm)	(Hz)	Height
1	3.92	1959.2	0.5503
2	3.02	1511.7	1.0000

Table of Multiplets

No.	Shift1 (ppm)	H's	Type	Atom1	Multiplet1	(ppm)
1	3.92	32	s	4	M01	3.85 .. 3.94
2	3.02	58	s	6	M02	2.98 .. 3.07

Table of Assignments

No.	Atom	Exp. Shift (ppm)	Multiplet
1	4	3.92	M01
2	6	3.02	M02

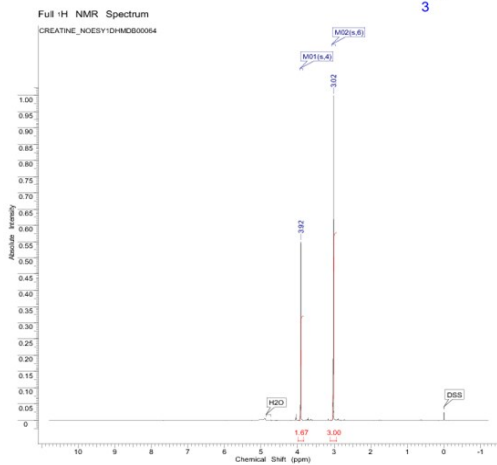
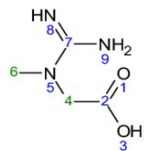
Spectra image with peak assignments

Creatine
HMDB00064

¹H NMR Spectrum : 500 MHz in H₂O

Sample : 50 mM at pH 7.0

Referenced to DSS



Creatine
HMDB00064

¹H NMR Spectrum : 500 MHz in H₂O

Sample : 50 mM at pH 7.0

Referenced to DSS

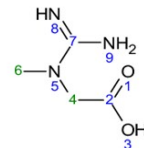


Table of Peaks

No.	Shift (ppm)	Integration	Height
1	3.92	1.67	0.5501
2	3.02	3.00	1.5000

Table of Multiplets

No.	Shift (ppm)	Integration	Type	Atom1	Multiplet1	Chemical Shift (ppm)
1	3.92	1.67	s	4	M01	[3.85 - 3.98]
2	3.02	3.00	s	6	M02	[2.98 - 3.07]

Table of Assignments

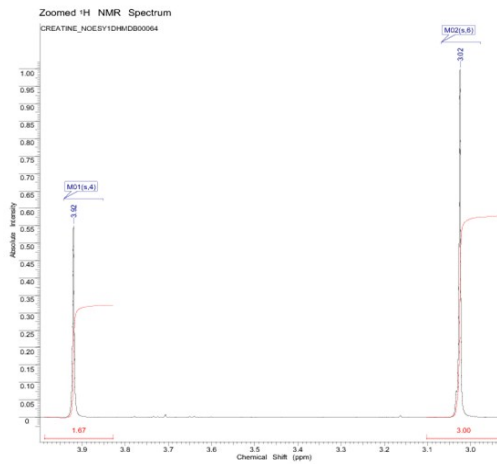
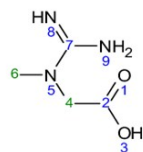
No.	Atom	Exp. Shift (ppm)	Multiplet
1	4	3.92	M01
2	6	3.02	M02

Creatine
HMDB00064

¹H NMR Spectrum : 500 MHz in H₂O

Sample : 50 mM at pH 7.0

Referenced to DSS



HMDB ID:HMDB00097

Compound name: Choline

Spectrum type: ¹H NMR Spectrum

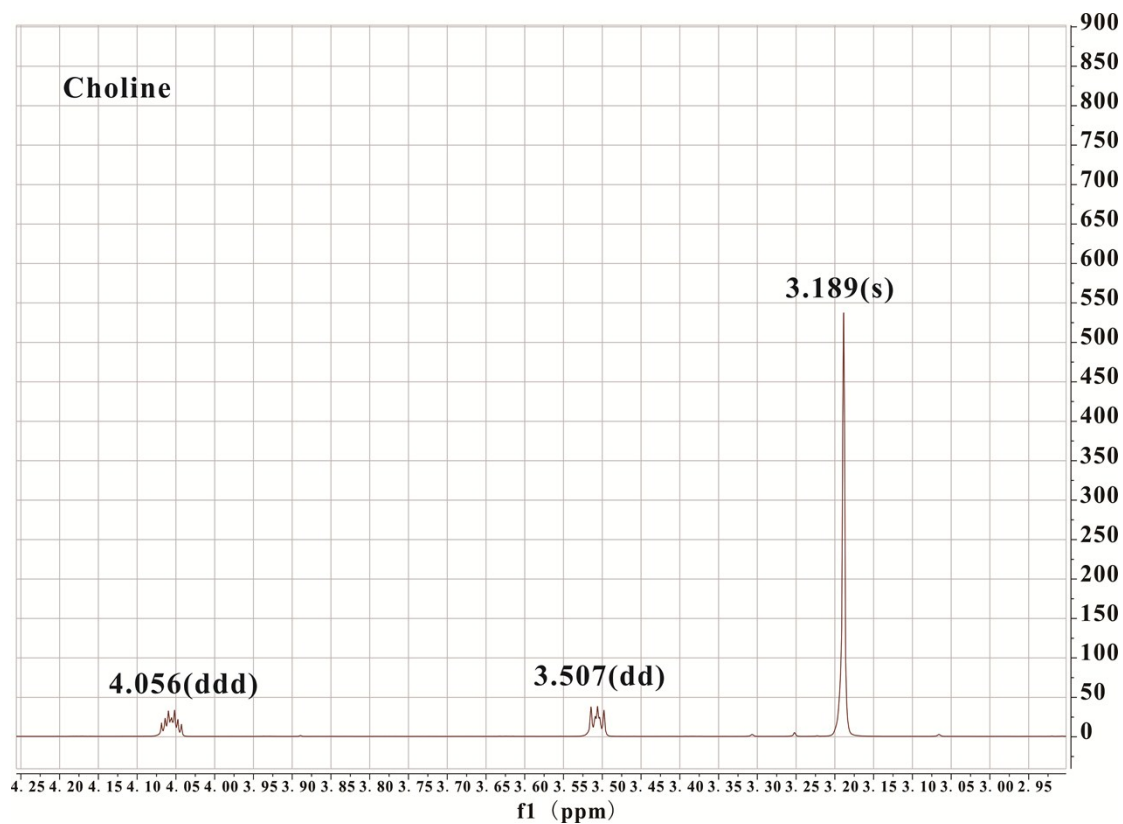


Table of Peaks

No.	(ppm)	(Hz)	Height
1	3.189	1912.4	1.0000
2	3.498	2097.7	0.0597
3	3.503	2101.0	0.2148
4	3.506	2102.7	0.0724
5	3.509	2104.4	0.0515
6	3.515	2107.7	0.0670
7	4.043	2424.6	0.0255
8	4.048	2427.5	0.0395
9	4.052	2430.0	0.0607
10	4.056	2432.4	0.0471
11	4.060	2434.8	0.0594
12	4.064	2437.2	0.0412
13	4.068	2440.0	

Table of Multiplets

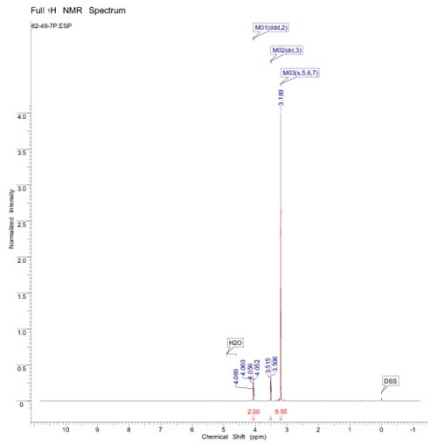
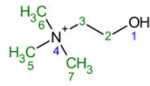
No.	Shift1 (ppm)	H's	Type	J (Hz)	Atom1	Multiplet1	(ppm)
1	3.189	66	s	-	6 6 7	M03	3.176 .. 3.205
2	3.507	14	dd	5.816 4.162	3	M02	3.492 .. 3.526
3	4.056	14	ddd	-	2	M01	4.034 .. 4.080

Table of Assignments

No.	Atom	Exp. Shift (ppm)	Multiplet
1	5	3.189	M03
2	6	3.189	M03
3	7	3.189	M03
4	3	3.507	M02
5	2	4.056	M01

Spectra image with peak assignments

Choline chloride
 HMDB00097
¹H NMR Spectrum: 600 MHz in H₂O
 Sample: 115 mM at pH 7.00
 Referenced to DSS



Choline chloride
 HMDB00097
¹H NMR Spectrum: 600 MHz in H₂O
 Sample: 115 mM at pH 7.00
 Referenced to DSS

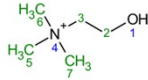


Table of Peaks

No.	(ppm)	(Hz)	Height
1	3.189	1912.4	4.0000
2	3.498	2097.8	0.2425
3	3.508	2102.8	0.2989
4	3.509	2104.4	0.2154
5	3.515	2107.9	0.2759
6	4.043	2424.7	0.1029
7	4.048	2427.6	0.1606
8	4.052	2430.1	0.2473
9	4.056	2432.4	0.1987
10	4.060	2434.8	0.2585
11	4.064	2437.2	0.1773
12	4.069	2440.0	0.1210

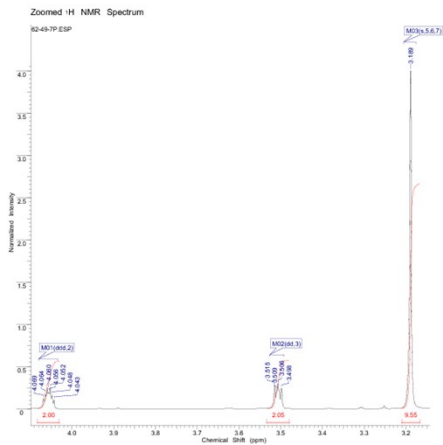
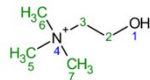
Table of Multiplets

No.	Shift (ppm)	F ₂	Type	J (Hz)	Atom1	Multiplet1	(ppm)
1	3.189	16	s	6, 6, 7	M02	(3.176 - 3.202)	
2	3.507	14	dd	8.816, 4.11	M02	(3.492 - 3.520)	
3	4.056	14	dd	-	M01	(4.034 - 4.083)	

Table of Assignments

No.	Atom	Exp. Shift (ppm)	Multiplet
1	5	3.189	M02
2	6	3.189	M02
3	7	3.189	M02
4	3	3.507	M02
5	2	4.056	M01

Choline chloride
 HMDB00097
¹H NMR Spectrum: 600 MHz in H₂O
 Sample: 115 mM at pH 7.00
 Referenced to DSS



HMDB ID:HMDB00925

Compound name: Trimethylamine N-oxide

Spectrum type: ¹H NMR Spectrum

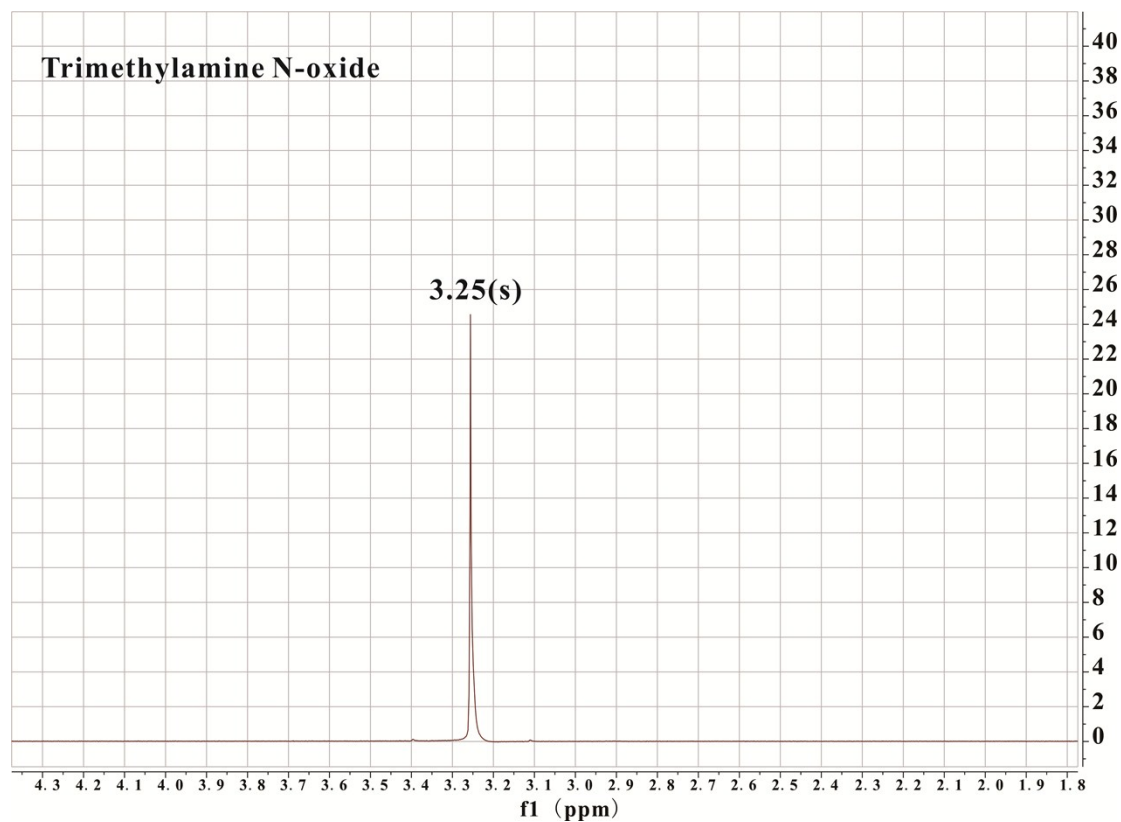


Table of Peaks

No.	(ppm)	(Hz)	Height
1	3.25	1626.5	1.0000

Table of Multiplets

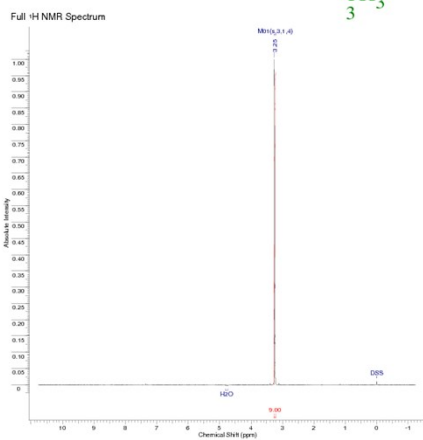
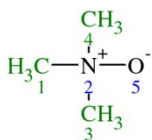
No.	Shift1 (ppm)	H's	Type	Atom1	Multiplet1	(ppm)
1	3.25	123	s	3 1 4	M01	3.22 .. 3.27

Table of Assignments

No.	Atom	Exp. Shift (ppm)	Multiplet
1	3	3.25	M01
2	1	3.25	M01
3	4	3.25	M01

Spectra image with peak assignments

Trimethylamine oxide
 HMDB00925
¹H NMR Spectrum: 500MHz in H₂O
 Sample: ~40mM in H₂O and pH 7.00
 Referenced to DSS



Trimethylamine oxide
 HMDB00925
¹H NMR Spectrum: 500MHz in H₂O
 Sample: ~40mM in H₂O and pH 7.00
 Referenced to DSS

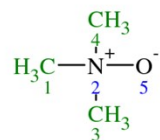


Table of Peaks

No.	ppm	Int.	Height
1	3.25	1426.5	1.0000

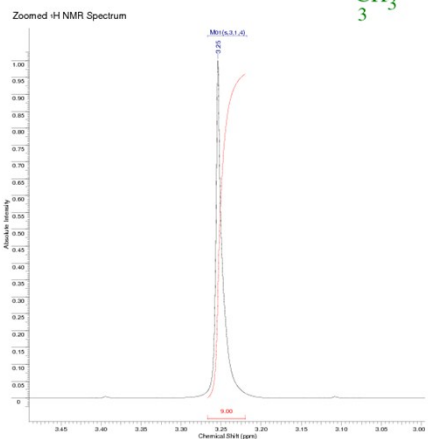
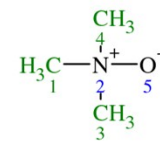
Table of Assignments

No.	Atom	Exp. Shift (ppm)	Multiplet
1	3	3.25	MR
2	1	3.25	MR
3	4	3.25	MR

Table of Multiplets

No.	Shift (ppm)	F ₂	Type	Atom	Multiplet	ppm
1	3.25	1.25	s	3, 1, 4	MR	[3.22 - 3.27]

Trimethylamine oxide
 HMDB00925
¹H NMR Spectrum: 500MHz in H₂O
 Sample: ~40mM in H₂O and pH 7.00
 Referenced to DSS



HMDB ID:HMDB00043

Compound name: Betaine

Spectrum type: ¹H NMR Spectrum

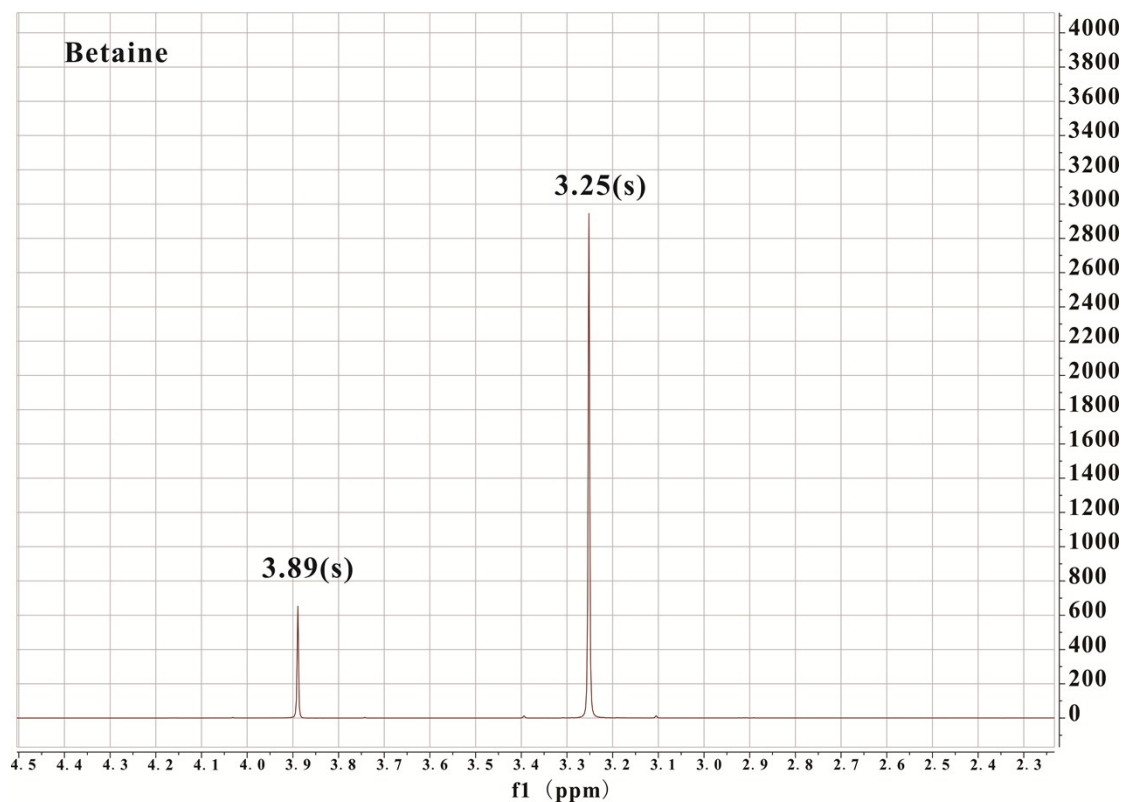


Table of Peaks

No.	(ppm)	(Hz)	Height
1	3.89	1943.8	0.1878
2	3.25	1625.3	1.0000

Table of Multiplets

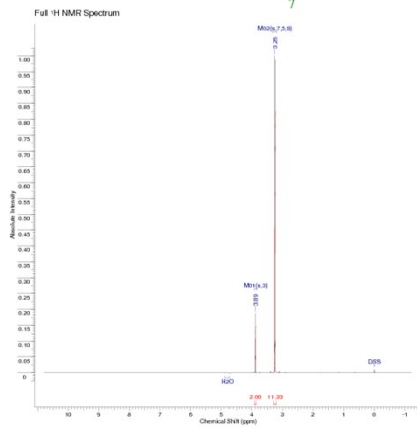
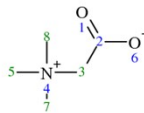
No.	Shift1 (ppm)	H's	Type	Atom1	Multiplet1	(ppm)
1	3.89	15	s	3	M01	3.84 .. 3.93
2	3.25	83	s	7 5 8	M02	3.19 .. 3.31

Table of Assignments

No.	Atom	Exp. Shift (ppm)	Multiplet
1	3	3.89	M01
2	5	3.25	M02
3	8	3.25	M02
4	7	3.25	M02

Spectra image with peak assignments

Betaine
 HMDB00043
¹H NMR Spectrum : 500 MHz in H₂O
 Sample : 50 mM at pH 7.0 in H₂O
 Referenced to DSS



Betaine
 HMDB00043
¹H NMR Spectrum : 500 MHz in H₂O
 Sample : 50 mM at pH 7.0 in H₂O
 Referenced to DSS

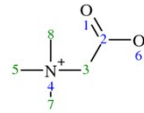


Table of Peaks

No.	Chemical Shift (ppm)	Integration	Height
1	3.25	2.00	0.1000
2	3.05	11.25	1.0000

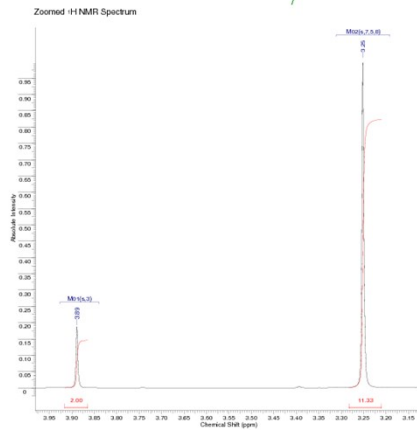
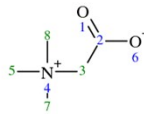
Table of Multiplets

No.	Chemical Shift (ppm)	Integration	Type	Atom	Multiplet	Height
1	3.25	2.00	s	3	triplet	0.1000
2	3.05	11.25	s	5, 6, 7	triplet	1.0000

Table of Assignments

No.	Atom	Chemical Shift (ppm)	Multiplet
1	3	3.25	triplet
2	5	3.05	triplet
3	6	3.05	triplet
4	7	3.05	triplet

Betaine
 HMDB00043
¹H NMR Spectrum : 500 MHz in H₂O
 Sample : 50 mM at pH 7.0 in H₂O
 Referenced to DSS



HMDB ID:HMDB00647

Compound name: L-Tyrosine

Spectrum type:1H NMR Spectrum

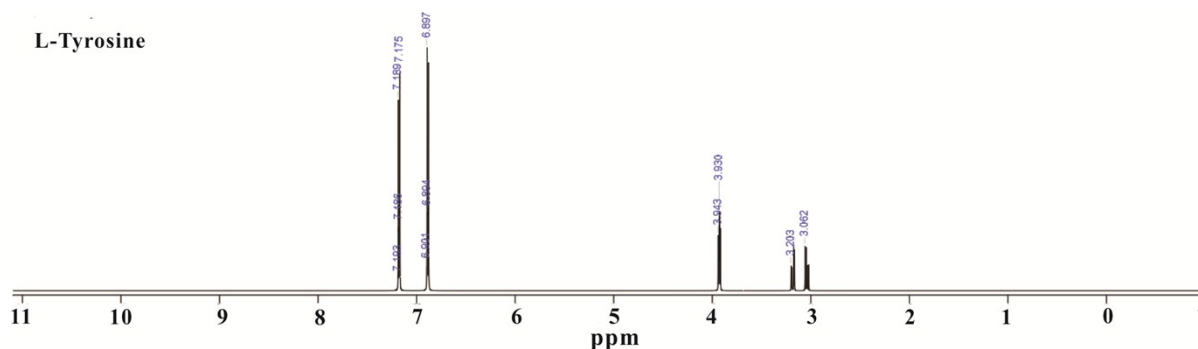


Table of Peaks

No.	(ppm)	Height	No.	(ppm)	Height
1	7.193	-0.0004	13	3.943	0.0077
2	7.189	0.0263	14	3.934	0.0096
3	7.186	0.0058	15	3.930	0.0106
4	7.178	0.0079	16	3.921	0.0087
5	7.175	0.0300	17	3.203	0.0035
6	7.170	0.0006	18	3.194	0.0033
7	6.901	0.0010	19	3.178	0.0064
8	6.897	0.0335	20	3.170	0.0057
9	6.894	0.0070	21	3.062	0.0063
10	6.886	0.0083	22	3.049	0.0061
11	6.883	0.0313	23	3.037	0.0036
12	6.877	0.0003	24	3.024	0.0037

Table of Multiplets

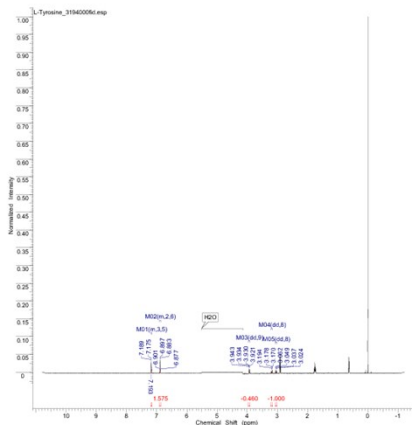
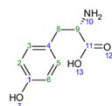
No.	Shift1 (ppm)	H's	Type	Atom1	Multiplet1	(ppm)
1	3.024	0	dd	8	M05	3.014 .. 3.072
2	3.170	0	dd	8	M04	3.161 .. 3.213
3	3.921	0	dd	9	M03	3.909 .. 3.954
4	6.877	2	m	2 6	M02	6.868 .. 6.909
5	7.710	2	m	3 5	M01	7.161 .. 7.201

Table of Assignments

No.	Atom	Exp. Shift (ppm)	Multiplet
1	8	3.024	M05
2	8	3.170	M04
3	9	3.921	M03
4	2	6.877	M02
5	6	6.877	M02
6	3	7.710	M01
7	5	7.710	M01

Spectra image with peak assignments

L-Tyrosine (HMDB00158)
 1H NMR spectrum: 600 MHz in H2O
 Sample: 2 mM at pH 7.0
 Referenced to DSS



L-Tyrosine (HMDB00158)
 1H NMR spectrum: 600 MHz in H2O
 Sample: 2 mM at pH 7.0
 Referenced to DSS

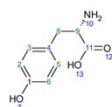


Table of Peaks

No.	(ppm)	Height
1	7.153	0.0004
2	7.189	0.0003
3	7.186	0.0004
4	7.178	0.0009
5	7.178	0.0005
6	7.170	0.0006
7	6.901	0.0010
8	6.887	0.0016
9	6.884	0.0010
10	6.880	0.0003
11	6.883	0.0013
12	6.877	0.0003
13	3.943	0.0027
14	3.934	0.0006
15	3.930	0.0106
16	3.921	0.0007
17	3.203	0.0035
18	3.194	0.0033
19	3.178	0.0004
20	3.170	0.0007
21	3.042	0.0063
22	3.048	0.0011
23	3.037	0.0038
24	3.024	0.0037

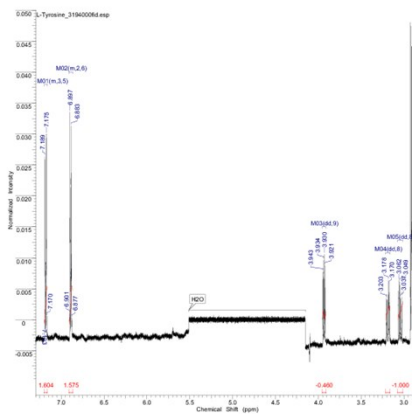
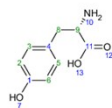
Table of Multiplets

No.	Start (ppm)	End (ppm)	Type	Assign1	Multiplet	(ppm)
1	3.024	0	qd	a	M05	(3.024 - 3.072)
2	3.170	0	qd	b	M04	(3.170 - 3.218)
3	3.192	0	qd	b	M03	(3.192 - 3.240)
4	6.877	2	m	c, d, e	M02	(6.877 - 6.901)
5	7.170	2	m	c, d, e	M01	(7.170 - 7.201)

Table of Assignments

No.	Atom	Exp. Shift (ppm)	Multiplet
1	O	3.024	M05
2	O	3.170	M04
3	O	3.192	M03
4	O	6.877	M02
5	O	6.877	M02
6	O	7.170	M01
7	O	7.170	M01

L-Tyrosine (HMDB00158)
 1H NMR spectrum: 600 MHz in H2O
 Sample: 2 mM at pH 7.0
 Referenced to DSS



HMDB ID:HMDB00094

Compound name: Citric acid

Spectrum type: ^1H NMR Spectrum

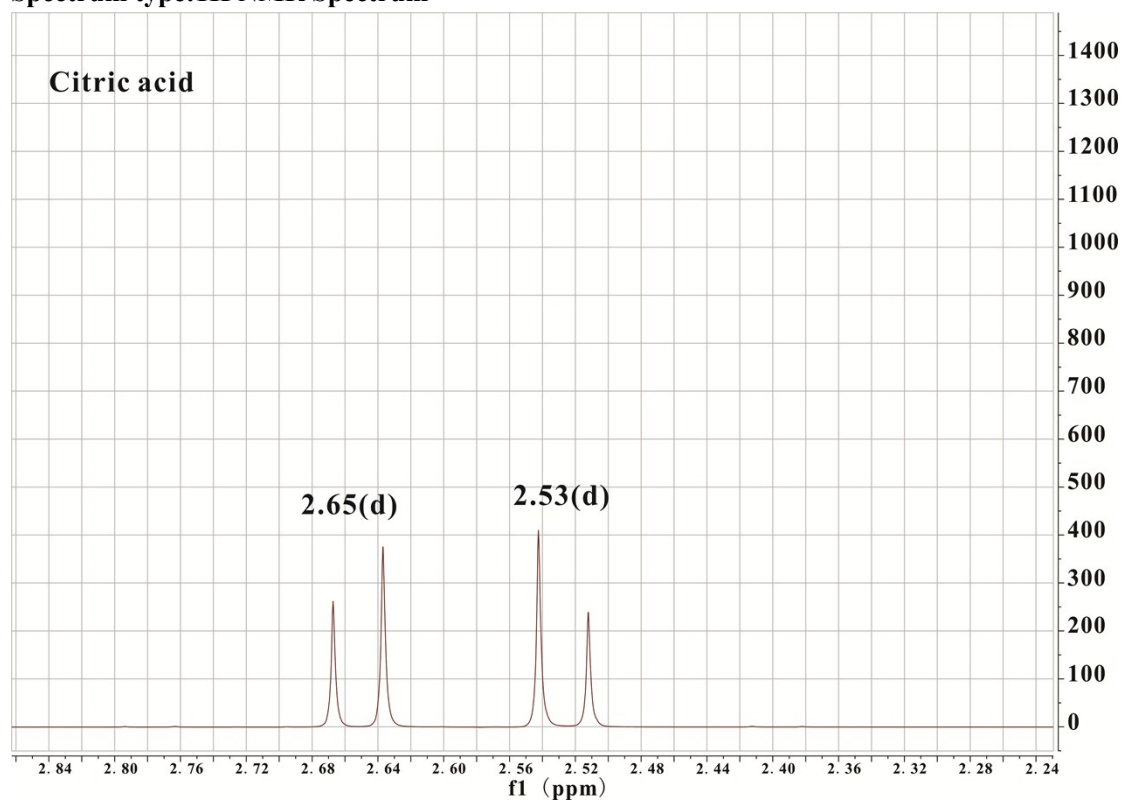


Table of Peaks

No.	(ppm)	(Hz)	Height
1	2.67	1333.2	0.6328
2	2.64	1318.1	0.9238
3	2.54	1270.8	1.0000
4	2.51	1255.7	0.5785

Table of Multiplets

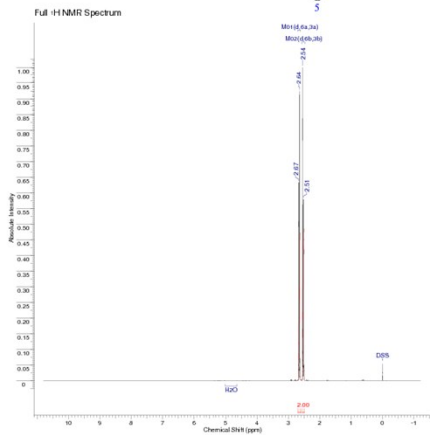
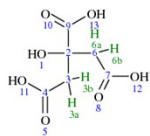
No.	Shift1 (ppm)	H' s	Type	J (Hz)	Atom1	Multiplet1	(ppm)
1	2.65	48	d	15.16	6a 3a	M01	2.61 .. 2.70
2	2.53	49	d	-	6b 3b	M02	2.48 .. 2.57

Table of Assignments

No.	Atom	Exp. Shift (ppm)	Multiplet
1	3a	2.65	M01
2	6a	2.65	M01
3	3b	2.53	M02
4	6b	2.53	M02

Spectra image with peak assignments

Citric acid
 HMDB00094
¹H NMR Spectrum : 500 MHz in H₂O
 Sample : 50 mM at pH 7.0 in H₂O
 Referenced to DSS



Citric acid
 HMDB00094
¹H NMR Spectrum : 500 MHz in H₂O
 Sample : 50 mM at pH 7.0 in H₂O
 Referenced to DSS

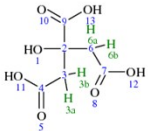


Table of Peaks

No.	Chem. Shift (ppm)	Integration	Multiplet
1	2.67	1.0000	t
2	2.54	1.0000	t
3	2.34	1.0000	t
4	2.21	0.5000	t

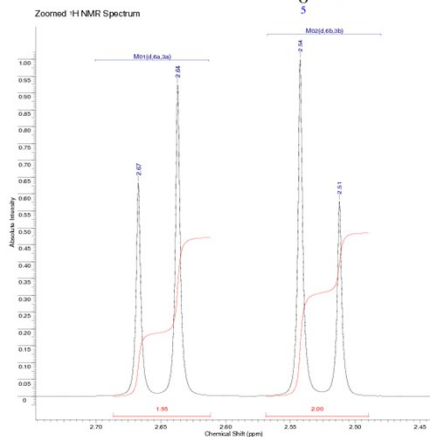
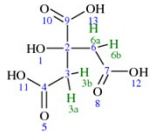
Table of Multiplets

No.	Chem. Shift (ppm)	Integration	Type	J (Hz)	Abundance	Multiplet	Chem. Shift (ppm)
1	2.65	1.00	d	15.10	6h, 3a	Triplet	(2.61, 2.70)
2	2.53	1.00	d	6h, 3a	Triplet	(2.49, 2.57)	

Table of Assignments

No.	Atom	Exp. Shift (ppm)	Multiplet
1	6a	2.65	Triplet
2	6b	2.53	Triplet
3	3a	2.34	Triplet
4	3b	2.21	Triplet

Citric acid
 HMDB00094
¹H NMR Spectrum : 500 MHz in H₂O
 Sample : 50 mM at pH 7.0 in H₂O
 Referenced to DSS



HMDB ID:HMDB00131

Compound name: Glycerol

Spectrum type: ¹H NMR Spectrum

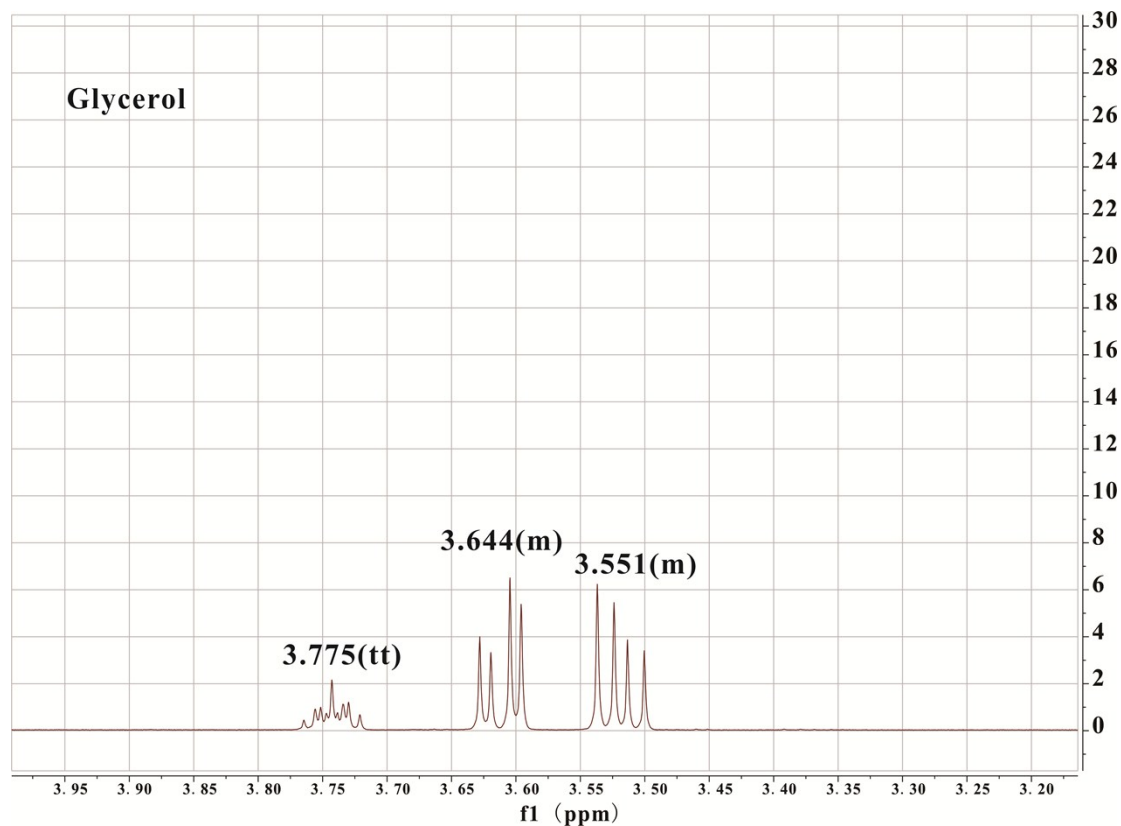


Table of Peaks

No.	(ppm)	(Hz)	Height
1	3.532	1765.6	2.1117
2	3.545	1772.1	2.3961
3	3.556	1777.3	3.4290
4	3.569	1783.9	3.8592
5	3.628	1813.4	3.4374
6	3.637	1817.7	4.0000
7	3.651	1825.1	2.1062
8	3.660	1825.9	2.4318
9	3.753	1875.9	0.4347
10	3.762	1880.3	0.8238
11	3.766	1882.4	0.8279
12	3.771	1884.7	0.6044
13	3.775	1886.8	1.3931
14	3.779	1888.9	0.5713
15	3.784	1891.1	0.6860
16	3.788	1893.2	0.6303
17	3.797	1897.6	0.2718

Table of Multiplets

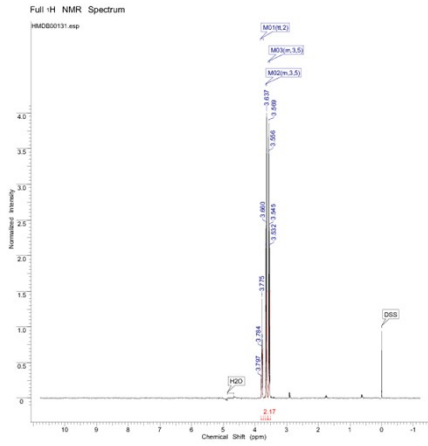
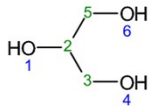
No.	Shift1 (ppm)	H's	Type	J (Hz)	Atom1	Multiplet1	(ppm)
1	3.551	37	m	-	3 5	M03	3.525 .. 3.577
2	3.644	38	m	-	3 5	M02	3.618 .. 3.670
3	3.775	18	tt	6.463 4.404	2	M01	3.720 .. 3.821

Table of Assignments

No.	Atom	Exp. Shift (ppm)	Multiplet
1	3	3.551	M03
2	5	3.551	M03
3	3	3.644	M02
4	5	3.644	M02
5	2	3.775	M01

Spectra image with peak assignments

Glycerol
HMDB00131
¹H NMR Spectrum: 500 MHz in H2O
Sample: 90 mM at pH 7.0
Referenced to DSS



Glycerol
HMDB00131
¹H NMR Spectrum: 500 MHz in H2O
Sample: 90 mM at pH 7.0
Referenced to DSS

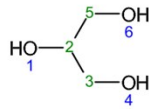


Table of Peaks

No.	ppm	Integration	Height
1	3.552	1.000	2.117
2	3.545	1.772	2.391
3	3.556	1.773	3.650
4	3.569	1.783	3.632
5	3.628	1.814	2.434
6	3.637	1.817	4.000
7	3.651	1.825	2.192
8	3.660	1.829	2.419
9	3.753	1.975	0.4347
10	3.762	1.983	0.628
11	3.789	1.982	0.6279
12	3.771	1.987	0.634
13	3.775	1.988	1.991
14	3.779	1.989	0.513
15	3.784	1.991	0.6880
16	3.788	1.992	0.630
17	3.797	1.997	0.2718

Table of Multiplets

No.	Start	End	Type	J (Hz)	AbsInt	Multiplet	ppm
1	3.551	3.7	m	-	3.5	M3	[3.529-3.577]
2	3.644	3.8	m	-	3.5	M2	[3.618-3.676]
3	3.775	3.8	d	6.465, 4.4	2	M1	[3.720-3.821]

Table of Assignments

No.	Atom	Exp. Shift (ppm)	Multiplet
1	1	3.551	M3
2	5	3.551	M3
3	3	3.644	M2
4	5	3.644	M2
5	2	3.775	M1

Glycerol
HMDB00131
¹H NMR Spectrum: 500 MHz in H2O
Sample: 90 mM at pH 7.0
Referenced to DSS

