Electronic Supplementary Material (ESI) for RSC Advances.

HMDB ID:HMDB00190

Compound name: L-Lactic acid

Spectrum type:1H NMR Spectrum

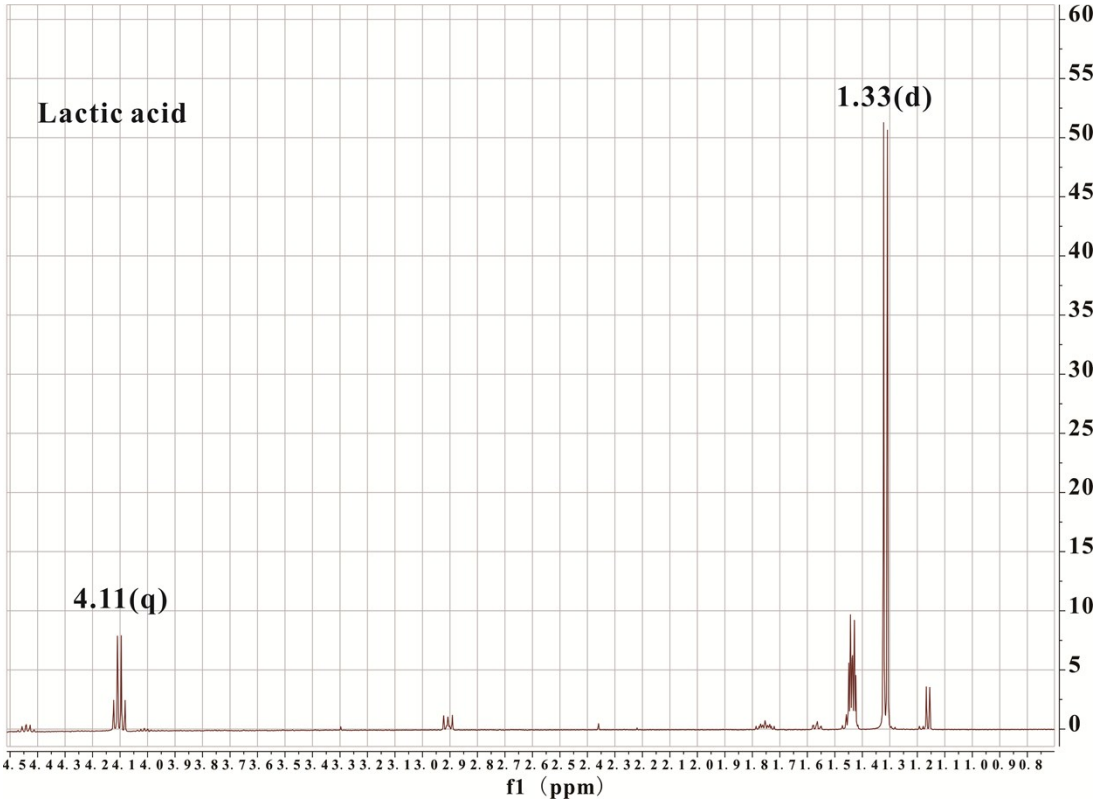


Table of Peaks

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

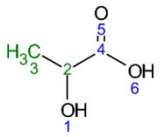
Lactic acid

HMDB00190

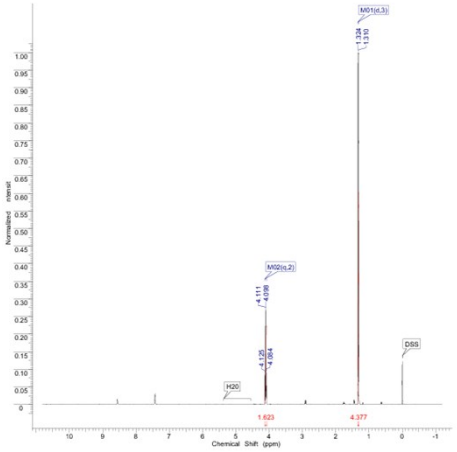
^{1}H NMR Spectrum: 500 Mhz D$_2$O n H

Sample: 50 mM at pH 7.0

Referenced to DSS



Full ^{1}H NMR spectrum



Lactic acid

HMDB00190

^{1}H NMR Spectrum: 500 Mhz D$_2$O n H

Sample: 50 mM at pH 7.0

Referenced to DSS

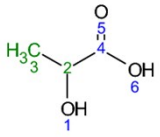


Table of Peaks

No.	(ppm)	Height
1	1.310	0.9981
2	1.324	1.0000
3	4.084	0.0903
4	4.098	0.2701
5	4.111	0.2953
6	4.125	0.0860

Table of Multiplets

No.	Shift1 (ppm)	H's	Type	J (Hz)	Atom1	Connected A	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, 6.9	2	7, 3	M02	7, M01	[4.08 - 4.13]

Table of Assignments

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

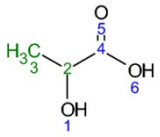
Lactic acid

HMDB00190

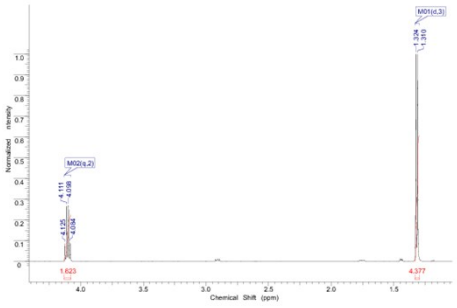
^{1}H NMR Spectrum: 500 Mhz D$_2$O n H

Sample: 50 mM at pH 7.0

Referenced to DSS



Zoomed ^{1}H NMR spectrum



HMDB ID:HMDB00883
Compound name:L-Valine
Spectrum type:1H NMR Spectrum

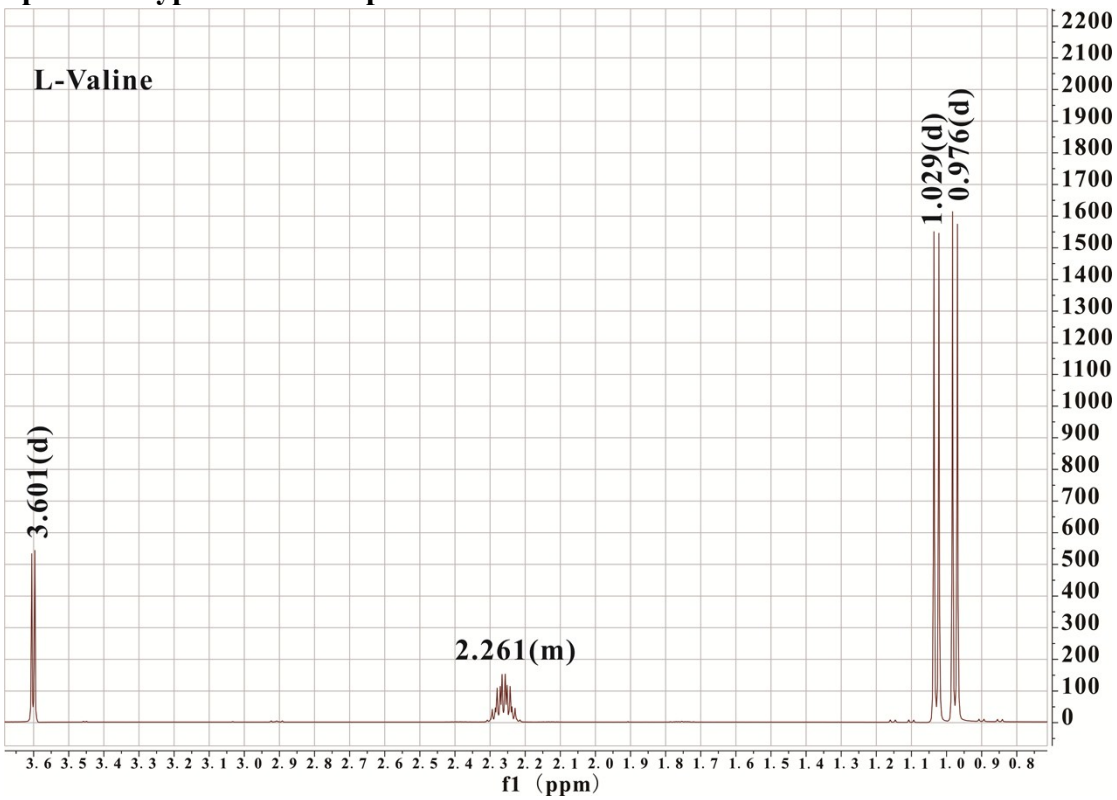


Table of Peaks

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

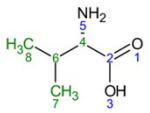
L-Valine

HMDB00883

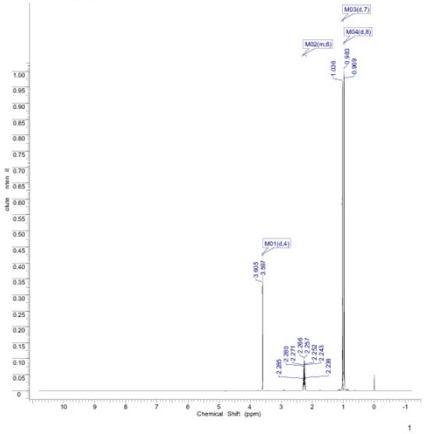
^{1}H NMR Spectrum: 500 MHz in H_2O

Sample: 50 mM at pH 7.0

Referenced to DSS



Full ^{1}H NMR Spectrum



L-Valine

HMDB00883

^{1}H NMR Spectrum: 500 MHz in H_2O

Sample: 50 mM at pH 7.0

Referenced to DSS

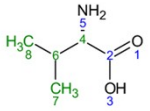


Table of Peaks

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	0.0276
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	0.0841
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	0.0260
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.	Shift (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	18.03, 7.01, 4.	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	0.976	M04
2	7	1.029	M03
3	6	2.261	M02
4	4	3.601	M01

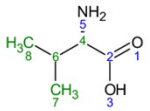
L-Valine

HMDB00883

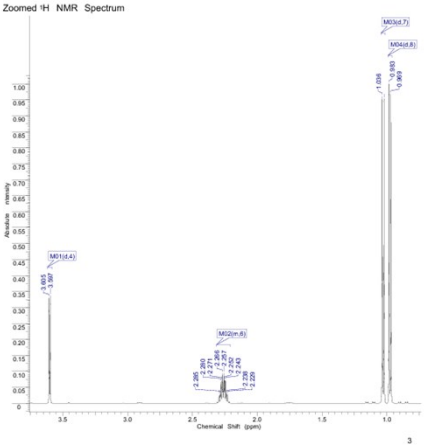
^{1}H NMR Spectrum: 500 MHz in H_2O

Sample: 50 mM at pH 7.0

Referenced to DSS



Zoomed ^{1}H NMR Spectrum



HMDB ID:HMDB00161

Compound name: L-Alanine

Spectrum type:1H NMR Spectrum

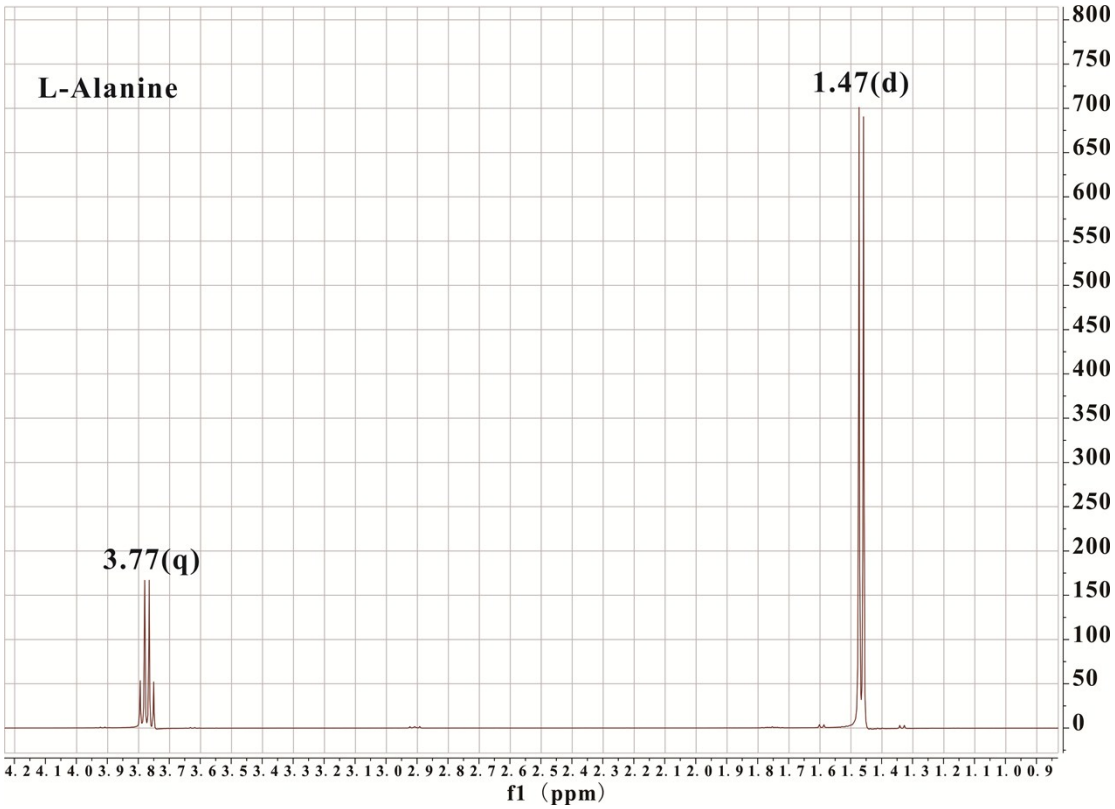


Table of Peaks

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

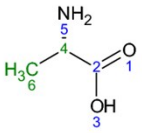
L-Alanine

HMDB00161

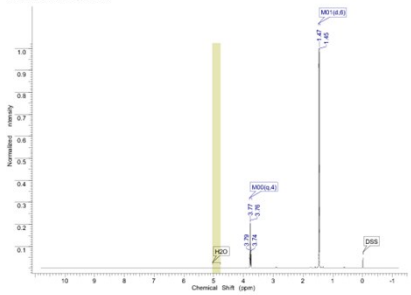
^{1}H NMR spectrum: 500 MHz in H_2O

Sample: 50 mM at pH 7.0

Referenced to DSS



Full ^{1}H NMR Spectrum



L-Alanine

HMDB00161

^{1}H NMR spectrum: 500 MHz in H_2O

Sample: 50 mM at pH 7.0

Referenced to DSS

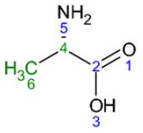


Table of Peaks

No.	(ppm)	(Hz)	Height
1	3.79	1892.8	0.0673
2	3.77	1885.4	0.2067
3	3.76	1878.1	0.2040
4	3.74	1871.0	0.0663
5	1.47	732.5	1.0000
6	1.45	725.3	0.9852

Table of Multiplets

No.	Shift1 (ppm)	H's	Type	J (Hz)	Atom1	Multiplet1	(ppm)
1	1.46	3	d	7.14	6	M01	[1.43 ... 1.49]
2	3.76	1	q	7.20	4	M00	[3.72 ... 3.80]

Table of Assignments

No.	Atom	Exp. Shift (ppm)	Multiplet
1	6	1.46	M01
2	4	3.76	M00

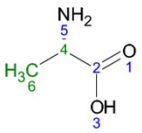
L-Alanine

HMDB00161

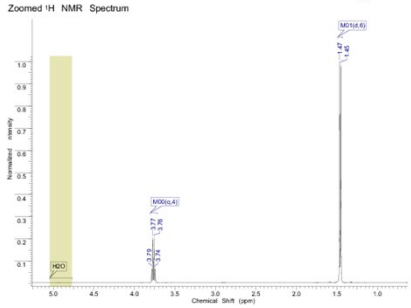
^{1}H NMR spectrum: 500 MHz in H_2O

Sample: 50 mM at pH 7.0

Referenced to DSS



Zoomed ^{1}H NMR Spectrum



HMDB ID:HMDB00042

Compound name: Acetic acid

Spectrum type:1H NMR Spectrum

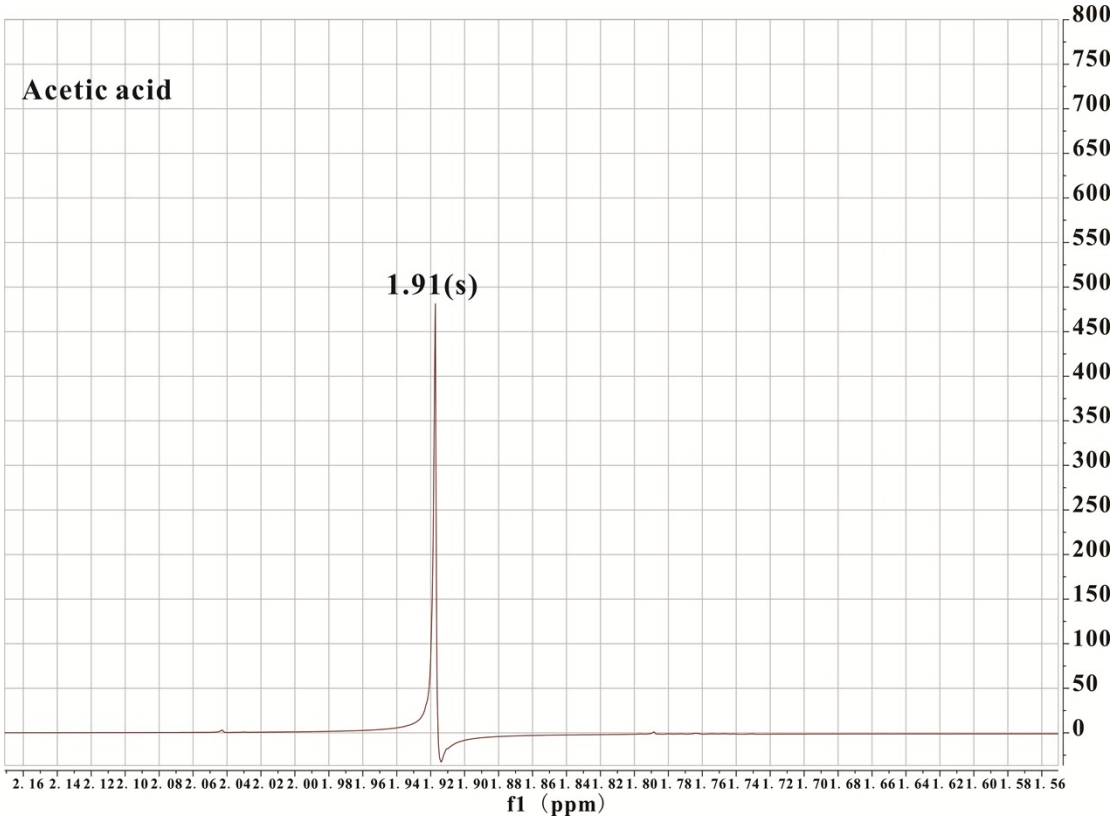


Table of Peaks

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

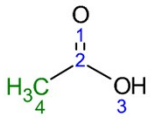
Acetic acid

HMDB00042

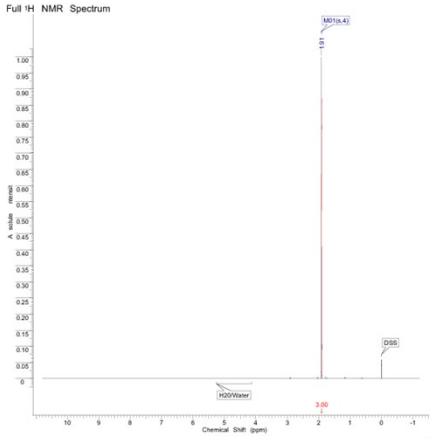
^{1}H NMR spectrum: 500 MHz in H_2O

Sample: 23 mM at pH 7.0

Referenced to DSS



Full ^{1}H NMR Spectrum



Acetic acid

HMDB00042

^{1}H NMR spectrum: 500 MHz in H_2O

Sample: 23 mM at pH 7.0

Referenced to DSS

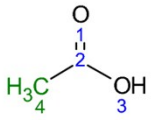


Table of Peaks

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

Table of Multiplets

No.	Shift (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

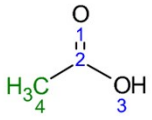
Acetic acid

HMDB00042

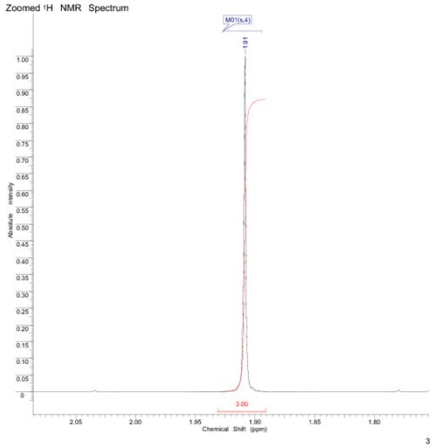
^{1}H NMR spectrum: 500 MHz in H_2O

Sample: 23 mM at pH 7.0

Referenced to DSS



Zoomed ^{1}H NMR Spectrum



HMDB ID:HMDB00696

Compound name: L-Methionine

Spectrum type:1H NMR Spectrum

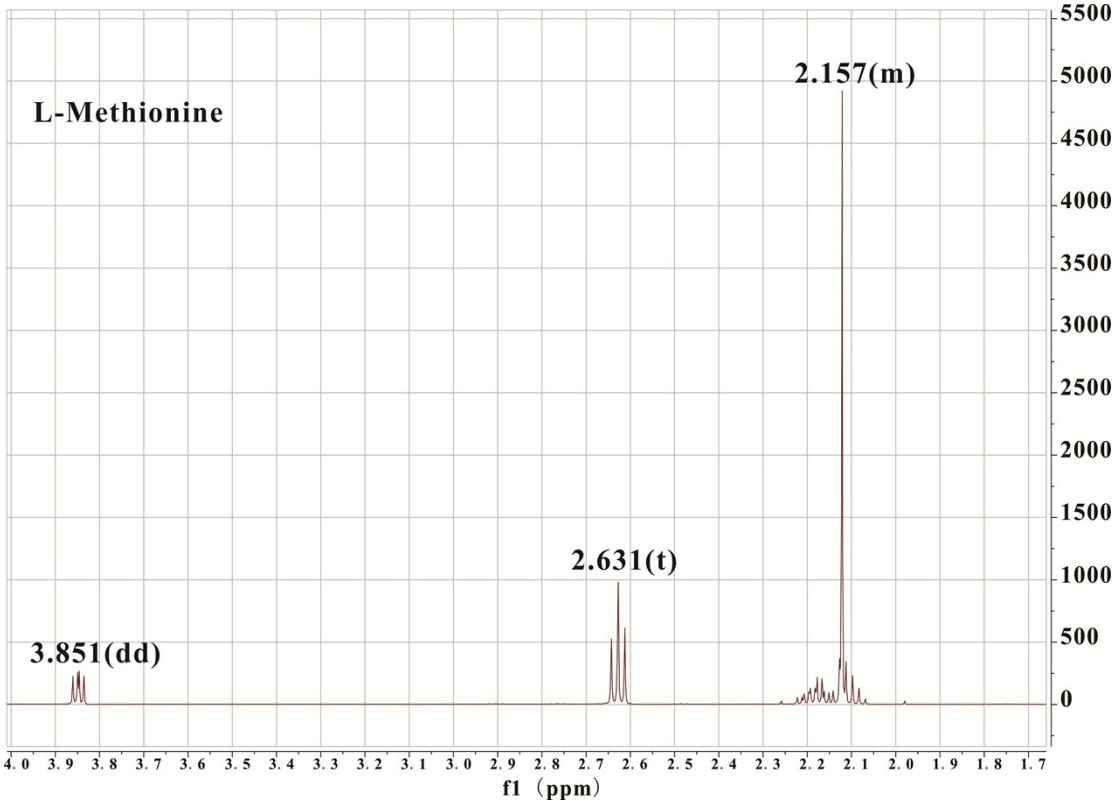


Table of Peaks

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

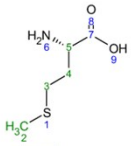
L-Methionine

HMDB00696

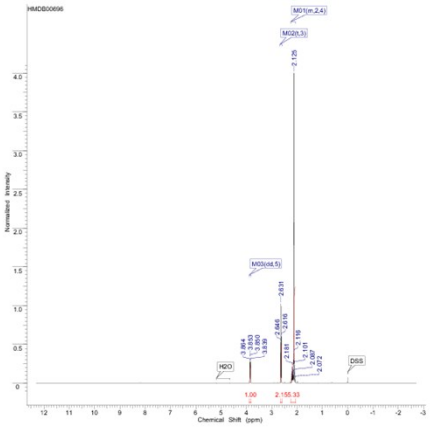
^{1}H NMR Spectrum: 500 MHz in H2O

Sample: 50 mM at pH 7.0

Referenced to DSS



Full ^{1}H NMR Spectrum



L-Methionine

HMDB00696

^{1}H NMR Spectrum: 500 MHz in H2O

Sample: 50 mM at pH 7.0

Referenced to DSS

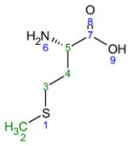


Table of Peaks

No.	(ppm)	(Hz)	Height
1	2.072	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
18	2.646	1322.7	0.5276
19	3.839	1918.7	0.2772
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	M01
2	4	2.157	M01
3	3	2.631	M02
4	5	3.851	M03

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	dd	7.100, 5.3(	5	M03	[3.818 ... 3.868]

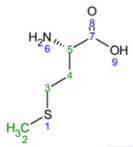
L-Methionine

HMDB00696

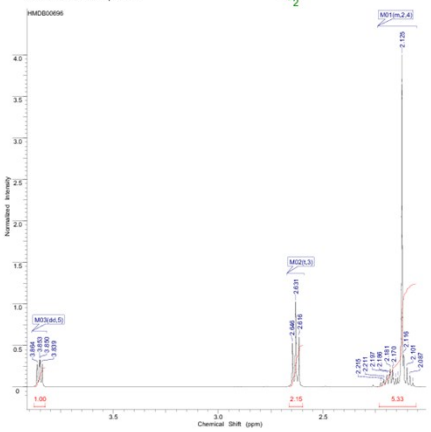
^{1}H NMR Spectrum: 500 MHz in H2O

Sample: 50 mM at pH 7.0

Referenced to DSS



Zoomed ^{1}H NMR Spectrum



HMDB ID:HMDB00357

Compound name: 3-Hydroxybutyric acid

Spectrum type:1H NMR Spectrum

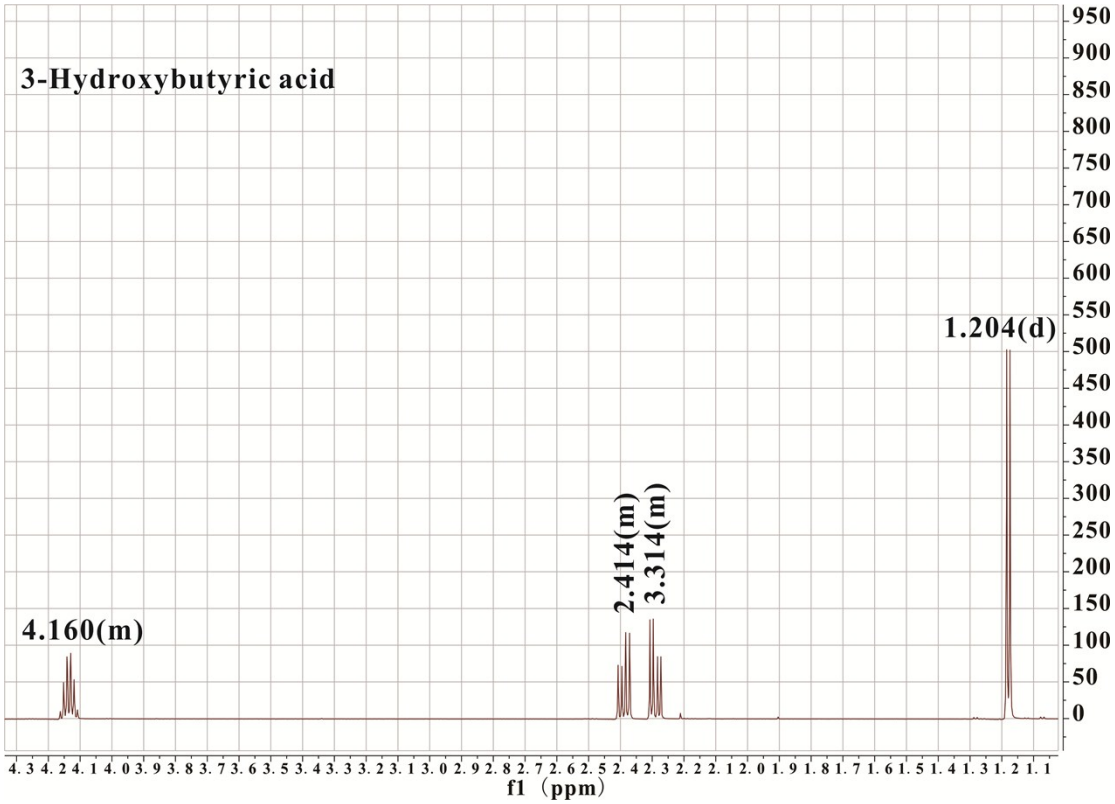


Table of Peaks

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

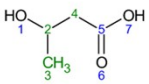
3-Hydroxybutyric acid

HMDB00357

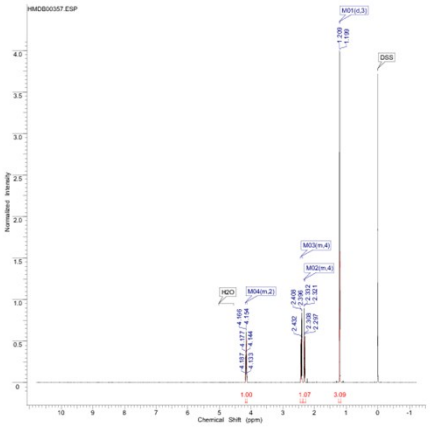
^{1}H NMR Spectrum: 500 MHz in H2O

Sample: 50 mM AT pH 7.0

Referenced to DSS



Full ^{1}H NMR Spectrum



3-Hydroxybutyric acid

HMDB00357

^{1}H NMR Spectrum: 500 MHz in H2O

Sample: 50 mM AT pH 7.0

Referenced to DSS

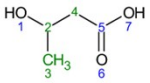


Table of Peaks

No.	(ppm)	(Hz)	Height
1	1.199	718.5	3.9858
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	0.8360
8	2.408	1443.3	0.8469
9	2.420	1450.4	0.5232
10	2.432	1457.7	0.5263
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.	Shift (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

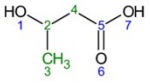
3-Hydroxybutyric acid

HMDB00357

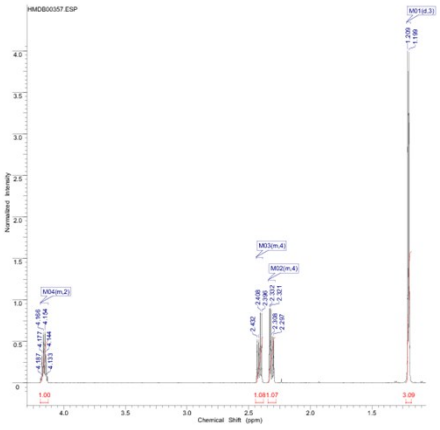
^{1}H NMR Spectrum: 500 MHz in H2O

Sample: 50 mM AT pH 7.0

Referenced to DSS



Zoomed ^{1}H NMR Spectrum



HMDB ID:HMDB00254

Compound name:Succinic acid

Spectrum type:1H NMR Spectrum

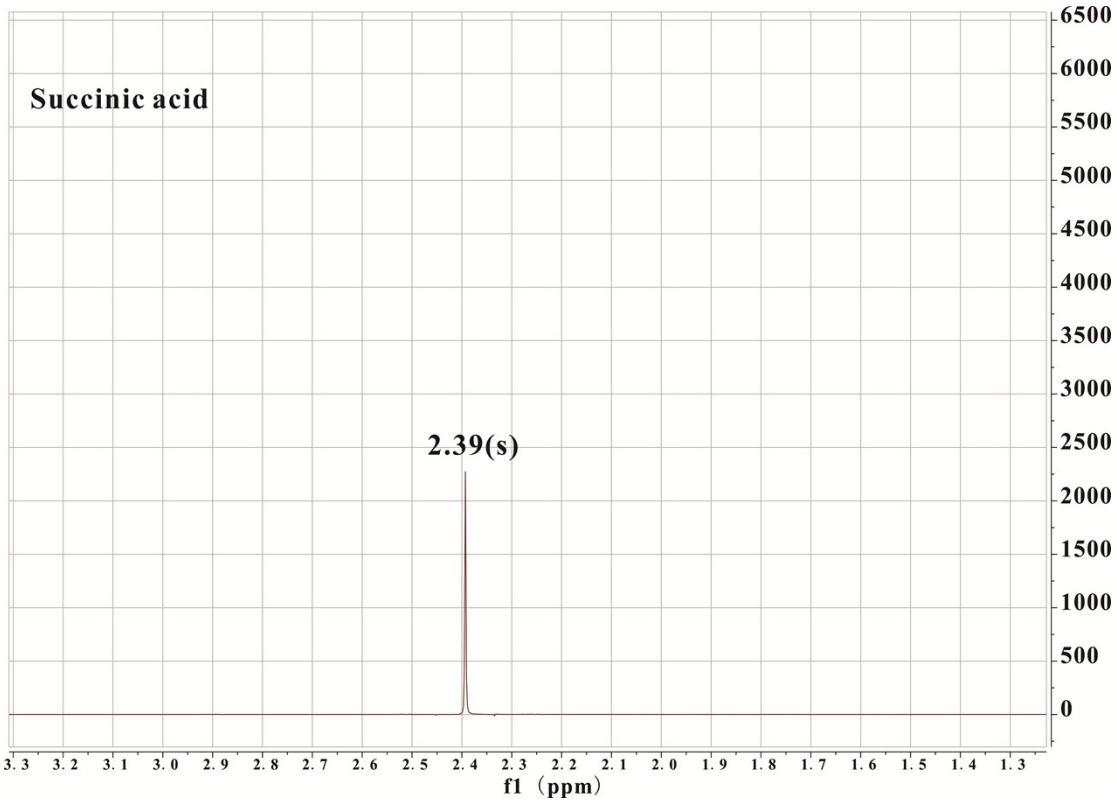


Table of Peaks

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

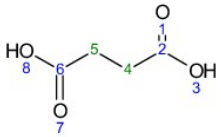
Succinic acid

HMDB00254

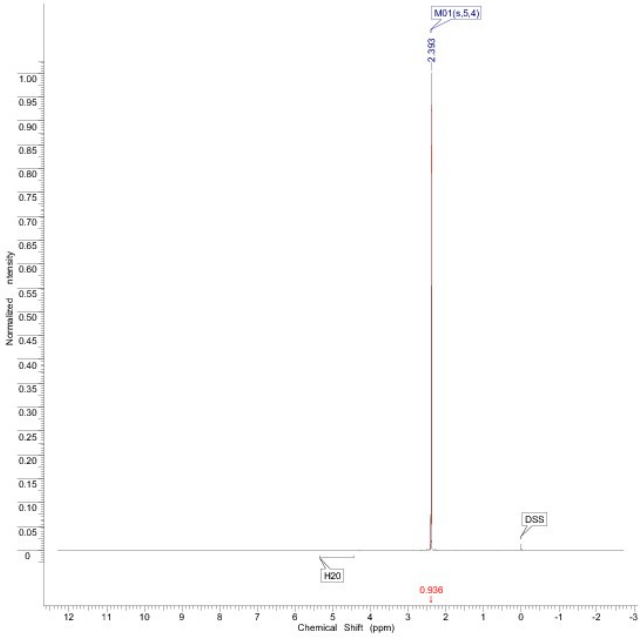
^{1}H NMR spectrum: 500 MHz D_2O in H

Sample: 50mM at pH 7.0

Referenced to DSS



Full ^{1}H NMR spectrum



Succinic acid

HMDB00254

^{1}H NMR spectrum: 500 MHz D_2O in H

Sample: 50mM at pH 7.0

Referenced to DSS

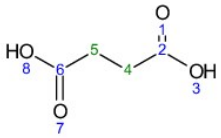


Table of Peaks

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

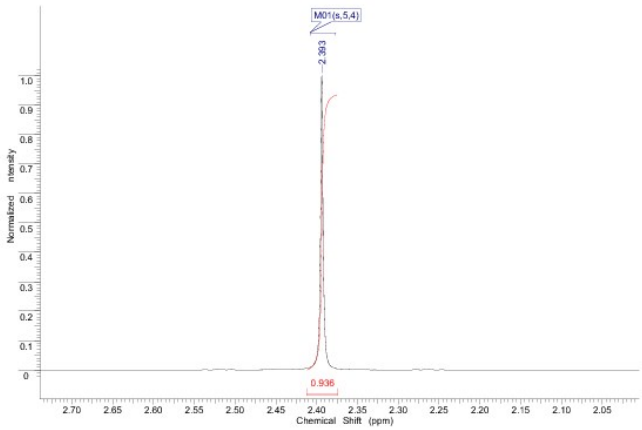
Table of Multiplets

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 ^{1}H NMR spectrum



HMDB ID:HMDB00641

Compound name: L-Glutamine

Spectrum type:1H NMR Spectrum

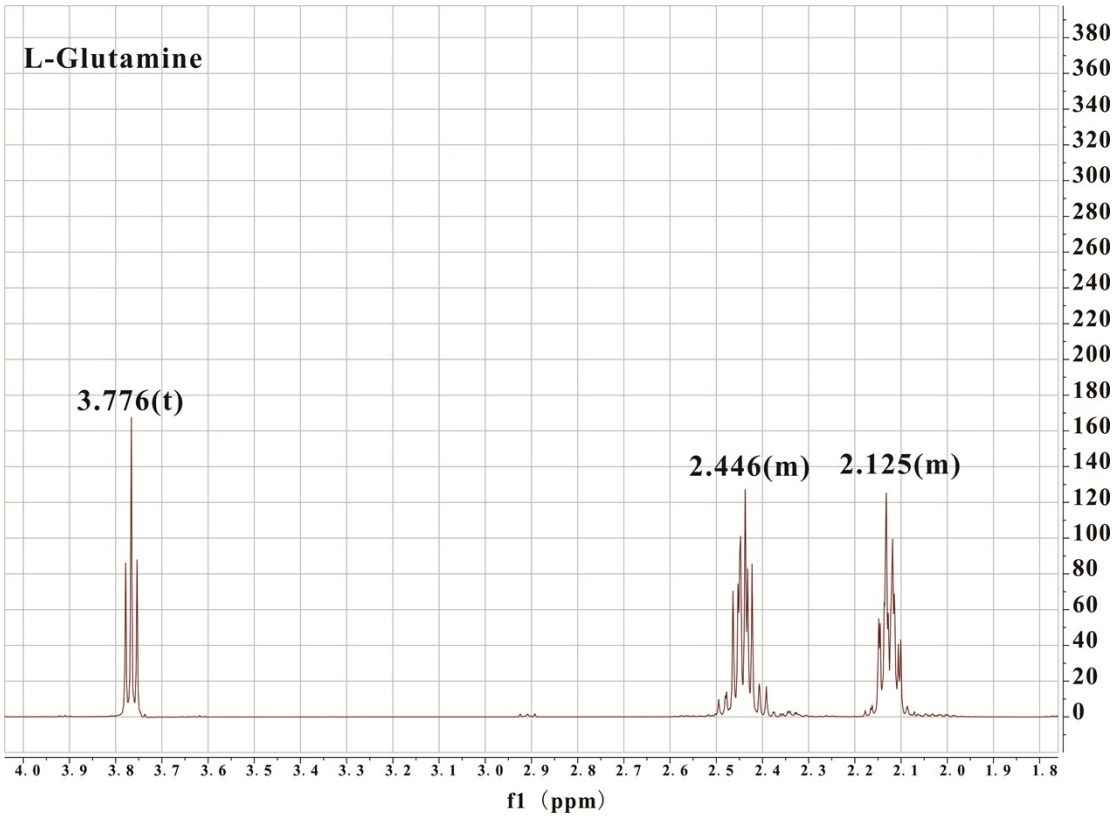


Table of Peaks

No.	(ppm)	(Hz)	Height
1	2.086	1042.87	0.0438
2	2.101	1049.97	0.3039
3	2.106	1052.58	0.2769
4	2.115	1057.07	0.4611
5	2.118	1058.76	0.6724
6	2.120	1059.49	0.5773
7	2.122	1060.64	0.4401
8	2.128	1063.52	0.3889
9	2.132	1065.67	0.8706
10	2.136	1067.83	0.4371
11	2.145	1072.22	0.3668
12	2.148	1073.82	0.3791
13	2.162	1080.78	0.0404
14	2.392	1195.39	0.1213

No.	(ppm)	(Hz)	Height
15	2.407	1203.22	0.1308
16	2.422	1210.82	0.6081
17	2.432	1215.58	0.5646
18	2.438	1218.38	0.8876
19	2.447	1223.18	0.6860
20	2.449	1224.19	0.6285
21	2.453	1226.07	0.5102
22	2.464	1231.47	0.4812
23	2.478	1238.48	0.0929
24	2.480	1239.81	0.0780
25	2.495	1246.95	0.0684
26	3.754	1876.22	0.5095
27	3.766	1882.40	1.0000
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

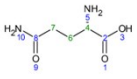
L-Glutamine

HMDB00641

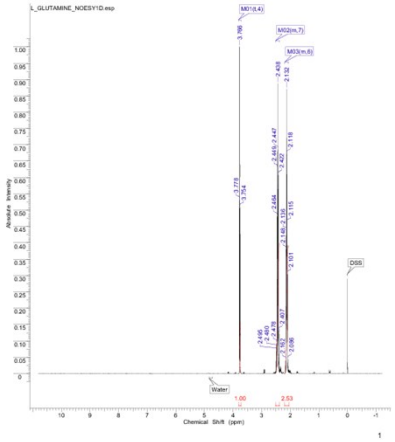
^{1}H NMR Spectrum: 500MHz in H_2O

Sample: 50 mM at pH 7.00

Referenced to DSS



Full ^{1}H NMR Spectrum



L-Glutamine

HMDB00641

^{1}H NMR Spectrum: 500MHz in H_2O

Sample: 50 mM at pH 7.00

Referenced to DSS

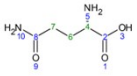


Table of Peaks

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	2.086	1042.87	0.0438	16	2.422	1210.82	0.6081
2	2.101	1049.97	0.3039	17	2.432	1215.58	0.5648
3	2.106	1052.58	0.2789	18	2.438	1218.38	0.6876
4	2.115	1057.07	0.4611	19	2.447	1223.18	0.6860
5	2.118	1058.76	0.6724	20	2.469	1234.19	0.6285
6	2.120	1059.49	0.5773	21	2.453	1226.07	0.5102
7	2.122	1060.64	0.4401	22	2.464	1231.47	0.4812
8	2.128	1063.52	0.3899	23	2.478	1238.48	0.0629
9	2.132	1065.67	0.8706	24	2.480	1239.81	0.0780
10	2.136	1067.83	0.4371	25	2.495	1246.95	0.0684
11	2.145	1072.22	0.3668	26	3.754	1876.22	0.5095
12	2.148	1073.82	0.3791	27	3.766	1882.40	1.0000
13	2.162	1080.78	0.0404	28	3.778	1888.58	0.5318
14	2.392	1195.39	0.1213				
15	2.407	1203.22	0.1308				

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	3.766	1	t	6.18	4	M01	[3.726 ... 3.810]

Table of Assignements

No.	Atom	Exp. Shift (ppm)	Multiplet
1	6	2.125	M03
2	7	2.446	M02
3	4	3.766	M01

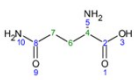
L-Glutamine

HMDB00641

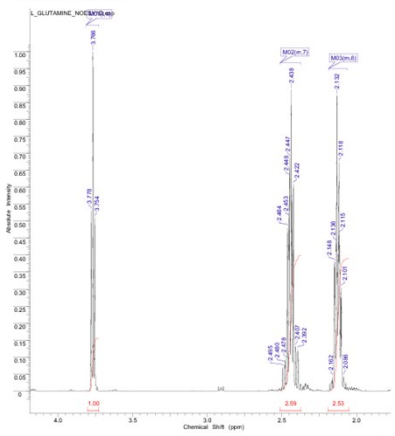
^{1}H NMR Spectrum: 500MHz in H_2O

Sample: 50 mM at pH 7.00

Referenced to DSS



Zoomed ^{1}H NMR Spectrum



HMDB ID:HMDB00064

Compound name: Creatine

Spectrum type:1H NMR Spectrum

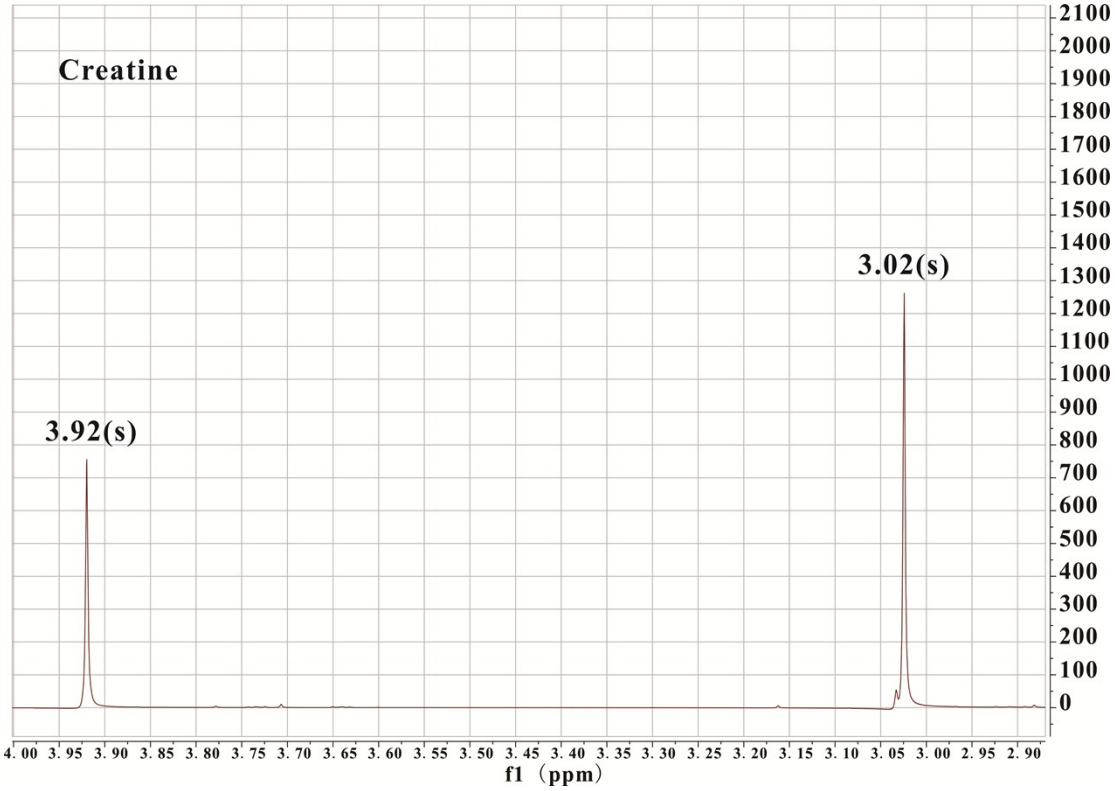


Table of Peaks

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

Table of Multiplets

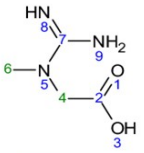
No.	Shift1 (ppm)	H's	Type	Atom1	Multiplet1	(ppm)
1	3.92	32	s	4	M01	3.85 .. 3.94
2	3.02	58	s	6	M02	2.98 .. 3.07

Table of Assignments

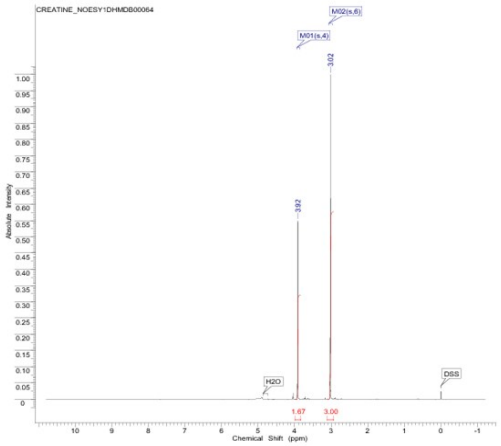
No.	Atom	Exp. Shift (ppm)	Multiplet
1	4	3.92	M01
2	6	3.02	M02

Spectra image with peak assignments

Creatine
HMDB00064
^{1}H NMR Spectrum : 500 MHz in H_2O
Sample : 50 mM at pH 7.0
Referenced to DSS



Full ^{1}H NMR Spectrum



Creatine
HMDB00064
^{1}H NMR Spectrum : 500 MHz in H_2O
Sample : 50 mM at pH 7.0
Referenced to DSS

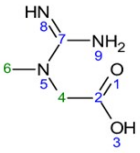


Table of Peaks

No.	(ppm)	(Hz)	Height
1	3.92	1958.2	0.5503
2	3.02	1511.7	1.0000

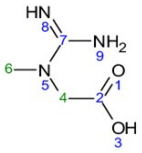
Table of Multiplets

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]

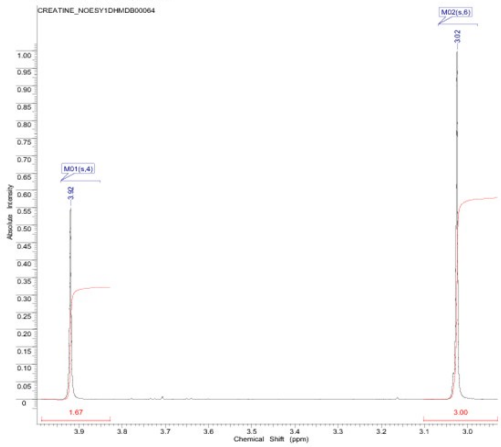
Table of Assignments

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

Creatine
HMDB00064
^{1}H NMR Spectrum : 500 MHz in H_2O
Sample : 50 mM at pH 7.0
Referenced to DSS



Zoomed ^{1}H NMR Spectrum



HMDB ID:HMDB00097

Compound name: Choline

Spectrum type:1H NMR Spectrum

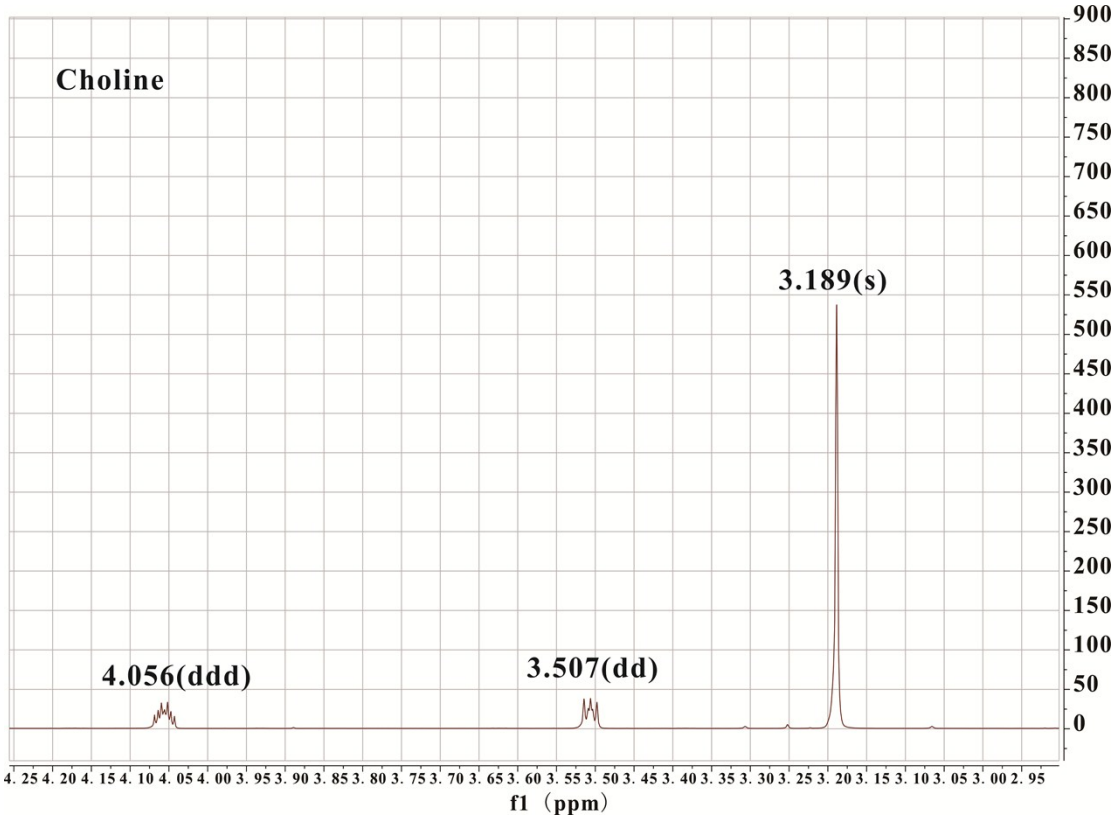


Table of Peaks

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

No.	(ppm)	(Hz)	Height
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

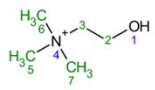
Choline chloride

HMDB00097

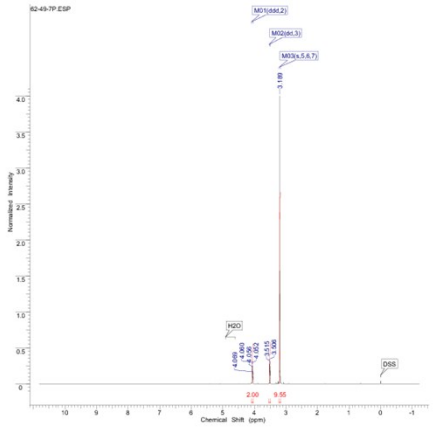
^{1}H NMR Spectrum: 600 MHz in H2O

Sample: 115 mM at pH 7.00

Referenced to DSS



Full ^{1}H NMR Spectrum



Choline chloride

HMDB00097

^{1}H NMR Spectrum: 600 MHz in H2O

Sample: 115 mM at pH 7.00

Referenced to DSS

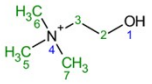


Table of Peaks

No.	(ppm)	(Hz)	Height
1	3.189	1912.4	4.0000
2	3.498	2097.8	0.2425
3	3.506	2102.8	0.2969
4	3.509	2104.4	0.2154
5	3.515	2107.8	0.2759
6	4.043	2424.7	0.1026
7	4.048	2427.6	0.1606
8	4.052	2430.1	0.2473
9	4.056	2432.4	0.1967
10	4.060	2434.8	0.2485
11	4.064	2437.2	0.1771
12	4.069	2440.0	0.1210

Table of Multiplets

No.	Shift1 (ppm)	H's	Type	J (Hz)	Atom1	Multiplet1	(ppm)
1	3.189	66	s	-	5, 6, 7	M03	[3.176 .. 3.205]
2	3.507	14	dd	5.816, 4.14	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

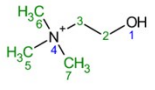
Choline chloride

HMDB00097

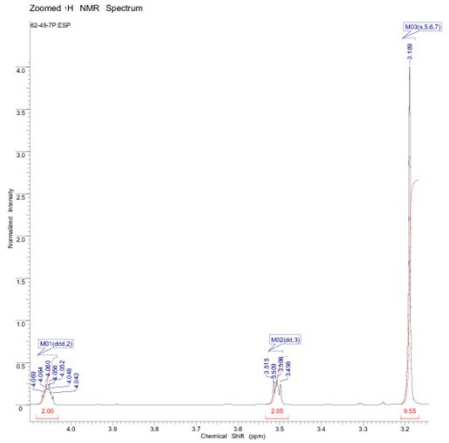
^{1}H NMR Spectrum: 600 MHz in H2O

Sample: 115 mM at pH 7.00

Referenced to DSS



Zoomed ^{1}H NMR Spectrum



HMDB ID:HMDB00925

Compound name: Trimethylamine N-oxide

Spectrum type:1H NMR Spectrum

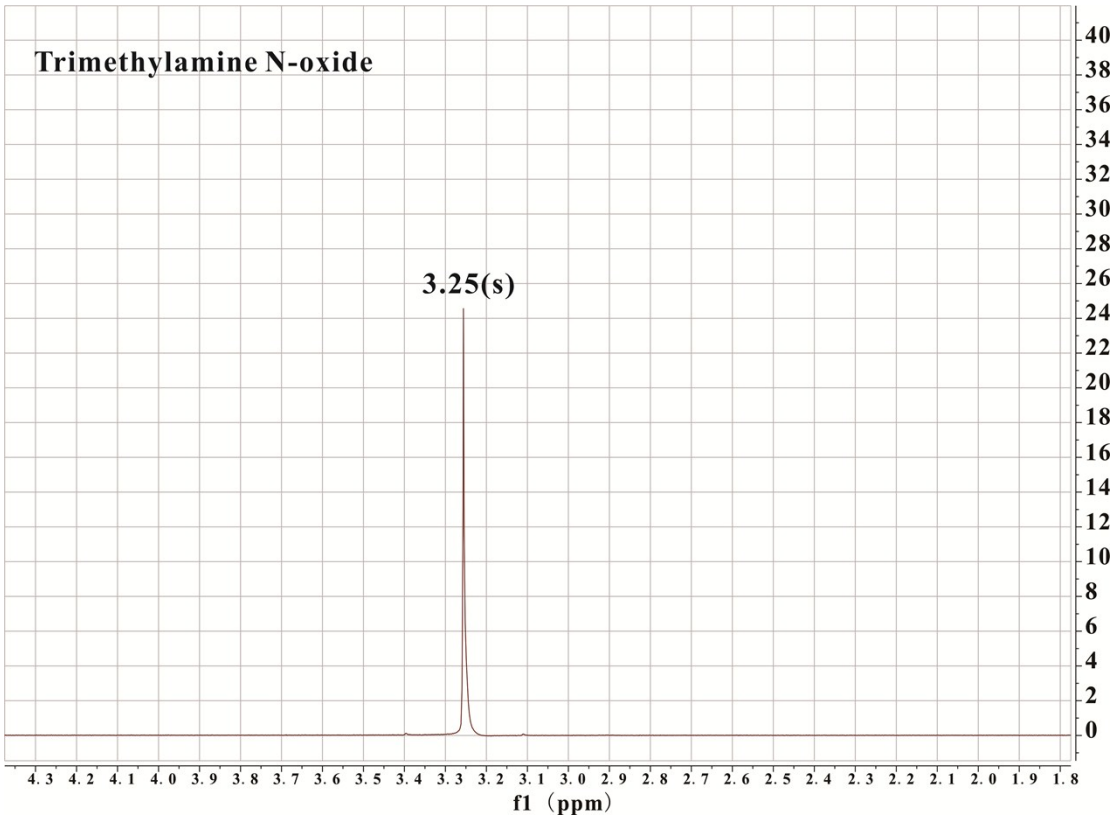


Table of Peaks

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

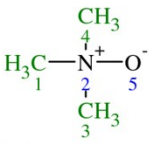
Trimethylamine oxide

HMDB00925

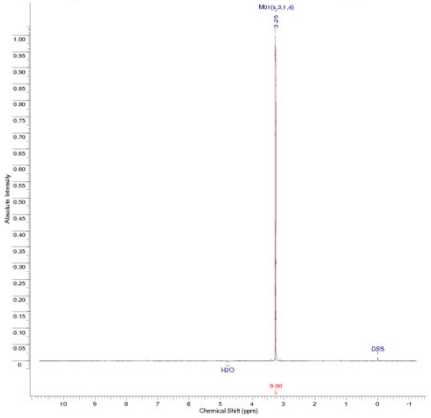
^{1}H NMR Spectrum: 500MHz in H2O

Sample: ~40mM in H2O and pH 7.00

Referenced to DSS



Full ^{1}H NMR Spectrum



Trimethylamine oxide

HMDB00925

^{1}H NMR Spectrum: 500MHz in H2O

Sample: ~40mM in H2O and pH 7.00

Referenced to DSS

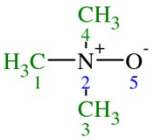


Table of Peaks

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

Table of Assignments

No.	Atom	Exp. Shift (ppm)	Multiplet
1	3	3.25	Mlt1
2	1	3.25	Mlt1
3	4	3.25	Mlt1

Table of Multiplets

No.	Shift (ppm)	H's	Type	Atom#	Multiplet	(ppm)
1	3.25	123	s	3, 1, 4	Mlt1	[3.22 , 3.27]

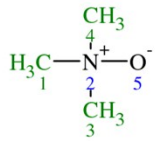
Trimethylamine oxide

HMDB00925

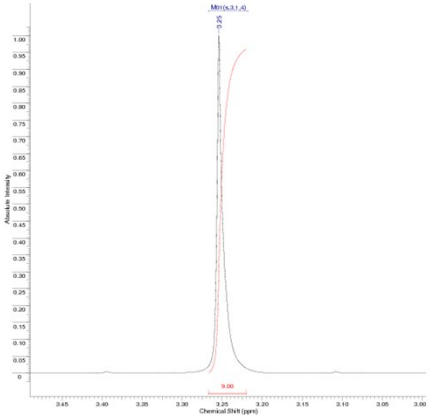
^{1}H NMR Spectrum: 500MHz in H2O

Sample: ~40mM in H2O and pH 7.00

Referenced to DSS



Zoomed ^{1}H NMR Spectrum



HMDB ID:HMDB00043

Compound name: Betaine

Spectrum type:1H NMR Spectrum

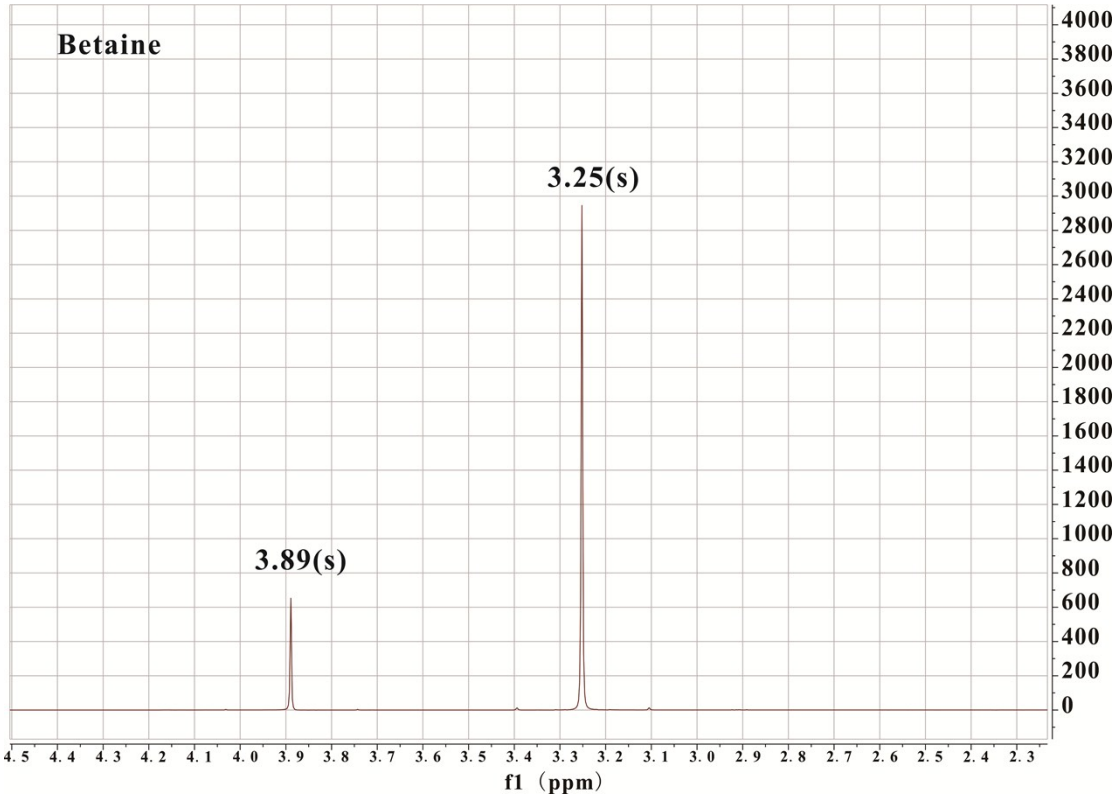


Table of Peaks

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

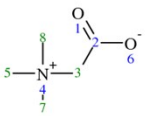
Betaine

HMDB00043

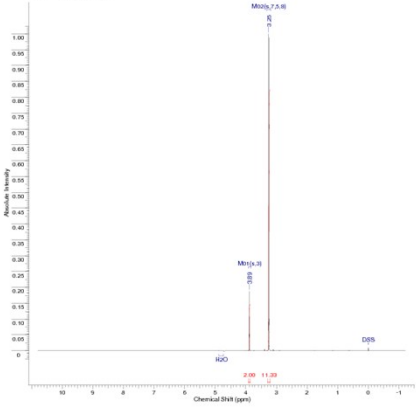
^{1}H NMR Spectrum : 500 MHz in H2O

Sample : 50 mM at pH 7.0 in H2O

Referenced to DSS



Full ^{1}H NMR Spectrum



Betaine

HMDB00043

^{1}H NMR Spectrum : 500 MHz in H2O

Sample : 50 mM at pH 7.0 in H2O

Referenced to DSS

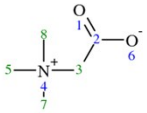


Table of Peaks

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

Table of Multiplets

No.	Shift (ppm)	Hs	Type	Atom1	Multiplet	(ppm)
1	3.89	15	s	3	Mln	[3.84 , 3.93]
2	3.25	83	s	7, 5, 8	Mlz	[3.19 , 3.31]

Table of Assignments

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

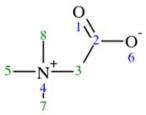
Betaine

HMDB00043

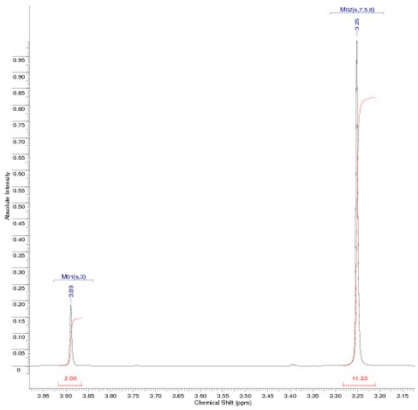
^{1}H NMR Spectrum : 500 MHz in H2O

Sample : 50 mM at pH 7.0 in H2O

Referenced to DSS



Zoomed ^{1}H NMR Spectrum



HMDB ID:HMDB00647

Compound name: L-Tyrosine

Spectrum type:1H NMR Spectrum

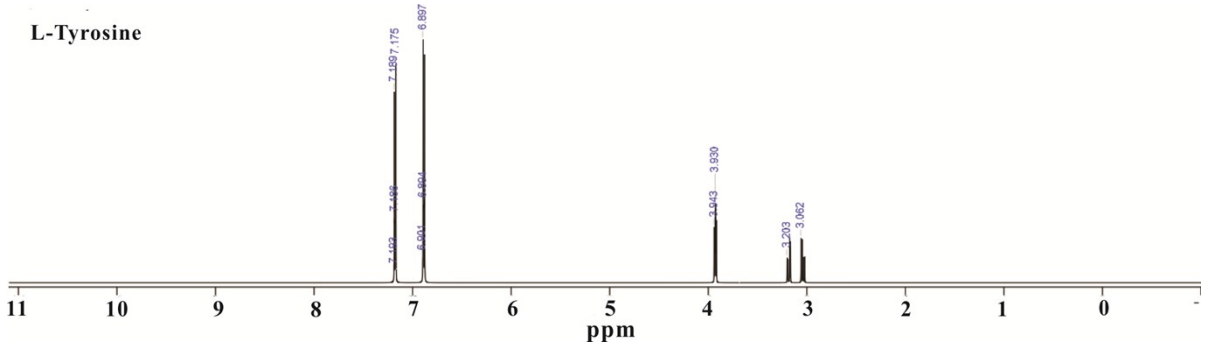


Table of Peaks

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

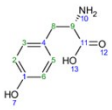
No.	Shift1 (ppm)	H's	Type	Atom1	Multiplet1	(ppm)
1	3.024	0	dd	8	M05	3.014 .. 3.072
2	3.170	0	dd	8	M04	3.161 .. 3.213
3	3.921	0	dd	9	M03	3.909 .. 3.954
4	6.877	2	m	2 6	M02	6.868 .. 6.909
5	7.710	2	m	3 5	M01	7.161 .. 7.201

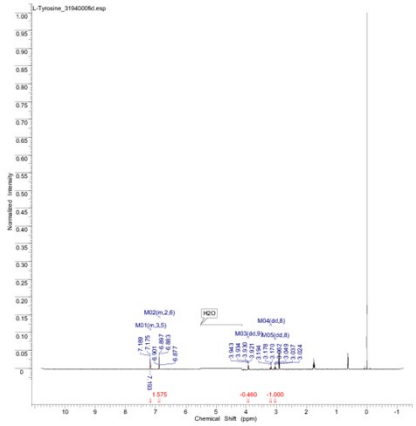
Table of Assignments

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

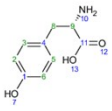


Table of Peaks

No.	(ppm)	Height
1	7.193	-0.0004
2	7.189	0.0263
3	7.186	0.0058
4	7.178	0.0079
5	7.175	0.0300
6	7.170	0.0006
7	6.901	0.0010
8	6.897	0.0335
9	6.894	0.0070
10	6.886	0.0083
11	6.883	0.0313
12	6.877	0.0003
13	3.943	0.0077
14	3.934	0.0096
15	3.930	0.0126
16	3.921	0.0087
17	3.203	0.0035
18	3.194	0.0033
19	3.178	0.0064
20	3.170	0.0057
21	3.062	0.0063
22	3.049	0.0081
23	3.037	0.0036
24	3.024	0.0037

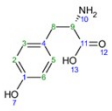
Table of Multiplets

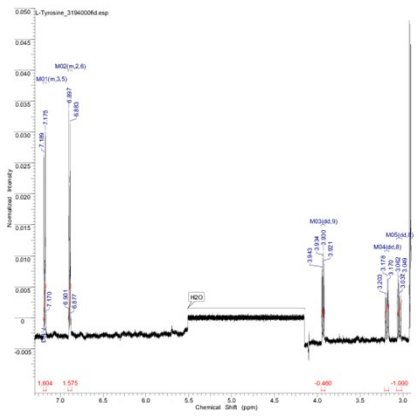
No.	Shift (ppm)	H's	Type	Atom1	Multiplet	(ppm)
1	3.024	0	dd	8	M05	[3.014 3.072]
2	3.170	0	dd	8	M04	[3.161 3.213]
3	3.921	0	dd	9	M03	[3.909 3.954]
4	6.877	2	m	2, 6	M02	[6.868 6.909]
5	7.170	2	m	3, 5	M01	[7.161 7.201]

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	7.170	M01
7	5	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

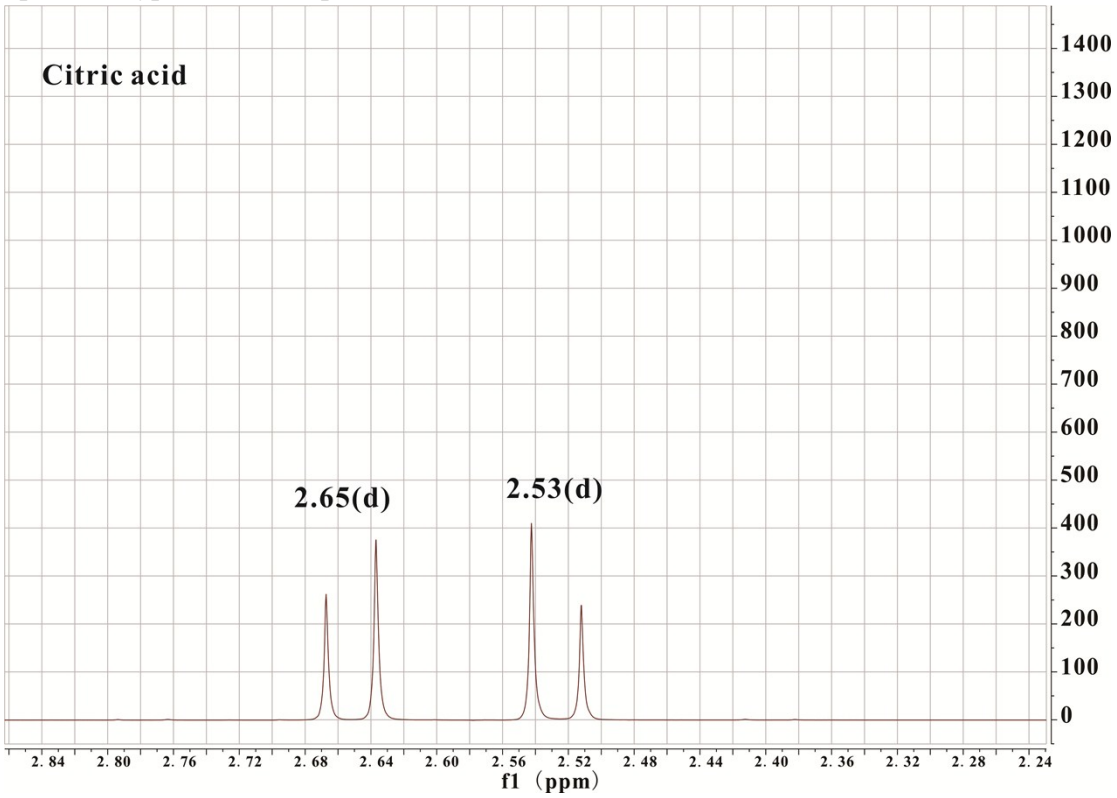


Table of Peaks

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

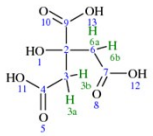
Citric acid

HMDB00094

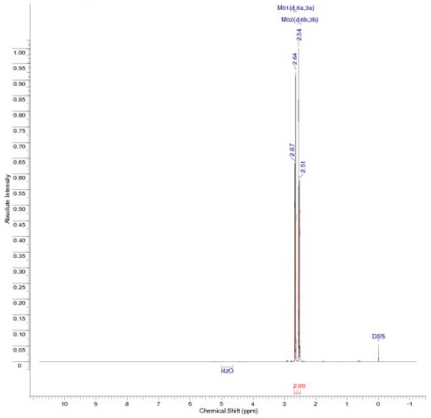
^{1}H NMR Spectrum : 500 MHz in H2O

Sample : 50 mM at pH 7.0 in H2O

Referenced to DSS



Full ^{1}H NMR Spectrum



Citric acid

HMDB00094

^{1}H NMR Spectrum : 500 MHz in H2O

Sample : 50 mM at pH 7.0 in H2O

Referenced to DSS

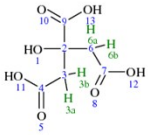


Table of Peaks

No.	(ppm)	(Hz)	Height
1	2.67	1333.2	0.5228
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.	Shift (ppm)	H's	Type	J (Hz)	Atom	Multiplet	(ppm)
1	2.65	4H	d	15.16	6a, 3a	Mlo1	[2.61 , 2.70]
2	2.53	4H	d	-	6b, 3b	Mlo2	[2.48 , 2.57]

Table of Assignments

No.	Atom	Exp. Shift (ppm)	Multiplet
1	3a	2.65	Mlo1
2	6a	2.65	Mlo1
3	3b	2.53	Mlo2
4	6b	2.53	Mlo2

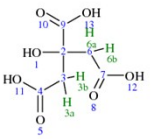
Citric acid

HMDB00094

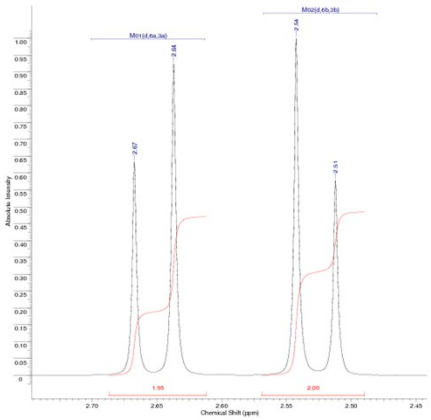
^{1}H NMR Spectrum : 500 MHz in H2O

Sample : 50 mM at pH 7.0 in H2O

Referenced to DSS



Zoomed ^{1}H NMR Spectrum



HMDB ID:HMDB00131

Compound name: Glycerol

Spectrum type:1H NMR Spectrum

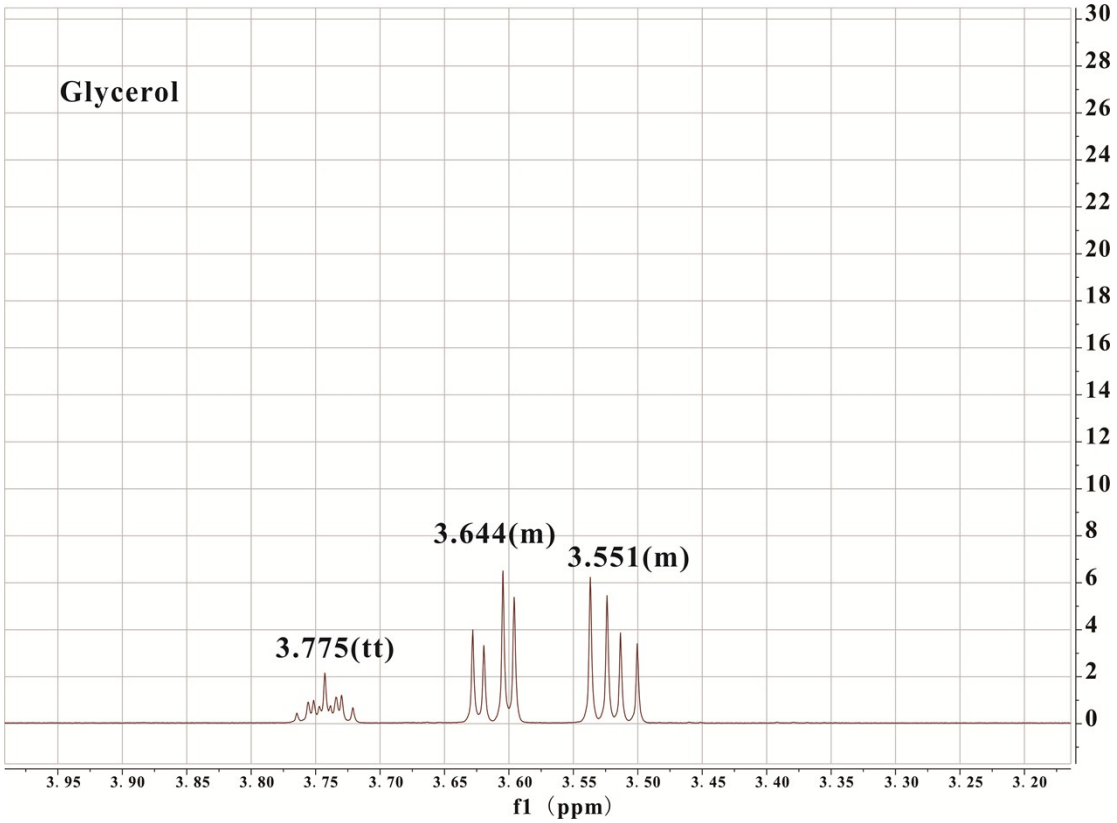


Table of Peaks

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

No.	(ppm)	(Hz)	Height
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

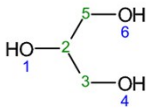
Glycerol

HMDB00131

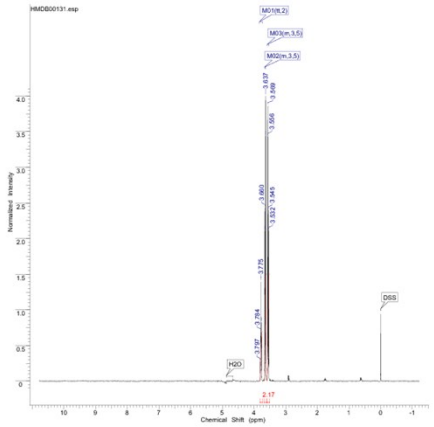
^{1}H NMR Spectrum: 500 MHz in H2O

Sample: 90 mM at pH 7.0

Referenced to DSS



Full ^{1}H NMR Spectrum



Glycerol

HMDB00131

^{1}H NMR Spectrum: 500 MHz in H2O

Sample: 90 mM at pH 7.0

Referenced to DSS

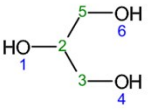


Table of Peaks

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	1829.5	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, 4.40	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

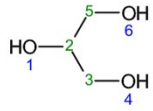
Glycerol

HMDB00131

^{1}H NMR Spectrum: 500 MHz in H2O

Sample: 90 mM at pH 7.0

Referenced to DSS



Zoomed ^{1}H NMR Spectrum