

Liquid-liquid equilibrium study of 1-Dodecyl-3-Methyl-Imidazolium

Dicyanamide + Inorganic salt + Water systems

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1) Appendix

2) Nuclear Magnetic Resonance Spectroscopy (Varian-INOVA 500MHz model):

- C-NMR: Table S1

- H-NMR: Table S2

3) Fourier Transform Infrared Spectroscopy (JASCO 4700 model): Table S3

4) Diffuse Reflection Spectroscopy (PerkinElmer L25 model): Table S4

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Appendix:

Thus, for the long-range term (the second term in Eq. (1) the activity coefficient of salt written as [9]

$$\ln \gamma_i^{\text{PDH}} = -A_x \left\{ \left(\frac{2z_i^2}{\rho} \right) \ln \left[\frac{(1+\rho I_x^{0.5})}{(1+\rho I_{x,0}^{0.5})} \right] + \frac{z_i^2 I_x^{0.5} + 2I_x^{1.5}}{1 + \rho I_x^{0.5}} \right\}; \quad i=\text{anion,cation} \quad (\text{A1})$$

$$A_x = \frac{1}{3} \left(\frac{2\pi N_A d}{M} \right)^{0.5} \left(\frac{e^2}{4\pi\epsilon_0\epsilon_r k_B T} \right)^{1.5} \quad (\text{A2})$$

$$I_x = \frac{1}{2} \sum_i z_i^2 x_i; \quad i=\text{anion,cation} \quad (\text{A3})$$

$$I_{x,0} = \lim_{x_m \rightarrow 0} I_x \quad (\text{A4})$$

Where z , I_x , ρ ($=14.9$), and N_A stand for the ion electric charge, mole fraction ionic strength, closet approach parameter, and Avogadro's number, respectively; e , k_B and ϵ_0 stand for the electron charge, Boltzmann constant and vacuum permeability factor, respectively. The dielectric constant of water is shown by ϵ . Besides, d and M represent the density and molar mass, respectively. Finally, $I_{x,0}$ shows the ionic strength of the solvent-free solution. x_m is the mole fraction of all molecular species.

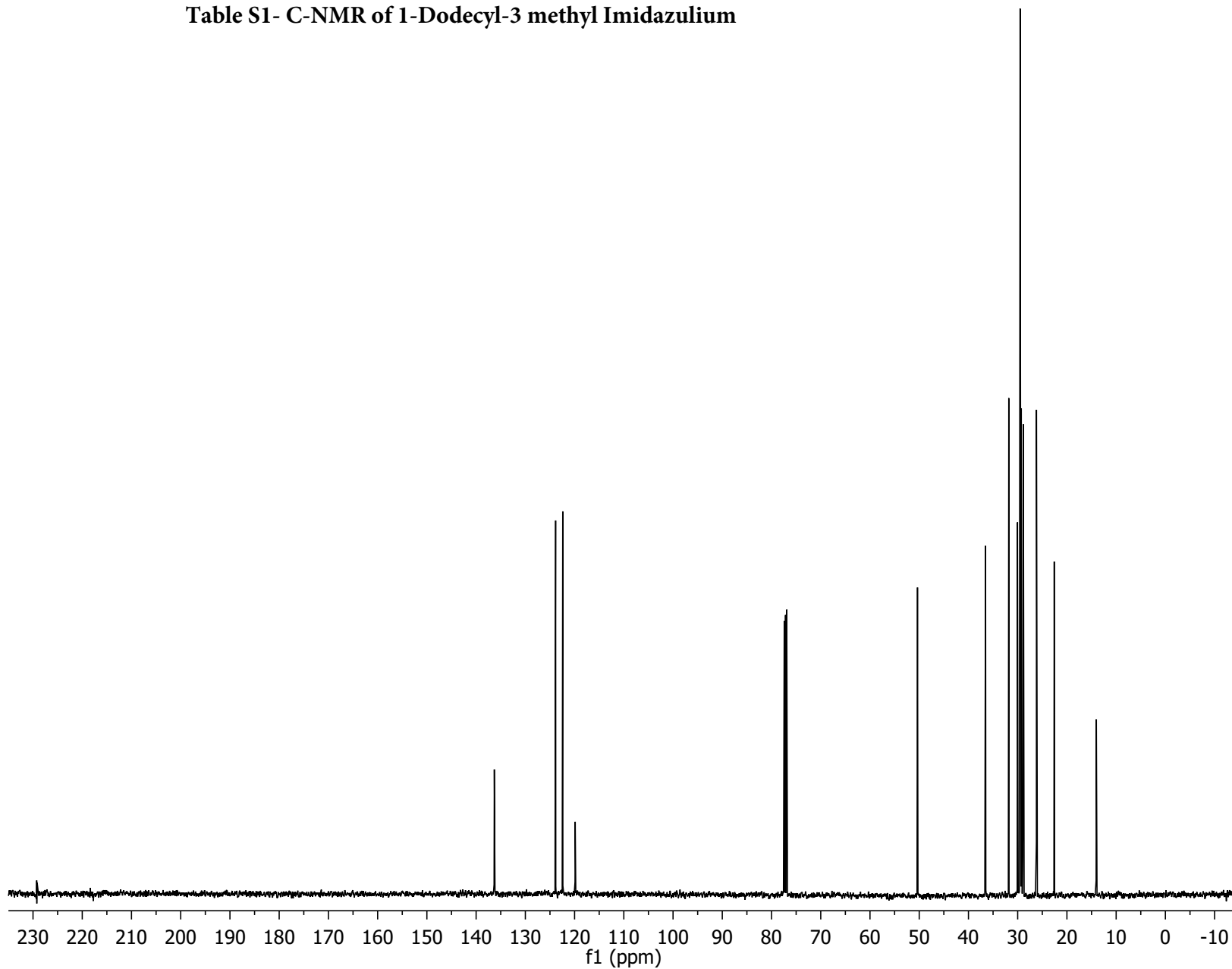


1-C



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3 Comment	
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	inova
8 Author	
9 Solvent	cdd3
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	416
13 Receiver Gain	60
14 Relaxation Delay	2.0000
15 Pulse Width	7.5000
16 Acquisition Time	1.0428
17 Acquisition Date	2018-09-06T11:42:50
18 Modification Date	2018-09-06T12:04:02
19 Spectrometer Frequency	125.68
20 Spectral Width	31421.8
21 Lowest Frequency	-1887.8
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

Table S1- C-NMR of 1-Dodecyl-3 methyl Imidazolium





1-C

— 50.3485

— 36.5268

— 31.8080

30.0414

29.5074

29.4158

29.2708

29.2291

28.8588

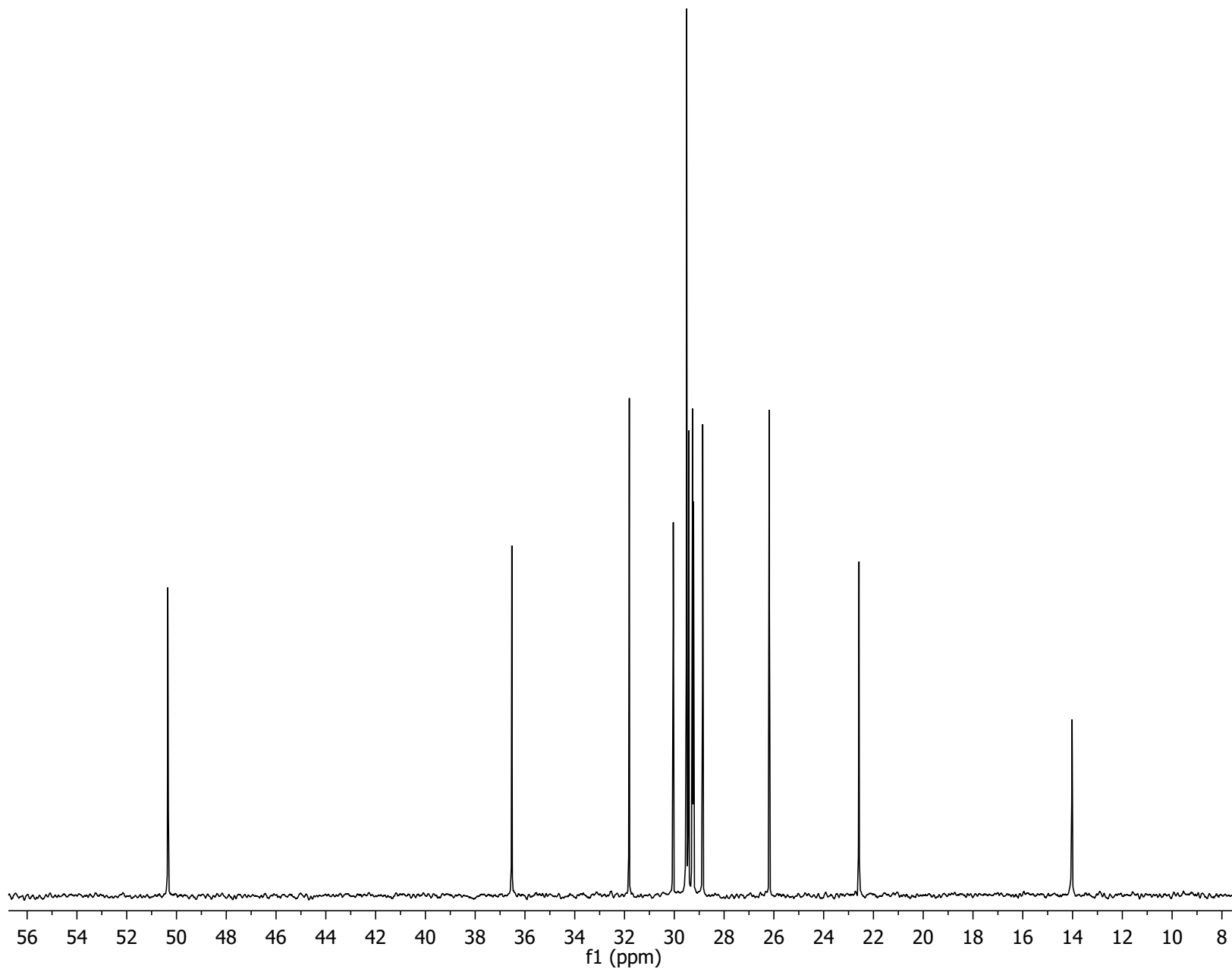
— 26.1859

— 22.5798

— 14.0185

Continued Table S1- C-NMR of 1-Dodecyl-3 methyl Imidazolium

Parameter	Value
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2 Title	1-C
3 Comment	
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	inova
8 Author	
9 Solvent	cdd3
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	416
13 Receiver Gain	60
14 Relaxation Delay	2.0000
15 Pulse Width	7.5000
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17 Acquisition Date	2018-09-06T11:42:50
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1-C

— 30.0414

— 29.5074

— 29.4158

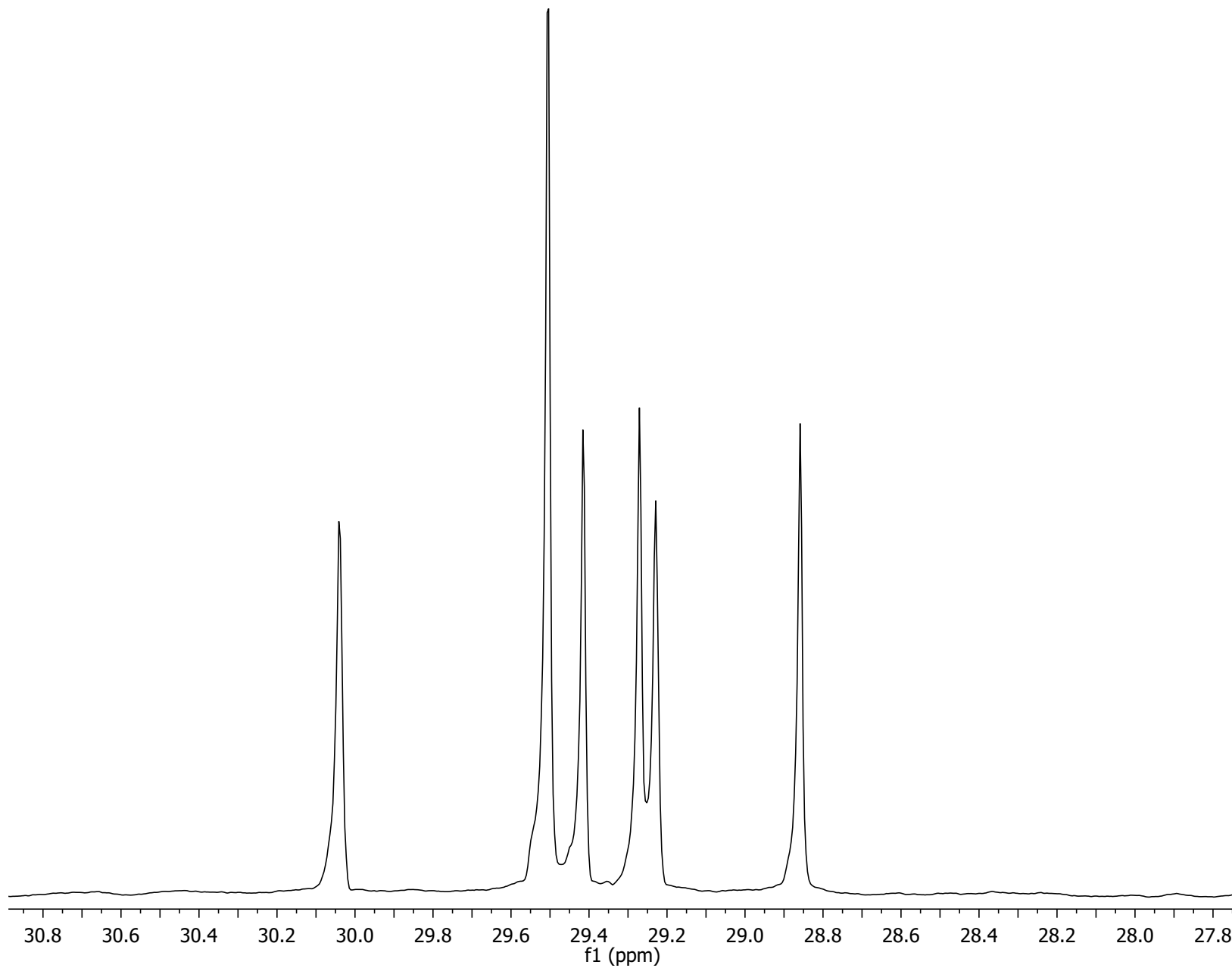
— 29.2708

— 29.2291

— 28.8588

Continued Table S1- C-NMR of 1-Dodecyl-3 methyl Imidazolium

Parameter	Value
1 Data File Name	F:/ 1397-06-14/ Taki/ 1-C.fid/ fid
2 Title	1-C
3 Comment	
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	inova
8 Author	
9 Solvent	cdd3
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	416
13 Receiver Gain	60
14 Relaxation Delay	2.0000
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16 Acquisition Time	1.0428
17 Acquisition Date	2018-09-06T11:42:50
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19 Spectrometer Frequency	125.68
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23 Acquired Size	32768
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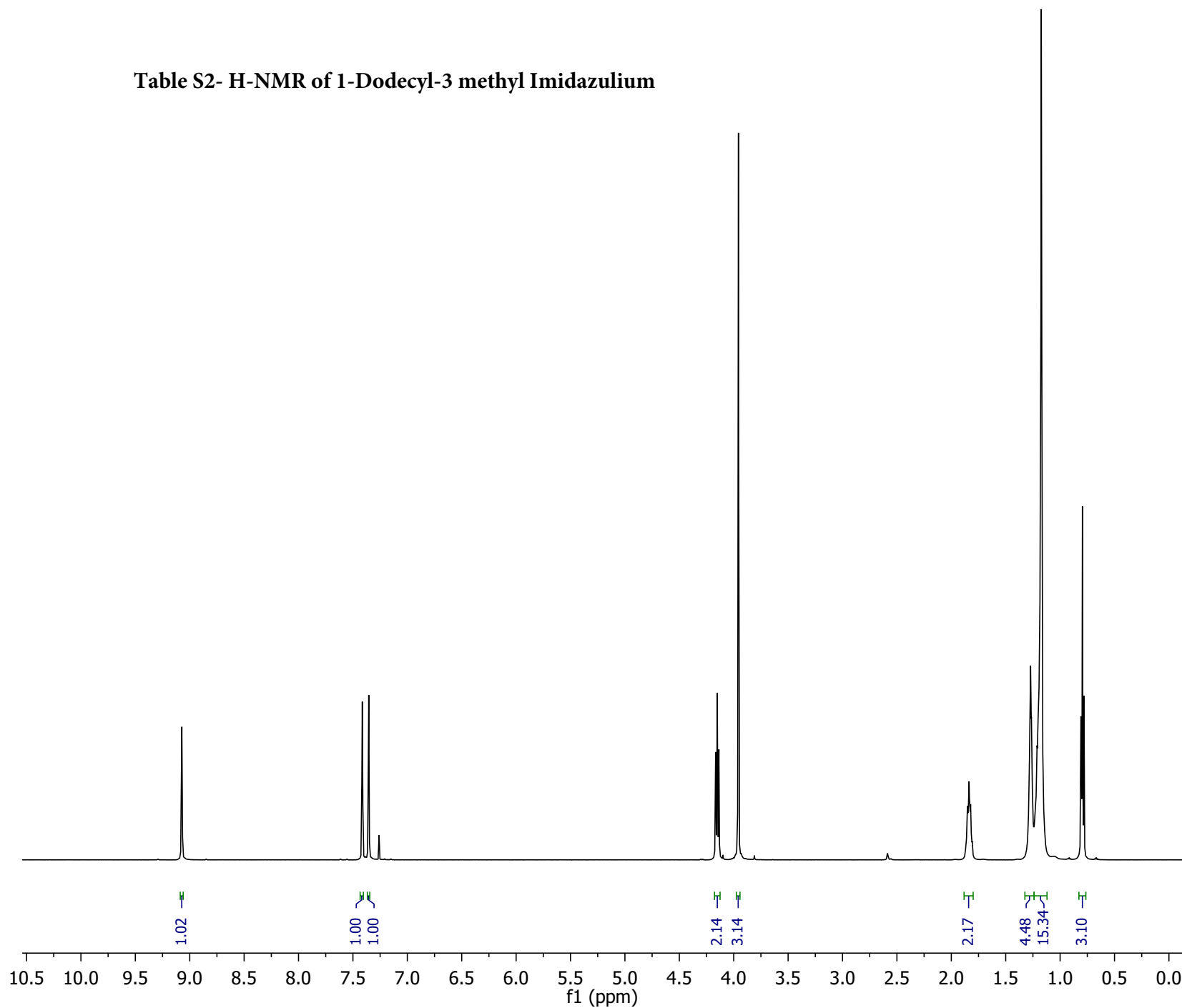


1-H

—9.0727

7.4178
7.4139
7.4101
7.3585
7.3546
7.3508
7.26014.1660
4.1510
4.1362
3.95661.8655
1.8513
1.8369
1.8224
1.8074
1.2786
1.2713
1.2626
1.2117
1.1967
1.1727
0.8080
0.7946
0.7805Table S2- ¹H-NMR of 1-Dodecyl-3 methyl Imidazolium

Parameter	Value
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2 Title	1-H
3 Comment	
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	inova
8 Author	
9 Solvent	cdd3
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	8
13 Receiver Gain	30
14 Relaxation Delay	1.0000
15 Pulse Width	5.0000
16 Acquisition Time	2.0490
17 Acquisition Date	2018-09-06T11:41:28
18 Modification Date	2018-09-06T11:42:26
19 Spectrometer Frequency	499.76
20 Spectral Width	7996.0
21 Lowest Frequency	-999.5
22 Nucleus	1H
23 Acquired Size	16384
24 Spectral Size	65536





1-H

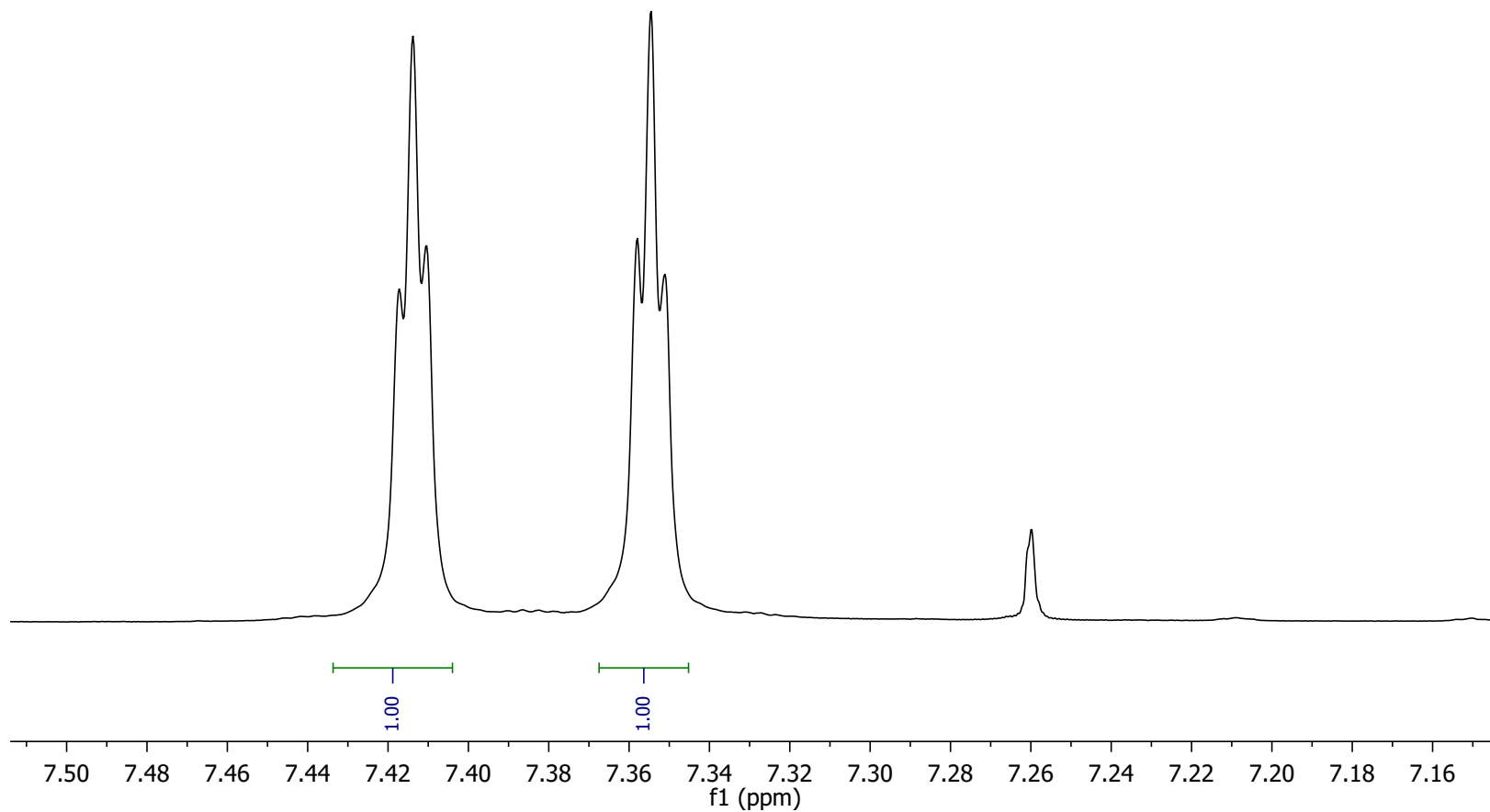
7.4178
7.4139
7.4101

7.3585
7.3546
7.3508

7.2601

Continued Table S2- ¹H-NMR of 1-Dodecyl-3 methyl Imidazolium

Parameter	Value
1 Data File Name	F:/ 1397-06-14/ Taki/ 1-H.fid/ fid
2 Title	1-H
3 Comment	
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	inova
8 Author	
9 Solvent	cdd3
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	8
13 Receiver Gain	30
14 Relaxation Delay	1.0000
15 Pulse Width	5.0000
16 Acquisition Time	2.0490
17 Acquisition Date	2018-09-06T11:41:28
18 Modification Date	2018-09-06T11:42:26
19 Spectrometer Frequency	499.76
20 Spectral Width	7996.0
21 Lowest Frequency	-999.5
22 Nucleus	¹ H
23 Acquired Size	16384
24 Spectral Size	65536





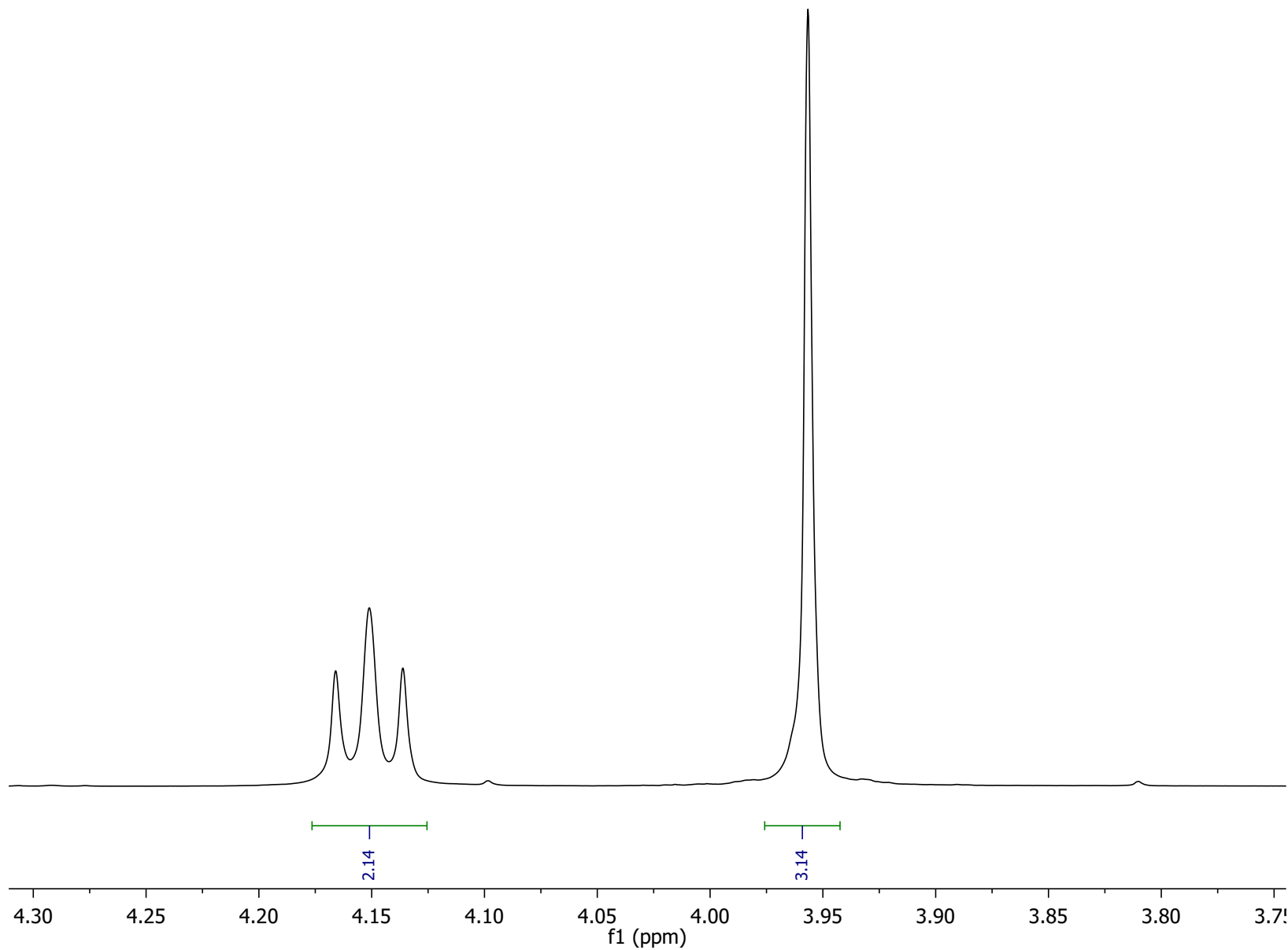
1-H

4.1660
4.1510
4.1362

3.9566

Continued Table S2- ¹H-NMR of 1-Dodecyl-3 methyl Imidazolium

Parameter	Value
1 Data File Name	F:/ 1397-06-14/ Taki/ 1-H.fid/ fid
2 Title	1-H
3 Comment	
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	inova
8 Author	
9 Solvent	cdd3
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	8
13 Receiver Gain	30
14 Relaxation Delay	1.0000
15 Pulse Width	5.0000
16 Acquisition Time	2.0490
17 Acquisition Date	2018-09-06T11:41:28
18 Modification Date	2018-09-06T11:42:26
19 Spectrometer Frequency	499.76
20 Spectral Width	7996.0
21 Lowest Frequency	-999.5
22 Nucleus	¹ H
23 Acquired Size	16384
24 Spectral Size	65536





1-H

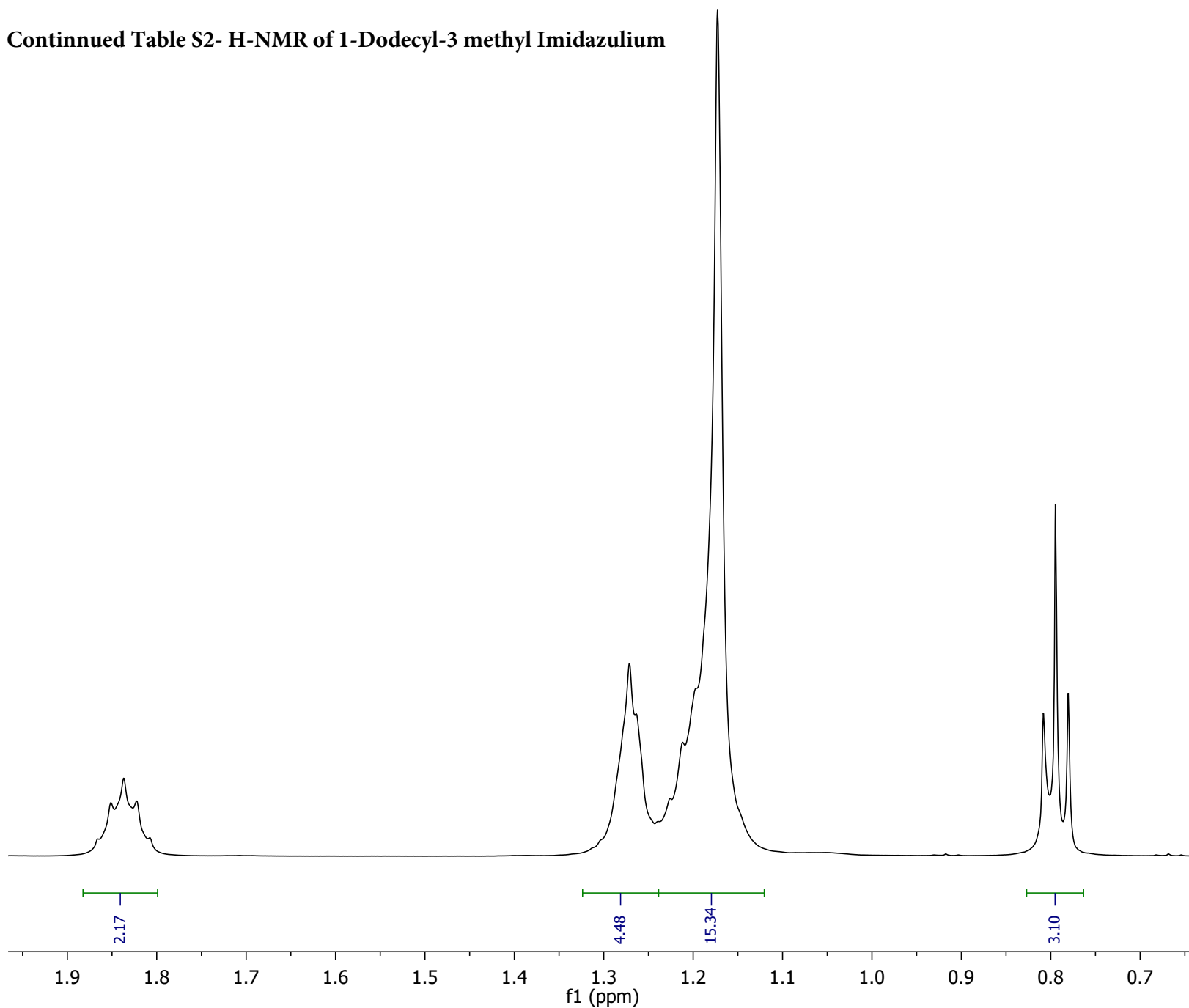
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1.8369
1.8224
1.8074

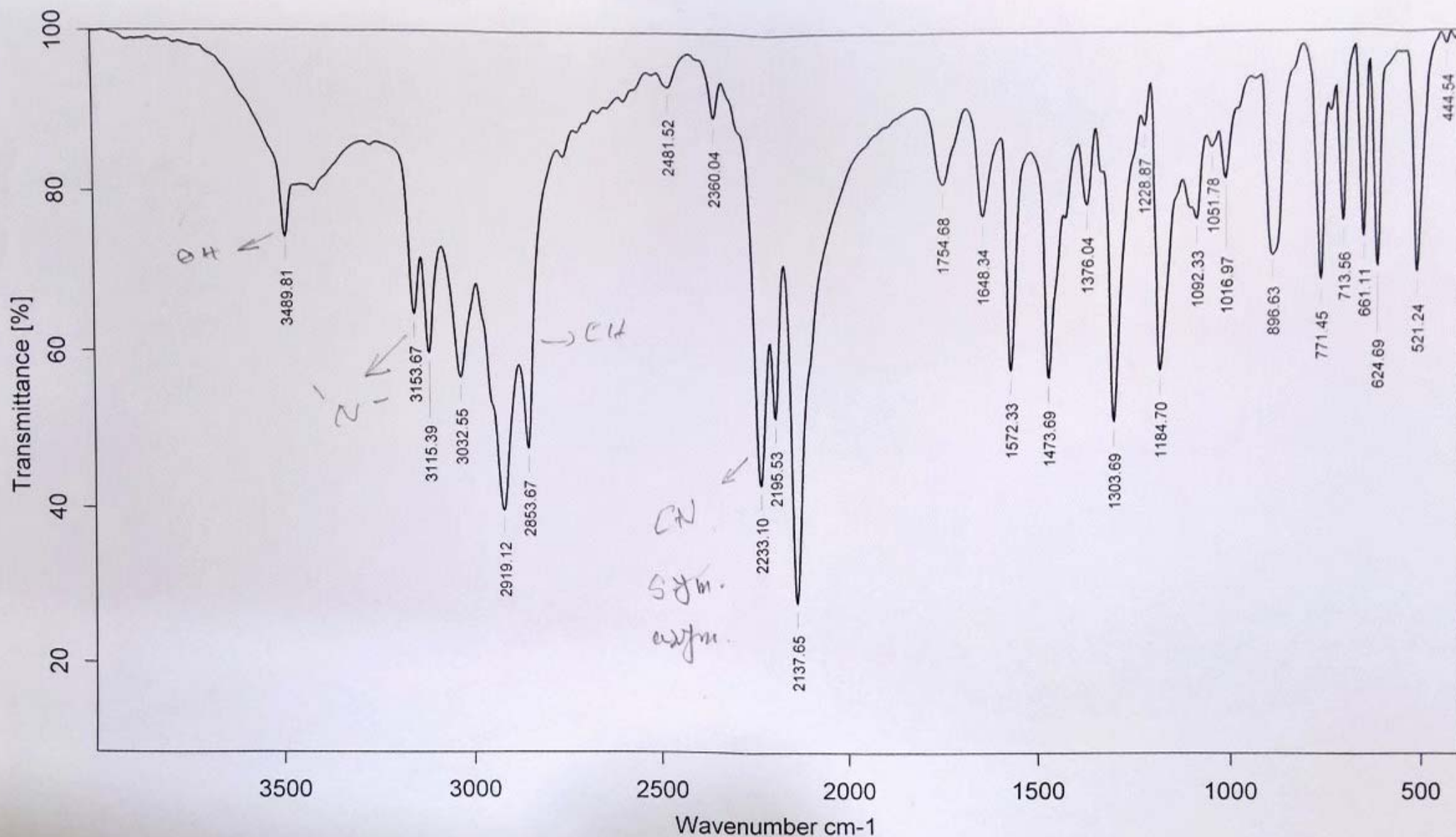
1.2786
1.2713
1.2626
1.2117
1.1967
1.1727

0.8080
0.7946
0.7805

Continued Table S2- ¹H-NMR of 1-Dodecyl-3 methyl Imidazolium

Parameter	Value
1 Data File Name	F:/ 1397-06-14/ Taki/ 1-H.fid/ fid
2 Title	1-H
3 Comment	
4 Origin	Varian
5 Owner	
6 Site	
7 Spectrometer	inova
8 Author	
9 Solvent	cdd3
10 Temperature	25.0
11 Pulse Sequence	s2pul
12 Number of Scans	8
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19 Spectrometer Frequency	499.76
20 Spectral Width	7996.0
21 Lowest Frequency	-999.5
22 Nucleus	¹ H
23 Acquired Size	16384
24 Spectral Size	65536





Sample : 00		Frequency Range : 3996.14 - 399.818		Measured on : 12/8/2018	
Technique :	Resolution : 4	Instrument : Alpha		Sample Scans : 16	
Customer : Default	Zerofilling : 2	Acquisition : Double Sided, For			

Table S3- Fourier Transform Infrared Spectroscopy of 1-Dodecyl-3 methyl Imidazulium

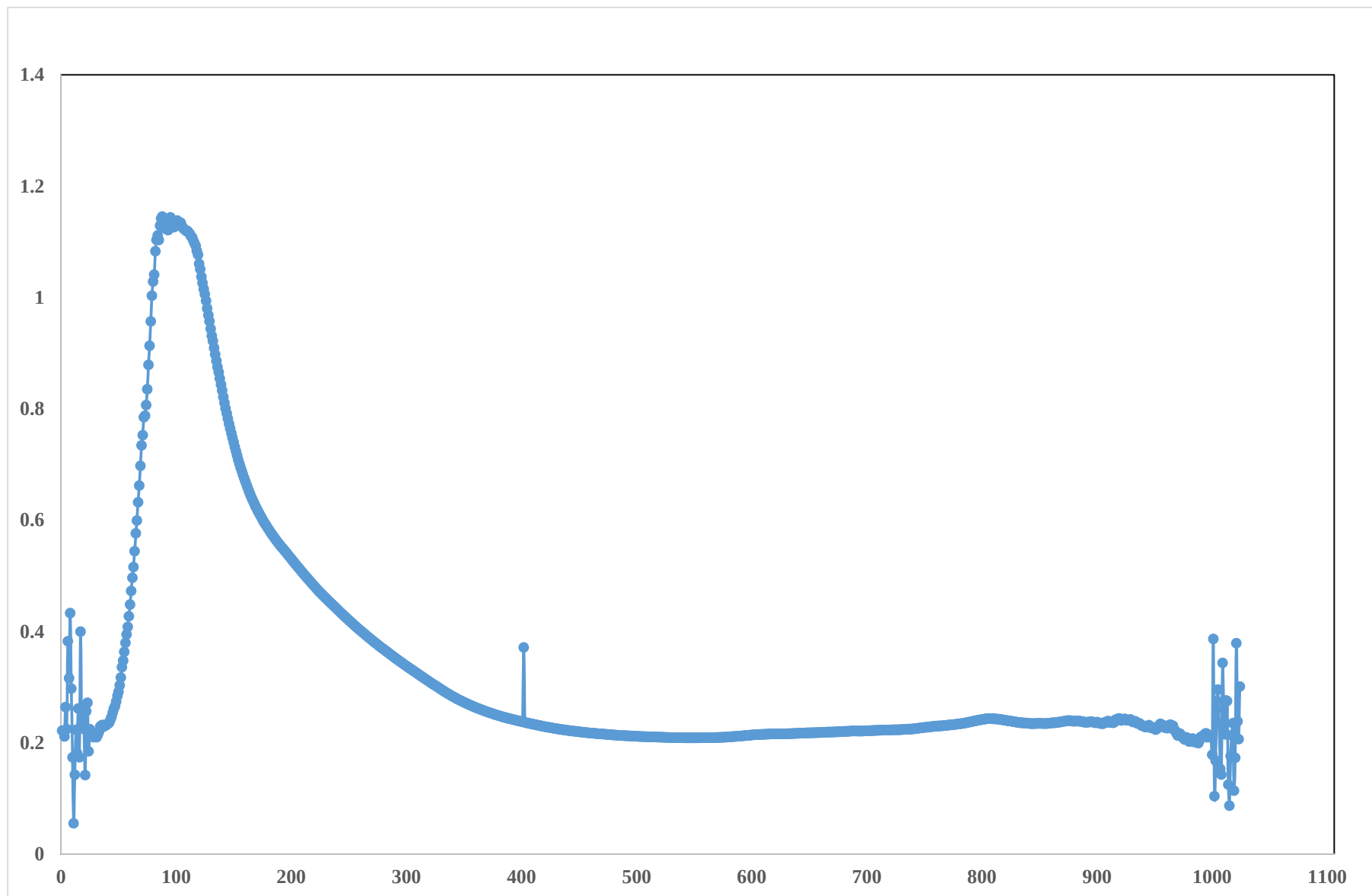


Table S4- 1-Dodecyl-3 methyl Imidazolium DRS Test Result