New Journal of Chemistry

Supporting Information

A novel core-shell Pd(0)@enSiO$_2$-Ni-TiO$_2$ nanocomposite with synergistic effect for efficient hydrogenations

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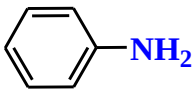
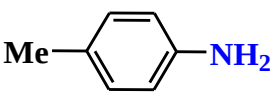
S1. Spectral details of compounds listed in Table 4

Aniline (2a)



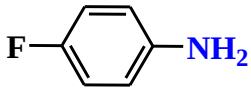
^{1}H NMR (400 MHz, CDCl$_3$): δ 3.68 (s, 2H, NH$_2$), 6.77 (d, *J*= 8 Hz, 2H, ArH), 6.89 (t, *J*= 7.3 Hz, 1H, ArH), 7.28 (t, *J*= 7.3 Hz, 2H, ArH); **^{13}C NMR (100 MHz, CDCl$_3$):** δ 115.24, 118.76, 129.43,146.59.

4-Methylaniline (2b)



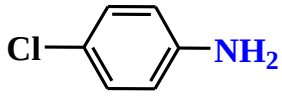
^{1}H NMR (400 MHz, CDCl$_3$): δ 2.28 (s, 3H, CH$_3$), 3.49 (s, 2H, NH$_2$), 6.65 (d, *J*= 8.2 Hz, 2H, ArH), 7.01 (d, *J*= 8.1 Hz, 2H, ArH); **^{13}C NMR (100 MHz, CDCl$_3$):** δ 20.50, 115.31, 127.84, 129.79, 143.82.

4-Fluoroaniline(2c)



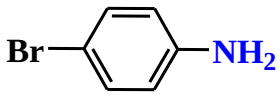
^{1}H NMR (400 MHz, $CDCl_3$): δ 3.60 (s, 2H, NH_2), 6.62(dd, *J*= 8.6 Hz, 4.5 Hz, 2H, ArH),6.89 (t, *J*= 8.0 Hz, 2H, ArH); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 115.69 (d, *J*= 22.4 Hz), 116.10 (d, *J*= 7.6 Hz), 142.57 (d, *J*= 2.0 Hz), 156.38 (d, *J*= 235.2 Hz).

4-Chloroaniline (2d)



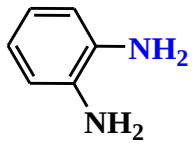
^{1}H NMR (400 MHz, $CDCl_3$): δ 3.68 (s, 2H, NH_2), 6.63 (d, *J*= 8.4 Hz, 2H, ArH),7.12 (d, *J*= 8.5 Hz, 2H, ArH); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 116.25, 123.16, 129.13, 144.95.

4-Bromoaniline (2e)



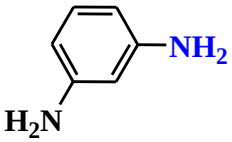
^{1}H NMR (400 MHz, $CDCl_3$): δ 3.69 (s, 2H, NH_2), 6.59 (d, *J*= 8.7 Hz, 2H, ArH),7.26 (d, *J*= 8.7 Hz, 2H, ArH); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 110.22, 116.72, 132.02, 145.41.

1,2-Diaminobenzene (2f)



^{1}H NMR (400 MHz, DMSO): δ 4.38 (s, 4H, NH_2), 6.36-6.48 (m, 2H, ArH), 6.49-6.52 (m, 2H, ArH); **^{13}C NMR (100 MHz, DMSO):** δ 114.98, 117.73, 135.39.

1,3-Diaminobenzene (2g)

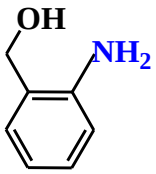


^{1}H NMR (400 MHz, $CDCl_3$): δ 3.55 (bs, 4H, NH_2), 6.05 (s, 1H, ArH),6.18 (d, *J*= 8.5 Hz, 2H, ArH),6.95 (t, *J*= 7.7 Hz, 1H, ArH); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 103.22, 106.79,132.07, 149.19.

1,4-Diaminobenzene (2h)

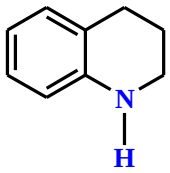
^{1}H NMR (400 MHz, $CDCl_3$): δ 3.23 (bs, 4H, NH_2), 6.60 (s, 4H, ArH); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 116.74, 138.59.

2-Aminobenzylalcohol (2i)



^{1}H NMR (400 MHz, DMSO): δ 3.36 (s, 2H, NH_2), 4.37 (d, *J*= 5.4 Hz, 2H, CH_2), 4.99 (t, *J*= 5.4 Hz, 1H, OH),6.51 (td, *J*= 7.3 Hz, 1.0 Hz, 1H, ArH), 6.61 (d, *J*= 7.9 Hz, 0.9 Hz, 1H, ArH),6.95 (td, *J*= 7.7 Hz, 1.5 Hz, 1H, ArH),7.04 (d, *J*= 7.4 Hz, 1H, ArH); **^{13}C NMR (100 MHz, DMSO)**: δ 61.60, 114.96,116.22, 125.80,128.07,146.78.

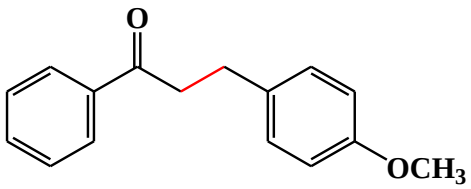
Quinoline (4a)



^{1}H NMR (400 MHz, $CDCl_3$): δ 1.94-2.00 (m, 2H, CH_2), 2.79 (t, *J*= 6.4Hz, 2H, CH_2), 3.32 (t, *J*= 6.5Hz, 2H, CH_2), 6.50 (d, *J*= 7.8Hz, 1H, ArH), 6.63 (t, *J*= 7.3Hz, 1H, ArH), 6.96-7.00 (m, 2H, ArH); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 22.23, 27.29, 41.98, 114.20, 117.20, 121.57, 126.90, 129.92, 144.98.

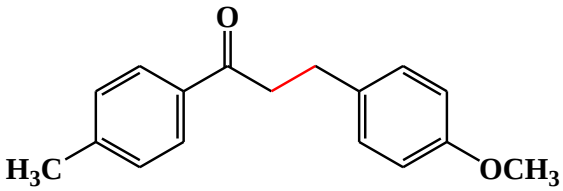
S2. Spectral details of compounds listed in Table 5

3-(4-Methoxylphenyl)-1-phenylpropan-1-one (6a)



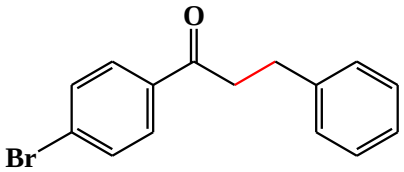
^{1}H NMR (400 MHz, $CDCl_3$): δ 3.04 (t, *J*= 7.7 Hz, 2H, CH_2), 3.30 (t, *J*= 7.7 Hz, 2H, CH_2),3.81 (s, 3H, OCH_3),6.87 (d, *J*= 8.6 Hz, 2H, ArH),7.20 (d, *J*= 8.6 Hz, 2H, ArH),7.48 (t, *J*= 7.6 Hz, 2H, ArH),7.58 (t, *J*= 7.9 Hz, 1H, ArH),7.98 (d, *J*= 7.2 Hz, 2H, ArH); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 29.28, 40.73,55.29,113.94,128.12,128.61,129.42,133.05,133.39,136.93,158.23, 199.49.

3-(4-Methoxyphenyl)-1-(4-methylphenyl)propan-1-one (6b)



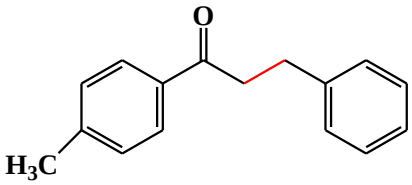
^{1}H NMR (400 MHz, $CDCl_3$): δ 2.43 (s, 3H, CH_3), 3.02 (t, *J*= 7.7 Hz, 2H, CH_2),3.27 (t, *J*= 7.7 Hz, 2H, CH_2),3.81 (s, 3H, OCH_3),6.86 (d, *J*= 8.6 Hz, 2H, ArH),7.19 (d, *J*= 8.5 Hz, 2H, ArH),7.27 (d, *J*= 8 Hz, 2H, ArH),7.88 (d, *J*= 8.2 Hz, 2H, ArH); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 21.73, 29.65, 40.74, 55.29, 113.91, 128.18, 129.29, 129.37, 133.43, 134.40,158.23, 199.21.

1-(4-Bromophenyl)-3-phenylpropan-1-one (6c)



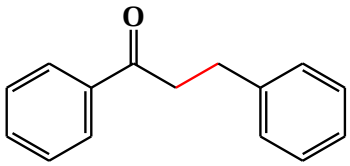
^{1}H NMR (400 MHz, $CDCl_3$): δ 3.10 (t, *J*= 4Hz, 2H, CH_2), 3.34 (t, *J*= 4Hz, 2H, CH_2), 7.22-7.61 (m, 7H, ArH), 7.99 (d, *J*= 4Hz,2H, ArH); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 30.14, 40.47, 126.15, 128.05, 128.44, 128.54, 128.62, 133.08, 136.86, 141.30, 199.21.

1-(4-Methylphenyl)-3-phenylpropan-1-one (6d)



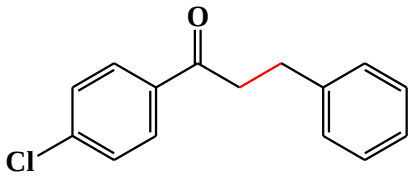
^{1}H NMR (400 MHz, $CDCl_3$): δ 2.44 (s, 3H, CH_3), 3.10(t, *J*= 7.7 Hz, 2H, CH_2),3.32 (t, *J*= 8 Hz, 2H, CH_2),7.23-7.36(m, 7H, ArH), 7.90 (d, *J*= 8.1 Hz, 2H, ArH); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 21.68, 30.32, 40.39, 126.14, 128.21, 128.47, 128.55, 129.32, 134.38, 141.47, 143.89, 198.98.

1,3-Diphenylpropan-1-one (6e)



^{1}H NMR (400 MHz, $CDCl_3$): δ 3.10 (t, *J*= 7.7 Hz, 2H, CH_2), 3.34 (t, *J*= 7.7 Hz, 2H, CH_2), 7.22-7.35 (m, 5H, ArH),7.48 (t, *J*= 7.6 Hz, 2H, ArH), 7.59 (t, *J*=7.4 Hz, 1H,ArH), 7.99 (d, *J*= 7.4 Hz, 2H, ArH); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 30.13, 40.48,126.15, 128.06, 128.45, 128.55, 128.64, 128.63,133.10,136.84,141.30, 199.29.

3-(4-Chlorophenyl)-1-phenylpropan-1-one (6f)



^{1}H NMR (400 MHz, $CDCl_3$): δ 3.06 (t, *J*= 8Hz,2H, CH_2), 3.20 (t, *J*= 8Hz, 2H,CH_2), 7.20-7.61 (m, 7H, ArH), 7.97 (d, *J*= 8Hz,2H, ArH); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 29.39, 40.13, 128.02, 128.61, 128.65, 129.83, 131.89, 133.16, 136.79, 139.75, 198.84.

S3. ^{1}H NMR and ^{13}C NMR spectra of compounds listed in **Table 4**

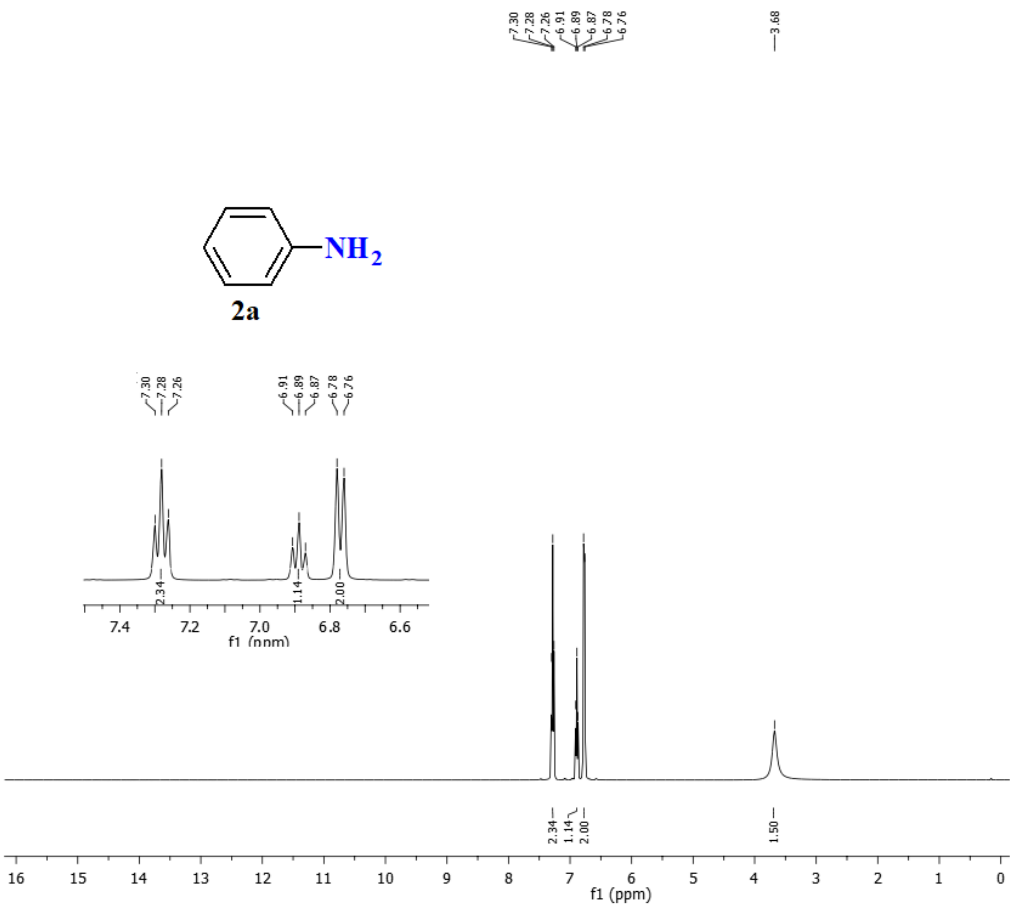


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Figure 1. ^{1}H NMR spectra of Aniline.

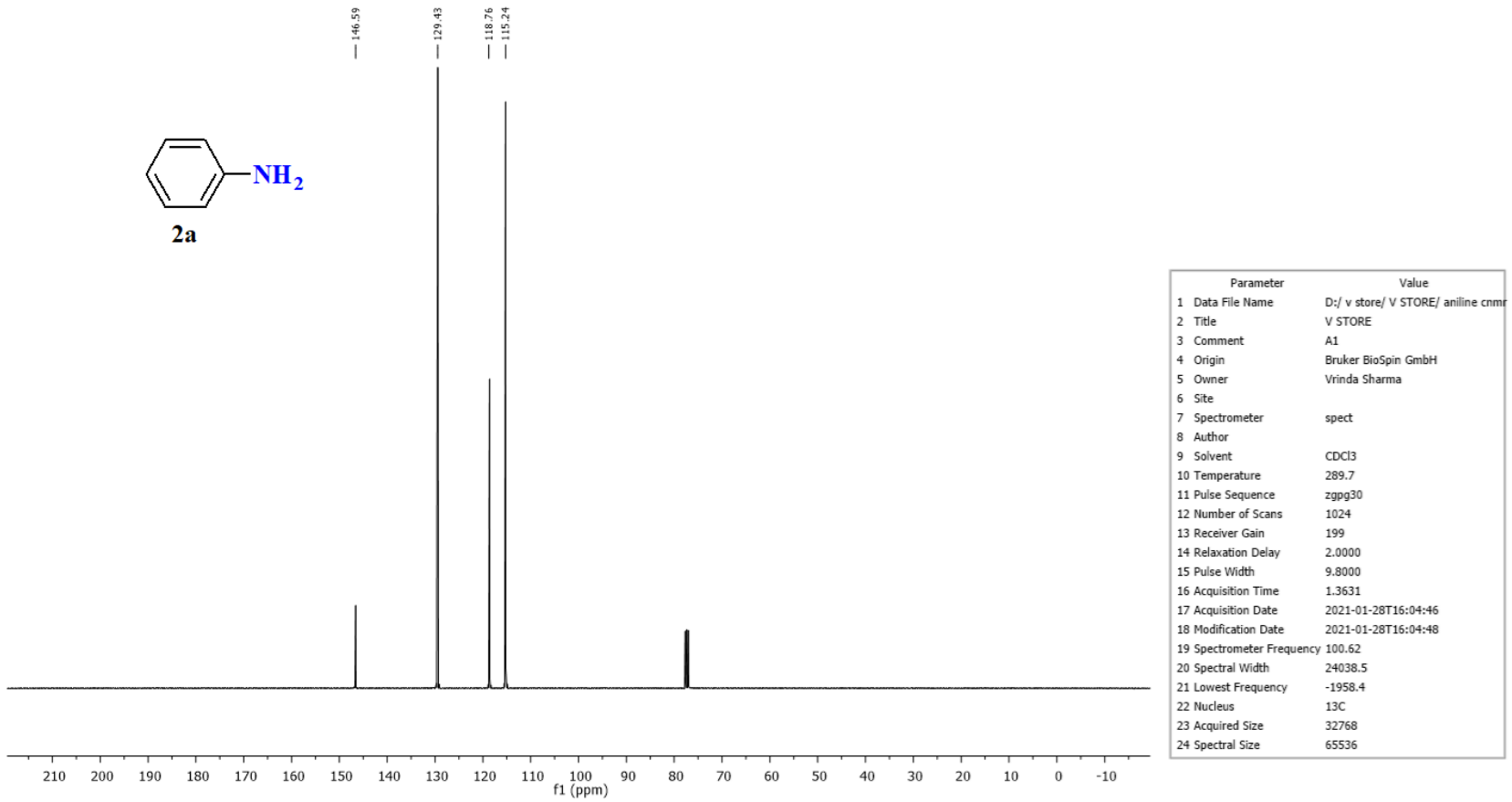

Figure 2. ^{13}C NMR spectra of Aniline.

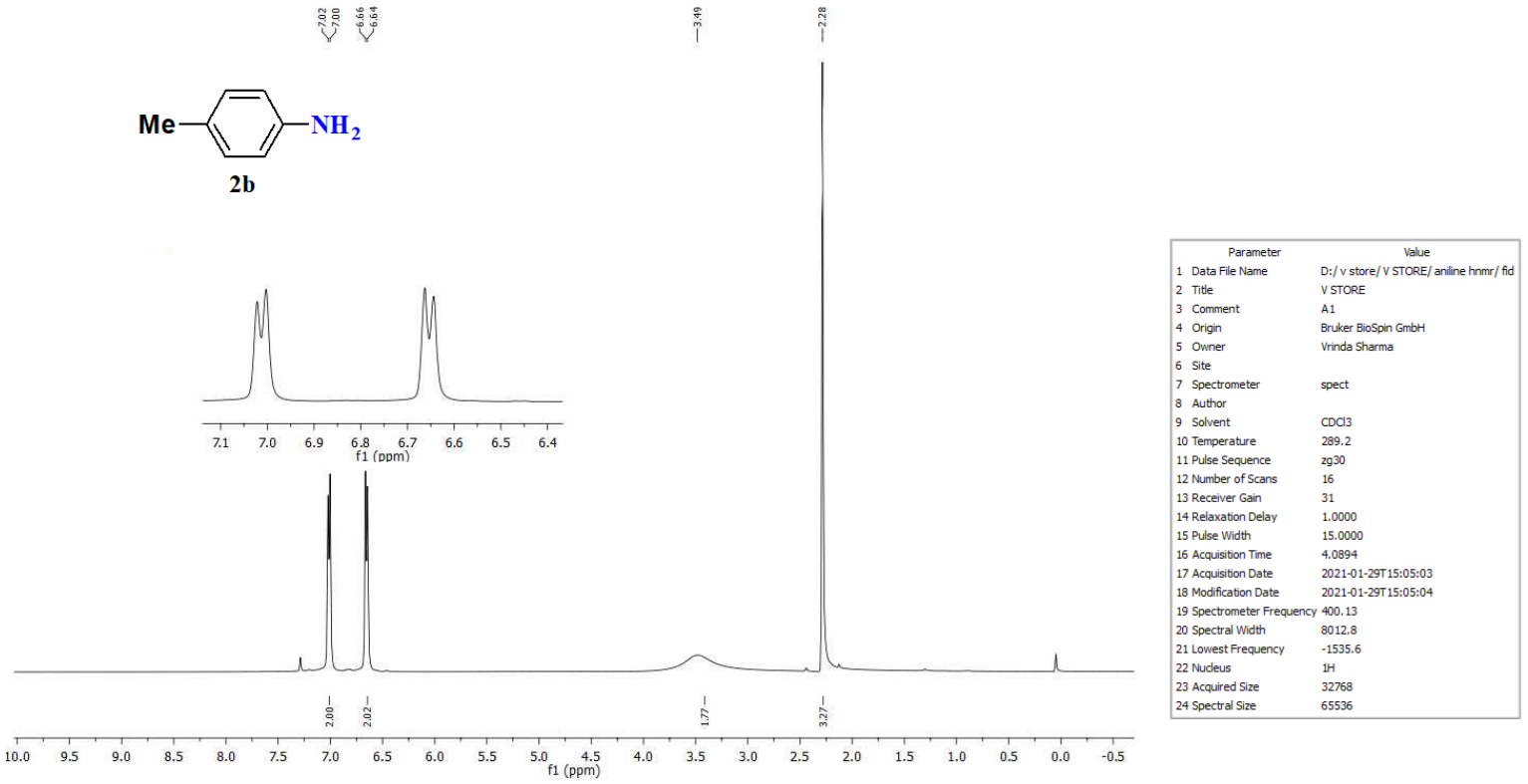

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Figure 3. ^{1}H NMR spectra of 4-Methylaniline.

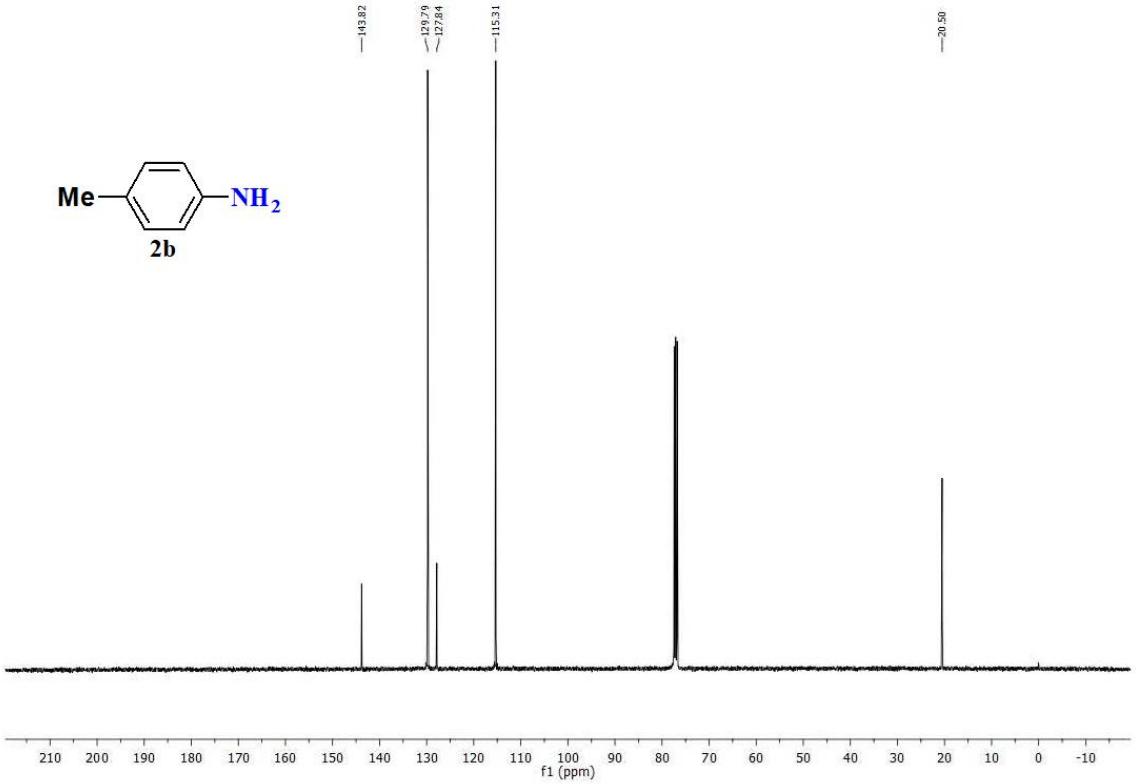

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Figure 4. ^{13}C NMR spectra of 4-Methylaniline.

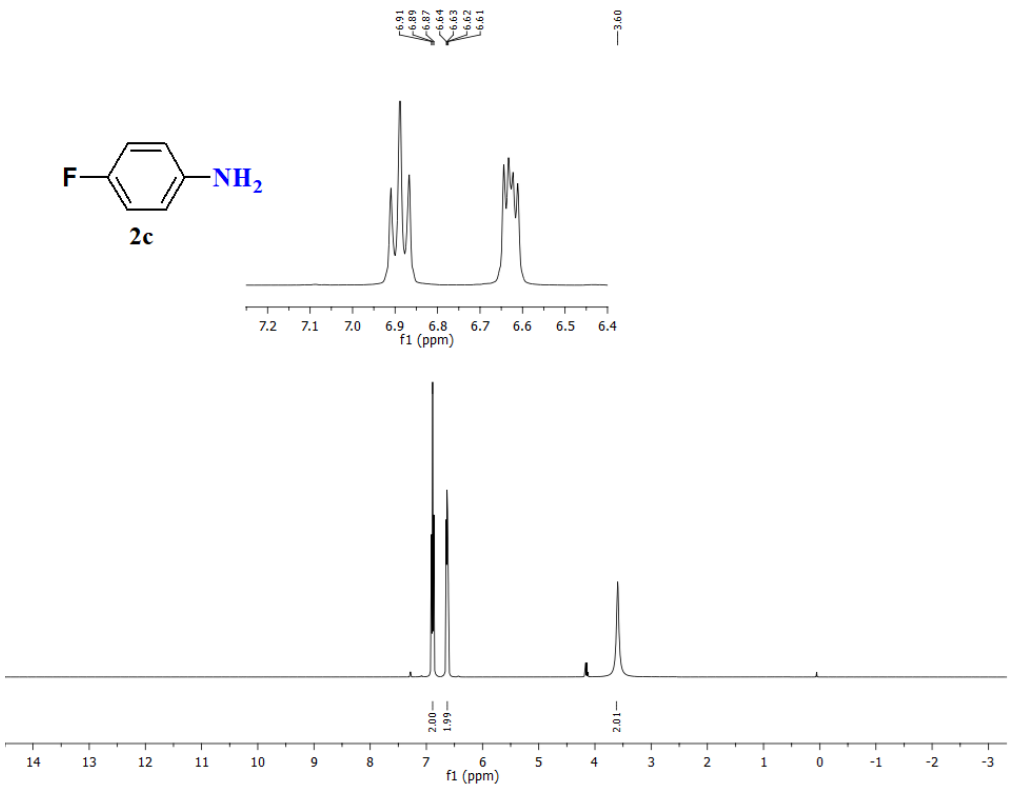

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Figure 5. ^{1}H NMR spectra of 4-Fluoroaniline.

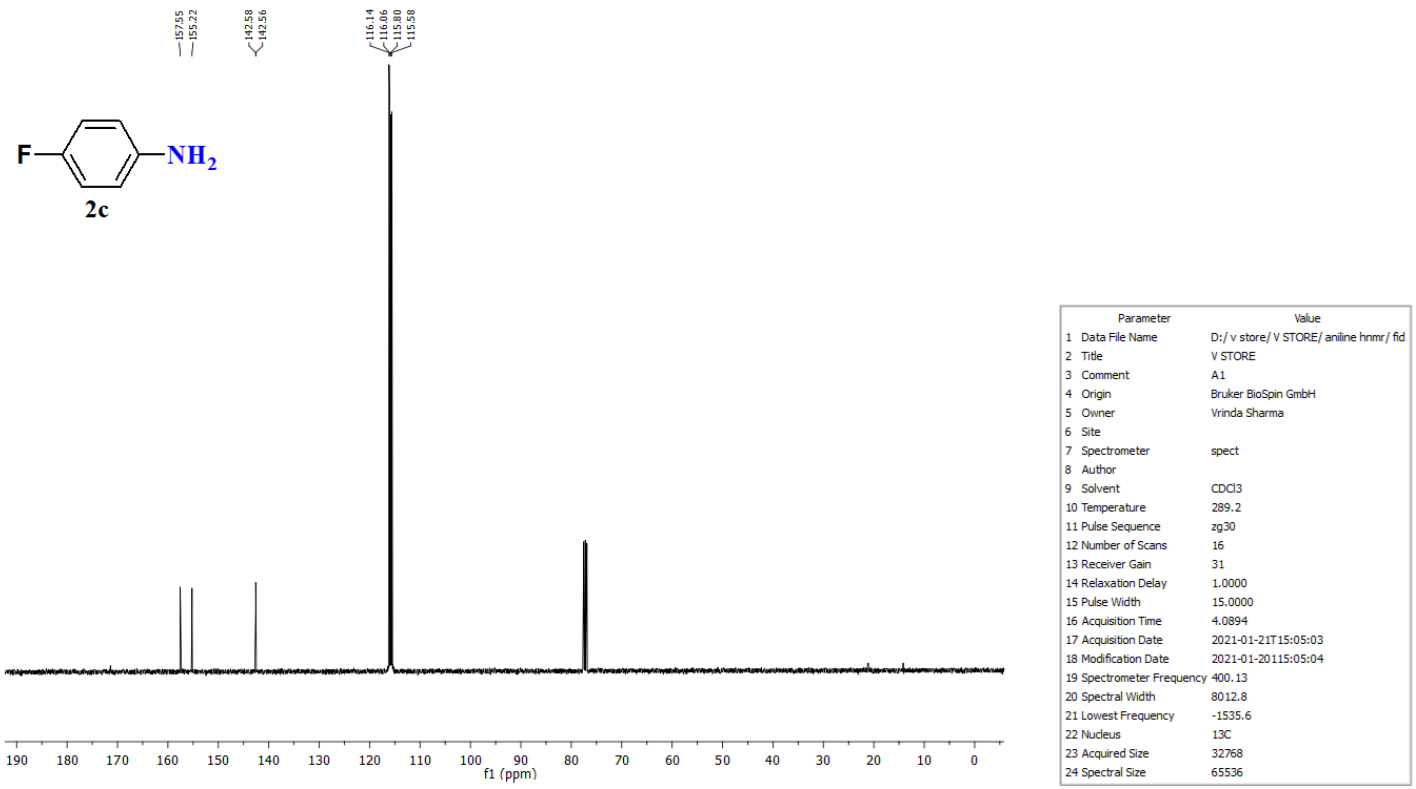

Figure 6. ^{13}C NMR spectra of 4-Fluoroaniline.

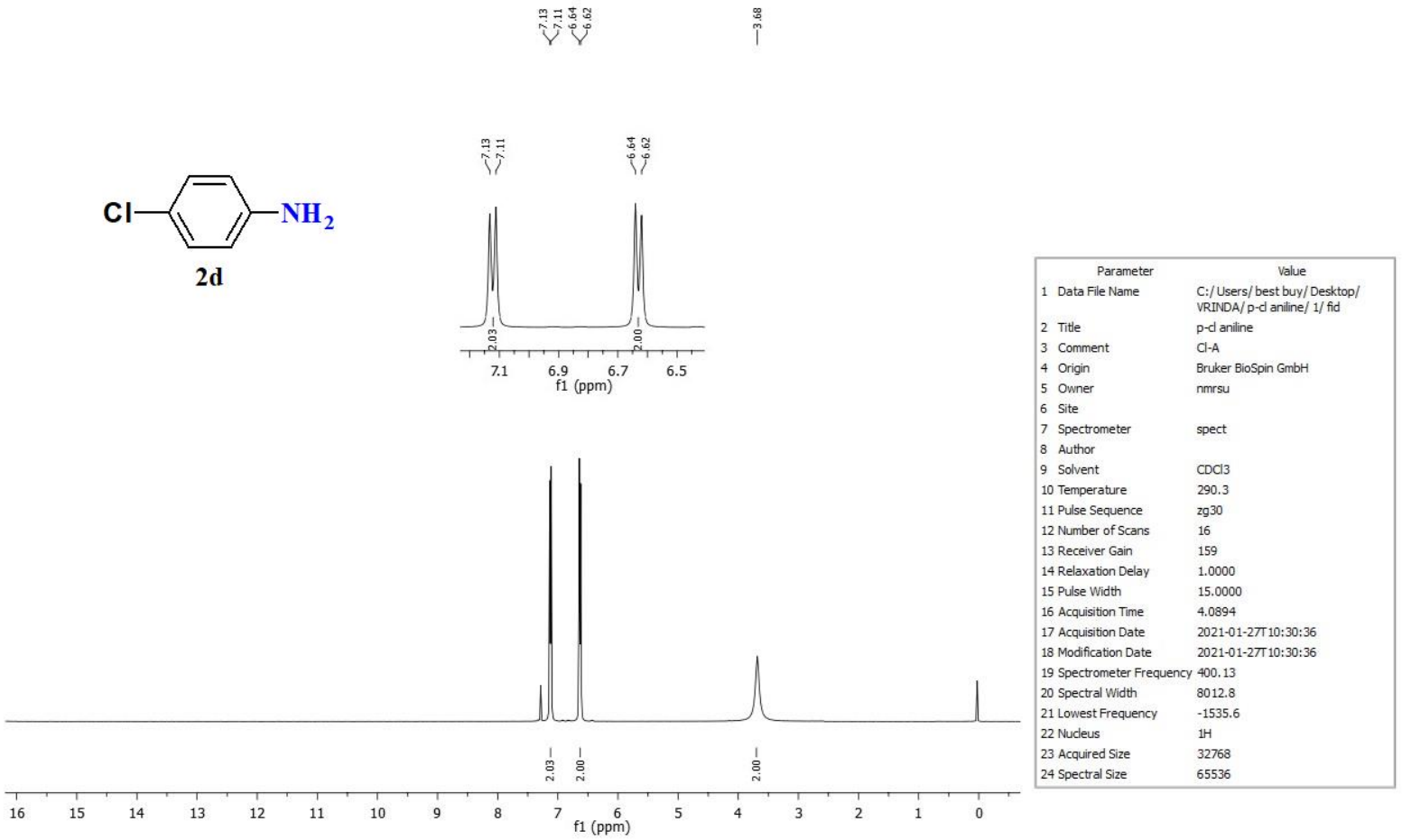

Figure 7. ^{1}H NMR spectra of 4-Chloroaniline.

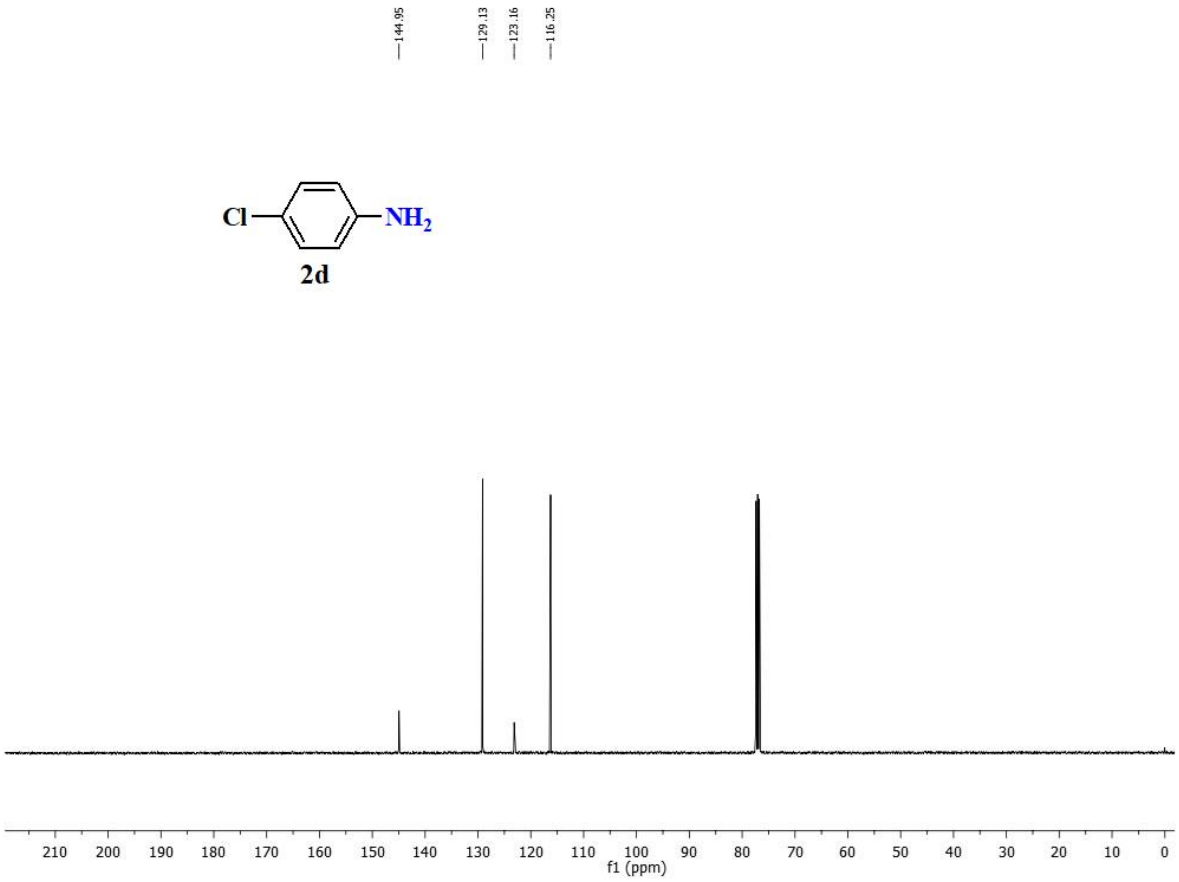

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Figure 8. ^{13}C NMR spectra of 4-Chloroaniline.

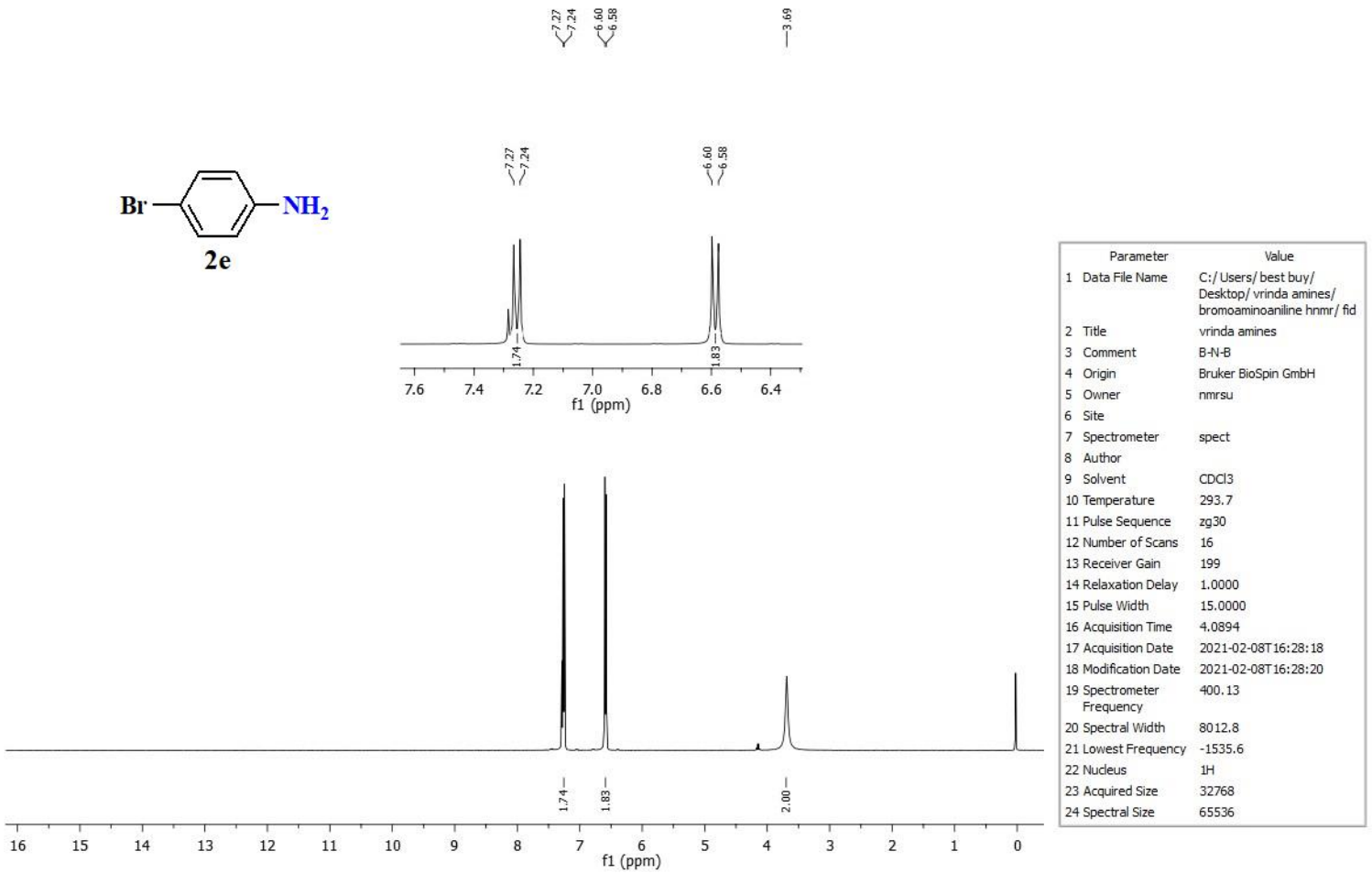

Figure 9. ^{1}H NMR spectra of 4-Bromoaniline.

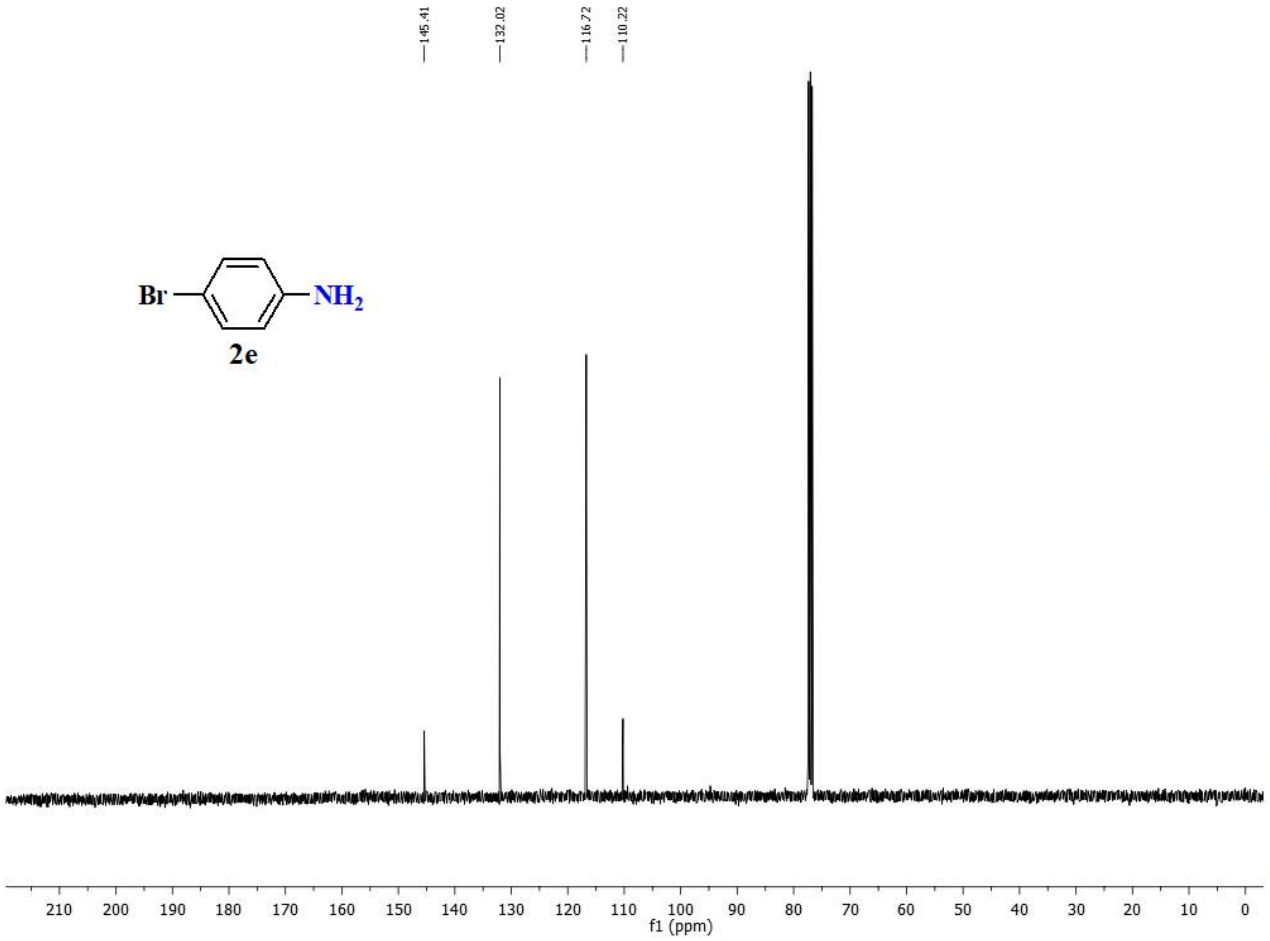

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Figure 10. ^{13}C NMR spectra of 4-Bromoaniline.

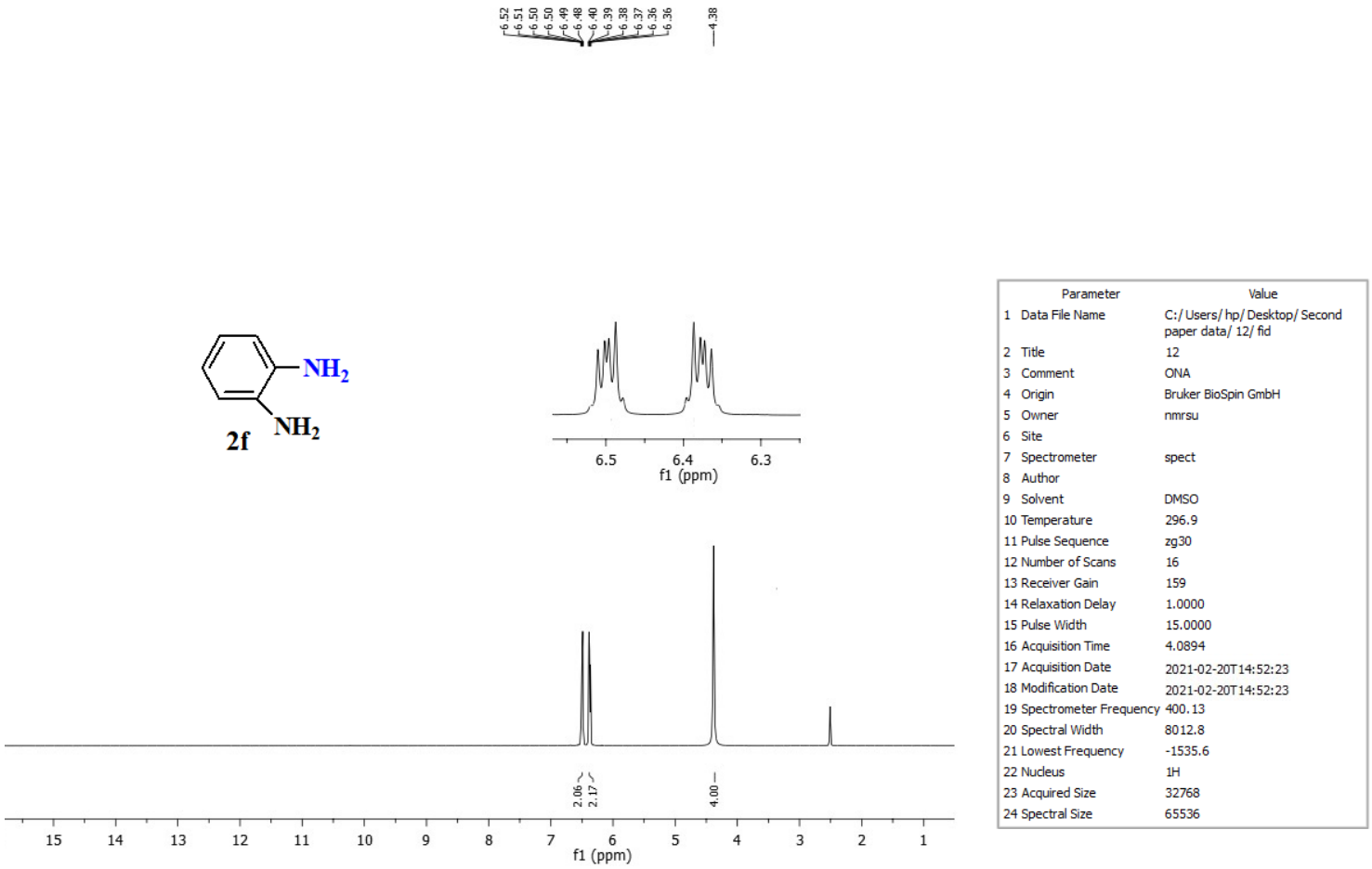
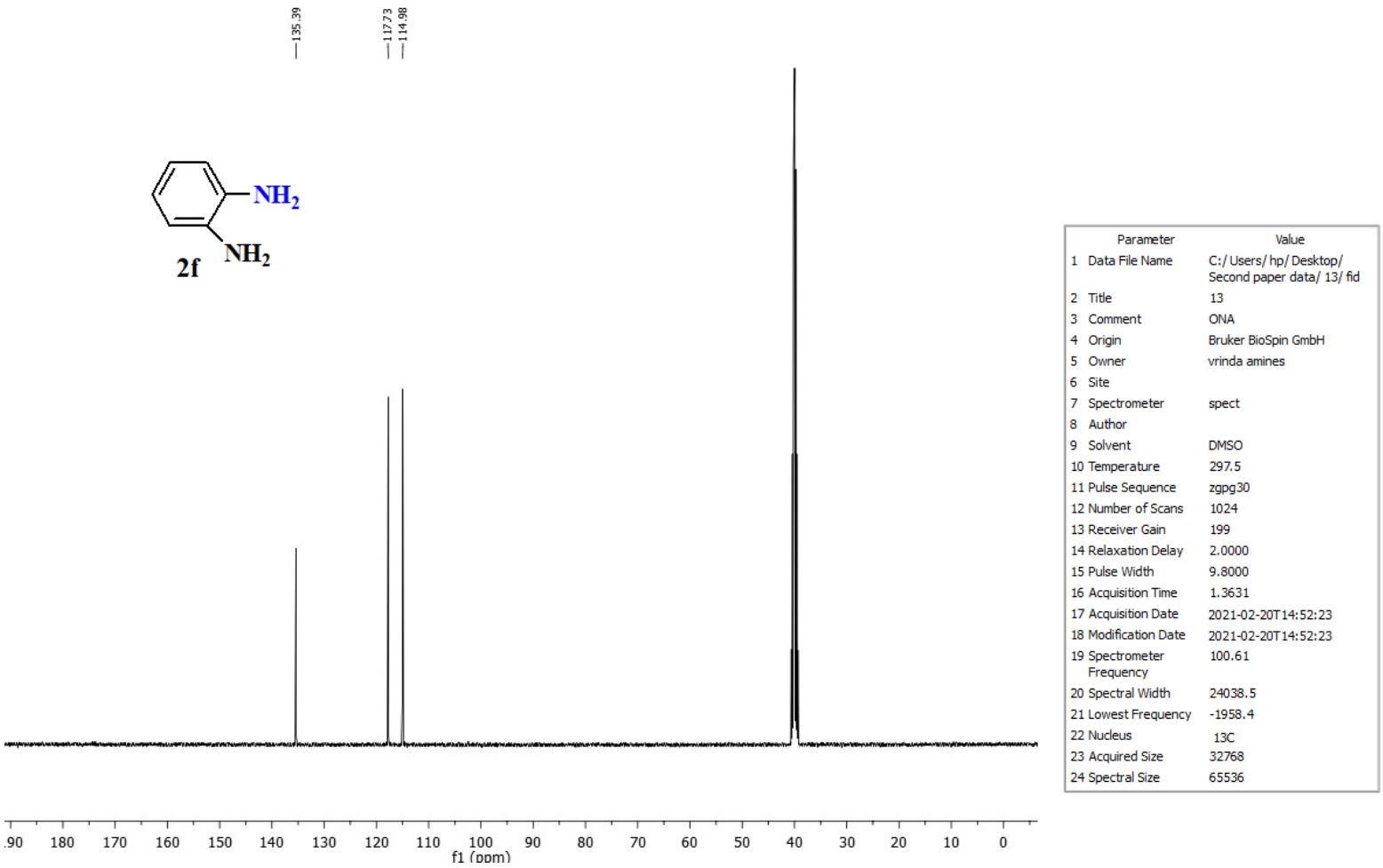


Figure 11. ^{1}H NMR spectra of 1,2-Diaminobenzene.



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5	Owner	vrinda amines
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	DMSO
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15	Pulse Width	9.8000
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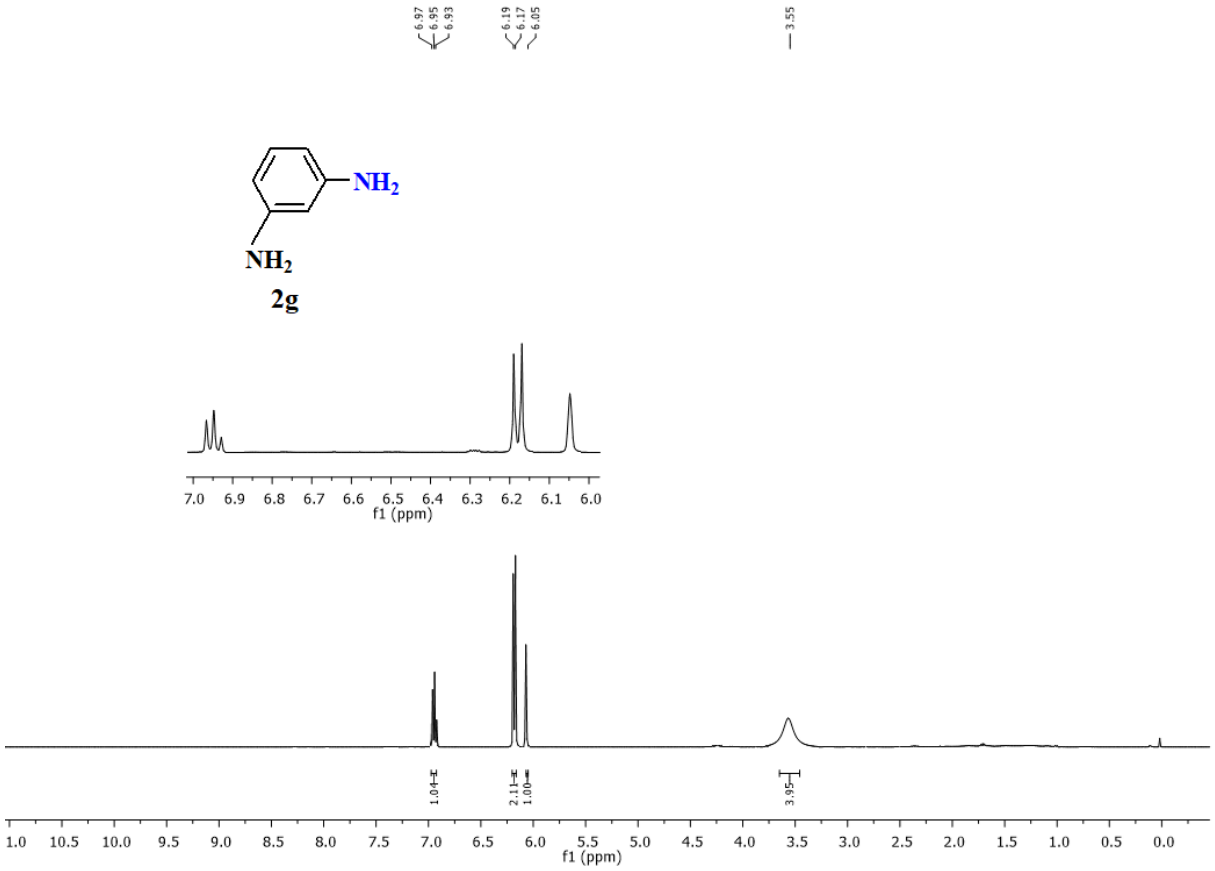
17	Acquisition Date	2021-02-20T14:52:23
18	Modification Date	2021-02-20T14:52:23
19	Spectrometer Frequency	100.61
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

Figure 12. ^{13}C NMR spectra of 1,2-Diaminobenzene.



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6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	289.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	31
14	Relaxation Delay	1.0000
15	Pulse Width	15.0000
16	Acquisition Time	4.0894
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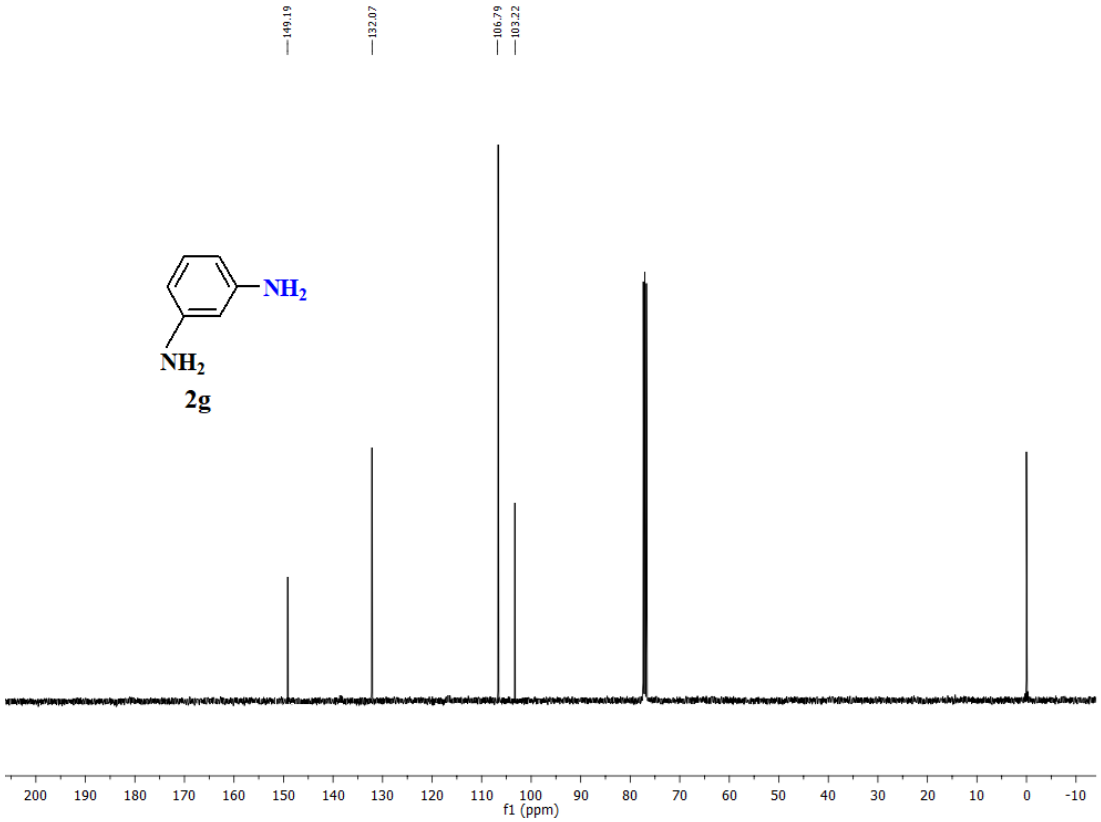
18	Modification Date	2021-02-22T15:03:45
19	Spectrometer Frequency	400.13
20	Spectral Width	8012.8
21	Lowest Frequency	-1535.6
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

Figure 13. ^{1}H NMR spectra of 1,3-Diaminobenzene.



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6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	289.2
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15 Pulse Width	15.0000
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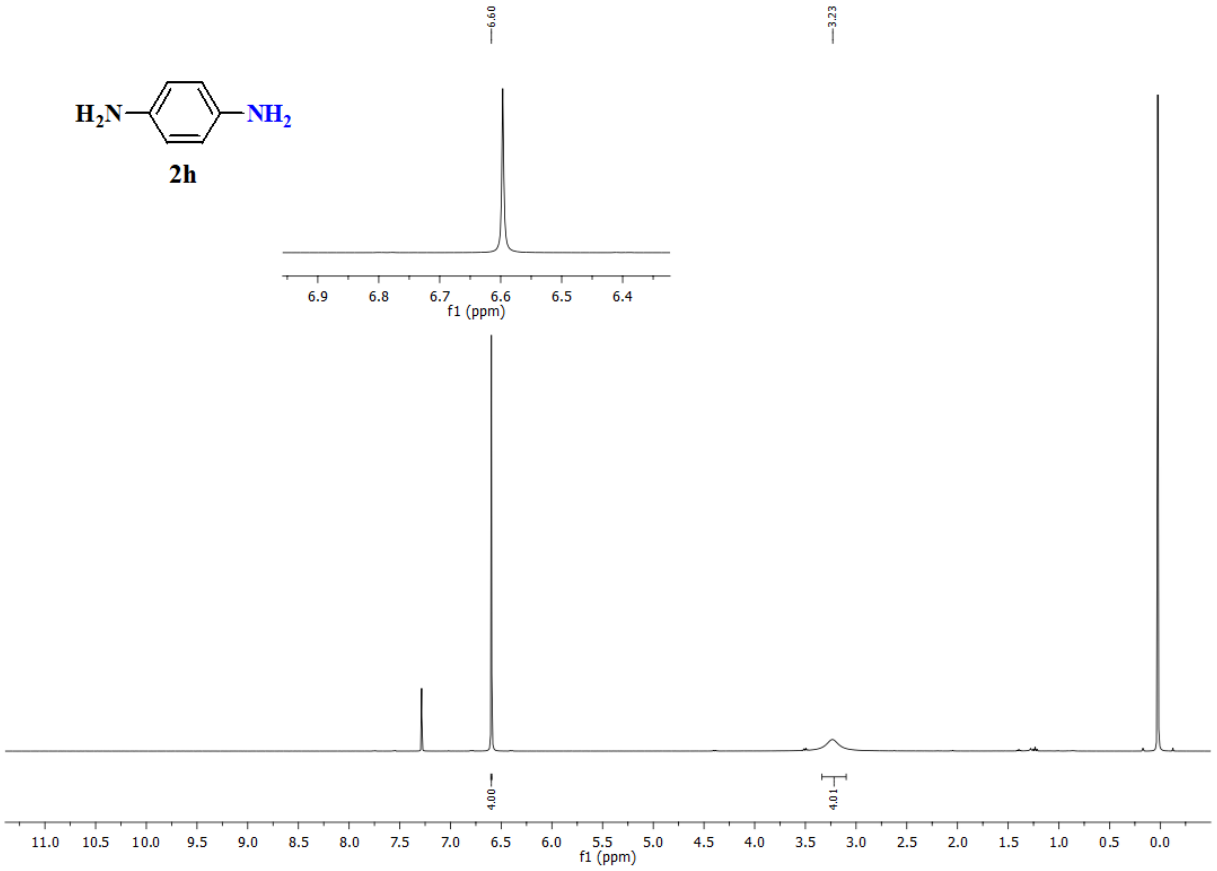
18 Modification Date	2021-02-22T15:03:45
19 Spectrometer Frequency	400.13
20 Spectral Width	8012.8
21 Lowest Frequency	-1535.6
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

Figure 14. ^{13}C NMR spectra of 1,3-Diaminobenzene.



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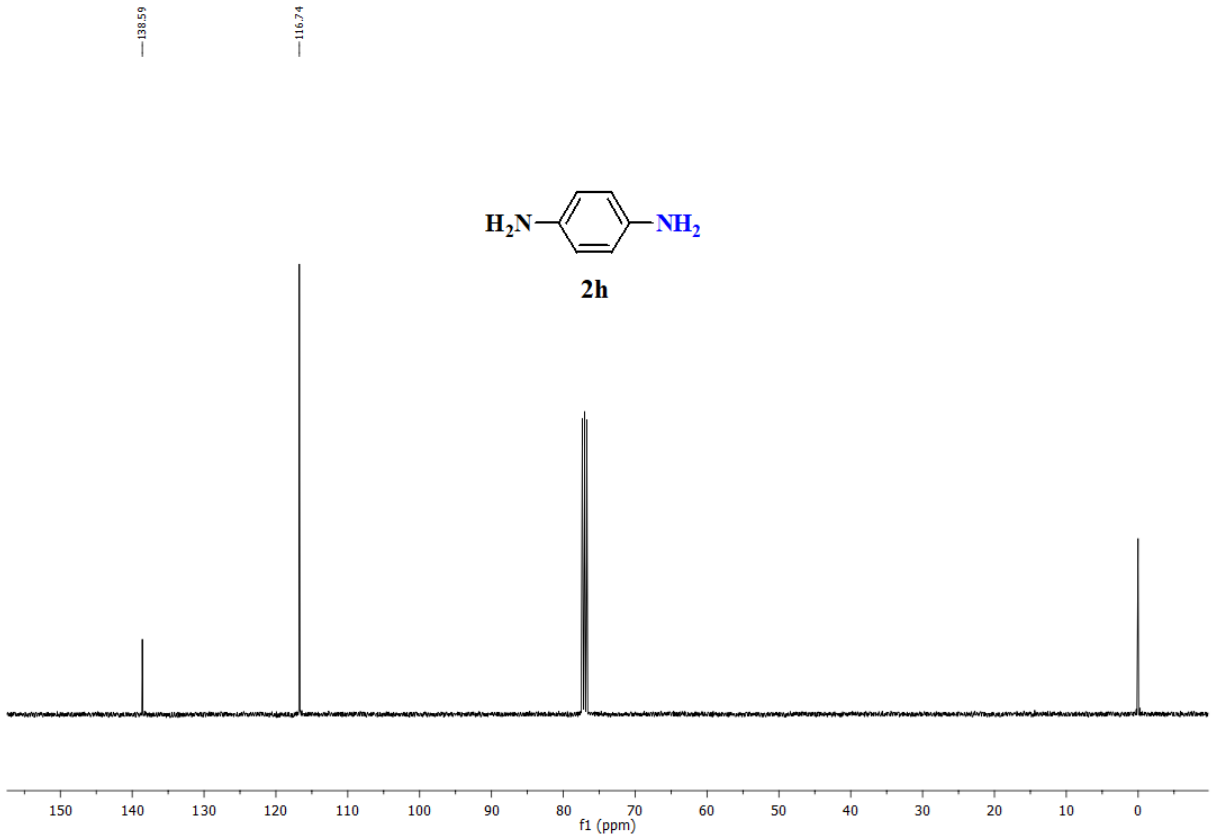
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	289.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	31
14	Relaxation Delay	1.0000
15	Pulse Width	15.0000
16	Acquisition Time	4.0894
17	Acquisition Date	2021-02-21T15:03:00
18	Modification Date	2021-02-21T15:03:02
19	Spectrometer Frequency	400.13
20	Spectral Width	8012.8
21	Lowest Frequency	-1535.6
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Figure 15. ^{1}H NMR spectra of 1,4-Diaminobenzene.



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3	Comment	A1
4	Origin	Bruker BioSpin GmbH
5	Owner	Vrinda Sharma
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	289.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	31
14	Relaxation Delay	1.0000
15	Pulse Width	15.0000
16	Acquisition Time	4.0894
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18	Modification Date	2021-02-21T15:03:45
19	Spectrometer Frequency	400.13
20	Spectral Width	8012.8
21	Lowest Frequency	-1535.6
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

Figure 16. ^{13}C NMR spectra of 1,4-Diaminobenzene.

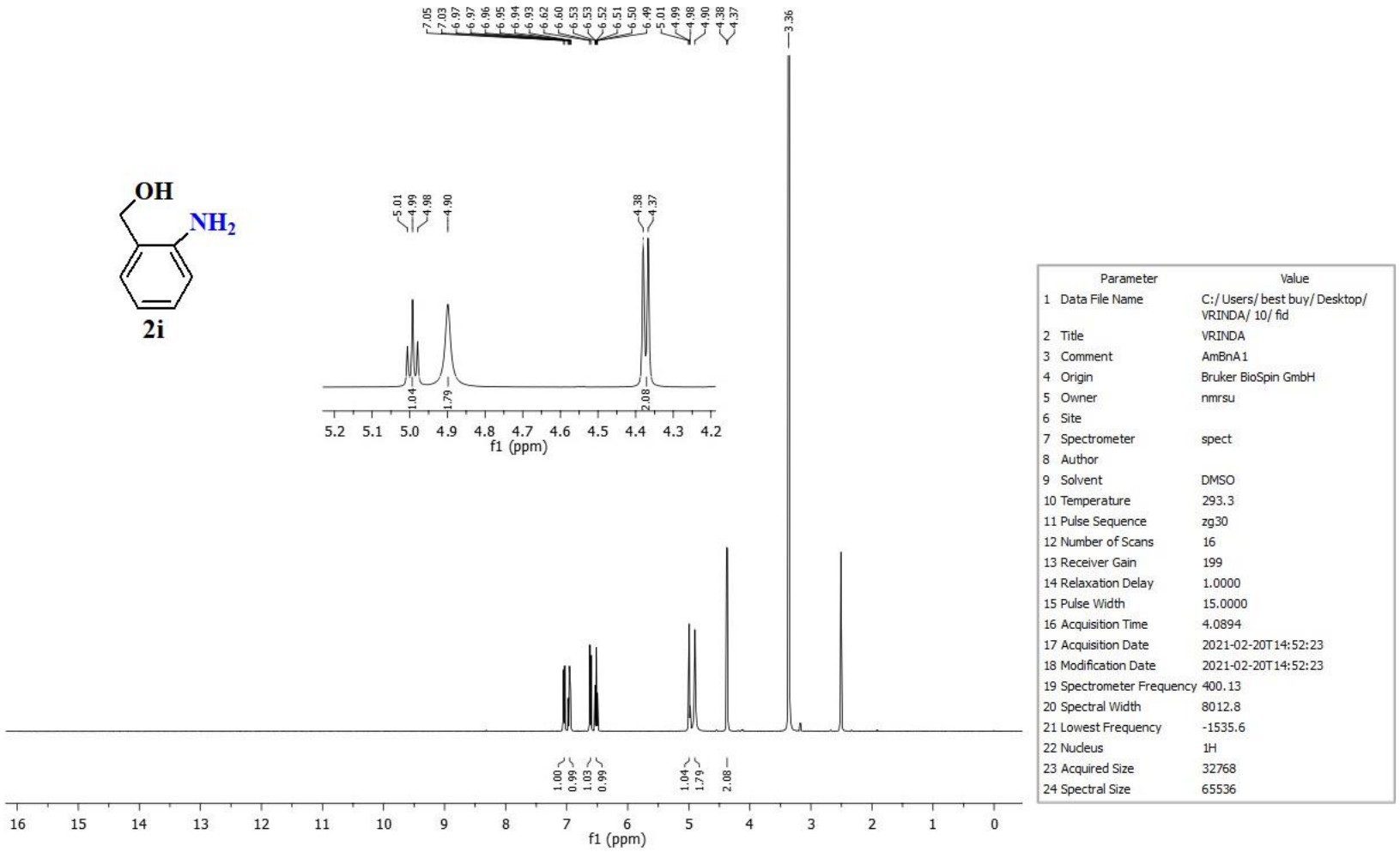
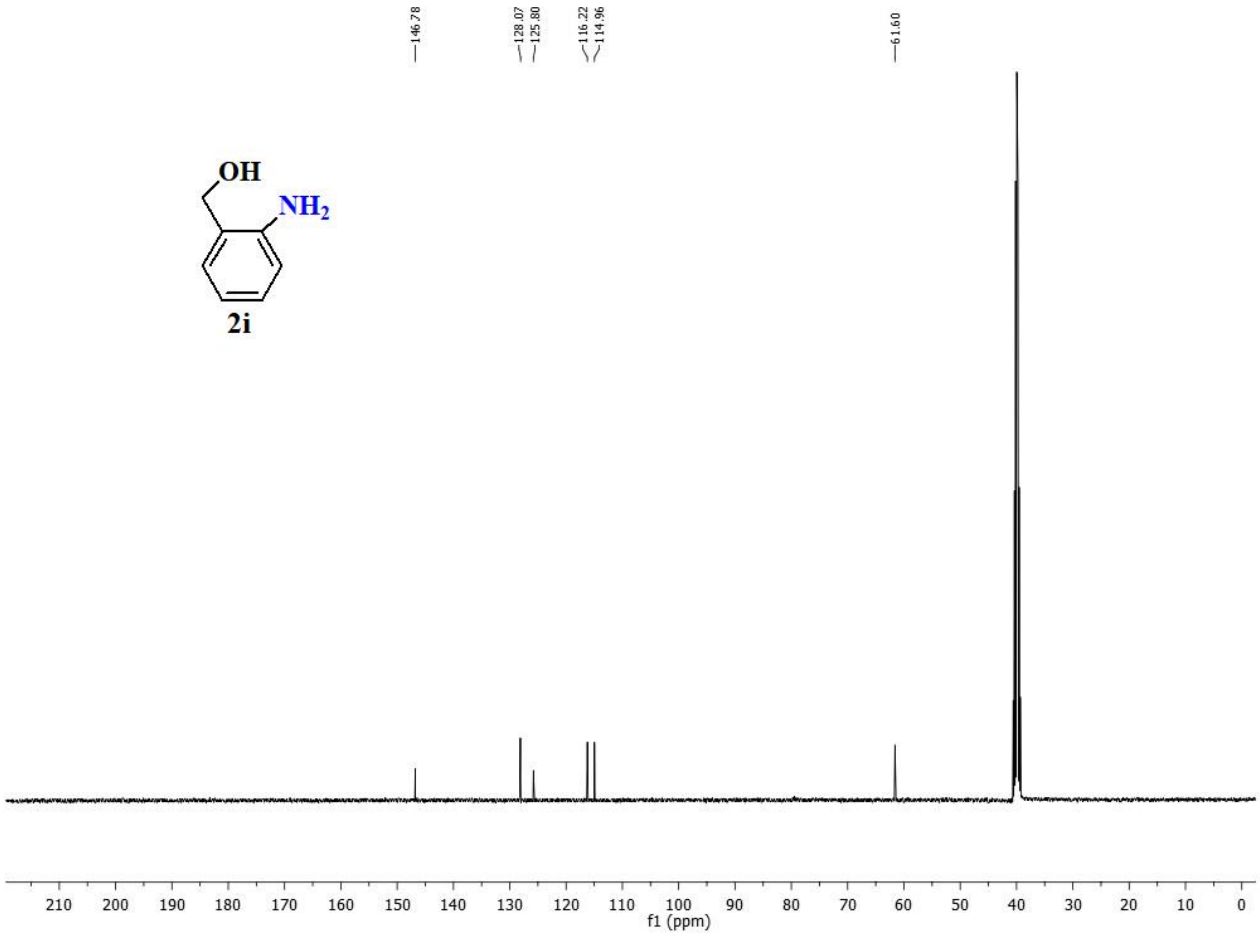


Figure 17. ^{1}H NMR spectra of 2-Aminobenzylalcohol.



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6 Site	
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8 Author	
9 Solvent	DMSO
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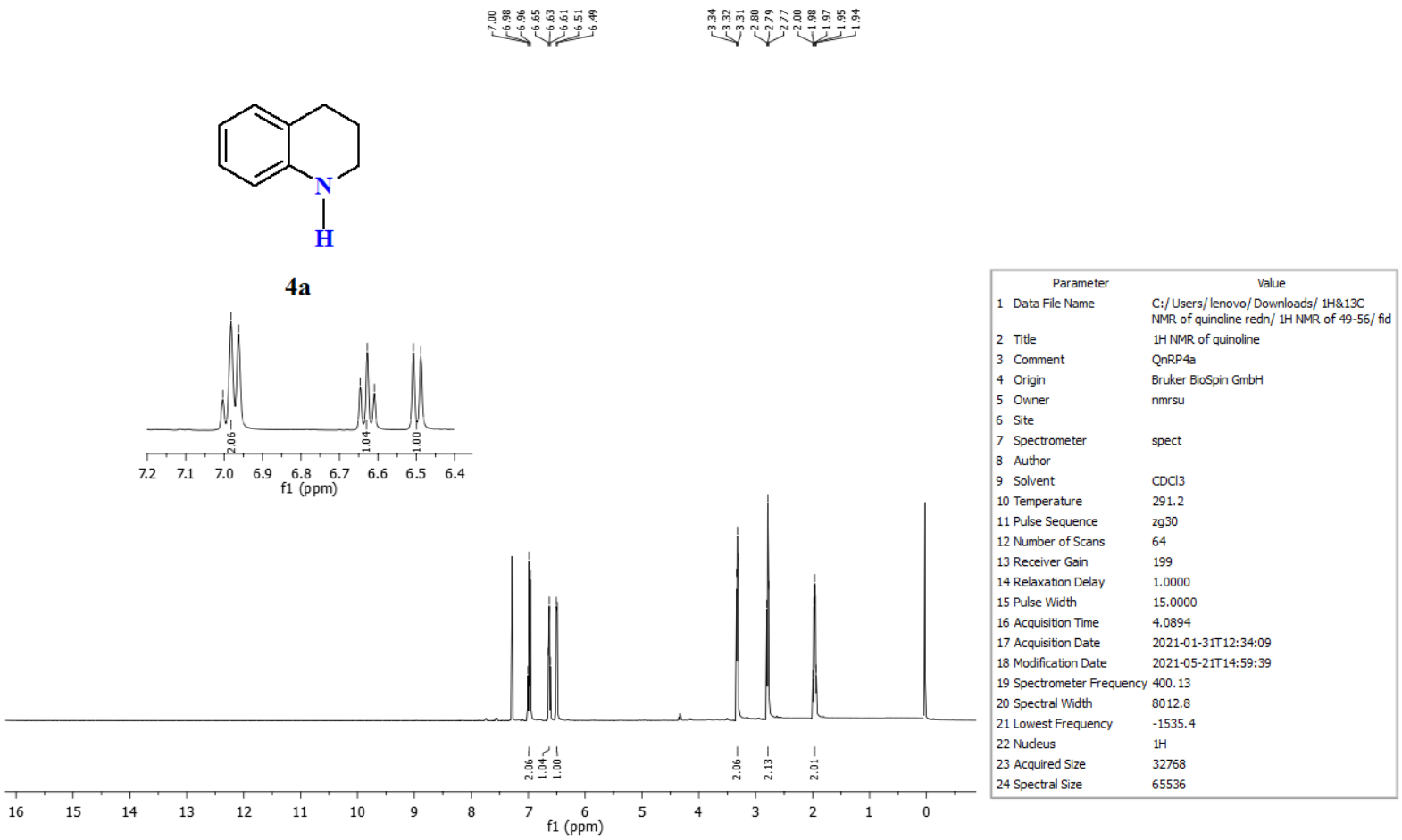
11 Pulse Sequence	zgpg30
12 Number of Scans	1024
13 Receiver Gain	199
14 Relaxation Delay	2.0000
15 Pulse Width	9.8000
16 Acquisition Time	1.3631
17 Acquisition Date	2021-02-20T15:52:05
18 Modification Date	2021-02-20T15:52:06
19 Spectrometer Frequency	100.61
20 Spectral Width	24038.5
21 Lowest Frequency	-1958.4
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	65536

Figure 18. ^{13}C NMR spectra of 2-Aminobenzylalcohol.



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5	Owner	nmrsu
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	291.2
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13	Receiver Gain	199
14	Relaxation Delay	1.0000
15	Pulse Width	15.0000
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18	Modification Date	2021-05-21T14:59:39
19	Spectrometer Frequency	400.13
20	Spectral Width	8012.8
21	Lowest Frequency	-1535.4
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Figure 19. ^{1}H NMR spectra of Quinoline.

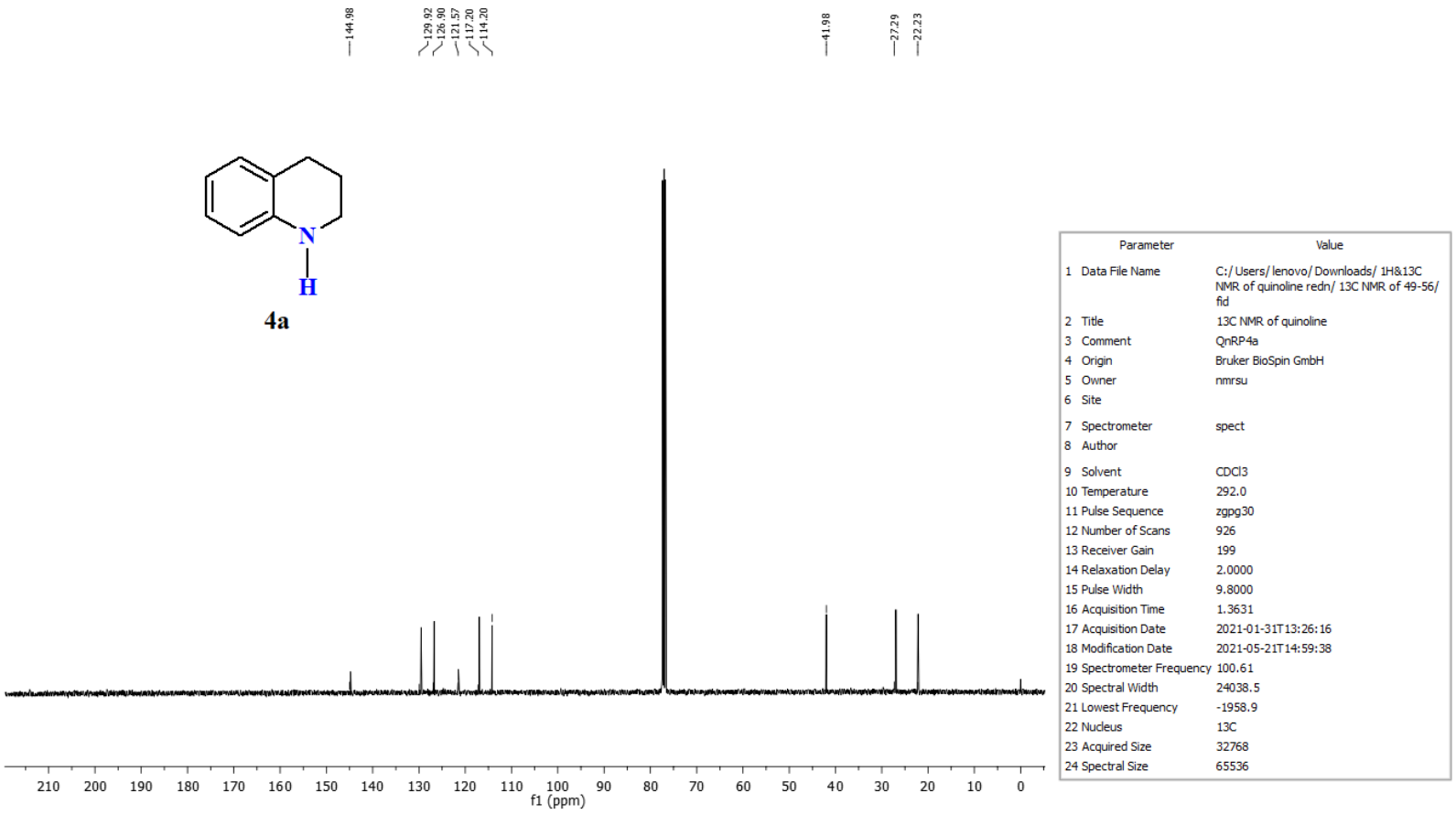


Figure 20. ^{13}C NMR spectra of Quinoline.

S4. ^{1}H NMR and ^{13}C NMR spectra of compounds listed in **Table 5**

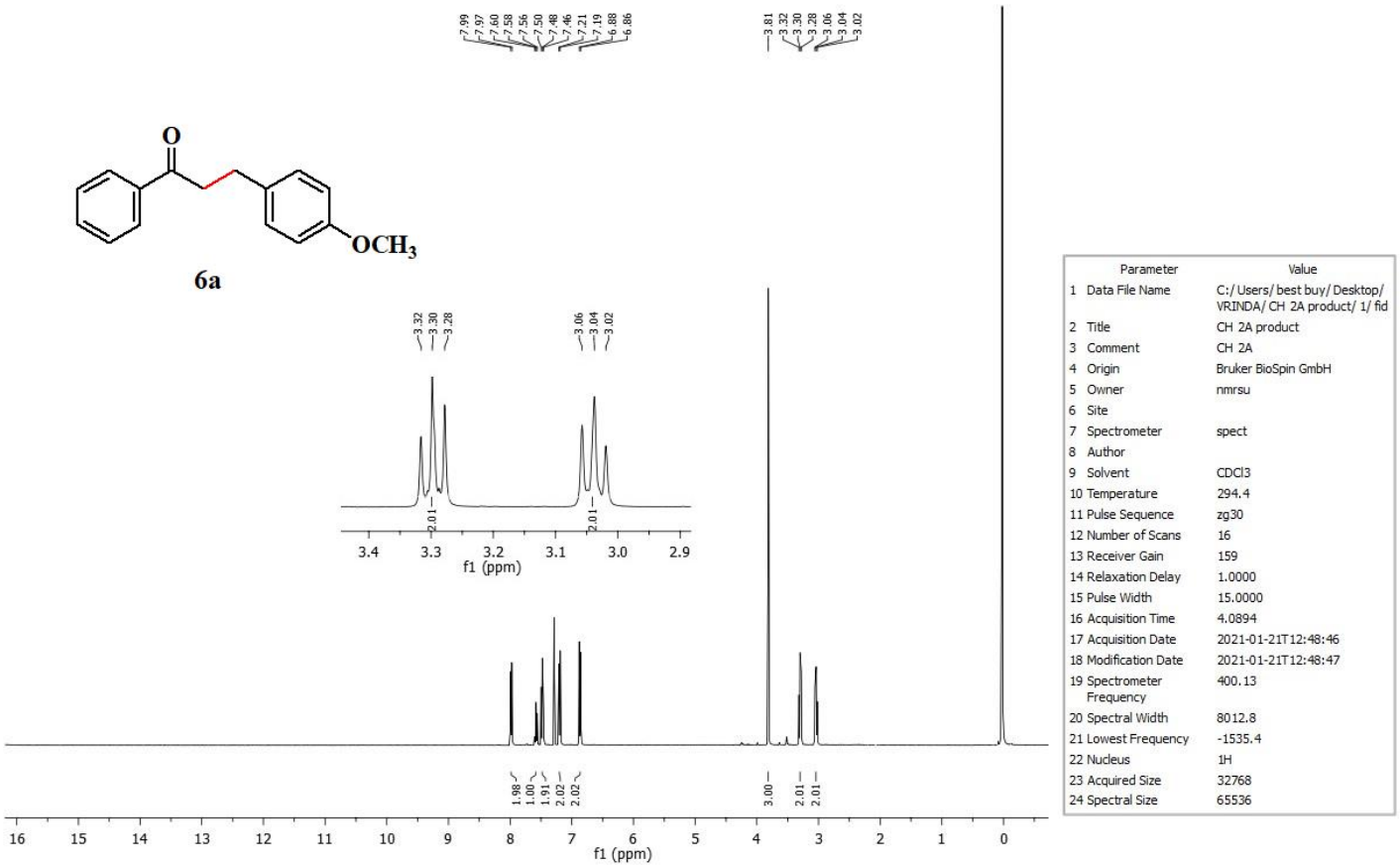
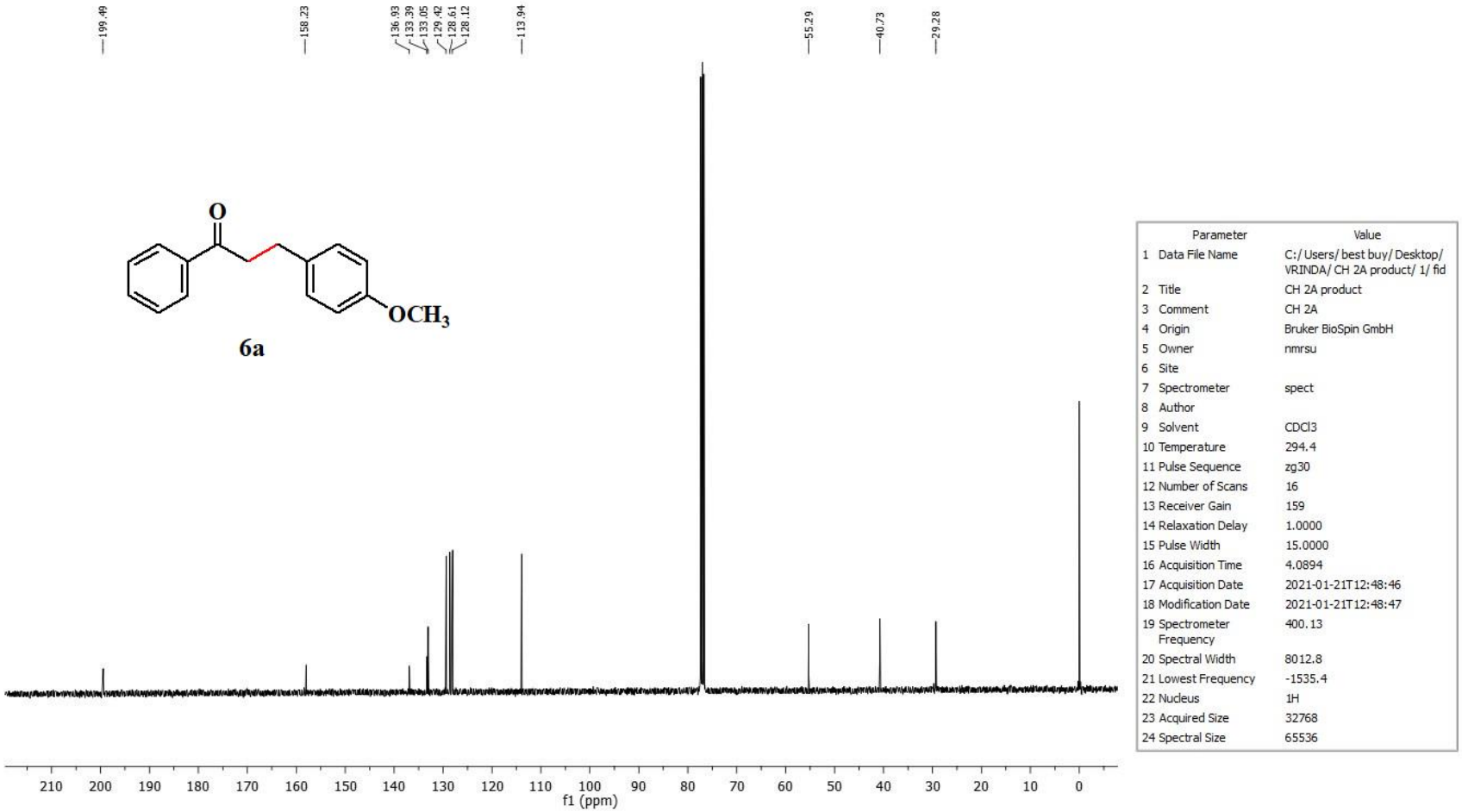


Figure 21. ^{1}H NMR spectra of 3-(4-Methoxylphenyl)-1-phenylpropan-1-one.



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6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	294.4
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	159
14	Relaxation Delay	1.0000
15	Pulse Width	15.0000
16	Acquisition Time	4.0894
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19	Spectrometer Frequency	400.13
20	Spectral Width	8012.8
21	Lowest Frequency	-1535.4
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Figure 22. ^{13}C NMR spectra of 3-(4-Methoxylphenyl)-1-phenylpropan-1-one.

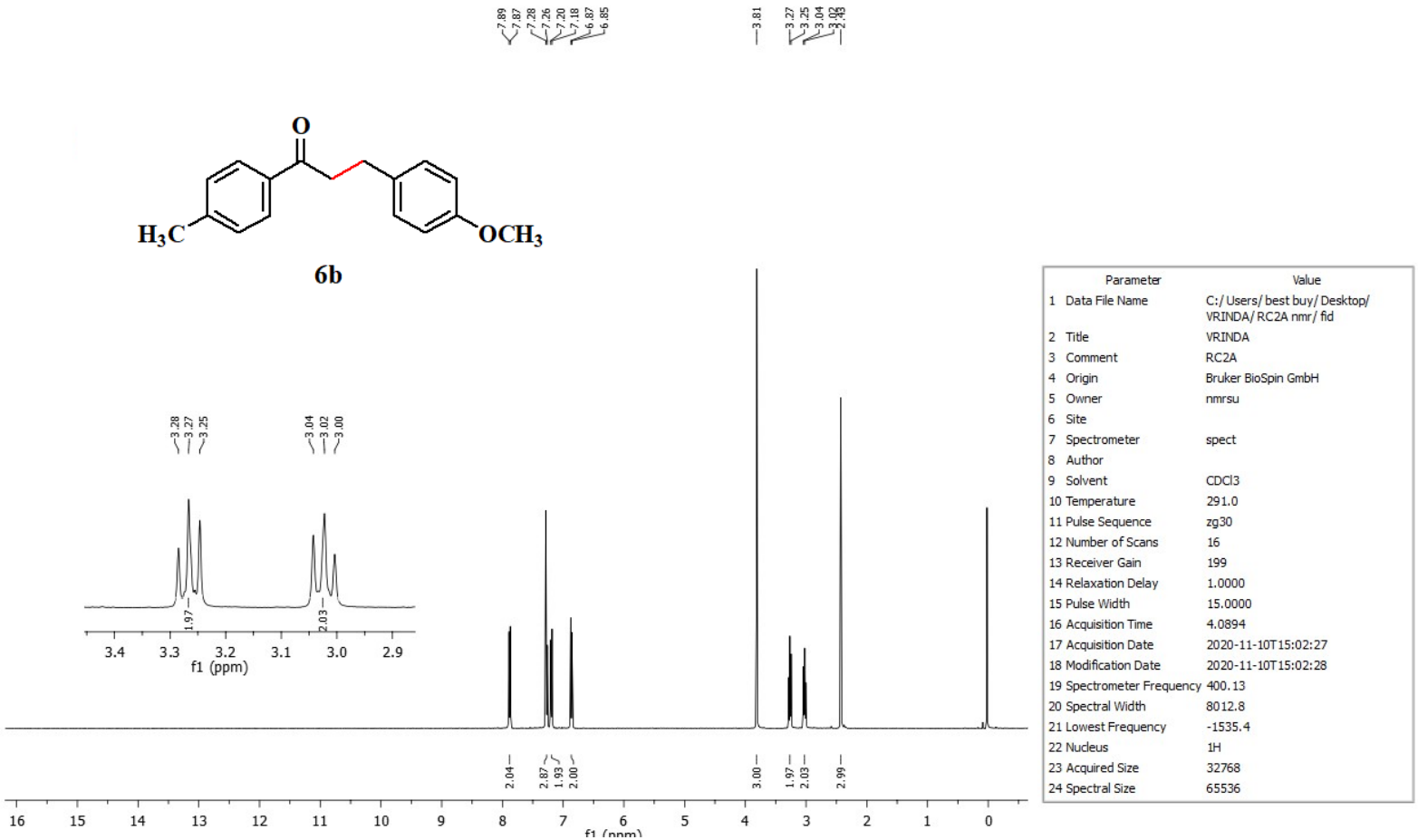
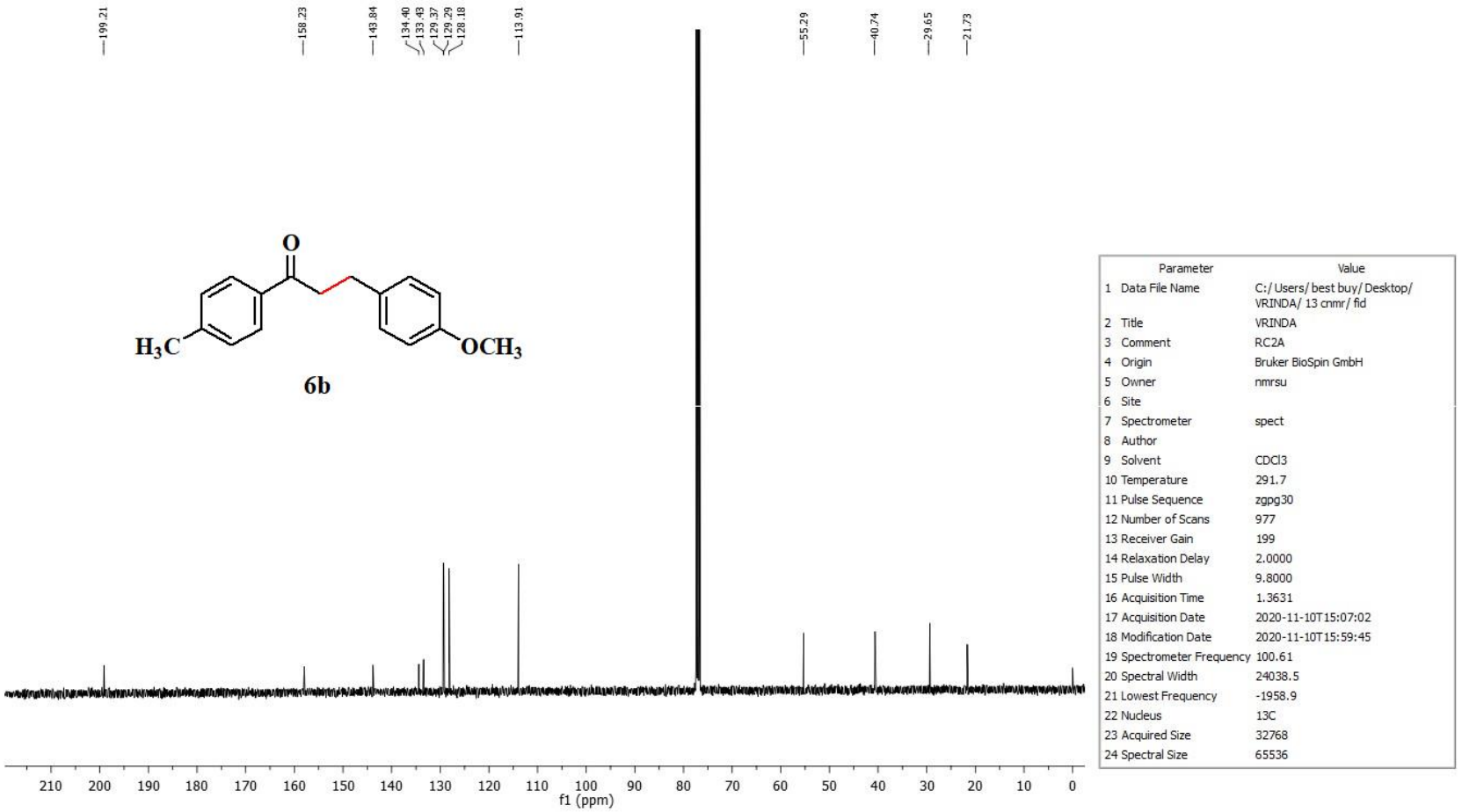


Figure 23. ^{1}H NMR spectra of 3-(4-Methoxyphenyl)-1-(4-methylphenyl)propan-1-one.



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8	Author	
9	Solvent	CDCl3
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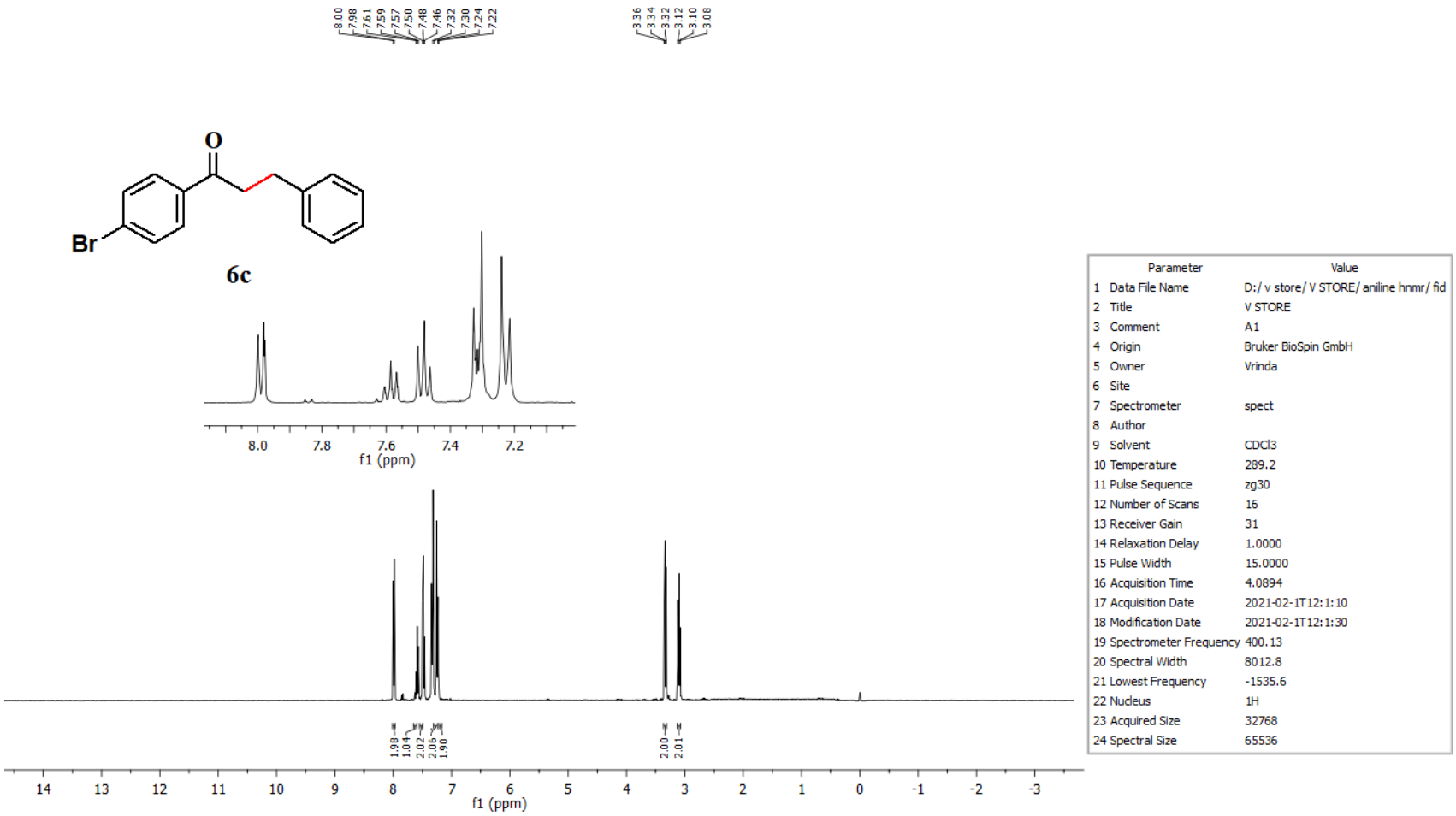
13	Receiver Gain	199
14	Relaxation Delay	2.0000
15	Pulse Width	9.8000
16	Acquisition Time	1.3631
17	Acquisition Date	2020-11-10T15:07:02
18	Modification Date	2020-11-10T15:59:45
19	Spectrometer Frequency	100.61
20	Spectral Width	24038.5
21	Lowest Frequency	-1958.9
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

Figure 24. ^{13}C NMR spectra of 3-(4-Methoxyphenyl)-1-(4-methylphenyl)propan-1-one.



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7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	289.2
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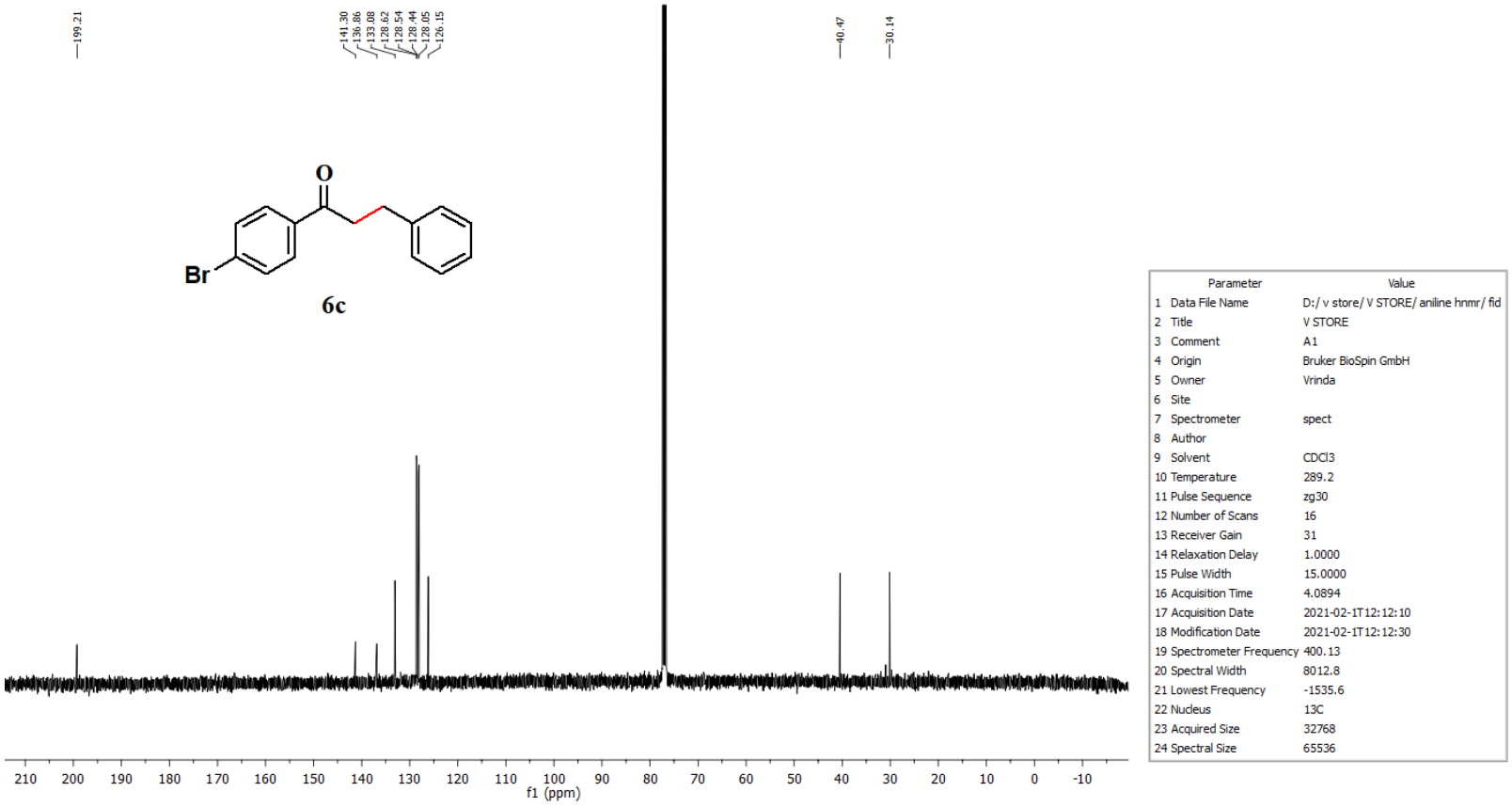
12	Number of Scans	16
13	Receiver Gain	31
14	Relaxation Delay	1.0000
15	Pulse Width	15.0000
16	Acquisition Time	4.0894
17	Acquisition Date	2021-02-1T12:1:10
18	Modification Date	2021-02-1T12:1:30
19	Spectrometer Frequency	400.13
20	Spectral Width	8012.8
21	Lowest Frequency	-1535.6
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

Figure 25. ^{1}H NMR spectra of 1-(4-Bromophenyl)-3-phenylpropan-1-one.



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6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	289.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	31
14	Relaxation Delay	1.0000
15	Pulse Width	15.0000
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19	Spectrometer Frequency	400.13
20	Spectral Width	8012.8
21	Lowest Frequency	-1535.6
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

Figure 26. ^{13}C NMR spectra of 1-(4-Bromophenyl)-3-phenylpropan-1-one.

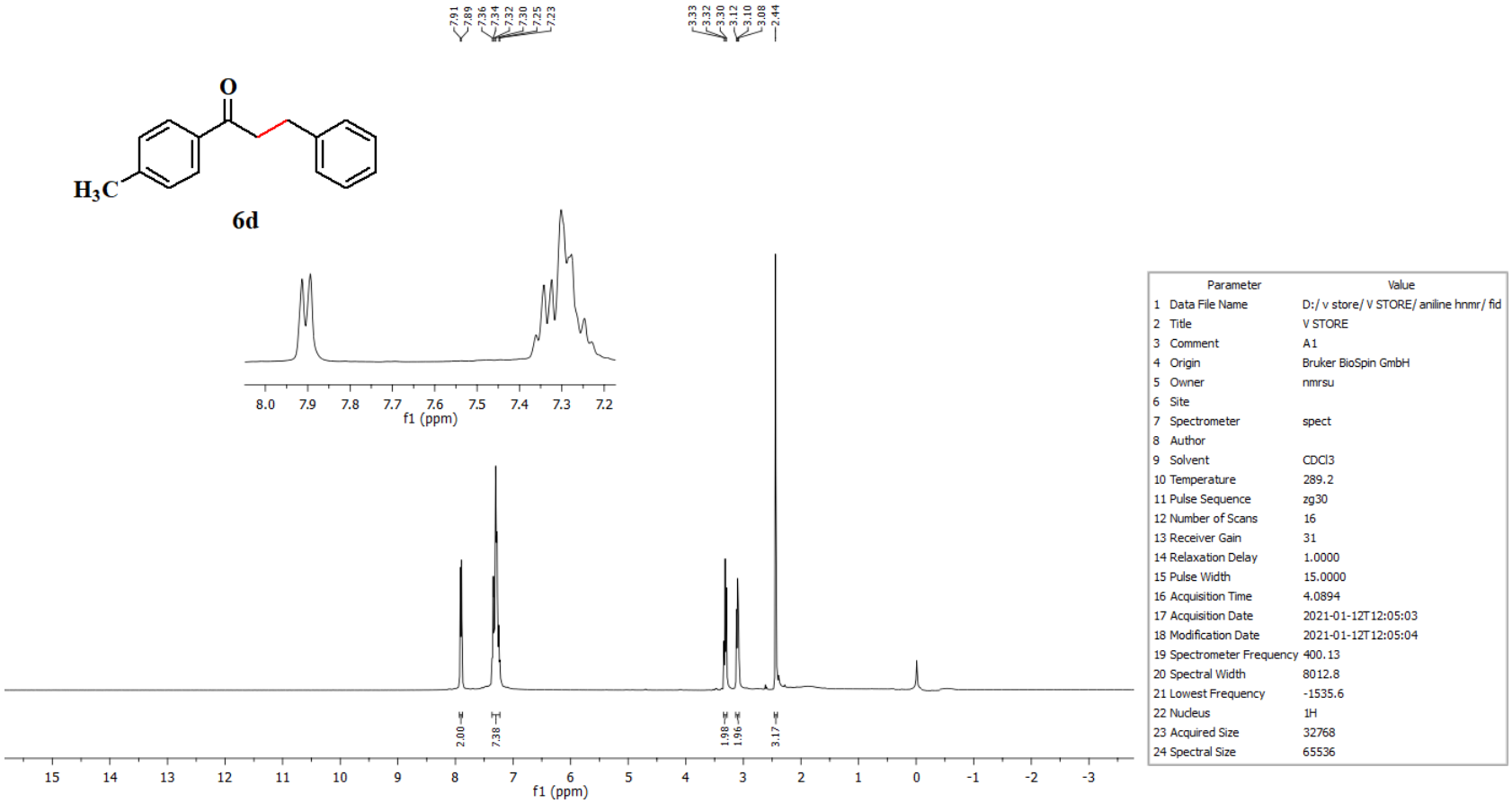
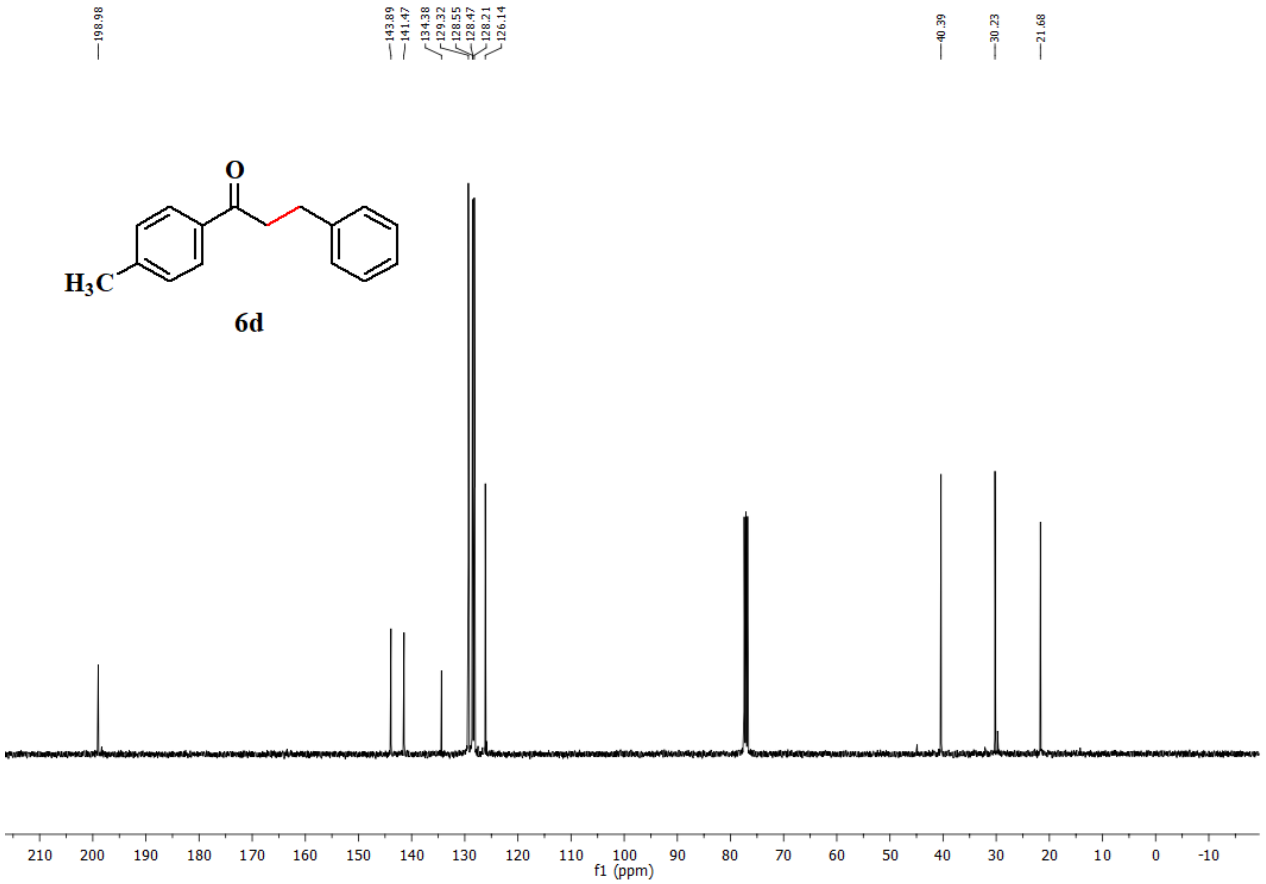


Figure 27. ^{1}H NMR spectra of 1-(4-Methylphenyl)-3-phenylpropan-1-one.



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6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	289.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	31
14	Relaxation Delay	1.0000
15	Pulse Width	15.0000
16	Acquisition Time	4.0894
17	Acquisition Date	2021-01-13T12:05:10
18	Modification Date	2021-01-13T12:05:30
19	Spectrometer Frequency	400.13
20	Spectral Width	8012.8
21	Lowest Frequency	-1535.6
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

Figure 28. ^{13}C NMR spectra of 1-(4-Methylphenyl)-3-phenylpropan-1-one.

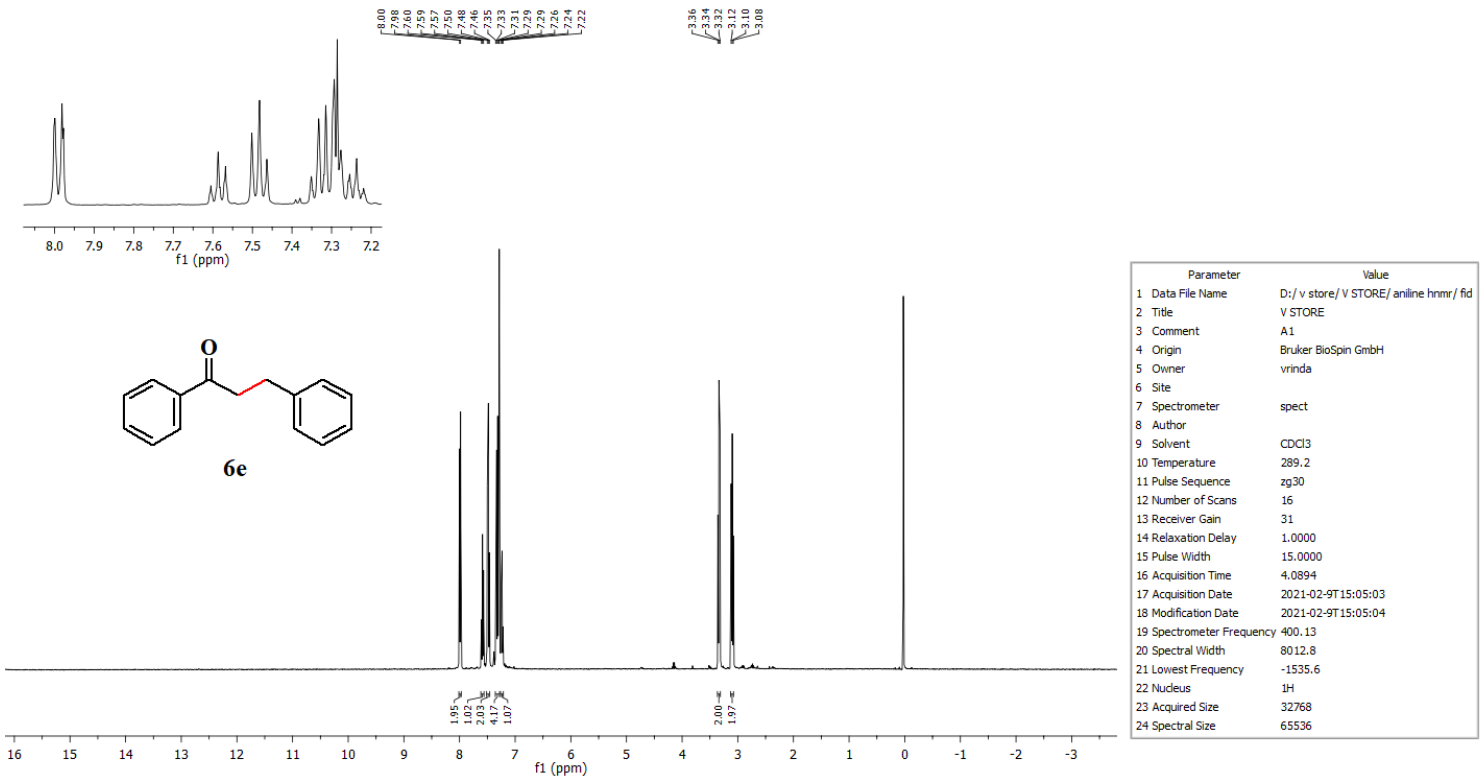


Figure 29. ^{1}H NMR spectra of 1,3-Diphenylpropan-1-one.

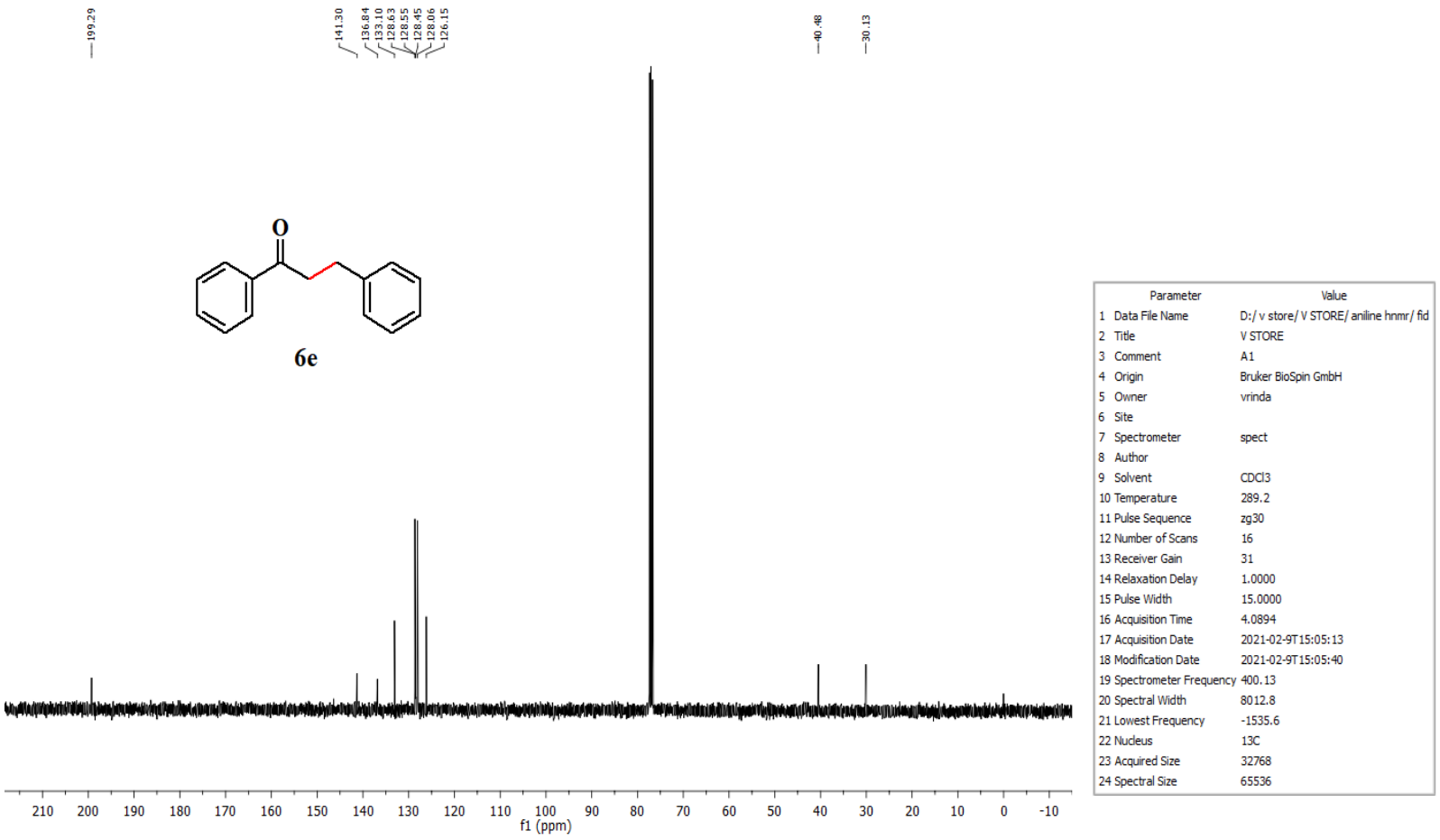


Figure 30. ^{13}C NMR spectra of 1,3-Diphenylpropan-1-one.

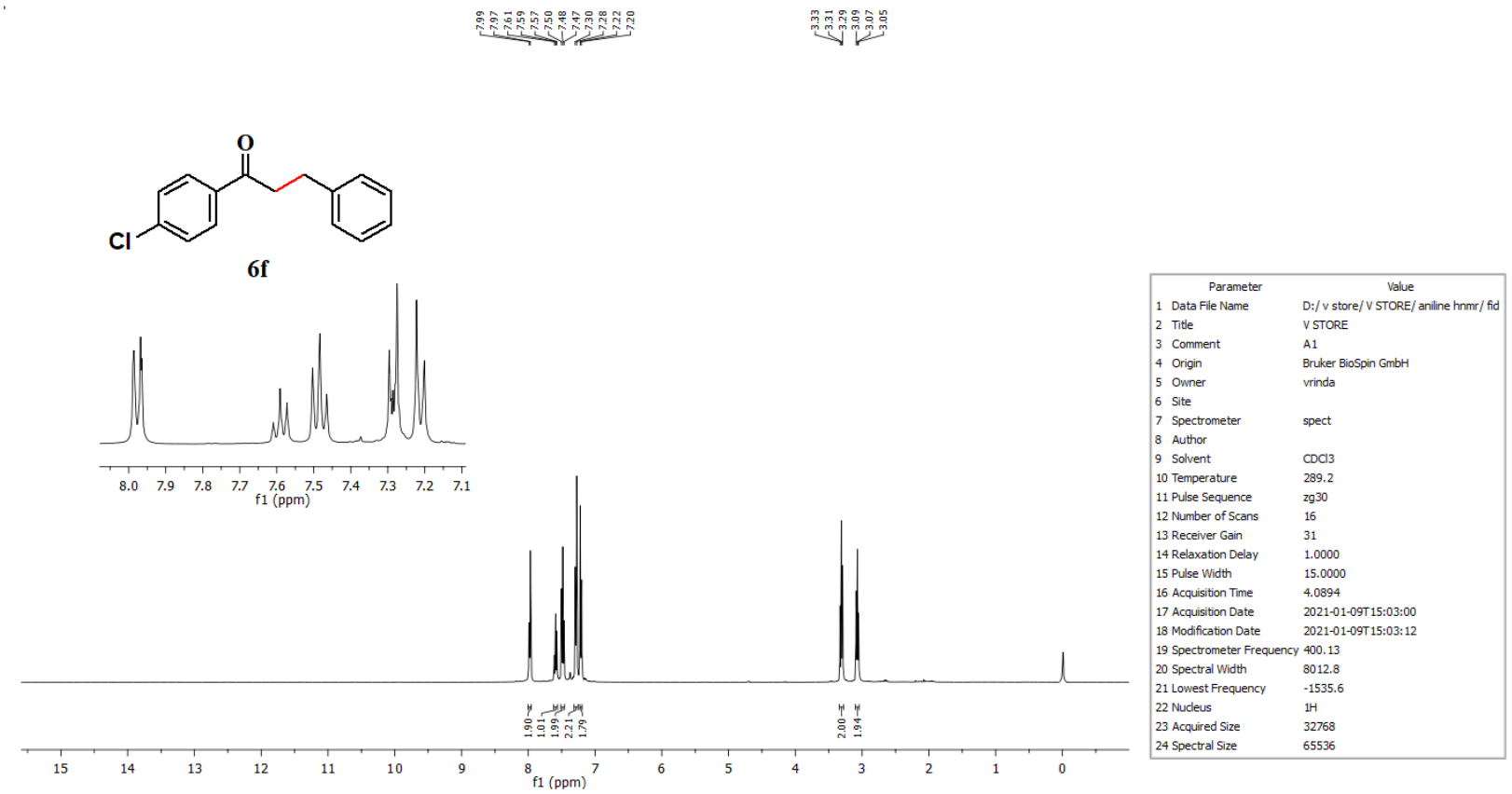
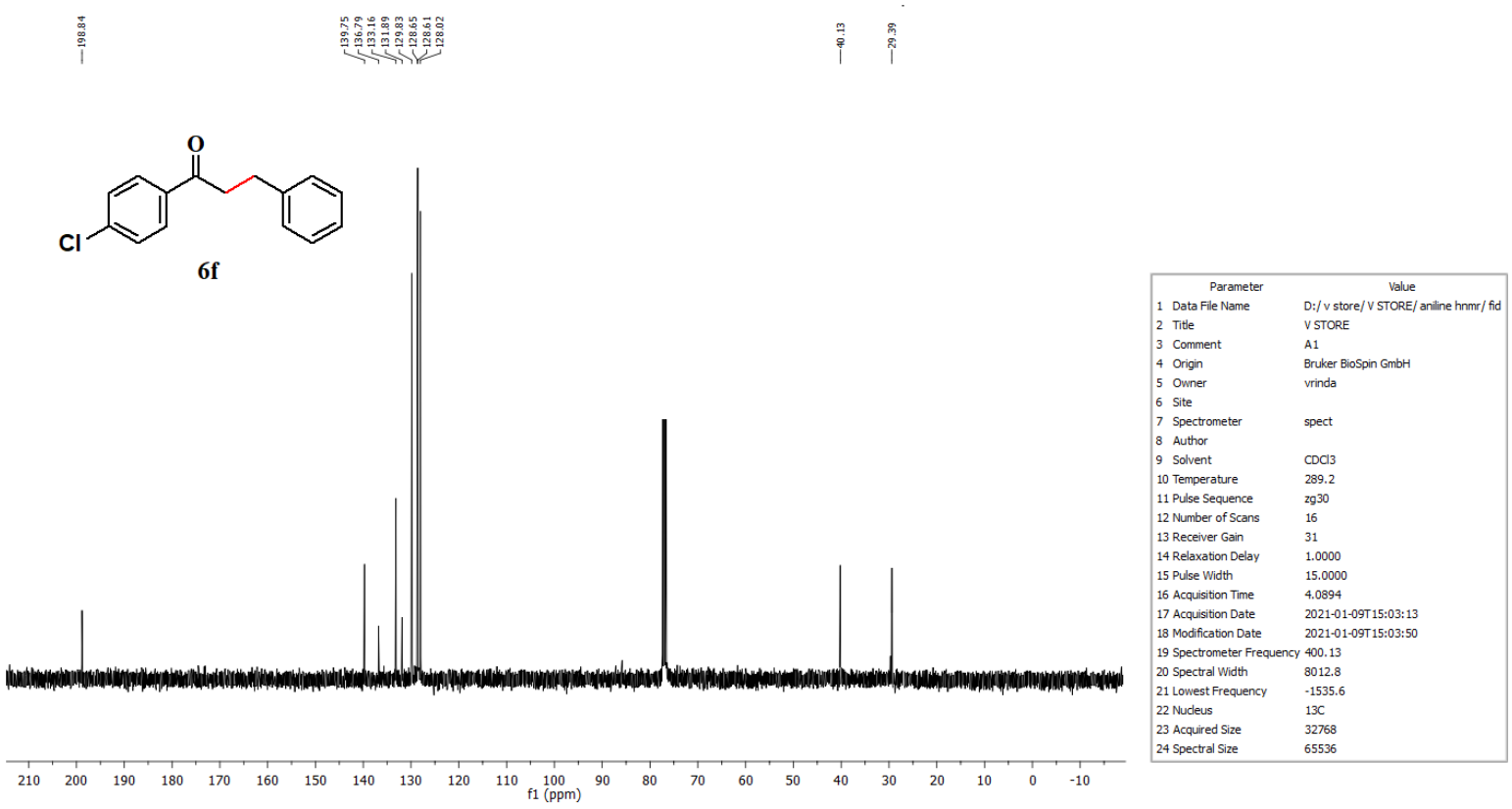


Figure 31. ^{1}H NMR spectra of 3-(4-Chlorophenyl)-1-phenylpropan-1-one.



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6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	289.2
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	31
14	Relaxation Delay	1.0000
15	Pulse Width	15.0000
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19	Spectrometer Frequency	400.13
20	Spectral Width	8012.8
21	Lowest Frequency	-1535.6
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

Figure 32. ^{13}C NMR spectra of 3-(4-Chlorophenyl)-1-phenylpropan-1-one