New Journal of Chemistry

Supplementary data

Synergistic promotion of Ag nanoparticles supported on magnetic Cu based metal organic framework for A^3-coupling and synthesis of benzopyranopyrimidines

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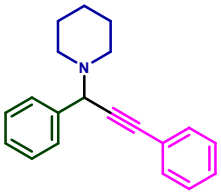
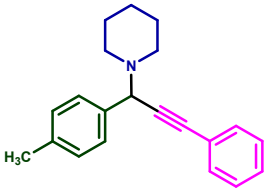
S1. Spectral data of the synthesized products 4(a-h)

1-(1,3-Diphenylprop-2-ynyl)piperidine (4a)



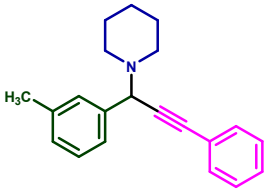
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.66 (d, *J* = 7.5 Hz, 2H, ArH), 7.56-7.53 (m, 2H, ArH), 7.40-7.30 (m, 6H, ArH), 4.84 (s, 1H, CH), 2.60 (br, 4H, $2CH_2$), 1.68-1.57 (m, 4H, $2CH_2$), 1.48-1.45 (m, 2H, CH_2); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 138.40, 131.82, 128.62, 128.29, 128.08, 127.52, 123.30, 87.85, 86.00, 62.35, 50.61, 26.10, 24.40.

1-(3-Phenyl-1-p-tolylprop-2-ynyl)piperidine (4b)



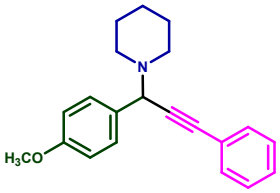
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.54-7.52 (m, 4H, ArH), 7.35-7.33 (m, 3H, ArH), 7.19 (d, *J* = 7.9 Hz, 2H, ArH), 4.79 (s, 1H, CH), 2.58 (t, *J* = 4.6 Hz, 4H, $2CH_2$), 2.38 (s, 3H, CH_3), 1.63-1.59 (m, 4H, $2CH_2$), 1.47-1.44 (m, 2H, CH_2); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 137.18, 135.48, 131.80, 128.77, 128.55, 128.26, 127.97, 123.37, 87.63, 86.28, 62.06, 50.62, 26.09, 24.41, 21.13.

1-(3-Phenyl-1-m-tolylprop-2-ynyl)piperidine (4c)



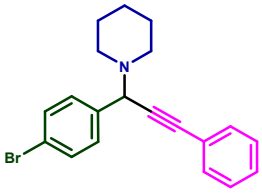
^{1}H NMR (400 MHz, $CDCl_3$):δ 7.56-7.52 (m, 2H), 7.45 (d, *J* = 1.7 Hz, 2H), 7.38-7.34 (m, 3H), 7.26 (d, *J* = 7.9 Hz, 1H), 7.13 (d, *J* = 7.5 Hz, 1H), 4.77 (s, 1H), 2.60-2.58 (m, 4H), 2.40 (s, 3H), 1.67-1.56 (m, 4H), 1.47 (dt, *J* = 8.8, 4.6 Hz, 2H);**^{13}C NMR (100 MHz, $CDCl_3$)**: δ 138.29, 137.70, 131.82, 129.29, 128.45, 128.27, 128.05, 127.95, 125.74, 123.36, 87.73, 86.21, 62.41, 50.78, 26.09, 24.40, 21.54.

1-(4-Methoxyphenyl)-3-phenylprop-2-ynyl)piperidine (4d)



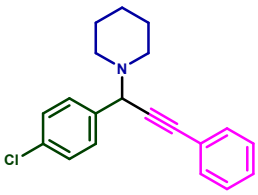
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60-7.56 (m, 4H, ArH), 7.39-7.35 (m, 3H, ArH), 6.94 (d, *J* = 8.6 Hz, 2H, ArH), 4.79 (s, 1H, CH), 3.84 (s, 3H, OCH_3), 2.60 (br, 4H, $2CH_2$), 1.69-1.58 (m, 4H, $2CH_2$), 1.50-1.47 (m, 2H, CH_2); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 159.02, 131.83, 130.73, 129.69, 128.31, 128.05, 123.43, 113.42, 87.67, 86.47, 61.82, 55.27, 50.64, 26.23, 24.54.

1-(4-Bromophenyl)-3-phenylprop-2-ynyl)piperidine (4e)



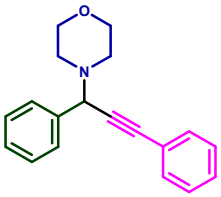
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.57-7.50 (m, 6H, ArH), 7.37-7.36 (m, 3H, ArH), 4.78 (s, 1H, CH), 2.57 (br, 4H, $2CH_2$), 1.68-1.56 (m, 4H, $2CH_2$), 1.49-1.48 (m, 2H, CH_2); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 137.81, 131.83, 131.18, 130.23, 128.35, 128.25, 123.07, 121.41, 88.29, 85.28, 61.78, 50.71, 26.15, 24.38.

1-(4-Chlorophenyl)-3-phenylprop-2-ynyl)piperidine (4f)



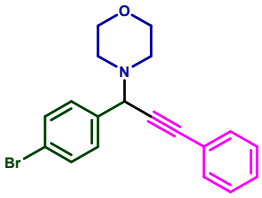
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.61 (d, *J* = 8.4 Hz, 2H, ArH), 7.55-7.53 (m, 2H, ArH), 7.37-7.34 (m, 5H, ArH), 4.79 (s, 1H, CH), 2.56 (t, *J* = 4.7 Hz, 4H, $2CH_2$), 1.65-1.58 (m, 4H, $2CH_2$), 1.48-1.45 (m, 2H, CH_2); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 137.32, 133.19, 131.82, 130.93, 129.83, 128.33, 128.20, 123.10, 88.24, 85.39, 61.73, 50.73, 26.16, 24.39.

4-(1,3-Diphenylprop-2-ynyl)morpholine (4g)



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.68 (d, *J* = 7.3 Hz, 2H, ArH), 7.58-7.55 (m, 2H, ArH), 7.43-7.33 (m, 6H, ArH), 4.84 (s, 1H, CH), 3.82-3.73 (m, 4H, $2CH_2$), 2.68 (br, 4H, $2CH_2$); **^{13}C NMR (100 MHz, $CDCl_3$)**: δ 137.84, 131.85, 128.63, 128.36, 128.30, 128.27, 127.82, 123.01, 88.53, 85.08, 67.20, 62.07, 49.91.

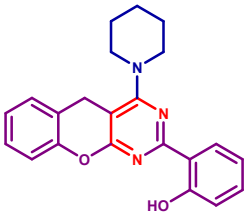
4-(1-(4-bromophenyl)-3-phenylprop-2-ynyl)morpholine (4h)



^{1}H NMR (400 MHz, $CDCl_3$):δ 7.56-7.50 (m, 6H), 7.38-7.35 (m, 3H), 4.77 (s, 1H), 3.80-3.71 (m, 4H), 2.64 (t, *J* = 4.4 Hz, 4H);**^{13}C NMR (100 MHz, $CDCl_3$)**: δ 136.96, 131.81, 131.35, 130.26, 128.44, 128.37, 122.67, 121.75, 88.93, 84.23, 67.11, 61.42, 49.77.

S2. Spectral data of the synthesized products 8(a-g)

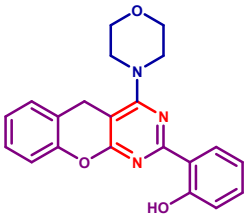
2-(4-(piperidin-1-yl)-5H-chromeno[2,3-d]pyrimidin-2-yl)phenol (8a)



^{1}H NMR (400 MHz, $CDCl_3$): δ 13.49 (brs, 1H, OH), 8.45 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.40-7.35 (m, 1H, Ar), 7.23 (dd, *J* = 8.9, 8.0 Hz, 3H, Ar), 7.15-7.13 (m, 1H, Ar), 7.00 (d, 1H, J= 8 Hz, Ar), 6.96-6.92 (m, 1H), 3.95 (s, 2H, CH_2), 3.48-3.45 [m, 4H, $N(CH_2)_2$], 1.81-1.76 (m, 6H, $3CH_2$); **^{13}C**

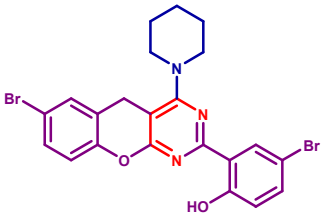
NMR (100 MHz, $CDCl_3$): δ 165.38, 164.50, 162.08, 160.44, 150.71, 132.84, 129.22, 128.54, 128.22, 124.40, 119.59, 118.84, 118.61, 117.55, 117.13, 97.62, 49.55, 25.99, 25.65, 24.36.

2-(4-morpholino-5H-chromeno[2,3-d]pyrimidin-2-yl)phenol (8b)



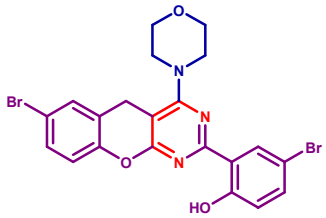
^{1}H NMR (400 MHz, $CDCl_3$): δ 13.12 (brs, 1H, OH), 8.39 (d, *J* = 7.9 Hz, 1H, Ar), 7.35 (t, *J* = 7.7 Hz, 1H, Ar), 7.25-7.17 (m, 3H, Ar), 7.11 (t, *J* = 7.2 Hz, 1H, Ar), 6.97 (d, *J* = 8.2 Hz, 1H, Ar), 6.91 (t, *J* = 6.8 Hz, 1H, Ar), 3.93-3.90 (m, 6H), 3.50 (s, 4H, $2CH_2$); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 164.84, 164.34, 162.16, 160.34, 150.42, 133.01, 129.19, 128.57, 128.37, 124.63, 119.09, 118.93, 118.43, 117.62, 117.11, 97.83, 66.74, 48.67, 25.93.

4-bromo-2-(7-bromo-4-piperidin-1-yl)-5H-chromeno[2,3-d]pyrimidin-2-yl)phenol (8c)



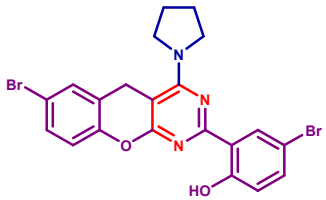
^{1}H NMR (400 MHz, $CDCl_3$): δ 13.39 (brs, 1H, OH), 8.52 (d, *J* = 8.0 Hz, 1H, Ar), 7.43 (dd, *J* = 8.7, 2.5 Hz, 1H, Ar), 7.38 (d, *J* = 8.1 Hz, 2H, Ar), 7.10 (d, *J* = 8.3 Hz, 1H, Ar), 6.88 (d, *J* = 8.7 Hz, 1H, Ar), 3.92 (s, 2H), 3.46 (t, *J* = 13.9 Hz, 4H), 1.78 (s, 6H); **^{13}C NMR (100 MHz, $CDCl_3$):** 165.18, 164.07, 160.97, 159.50, 149.73, 135.55, 131.33, 131.30, 131.26, 121.59, 120.08, 119.55, 118.92, 116.95, 111.02, 97.25, 49.54, 25.91, 25.50, 24.27.

4-bromo-2-(7-bromo-4-morpholino-5H-chromeno[2,3-d]pyrimidin-2-yl)phenol (8d)



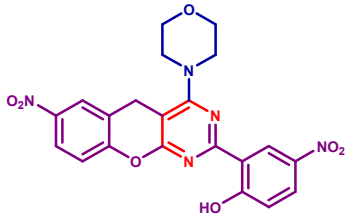
^{1}H NMR (400 MHz, $CDCl_3$): δ 13.03 (brs, 1H, OH), 8.46 (d, *J* = 7.9 Hz, 1H, Ar), 7.43-7.37 (m, 3H, Ar), 7.07 (d, *J* = 8.3 Hz, 1H, Ar), 6.85 (d, *J* = 8.8 Hz, 1H, Ar), 3.94-3.89 (m, 6H), 3.51 (t, J = 4 Hz, 2H, CH_2); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 164.80, 163.66, 161.06, 159.43, 149.35, 135.72, 131.94, 131.47, 131.38, 131.30, 121.02, 119.66, 118.82, 117.08, 110.96, 97.51, 66.74, 48.65, 25.26.

4-bromo-2-(7-bromo-4-(pyrrolidin-1-yl)-5H-chromeno[2,3-d]pyrimidin-2-yl)phenol (8e)



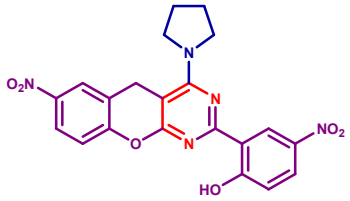
^{1}H NMR (400 MHz, $CDCl_3$): δ 13.64 (brs, 1H, OH), 8.52 (d, *J* = 8.0 Hz, 1H, Ar), 7.42 (dd, *J* = 8.7, 2.2 Hz, 1H, Ar), 7.36 (d, *J* = 9.0 Hz, 1H, Ar), 7.33 (s, 1H, Ar), 7.07 (d, *J* = 8.6 Hz, 1H, Ar), 6.86 (d, *J* = 8.7 Hz, 1H, Ar), 4.26 (s, 2H, CH_2), 3.84 (t, *J* = 6.0 Hz, 4H), 1.28 (t, *J* = 7.1 Hz, 4H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 161.24, 160.80, 160.32, 159.57, 149.27, 135.34, 131.34, 131.30, 130.87, 121.25, 120.14, 119.43, 118.76, 116.54, 110.88, 91.44, 60.73, 50.01, 25.63.

4-nitro-2-(7-nitro-4-morpholino-5H-chromeno[2,3-d]pyrimidin-2-yl)phenol (8f)



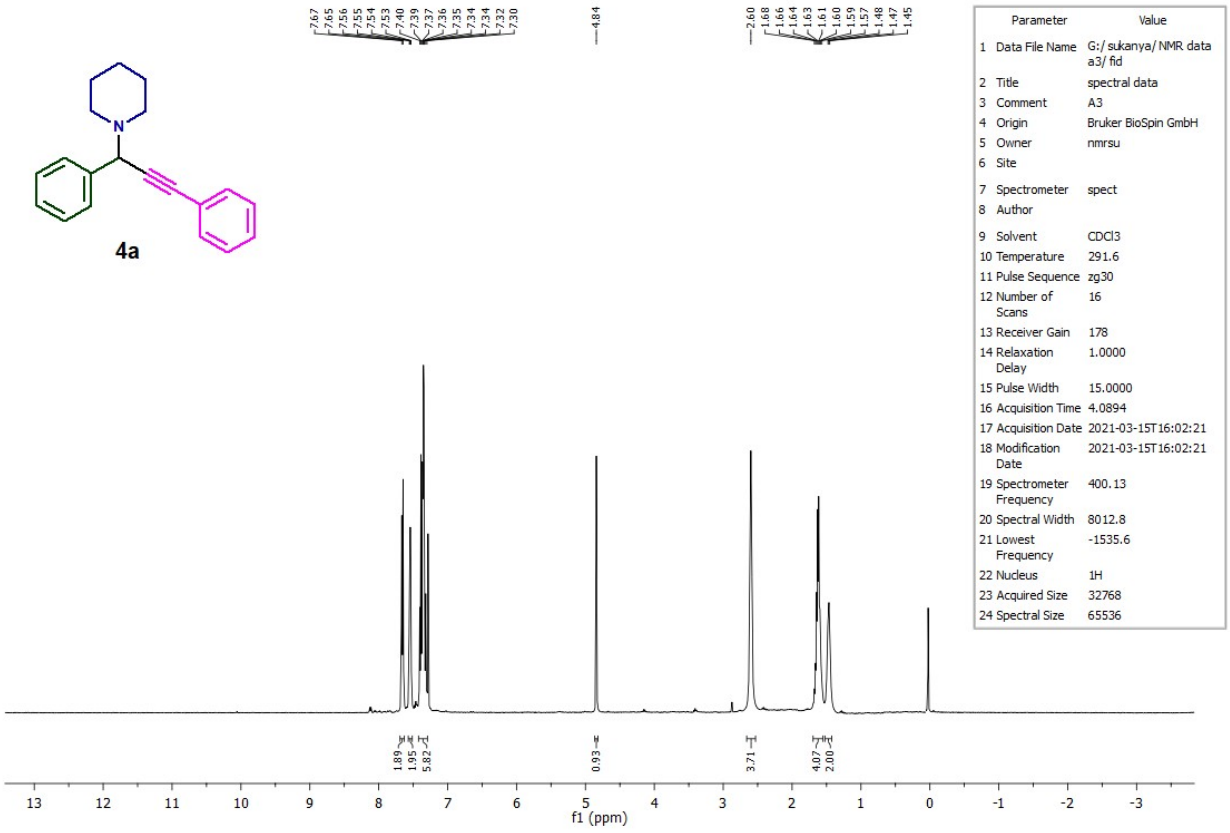
^{1}H NMR (400 MHz, $CDCl_3$): δ 13.82 (brs, 1H, OH), 9.32 (d, *J* = 8.0 Hz, 1H, Ar), 8.28 (dd, *J* = 9.2, 2.8 Hz, 1H), 8.23 (d, *J* = 7.6 Hz, 2H), 7.36 (d, *J* = 9.8 Hz, 1H), 7.15-7.12 (m, 1H), 4.11 (s, 2H), 3.97 (t, J = 4 Hz, 4H), 3.63 (s, 4H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 165.99, 156.64, 155.31, 155.13, 154.77, 144.48, 140.32, 128.45, 128.33, 125.89, 124.69, 124.61, 120.13, 118.73, 118.14, 105.46, 66.76, 48.67, 25.93.

4-nitro-2-(7-nitro-4-(pyrrolidin-1-yl)-5H-chromeno[2,3-d]pyrimidin-2-yl)phenol (8g)



^{1}H NMR (400 MHz, $CDCl_3$): δ 14.43 (brs, 1H, OH), 9.33 (s, 1H, Ar), 8.25 (d, *J* = 7.8 Hz, 1H, Ar), 8.20-8.16 (m, 2H, Ar), 6.93 (d, *J* = 8 Hz, 1H, Ar), 7.05 (d, *J* = 9.1 Hz, 1H), 4.42 (s, 2H), 3.92 (s, 4H), 1.28 (s, 4H); **^{13}C NMR (100 MHz, $CDCl_3$):** δ 166.01, 157.08, 155.86, 155.64 153.51, 142.26, 140.31, 127.92, 125.81, 124.77, 124.43, 118.41, 117.87, 111.63, 60.71, 50.33, 25.64.

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



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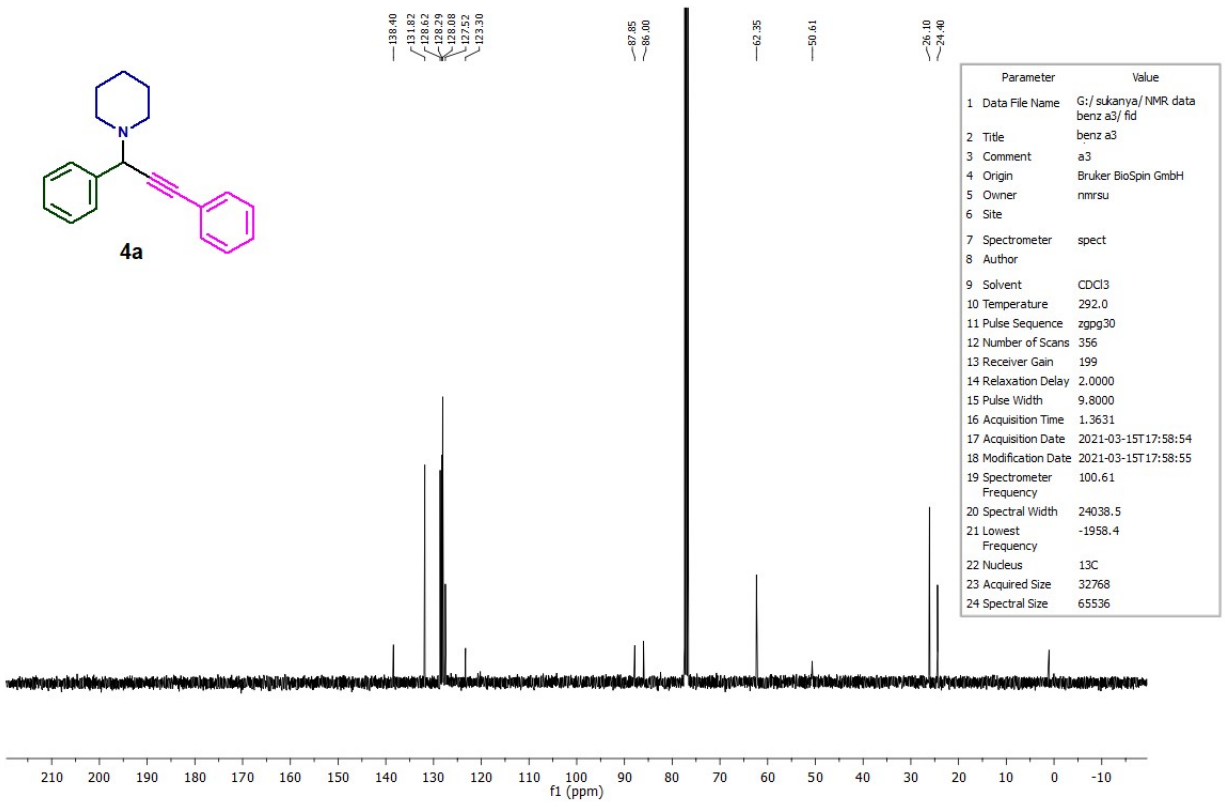
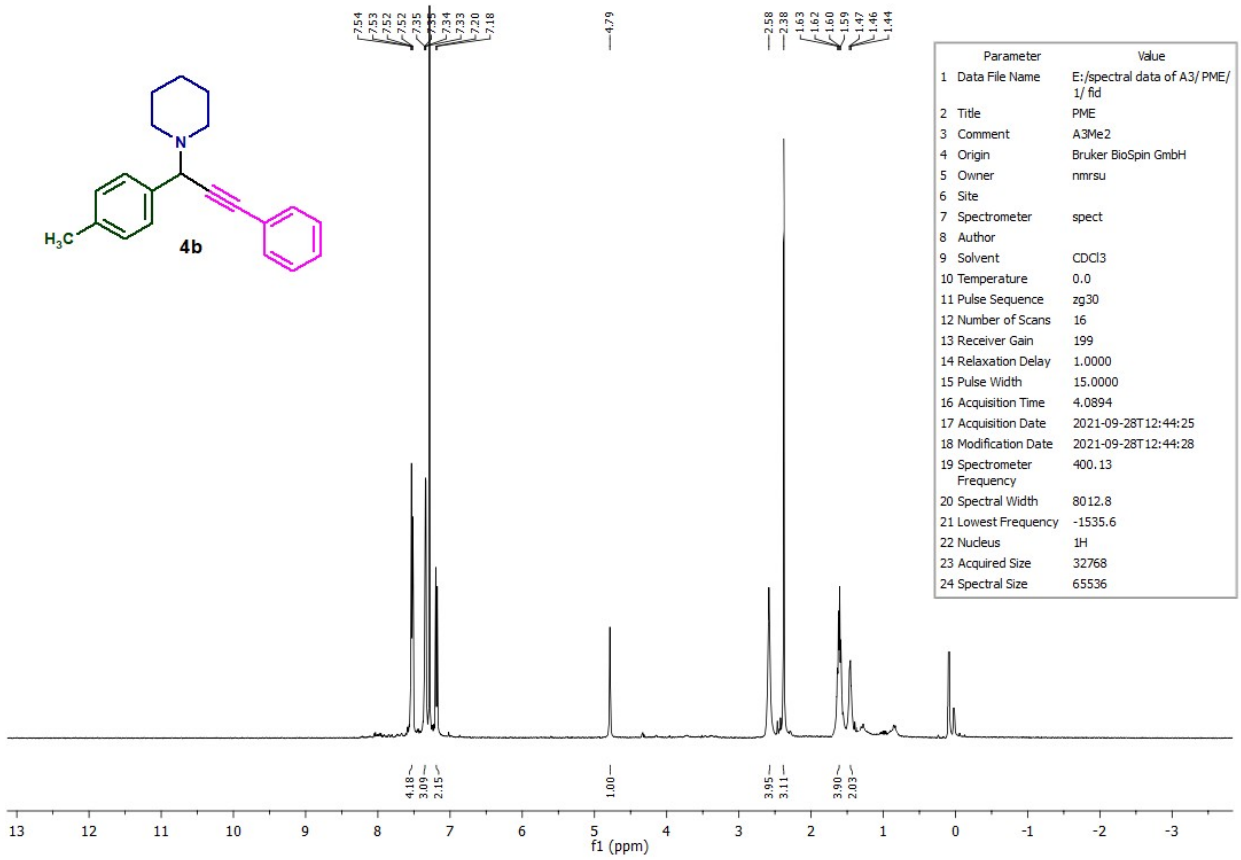
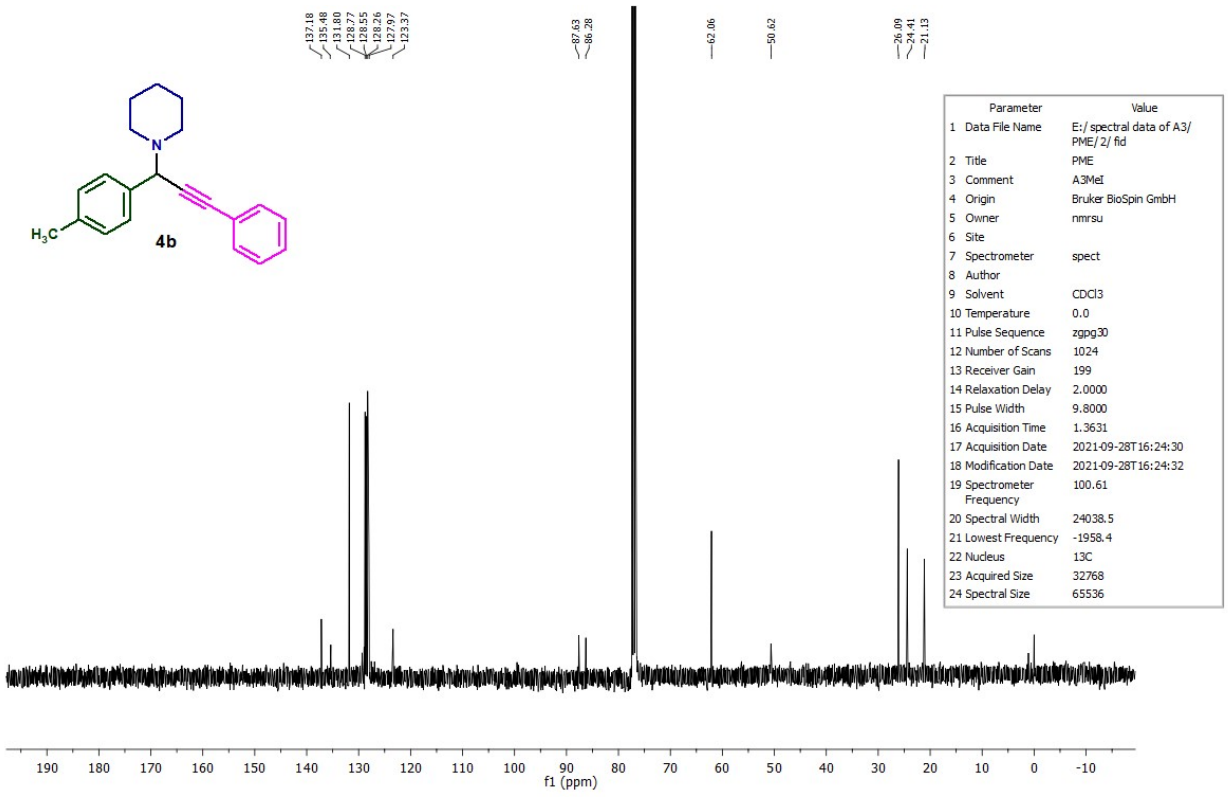
^{1}H NMR spectra of product (4a)



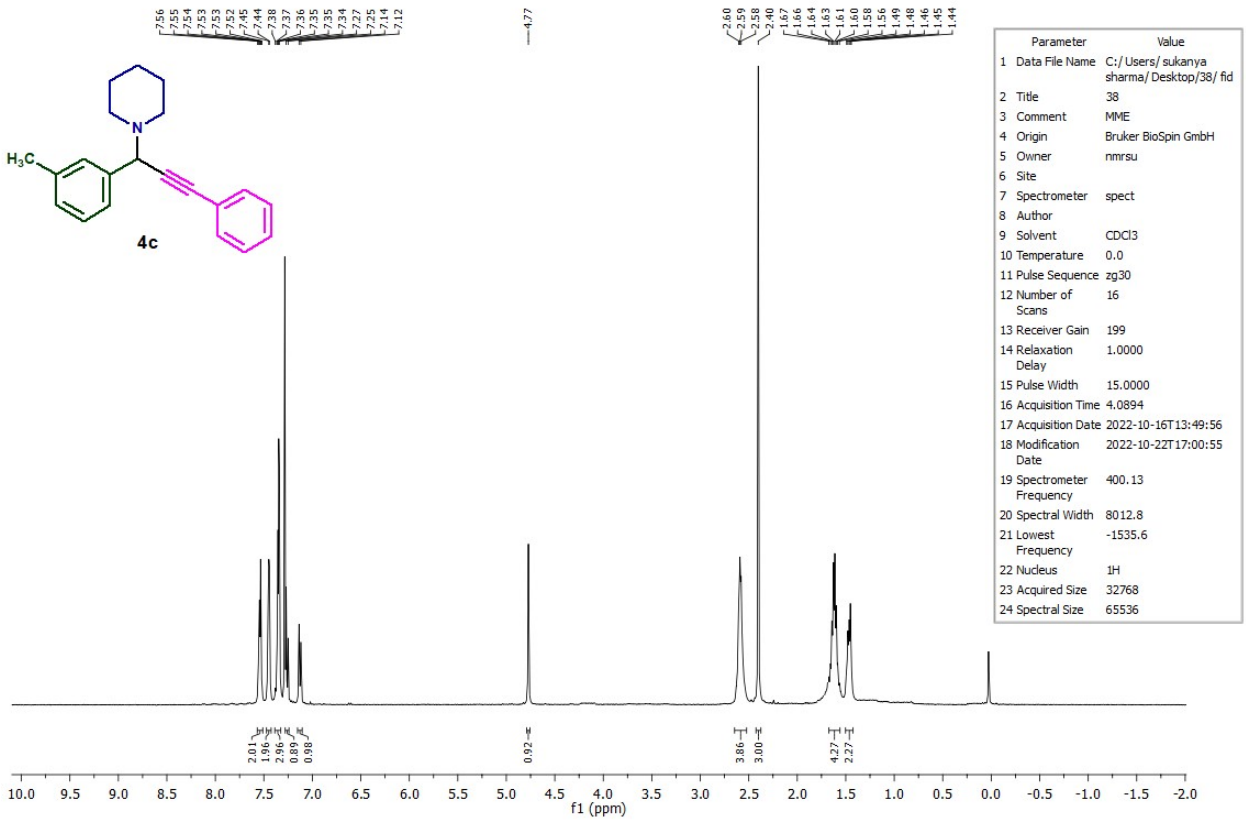
^{13}C NMR spectra of product (4a)



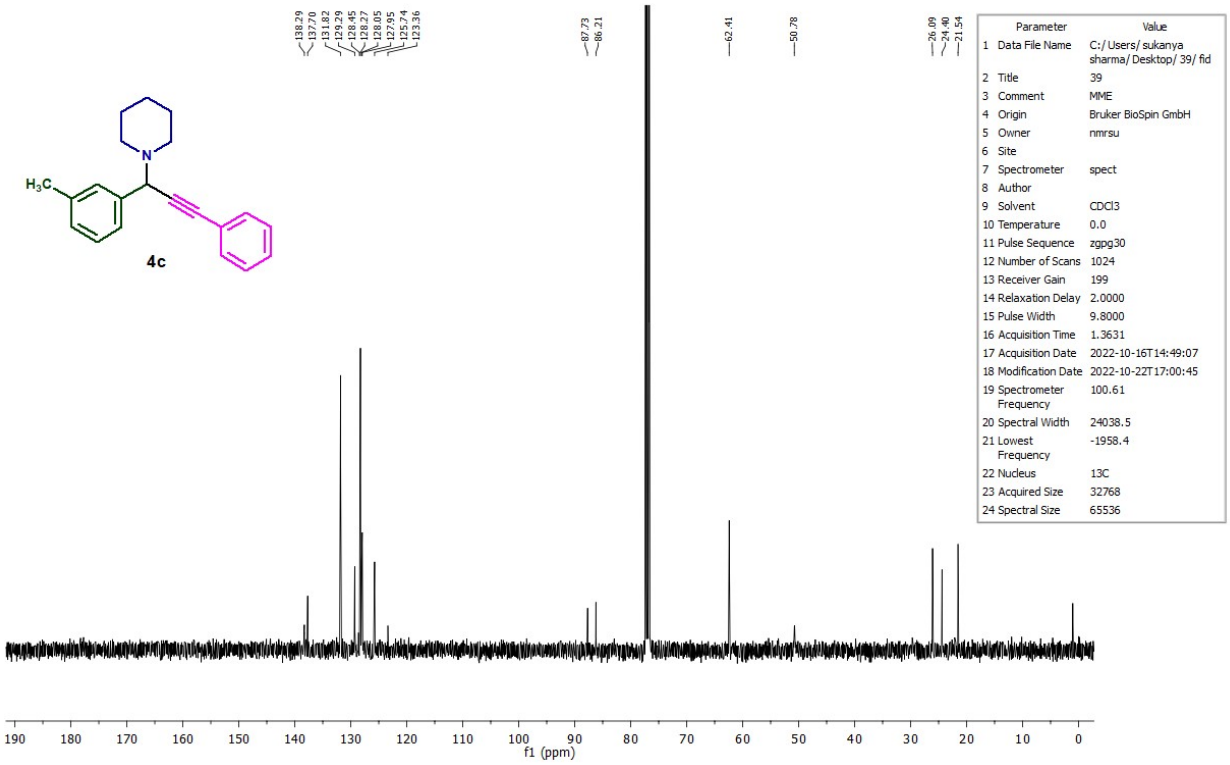
^{1}H NMR spectra of product (4b)



^{13}C NMR spectra of product (4b)



^{1}H NMR spectra of product (4c)



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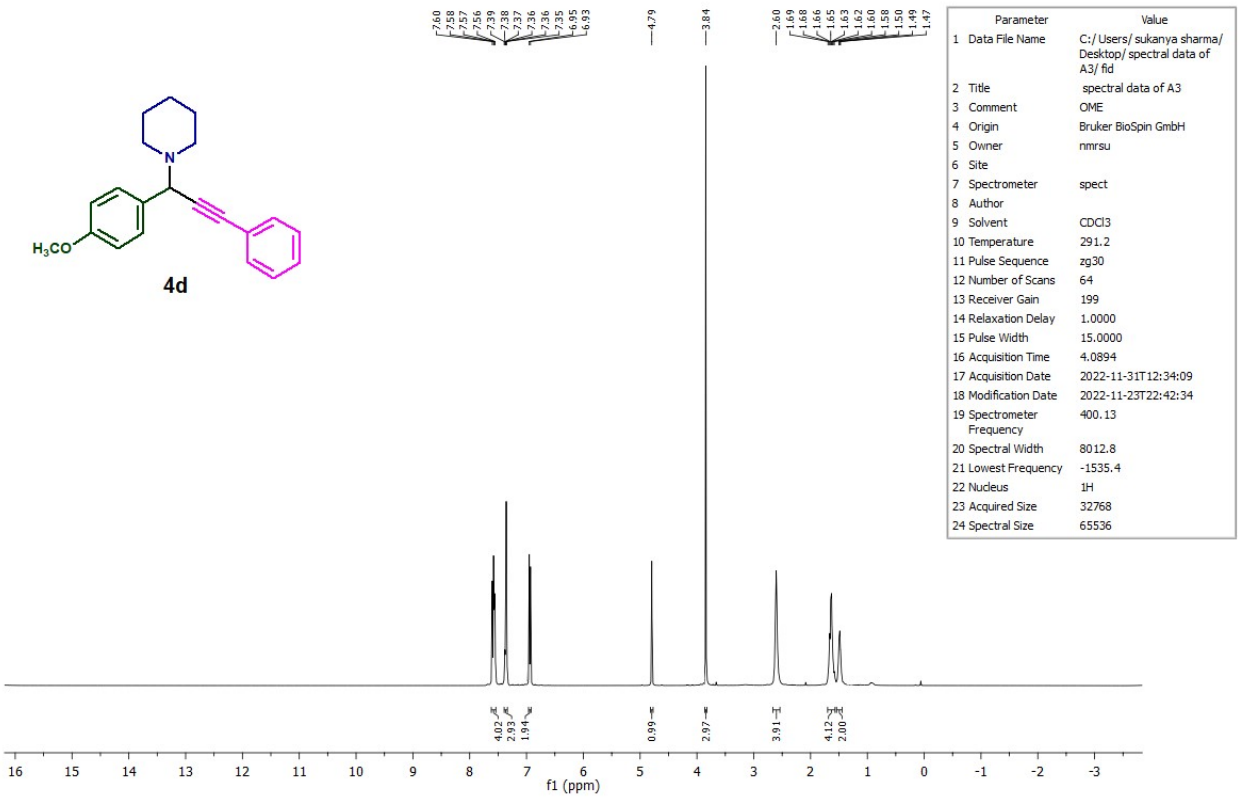
^{13}C NMR spectra of product (4c)



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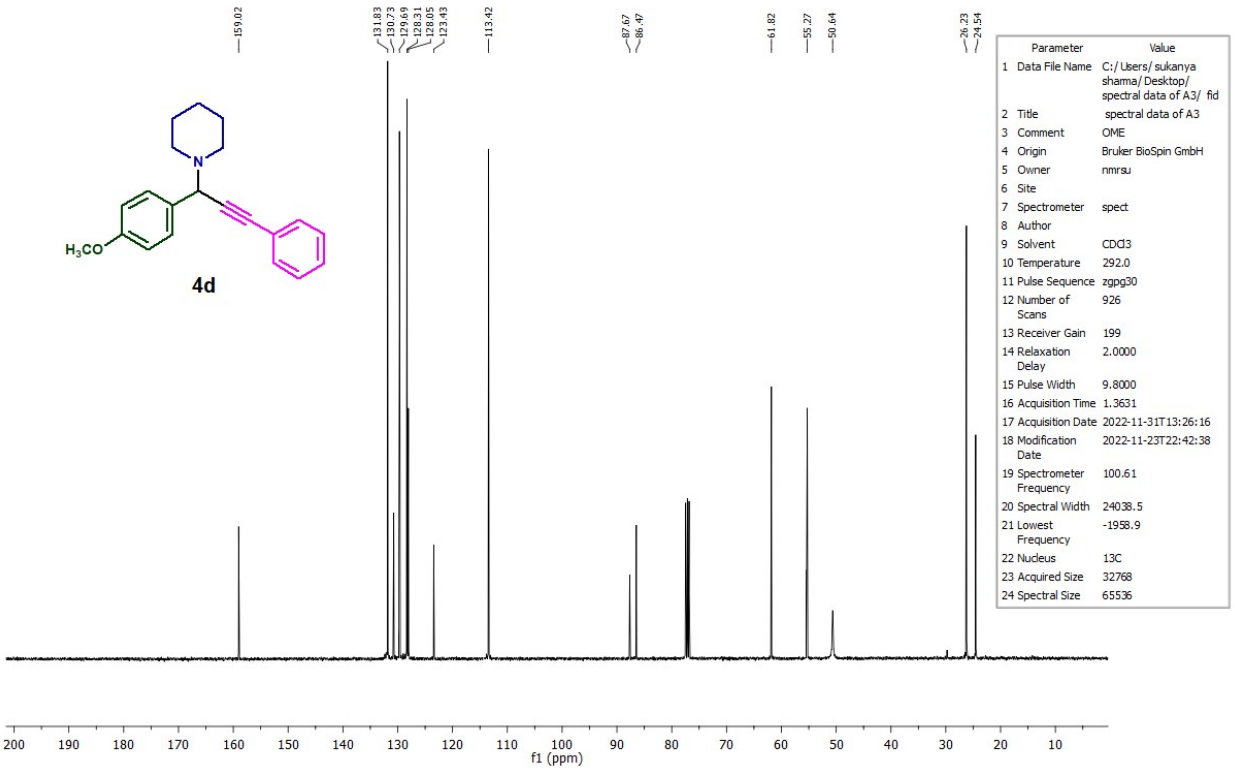
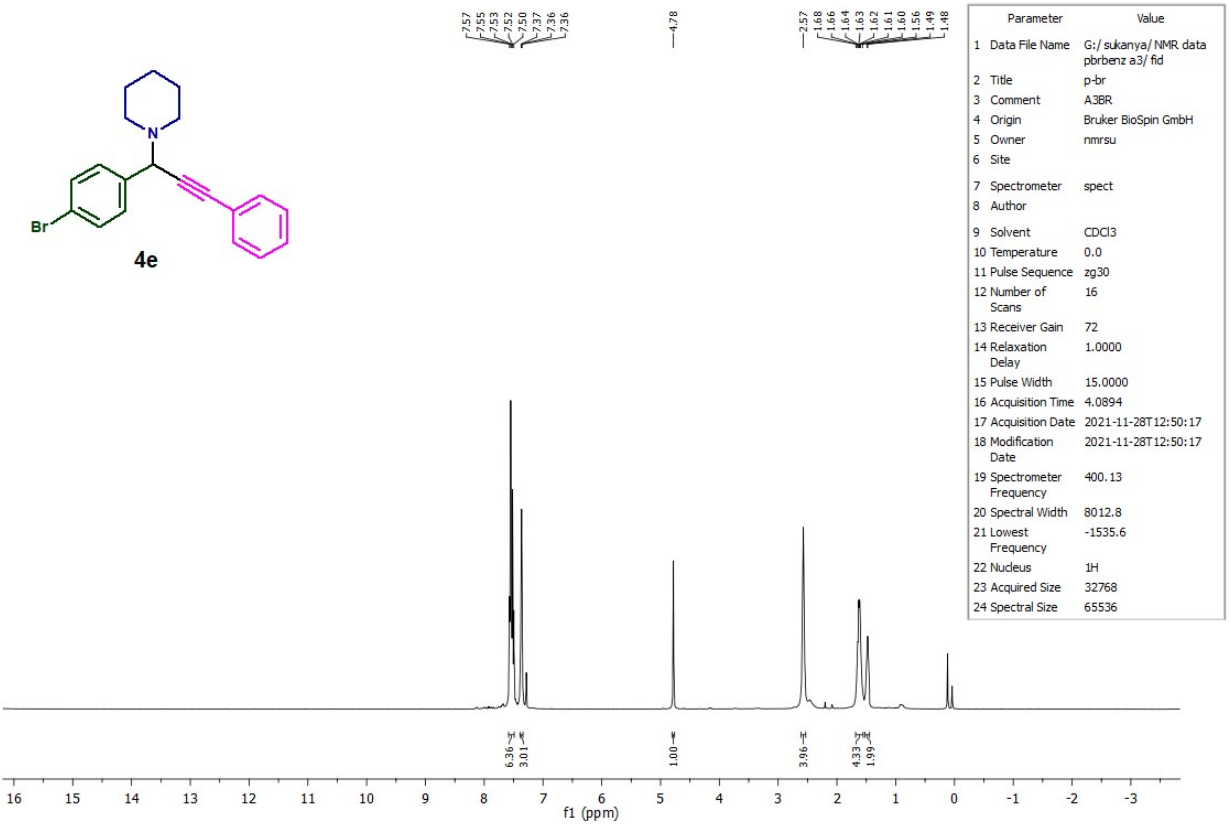
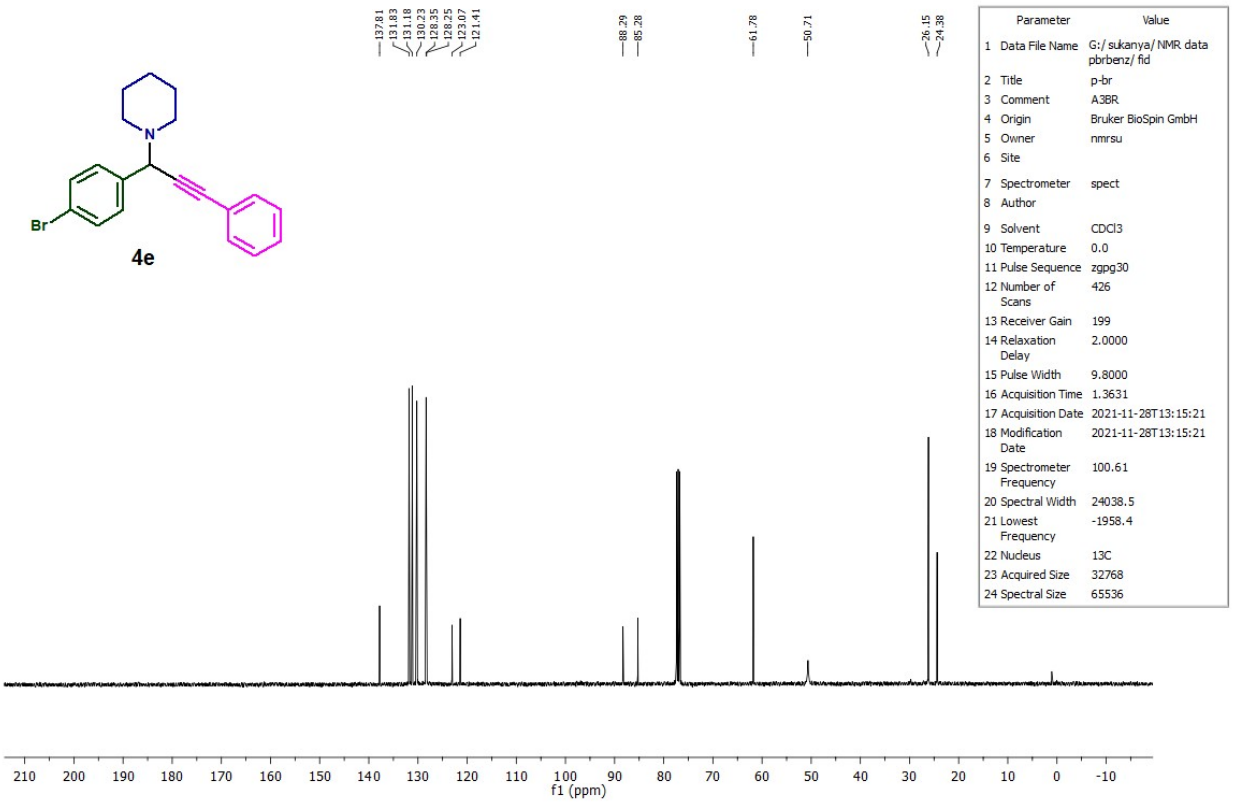
^{1}H NMR spectra of product (4d)



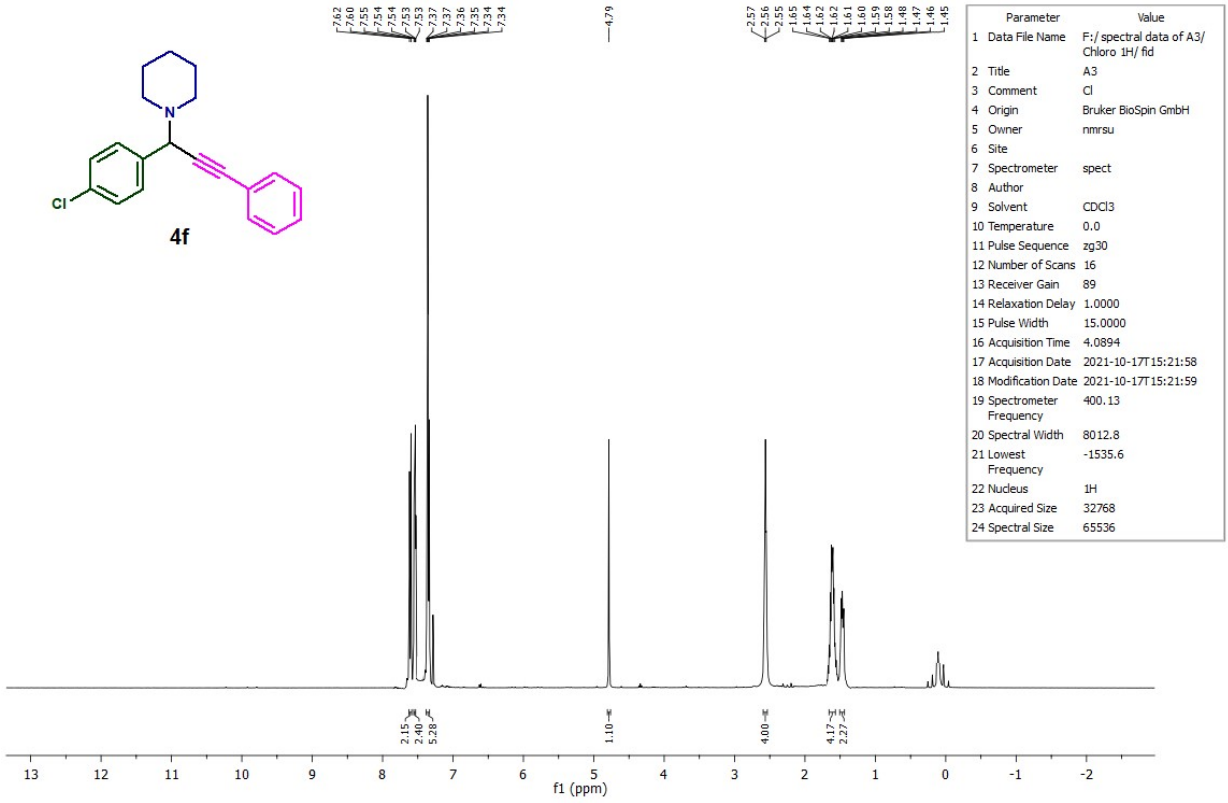
^{13}C NMR spectra of product (4d)



^{1}H NMR spectra of product (4e)



^{13}C NMR spectra of product (4e)



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8 Author	
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11 Pulse Sequence	zg30
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17 Acquisition Date	2021-10-17T15:21:58
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21 Lowest Frequency	-1535.6
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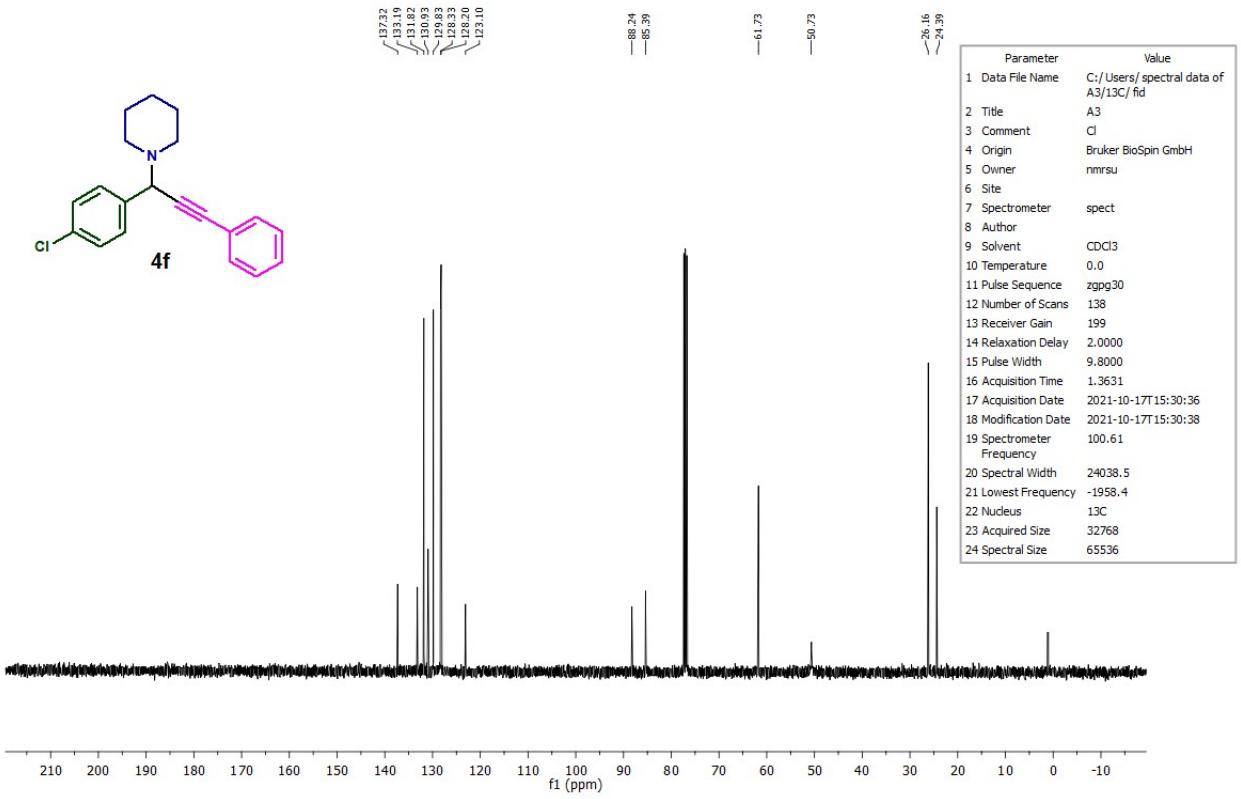
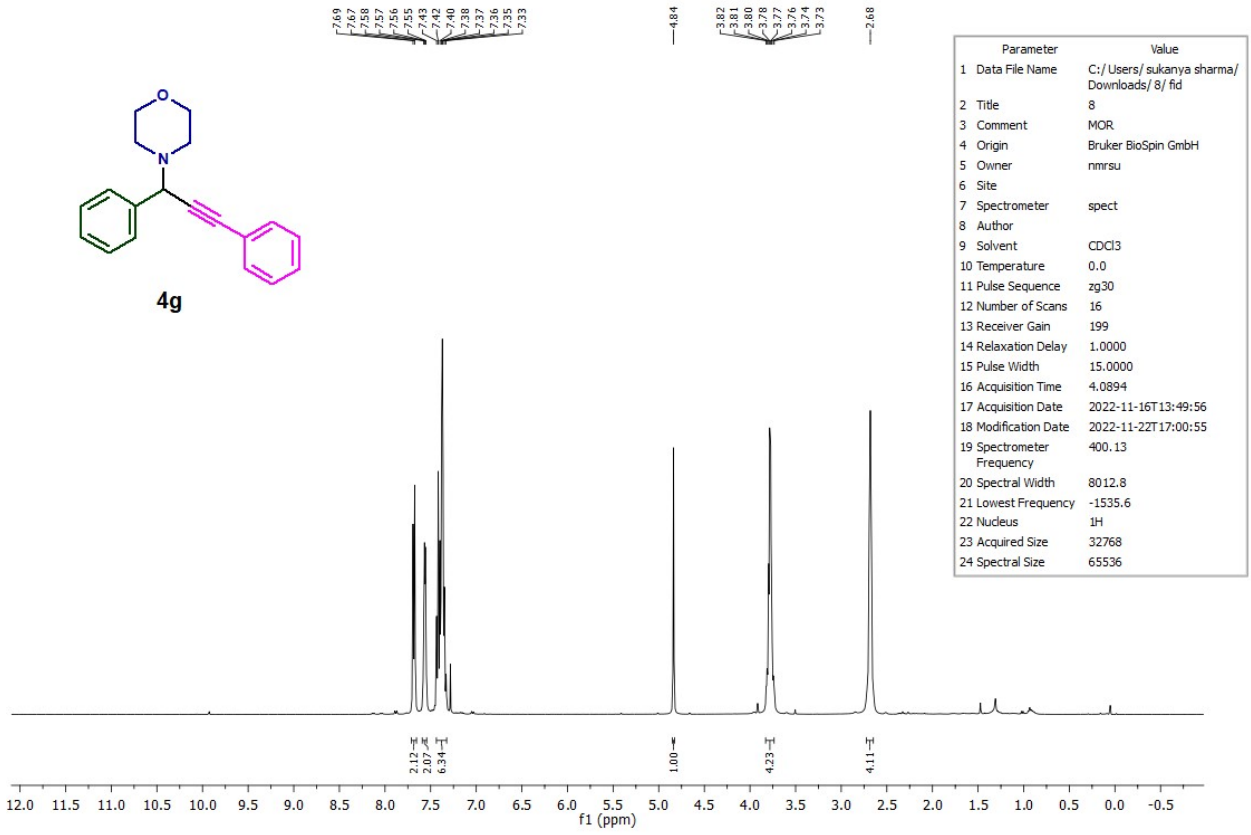
^{1}H NMR spectra of product (4f)



^{13}C NMR spectra of product (4f)



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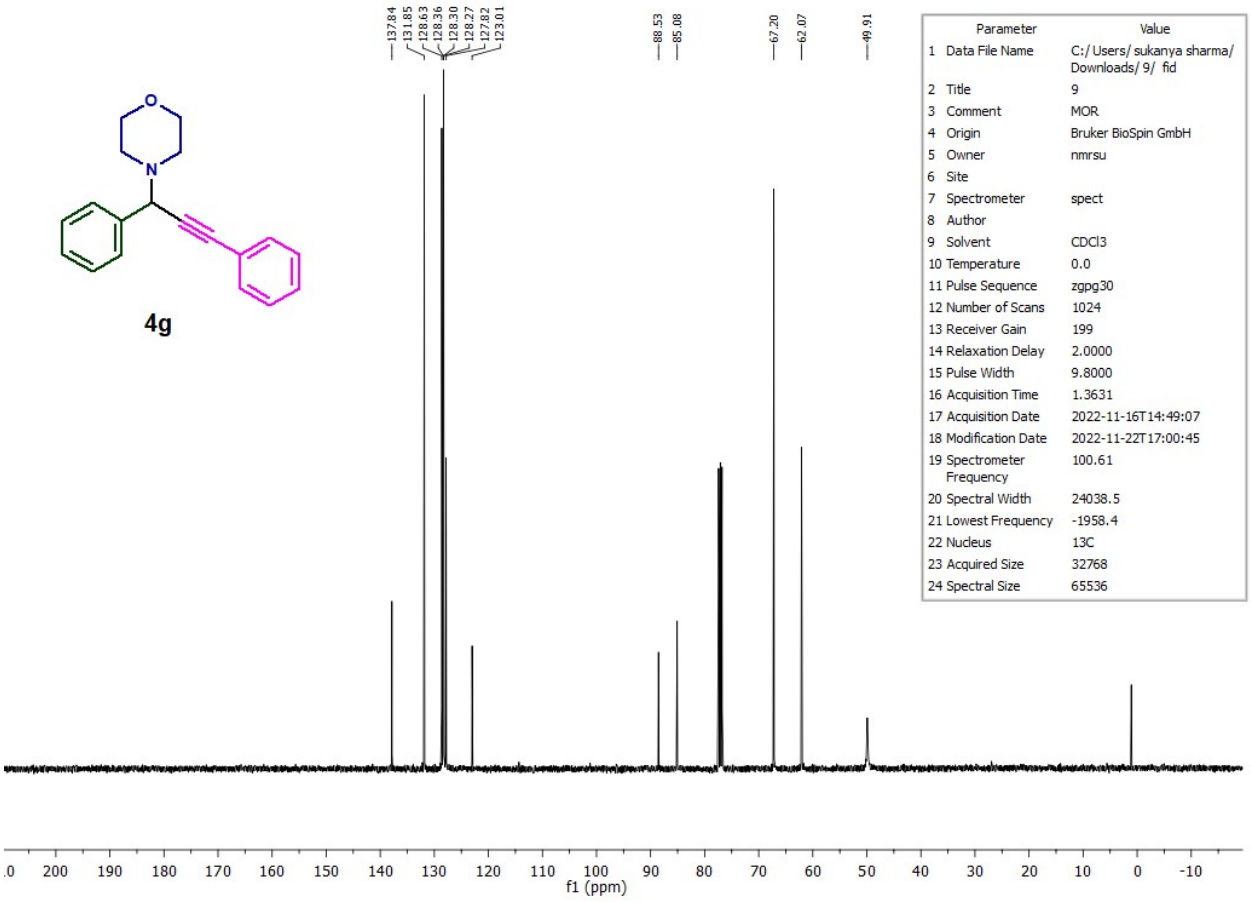
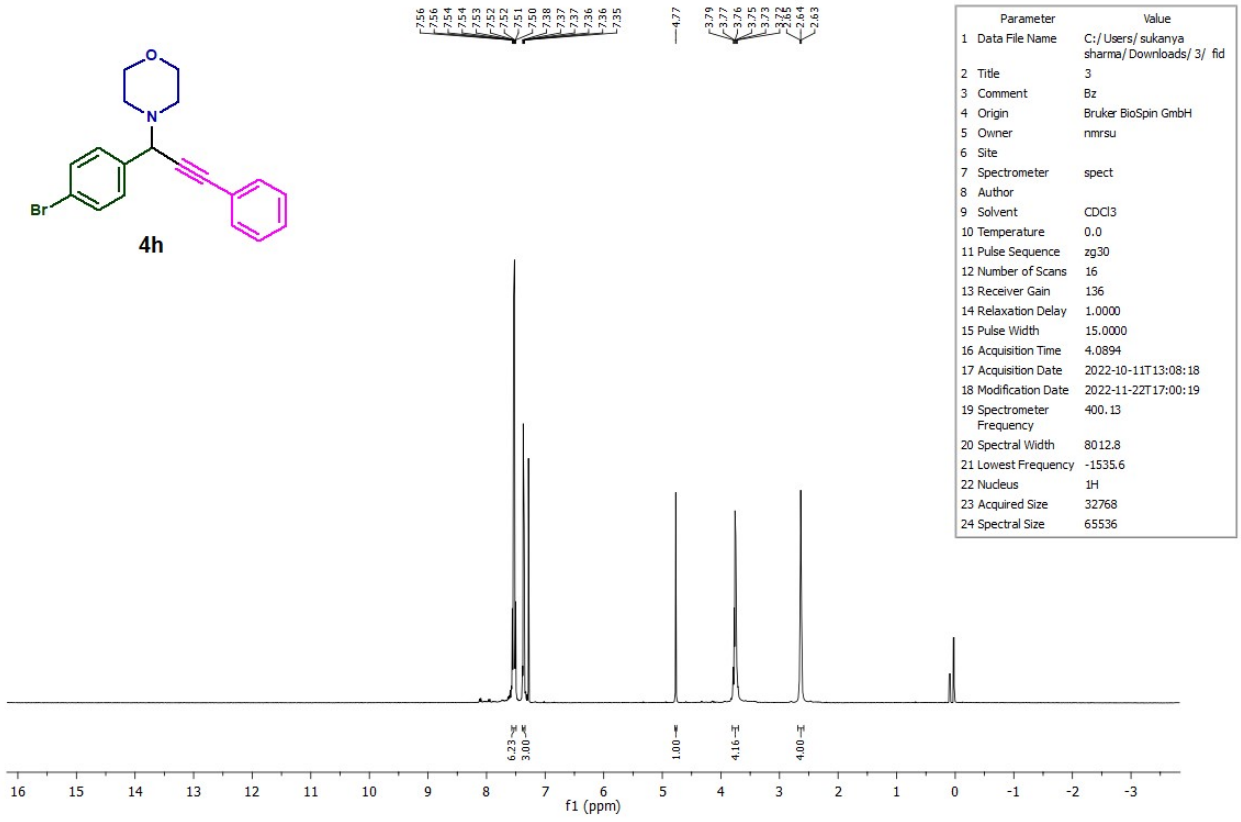
24	Spectral Size	65536

^{1}H NMR spectra of product (4g)



^{13}C NMR spectra of product (4g)



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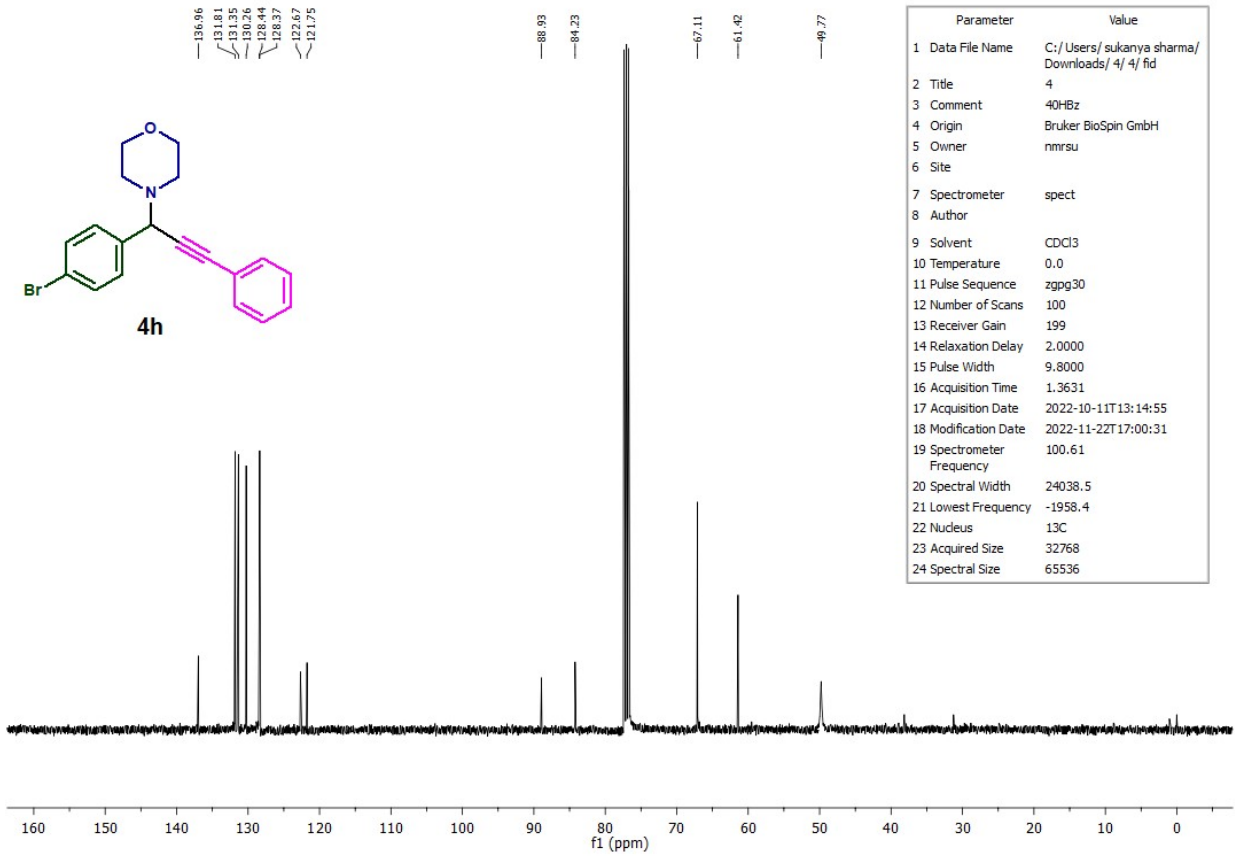
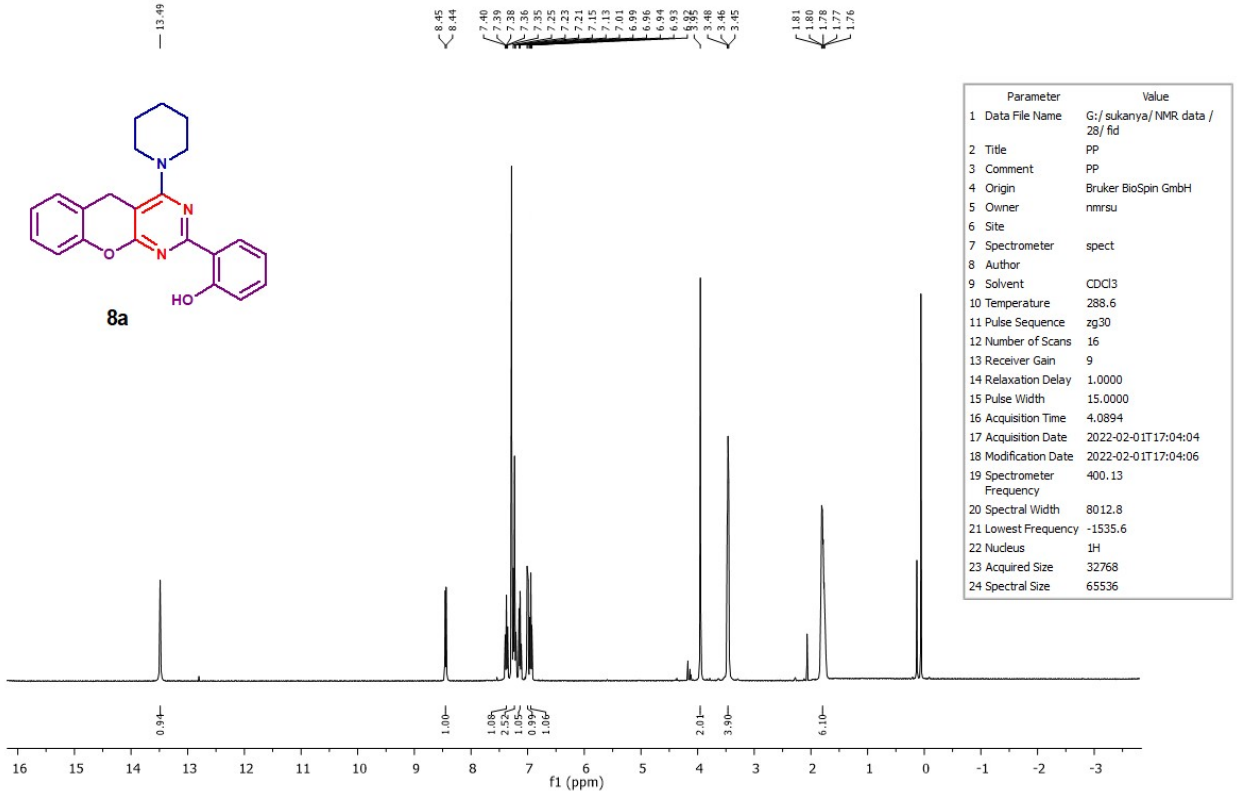
^{1}H NMR spectra of product (4h)

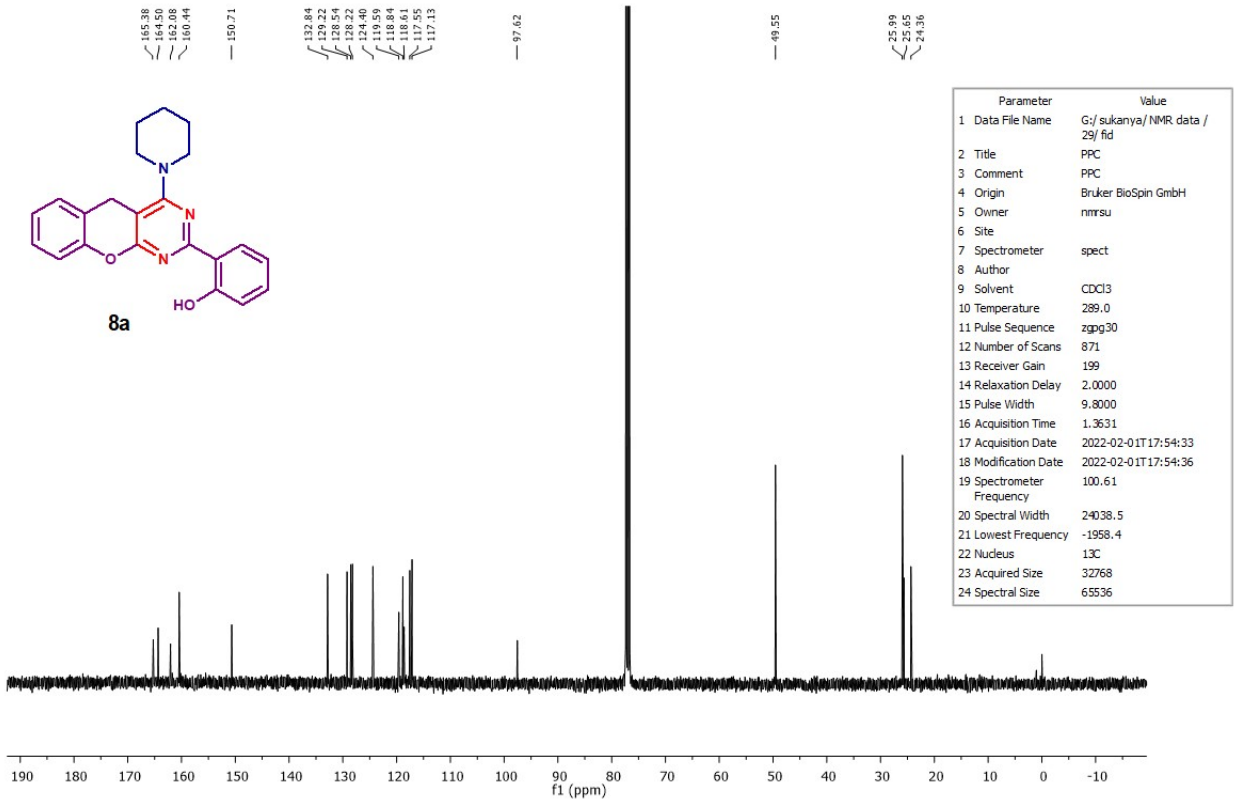


^{13}C NMR spectra of product (4h)

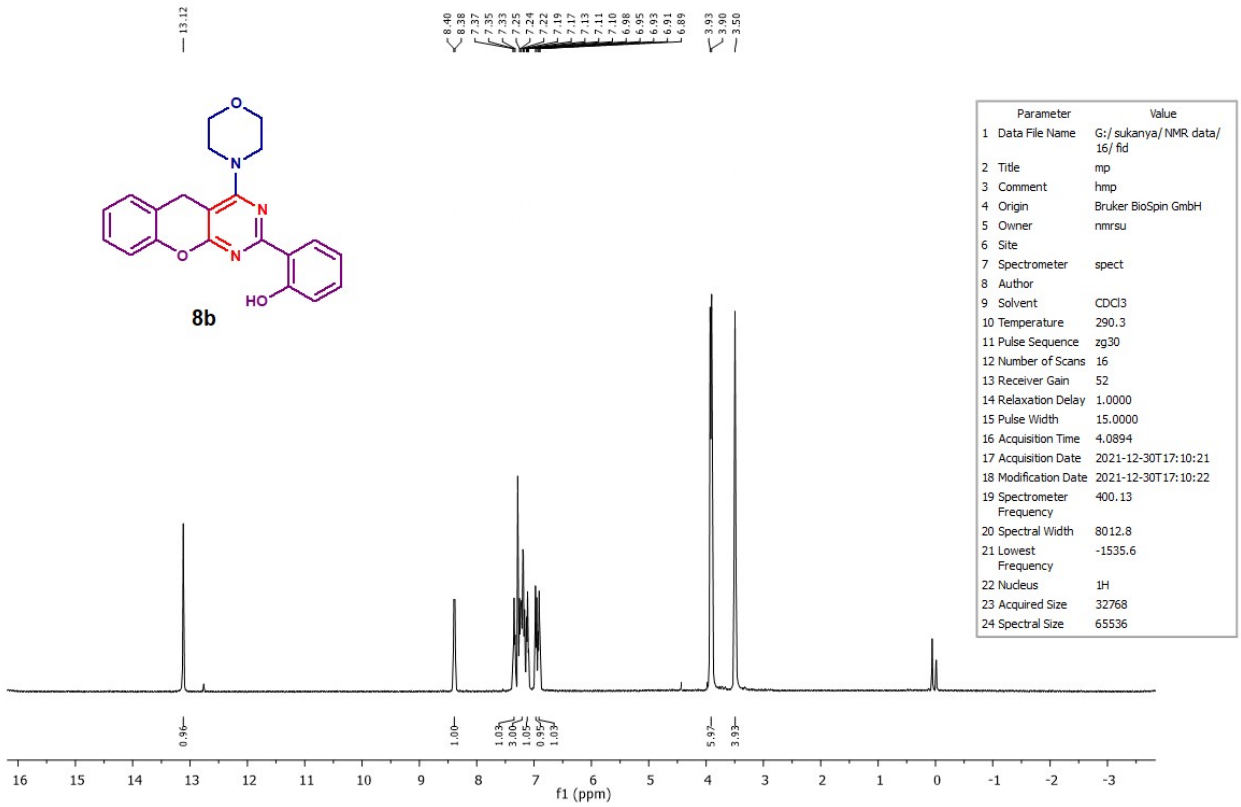
S4. ^{1}H and ^{13}C NMR spectra of compounds listed in Table 7



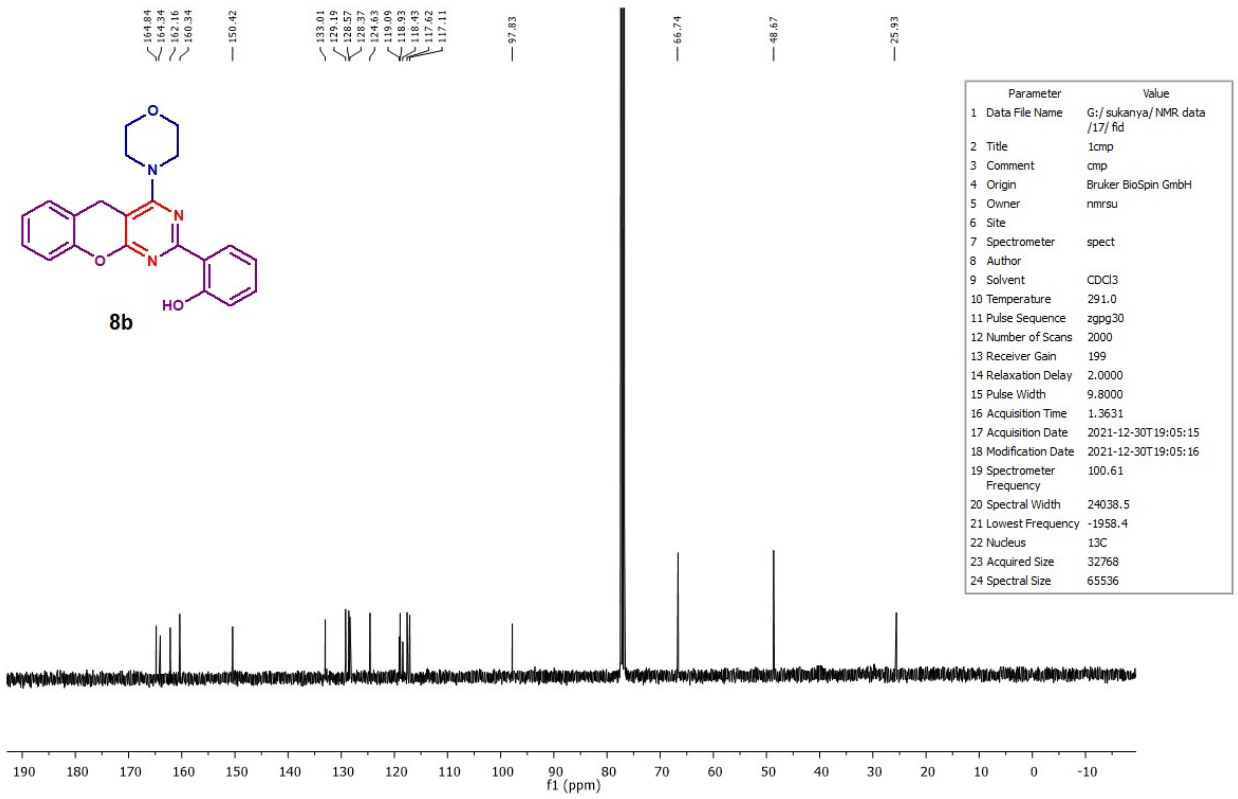
^{1}H NMR spectra of product (8a)



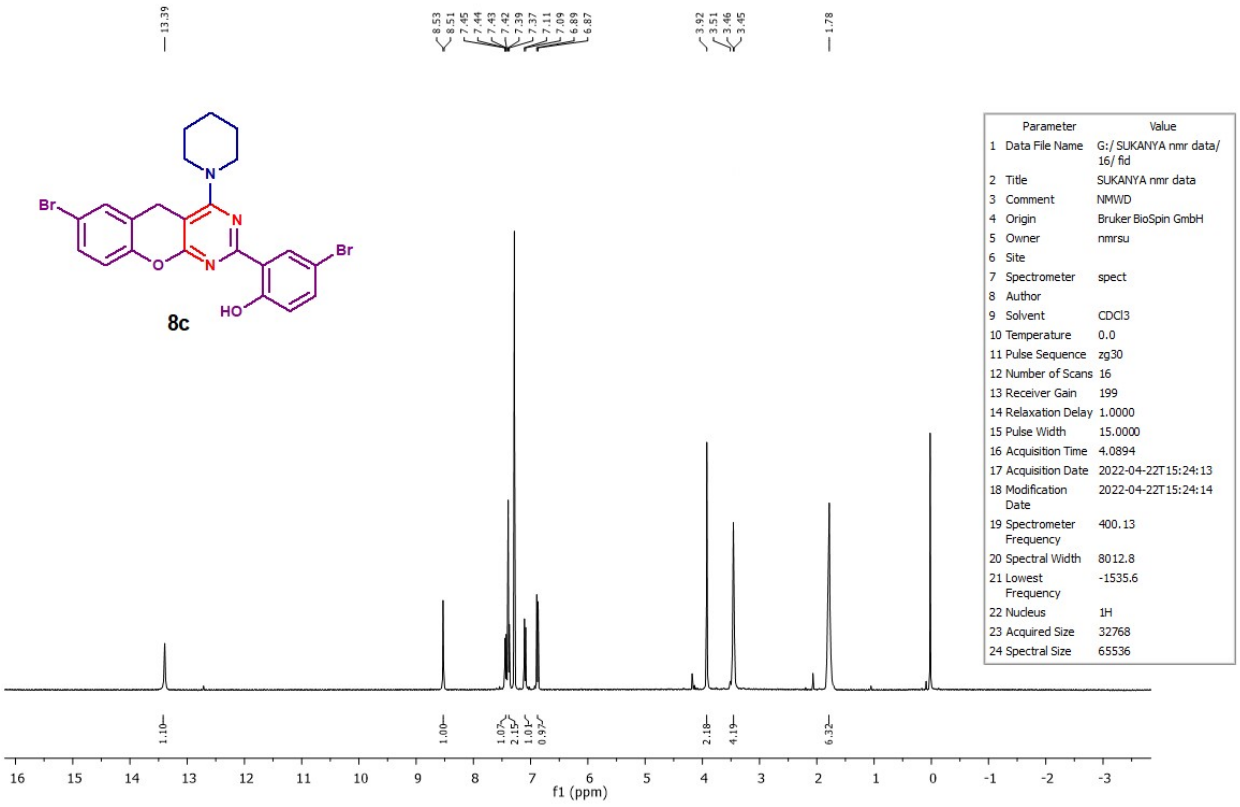
^{13}C NMR spectra of product (8a)



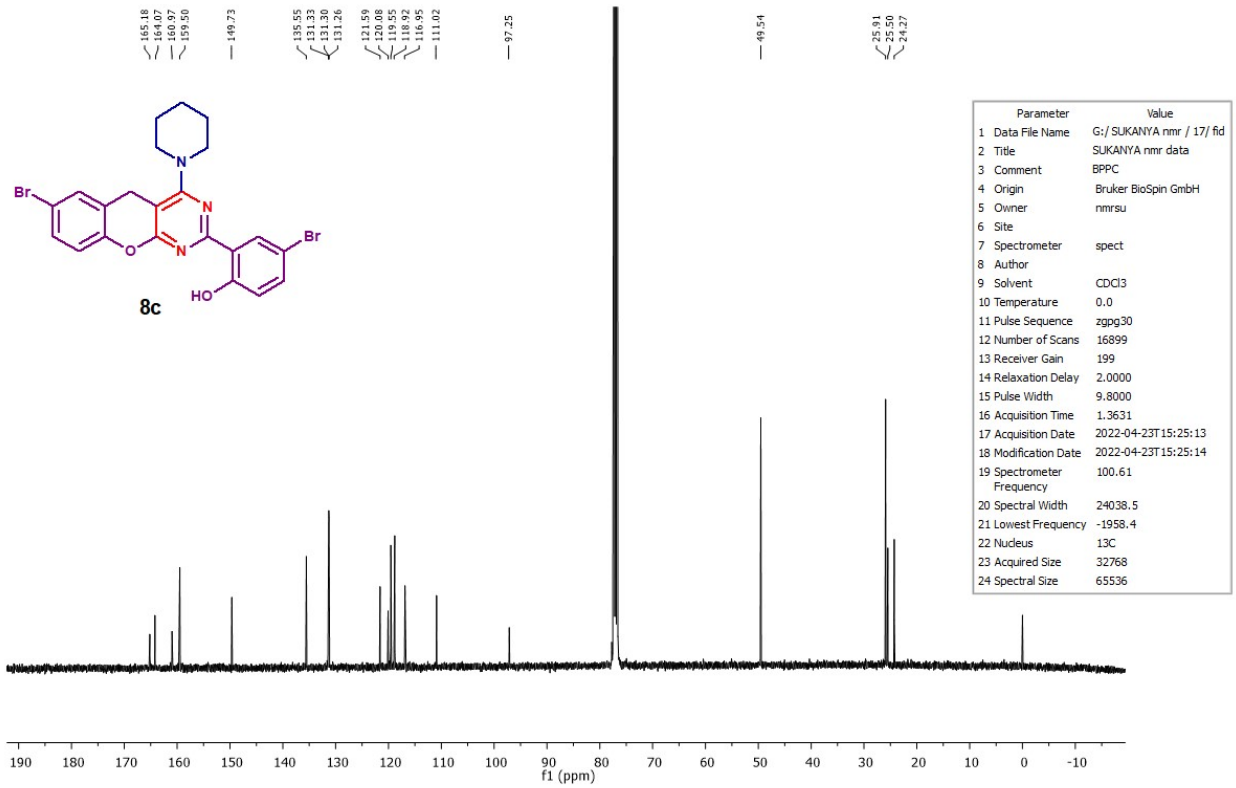
^{1}H NMR spectra of product (8b)



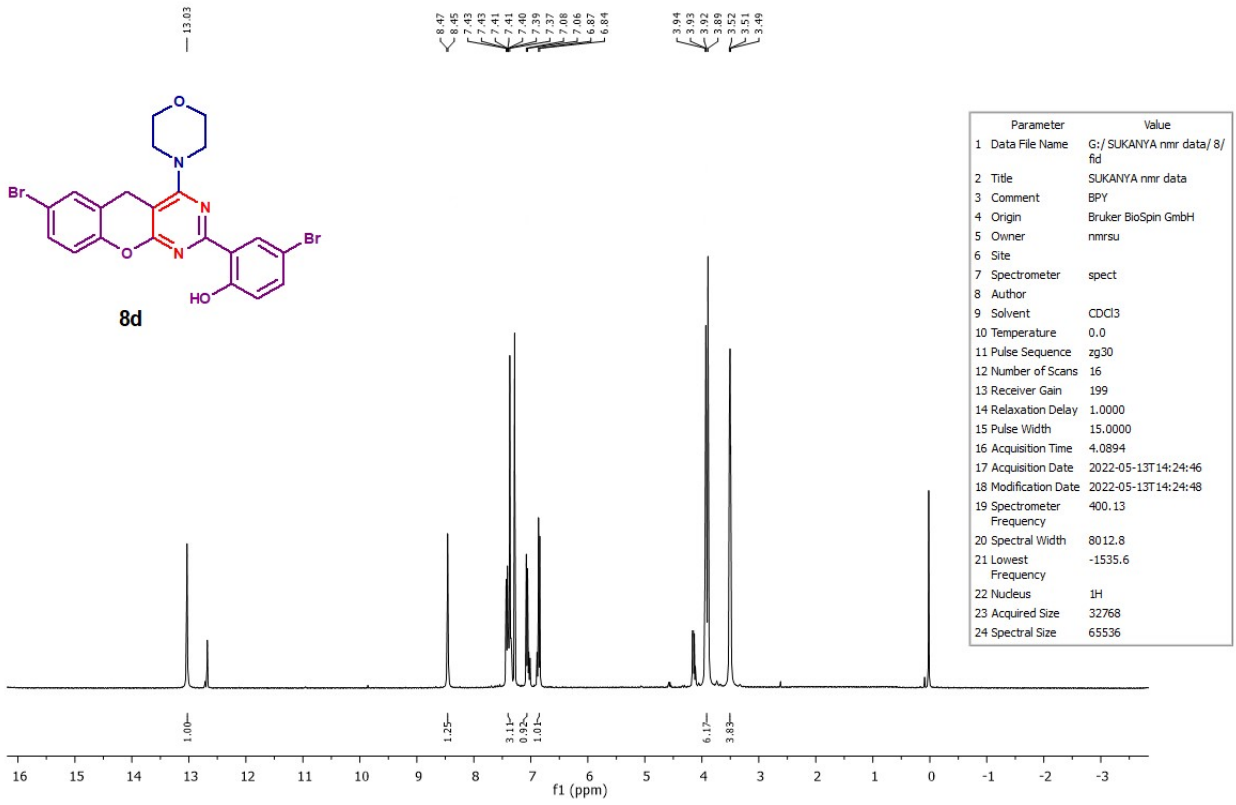
^{13}C NMR spectra of product (8b)



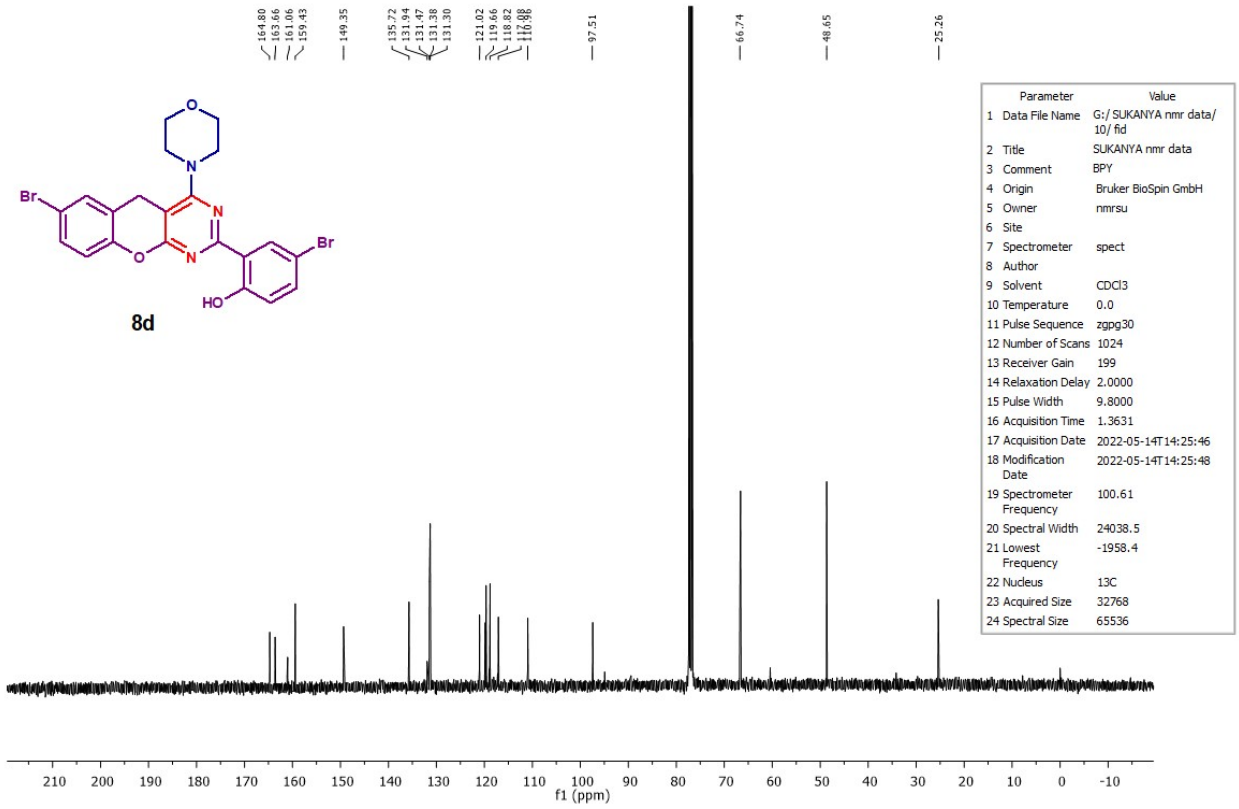
^{1}H NMR spectra of product (8c)



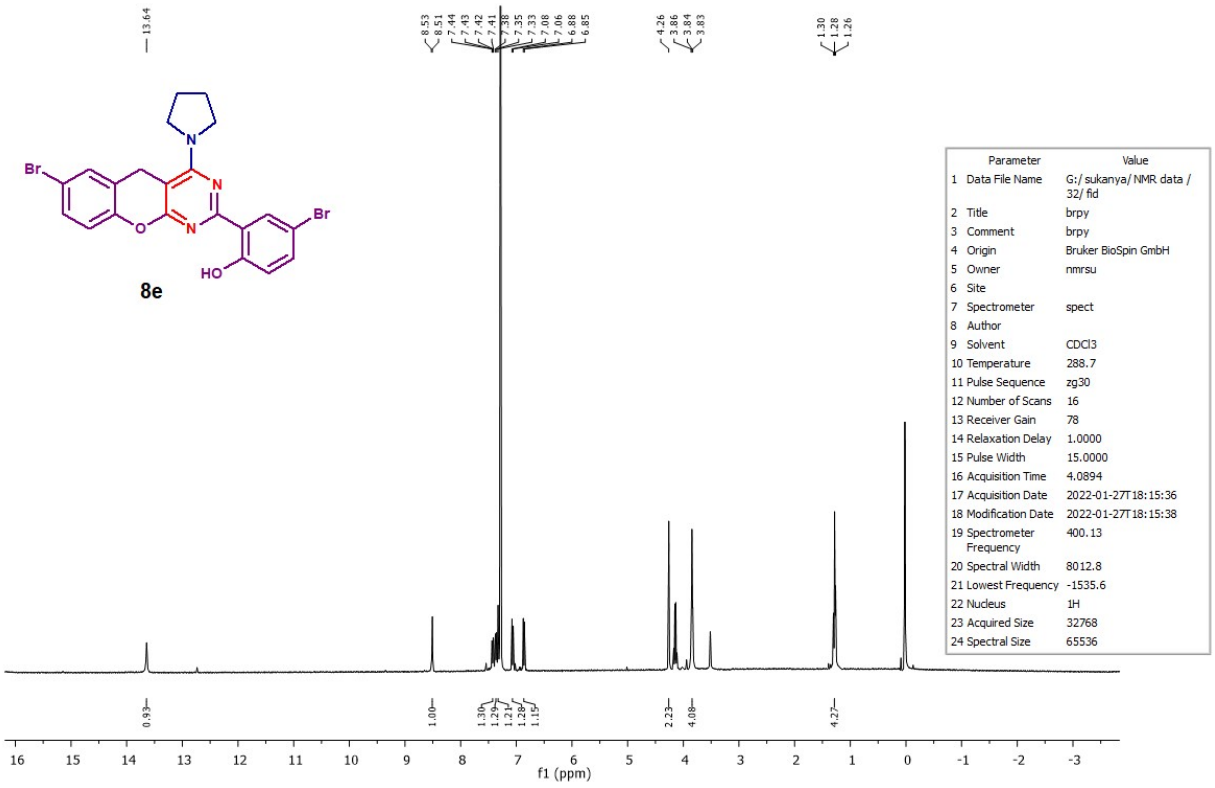
^{13}C NMR spectra of product (8c)



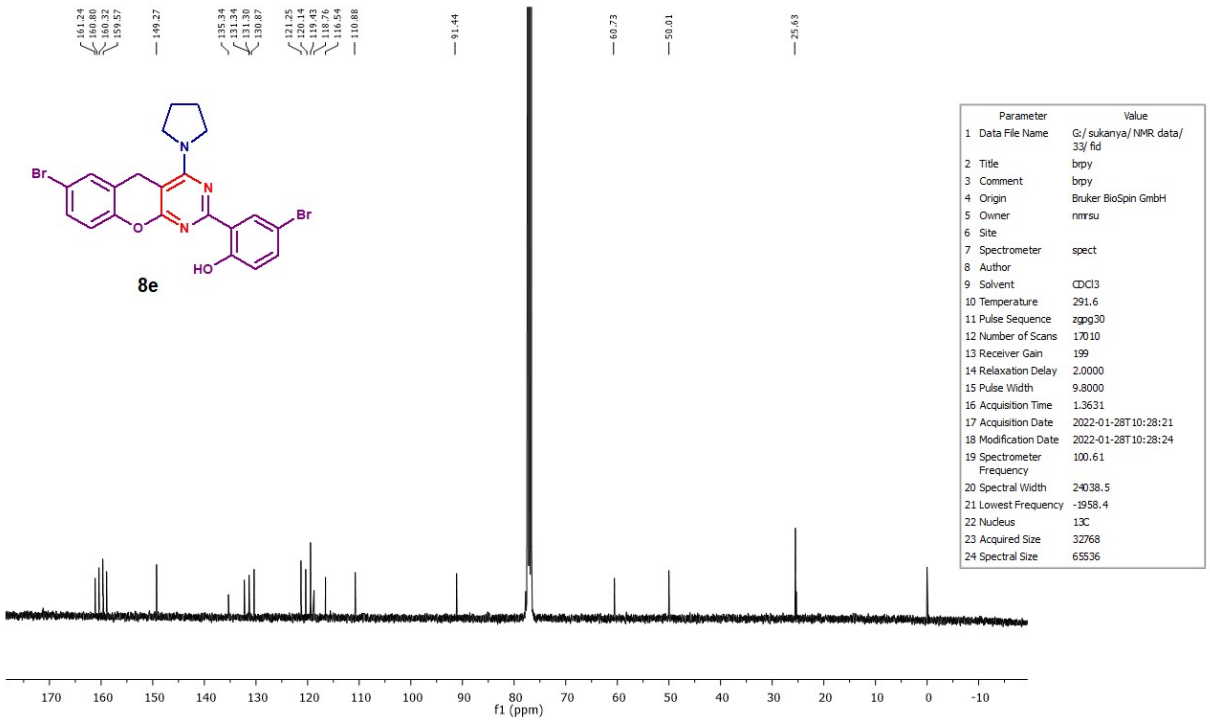
^{1}H NMR spectra of product (8d)



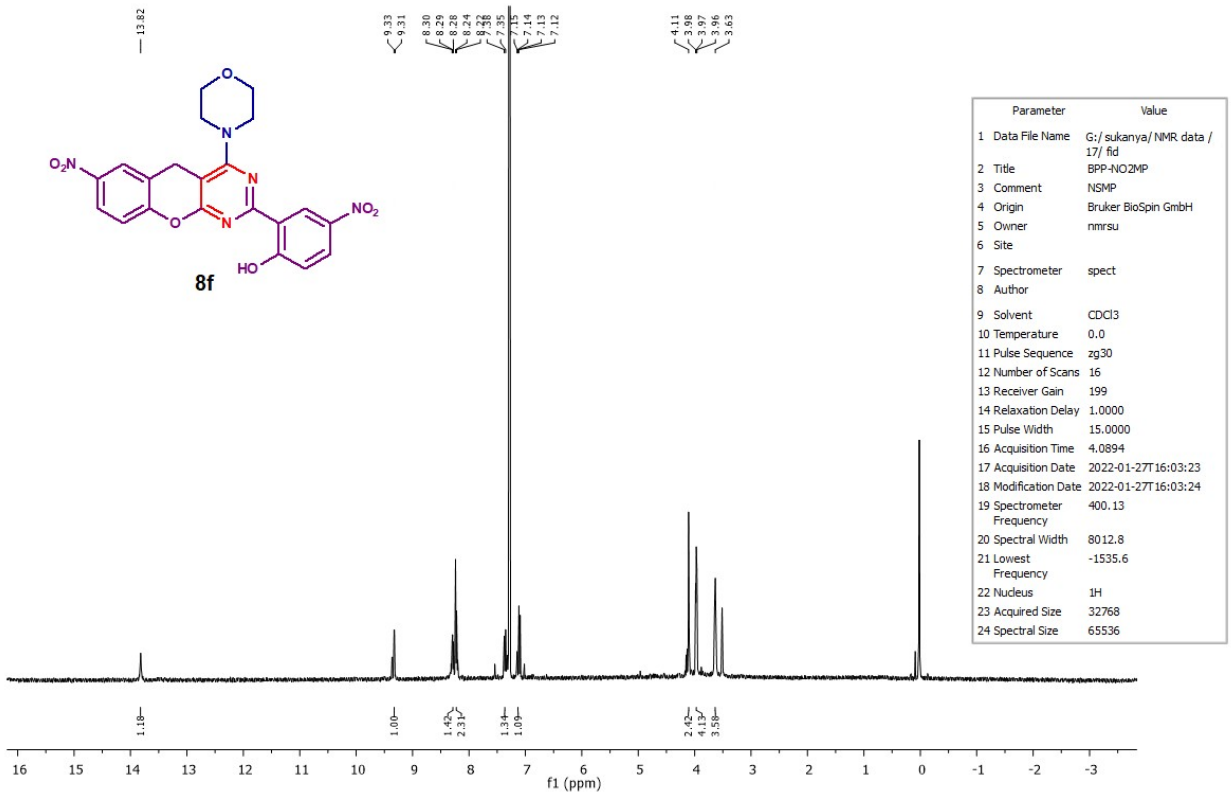
^{13}C NMR spectra of product (8d)



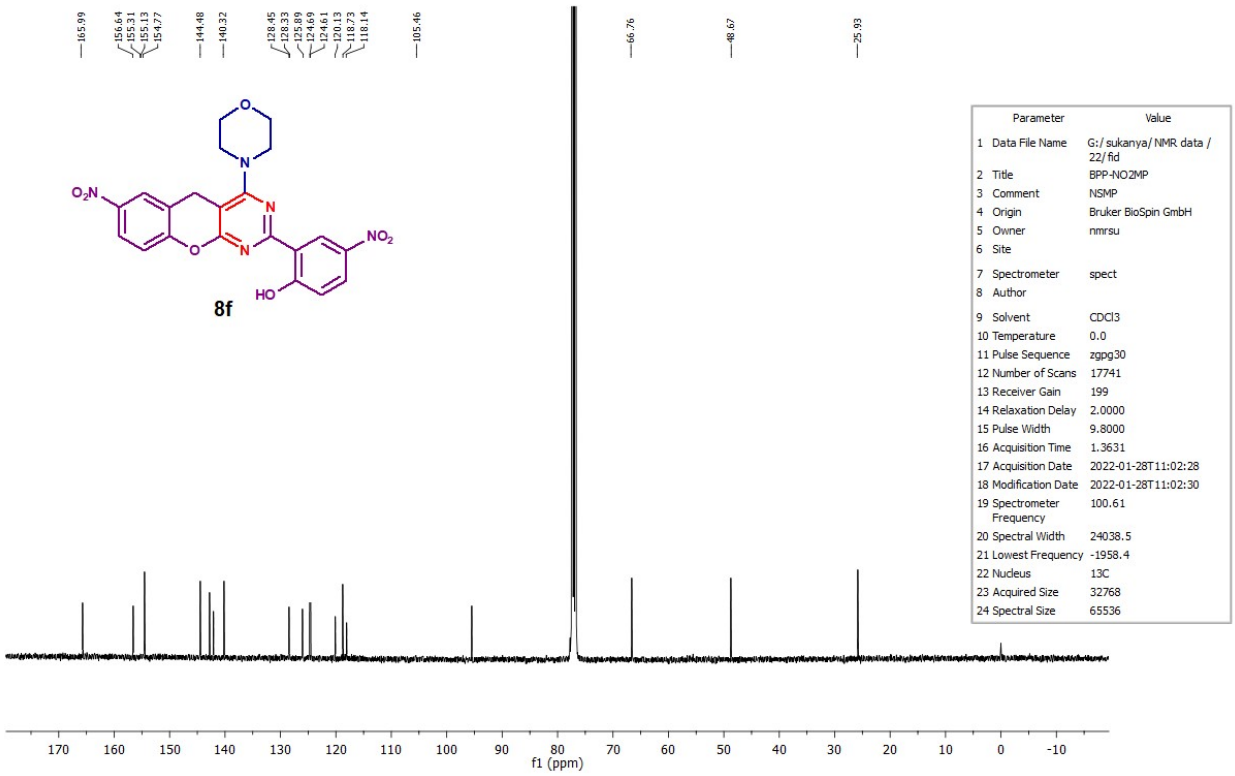
^{1}H NMR spectra of product (8e)



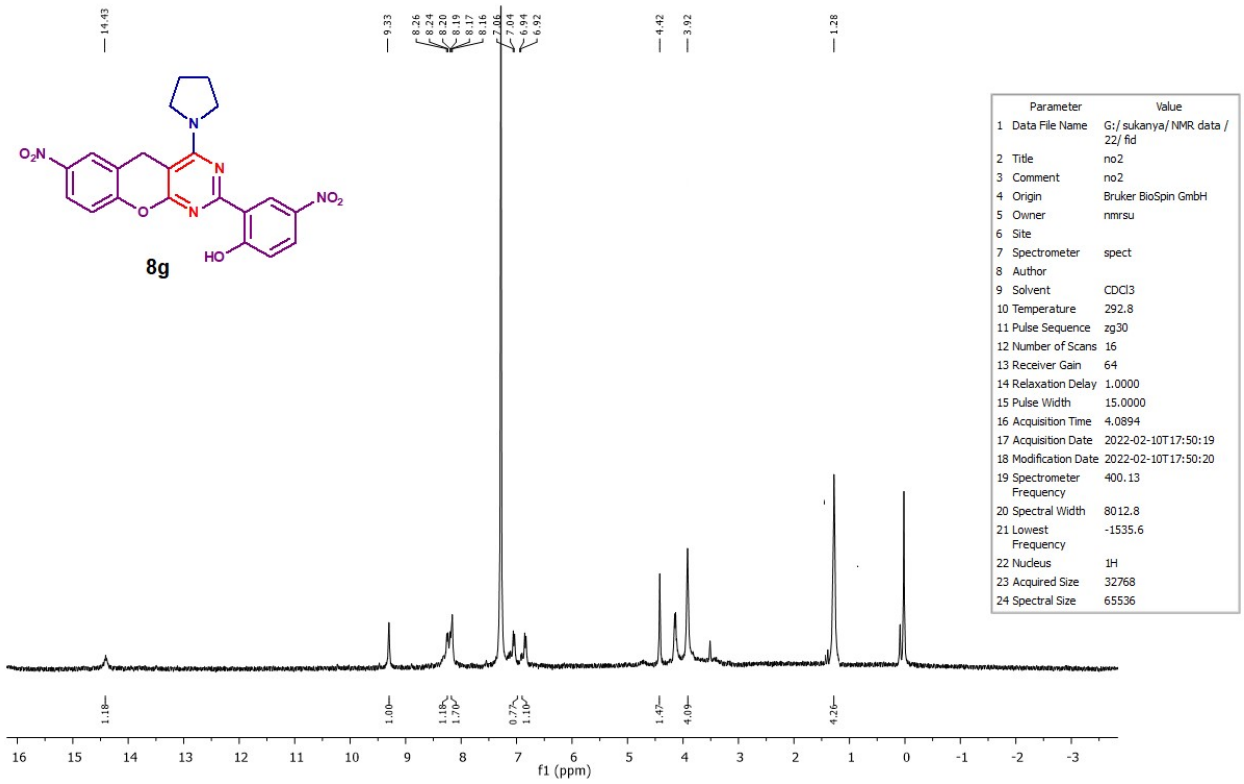
^{13}C NMR spectra of product (8e)



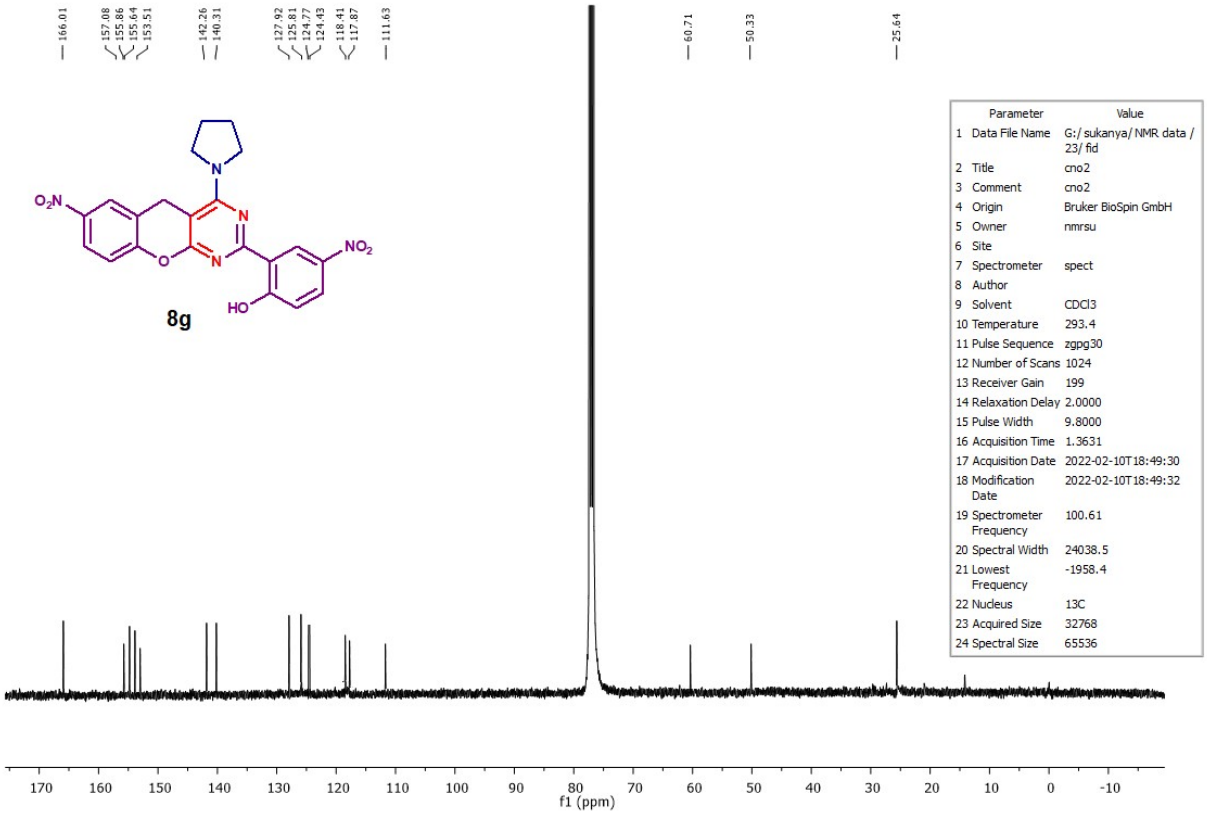
^{1}H NMR spectra of product (8f)



^{13}C NMR spectra of product (8f)



^{1}H NMR spectra of product (8g)



^{13}C NMR spectra of product (8g)