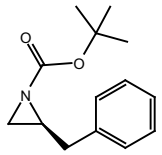
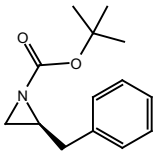
Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zg30
4 Experiment	1D
5 Number of Scans	64
6 Relaxation Delay	1.0000
7 Spectrometer Frequency	400.13
8 Nucleus	1H

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.34 (dd, J = 8.2, 1.7 Hz, 2H), 7.32 – 7.27 (m, 2H), 7.25 – 7.19 (m, 1H), 2.81 – 2.74 (m, 1H), 2.67 (d, J = 5.8 Hz, 1H), 2.63 (dt, J = 6.0, 3.1 Hz, 1H), 2.25 (d, J = 5.9 Hz, 1H), 2.01 (d, J = 3.2 Hz, 1H), 1.37 (s, 10H).

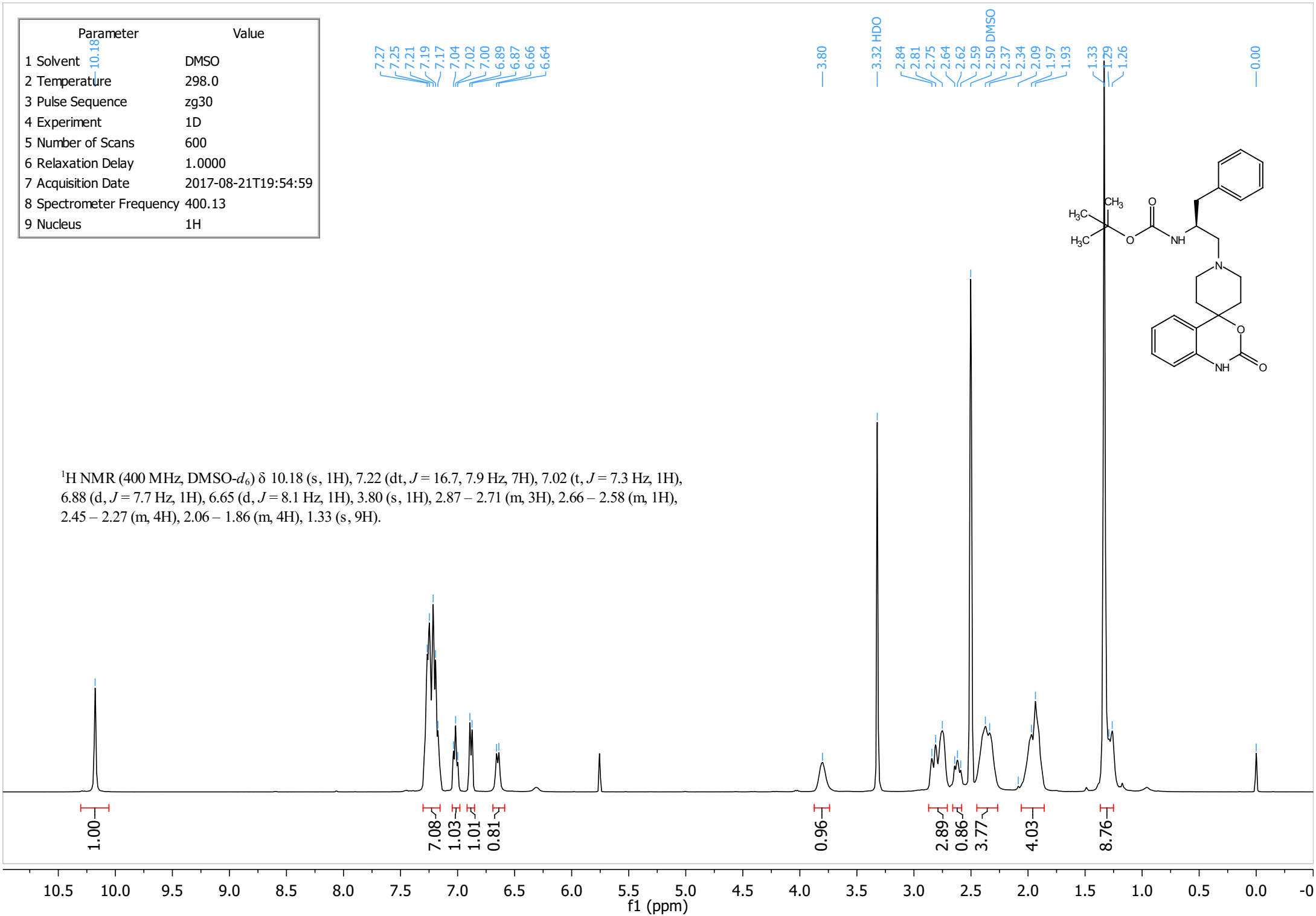


Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zgpg30
4 Experiment	1D
5 Number of Scans	2056
6 Relaxation Delay	2.0000
7 Spectrometer Frequency	100.61
8 Nucleus	13C

^{13}C NMR (101 MHz, DMSO-d_6) δ
161.58, 138.21, 128.71, 128.20, 126.27,
80.10, 37.67, 37.59, 30.76, 27.54.



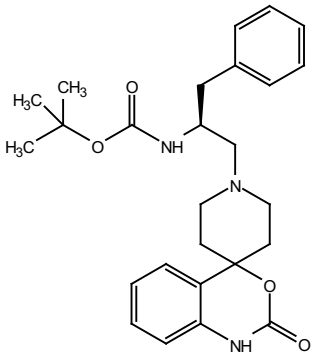
Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zg30
4 Experiment	1D
5 Number of Scans	600
6 Relaxation Delay	1.0000
7 Acquisition Date	2017-08-21T19:54:59
8 Spectrometer Frequency	400.13
9 Nucleus	1H



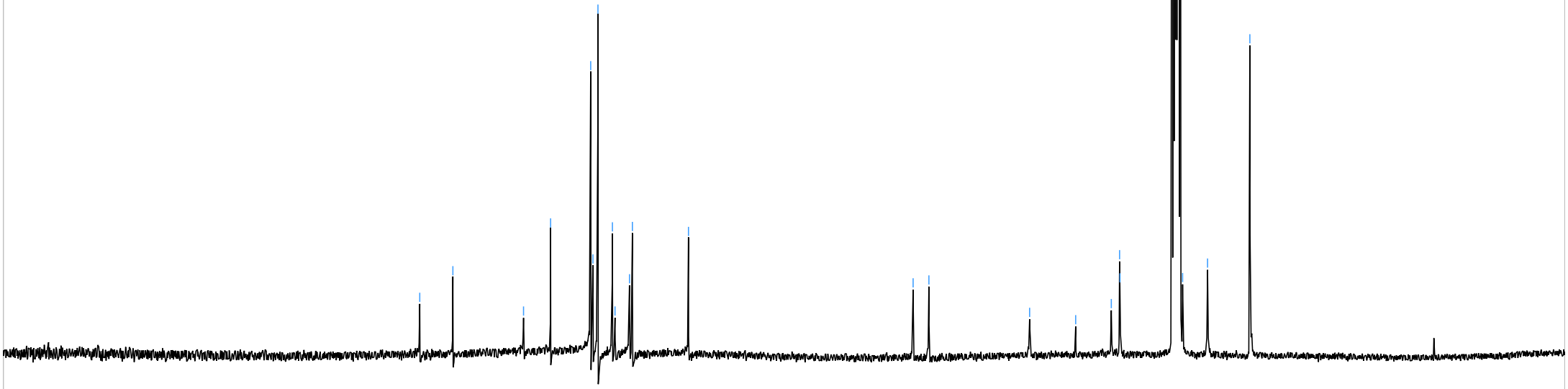
^{1}H NMR (400 MHz, DMSO-d_6) δ 10.18 (s, 1H), 7.22 (dt, J = 16.7, 7.9 Hz, 7H), 7.02 (t, J = 7.3 Hz, 1H), 6.88 (d, J = 7.7 Hz, 1H), 6.65 (d, J = 8.1 Hz, 1H), 3.80 (s, 1H), 2.87 – 2.71 (m, 3H), 2.66 – 2.58 (m, 1H), 2.45 – 2.27 (m, 4H), 2.06 – 1.86 (m, 4H), 1.33 (s, 9H).

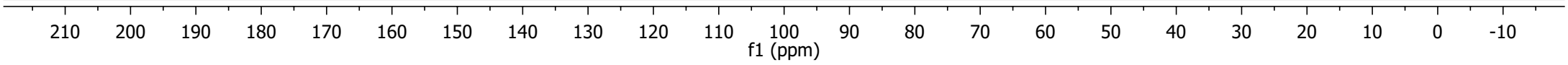
Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zgpg30
4 Experiment	1D
5 Number of Scans	2000
6 Relaxation Delay	2.0000
7 Acquisition Date	2017-08-21T21:50:35
8 Spectrometer Frequency	100.61
9 Nucleus	13C

155.75, 150.68, 139.87, 135.73, 129.59, 129.26, 128.48, 126.27, 125.87, 123.66, 123.22, 114.63, 80.26, 77.85, 62.44, 55.39, 49.94, 48.67, 48.61, 39.03, 35.21, 28.74

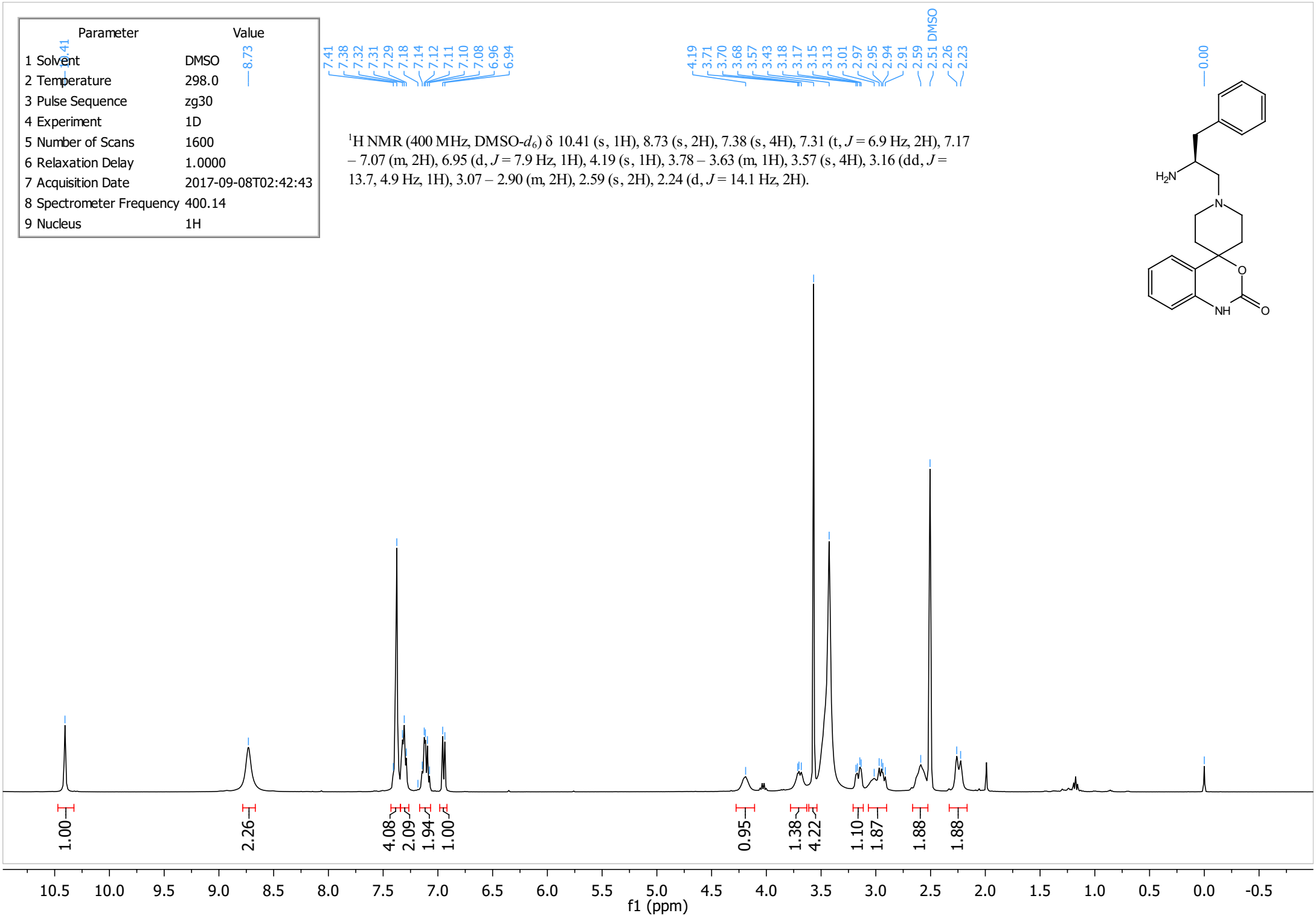


^{13}C NMR (101 MHz, DMSO-d_6) δ 155.75, 150.68, 139.87, 135.73, 129.59, 129.26, 128.48, 126.27, 125.87, 123.66, 123.22, 114.63, 80.26, 77.85, 62.44, 55.39, 49.94, 48.67, 48.61, 39.03, 35.21, 28.74.





Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zg30
4 Experiment	1D
5 Number of Scans	1600
6 Relaxation Delay	1.0000
7 Acquisition Date	2017-09-08T02:42:43
8 Spectrometer Frequency	400.14
9 Nucleus	1H

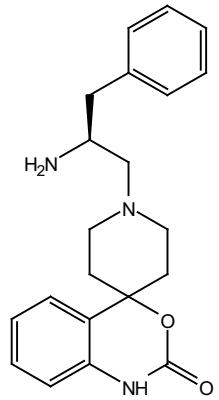


^{1}H NMR (400 MHz, DMSO-d_6) δ 10.41 (s, 1H), 8.73 (s, 2H), 7.38 (s, 4H), 7.31 (t, J = 6.9 Hz, 2H), 7.17 – 7.07 (m, 2H), 6.95 (d, J = 7.9 Hz, 1H), 4.19 (s, 1H), 3.78 – 3.63 (m, 1H), 3.57 (s, 4H), 3.16 (dd, J = 13.7, 4.9 Hz, 1H), 3.07 – 2.90 (m, 2H), 2.59 (s, 2H), 2.24 (d, J = 14.1 Hz, 2H).

Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zgpg30
4 Experiment	1D
5 Number of Scans	6144
6 Relaxation Delay	2.0000
7 Acquisition Date	2017-09-08T00:24:58
8 Spectrometer Frequency	100.62
9 Nucleus	13C

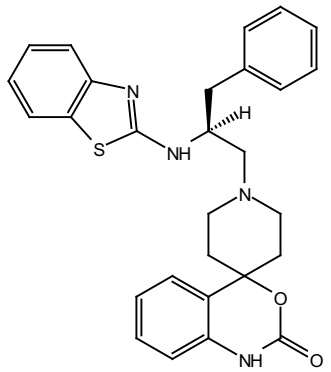
149.57 135.54 135.49 129.97 129.92 129.26 127.74 123.55 123.44 115.01 77.86 66.82 58.03 49.92 47.74 47.44 36.97 32.85 32.73

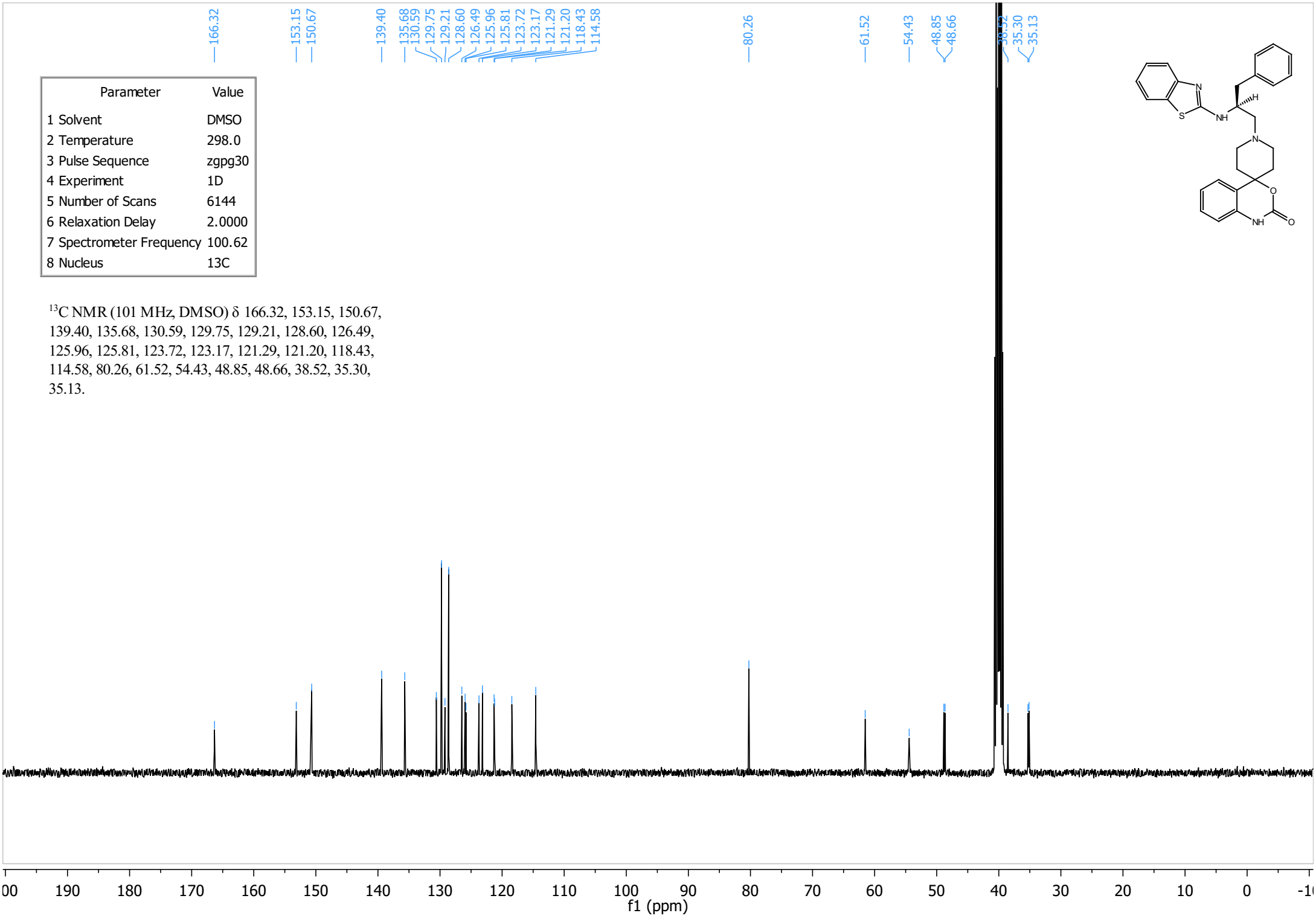
^{13}C NMR (101 MHz, DMSO-d_6) δ 149.57, 135.54, 135.49, 129.97, 129.92, 129.26, 127.74, 123.55, 123.44, 115.01, 77.86, 66.82, 58.03, 49.92, 47.74, 47.44, 36.97, 32.85, 32.73.



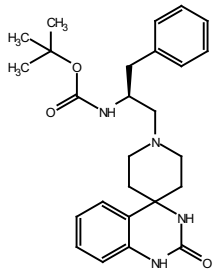
Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zg30
4 Experiment	1D
5 Number of Scans	1600
6 Relaxation Delay	1.0000
7 Acquisition Date	2017-09-18T21:54:24
8 Spectrometer Frequency	400.14
9 Nucleus	1H

^{1}H NMR (400 MHz, DMSO-d_6) δ 10.10 (s, 1H), 7.89 (d, J = 7.8 Hz, 1H), 7.57 (d, J = 7.7 Hz, 1H), 7.30 (d, J = 8.0 Hz, 1H), 7.21 (d, J = 3.9 Hz, 4H), 7.16 – 7.11 (m, 2H), 7.06 (d, J = 7.7 Hz, 1H), 6.91 (dt, J = 14.2, 7.6 Hz, 2H), 6.80 (d, J = 7.9 Hz, 1H), 4.22 – 4.08 (m, 1H), 2.95 (dd, J = 13.6, 5.0 Hz, 1H), 2.84 – 2.67 (m, 3H), 2.47 (d, J = 6.8 Hz, 1H), 2.42 – 2.28 (m, 3H), 1.85 (p, J = 14.0, 13.1 Hz, 4H).




166.32
153.15
150.67
139.40
135.68
130.59
129.75
129.21
128.60
126.49
125.96
125.81
123.72
123.17
121.29
121.20
118.43
114.58
80.26
61.52
54.43
48.85
48.66
38.52
35.30
35.13
Parameter Value
1 Solvent DMSO
2 Temperature 298.0
3 Pulse Sequence zgpg30
4 Experiment 1D
5 Number of Scans 6144
6 Relaxation Delay 2.0000
7 Spectrometer Frequency 100.62
8 Nucleus 13C
13C NMR (101 MHz, DMSO) δ 166.32, 153.15, 150.67, 139.40, 135.68, 130.59, 129.75, 129.21, 128.60, 126.49, 125.96, 125.81, 123.72, 123.17, 121.29, 121.20, 118.43, 114.58, 80.26, 61.52, 54.43, 48.85, 48.66, 38.52, 35.30, 35.13.
N
S
NH
H
N
O
NH
O
f1 (ppm)

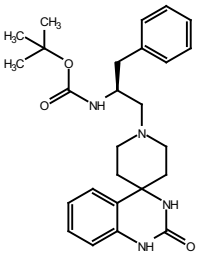
Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zg30
4 Experiment	1D
5 Number of Scans	1600
6 Relaxation Delay	1.0000
7 Acquisition Date	2017-09-09T02:43:39
8 Spectrometer Frequency	400.14
9 Nucleus	1H



^{1}H NMR (400 MHz, DMSO-d_6) δ 9.18 (s, 1H), 7.27 (t, J = 7.3 Hz, 2H), 7.20 (d, J = 6.9 Hz, 3H), 7.12 (t, J = 7.6 Hz, 1H), 6.89 (t, J = 7.5 Hz, 1H), 6.80 (d, J = 7.9 Hz, 1H), 6.61 (d, J = 8.5 Hz, 1H), 3.85 – 3.71 (m, 1H), 2.87 – 2.77 (m, 1H), 2.60 (d, J = 31.3 Hz, 3H), 2.42 – 2.25 (m, 2H), 1.86 (d, J = 12.1 Hz, 2H), 1.68 (d, J = 10.5 Hz, 2H), 1.33 (s, 9H).

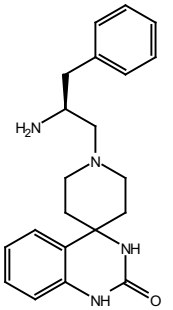
Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zgpg30
4 Experiment	1D
5 Number of Scans	6144
6 Relaxation Delay	2.0000
7 Acquisition Date	2017-09-09T00:25:40
8 Spectrometer Frequency	100.62
9 Nucleus	13C

^{13}C NMR (101 MHz, DMSO) δ 155.73, 153.67, 139.94, 137.69, 129.57, 128.47, 128.16, 127.13, 126.23, 123.90, 121.73, 114.32, 77.80, 62.28, 54.02, 49.84, 48.14, 47.99, 39.01, 37.30, 28.75.



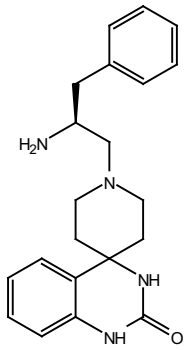
Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zg30
4 Experiment	1D
5 Number of Scans	600
6 Relaxation Delay	1.0000
7 Acquisition Date	2017-08-30T19:24:55
8 Spectrometer Frequency	400.14
9 Nucleus	1H

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.12 (s, 1H), 7.18 (dt, J = 21.6, 7.5 Hz, 5H), 7.05 (t, J = 7.6 Hz, 1H), 6.82 (t, J = 7.5 Hz, 1H), 6.74 (d, J = 3.8 Hz, 2H), 3.26 (s, 2H), 3.04 (s, 1H), 2.63 – 2.49 (m, 4H), 2.36 (d, J = 35.4 Hz, 2H), 2.23 – 2.07 (m, 2H), 1.86 (dq, J = 23.8, 13.0, 10.8 Hz, 2H), 1.60 (d, J = 12.8 Hz, 2H), 1.44 (s, 1H).



Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zgpg30
4 Experiment	1D
5 Number of Scans	1024
6 Relaxation Delay	2.0000
7 Acquisition Date	2017-08-30T20:24:59
8 Spectrometer Frequency	100.62
9 Nucleus	13C

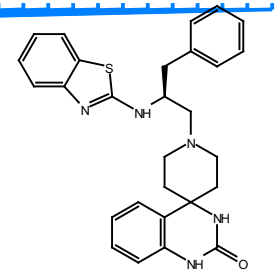
153.72, 140.31, 137.67, 129.70, 128.56, 128.14, 127.17, 126.23, 124.03, 121.75, 114.29, 64.99, 54.09, 49.73, 49.15, 47.41, 42.46, 37.33



^{13}C NMR (101 MHz, DMSO-d_6) δ 153.72, 140.31, 137.67, 129.70, 128.56, 128.14, 127.17, 126.23, 124.03, 121.75, 114.29, 64.99, 54.09, 49.73, 49.15, 47.41, 42.46, 37.33.

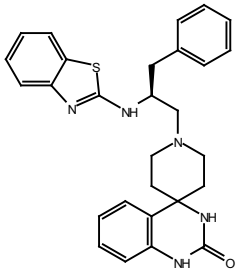
Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zg30
4 Experiment	1D
5 Number of Scans	64
6 Relaxation Delay	1.0000
7 Spectrometer Frequency	400.13
8 Nucleus	1H

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.38 (d, J = 1.9 Hz, 1H), 9.29 (s, 1H), 8.28 (d, J = 8.1 Hz, 1H), 7.70 (dd, J = 7.7, 1.2 Hz, 1H), 7.42 (dd, J = 7.8, 1.0 Hz, 1H), 7.35 – 7.32 (m, 4H), 7.28 – 7.22 (m, 2H), 7.17 (td, J = 7.7, 1.3 Hz, 1H), 7.11 (d, J = 7.6 Hz, 1H), 7.07 (td, J = 7.7, 1.3 Hz, 1H), 6.92 (td, J = 7.7, 1.3 Hz, 1H), 6.83 (dd, J = 7.9, 1.3 Hz, 1H), 4.61 (s, 2H), 3.81 (s, 1H), 3.65 – 3.53 (m, 1H), 3.50 – 3.40 (m, 2H), 3.34 – 3.24 (m, 1H), 3.01 (dq, J = 14.0, 7.6, 7.1 Hz, 2H), 2.37 – 2.29 (m, 1H), 2.20 – 2.11 (m, 1H), 2.01 – 1.88 (m, 2H).



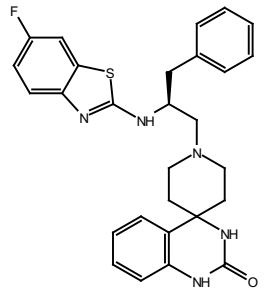
Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zgpg30
4 Experiment	1D
5 Number of Scans	1024
6 Relaxation Delay	2.0000
7 Spectrometer Frequency	100.61
8 Nucleus	13C

^{13}C NMR (101 MHz, DMSO-d_6) δ 166.32, 158.73, 158.39, 153.05, 152.25, 137.64, 137.34, 130.81, 129.69, 128.98, 128.94, 127.17, 126.21, 124.40, 124.08, 122.04, 121.61, 118.82, 114.68, 52.61, 51.64, 48.95, 47.35, 38.46, 35.15.



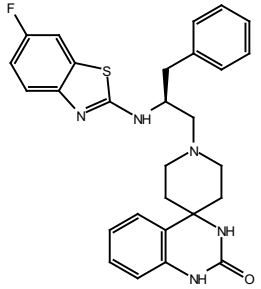
Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zg30
4 Experiment	1D
5 Number of Scans	64
6 Relaxation Delay	1.0000
7 Spectrometer Frequency	400.13
8 Nucleus	1H

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.16 (s, 1H), 7.90 (d, J = 8.2 Hz, 1H), 7.58 (dd, J = 8.8, 2.8 Hz, 1H), 7.34 (dd, J = 8.8, 4.9 Hz, 1H), 7.27 (d, J = 5.1 Hz, 4H), 7.17 (ddd, J = 9.0, 5.7, 3.5 Hz, 1H), 7.09 (dd, J = 13.6, 7.3 Hz, 2H), 7.05 – 6.99 (m, 1H), 6.84 (t, J = 7.6 Hz, 1H), 6.80 – 6.76 (m, 2H), 4.20 (q, J = 7.3 Hz, 1H), 3.00 (dd, J = 13.7, 5.3 Hz, 1H), 2.84 (dd, J = 13.7, 7.3 Hz, 1H), 2.76 – 2.60 (m, 3H), 2.61 – 2.52 (m, 2H), 2.45 (d, J = 1.5 Hz, 1H), 1.89 – 1.80 (m, 2H), 1.65 (t, J = 15.6 Hz, 2H).



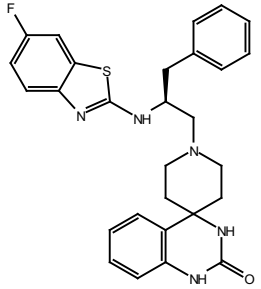
Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zgpg30
4 Experiment	1D
5 Number of Scans	1024
6 Relaxation Delay	2.0000
7 Spectrometer Frequency	100.61
8 Nucleus	13C

166.32 153.63 149.82 139.44 137.63 131.70 129.73 128.61 128.15 127.04 126.49 123.98 121.68 118.85 118.76 114.29 113.33 113.09 108.38 108.11 61.35 54.41 53.97 48.21 48.11 38.46 37.44 37.20



^{13}C NMR (101 MHz, DMSO-d_6) δ 166.32, 153.63, 149.82, 139.44, 137.63, 131.70, 129.73, 128.61, 128.15, 127.04, 126.49, 123.98, 121.68, 118.85, 118.76, 114.29, 113.33, 113.09, 108.38, 108.11, 61.35, 54.41, 53.97, 48.21, 48.11, 38.46, 37.44, 37.20.

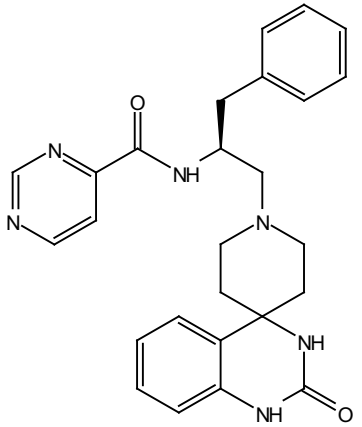
Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zgfhigqn.2
4 Experiment	1D
5 Number of Scans	64
6 Relaxation Delay	1.0000
7 Spectrometer Frequency	376.50
8 Nucleus	19F



^{19}F NMR (376 MHz, DMSO-d_6) δ -122.47.

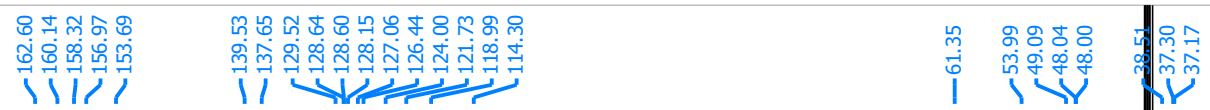
Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zg30
4 Experiment	1D
5 Number of Scans	16
6 Relaxation Delay	1.0000
7 Spectrometer Frequency	400.13
8 Nucleus	1H

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.33 (d, J = 1.3 Hz, 1H), 9.18 (d, J = 2.0 Hz, 1H), 9.04 (d, J = 5.0 Hz, 1H), 8.82 (d, J = 8.8 Hz, 1H), 7.98 – 7.95 (m, 1H), 7.23 (d, J = 4.4 Hz, 4H), 7.19 – 7.07 (m, 3H), 6.87 (t, J = 7.6 Hz, 1H), 6.80 (d, J = 8.3 Hz, 2H), 4.39 (h, J = 7.5 Hz, 1H), 3.00 – 2.91 (m, 2H), 2.73 – 2.66 (m, 2H), 2.62 (dt, J = 11.2, 5.5 Hz, 2H), 2.58 – 2.52 (m, 2H), 1.86 (dtd, J = 17.1, 12.9, 4.7 Hz, 2H), 1.66 (ddd, J = 13.9, 5.6, 2.7 Hz, 2H).

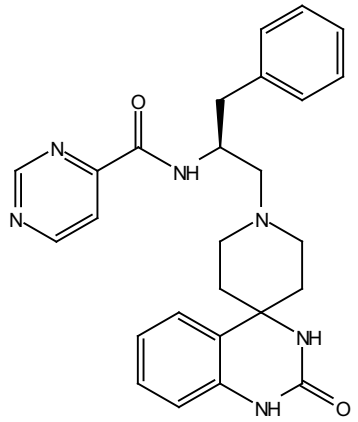


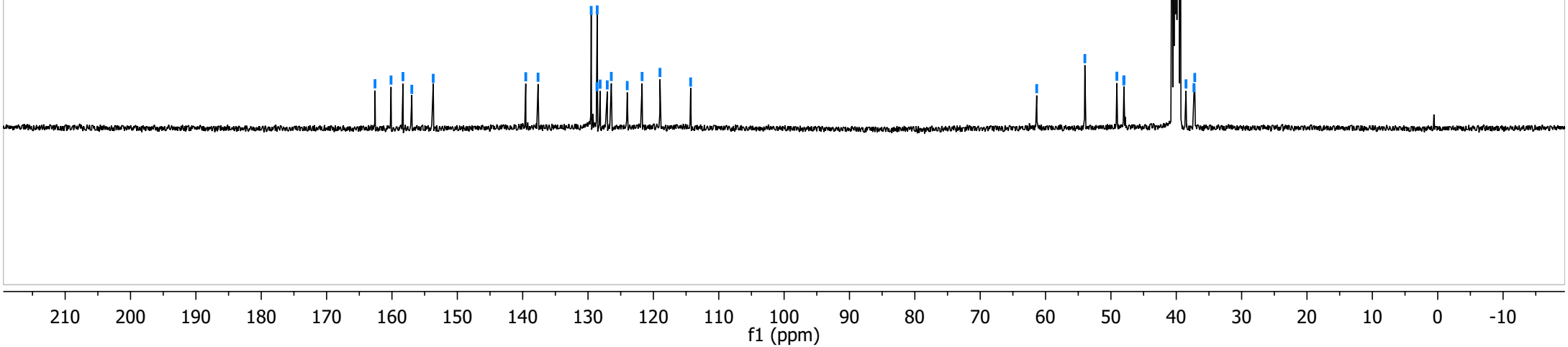
1D — Aug29-2017.121.1.1r — SampleID DOGRAAB1-008-EXP017-1-13C

Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zgpg30
4 Experiment	1D
5 Number of Scans	256
6 Relaxation Delay	2.0000
7 Spectrometer Frequency	100.61
8 Nucleus	13C



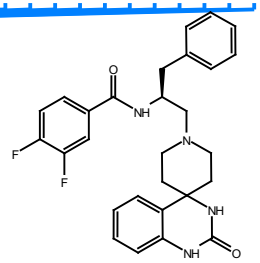
^{13}C NMR (101 MHz, DMSO-d_6) δ 162.60, 160.14, 158.32, 156.97, 153.69, 139.53, 137.65, 129.52, 128.64, 128.60, 128.15, 127.06, 126.44, 124.00, 121.73, 118.99, 114.30, 61.35, 53.99, 49.09, 48.04, 48.00, 38.51, 37.30, 37.17.





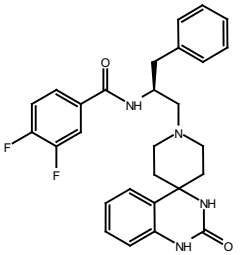
Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zg30
4 Experiment	1D
5 Number of Scans	64
6 Relaxation Delay	1.0000
7 Spectrometer Frequency	400.13
8 Nucleus	1H

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.20 – 9.14 (m, 1H), 8.34 – 8.27 (m, 1H), 7.82 (ddd, J = 11.6, 7.8, 2.1 Hz, 1H), 7.68 (ddt, J = 7.8, 4.8, 1.6 Hz, 1H), 7.54 (dt, J = 10.4, 8.3 Hz, 1H), 7.25 (d, J = 5.7 Hz, 4H), 7.20 (dd, J = 7.9, 1.3 Hz, 1H), 7.16 (td, J = 6.0, 2.7 Hz, 1H), 7.12 (td, J = 7.6, 1.2 Hz, 1H), 6.90 – 6.86 (m, 1H), 6.81 – 6.79 (m, 1H), 6.79 (s, 1H), 4.35 (q, J = 7.3 Hz, 1H), 2.98 (dd, J = 13.8, 5.0 Hz, 1H), 2.79 (dd, J = 13.8, 8.6 Hz, 1H), 2.73 – 2.65 (m, 2H), 2.63 – 2.51 (m, 4H), 1.88 (qd, J = 12.5, 4.4 Hz, 2H), 1.69 (dt, J = 14.9, 5.0 Hz, 2H).



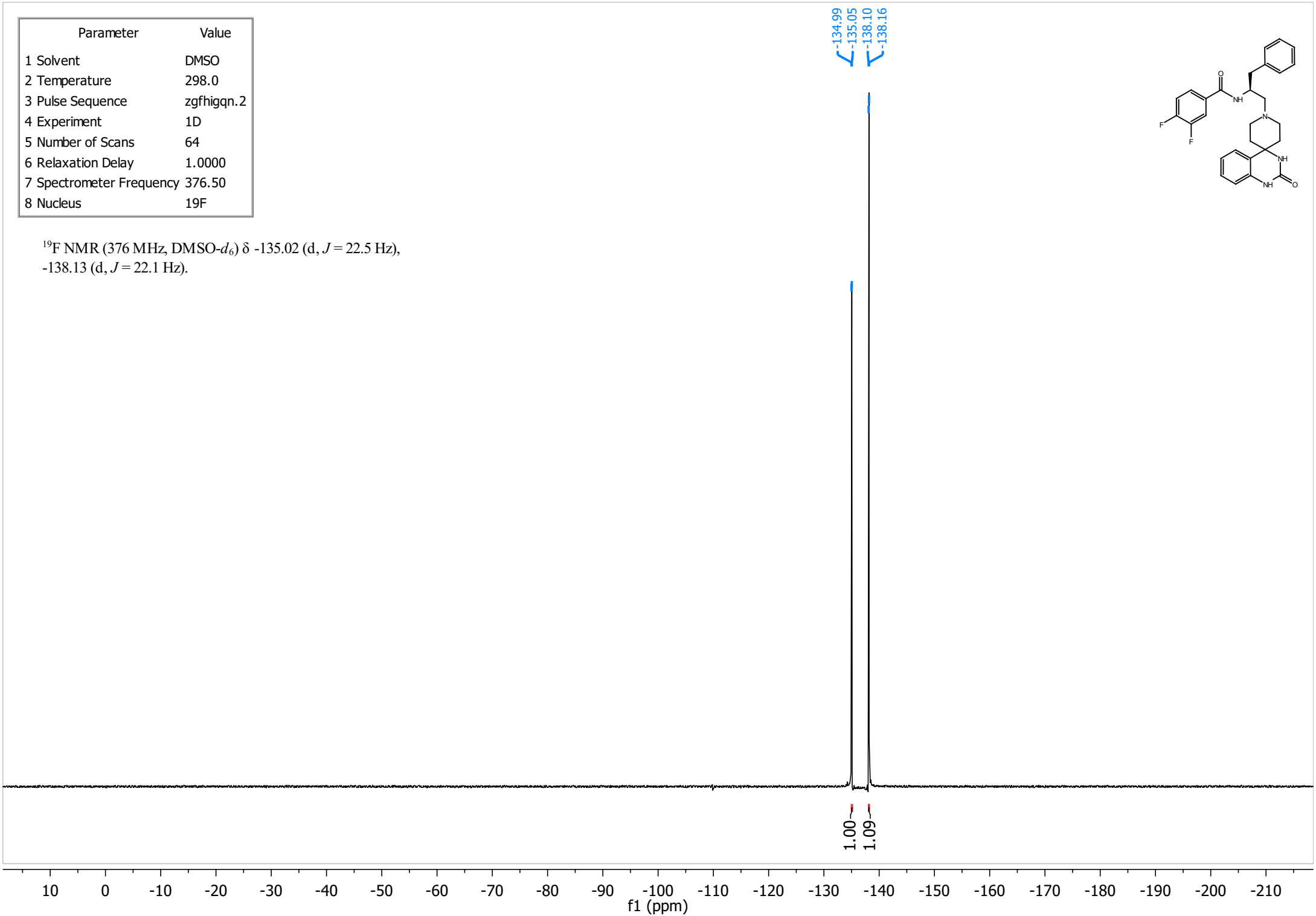
Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zgpg30
4 Experiment	1D
5 Number of Scans	1024
6 Relaxation Delay	2.0000
7 Spectrometer Frequency	100.61
8 Nucleus	13C

^{13}C NMR (101 MHz, DMSO-d_6) δ 164.14, 153.68, 150.83, 148.39, 139.70, 137.66, 132.66, 129.57, 128.57, 128.17, 127.08, 126.40, 125.09, 124.01, 121.74, 118.04, 117.87, 117.08, 116.90, 114.32, 61.69, 54.00, 49.39, 48.26, 47.85, 38.74, 37.34, 37.19.



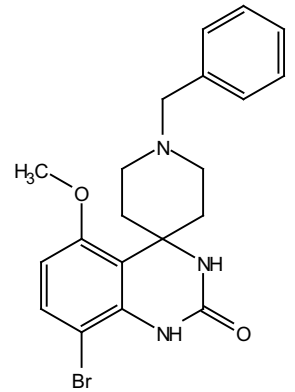
Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zgfhigqn.2
4 Experiment	1D
5 Number of Scans	64
6 Relaxation Delay	1.0000
7 Spectrometer Frequency	376.50
8 Nucleus	19F

^{19}F NMR (376 MHz, DMSO-d_6) δ -135.02 (d, J = 22.5 Hz), -138.13 (d, J = 22.1 Hz).



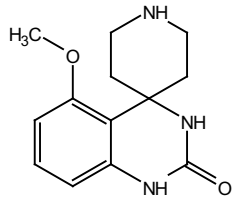
Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zg30
4 Experiment	1D
5 Number of Scans	16
6 Relaxation Delay	1.0000
7 Spectrometer Frequency	400.13
8 Nucleus	1H

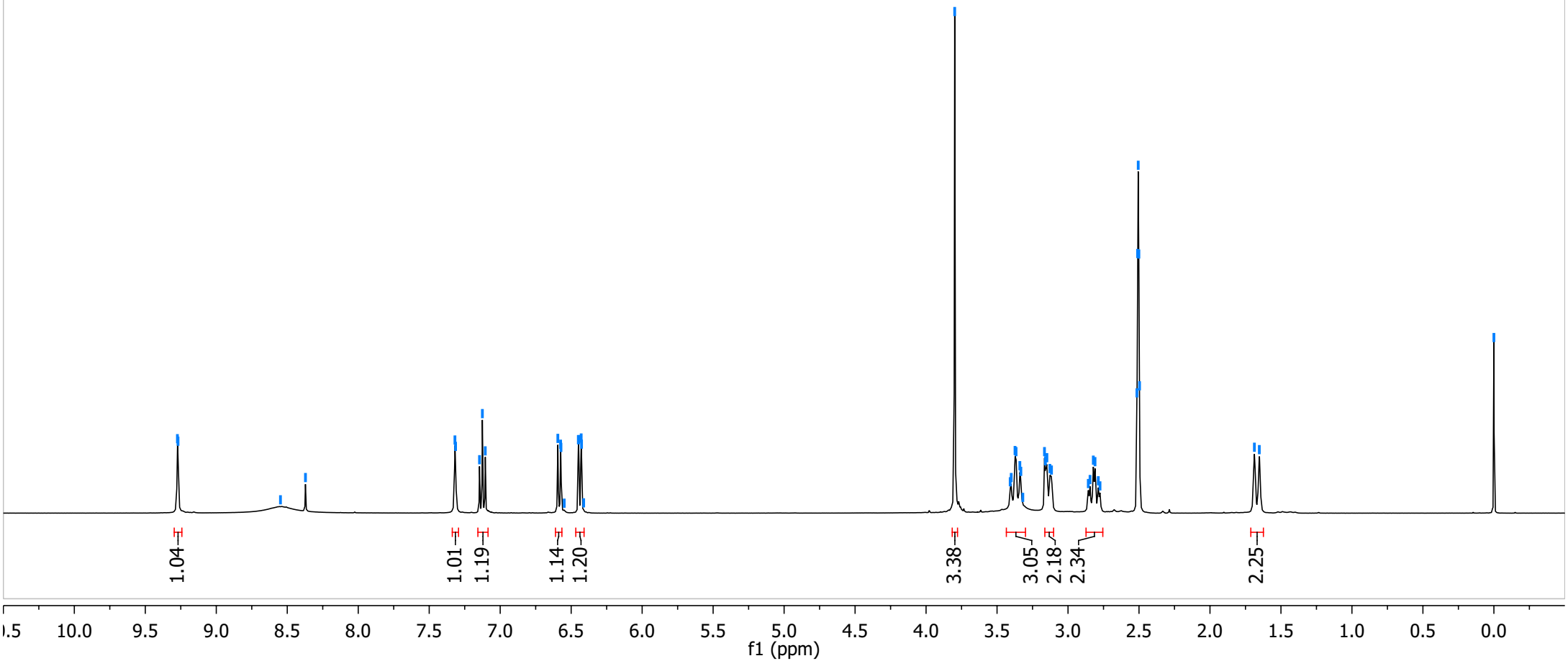
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.60 (d, J = 2.1 Hz, 1H), 7.45 (d, J = 9.0 Hz, 1H), 7.33 (d, J = 5.8 Hz, 4H), 7.25 (pd, J = 5.1, 2.5 Hz, 1H), 7.09 (d, J = 2.2 Hz, 1H), 6.65 (d, J = 9.0 Hz, 1H), 3.82 (s, 3H), 3.17 (d, J = 5.3 Hz, 1H), 2.68 (td, J = 12.6, 5.2 Hz, 2H), 2.60 – 2.55 (m, 3H), 1.53 (d, J = 12.7 Hz, 2H).



Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zg30
4 Experiment	1D
5 Number of Scans	16
6 Relaxation Delay	1.0000
7 Spectrometer Frequency	400.13
8 Nucleus	1H

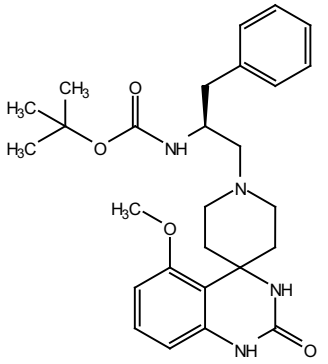
^{1}H NMR (400 MHz, DMSO-d_6) δ 9.27 (d, J = 1.7 Hz, 1H), 7.32 (d, J = 1.8 Hz, 1H), 7.13 (t, J = 8.1 Hz, 1H), 6.61 – 6.57 (m, 1H), 6.44 (dd, J = 8.1, 1.0 Hz, 1H), 3.80 (s, 3H), 3.37 (td, J = 13.5, 2.9 Hz, 3H), 3.14 (dd, J = 12.8, 4.4 Hz, 2H), 2.82 (td, J = 14.1, 4.9 Hz, 2H), 1.67 (d, J = 13.9 Hz, 2H).





Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zg30
4 Experiment	1D
5 Number of Scans	64
6 Relaxation Delay	1.0000
7 Spectrometer Frequency	400.13
8 Nucleus	1H

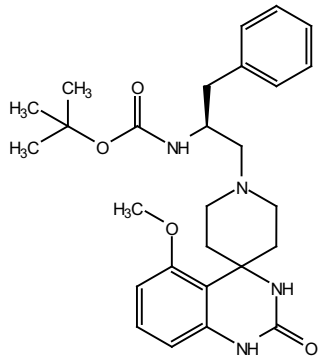
^{1}H NMR (400 MHz, DMSO-d_6) δ 9.09 (s, 1H), 7.27 (t, J = 7.5 Hz, 2H), 7.24 – 7.14 (m, 3H), 7.07 (t, J = 8.1 Hz, 1H), 6.62 (d, J = 8.7 Hz, 1H), 6.59 – 6.50 (m, 2H), 6.42 (d, J = 7.9 Hz, 1H), 3.85 – 3.77 (m, 1H), 3.74 (s, 3H), 2.82 (dd, J = 13.8, 5.0 Hz, 1H), 2.71 – 2.54 (m, 6H), 2.34 (ddd, J = 48.9, 12.3, 7.1 Hz, 3H), 1.46 (t, J = 10.9 Hz, 2H), 1.34 (s, 9H).

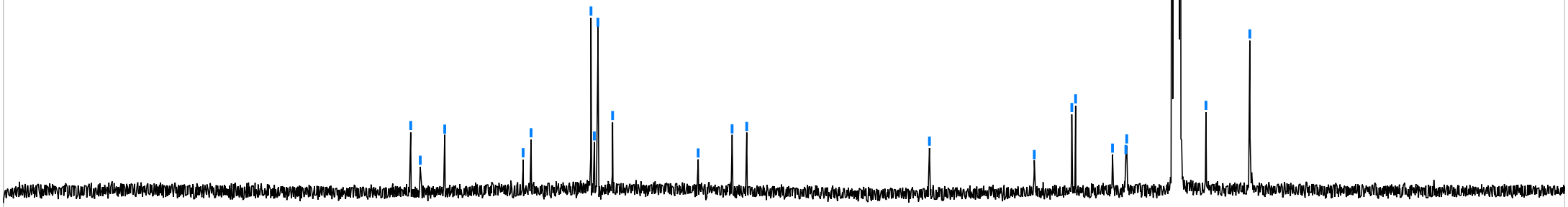


Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zgpg30
4 Experiment	1D
5 Number of Scans	256
6 Relaxation Delay	2.0000
7 Spectrometer Frequency	100.61
8 Nucleus	13C

157.13 155.67 151.93 139.93 138.72 129.55 129.04 128.49 126.24 113.15 107.96 105.72 77.77 61.72 55.98 55.40 49.75 47.71 47.58 35.46 28.75

^{13}C NMR (101 MHz, DMSO-d_6) δ 157.13, 155.67, 151.93, 139.93, 138.72, 129.55, 129.04, 128.49, 126.24, 113.15, 107.96, 105.72, 77.77, 61.72, 55.98, 55.40, 49.75, 47.71, 47.58, 35.46, 28.75.



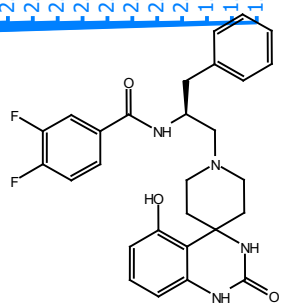


210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10

f1 (ppm)

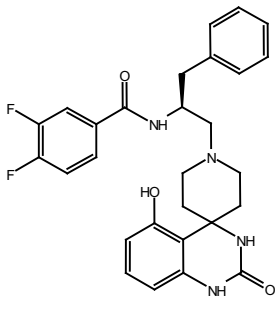
Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zg30
4 Experiment	1D
5 Number of Scans	64
6 Relaxation Delay	1.0000
7 Spectrometer Frequency	400.13
8 Nucleus	1H

^{1}H NMR (400 MHz, DMSO-d_6) δ 9.54 (s, 1H), 8.99 (s, 1H), 8.31 (d, J = 8.4 Hz, 1H), 7.80 (ddd, J = 11.5, 7.8, 2.1 Hz, 1H), 7.67 (dt, J = 10.4, 3.6 Hz, 1H), 7.54 (dt, J = 10.5, 8.3 Hz, 1H), 7.25 (d, J = 6.3 Hz, 4H), 7.16 (td, J = 6.1, 2.7 Hz, 1H), 6.88 (t, J = 7.9 Hz, 1H), 6.49 (s, 1H), 6.33 (d, J = 8.0 Hz, 1H), 6.24 (d, J = 7.9 Hz, 1H), 4.39 – 4.31 (m, 1H), 2.97 (dd, J = 13.7, 4.8 Hz, 1H), 2.78 (dd, J = 13.9, 8.8 Hz, 4H), 2.71 – 2.62 (m, 2H), 2.61 – 2.51 (m, 3H), 2.45 (d, J = 5.3 Hz, 1H), 1.45 (t, J = 12.5 Hz, 2H).



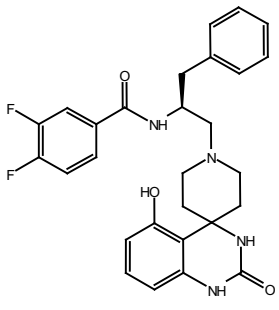
Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zgpg30
4 Experiment	1D
5 Number of Scans	1024
6 Relaxation Delay	2.0000
7 Spectrometer Frequency	100.61
8 Nucleus	13C

^{13}C NMR (101 MHz, DMSO-d_6) δ 164.13, 154.95, 151.98, 148.25, 139.69, 138.79, 132.72, 129.57, 128.58, 126.40, 125.07, 118.03, 117.85, 117.08, 116.90, 111.59, 110.01, 105.92, 61.56, 55.10, 49.35, 47.92, 47.64, 38.78, 35.34.



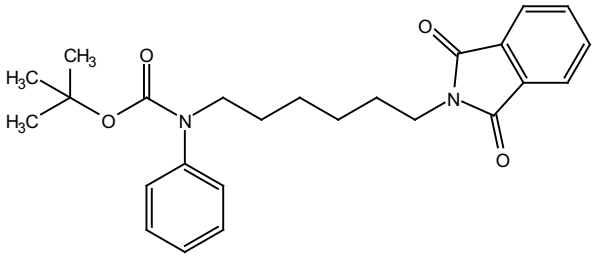
Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zgfhigqn.2
4 Experiment	1D
5 Number of Scans	64
6 Relaxation Delay	1.0000
7 Spectrometer Frequency	376.50
8 Nucleus	19F

^{19}F NMR (376 MHz, DMSO-d_6) δ -135.08 (d, J = 22.0 Hz), -138.11 (d, J = 22.1 Hz).



Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zg30
4 Experiment	1D
5 Number of Scans	16
6 Relaxation Delay	1.0000
7 Spectrometer Frequency	400.13
8 Nucleus	1H

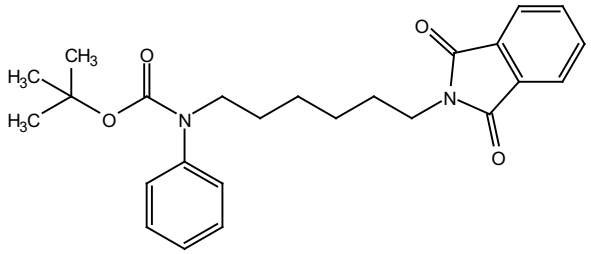
^{1}H NMR (400 MHz, DMSO-d_6) δ 7.90 – 7.79 (m, 4H), 7.37 – 7.29 (m, 2H), 7.23 – 7.15 (m, 3H), 3.55 (q, J = 7.1 Hz, 4H), 1.55 (p, J = 7.0 Hz, 2H), 1.41 (q, J = 7.3 Hz, 2H), 1.35 (s, 9H), 1.25 (dd, J = 7.1, 3.5 Hz, 4H).

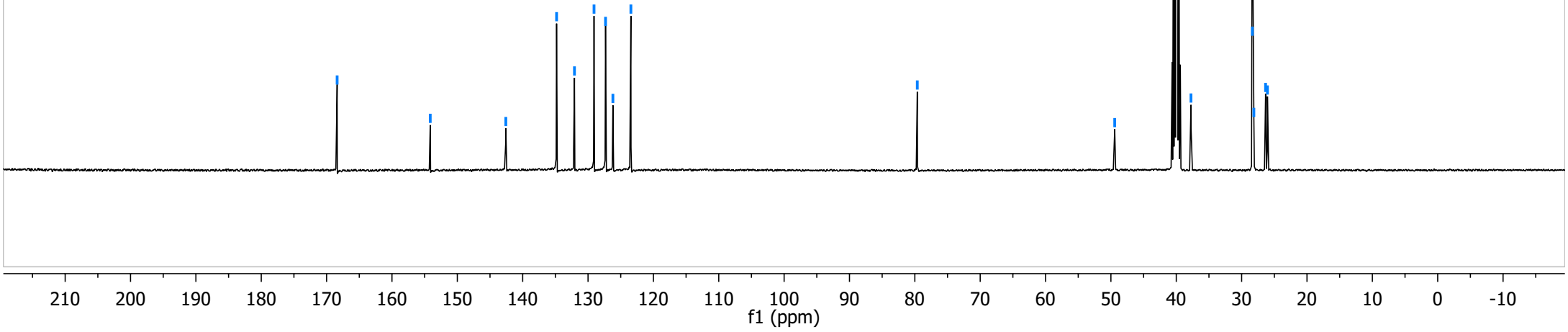


Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zgpg30
4 Experiment	1D
5 Number of Scans	256
6 Relaxation Delay	2.0000
7 Spectrometer Frequency	100.61
8 Nucleus	13C

168.39 154.14 142.58 134.81 132.08 129.08 127.32 126.20 123.45 79.62 49.42 37.75 28.38 28.36 28.13 26.34 26.05

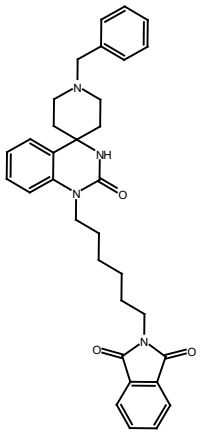
^{13}C NMR (101 MHz, DMSO-d_6) δ 168.39, 154.14, 142.58, 134.81, 132.08, 129.08, 127.32, 126.20, 123.45, 79.62, 49.42, 37.75, 28.38, 28.36, 28.13, 26.34, 26.05.





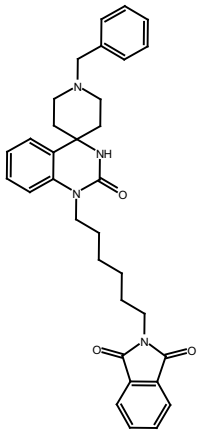
Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zg30
4 Experiment	1D
5 Number of Scans	128
6 Relaxation Delay	1.0000
7 Spectrometer Frequency	400.14
8 Nucleus	1H

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.87 – 7.80 (m, 4H), 7.34 (s, 1H), 7.31 (d, J = 4.5 Hz, 4H), 7.23 (ddd, J = 7.9, 5.2, 3.0 Hz, 2H), 6.98 (ddd, J = 9.8, 7.9, 1.6 Hz, 2H), 6.94 (s, 1H), 3.79 (t, J = 7.5 Hz, 2H), 3.55 (d, J = 7.1 Hz, 4H), 2.64 – 2.51 (m, 4H), 1.92 (td, J = 12.7, 4.6 Hz, 2H), 1.66 (d, J = 12.9 Hz, 2H), 1.54 (dt, J = 21.7, 7.2 Hz, 4H), 1.37 – 1.26 (m, 4H).



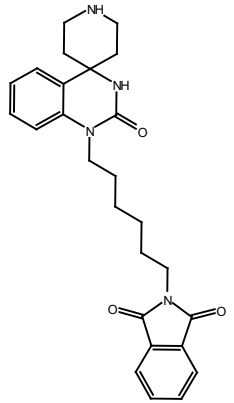
Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zgpg30
4 Experiment	1D
5 Number of Scans	2056
6 Relaxation Delay	2.0000
7 Spectrometer Frequency	100.62
8 Nucleus	13C

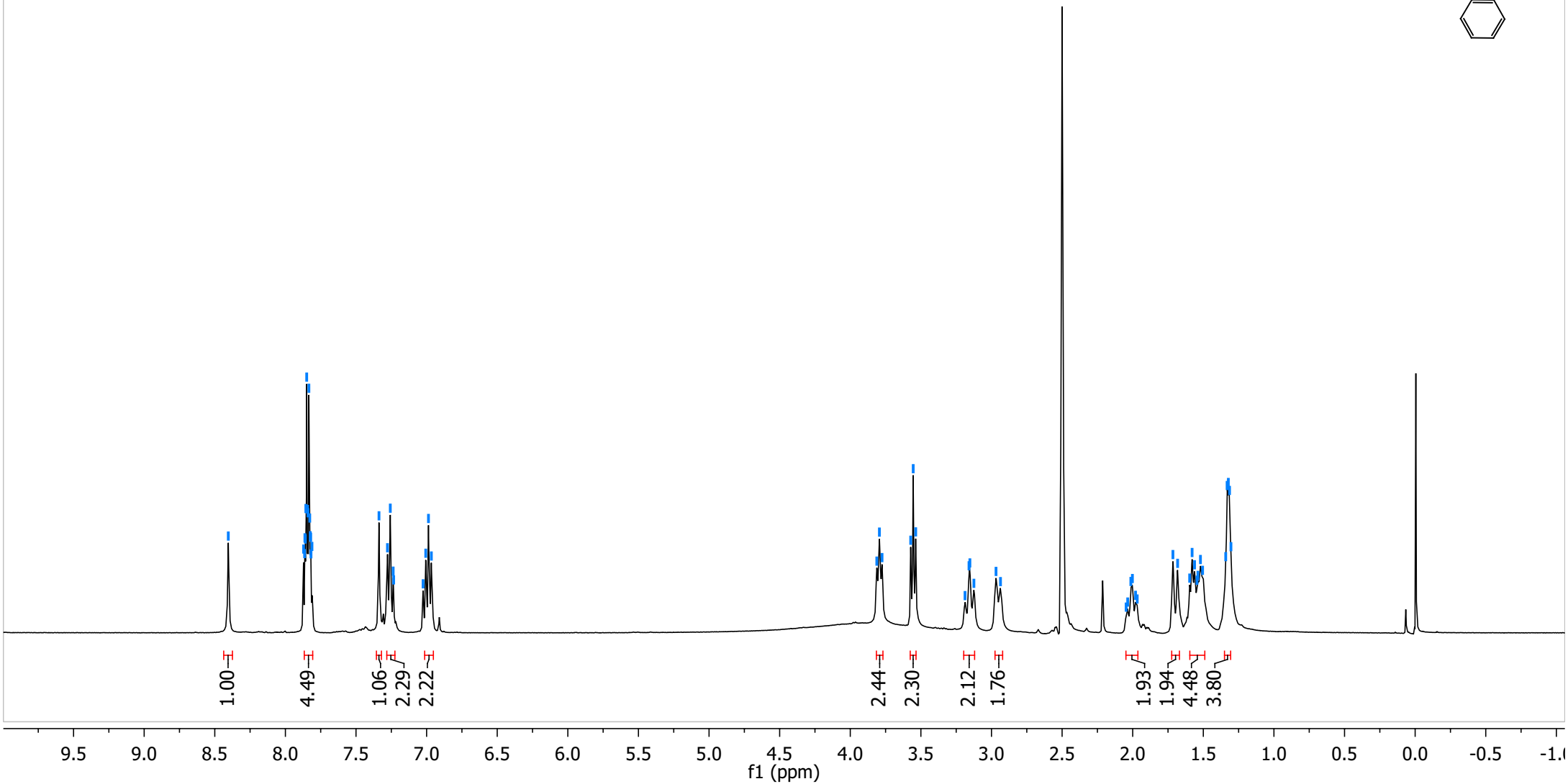
^{13}C NMR (101 MHz, DMSO-d_6)
δ 167.93, 153.19, 138.67, 137.23, 134.35, 131.61, 129.33, 128.79, 128.15, 127.92, 126.82, 123.42, 122.98, 121.65, 113.18, 62.01, 52.32, 47.38, 40.69, 37.32, 36.16, 27.92, 26.55, 25.98, 25.88.



Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zg30
4 Experiment	1D
5 Number of Scans	128
6 Relaxation Delay	1.0000
7 Spectrometer Frequency	400.14
8 Nucleus	1H

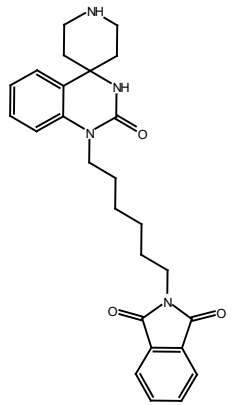
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.40 (s, 1H), 7.87 – 7.81 (m, 4H), 7.34 (s, 1H), 7.26 (t, J = 8.1 Hz, 2H), 6.99 (t, J = 7.9 Hz, 2H), 3.79 (t, J = 7.4 Hz, 2H), 3.55 (t, J = 7.1 Hz, 2H), 3.20 – 3.12 (m, 2H), 2.95 (d, J = 12.7 Hz, 2H), 2.01 (td, J = 13.5, 4.6 Hz, 2H), 1.70 (d, J = 13.3 Hz, 2H), 1.60 – 1.49 (m, 4H), 1.35 – 1.31 (m, 4H).





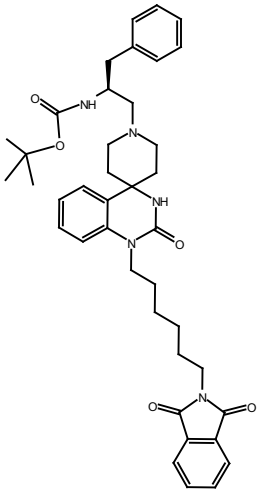
Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zgpg30
4 Experiment	1D
5 Number of Scans	2056
6 Relaxation Delay	2.0000
7 Spectrometer Frequency	100.62
8 Nucleus	13C

^{13}C NMR (101 MHz, DMSO-d_6) δ 167.96, 152.97, 136.96, 134.36, 131.62, 128.61, 128.20, 123.56, 122.99, 121.71, 113.30, 52.29, 40.75, 37.33, 35.27, 27.93, 26.55, 26.01, 25.87.



Parameter	Value
1 Solvent	CDCl3
2 Temperature	298.0
3 Pulse Sequence	zg30
4 Experiment	1D
5 Number of Scans	128
6 Relaxation Delay	1.0000
7 Spectrometer Frequency	400.14
8 Nucleus	1H

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.80 (dt, *J* = 5.3, 2.6 Hz, 2H), 7.71 – 7.62 (m, 2H), 7.29 – 7.16 (m, 8H), 7.04 – 6.95 (m, 1H), 6.86 (d, *J* = 8.1 Hz, 1H), 6.01 (d, *J* = 11.2 Hz, 1H), 4.74 (d, *J* = 37.7 Hz, 1H), 4.42 – 4.32 (m, 0H), 4.15 – 4.05 (m, 1H), 4.01 – 3.90 (m, 1H), 3.84 (t, *J* = 7.7 Hz, 2H), 3.65 (t, *J* = 7.3 Hz, 2H), 2.93 – 2.72 (m, 5H), 2.38 (ddt, *J* = 22.9, 16.3, 12.2 Hz, 4H), 2.03 (d, *J* = 7.1 Hz, 2H), 1.84 – 1.76 (m, 2H), 1.66 (q, *J* = 7.0 Hz, 4H), 1.46 – 1.34 (m, 13H).

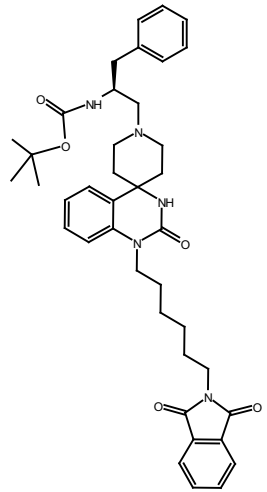


Parameter	Value
1 Solvent	CDCl3
2 Temperature	298.0
3 Pulse Sequence	zgpg30
4 Experiment	1D
5 Number of Scans	2056
6 Relaxation Delay	2.0000
7 Spectrometer Frequency	100.62
8 Nucleus	13C

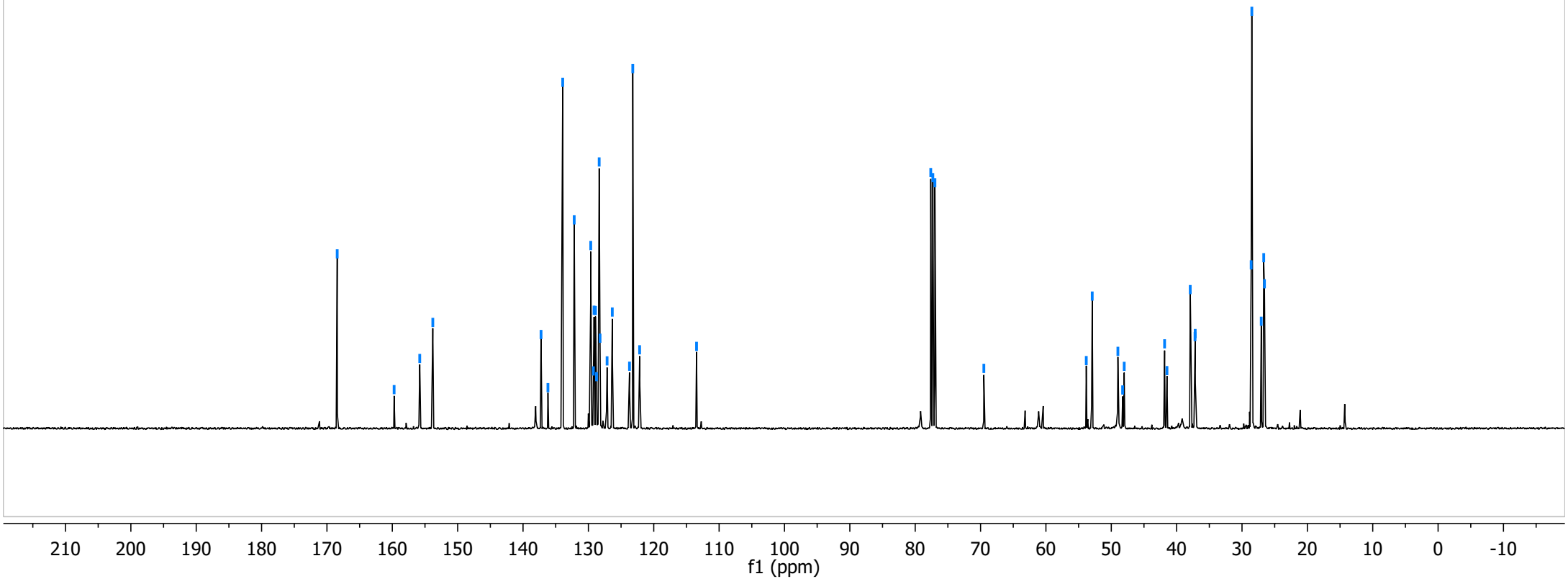
168.43 159.72 155.80 153.80 137.24 136.19 133.93 132.17 129.64 129.24 129.14 128.92 128.76 128.35 128.22 127.14 126.34 123.71 123.21 122.16 113.45

77.62 77.30 76.98 69.50

53.83 52.92 48.99 48.26 48.02 41.84 41.48 37.92 37.19 37.16 28.60 28.50 27.06 26.68 26.57

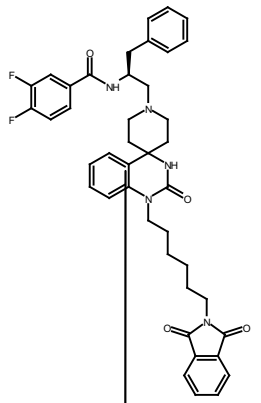


^{13}C NMR (101 MHz, Chloroform-*d*) δ 168.43, 159.72, 155.80, 153.80, 137.24, 136.19, 133.93, 132.17, 129.64, 129.24, 129.14, 128.92, 128.76, 128.35, 128.22, 127.14, 126.34, 123.71, 123.21, 122.16, 113.45, 77.62, 77.30, 76.98, 69.50, 53.83, 52.92, 48.99, 48.26, 48.02, 41.84, 41.48, 37.92, 37.19, 37.16, 28.60, 28.50, 27.06, 26.68, 26.57.



Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zg30
4 Experiment	1D
5 Number of Scans	16
6 Relaxation Delay	1.0000
7 Spectrometer Frequency	400.13
8 Nucleus	1H

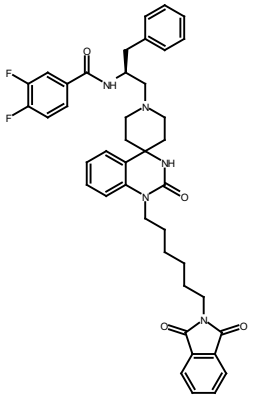
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.32 (d, J = 8.4 Hz, 1H), 7.87 – 7.84 (m, 2H), 7.84 – 7.80 (m, 3H), 7.69 – 7.64 (m, 1H), 7.54 (dt, J = 10.5, 8.3 Hz, 1H), 7.27 – 7.21 (m, 6H), 7.15 (td, J = 5.9, 2.6 Hz, 1H), 6.99 – 6.94 (m, 3H), 4.34 (q, J = 7.3 Hz, 1H), 3.79 (t, J = 7.5 Hz, 2H), 3.57 – 3.52 (m, 2H), 2.97 (dd, J = 13.7, 4.9 Hz, 1H), 2.78 (dd, J = 13.7, 8.6 Hz, 1H), 2.73 – 2.64 (m, 2H), 2.61 – 2.53 (m, 2H), 1.87 (p, J = 11.7, 9.4 Hz, 2H), 1.69 – 1.62 (m, 2H), 1.57 (t, J = 6.9 Hz, 2H), 1.54 – 1.47 (m, 2H), 1.35 – 1.28 (m, 4H).



f1 (ppm)

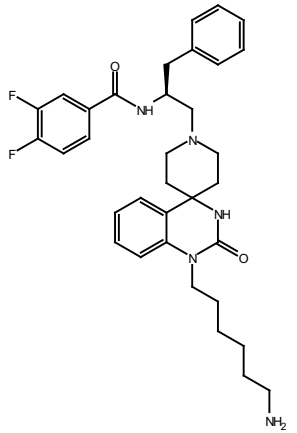
Parameter	Value
1 Solvent	CDCl3
2 Temperature	298.0
3 Pulse Sequence	zgfhigqn
4 Experiment	1D
5 Number of Scans	32
6 Relaxation Delay	1.0000
7 Spectrometer Frequency	376.50
8 Nucleus	19F

^{19}F NMR (376 MHz, Chloroform-*d*) δ -69.95 (d, *J* = 8.4 Hz), -71.84 (d, *J* = 7.8 Hz).



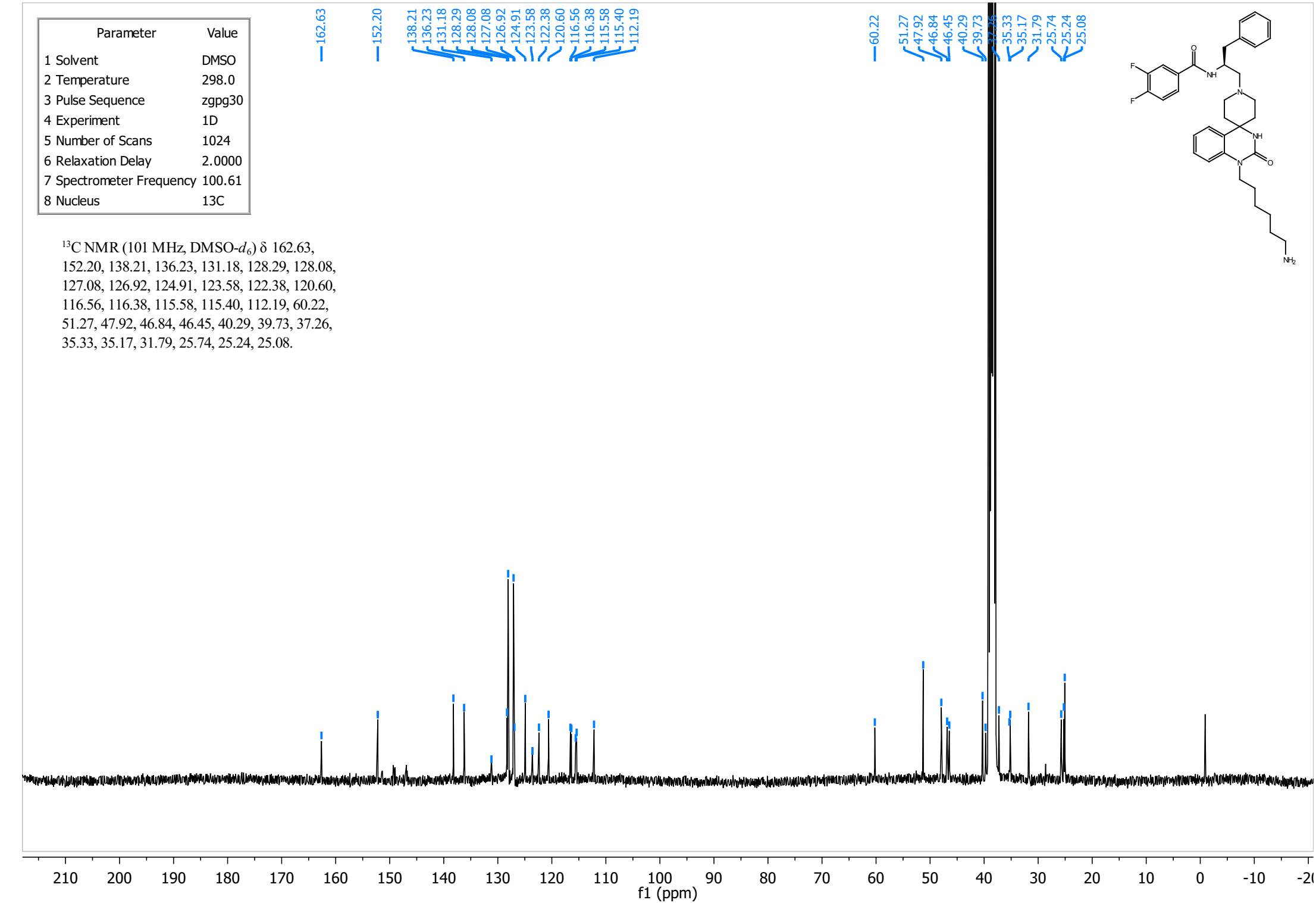
Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zg30
4 Experiment	1D
5 Number of Scans	64
6 Relaxation Delay	1.0000
7 Spectrometer Frequency	400.13
8 Nucleus	1H

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.31 (d, J = 8.4 Hz, 1H), 7.81 (ddd, J = 11.7, 7.8, 2.2 Hz, 1H), 7.68 (ddd, J = 9.4, 4.4, 1.9 Hz, 1H), 7.54 (dt, J = 10.6, 8.4 Hz, 1H), 7.29 – 7.26 (m, 1H), 7.24 (d, J = 2.9 Hz, 5H), 7.16 (dq, J = 6.1, 3.9, 3.2 Hz, 1H), 6.97 (dt, J = 7.3, 3.3 Hz, 2H), 6.93 (s, 1H), 4.34 (td, J = 8.0, 5.2 Hz, 1H), 3.83 – 3.77 (m, 2H), 3.40 – 3.32 (m, 2H), 2.97 (dd, J = 13.8, 4.9 Hz, 1H), 2.79 (dd, J = 13.7, 8.6 Hz, 1H), 2.74 – 2.65 (m, 2H), 2.62 – 2.52 (m, 4H), 1.88 (qd, J = 14.7, 14.1, 4.3 Hz, 3H), 1.65 (ddd, J = 13.9, 6.1, 2.9 Hz, 2H), 1.53 (t, J = 7.3 Hz, 2H), 1.31 (q, J = 7.5, 5.1 Hz, 8H).



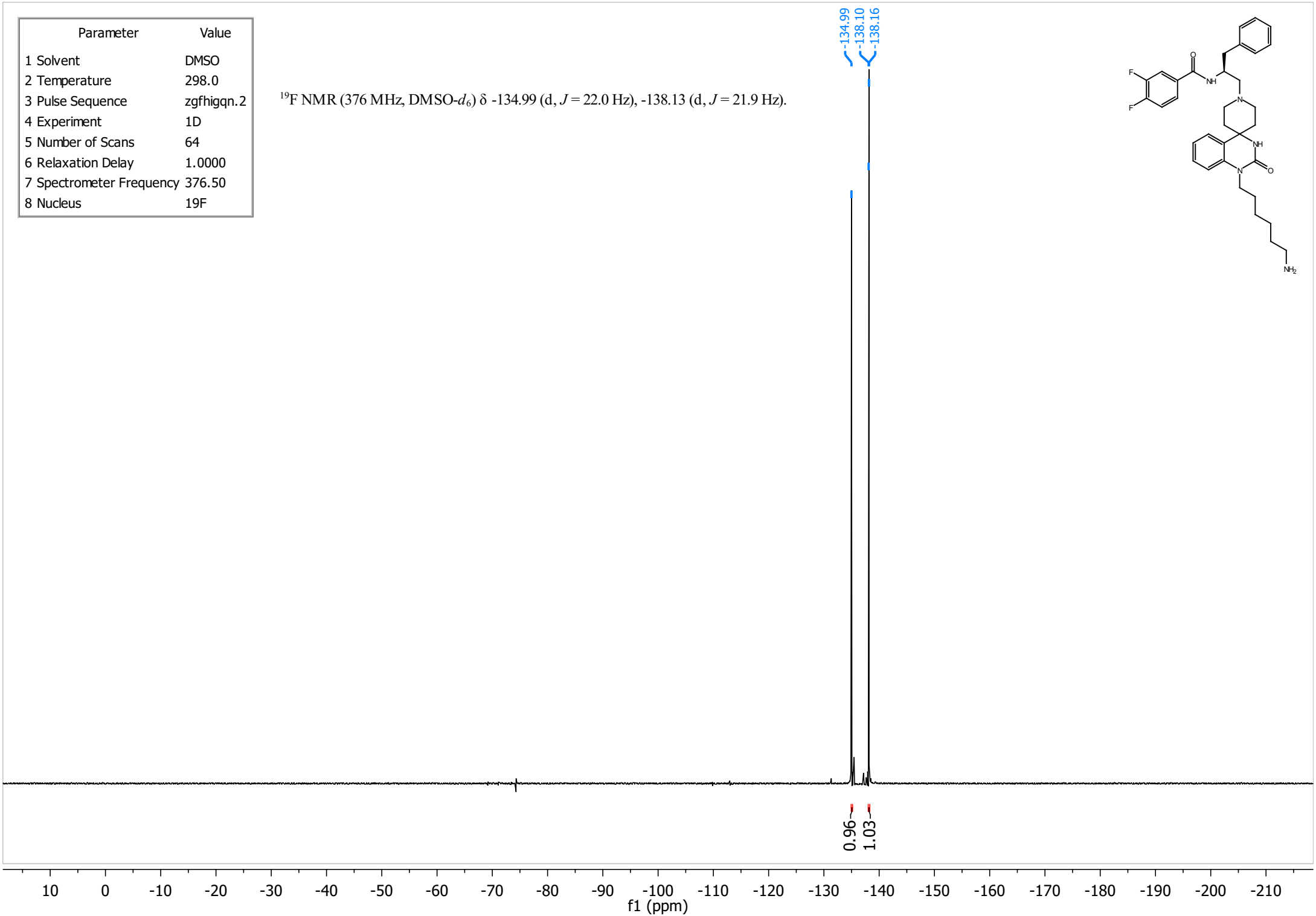
Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zgpg30
4 Experiment	1D
5 Number of Scans	1024
6 Relaxation Delay	2.0000
7 Spectrometer Frequency	100.61
8 Nucleus	13C

^{13}C NMR (101 MHz, DMSO-d_6) δ 162.63, 152.20, 138.21, 136.23, 131.18, 128.29, 128.08, 127.08, 126.92, 124.91, 123.58, 122.38, 120.60, 116.56, 116.38, 115.58, 115.40, 112.19, 60.22, 51.27, 47.92, 46.84, 46.45, 40.29, 39.73, 37.26, 35.33, 35.17, 31.79, 25.74, 25.24, 25.08.



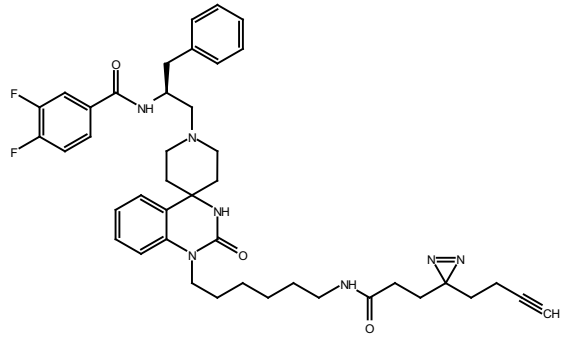
Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zgfhigqn.2
4 Experiment	1D
5 Number of Scans	64
6 Relaxation Delay	1.0000
7 Spectrometer Frequency	376.50
8 Nucleus	19F

^{19}F NMR (376 MHz, DMSO-d_6) δ -134.99 (d, J = 22.0 Hz), -138.13 (d, J = 21.9 Hz).



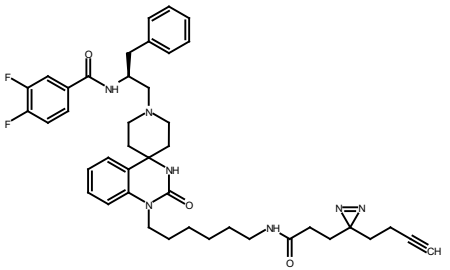
Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zg30
4 Experiment	1D
5 Number of Scans	256
6 Relaxation Delay	1.0000
7 Spectrometer Frequency	400.14
8 Nucleus	1H

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.31 (d, J = 8.4 Hz, 1H), 7.85 – 7.77 (m, 2H), 7.68 (ddt, J = 8.0, 4.6, 1.5 Hz, 1H), 7.54 (dt, J = 10.5, 8.3 Hz, 1H), 7.29 – 7.22 (m, 6H), 7.15 (ddd, J = 6.6, 5.7, 2.8 Hz, 1H), 6.97 (dd, J = 14.8, 7.1 Hz, 3H), 4.35 (td, J = 8.0, 5.2 Hz, 1H), 3.80 (t, J = 7.5 Hz, 2H), 2.99 (dq, J = 10.4, 5.6, 4.9 Hz, 3H), 2.83 – 2.75 (m, 2H), 2.69 (dq, J = 11.6, 5.9, 3.2 Hz, 2H), 2.58 – 2.53 (m, 2H), 1.97 (td, J = 7.4, 2.7 Hz, 2H), 1.87 (dd, J = 8.6, 6.8 Hz, 4H), 1.68 – 1.66 (m, 1H), 1.63 (dd, J = 8.6, 6.7 Hz, 3H), 1.55 (t, J = 7.4 Hz, 5H), 1.38 (p, J = 6.8 Hz, 2H), 1.30 (dd, J = 6.8, 3.5 Hz, 5H).



Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zgpg30
4 Experiment	1D
5 Number of Scans	2056
6 Relaxation Delay	2.0000
7 Spectrometer Frequency	100.62
8 Nucleus	13C

^{13}C NMR (101 MHz, DMSO-d_6) δ 170.36, 163.64, 153.20, 149.87, 147.90, 147.78, 139.22, 137.23, 132.15, 129.29, 129.08, 128.08, 127.92, 125.91, 124.58, 123.39, 121.61, 117.56, 117.38, 116.59, 116.41, 113.17, 83.14, 71.71, 61.23, 52.29, 48.92, 47.85, 47.46, 40.77, 38.40, 38.26, 36.34, 36.18, 31.46, 29.49, 29.02, 28.25, 28.14, 26.68, 26.11, 26.06, 12.65.



Parameter	Value
1 Solvent	DMSO
2 Temperature	298.0
3 Pulse Sequence	zgfhigqn.2
4 Experiment	1D
5 Number of Scans	64
6 Relaxation Delay	1.0000
7 Spectrometer Frequency	376.51
8 Nucleus	19F

^{19}F NMR (377 MHz, DMSO-d_6) δ -135.01 (d, J = 21.9 Hz), -138.12 (d, J = 22.6 Hz).