

Supplementary Materials

Pyrazolo[4,3-*e*]tetrazolo[1,5-*b*][1,2,4]triazine Sulfonamides as Novel Potential Anticancer Agents: Cytotoxic and Genotoxic Activities In Vitro

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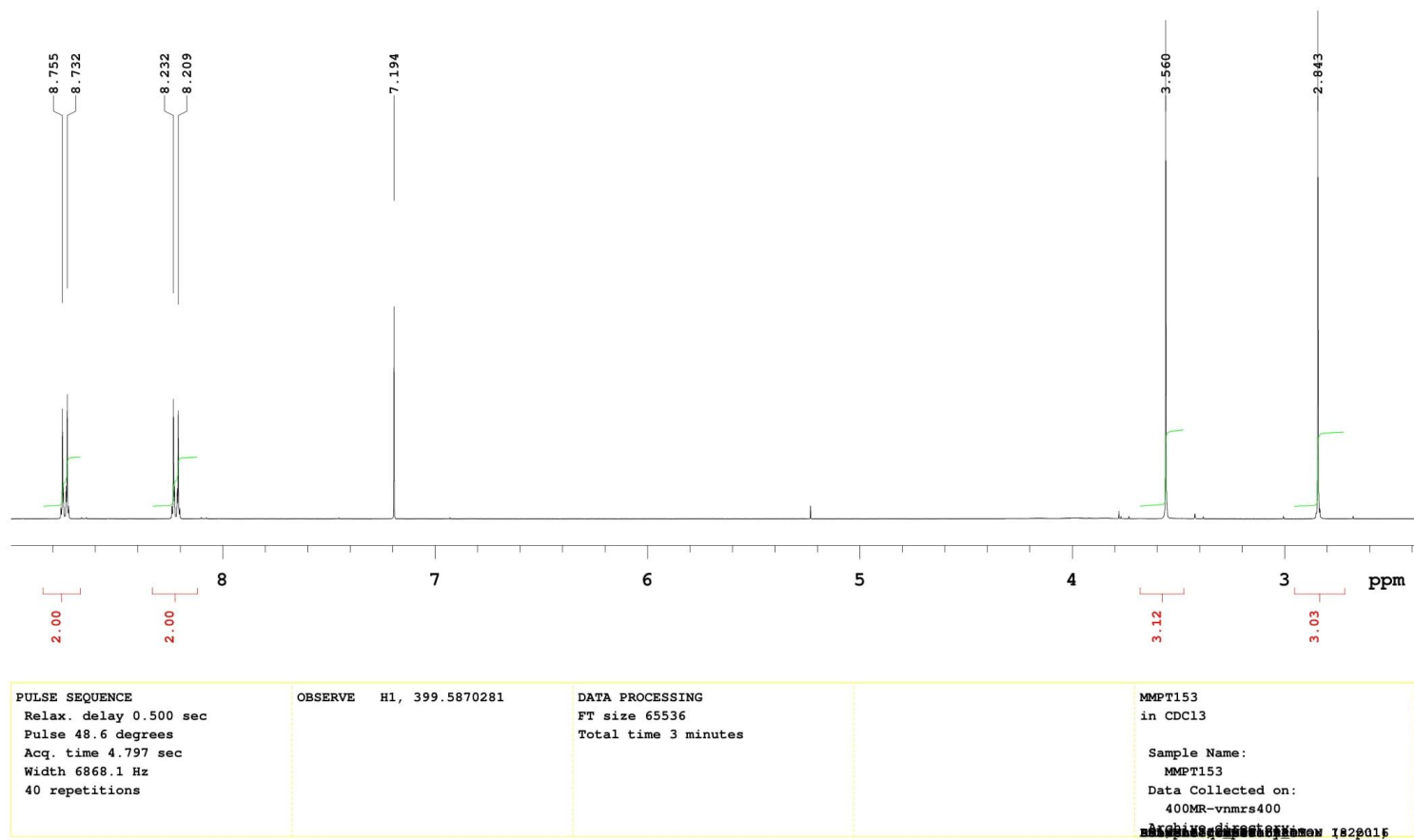
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Figure S1: ^1H -NMR in CDCl_3 for derivative 1



Chemical Shift (ppm)	Integration
8.135 - 8.672	1.96
8.140 - 8.157	1.99
7.260	1.94
5.300	2.92
3.154 - 4.529	1.20, 5.38, 0.72, 3.17, 0.99
2.278	1.20

PULSE SEQUENCE
 Relax. delay 0.500 sec
 Pulse 48.6 degrees
 Acq. time 4.797 sec
 Width 6793.5 Hz
 40 repetitions

OBSERVE H1, 399.5428928

DATA PROCESSING
 FT size 65536
 Total time 3 minutes

MMPT223
 in CDC13

Sample Name:
 MMPT223
 Data Collected on:
 400MR-vnmrs400

Figure S3: ^1H -NMR in acetone for derivative 2a

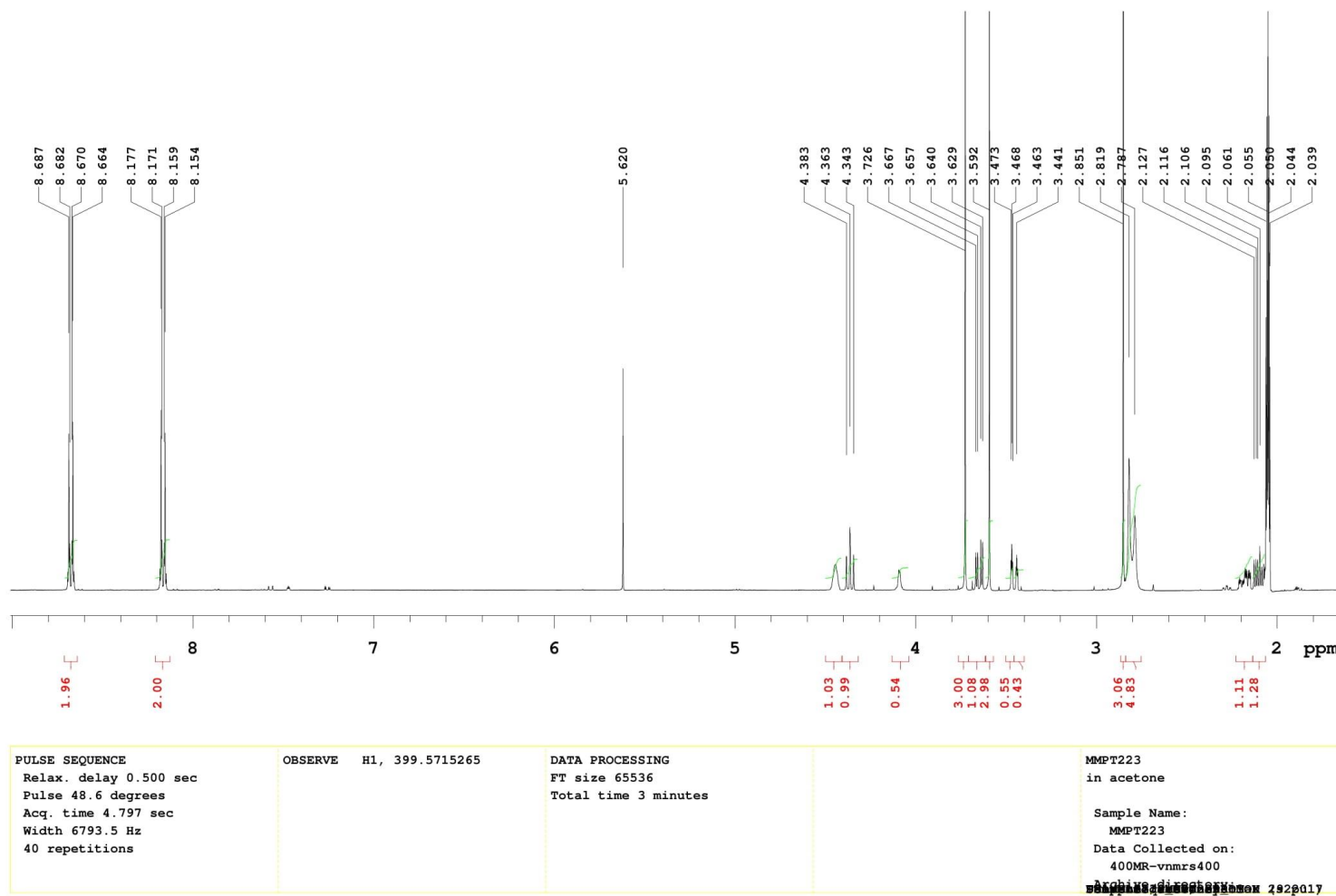


Figure S4: ^{13}C -NMR in acetone for derivative 2a

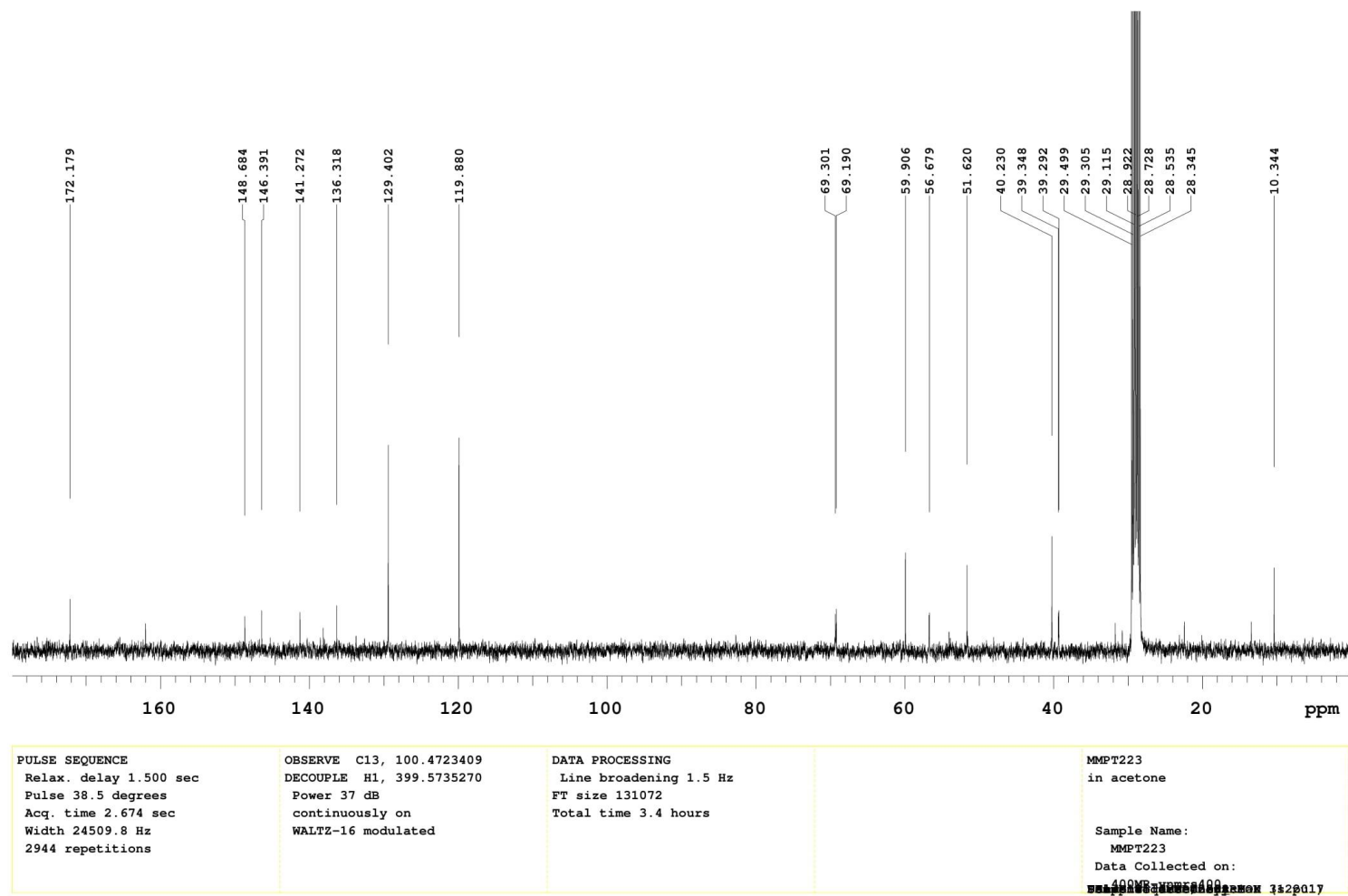


Figure S5: HRMS for derivative 2a

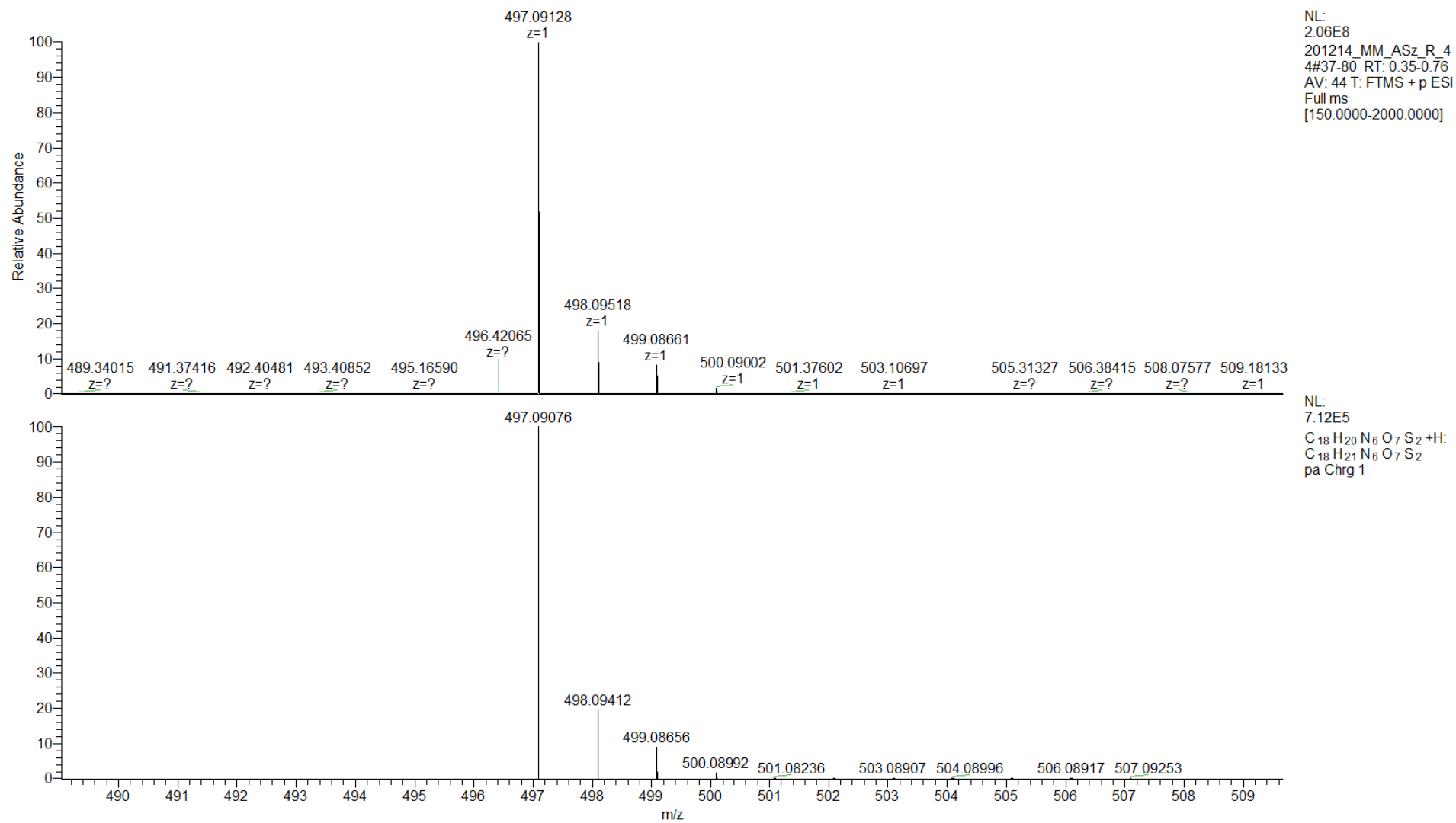


Figure S6: ^1H -NMR in DMSO for derivative **2b**

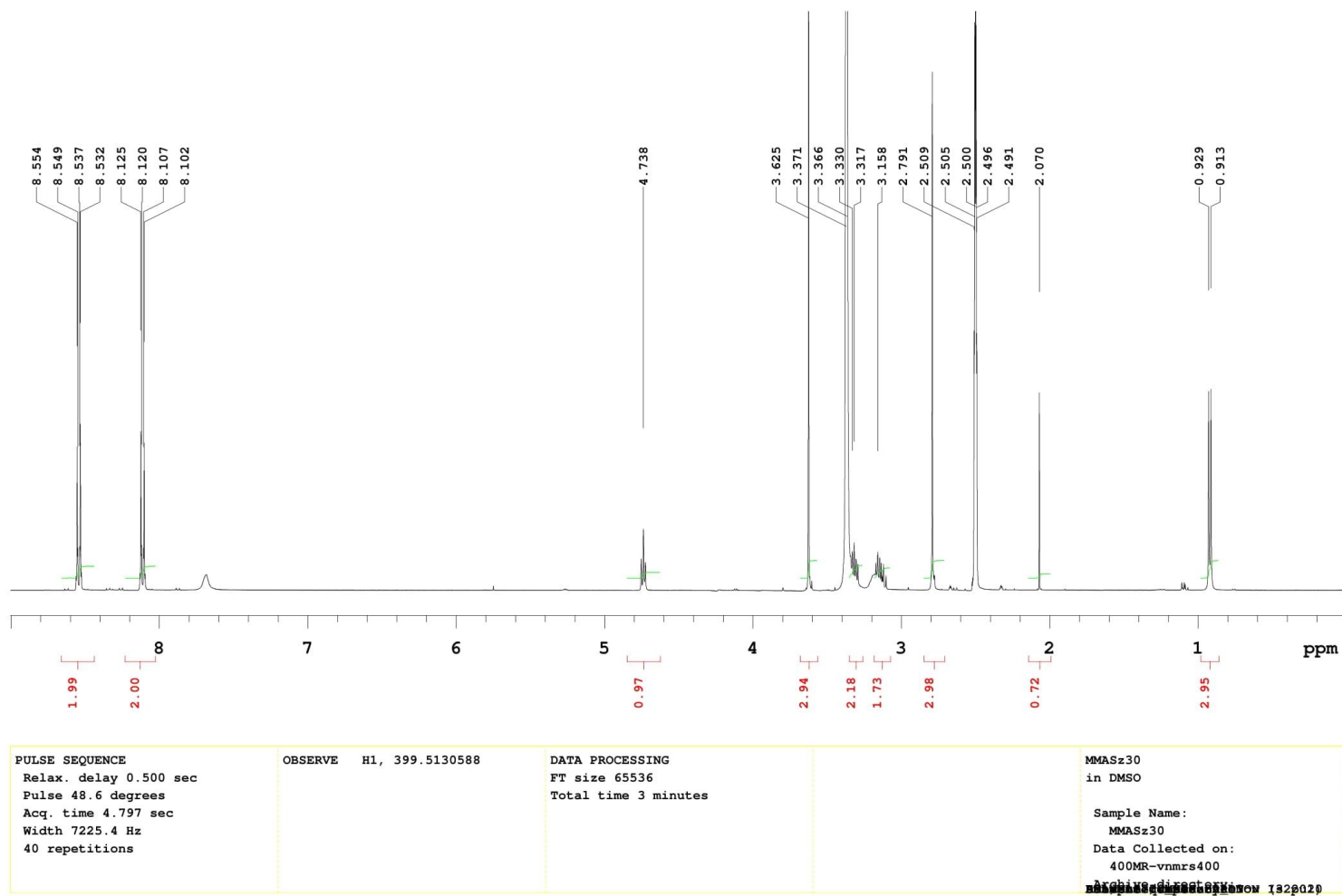


Figure S7: ^1H -NMR for derivative **2b** in DMSO with one drop of D_2O

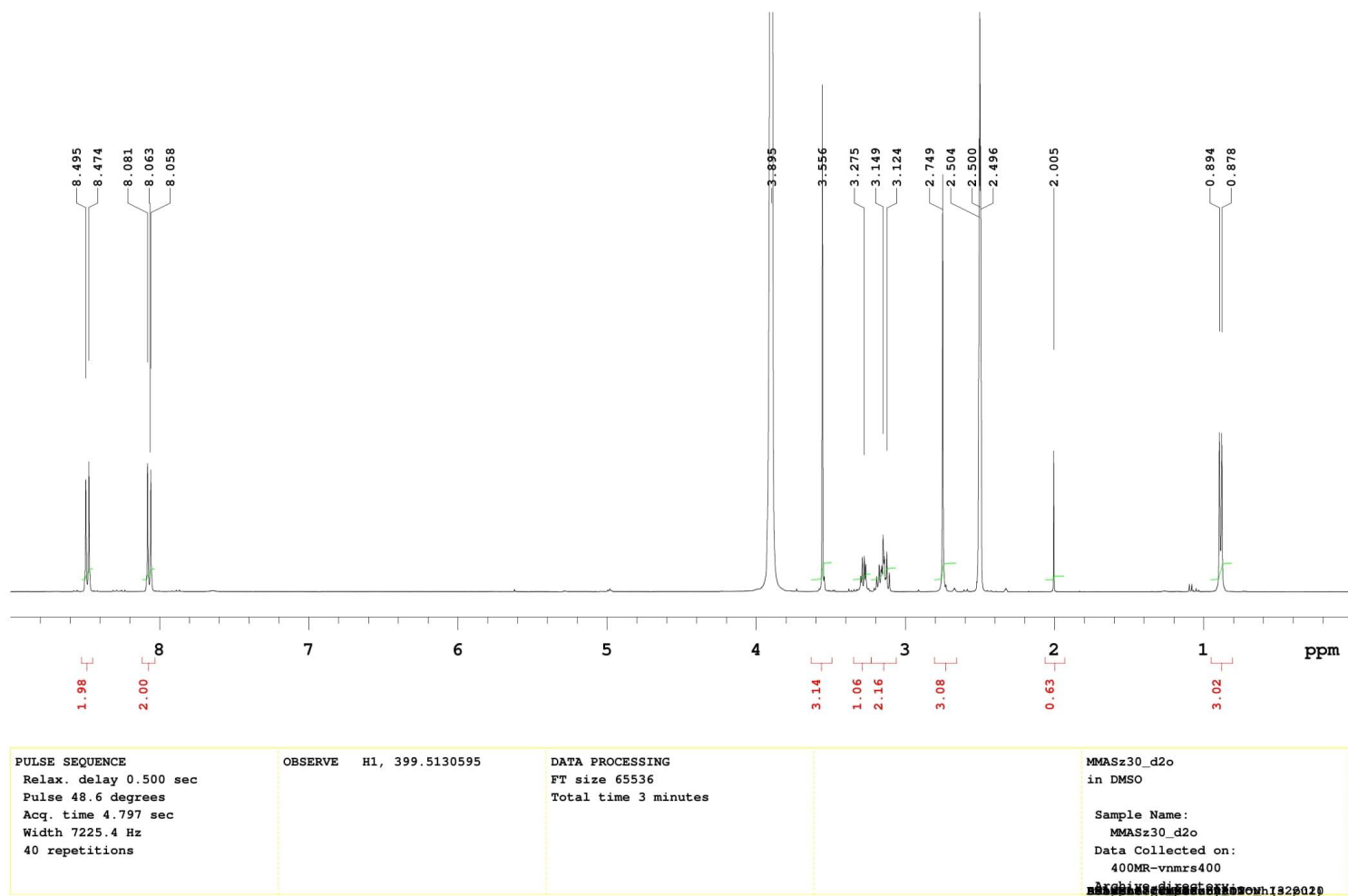


Figure S8: ^{13}C -NMR for derivative **2b**

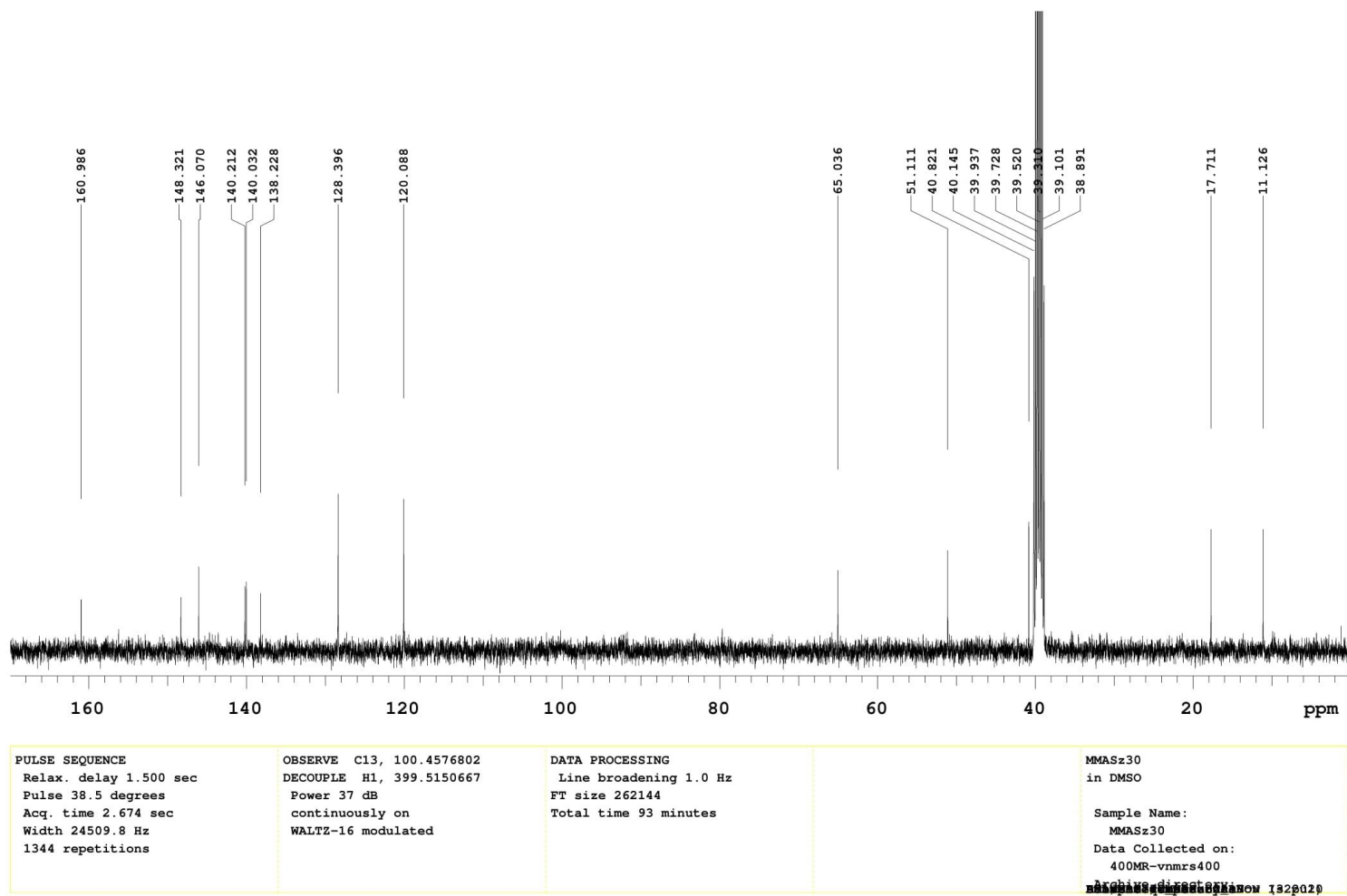


Figure S9: HRMS for 2b

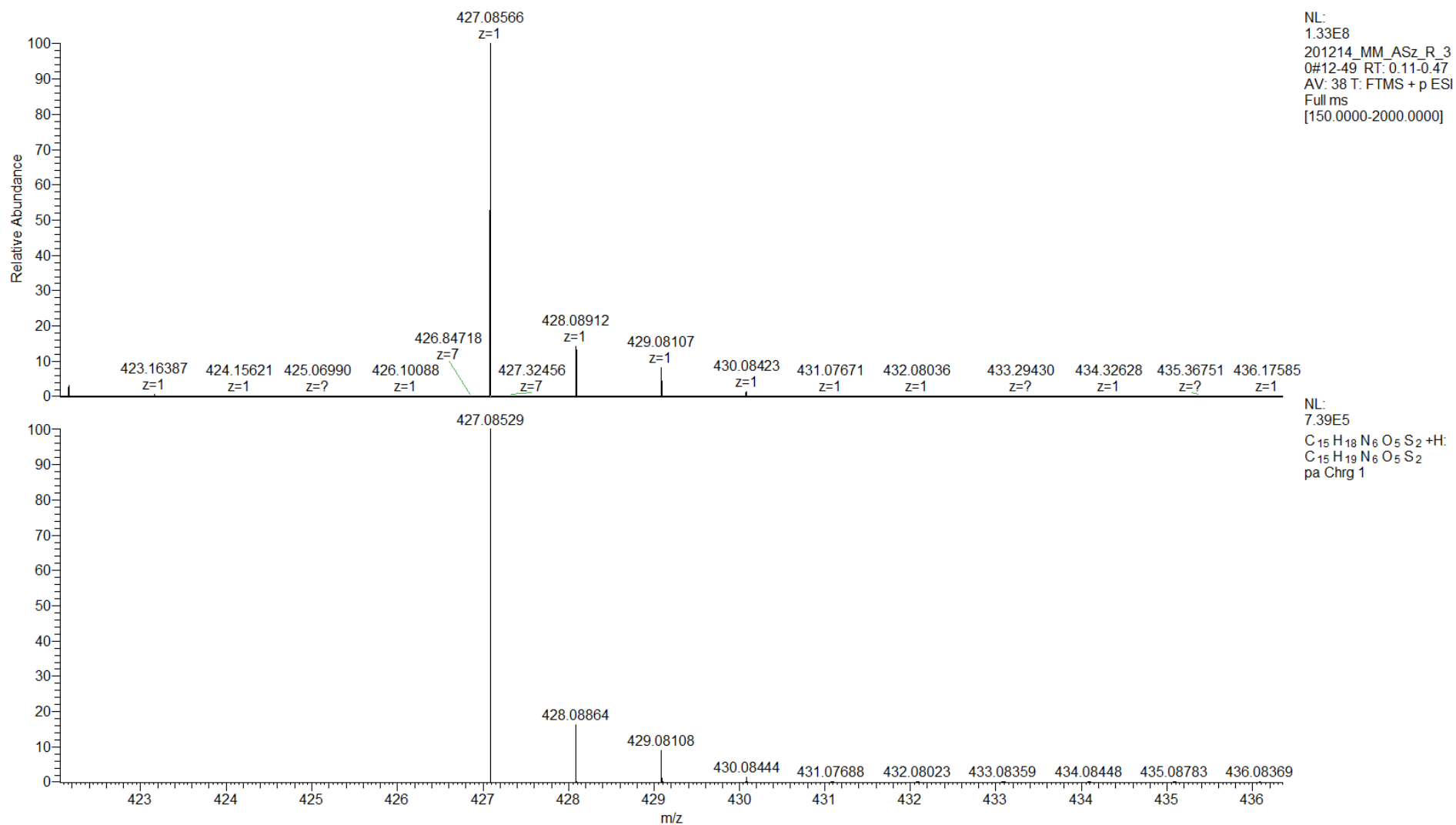


Figure S10: ^1H -NMR for derivative 2c

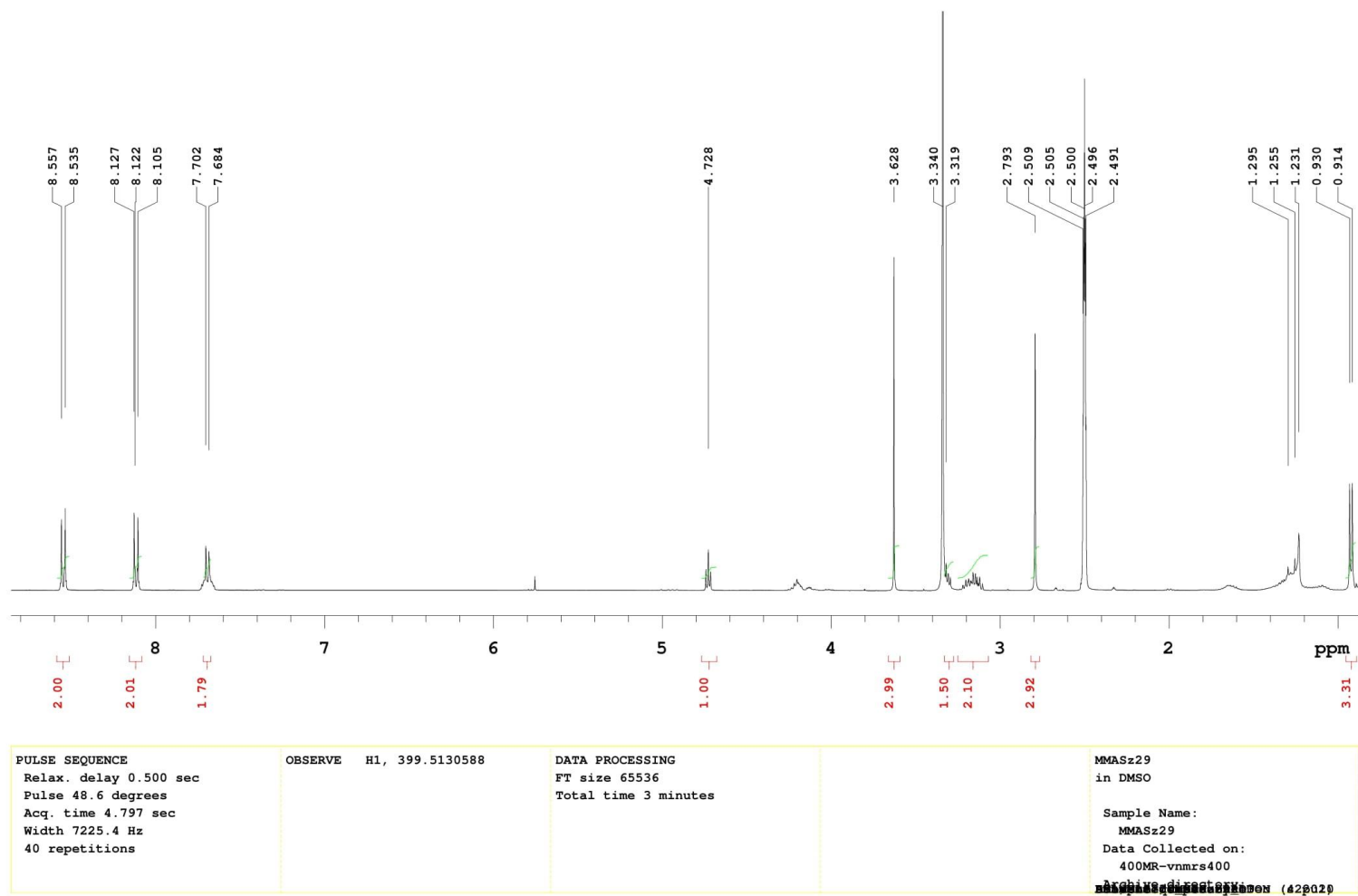
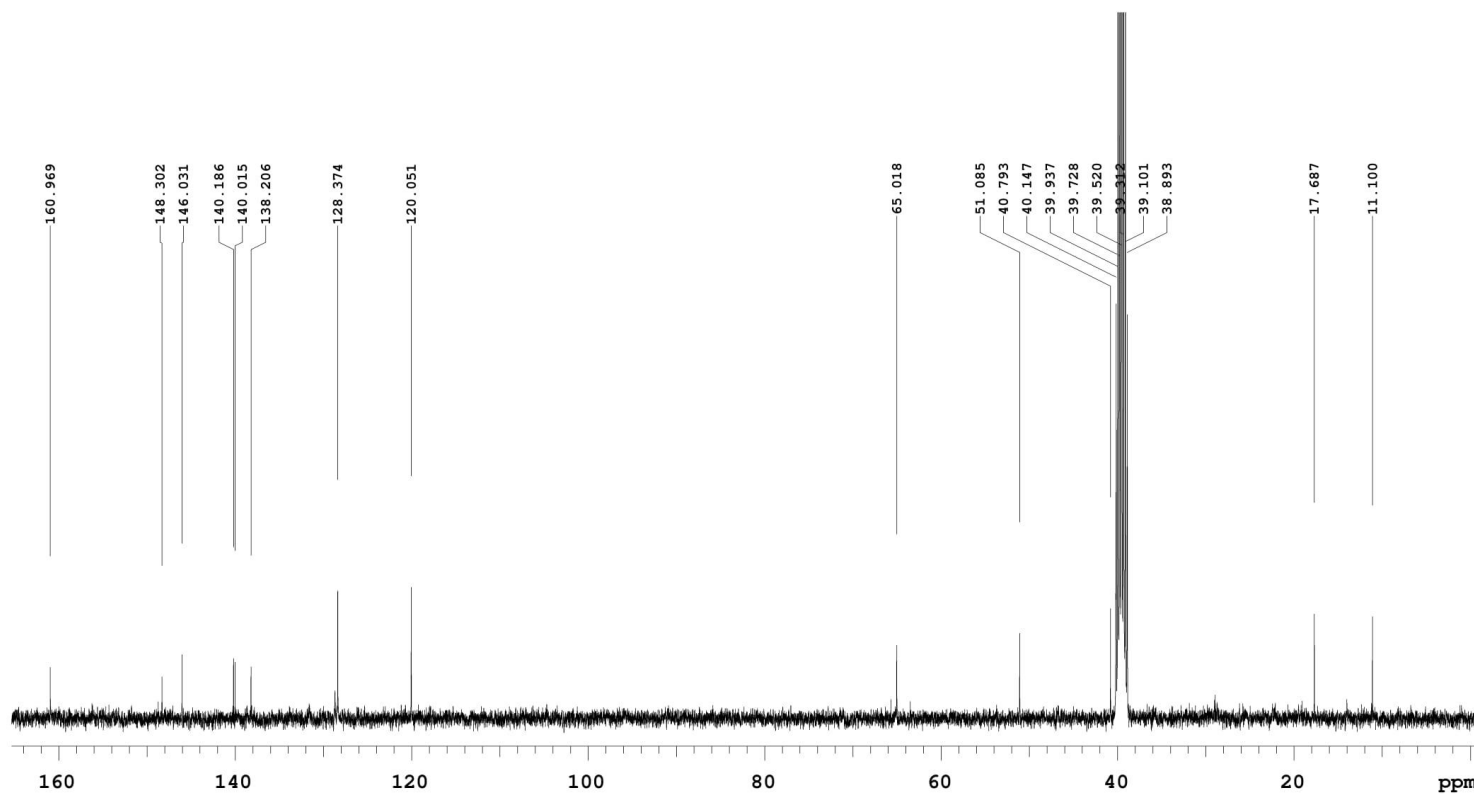


Figure S11: ^{13}C -NMR for derivative 2c



PULSE SEQUENCE
Relax. delay 1.500 sec
Pulse 38.5 degrees
Acq. time 2.674 sec
Width 24509.8 Hz
2416 repetitions

OBSERVE C13, 100.4576830
DECOUPLE H1, 399.5150667
Power 37 dB
continuously on
WALTZ-16 modulated

DATA PROCESSING
Line broadening 1.0 Hz
FT size 262144
Total time 2.8 hours

MMASz29
in DMSO

Sample Name:
MMASz29
Data Collected on:
400MR-vnmrs400

DATE: 2018-04-20 10:00:00 (428020)

Figure S12: HRMS for 2c

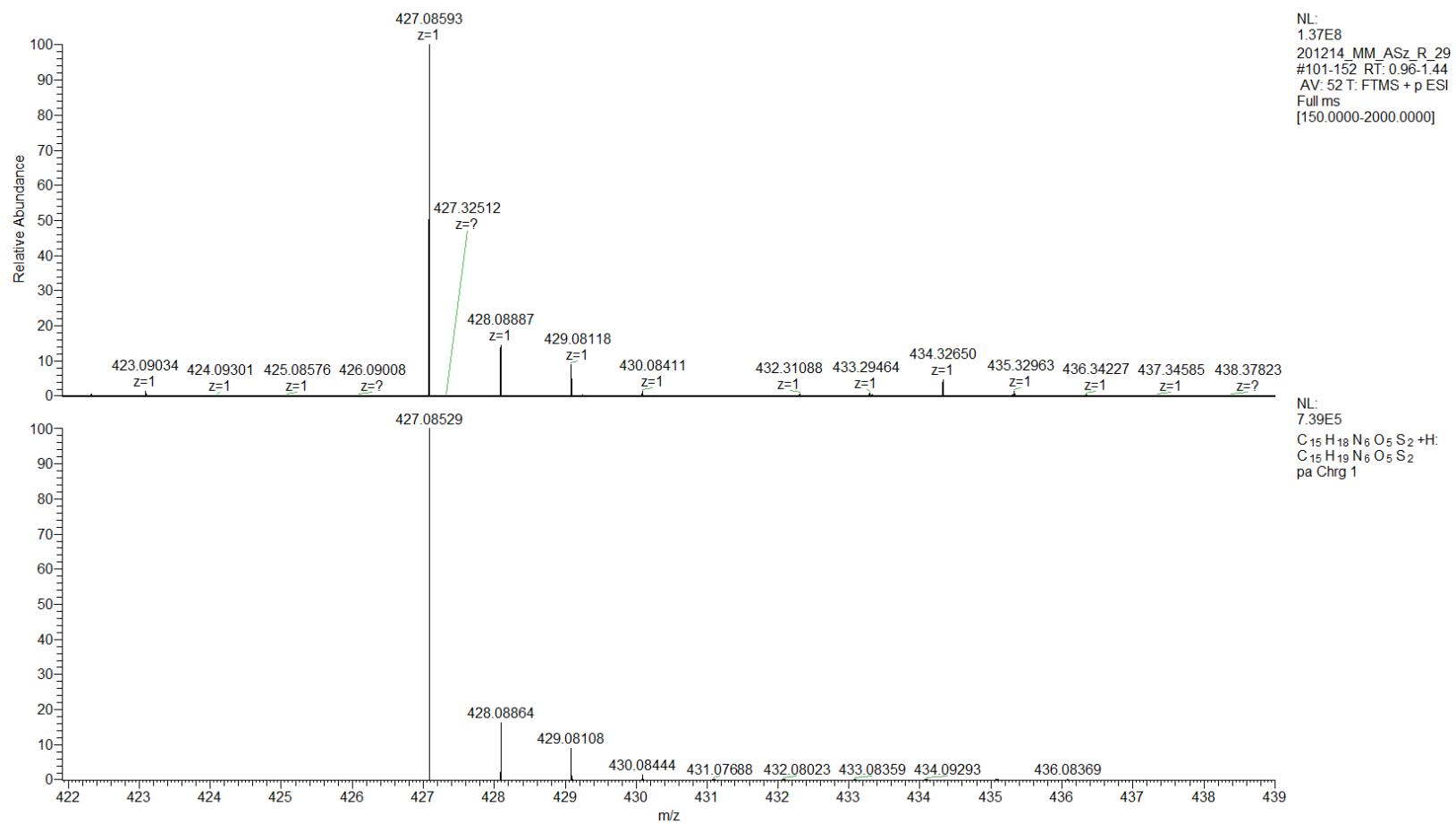


Figure S13: ^1H -NMR in $\text{MeOH-}d_4$ for derivative MM129

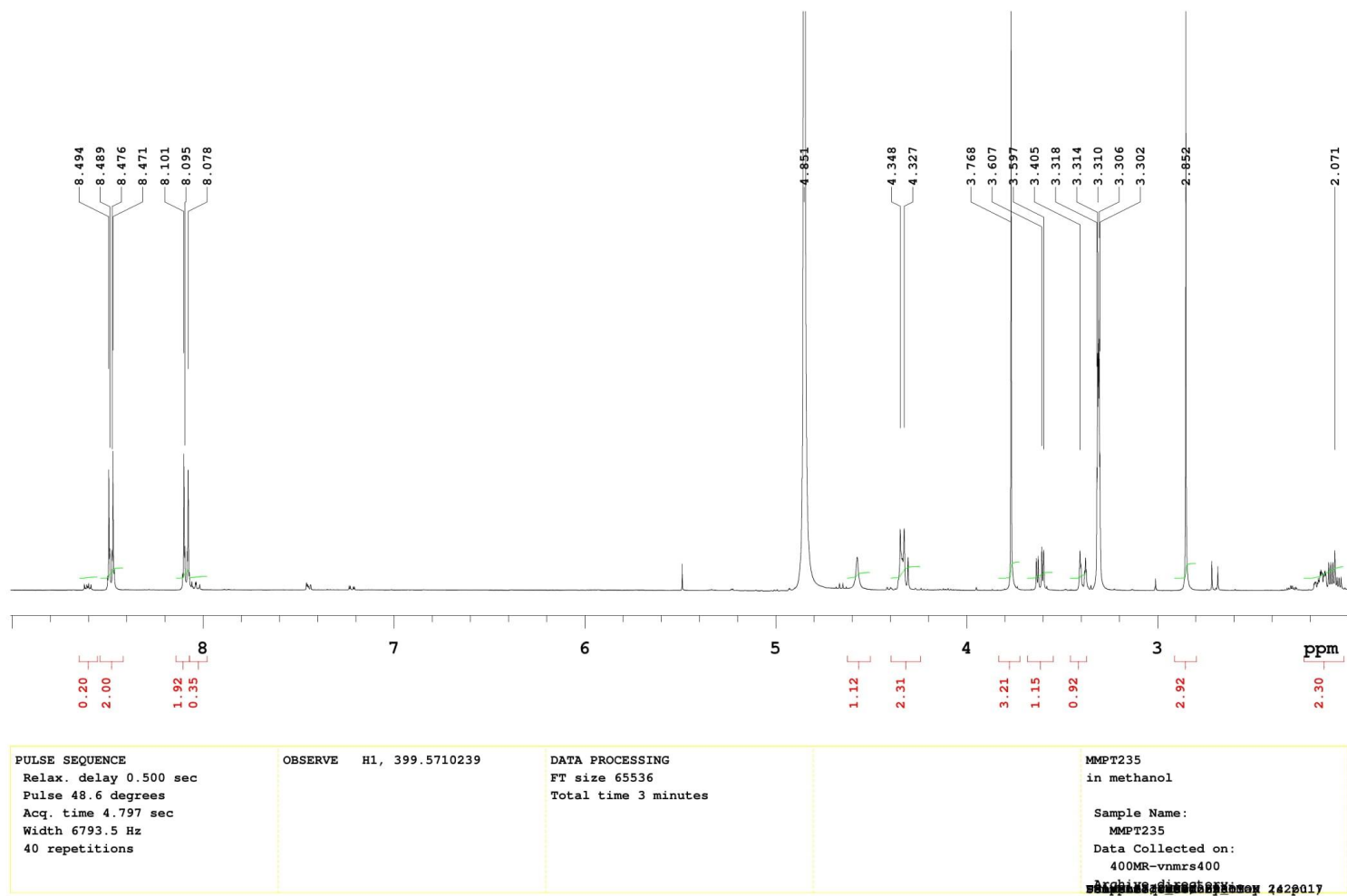
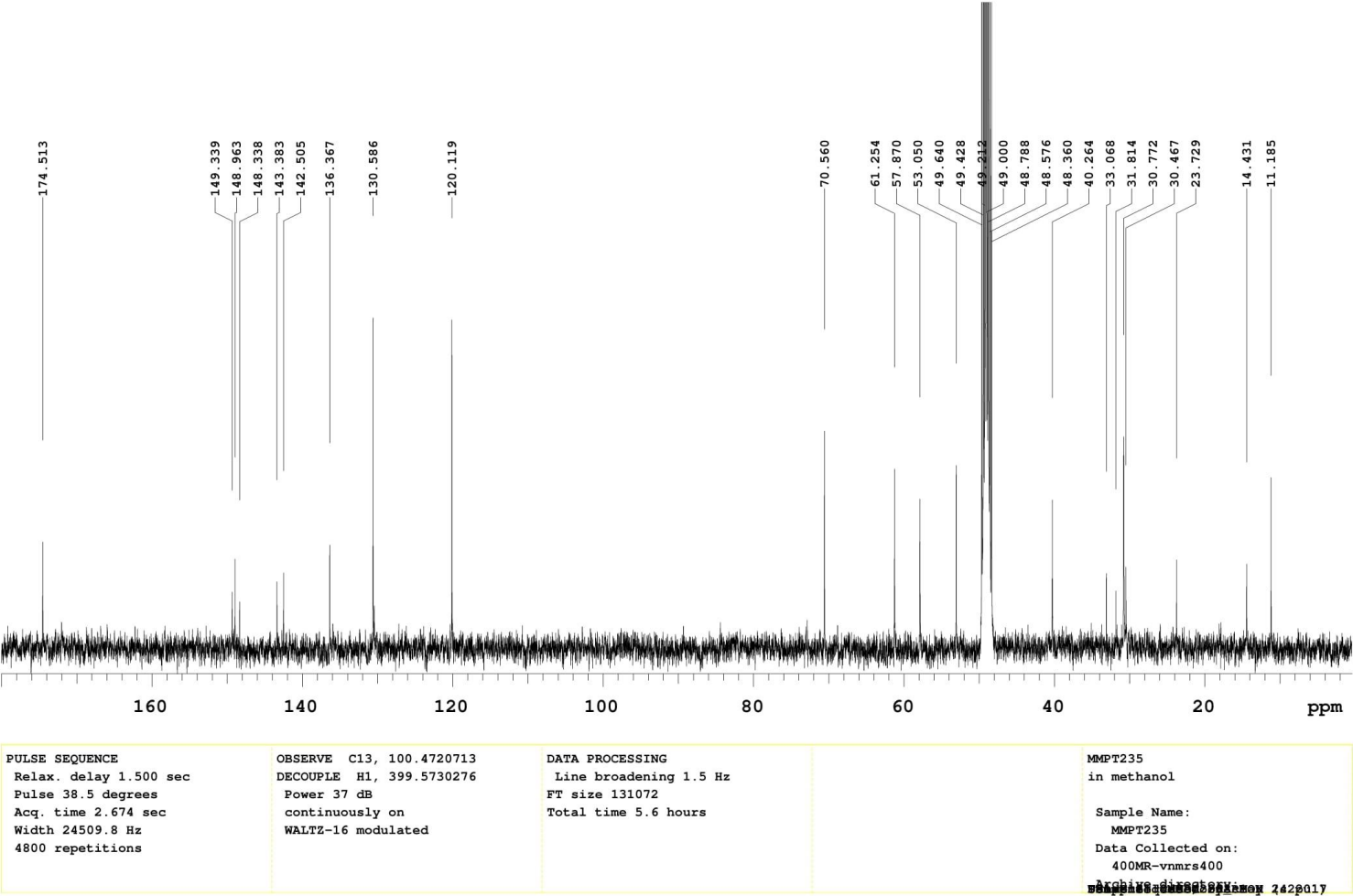


Figure S14: ^{13}C -NMR in $\text{MeOH-}d_4$ for derivative MM129



1H NMR Spectrum Data:

Chemical Shift (ppm)	Integration
8.671, 8.649	1.98
8.156, 8.134	2.00
7.260	-
5.300	-
4.528, 4.508, 4.488	2.00
3.789, 3.682, 3.673, 3.654, 3.644, 3.619, 3.531, 3.502	3.01, 1.10, 2.99, 1.08
2.891	3.00
2.278, 2.259, 2.186, 2.175, 2.165, 2.154	1.08, 1.11

Sample Information:
 Sample Name: MMPT288
 Data Collected on: 400MR-vnmrs400

Acquisition Parameters:
 PULSE SEQUENCE: Relax. delay 0.500 sec
 Pulse 48.6 degrees
 Acq. time 4.797 sec
 Width 6793.5 Hz
 32 repetitions

Processing Parameters:
 OBSERVE H1, 399.5428928
 DATA PROCESSING: FT size 65536
 Total time 2 minutes

Figure S16: ^1H -NMR in $\text{MeOH-}d_4$ for derivative MM130

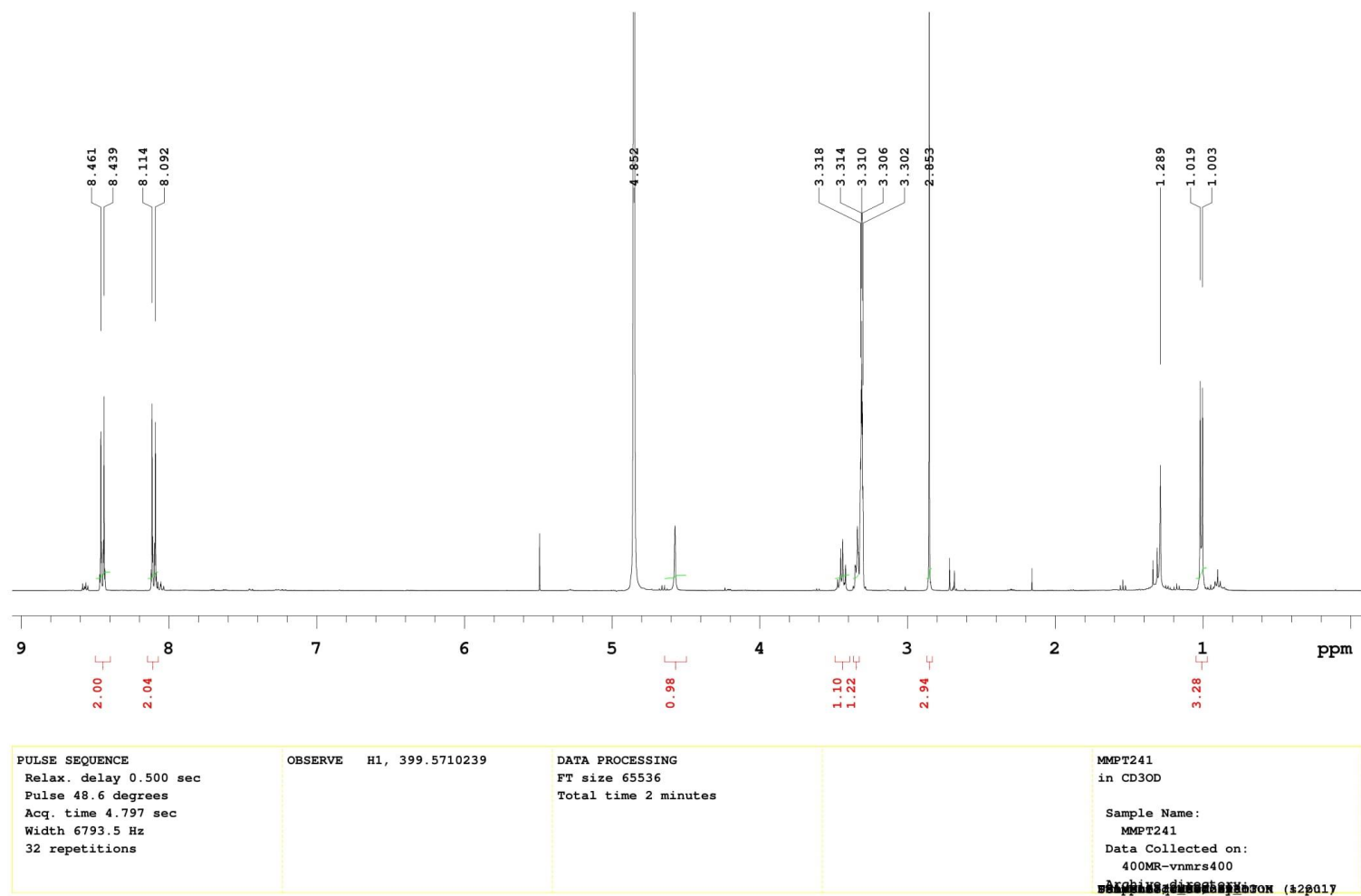
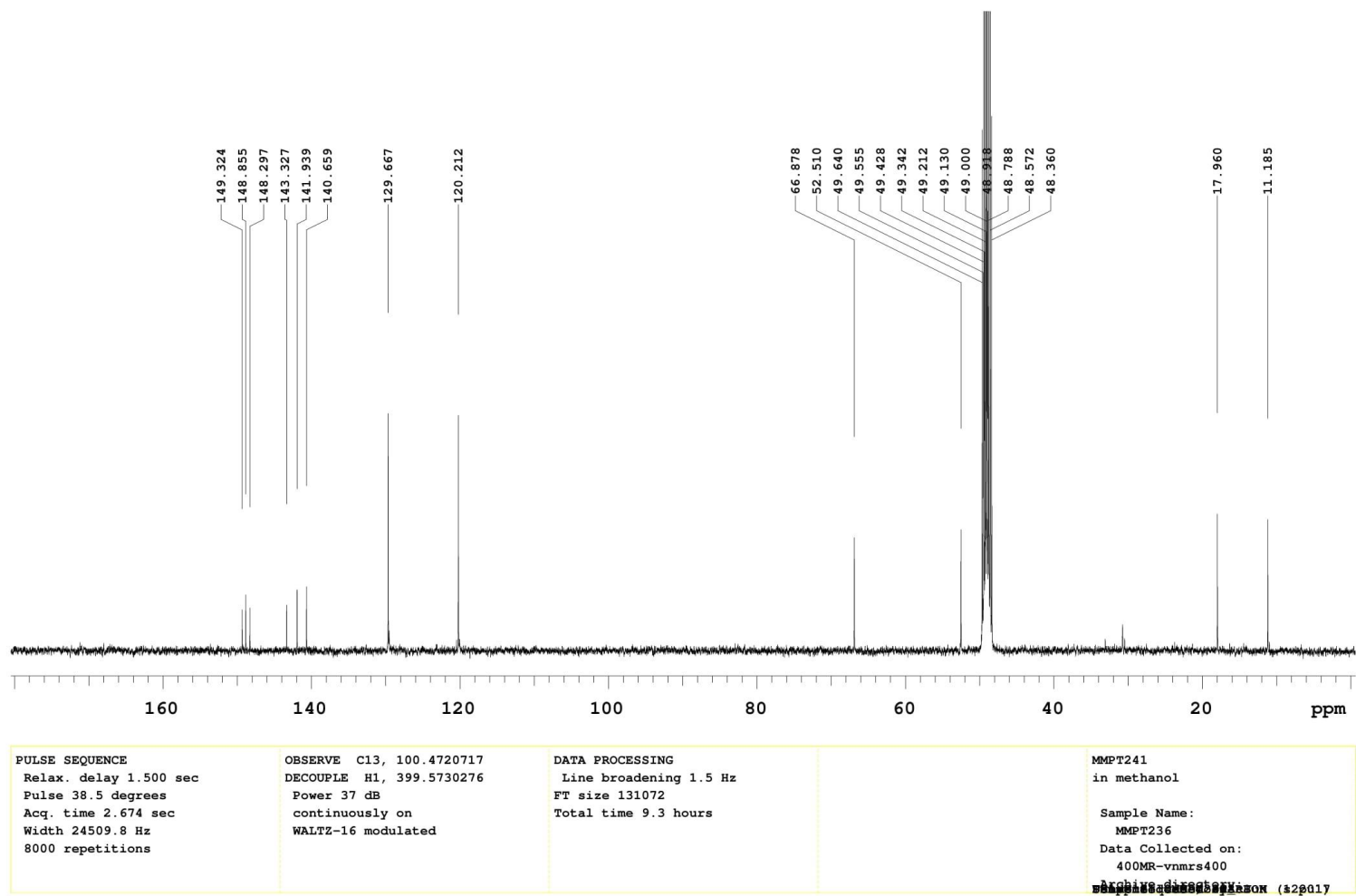


Figure S17: ^{13}C -NMR in $\text{MeOH-}d_4$ for derivative MM130



1H NMR spectrum of MMPT233 in methanol. The spectrum shows peaks from 2.8 to 8.5 ppm. Integration values are shown below the peaks: 1.93, 2.00, 0.66, 1.01, 2.04, 0.41, 0.57, 0.24, 3.00. Peak labels are at the top: 8.471, 8.465, 8.453, 8.448, 8.103, 8.098, 8.086, 8.081, 5.491, 4.850, 4.573, 3.674, 3.661, 3.658, 3.644, 3.498, 3.488, 3.485, 3.473, 3.318, 3.314, 3.310, 3.306, 3.302, 3.092, 3.079, 3.058, 3.046, 2.902, 2.885, 2.869, 2.853. The x-axis is labeled 'ppm'.

Chemical Shift (ppm)	Integration
8.471	1.93
8.465	1.93
8.453	1.93
8.448	1.93
8.103	2.00
8.098	2.00
8.086	2.00
8.081	2.00
5.491	0.66
4.850	0.66
4.573	0.66
3.674	1.01
3.661	1.01
3.658	1.01
3.644	1.01
3.498	1.01
3.488	1.01
3.485	1.01
3.473	1.01
3.318	2.04
3.314	2.04
3.310	2.04
3.306	2.04
3.302	2.04
3.092	0.41
3.079	0.41
3.058	0.41
3.046	0.41
2.902	0.57
2.885	0.57
2.869	0.24
2.853	0.24

PULSE SEQUENCE
Relax. delay 0.500 sec
Pulse 48.6 degrees
Acq. time 4.797 sec
Width 6793.5 Hz
40 repetitions

OBSERVE H1, 399.5710239

DATA PROCESSING
FT size 65536
Total time 3 minutes

MMPT233
in methanol

Sample Name:
MMPT233
Data Collected on:
400MR-vnmrs400

2429017

Region	Chemical Shift (ppm)	Assignment
Aromatic/Quaternary	149.324, 148.885, 148.304, 143.339, 142.043, 139.341	Aromatic and quaternary carbons
Aliphatic	129.775, 120.264	Aliphatic carbons
Methoxy	3.8	Methoxy group (-OCH ₃)
Methine	4.6	Methine group (-CH-)
Solvent	49.0	Methanol (CD ₃ OH)
Methyl	11.2	Methyl group (-CH ₃)

PULSE SEQUENCE
 Relax. delay 1.500 sec
 Pulse 38.5 degrees
 Acq. time 2.674 sec
 Width 24509.8 Hz
 1328 repetitions

OBSERVE C13, 100.4720717
 DECOUPLE H1, 399.5730276
 Power 37 dB
 continuously on
 WALTZ-16 modulated

DATA PROCESSING
 Line broadening 1.5 Hz
 FT size 131072
 Total time 92 minutes

MMPT233
 in methanol

Sample Name:
 MMPT233
 Data Collected on:
 400MR-vnmrs400