Supporting information

Cholic acid-based antimicrobial peptide mimics as antibacterial agents

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[3] School of Life Sciences, University of Technology Sydney, PO Box 123, Ultimo 2007, Australia
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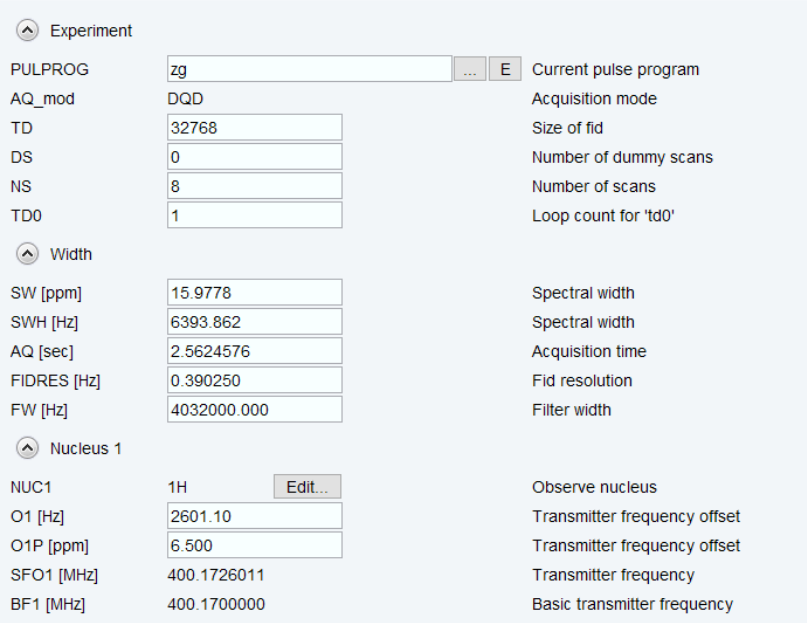
^{1}H NMR and ^{13}C NMR spectra of synthesised compounds

Acquisition parameters for ^{1}H NMR and ^{13}C NMR spectra

^{1}H NMR:

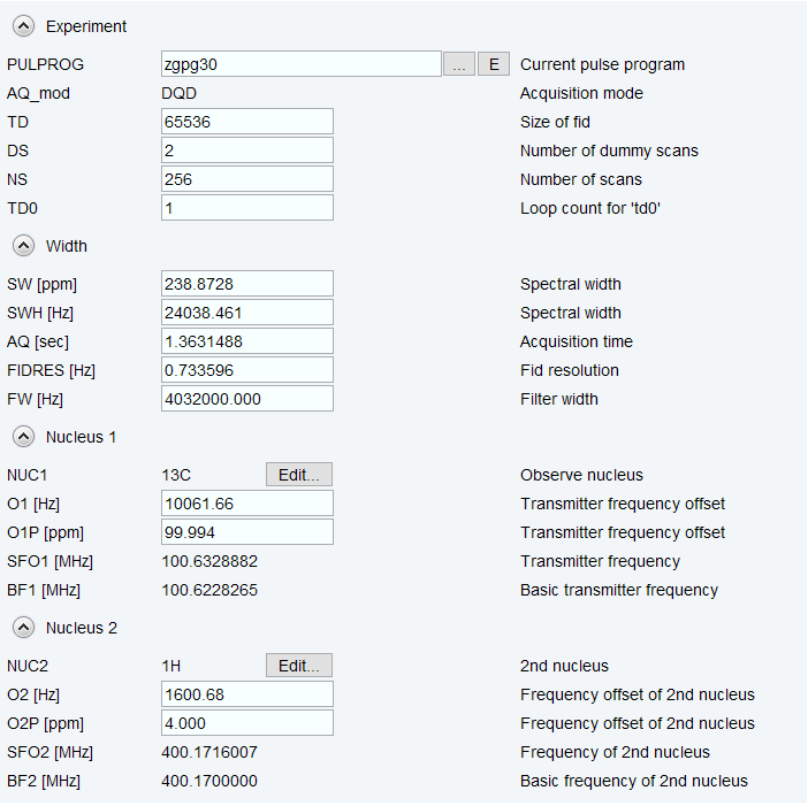
Standard Bruker pulse program “zg” was used and the delay (D1) was set to 5 s.



Experiment		
PULPROG	zg ... E	Current pulse program
AQ_mod	DQD	Acquisition mode
TD	32768	Size of fid
DS	0	Number of dummy scans
NS	8	Number of scans
TD0	1	Loop count for 'td0'
Width		
SW [ppm]	15.9778	Spectral width
SWH [Hz]	6393.862	Spectral width
AQ [sec]	2.5624576	Acquisition time
FIDRES [Hz]	0.390250	Fid resolution
FW [Hz]	4032000.000	Filter width
Nucleus 1		
NUC1	1H Edit...	Observe nucleus
O1 [Hz]	2601.10	Transmitter frequency offset
O1P [ppm]	6.500	Transmitter frequency offset
SFO1 [MHz]	400.1726011	Transmitter frequency
BF1 [MHz]	400.1700000	Basic transmitter frequency

^{13}C{^{1}H} NMR:

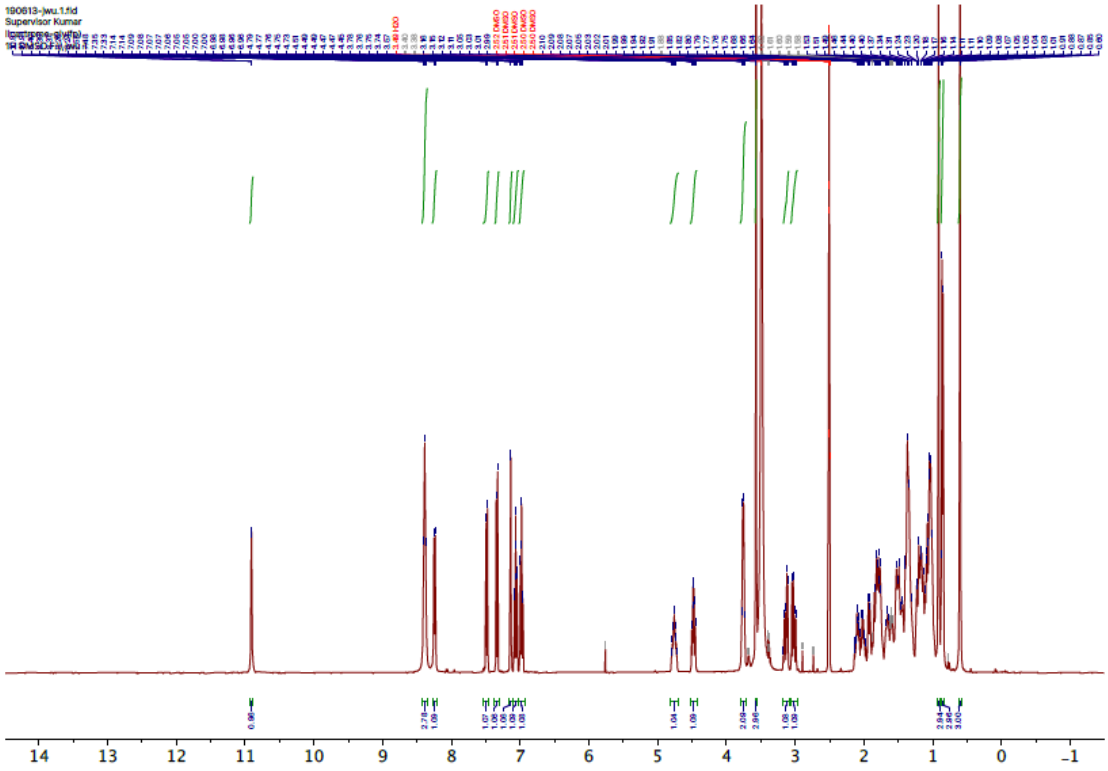
Standard Bruker pulse program “zgpg30” was used and the delay (D1) was set to 1 s.



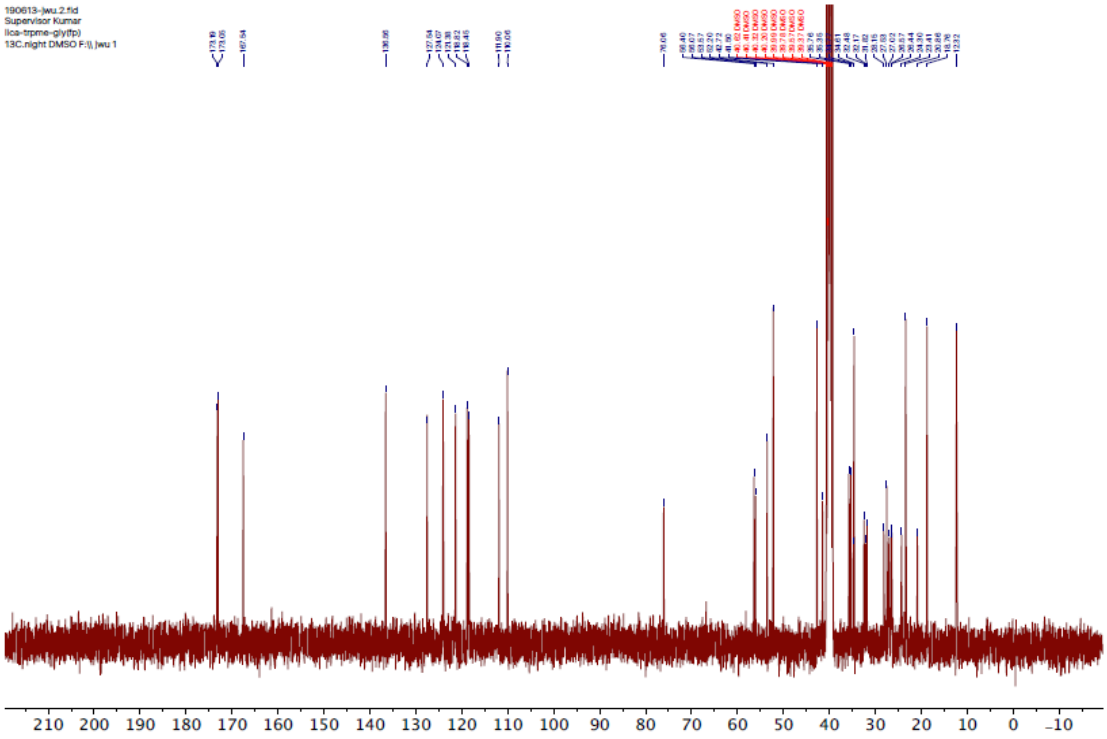
Experiment		
PULPROG	zgpg30 ... E	Current pulse program
AQ_mod	DQD	Acquisition mode
TD	65536	Size of fid
DS	2	Number of dummy scans
NS	256	Number of scans
TD0	1	Loop count for 'td0'
Width		
SW [ppm]	238.8728	Spectral width
SWH [Hz]	24038.461	Spectral width
AQ [sec]	1.3631488	Acquisition time
FIDRES [Hz]	0.733596	Fid resolution
FW [Hz]	4032000.000	Filter width
Nucleus 1		
NUC1	13C Edit...	Observe nucleus
O1 [Hz]	10061.66	Transmitter frequency offset
O1P [ppm]	99.994	Transmitter frequency offset
SFO1 [MHz]	100.6328882	Transmitter frequency
BF1 [MHz]	100.6228265	Basic transmitter frequency
Nucleus 2		
NUC2	1H Edit...	2nd nucleus
O2 [Hz]	1600.68	Frequency offset of 2nd nucleus
O2P [ppm]	4.000	Frequency offset of 2nd nucleus
SFO2 [MHz]	400.1716007	Frequency of 2nd nucleus
BF2 [MHz]	400.1700000	Basic frequency of 2nd nucleus

2-(((3*R*,5*R*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl)oxy)-2-oxoethan-1-aminium **(16a)**

^{1}H NMR (400 MHz, DMSO-d_6):

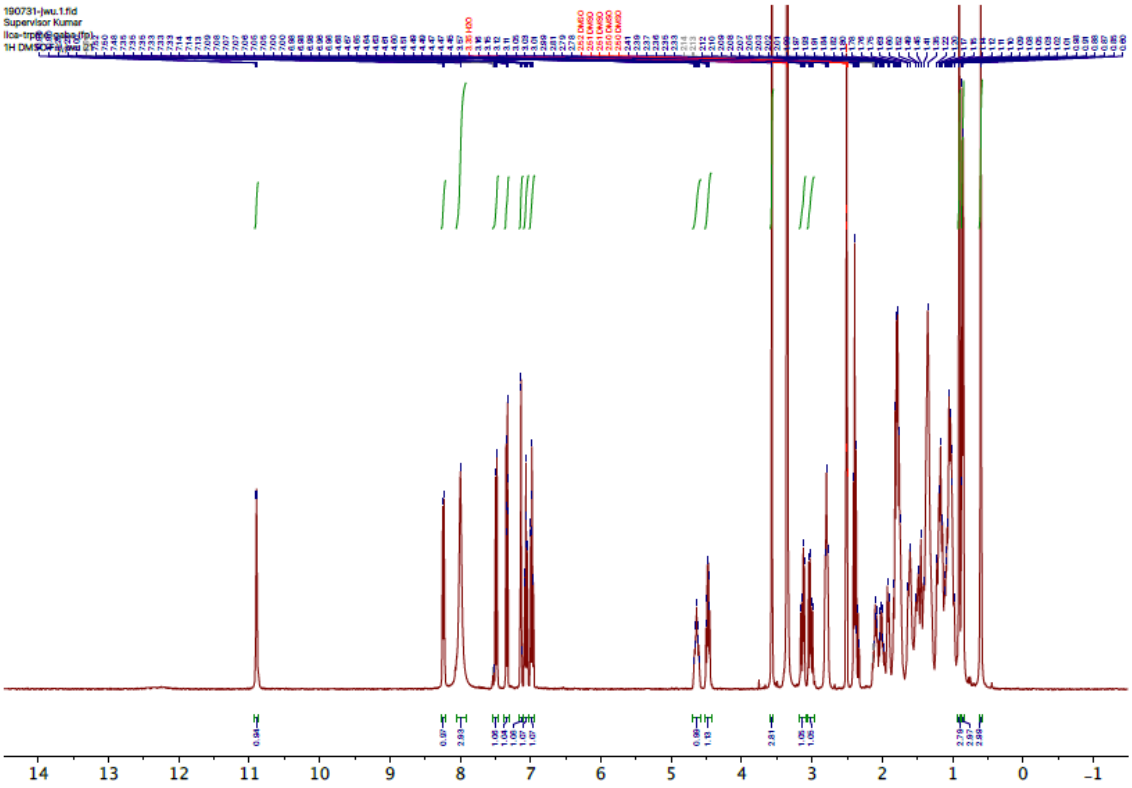


^{13}C NMR (100 MHz, DMSO-d_6):

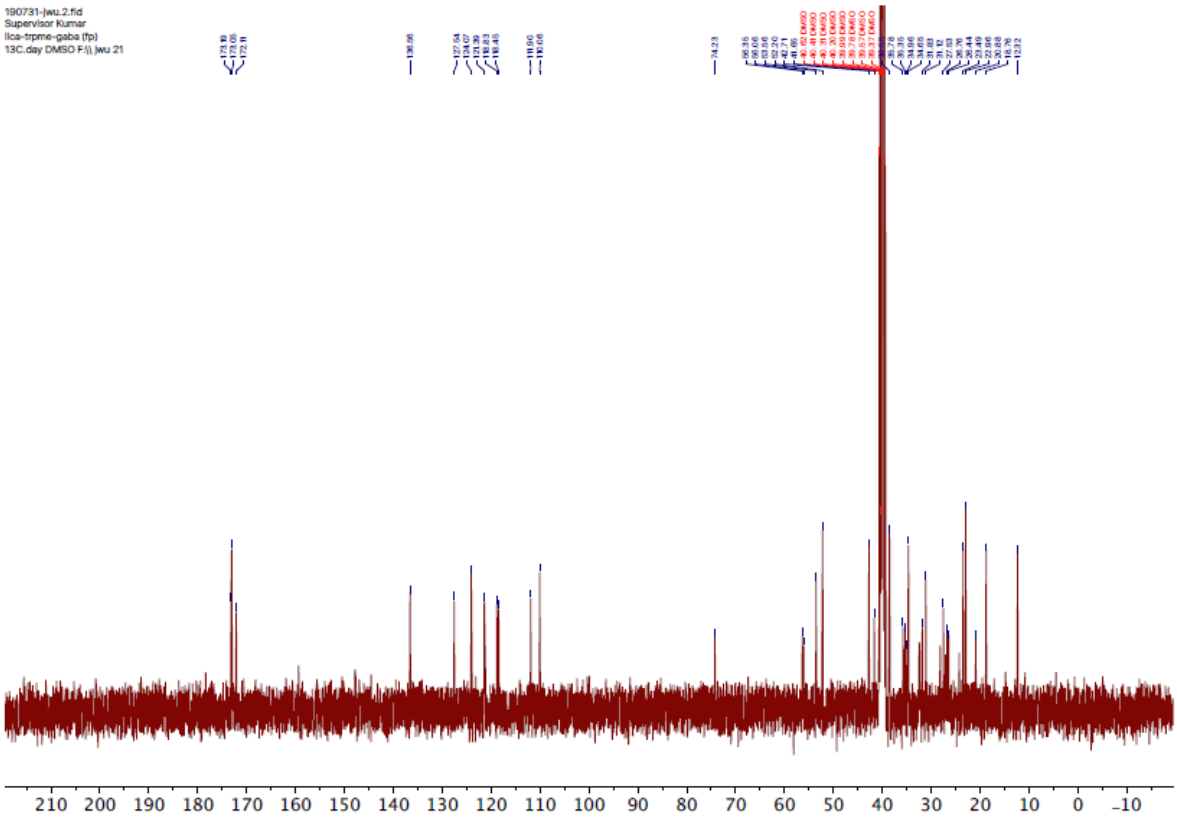


4-(((3*R*,5*R*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl)oxy)-4-oxobutan-1-aminium **(16b)**

^{1}H NMR (400 MHz, DMSO-d_6):

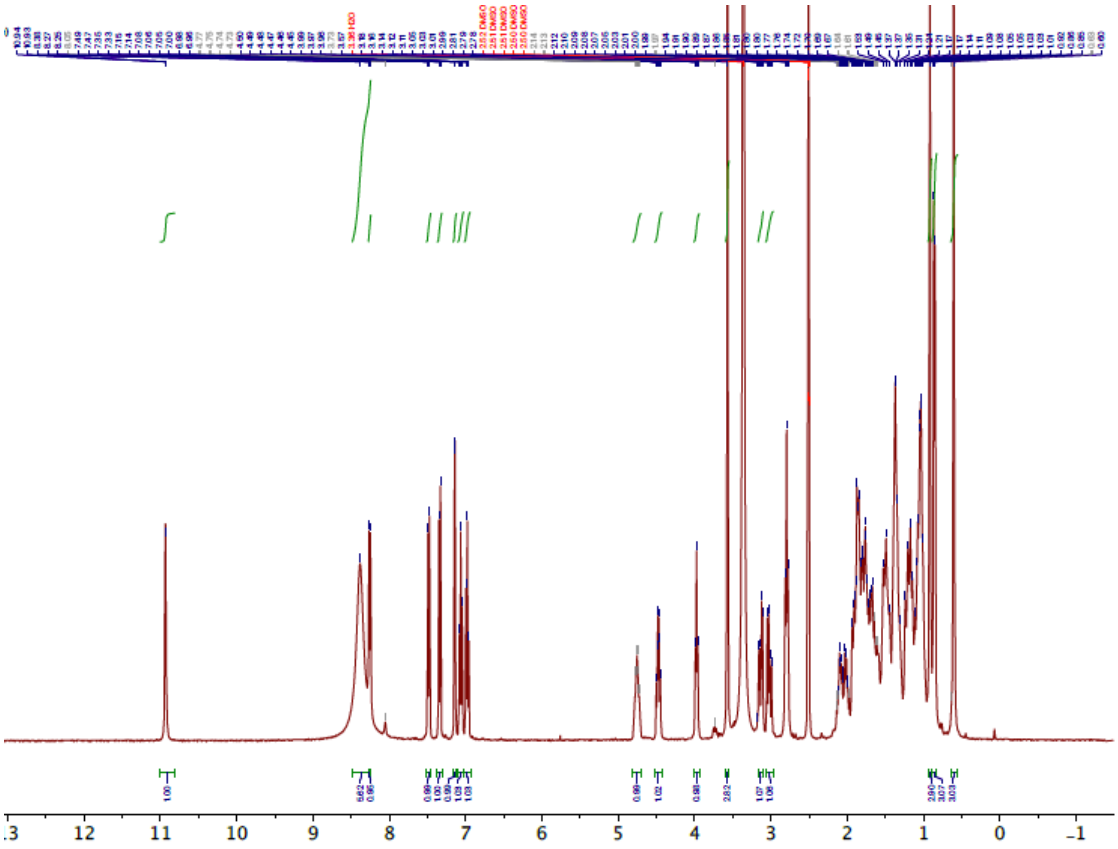


^{13}C NMR (100 MHz, DMSO-d_6):

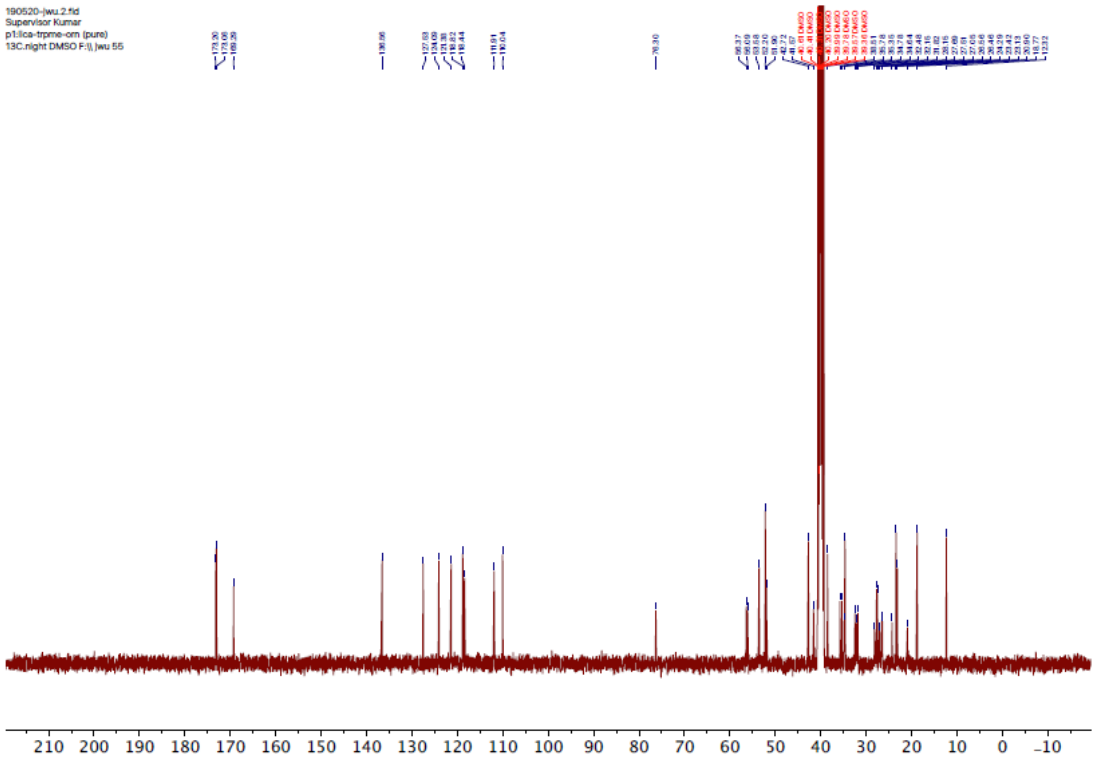


(*S*)-5-(((3*R*,5*R*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl)oxy)-5-oxopentane-1,4-diaminium **(16c)**

^{1}H NMR (400 MHz, DMSO-d_6):

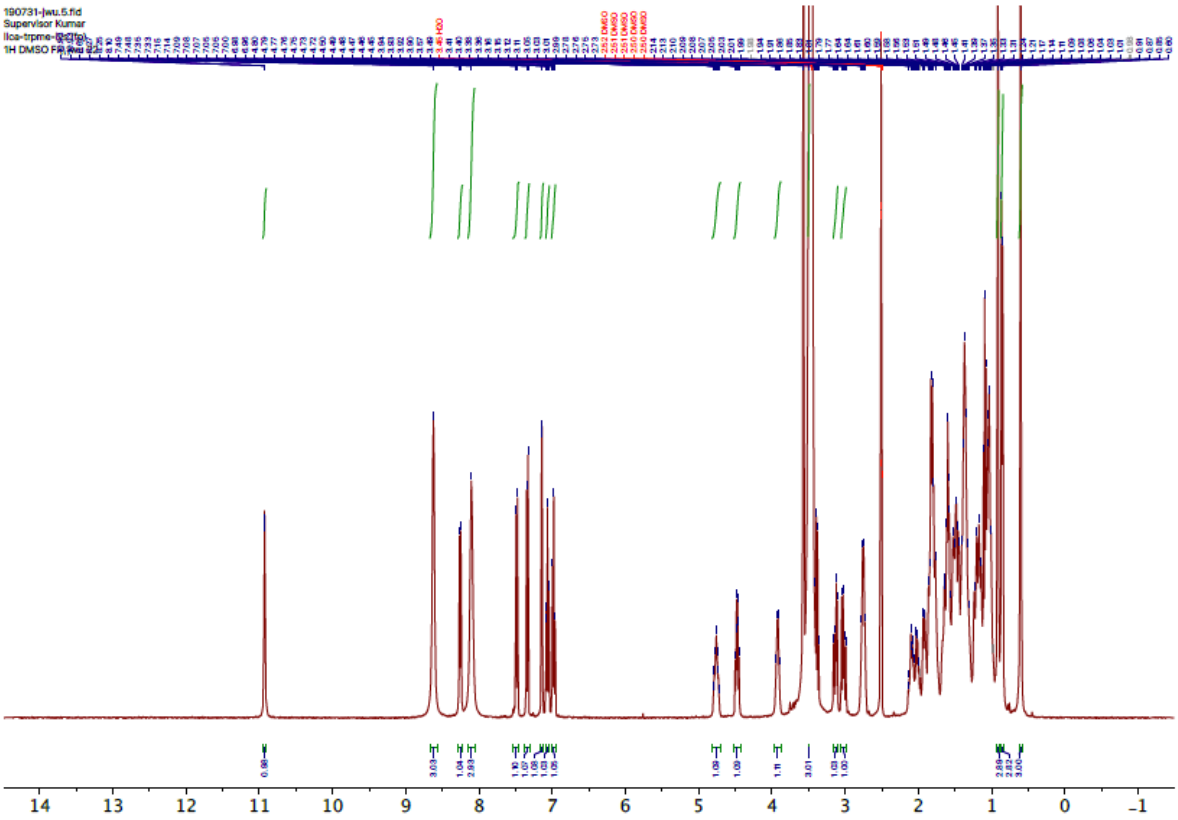


^{13}C NMR (100 MHz, DMSO-d_6):

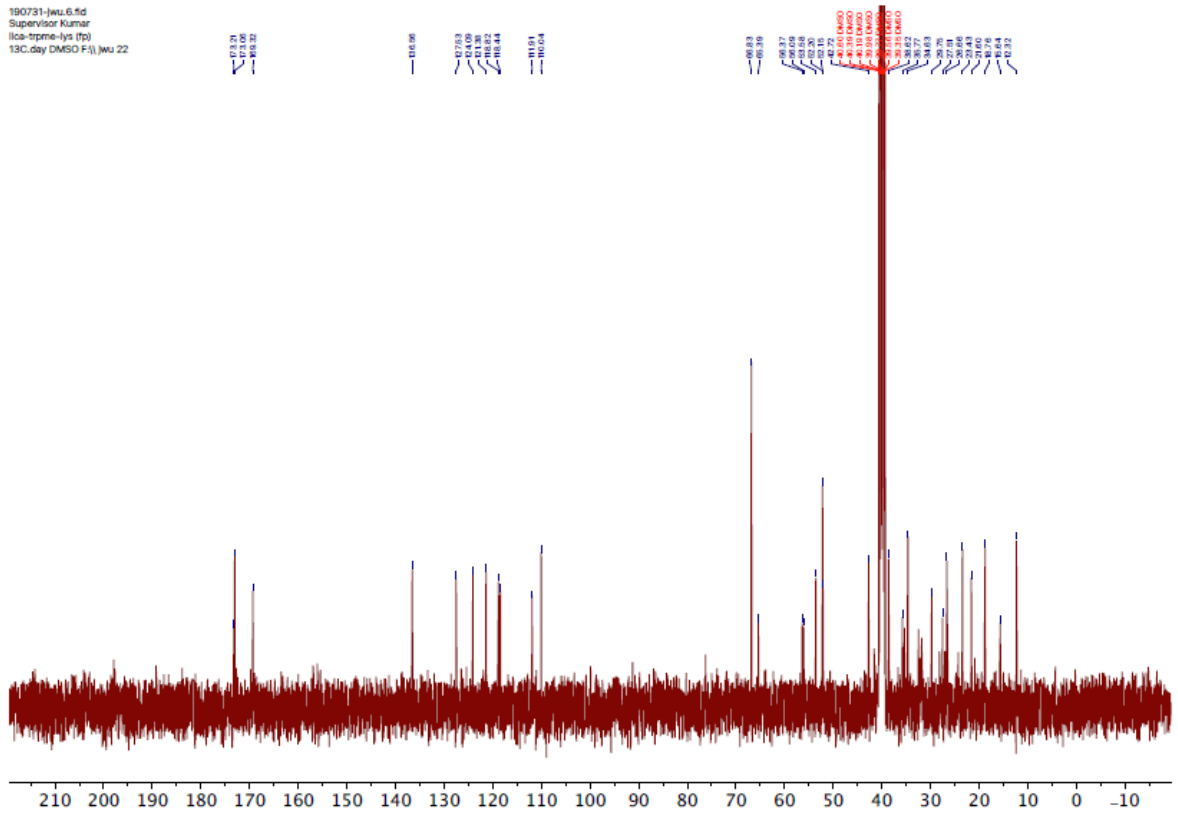


(*S*)-6-(((3*R*,5*R*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl)oxy)-6-oxohexane-1,5-diaminium **(16d)**

^{1}H NMR (400 MHz, DMSO-d_6):

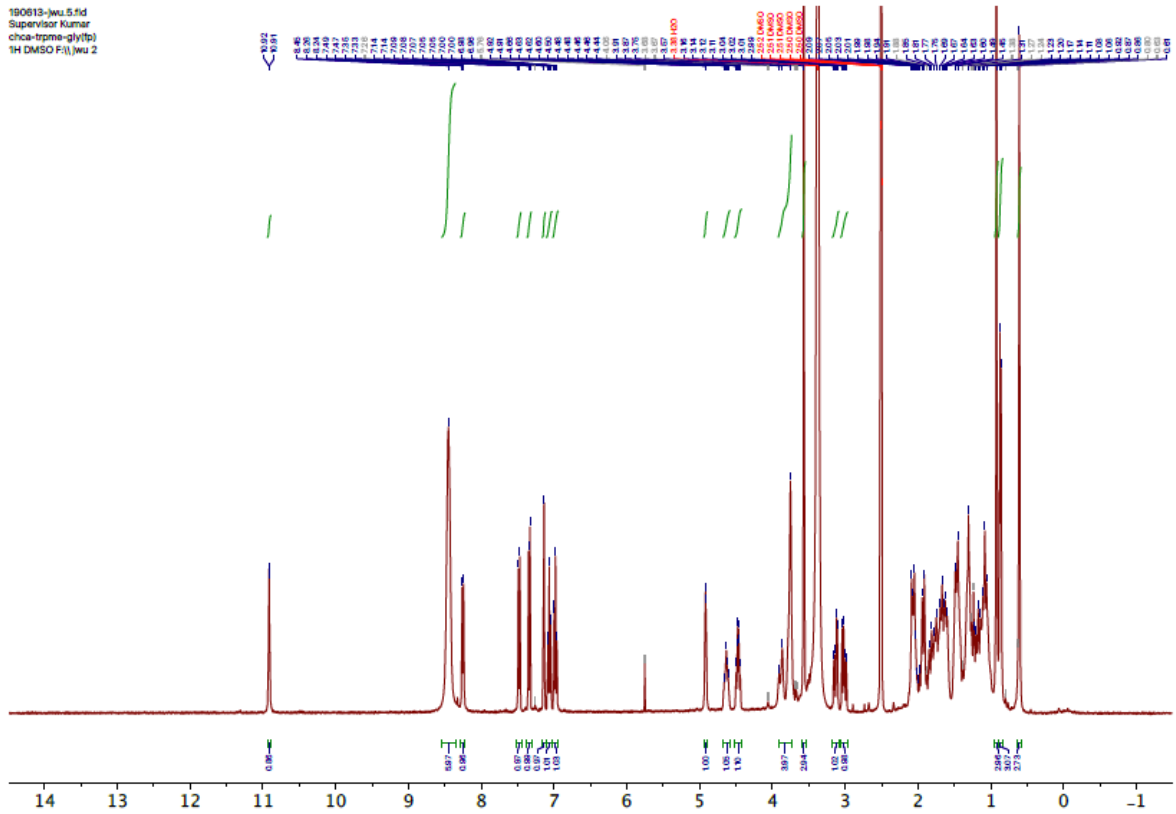


^{13}C NMR (75 MHz, DMSO-d_6):

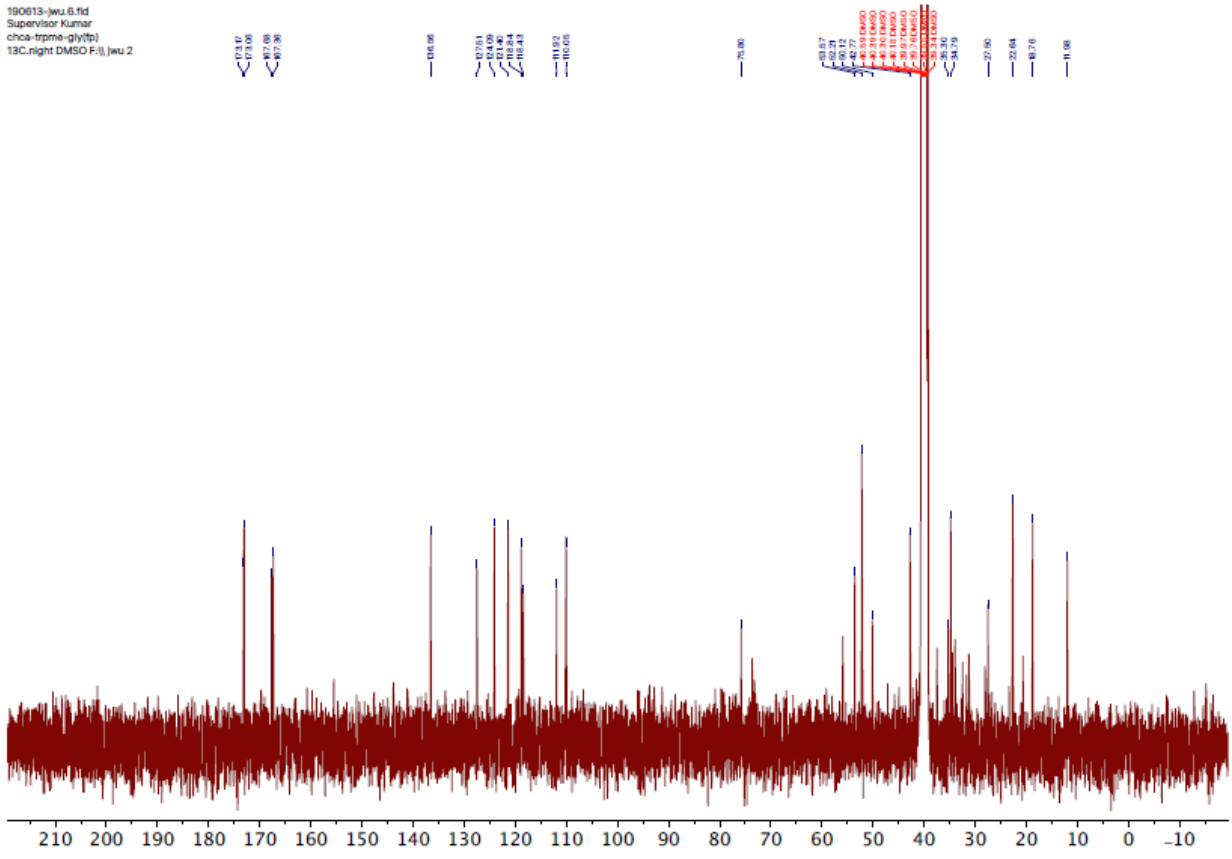


2,2'-(((3*R*,5*S*,7*R*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthrene-3,7-diyl)bis(oxy))bis(2-oxoethan-1-aminium) **(17a)**

^{1}H NMR (400 MHz, DMSO-d_6):

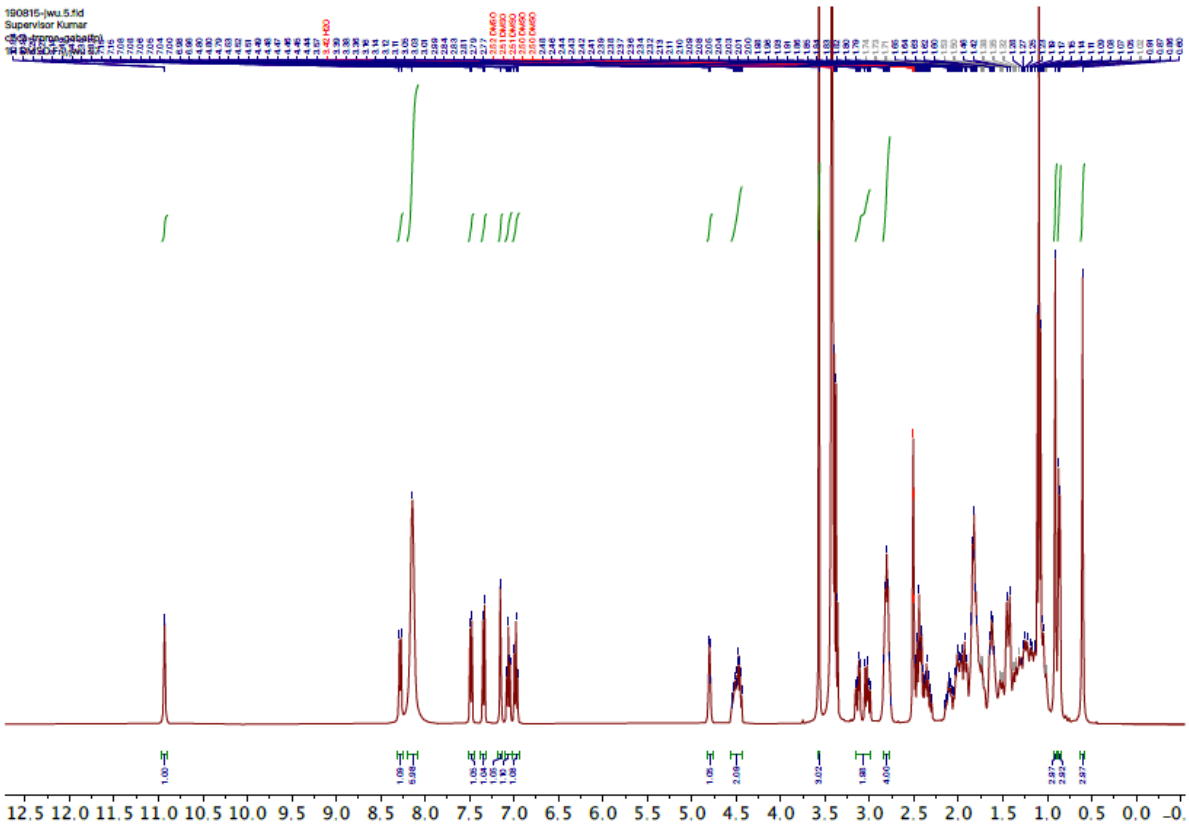


^{13}C NMR (100 MHz, DMSO-d_6):

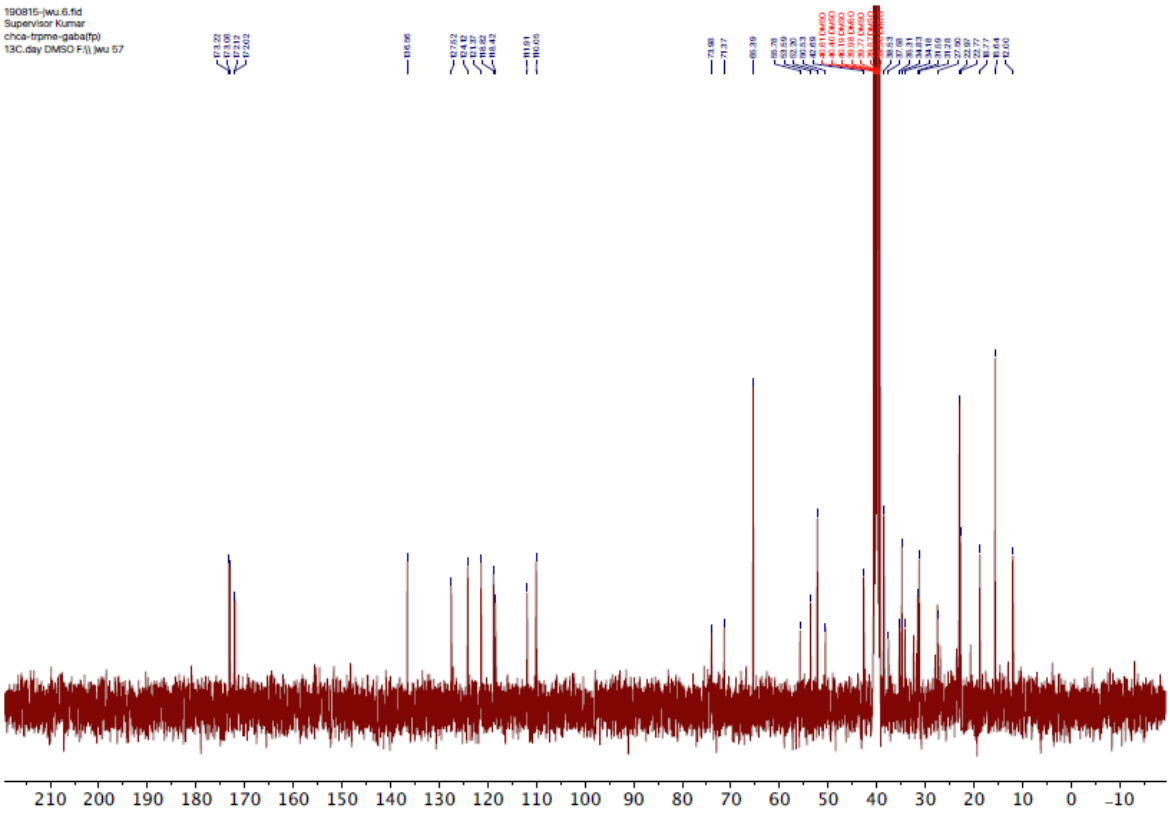


4,4'-(((3*R*,5*S*,7*R*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthrene-3,7-diyl)bis(oxy))bis(4-oxobutan-1-aminium) **(17b)**

^{1}H NMR (400 MHz, DMSO-d_6):

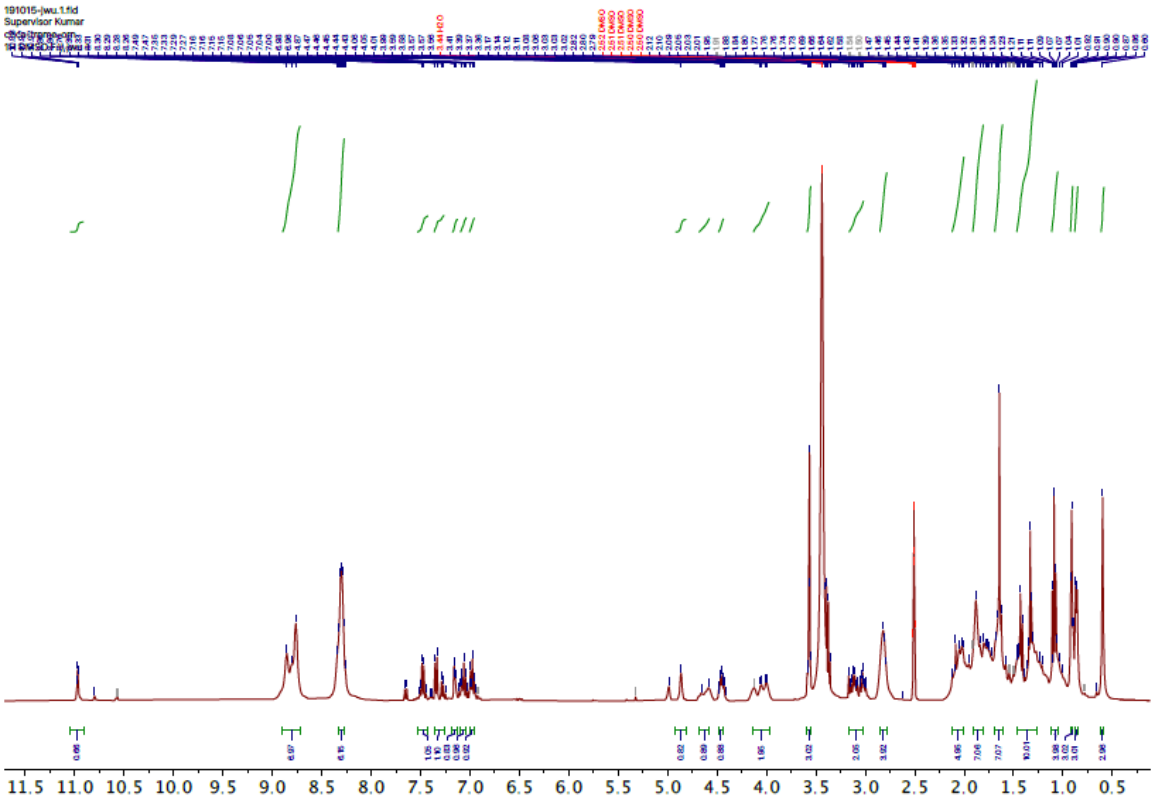


^{13}C NMR (100 MHz, DMSO-d_6):

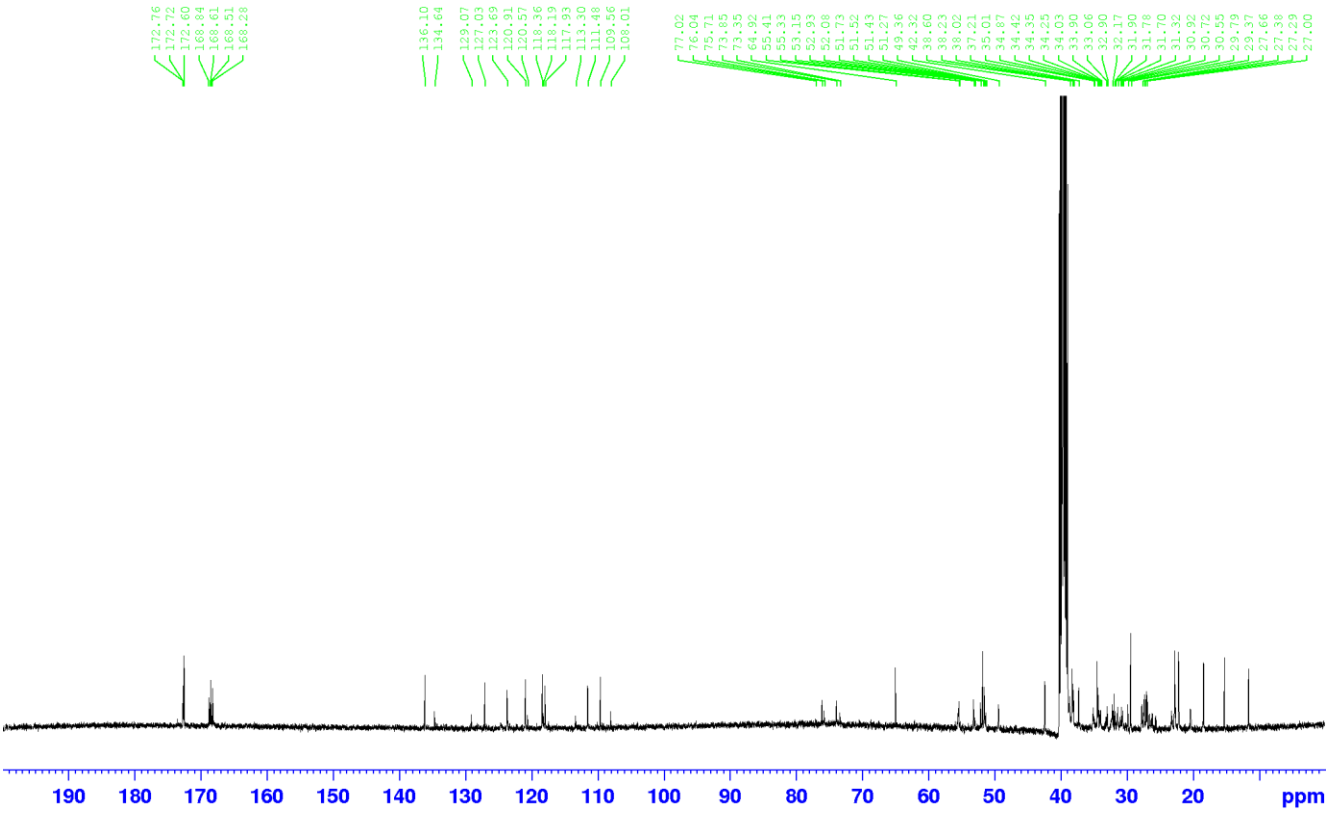


(4*S*,4'*S*)-5,5'-(((3*R*,5*S*,7*R*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthrene-3,7-diyl)bis(oxy))bis(5-oxopentane-1,4-diaminium) **(17c)**

^{1}H NMR (400 MHz, DMSO-d_6):

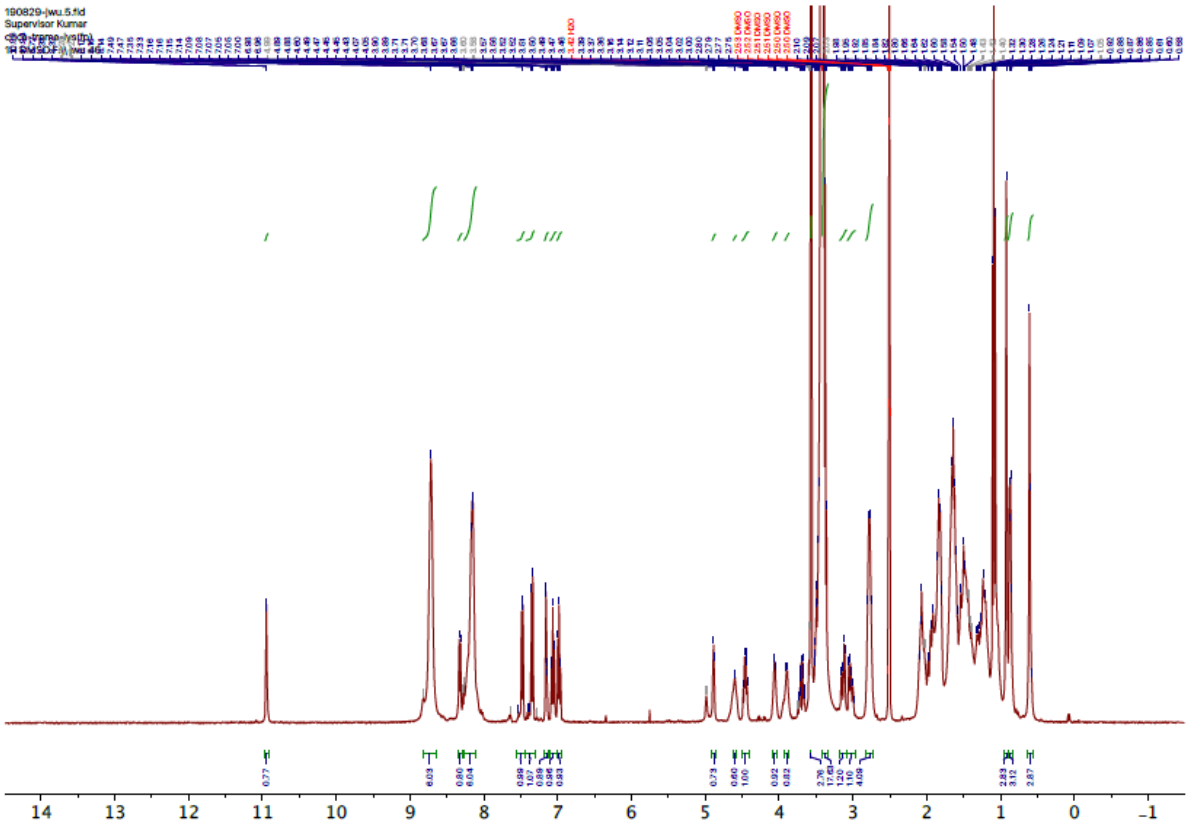


^{13}C NMR (100 MHz, DMSO-d_6):

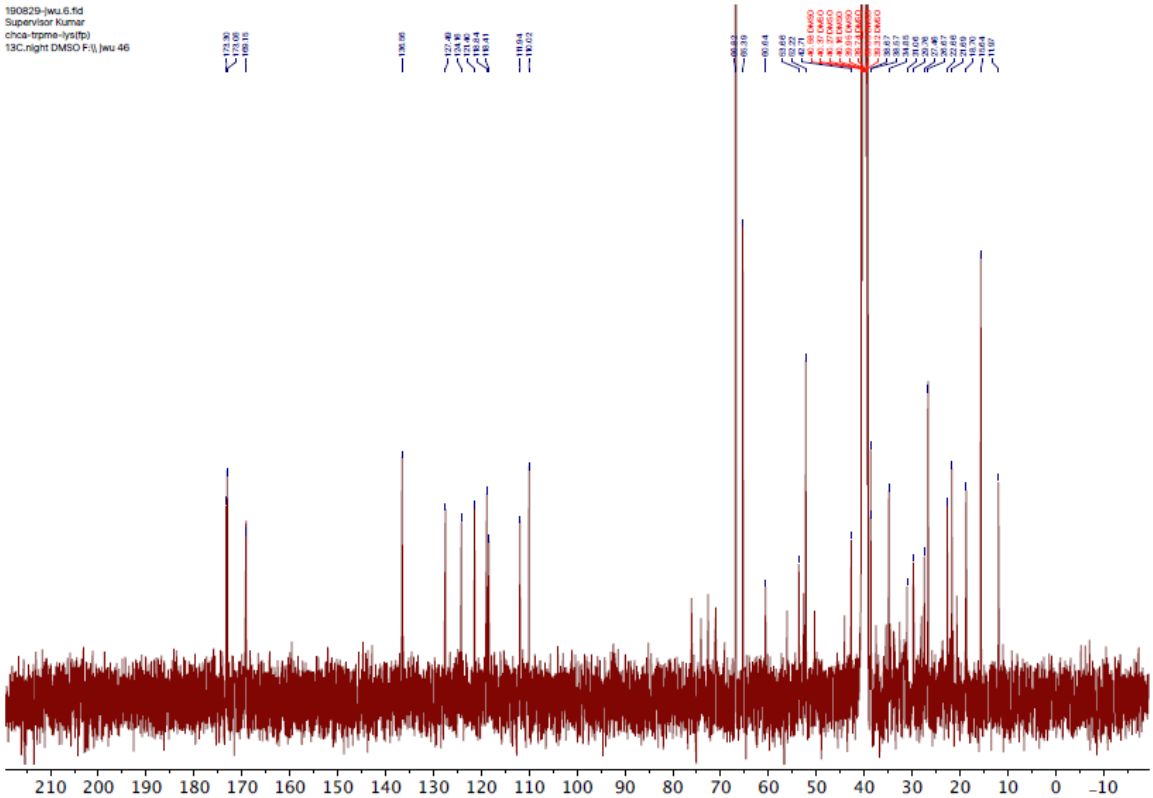


(5*S*,5'*S*)-6,6'-(((3*R*,5*S*,7*R*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthrene-3,7-diyl)bis(oxy))bis(6-oxohexane-1,5-diaminium) **(17d)**

^{1}H NMR (600 MHz, DMSO-d_6):

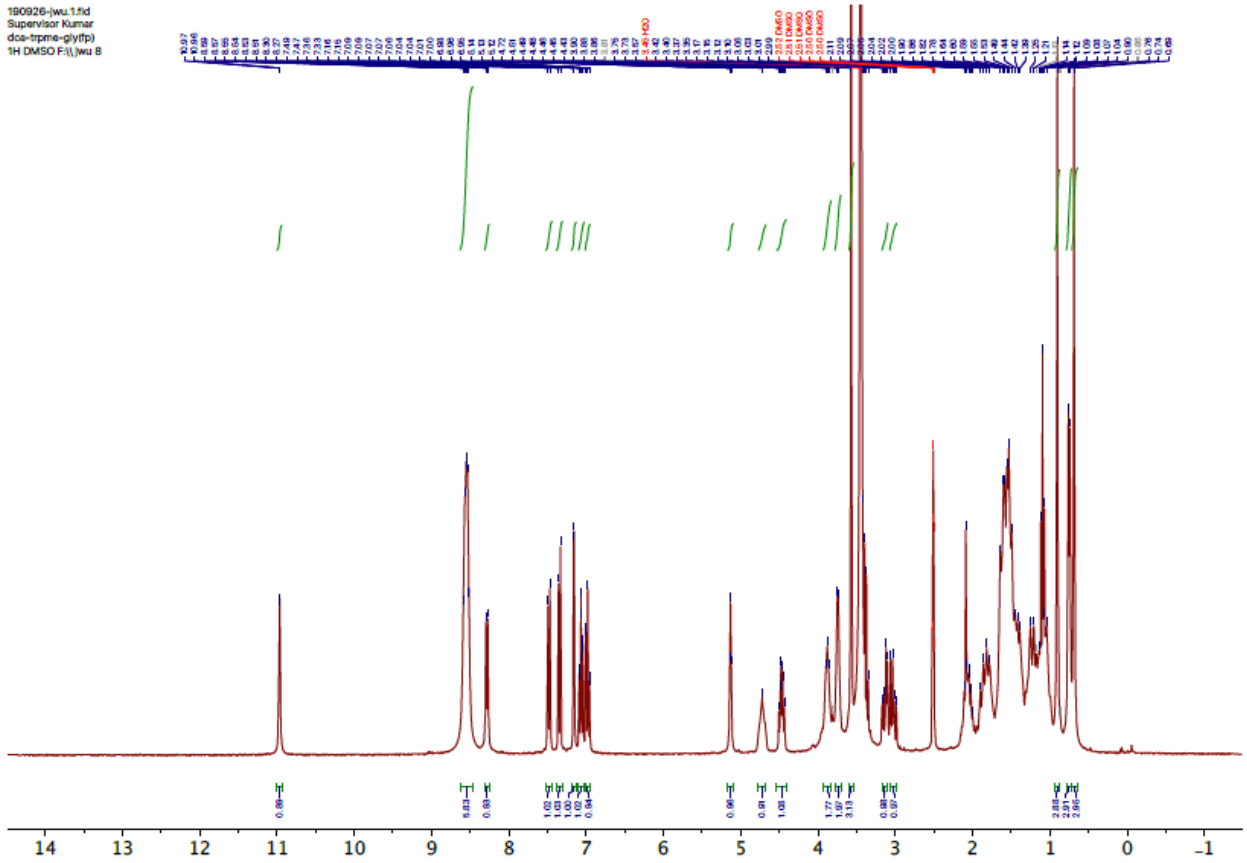


^{13}C NMR (150 MHz, DMSO-d_6):

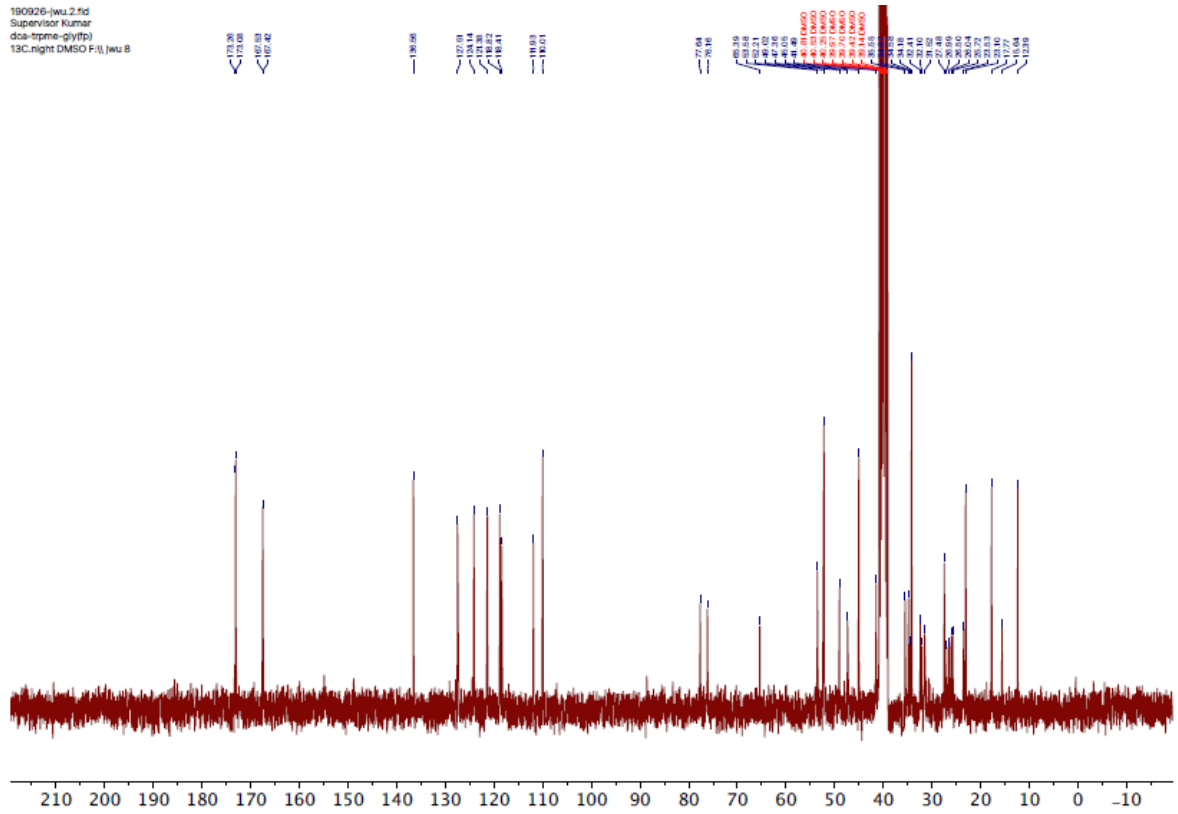


2,2'-(((3*R*,5*R*,8*R*,9*S*,10*S*,12*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthrene-3,12-diyl)bis(oxy))bis(2-oxoethan-1-aminium) **(18a)**

^{1}H NMR (300 MHz, DMSO-d_6):

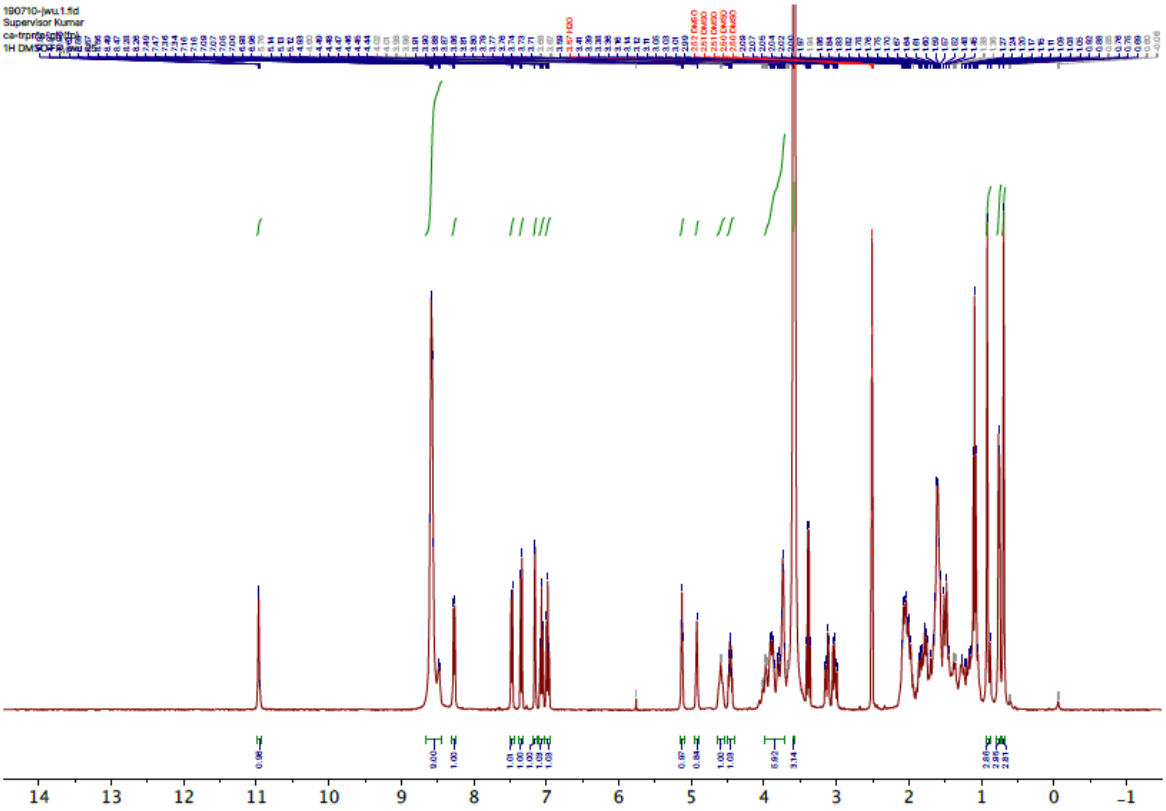


^{13}C NMR (75 MHz, DMSO-d_6):

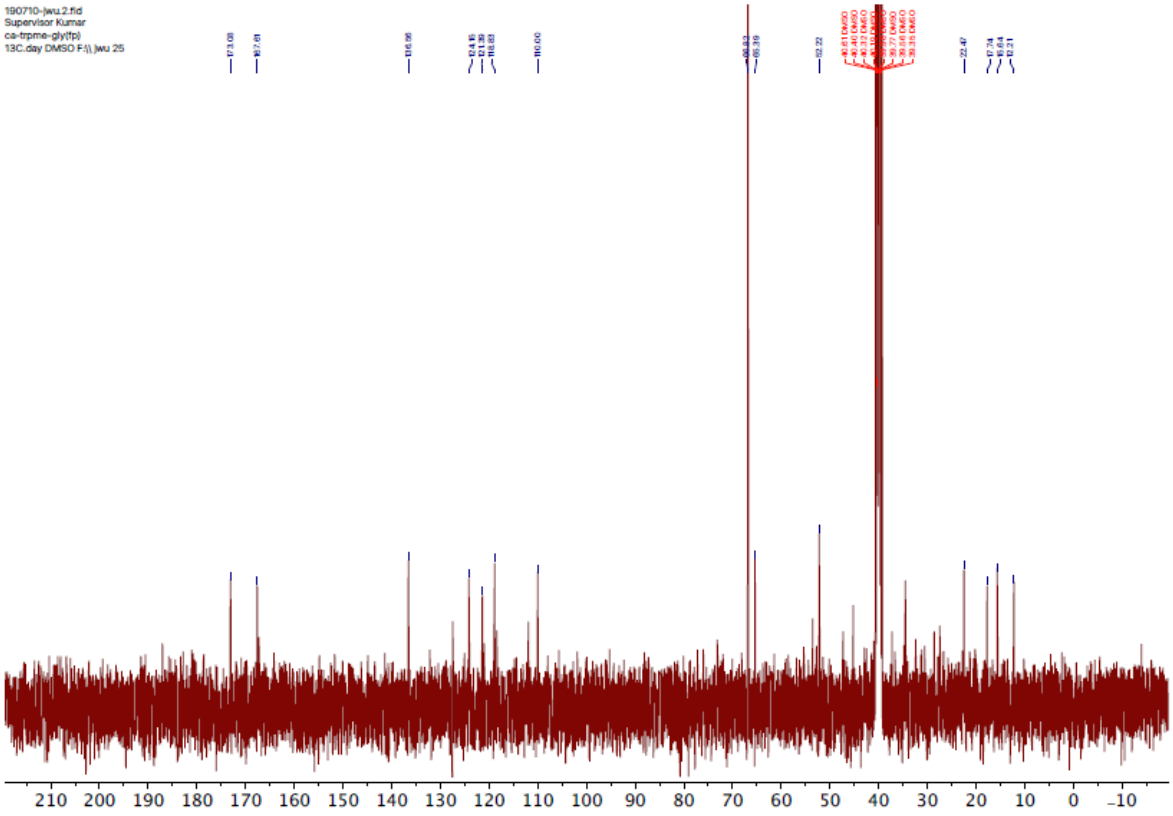


2,2'-(((3*R*,5*S*,7*R*,8*R*,9*S*,10*S*,12*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-3-(2-aminoacetoxy)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthrene-7,12-diyl)bis(oxy))bis(2-oxoethan-1-aminium) **(19a)**

^{1}H NMR (400 MHz, DMSO-d_6):

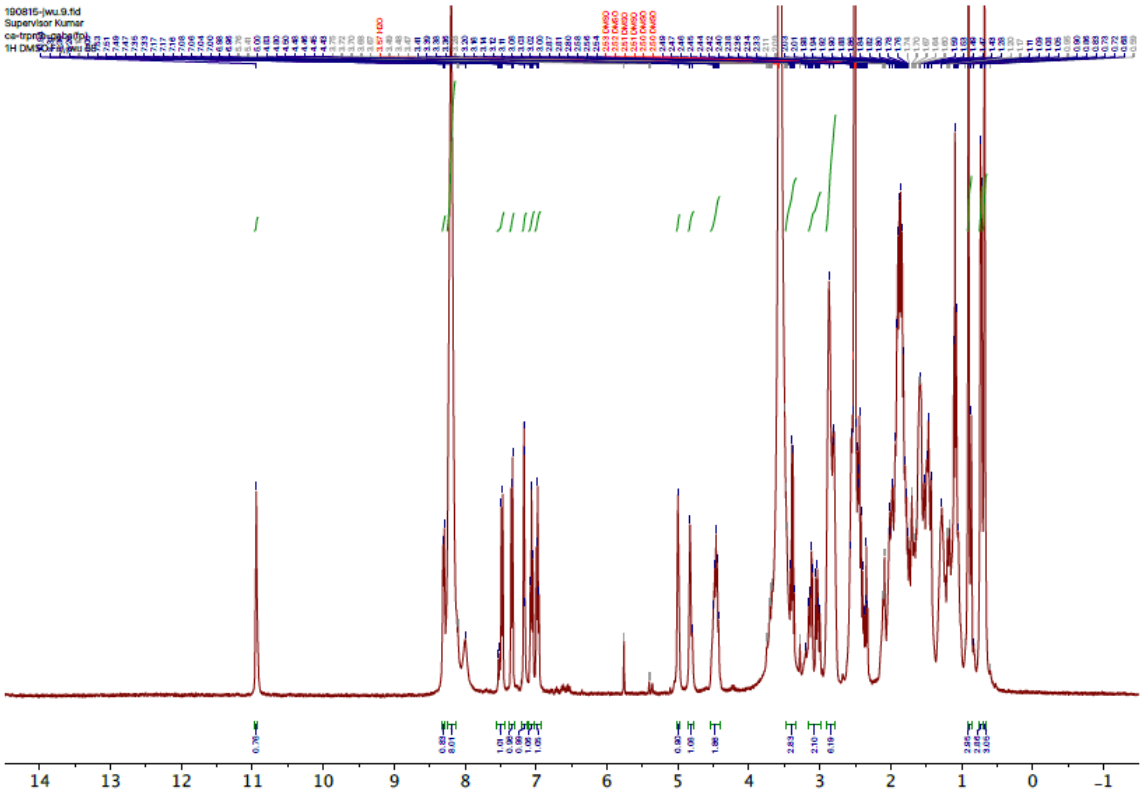


^{13}C NMR (100 MHz, DMSO-d_6):

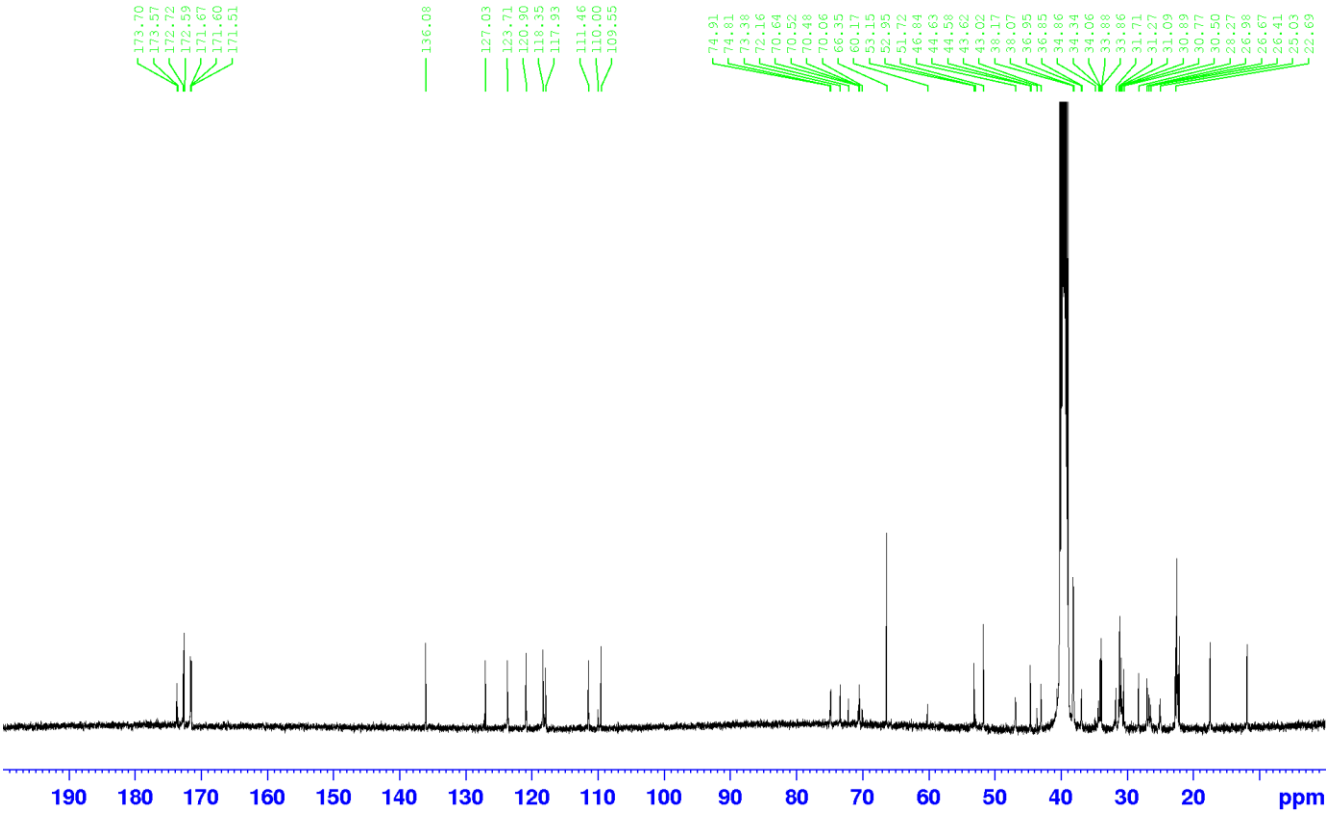


4,4',4"-(((3*R*,5*S*,7*R*,8*R*,9*S*,10*S*,12*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthrene-3,7,12-triyl)tris(oxy))tris(4-oxobutan-1-aminium) **(19b)**

^{1}H NMR (400 MHz, DMSO-d_6):

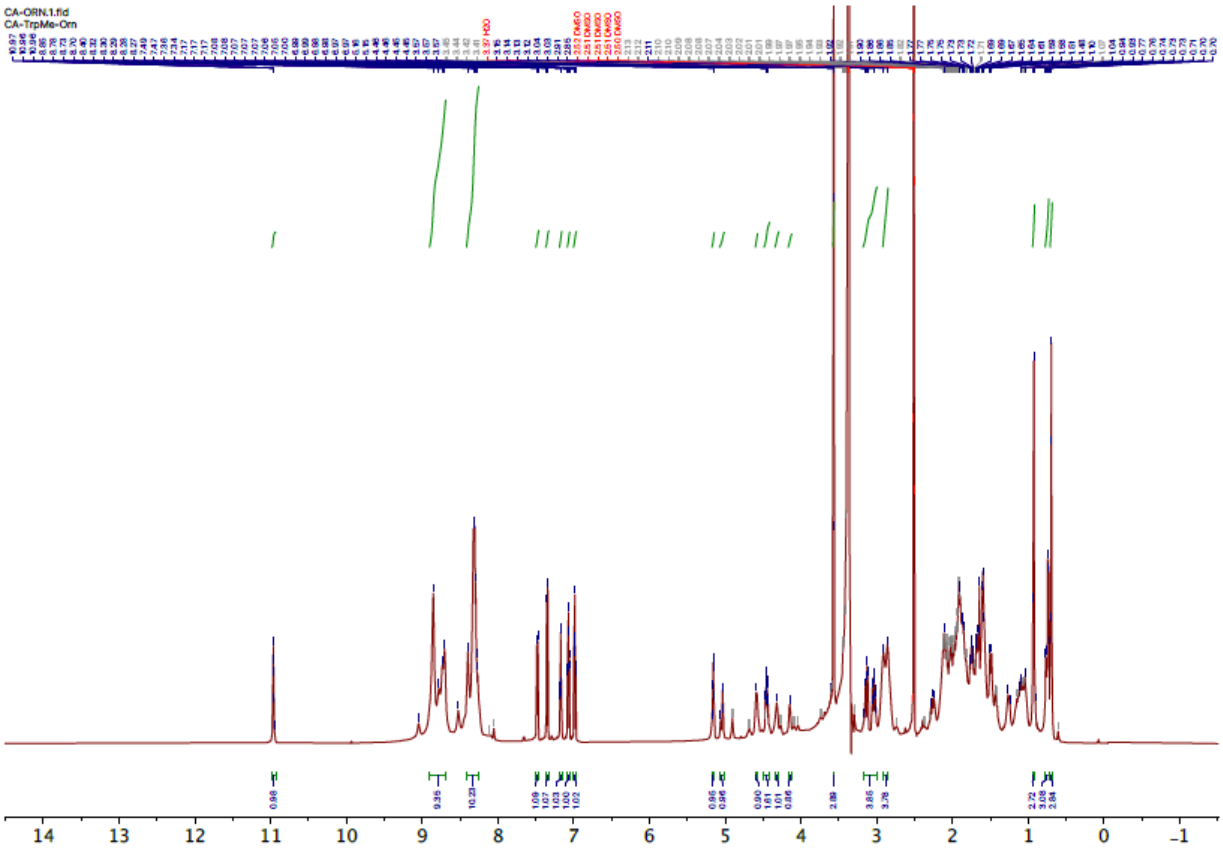


^{13}C NMR (100 MHz, DMSO-d_6):

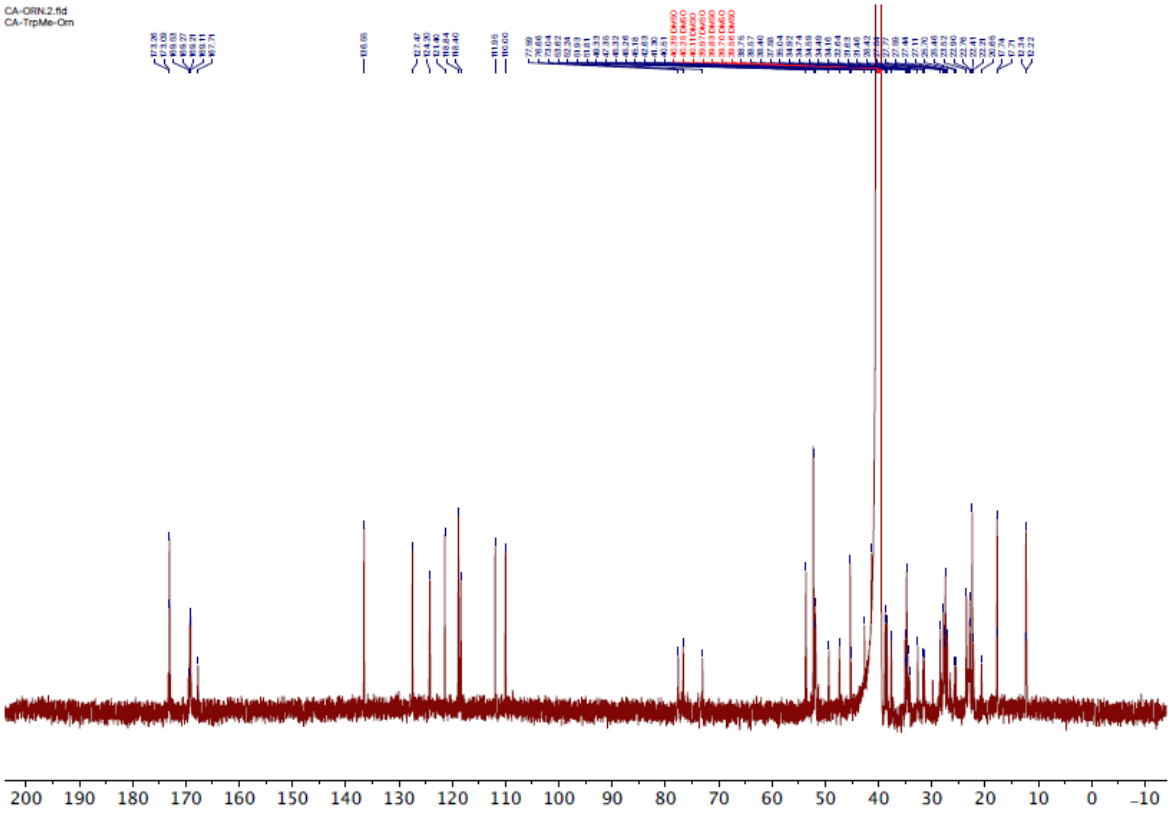


(4*S*,4'*S*,4"*S*)-5,5',5"-(((3*R*,5*S*,7*R*,8*R*,9*S*,10*S*,12*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthrene-3,7,12-triyl)tris(oxy))tris(5-oxopentane-1,4-diaminium) **(19c)**

^{1}H NMR (600 MHz, DMSO-d_6):

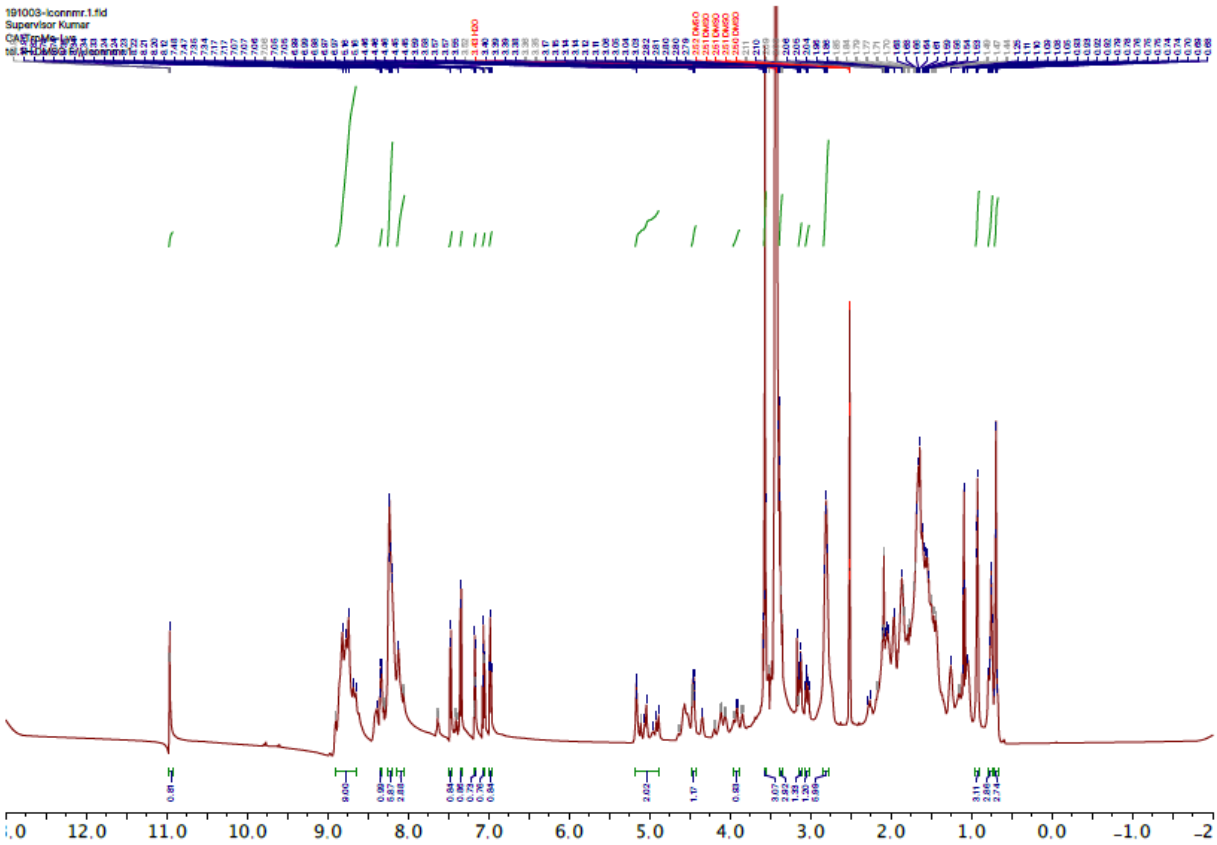


^{13}C NMR (150 MHz, DMSO-d_6):

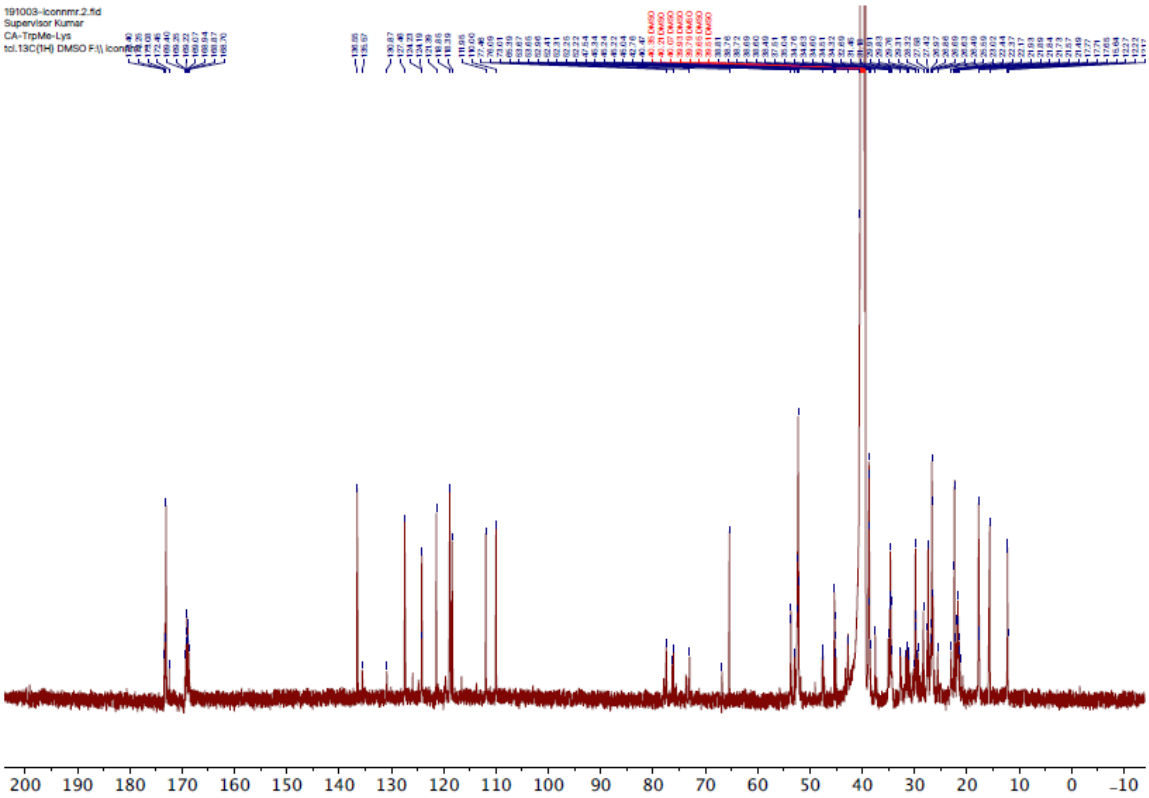


(5*S*,5'*S*,5"*S*)-6,6',6"-(((3*R*,5*S*,7*R*,8*R*,9*S*,10*S*,12*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthrene-3,7,12-triyl)tris(oxy))tris(6-oxohexane-1,5-diaminium) **(19d)**

^{1}H NMR (600 MHz, DMSO-d_6):

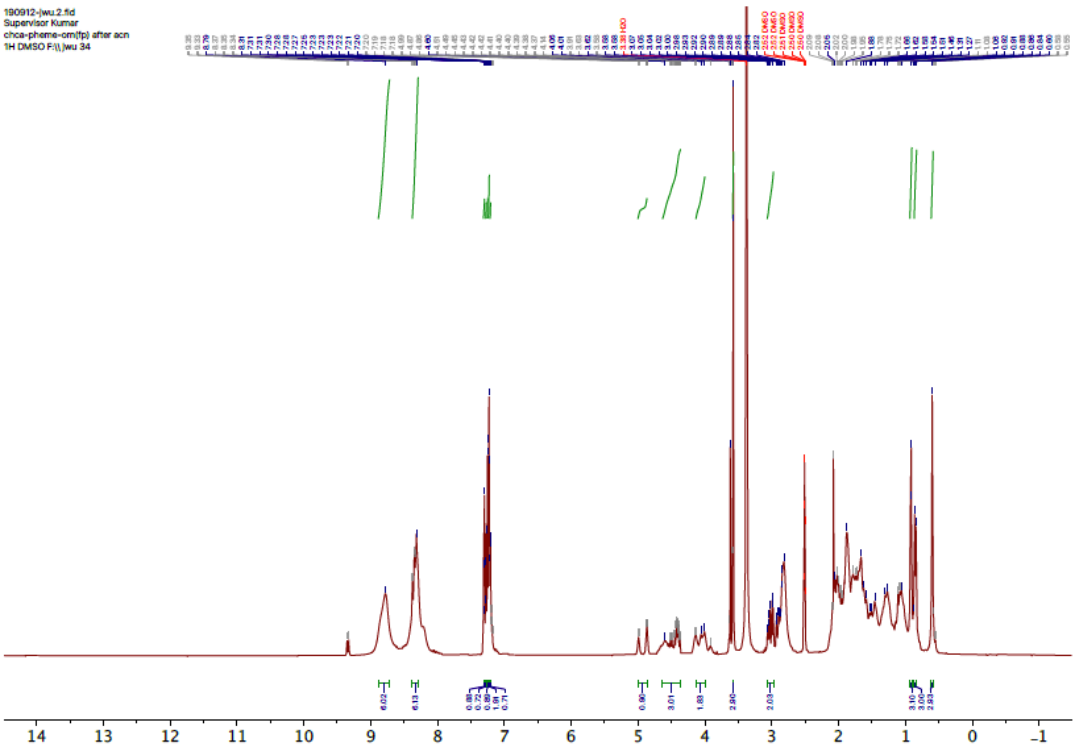


^{13}C NMR (150 MHz, DMSO-d_6):



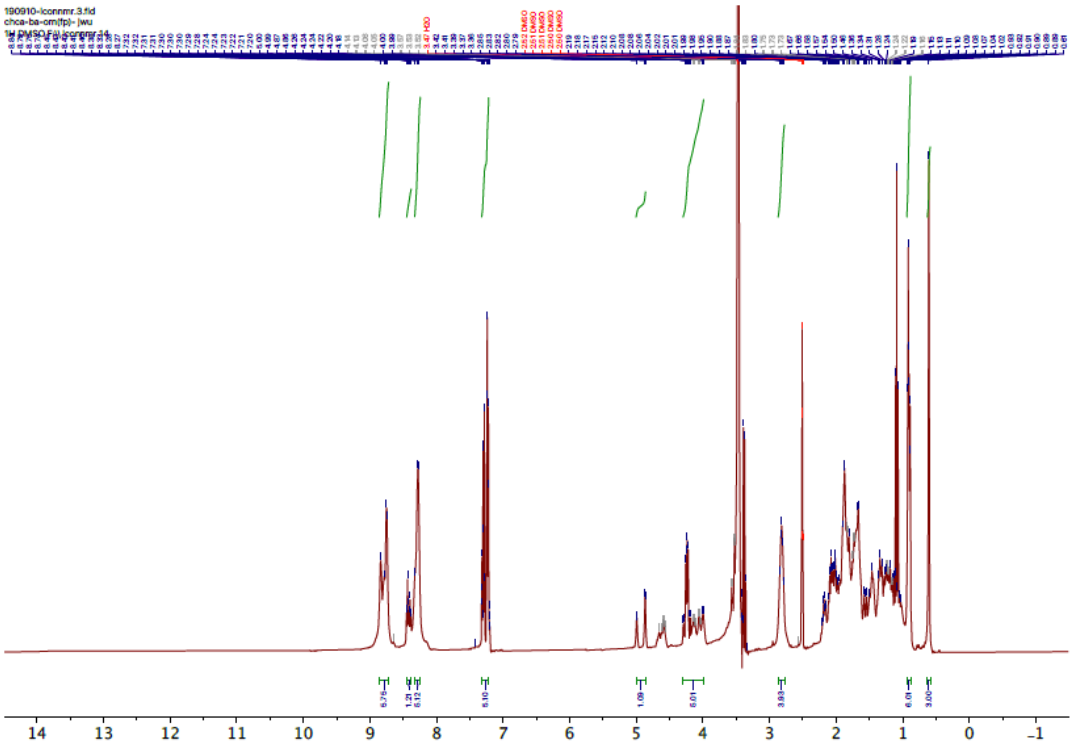
(4*S*,4'*S*)-5,5'-(((3*R*,5*S*,7*R*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-1-Methoxy-1-oxo-3-phenylpropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthrene-3,7-diyl)bis(oxy))bis(5-oxopentane-1,4-diaminium) **(20)**

^{1}H NMR (400 MHz, DMSO-d_6):



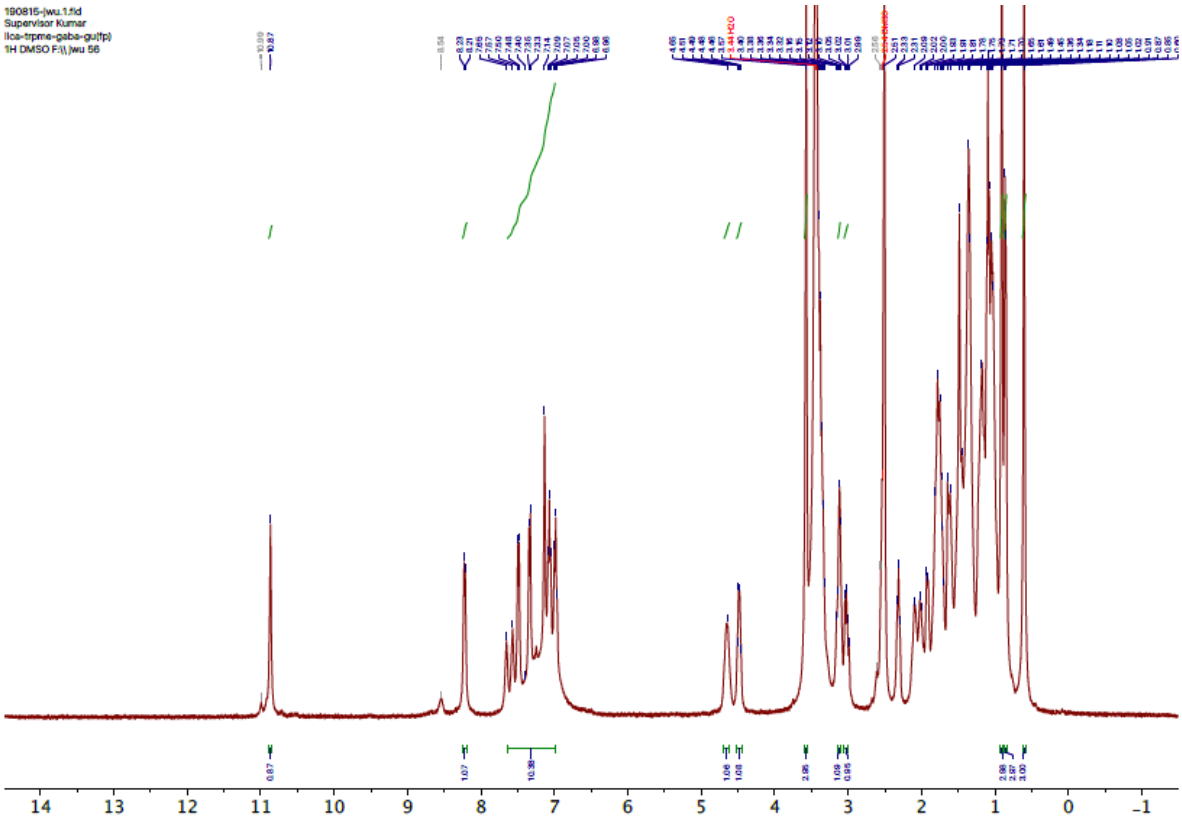
(4*S*,4'*S*)-5,5'-(((3*R*,5*S*,7*R*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(Benzylamino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthrene-3,7-diyl)bis(oxy))bis(5-oxopentane-1,4-diaminium) **(21)**

^{1}H NMR (400 MHz, DMSO-d_6):

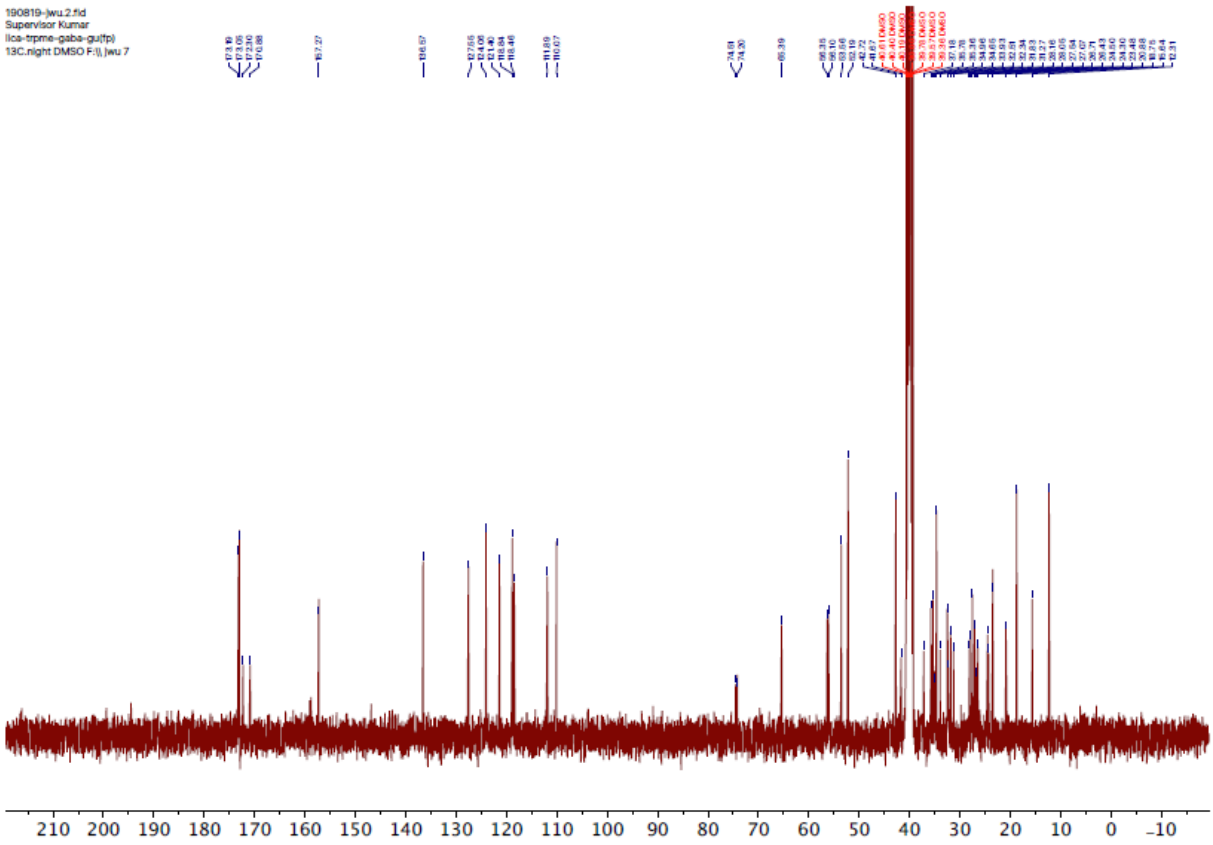


((4-(((3*R*,5*R*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl)oxy)-4-oxobutyl)amino)(amino)methaniminium **(23)**

^{1}H NMR (400 MHz, DMSO-d_6):

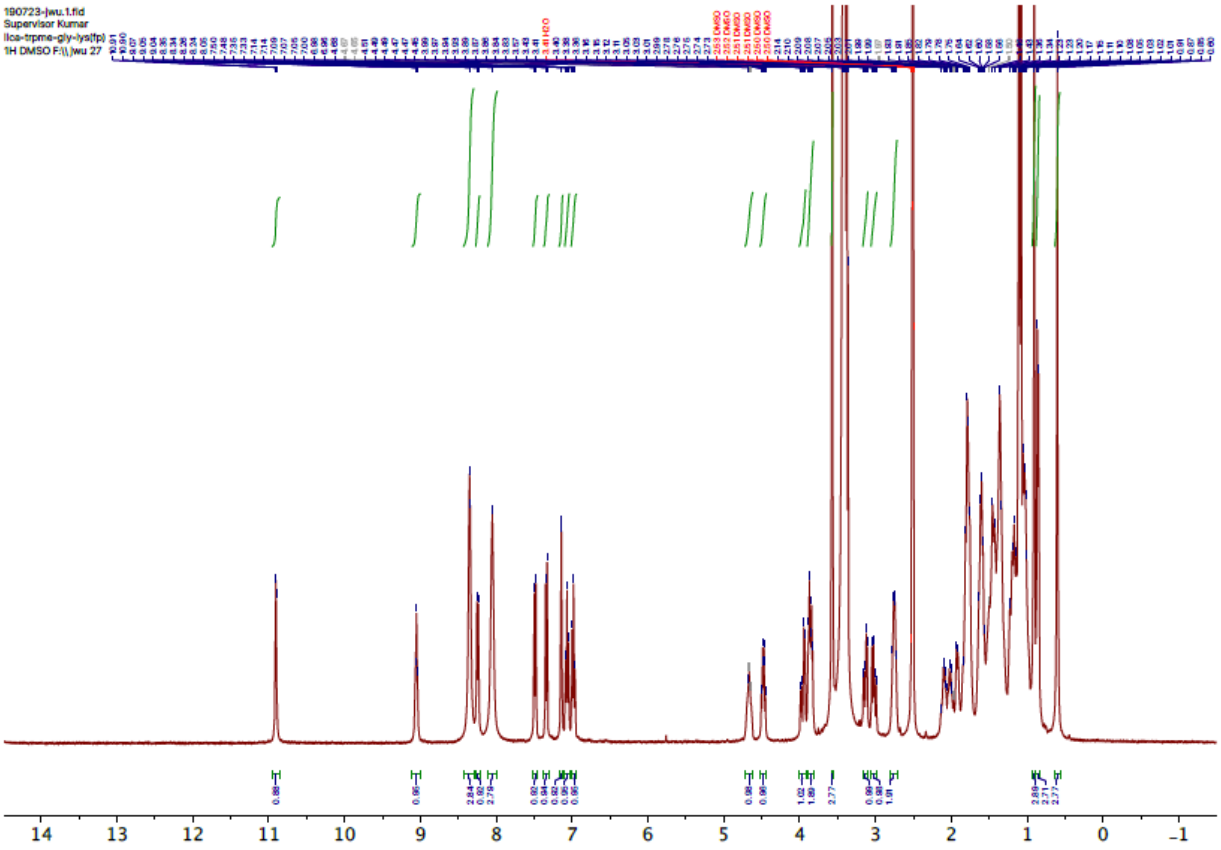


^{13}C NMR (75 MHz, DMSO-d_6):

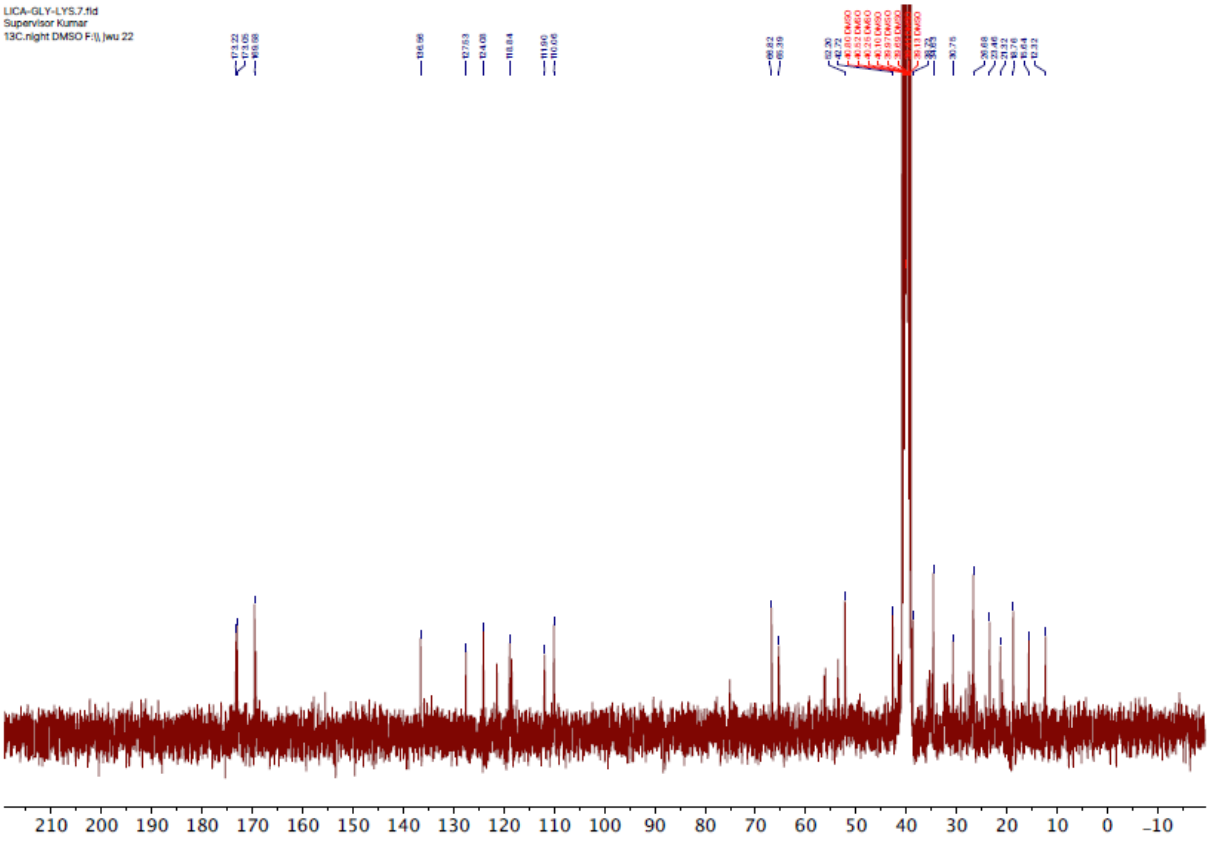


Methyl ((*R*)-4-((3*R*,5*R*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-3-((L-lysylglycyl)oxy)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthren-17-yl)pentanoyl)-L-tryptophanate **(25)**

^{1}H NMR (400 MHz, DMSO-d_6):

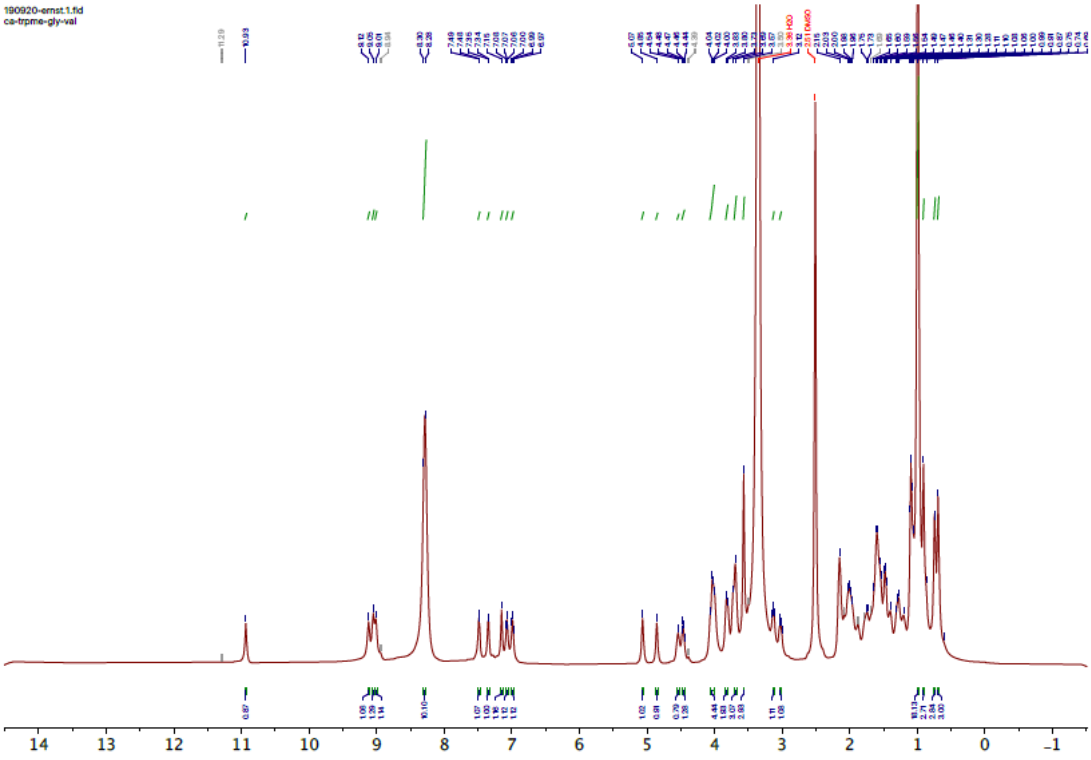


^{13}C NMR (75 MHz, DMSO-d_6):



1,1',1''-(((((3*R*,5*S*,7*R*,8*R*,9*S*,10*S*,12*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthrene-3,7,12-triyl)tris(oxy))tris(2-oxoethane-2,1-diyl))tris(azanediyl))tris(3-methyl-1-oxobutan-2-aminium) **(27)**

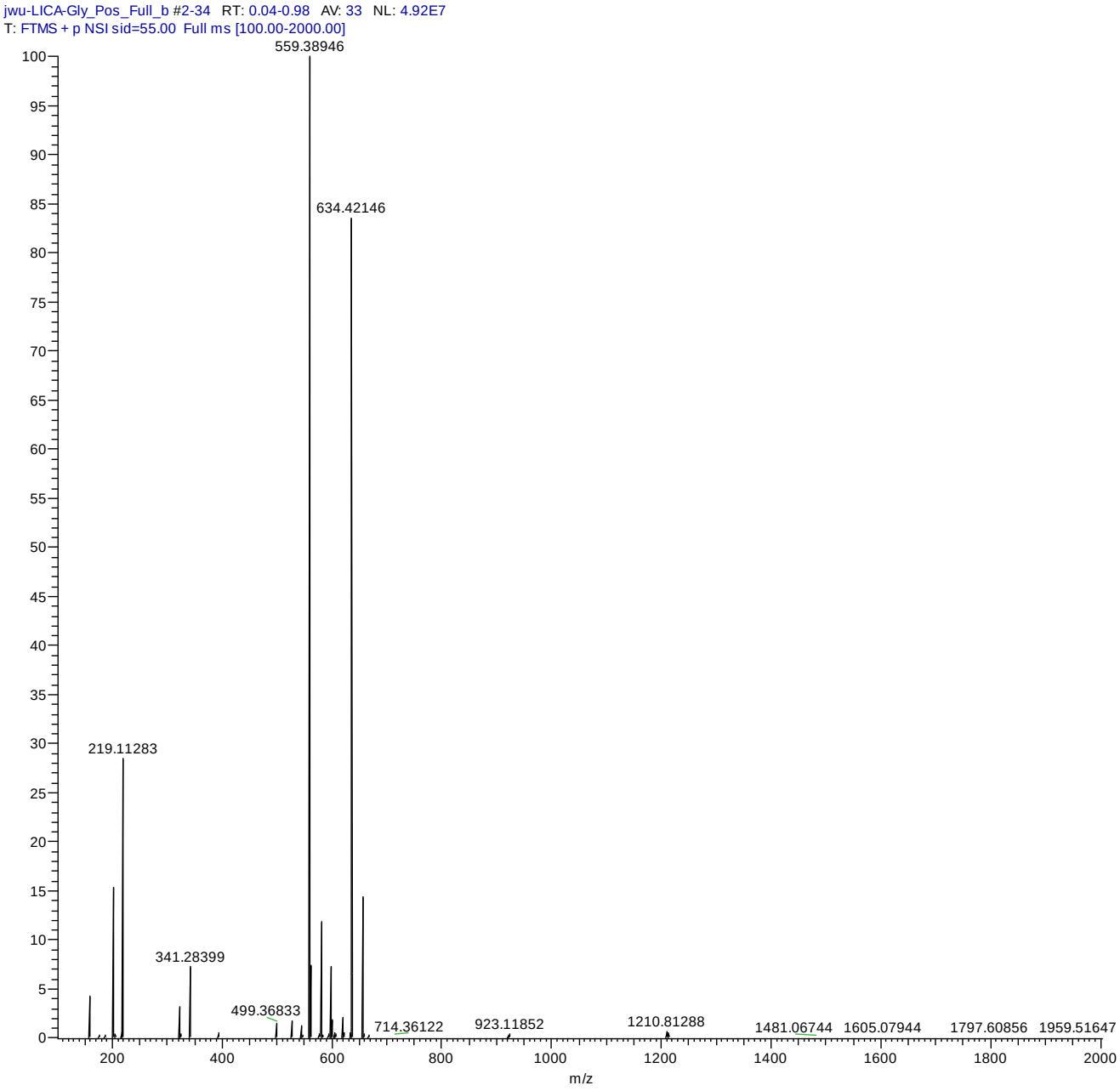
^{1}H NMR (600 MHz, DMSO-d_6):



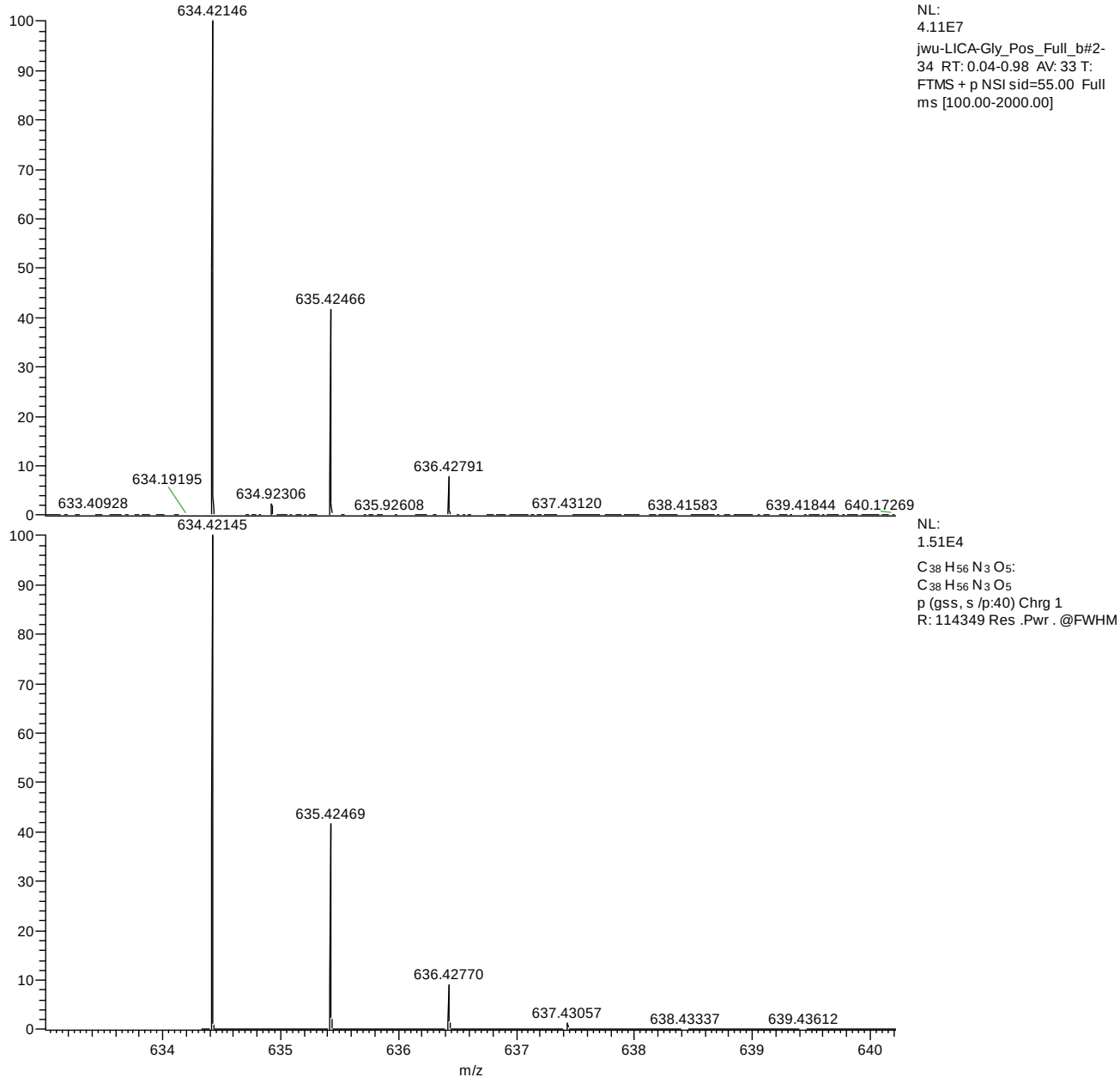
High resolution mass spectra (HRMS) of synthesised compounds

2-(((3*R*,5*R*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl)oxy)-2-oxoethan-1-aminium **(16a)**

Full spectrum

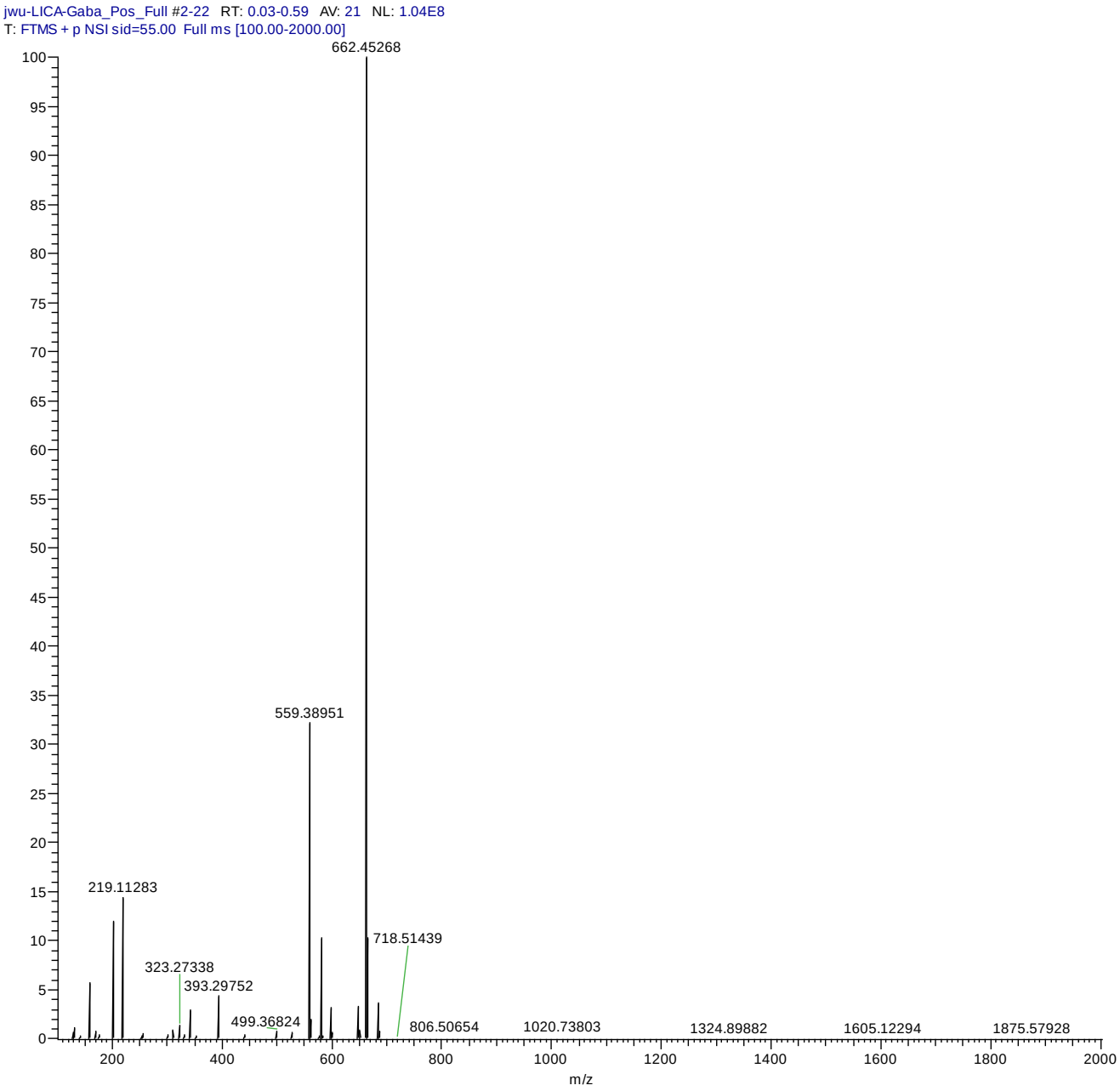


Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)

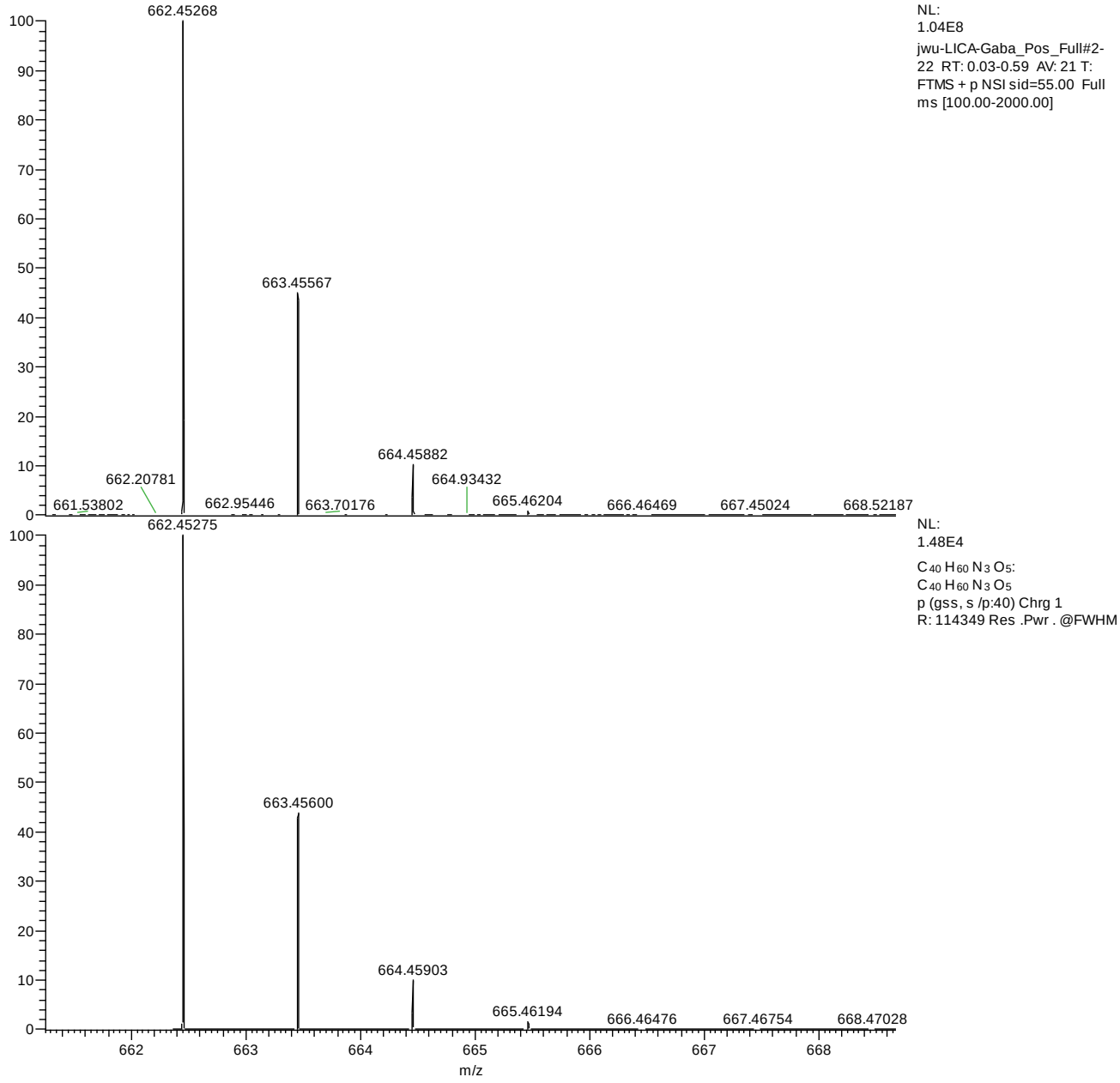


4-(((3*R*,5*R*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl)oxy)-4-oxobutan-1-aminium **(16b)**

Full spectrum

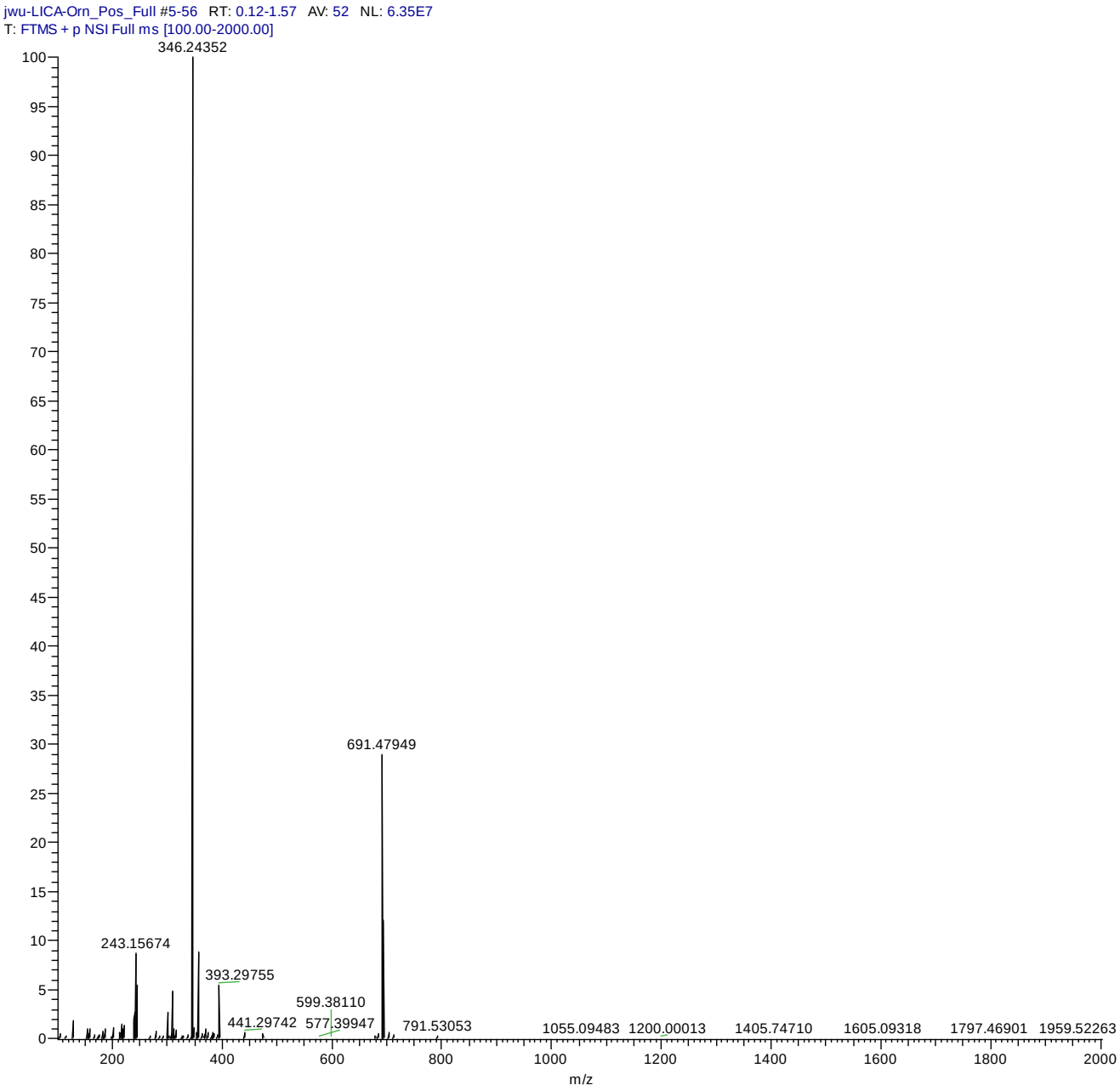


Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)

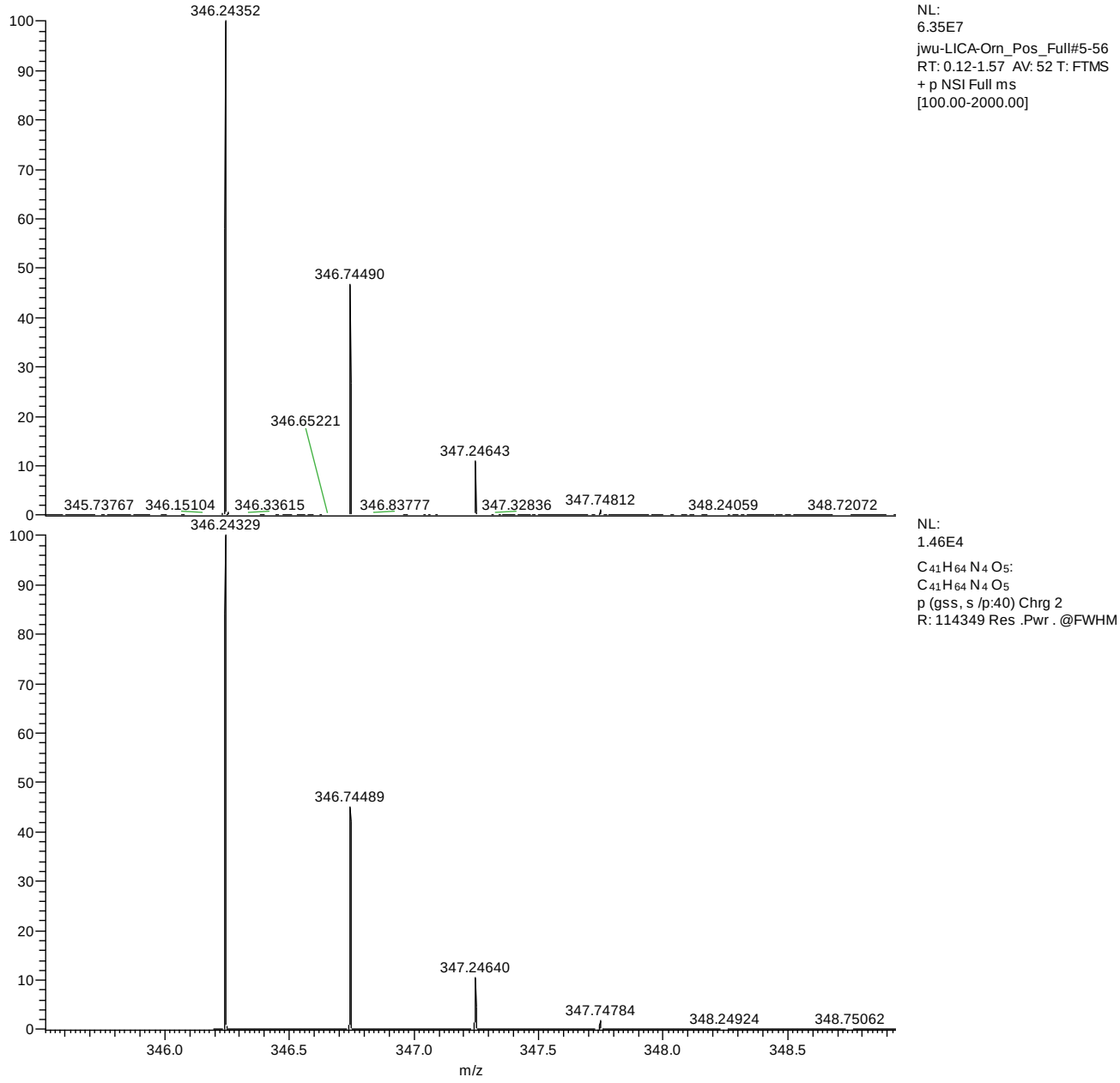


(*S*)-5-(((3*R*,5*R*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl)oxy)-5-oxopentane-1,4-diaminium **(16c)**

Full spectrum

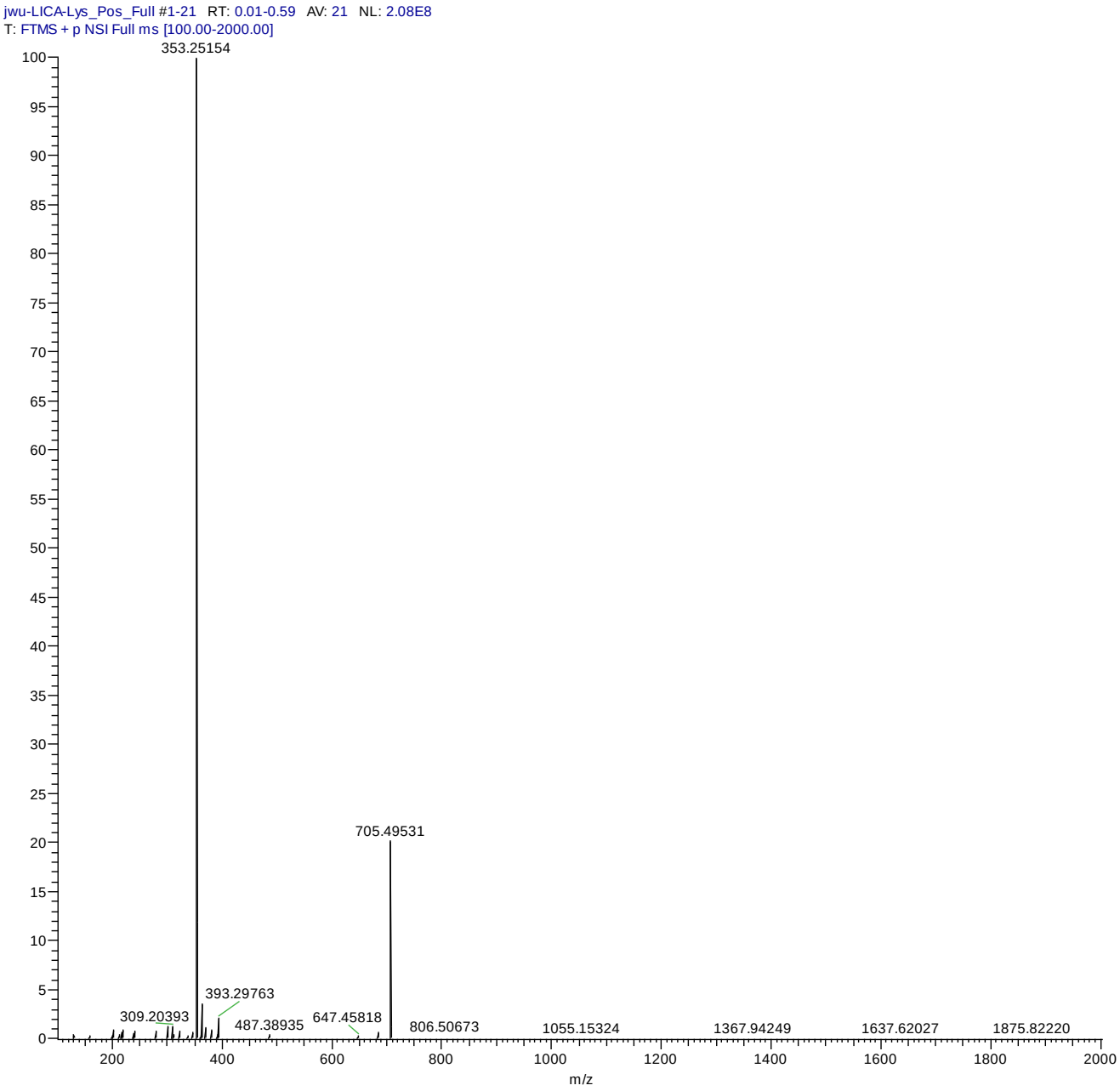


Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)

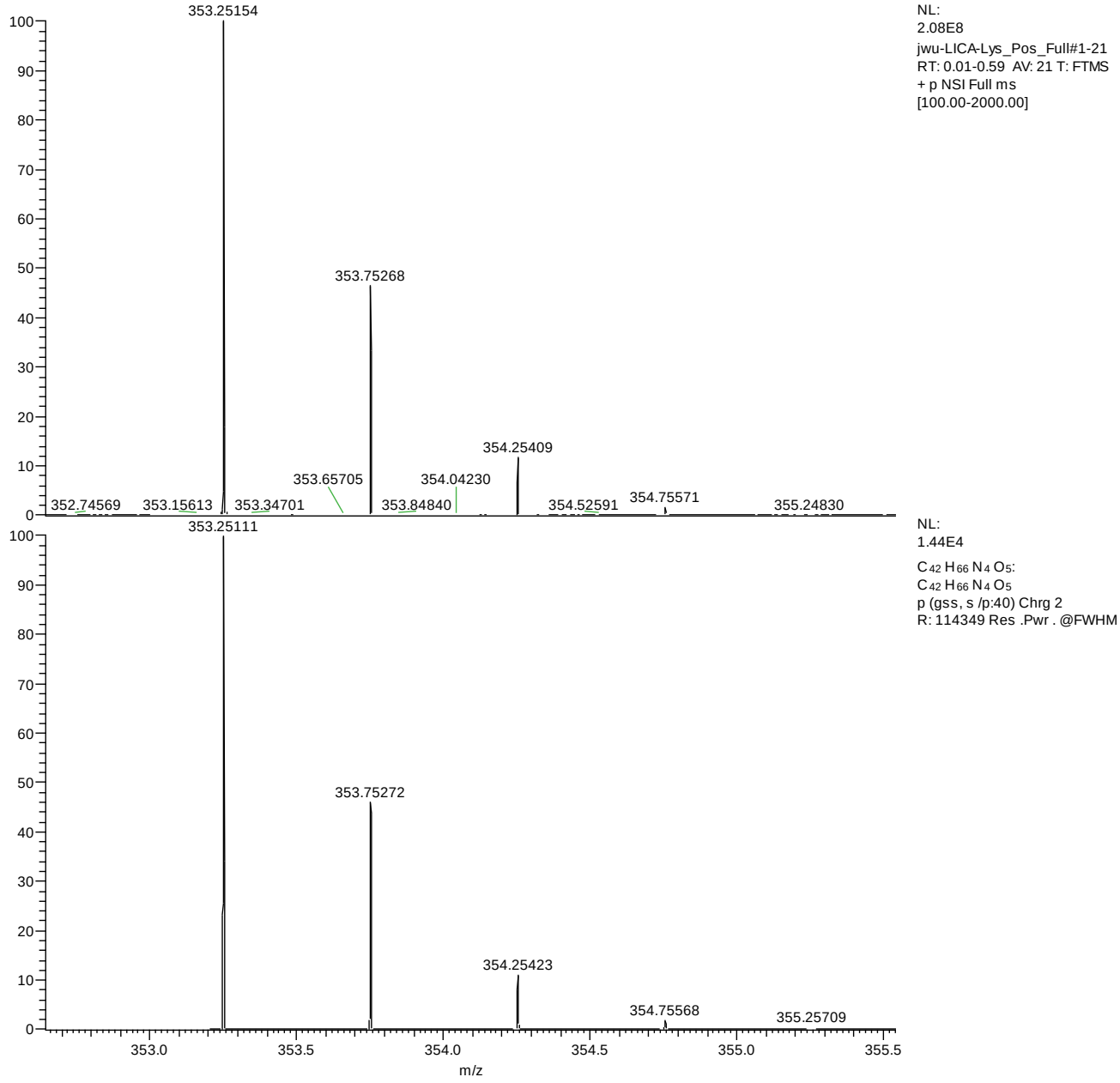


(*S*)-6-(((3*R*,5*R*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl)oxy)-6-oxohexane-1,5-diaminium **(16d)**

Full spectrum

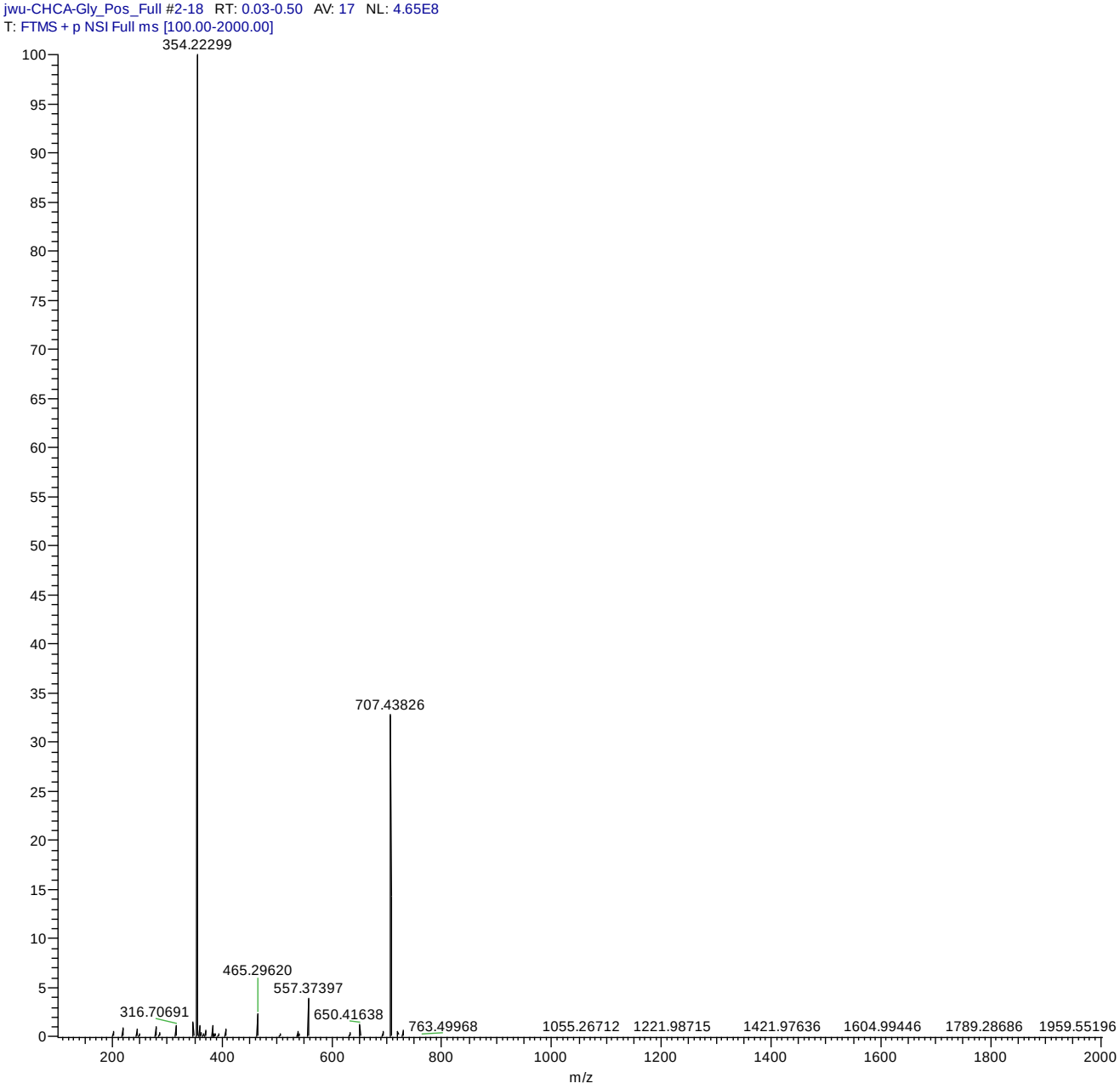


Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)

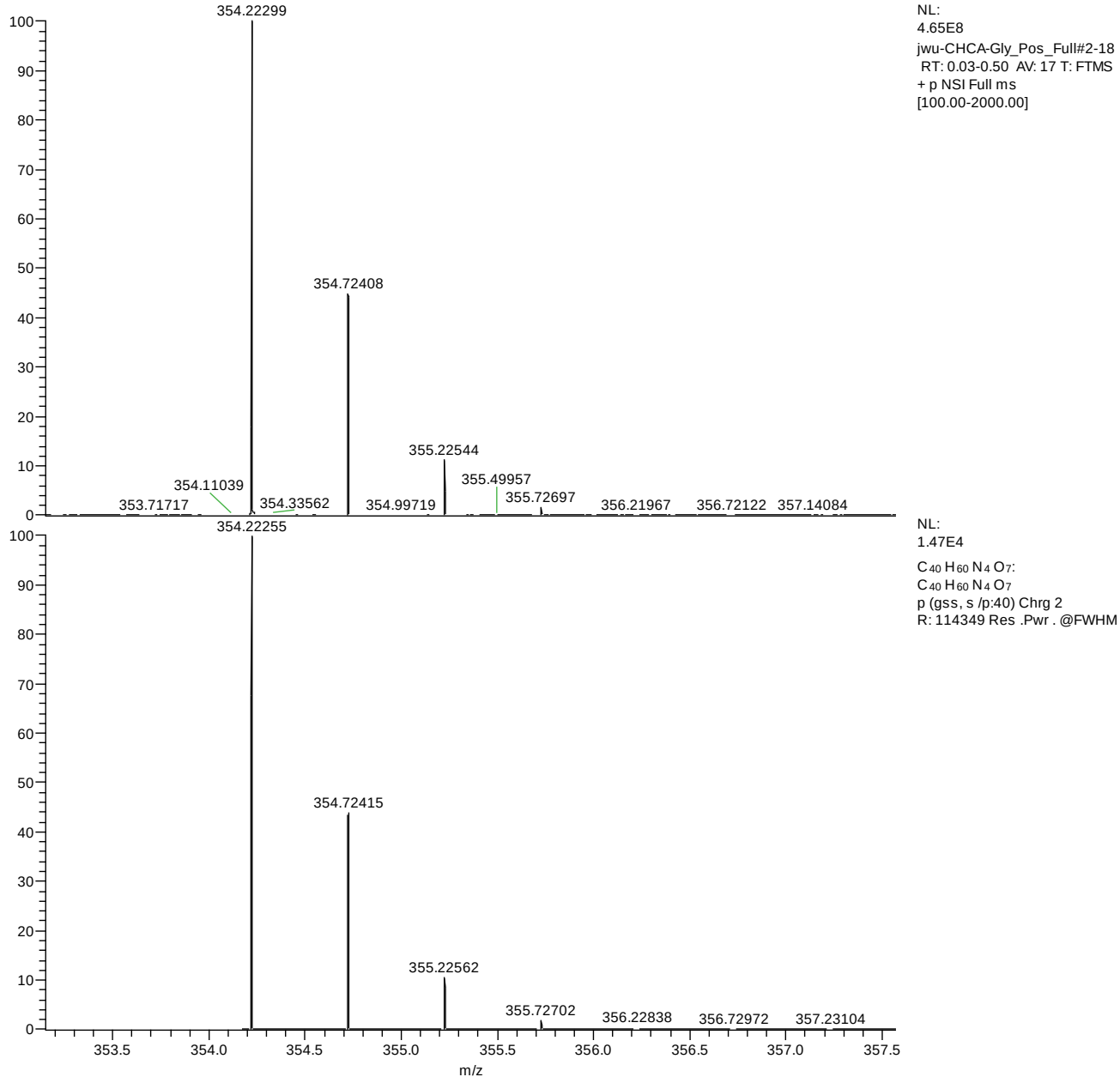


2,2'-(((3*R*,5*S*,7*R*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthrene-3,7-diyl)bis(oxy))bis(2-oxoethan-1-aminium) **(17a)**

Full spectrum

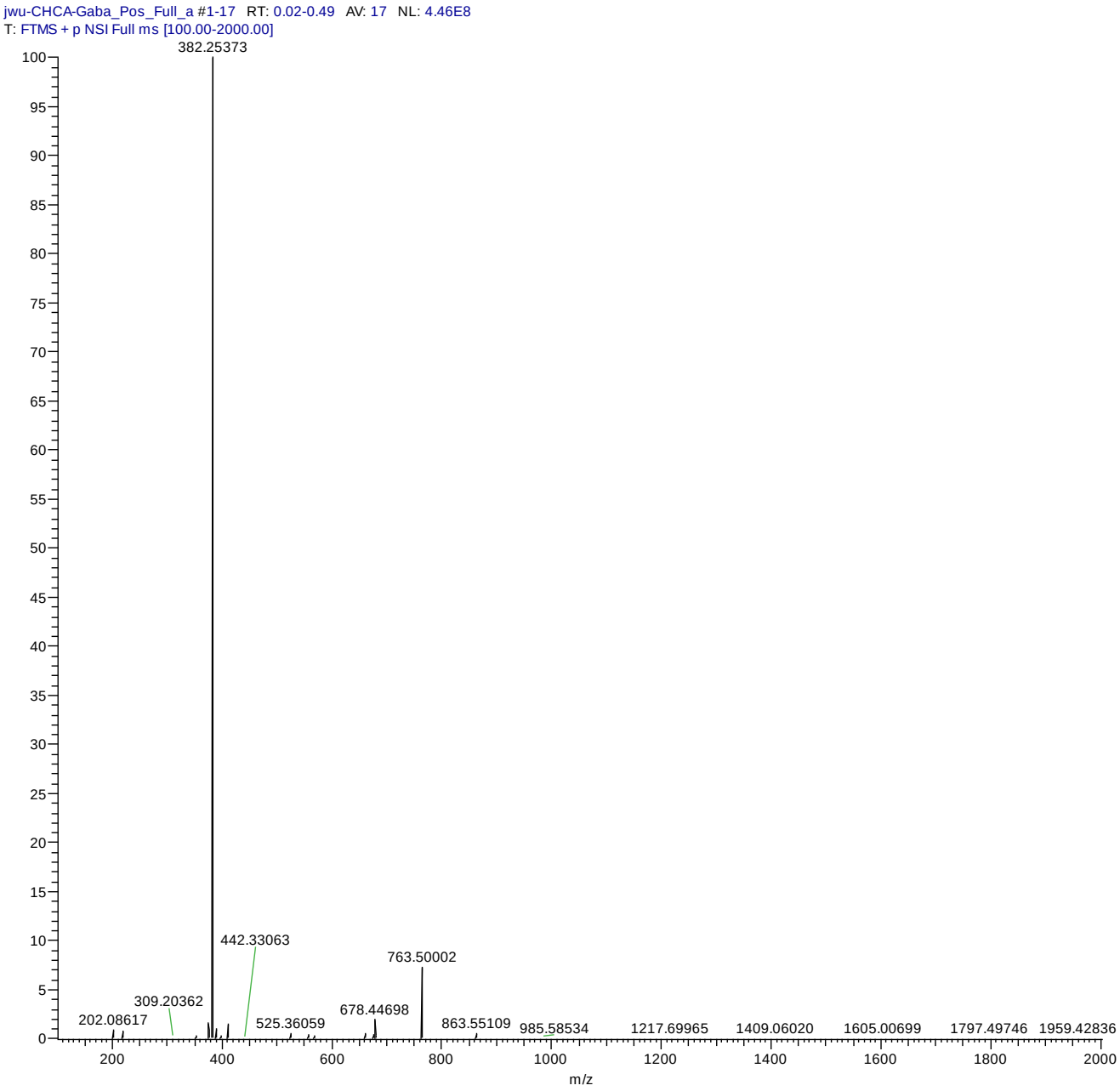


Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)

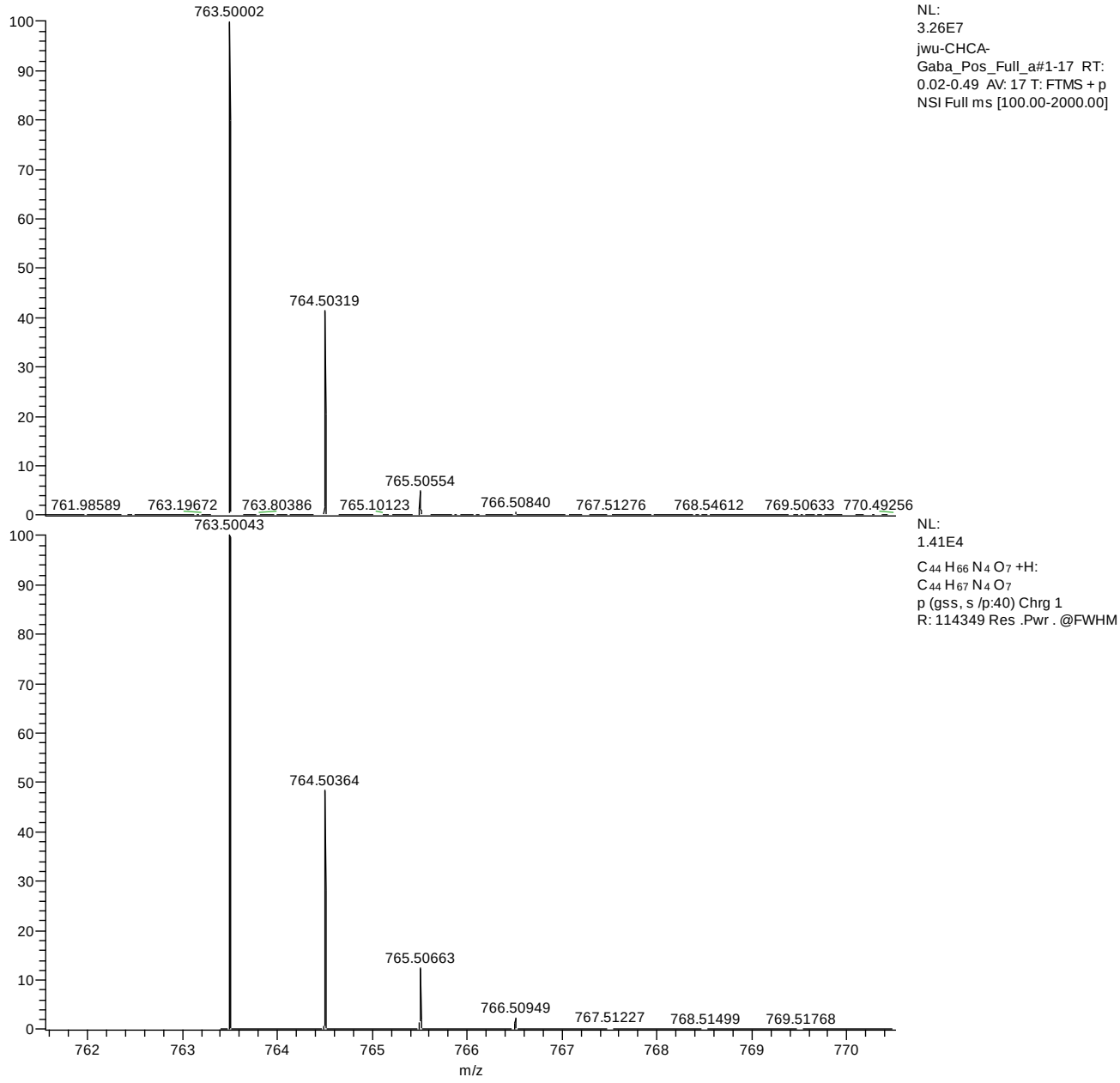


4,4'-(((3*R*,5*S*,7*R*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthrene-3,7-diyl)bis(oxy))bis(4-oxobutan-1-aminium) **(17b)**

Full spectrum

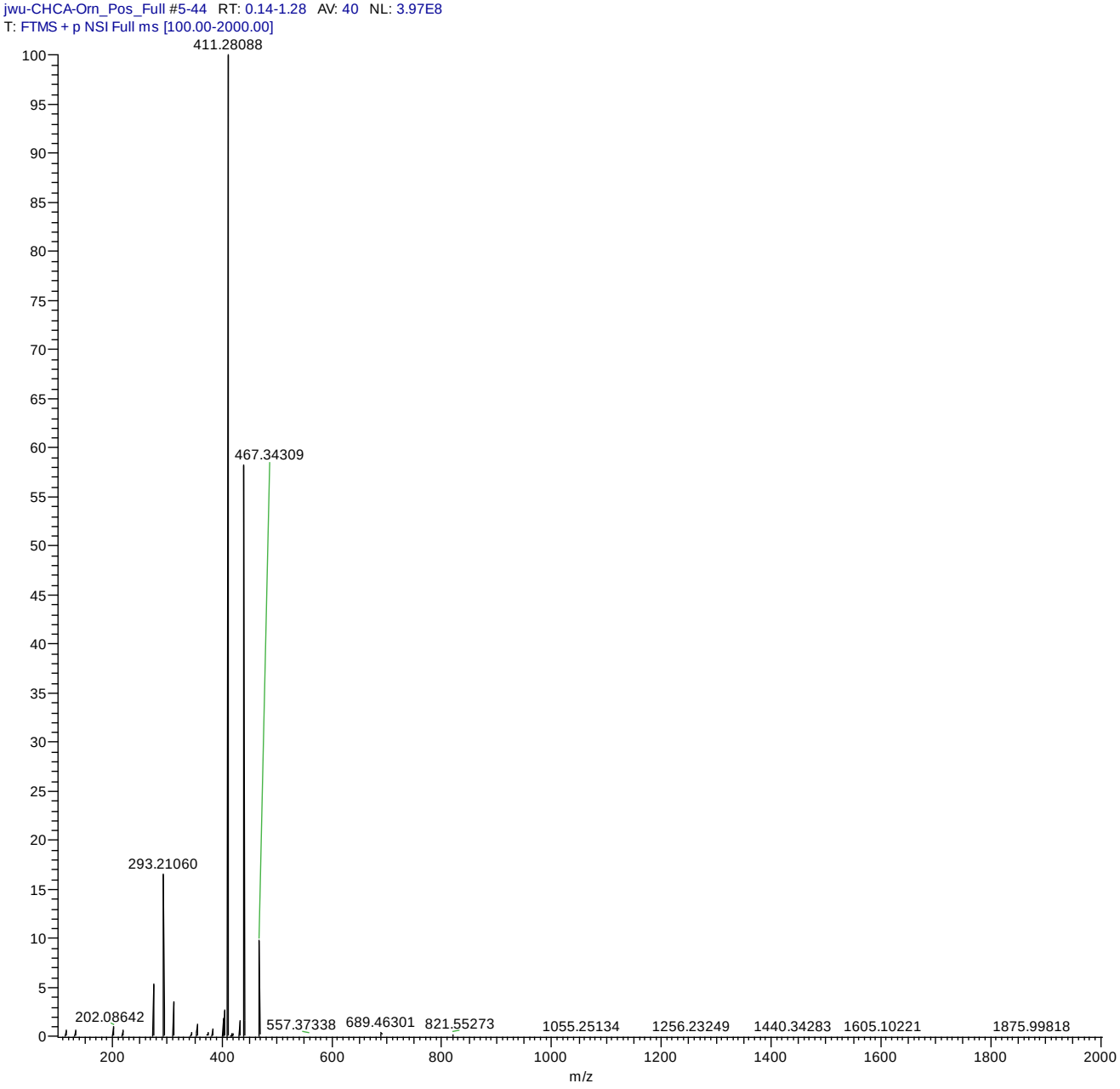


Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)

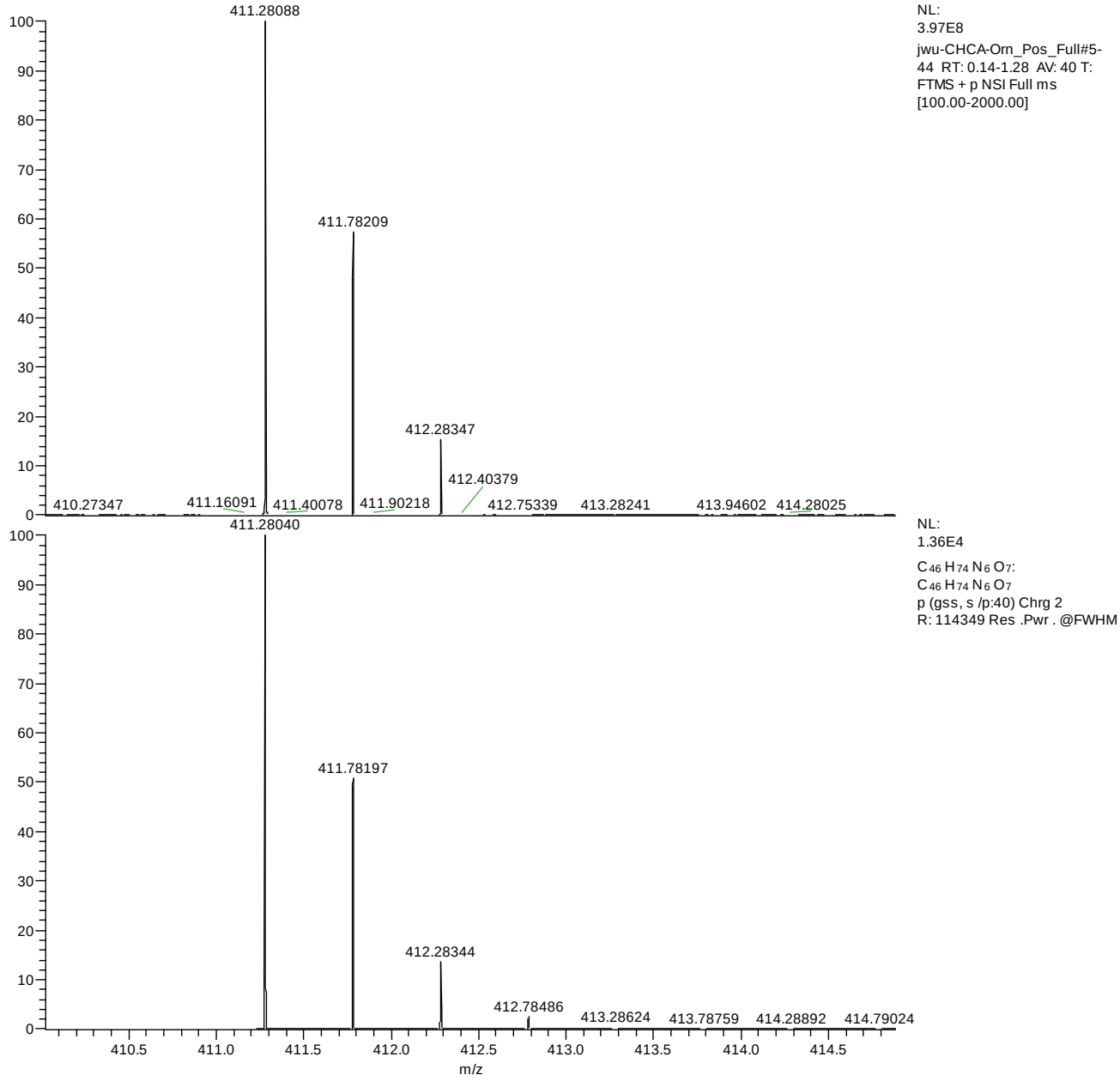


(4*S*,4'*S*)-5,5'-(((3*R*,5*S*,7*R*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthrene-3,7-diyl)bis(oxy))bis(5-oxopentane-1,4-diaminium) **(17c)**

Full spectrum

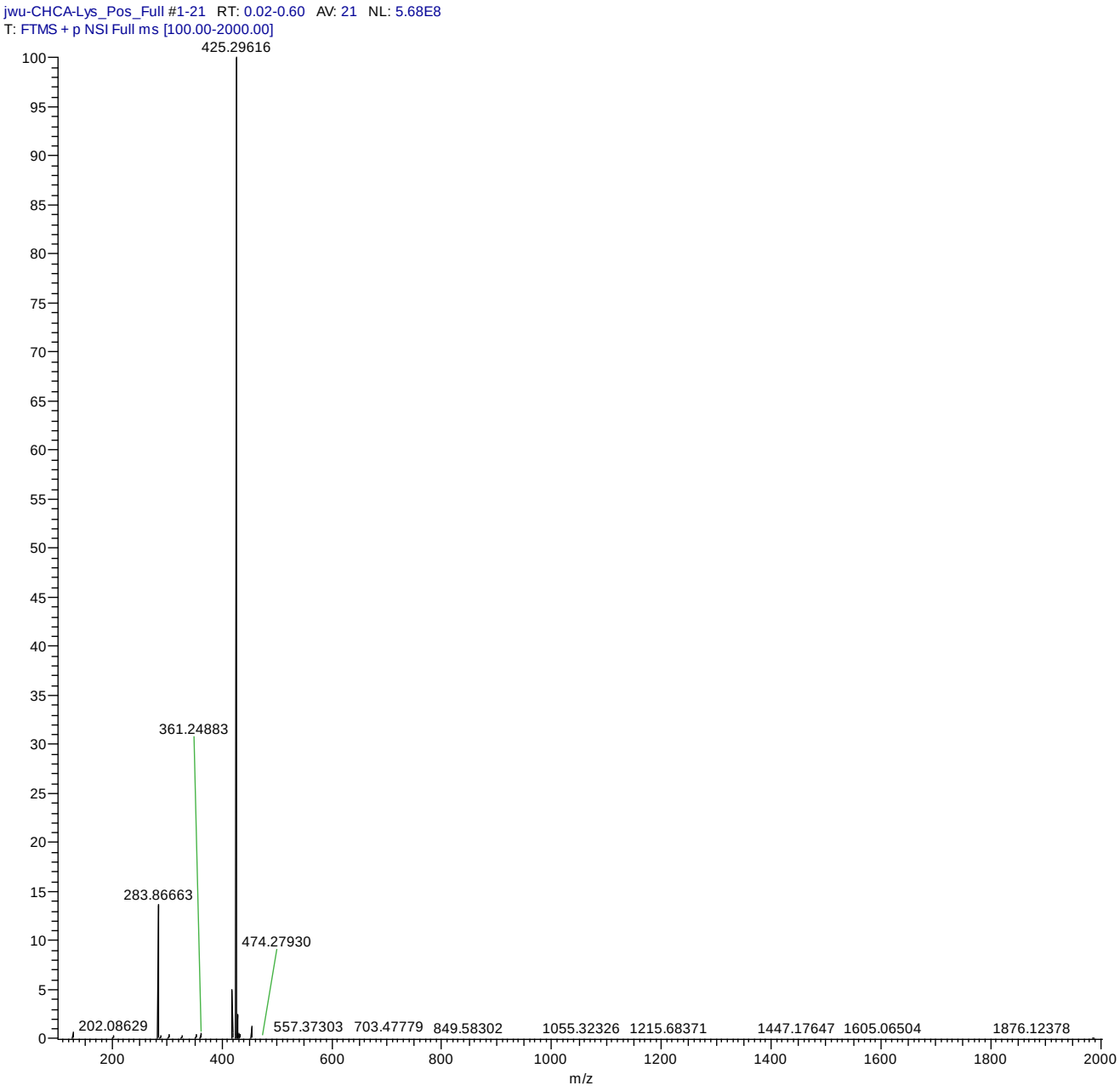


Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)

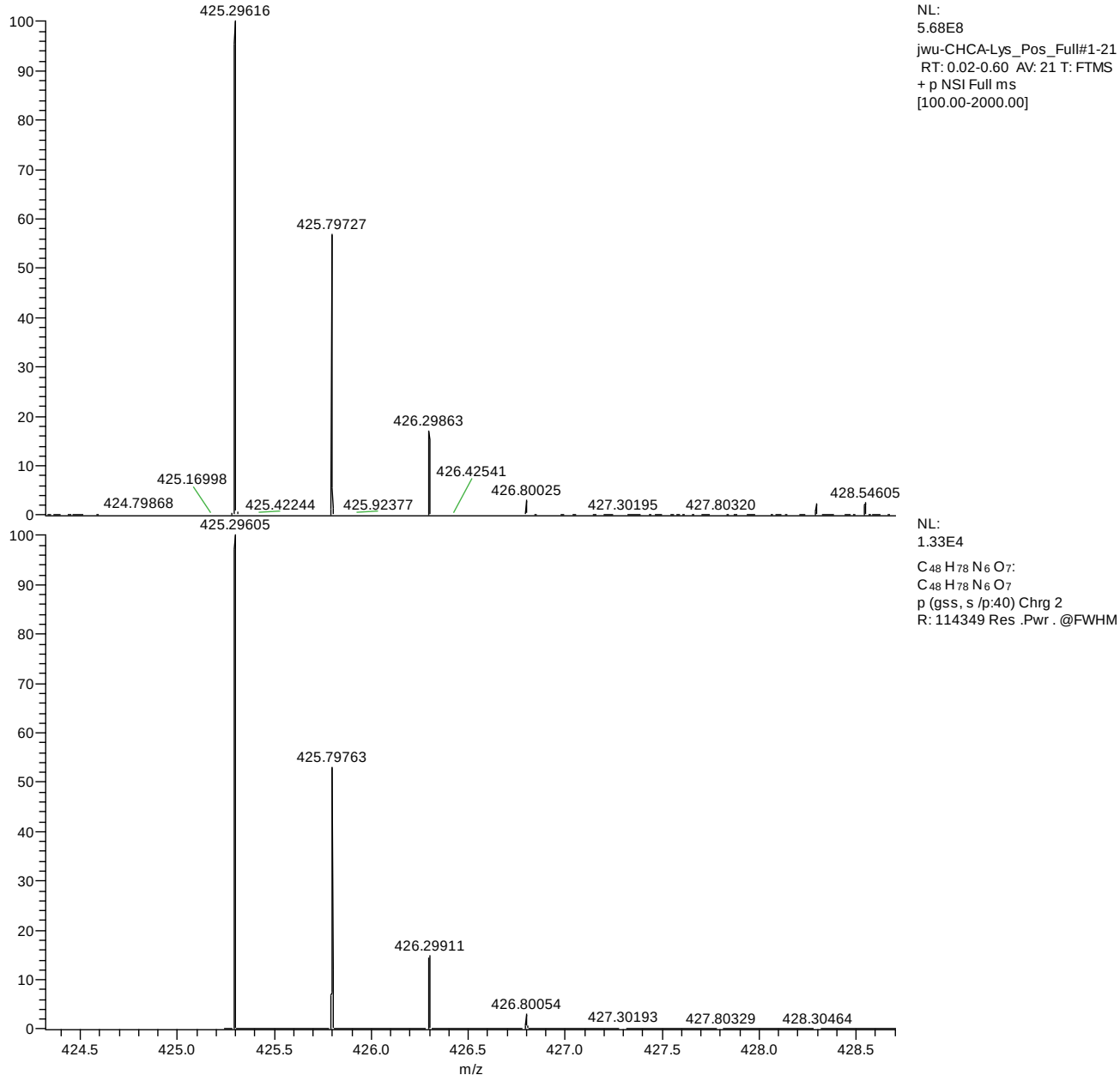


(5*S*,5'*S*)-6,6'-(((3*R*,5*S*,7*R*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthrene-3,7-diyl)bis(oxy))bis(6-oxohexane-1,5-diaminium) **(17d)**

Full spectrum

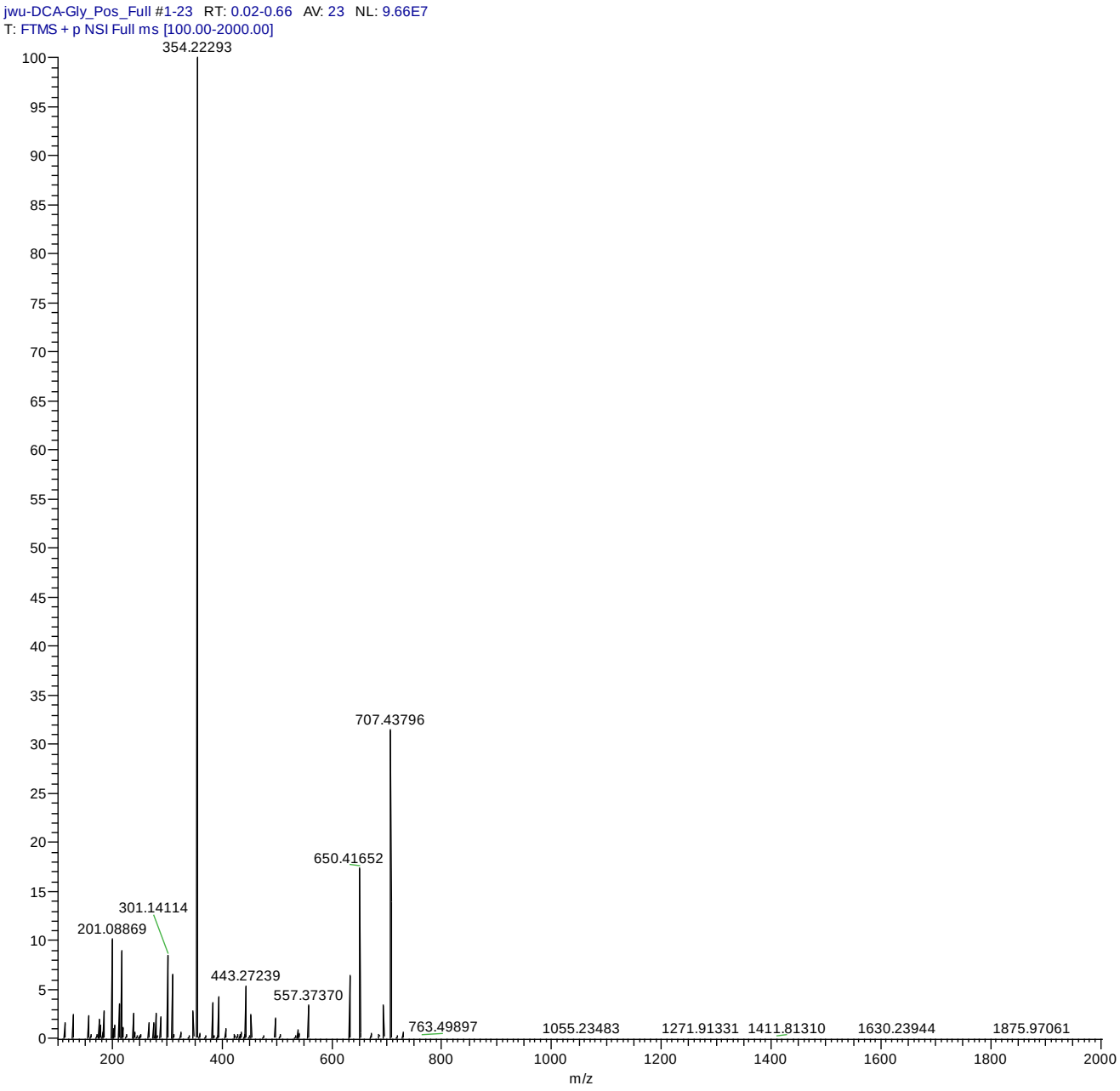


Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)

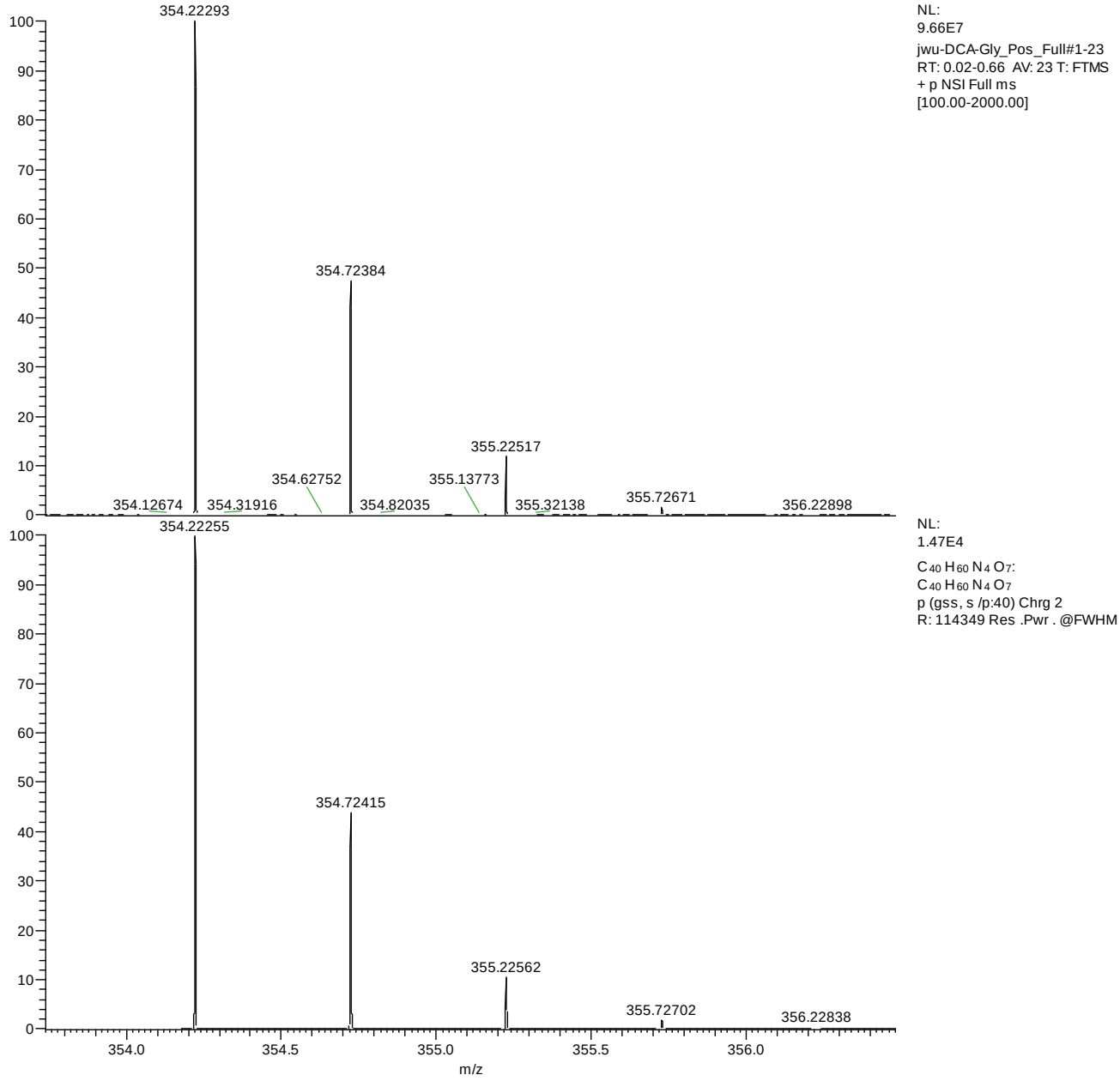


2,2'-(((3*R*,5*R*,8*R*,9*S*,10*S*,12*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthrene-3,12-diyl)bis(oxy))bis(2-oxoethan-1-aminium) **(18a)**

Full spectrum

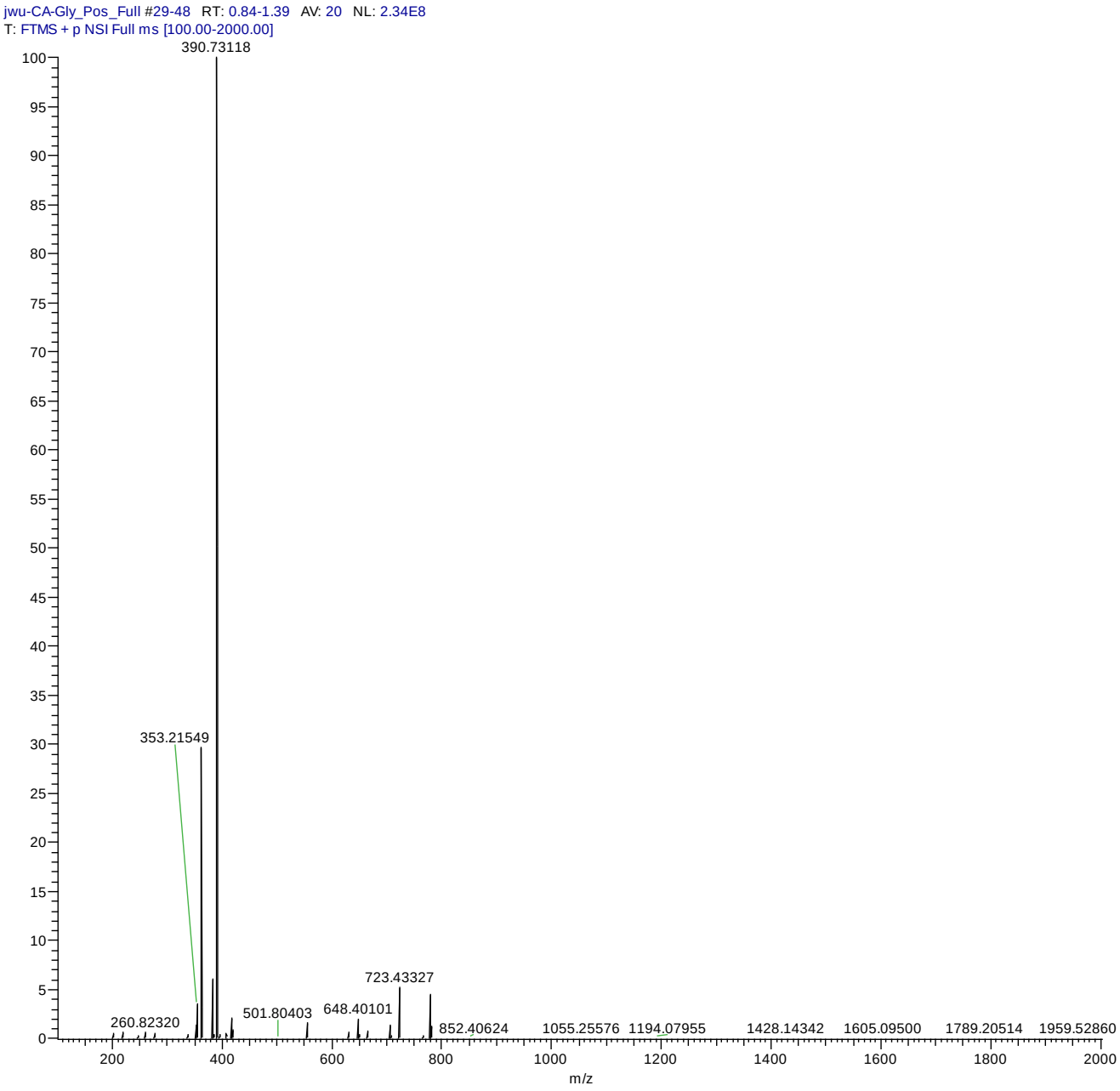


Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)

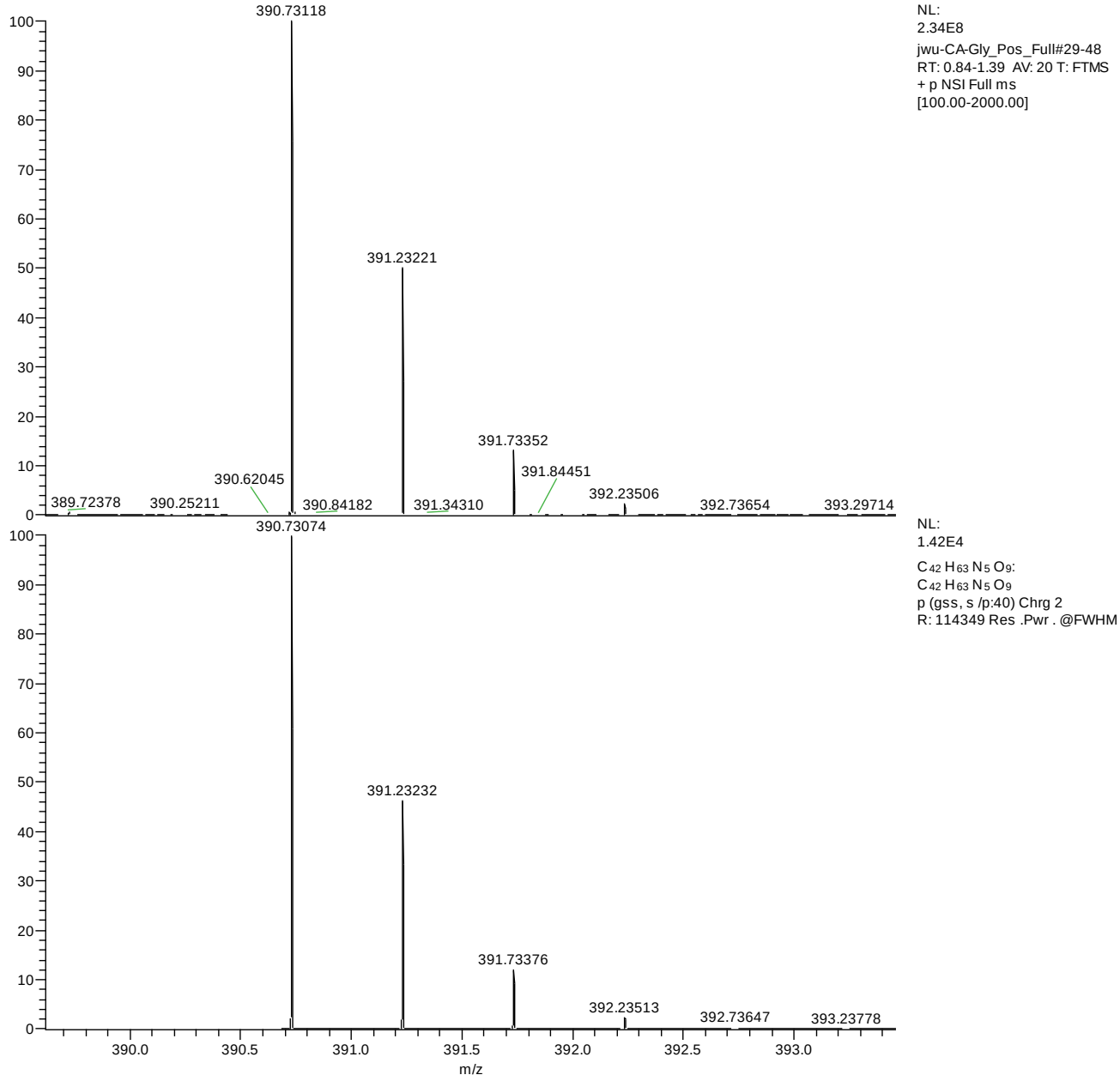


2,2'-(((3*R*,5*S*,7*R*,8*R*,9*S*,10*S*,12*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-3-(2-aminoacetoxy)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthrene-7,12-diyl)bis(oxy))bis(2-oxoethan-1-aminium) **(19a)**

Full spectrum

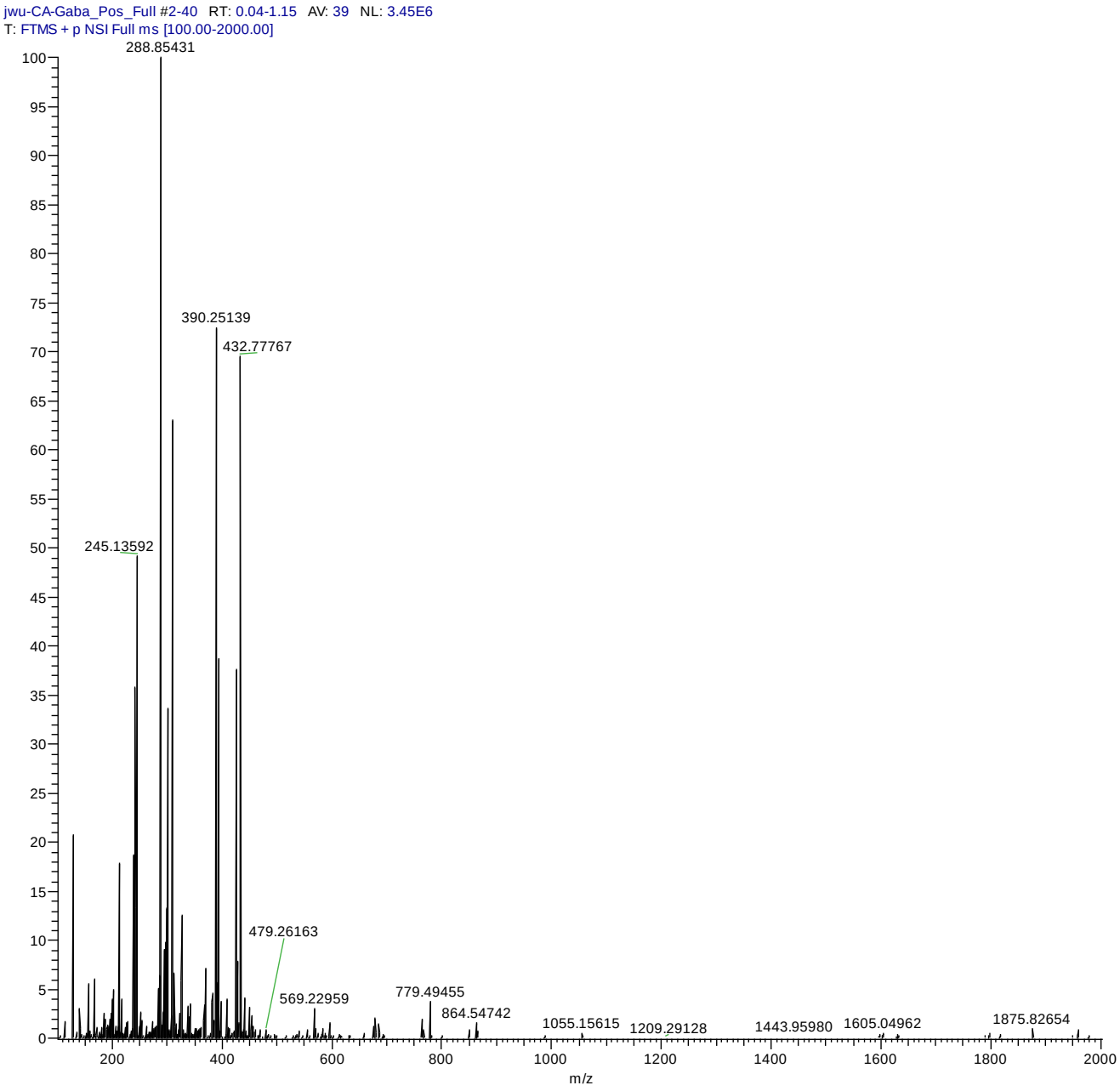


Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)

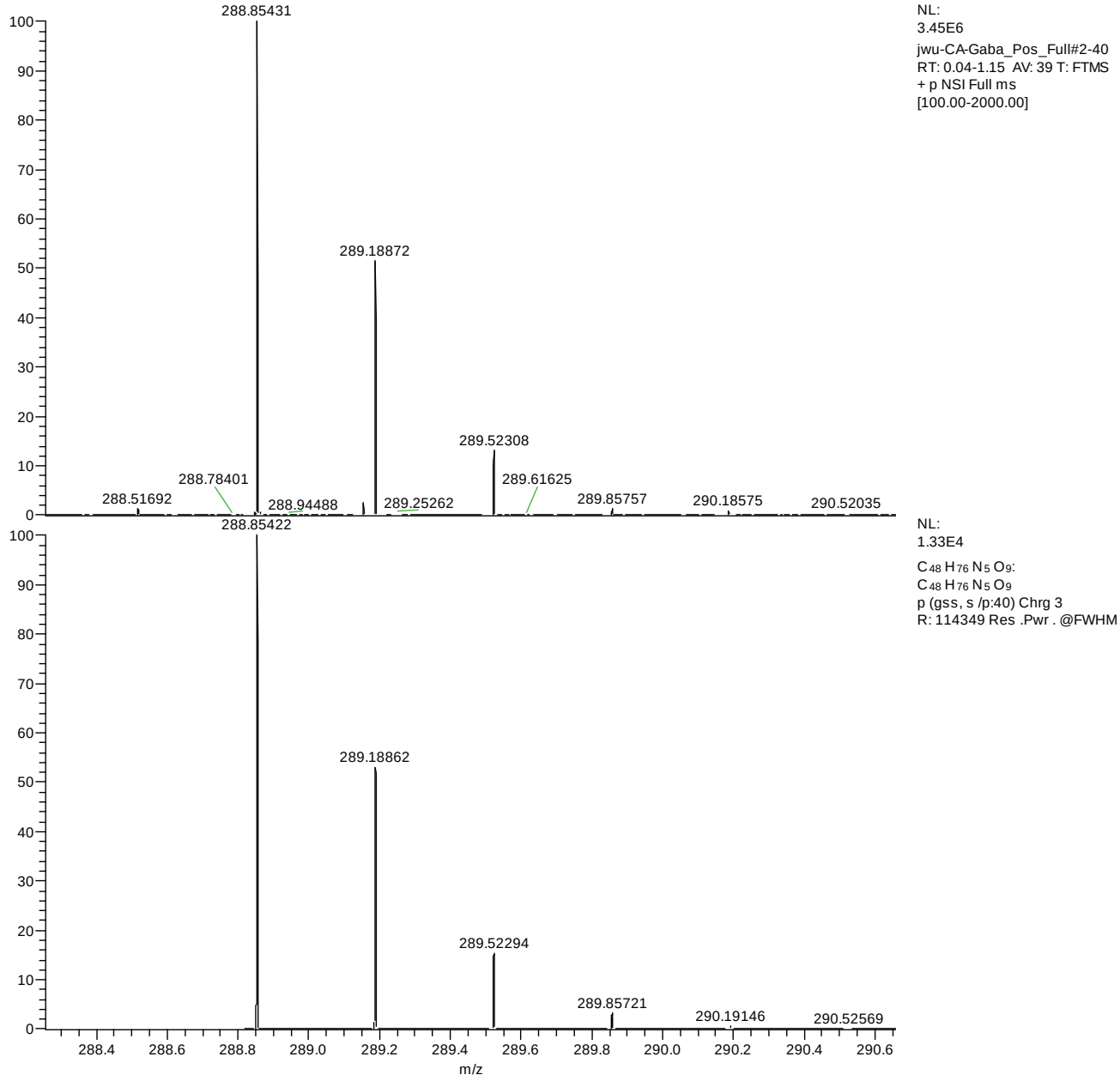


4,4',4"-(((3*R*,5*S*,7*R*,8*R*,9*S*,10*S*,12*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthrene-3,7,12-triyl)tris(oxy))tris(4-oxobutan-1-aminium) **(19b)**

Full spectrum

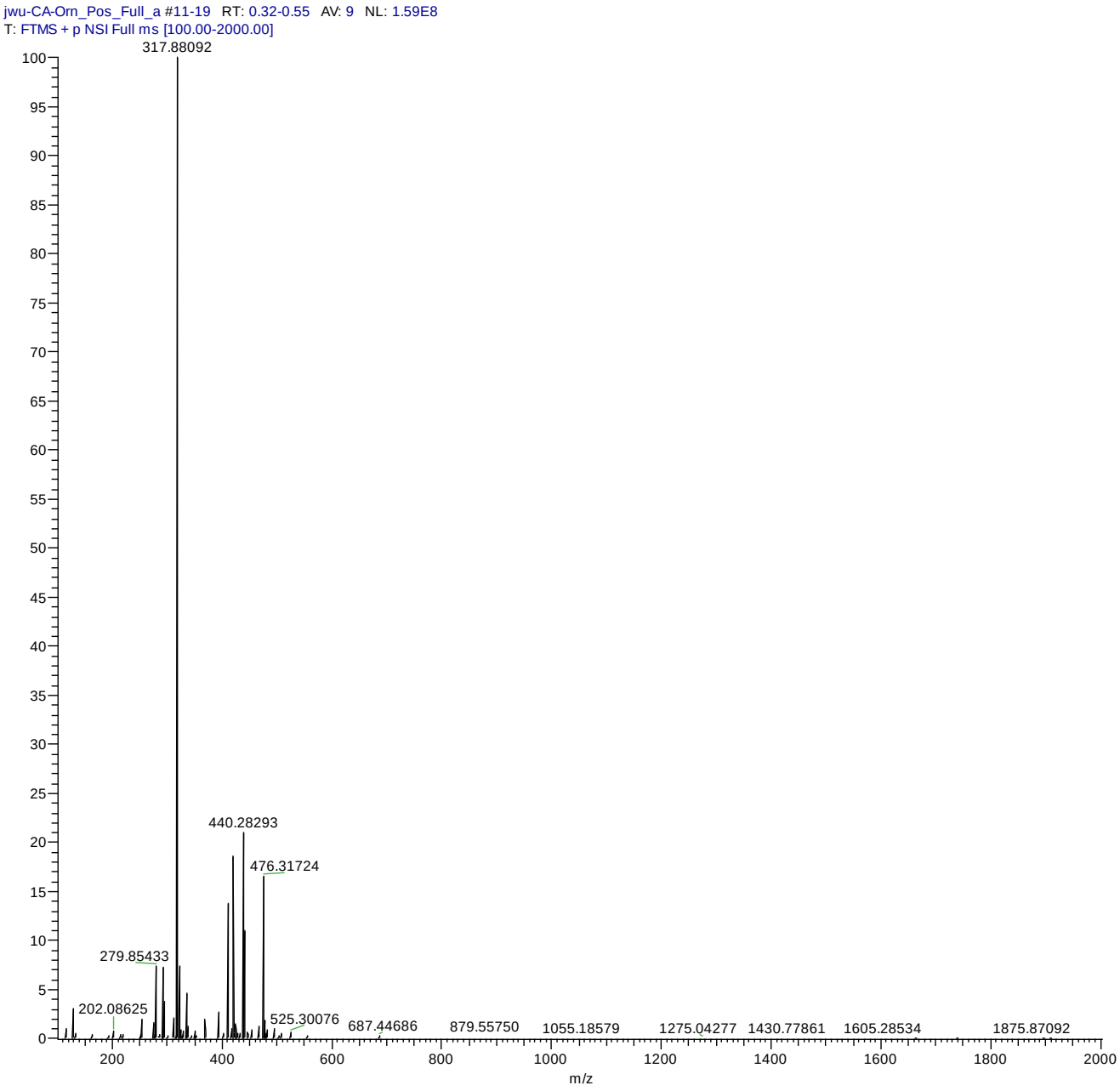


Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)

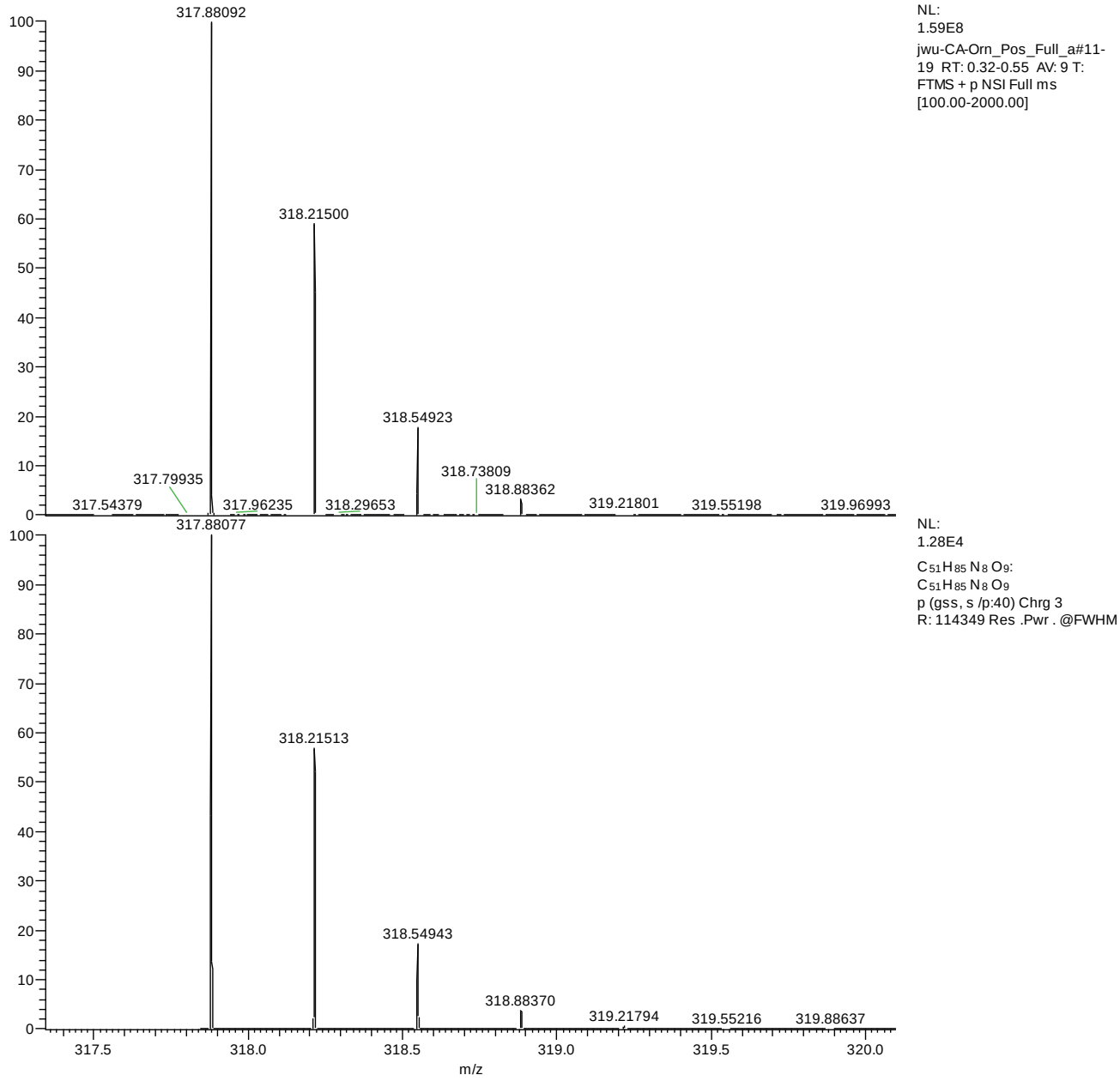


(4*S*,4'*S*,4"*S*)-5,5',5"-(((3*R*,5*S*,7*R*,8*R*,9*S*,10*S*,12*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthrene-3,7,12-triyl)tris(oxy))tris(5-oxopentane-1,4-diaminium) **(19c)**

Full spectrum

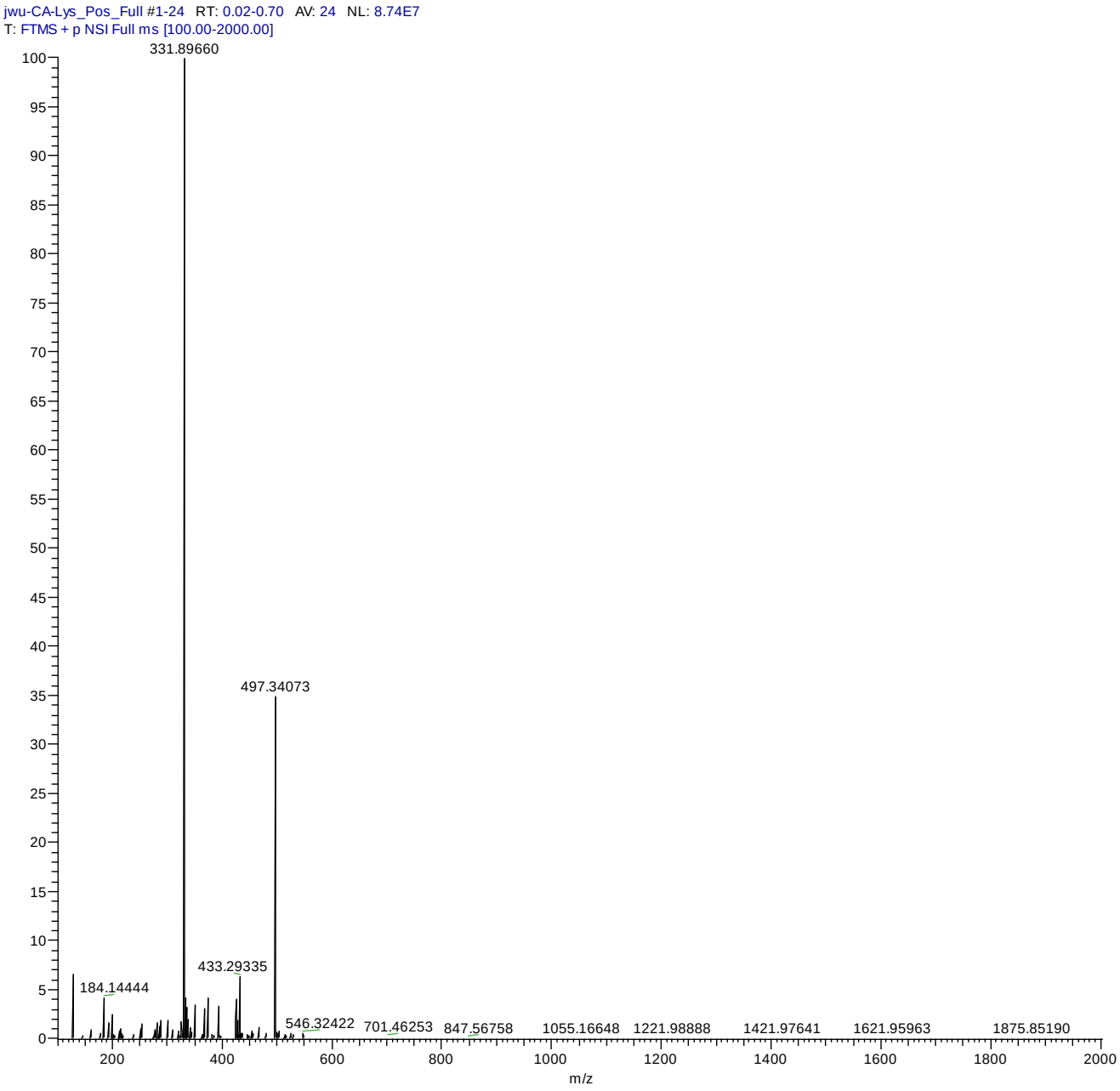


Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)

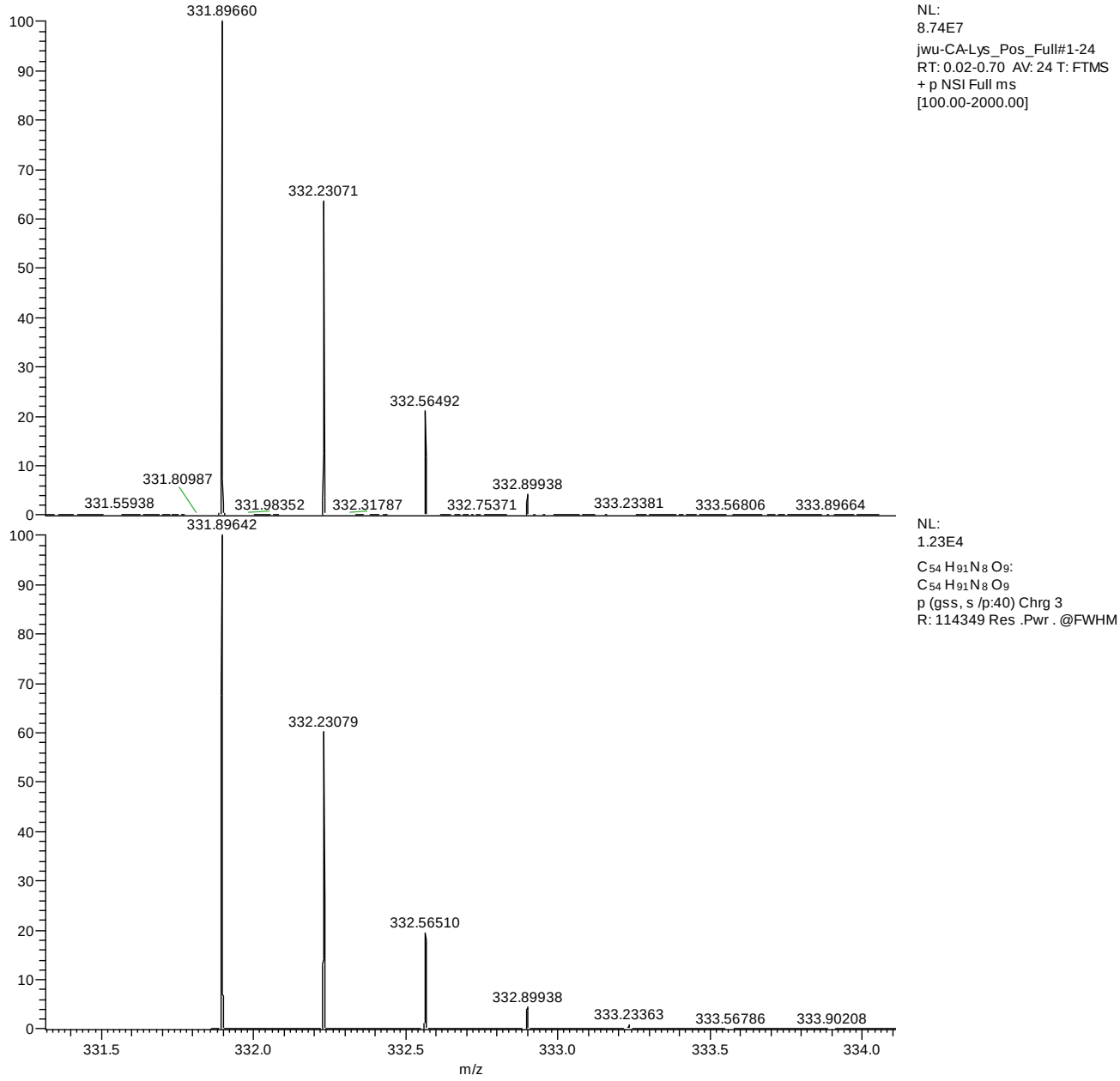


(5*S*,5'*S*,5"*S*)-6,6',6"-(((3*R*,5*S*,7*R*,8*R*,9*S*,10*S*,12*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthrene-3,7,12-triyl)tris(oxy))tris(6-oxohexane-1,5-diaminium) **(19d)**

Full spectrum

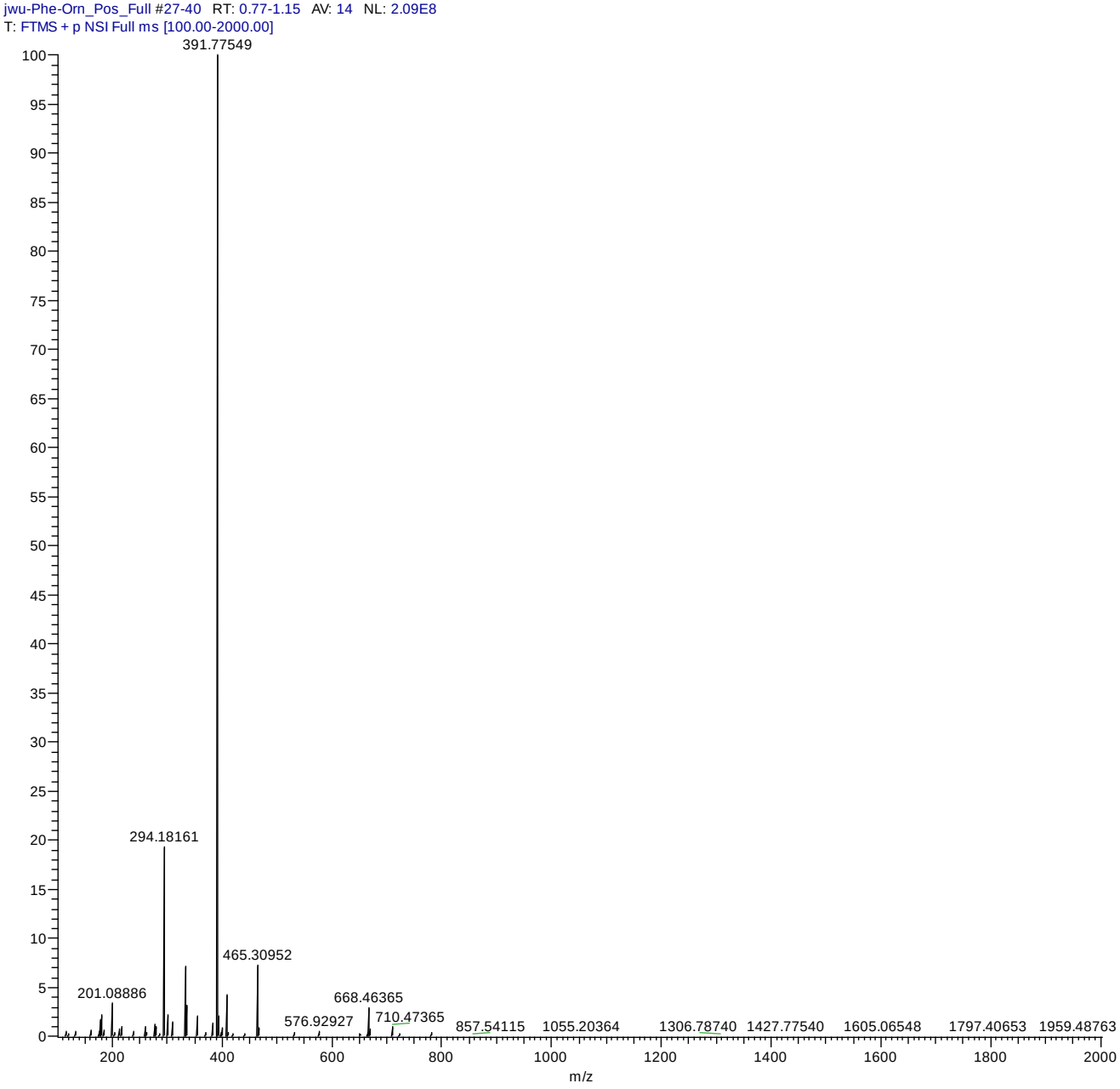


Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)

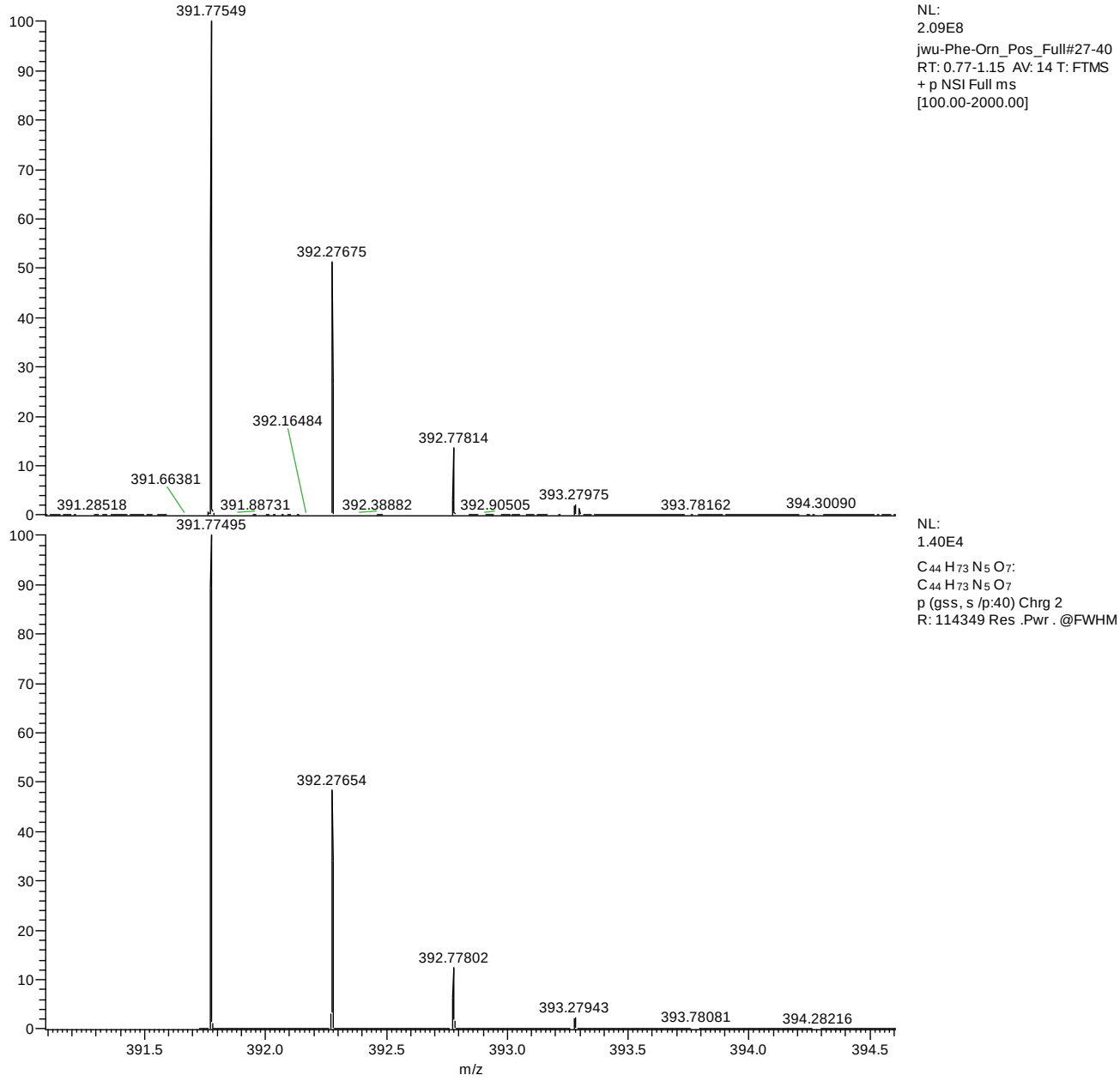


(4*S*,4'*S*)-5,5'-(((3*R*,5*S*,7*R*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-1-Methoxy-1-oxo-3-phenylpropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthrene-3,7-diyl)bis(oxy))bis(5-oxopentane-1,4-diaminium) **(20)**

Full spectrum

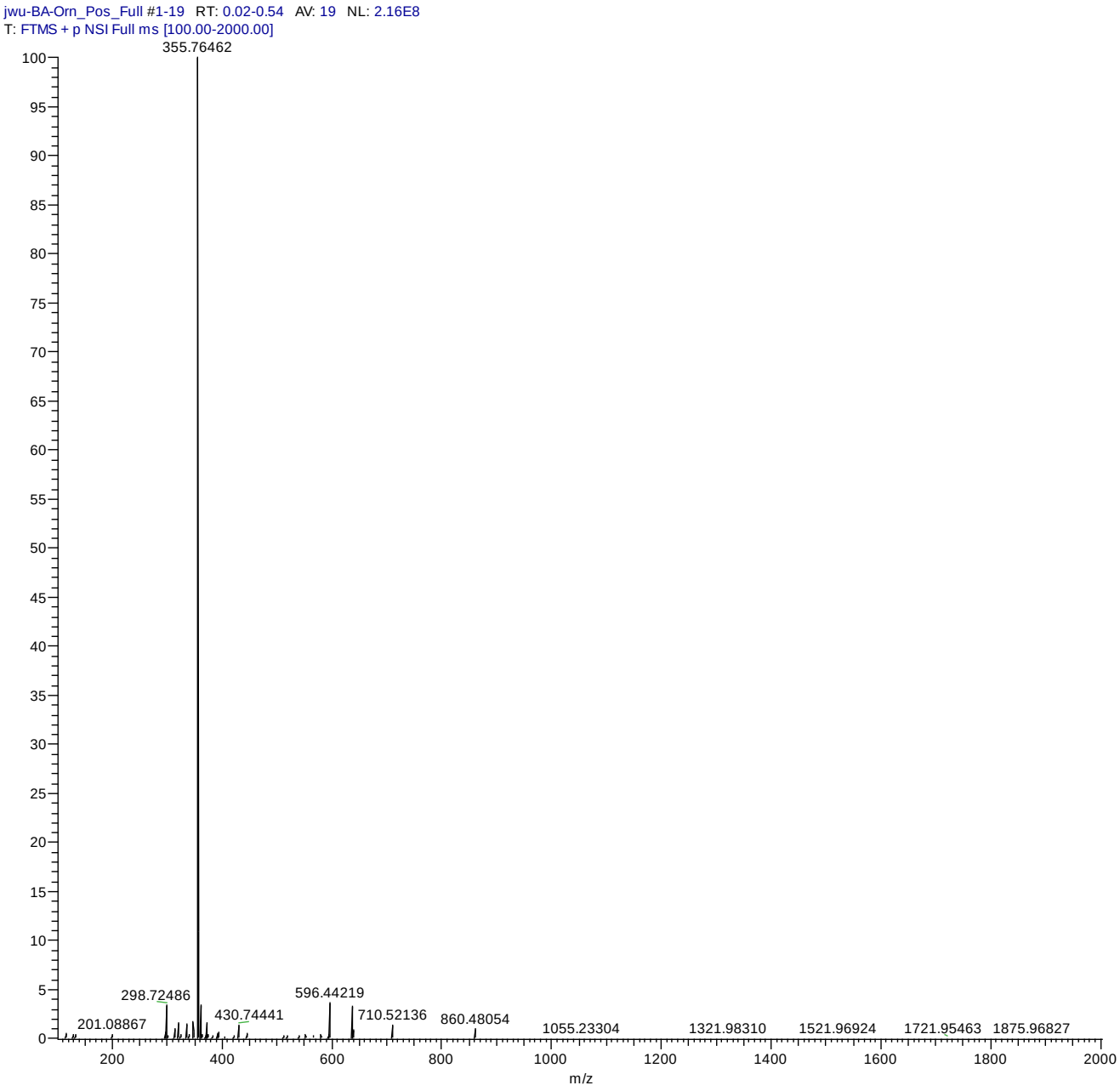


Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)

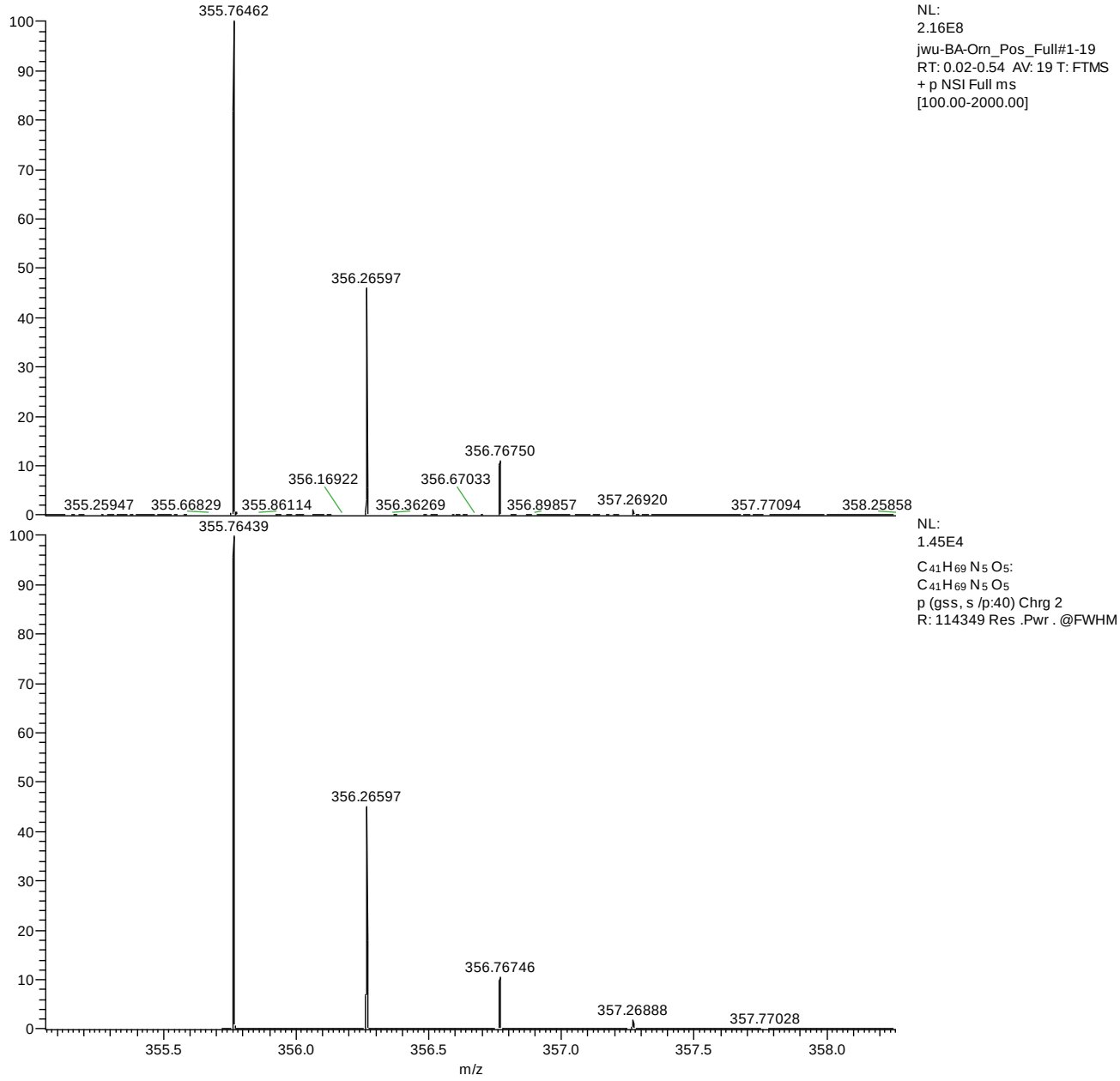


(4*S*,4'*S*)-5,5'-(((3*R*,5*S*,7*R*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(Benzylamino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthrene-3,7-diyl)bis(oxy))bis(5-oxopentane-1,4-diaminium) **(21)**

Full spectrum

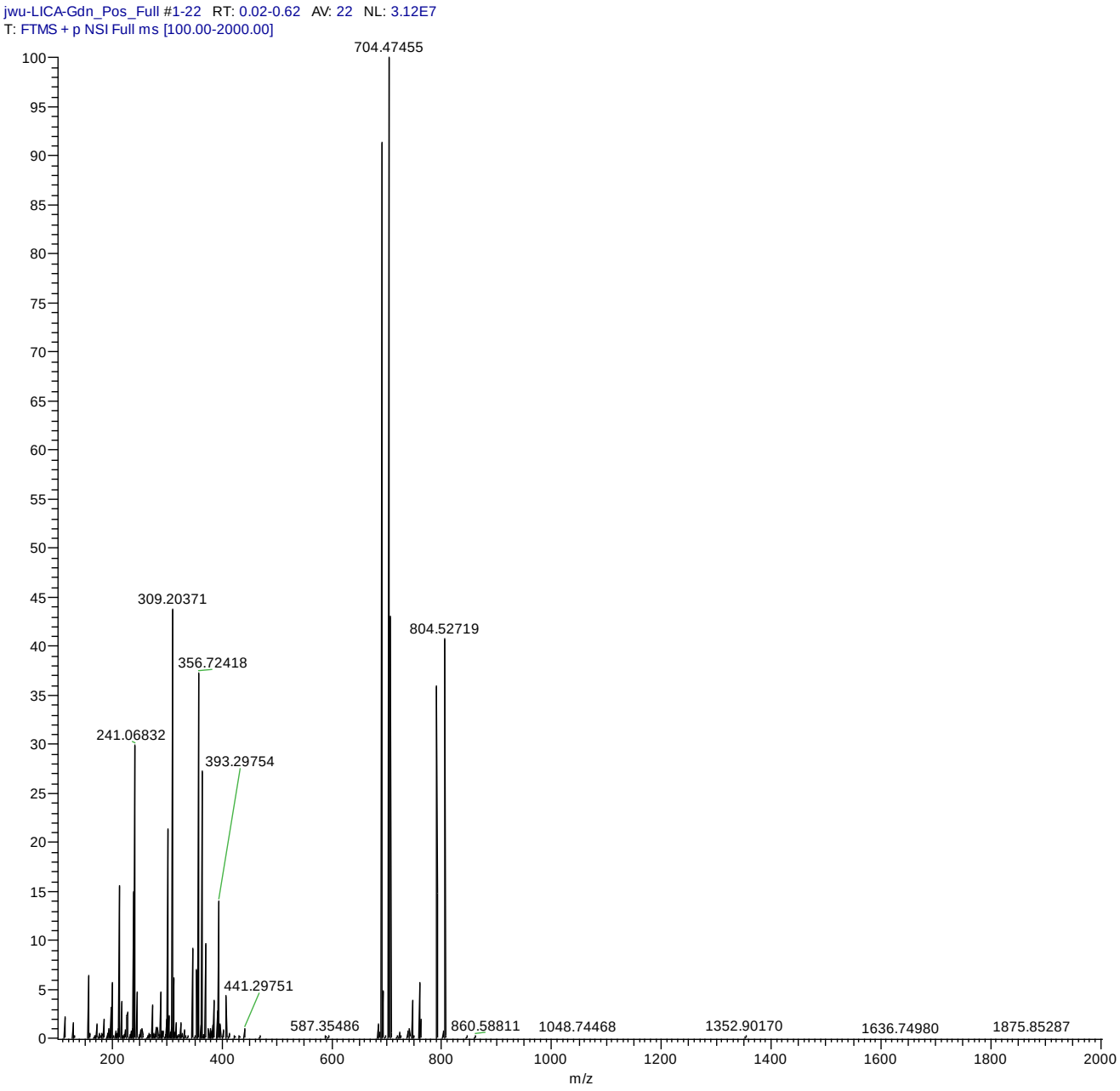


Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)

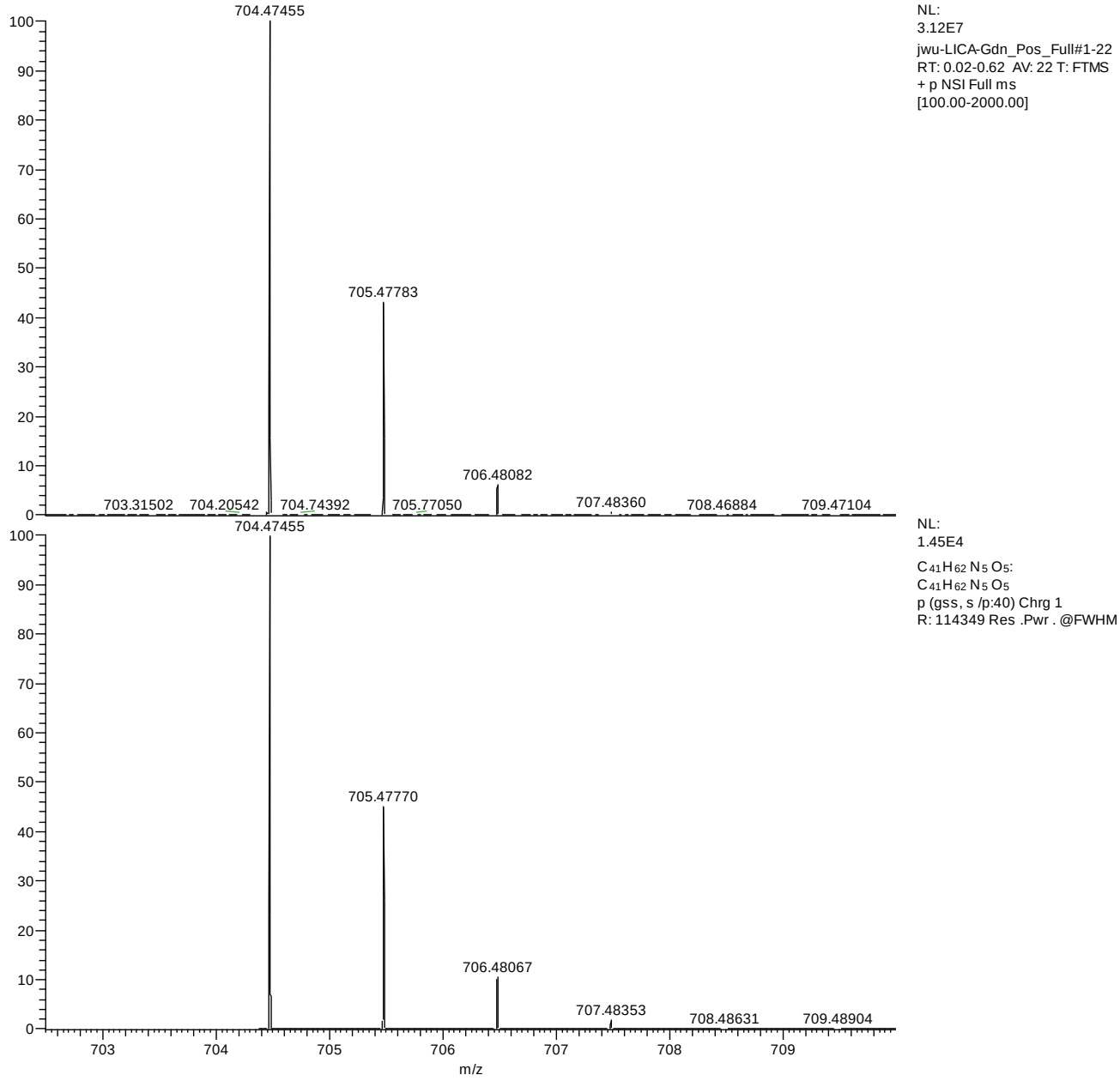


((4-(((3*R*,5*R*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthren-3-yl)oxy)-4-oxobutyl)amino)(amino)methaniminium **(23)**

Full spectrum

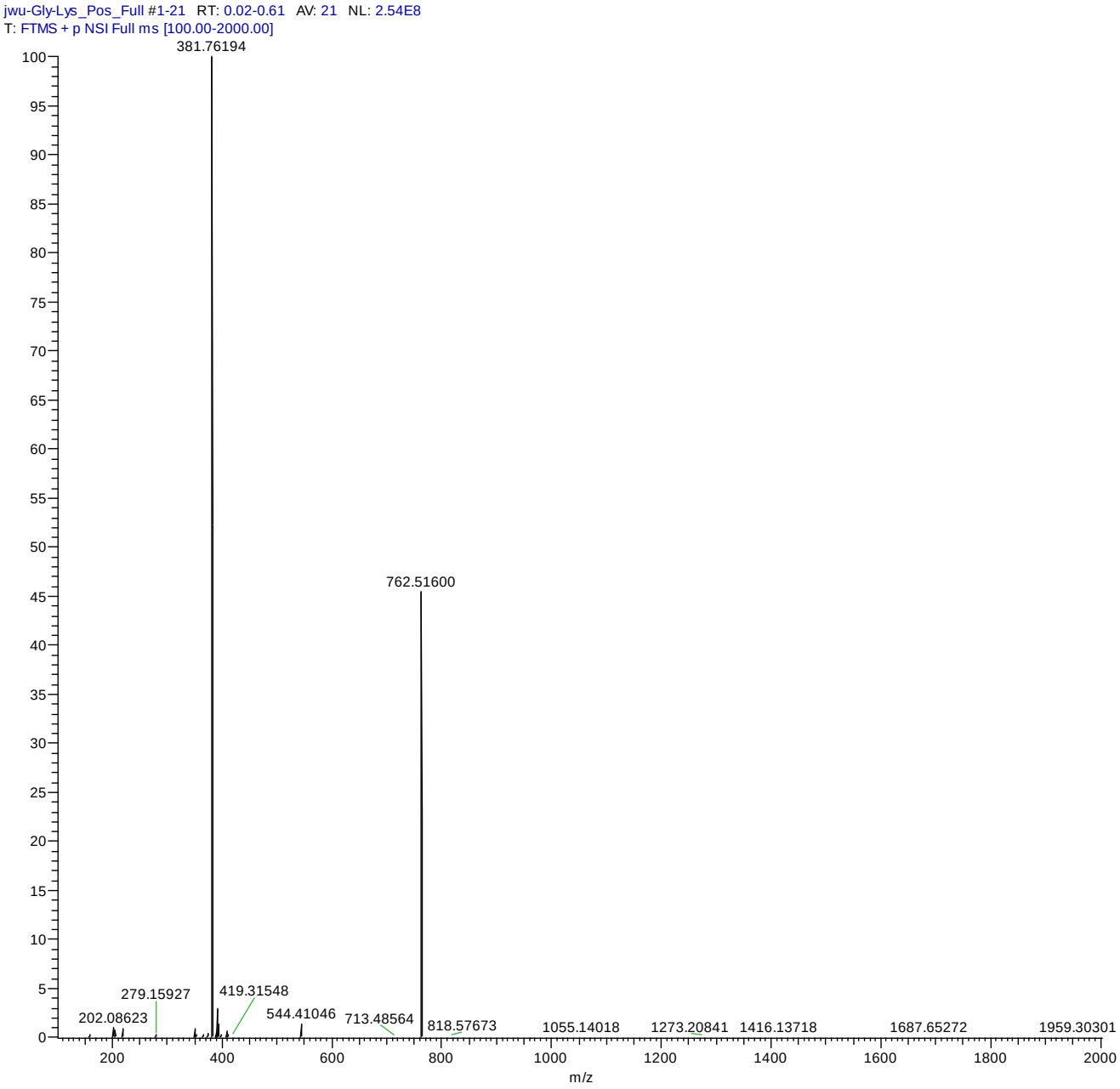


Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)

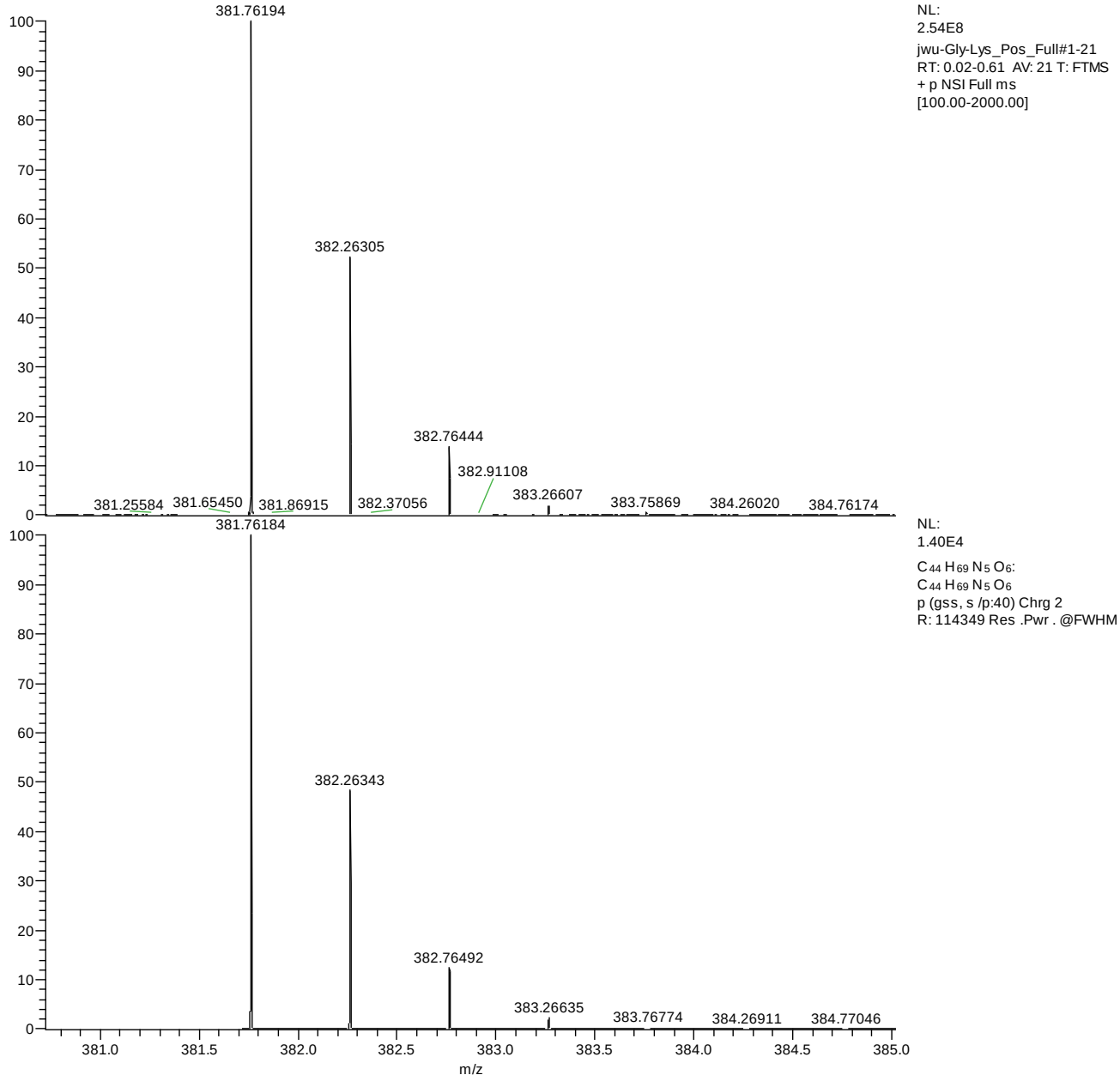


Methyl ((*R*)-4-((3*R*,5*R*,8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-3-((L-lysylglycyl)oxy)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthren-17-yl)pentanoyl)-L-tryptophanate **(25)**

Full spectrum

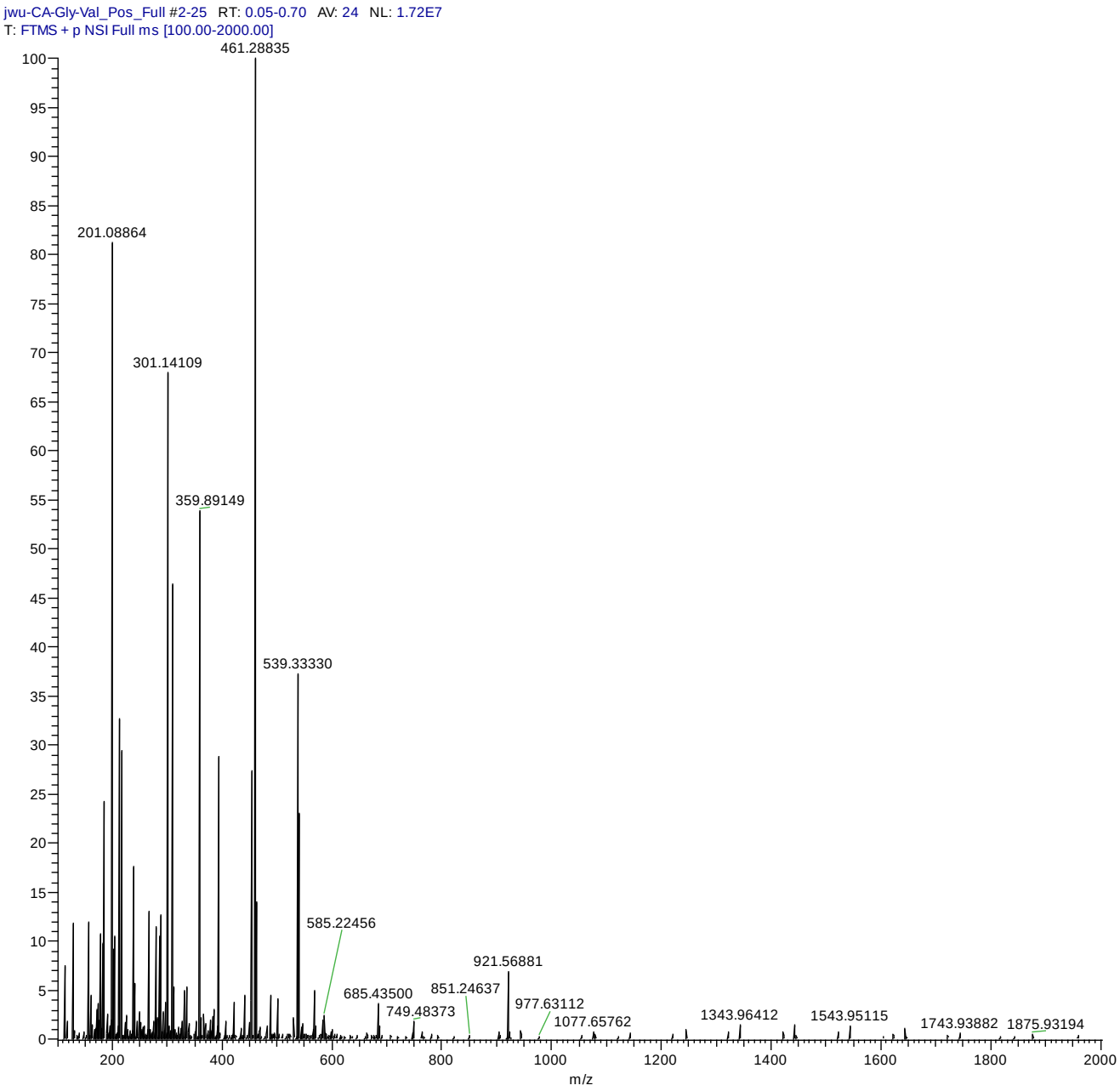


Zoomed spectrum



1,1',1''-(((((3*R*,5*S*,7*R*,8*R*,9*S*,10*S*,12*S*,13*R*,14*S*,17*R*)-17-((*R*)-5-(((*S*)-3-(1*H*-Indol-3-yl)-1-methoxy-1-oxopropan-2-yl)amino)-5-oxopentan-2-yl)-10,13-dimethylhexadecahydro-1*H*-cyclopenta[*a*]phenanthrene-3,7,12-triyl)tris(oxy))tris(2-oxoethane-2,1-diyl))tris(azanediyl))tris(3-methyl-1-oxobutan-2-aminium) **(27)**

Full spectrum



Zoomed spectrum (Top spectrum: measured mass; bottom spectrum: calculated mass)