Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

SUPPORTING INFORMATION

Tight-binding Inhibition of Jack bean α-Mannosidase by Glycoimidazole Clusters

Maëva M. Pichon, Fabien Stauffert, Anne Bodlenner, and Philippe Compain*

Tables of contents

Copies of ^{1}H NMR, ^{13}C NMR and HRMS spectra

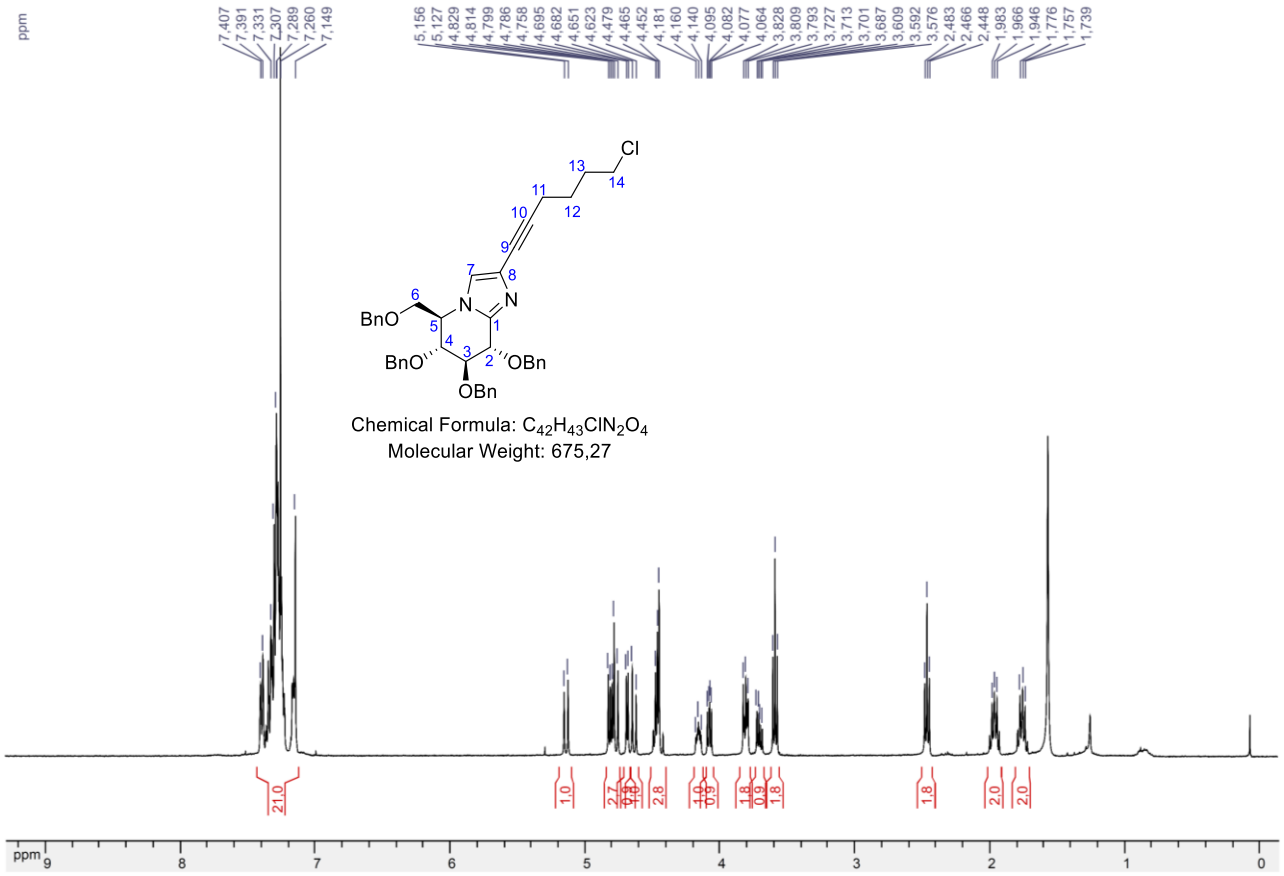

Fig S1. ^{1}H NMR (400 MHz, CDCl3) spectrum of compound **9a**

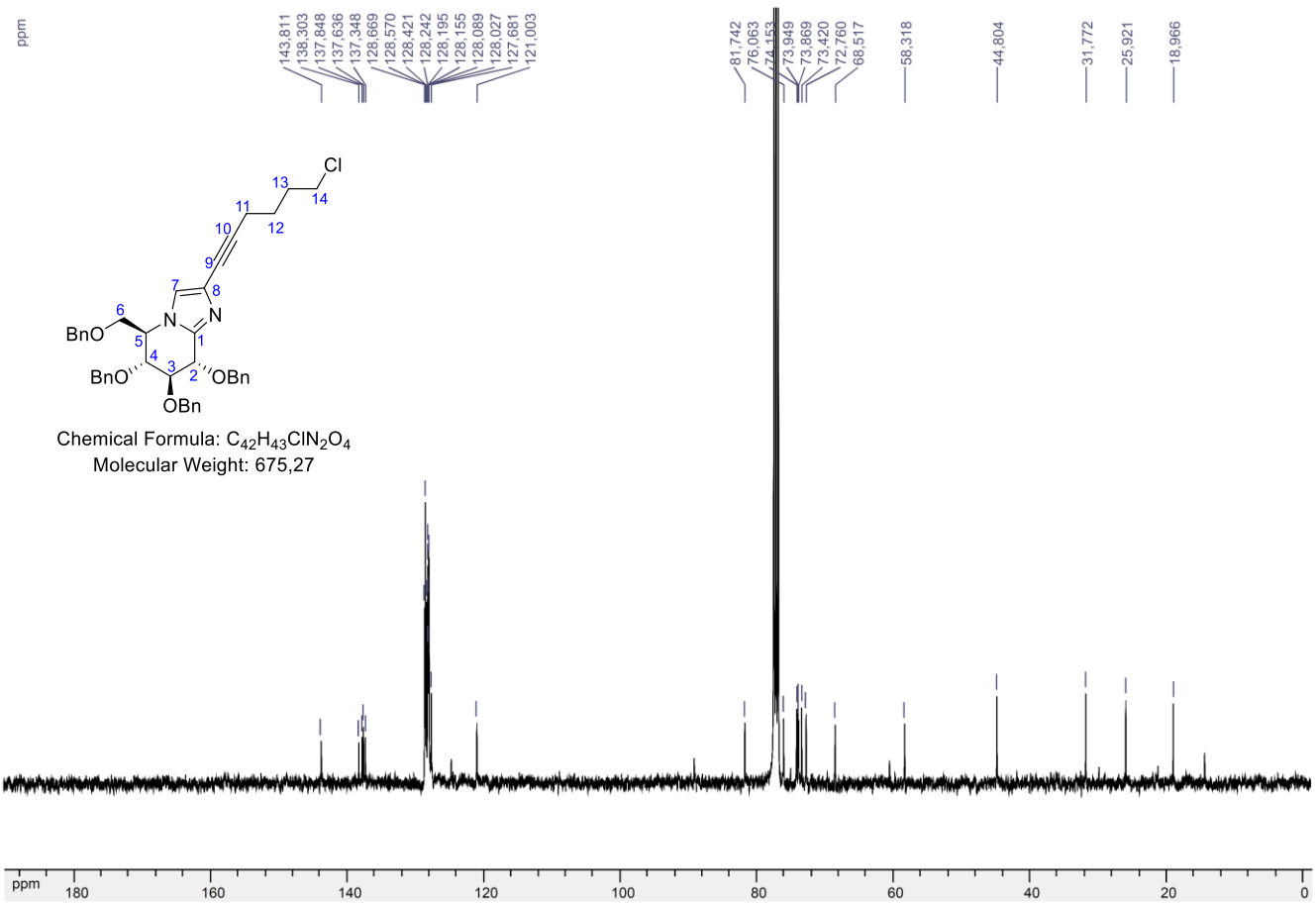

Fig S2. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **9a**

Mass Spectrum HR Report

Analysis Info

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Sample Name	MP0198	Instrument	micrOTOF II 8213750.1045
Comment			1

Acquisition Parameter

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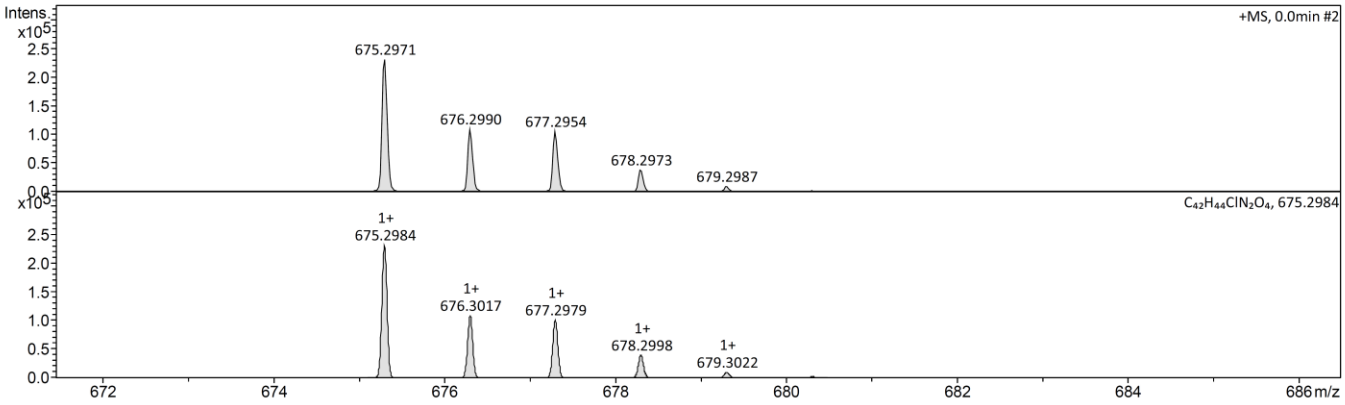

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675.297071	1	C42H44ClN2O4	675.298412	2.0	3.4	21.5	ok	even	8.1	7.8	n.a.	n.a.	n.a.	n.a.	

Fig S3. HRMS (ESI-MS) spectrum of compound **9a**

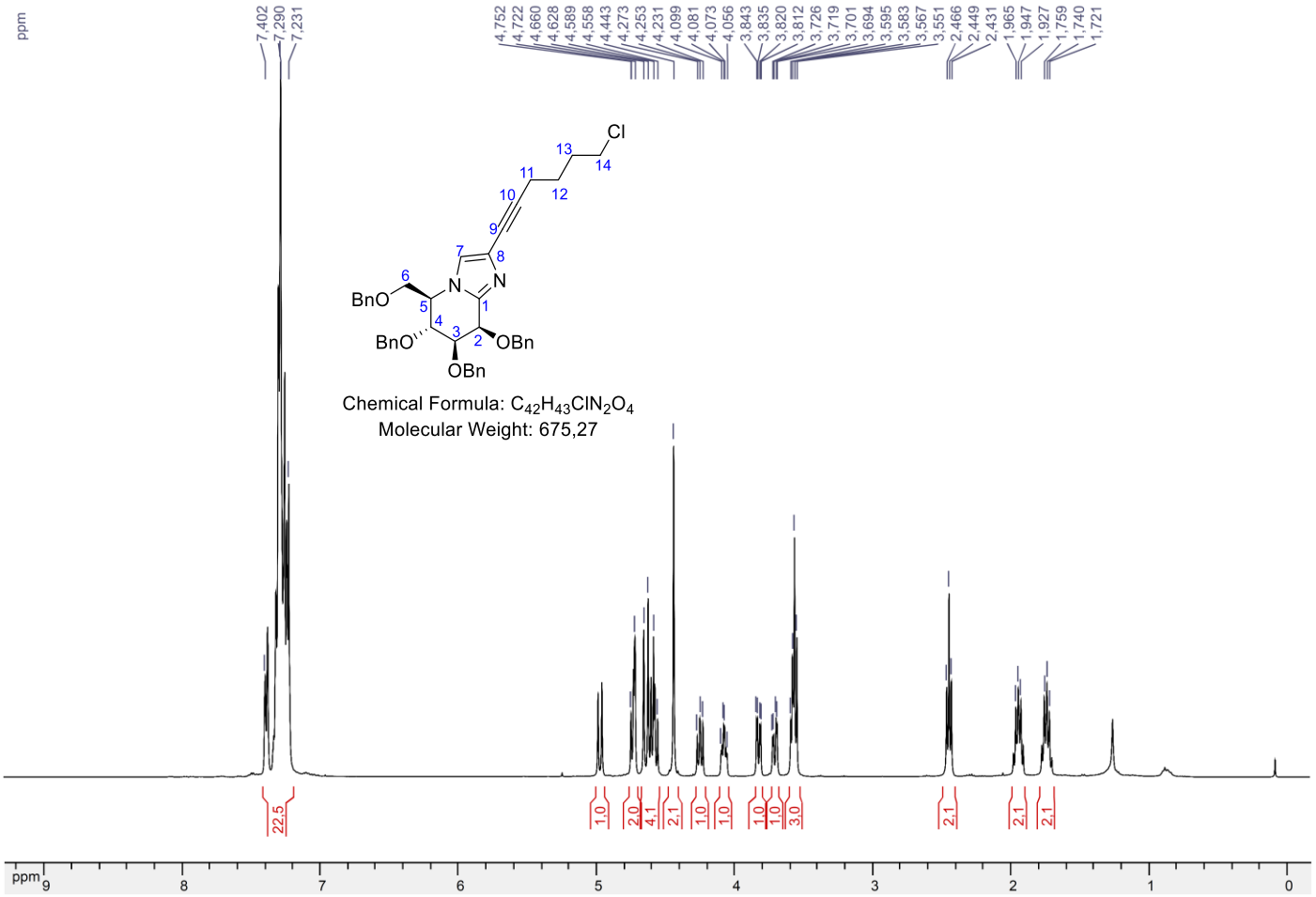

Fig S4. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **9b**

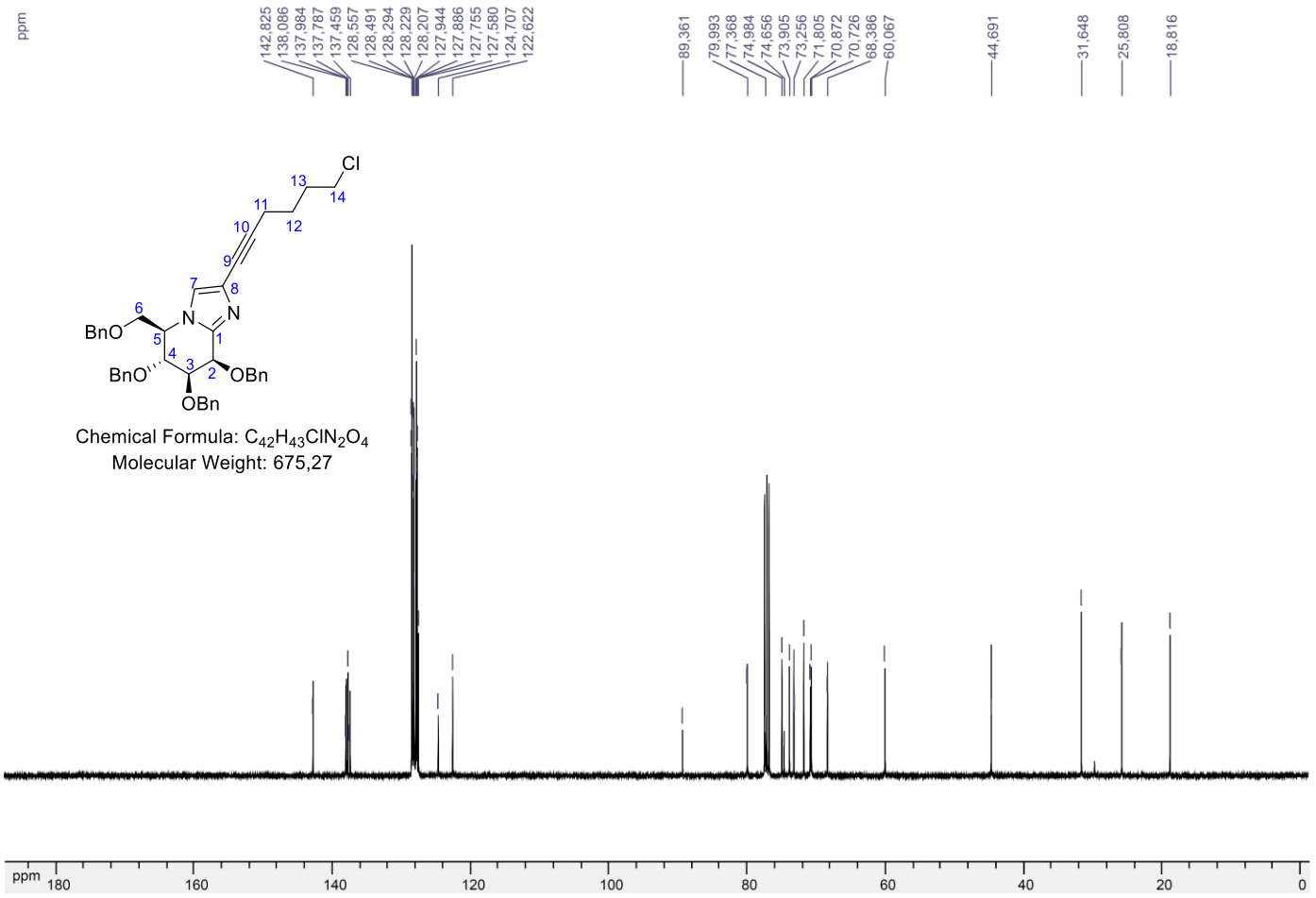

Fig S5. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **9b**

Mass Spectrum HR Report

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Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Corrector Fill	59.0 V
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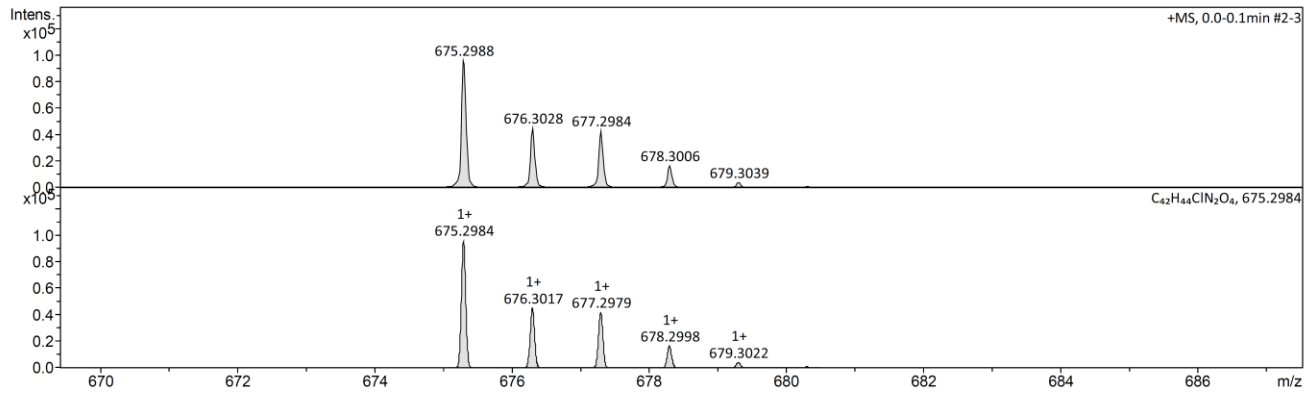
		n/a	n/a	Set Detector TOF	1953.3 V



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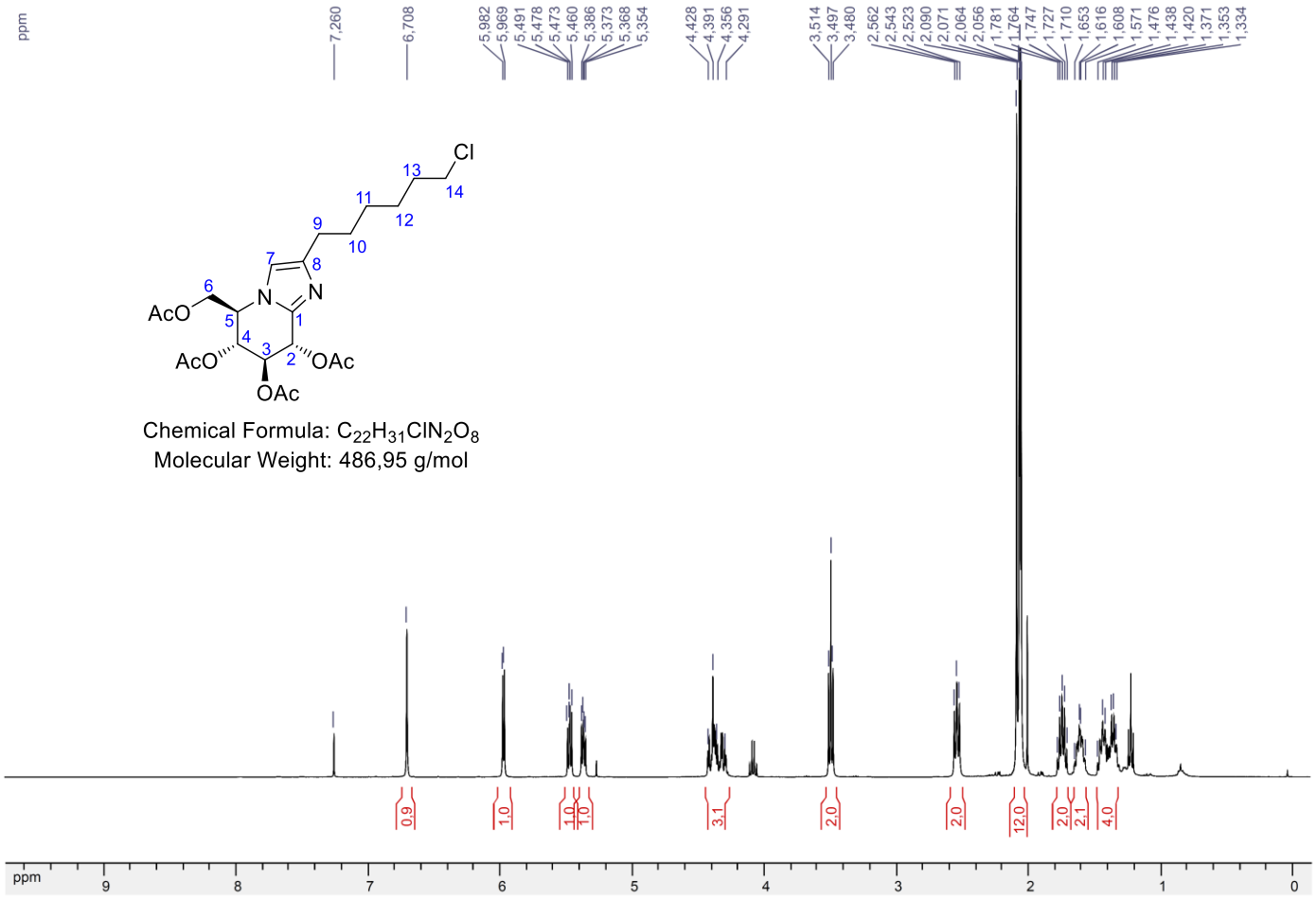
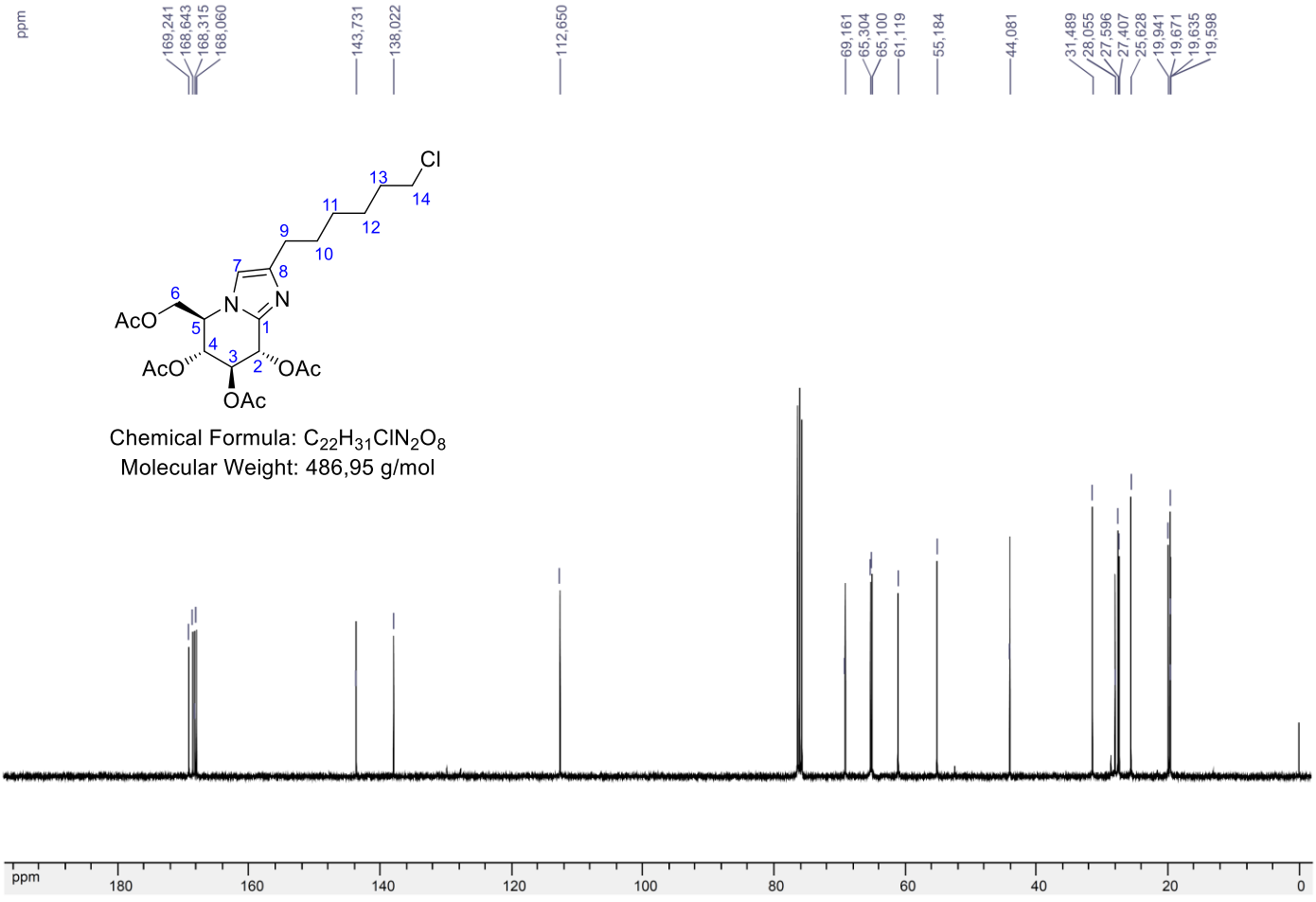
675.298793	1	C42H44ClN2O4	675.298412	-0.6	-1.1	21.5	ok	even	5.8	6.1	n.a.	n.a.	n.a.	n.a.	

Fig S6. HRMS (ESI-MS) spectrum of compound **9b**



Chemical Formula: $C_{22}H_{31}ClN_2O_8$
Molecular Weight: 486,95 g/mol

Fig S7. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **10a**



Chemical Formula: $C_{22}H_{31}ClN_2O_8$
Molecular Weight: 486,95 g/mol

Fig S8. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **10a**

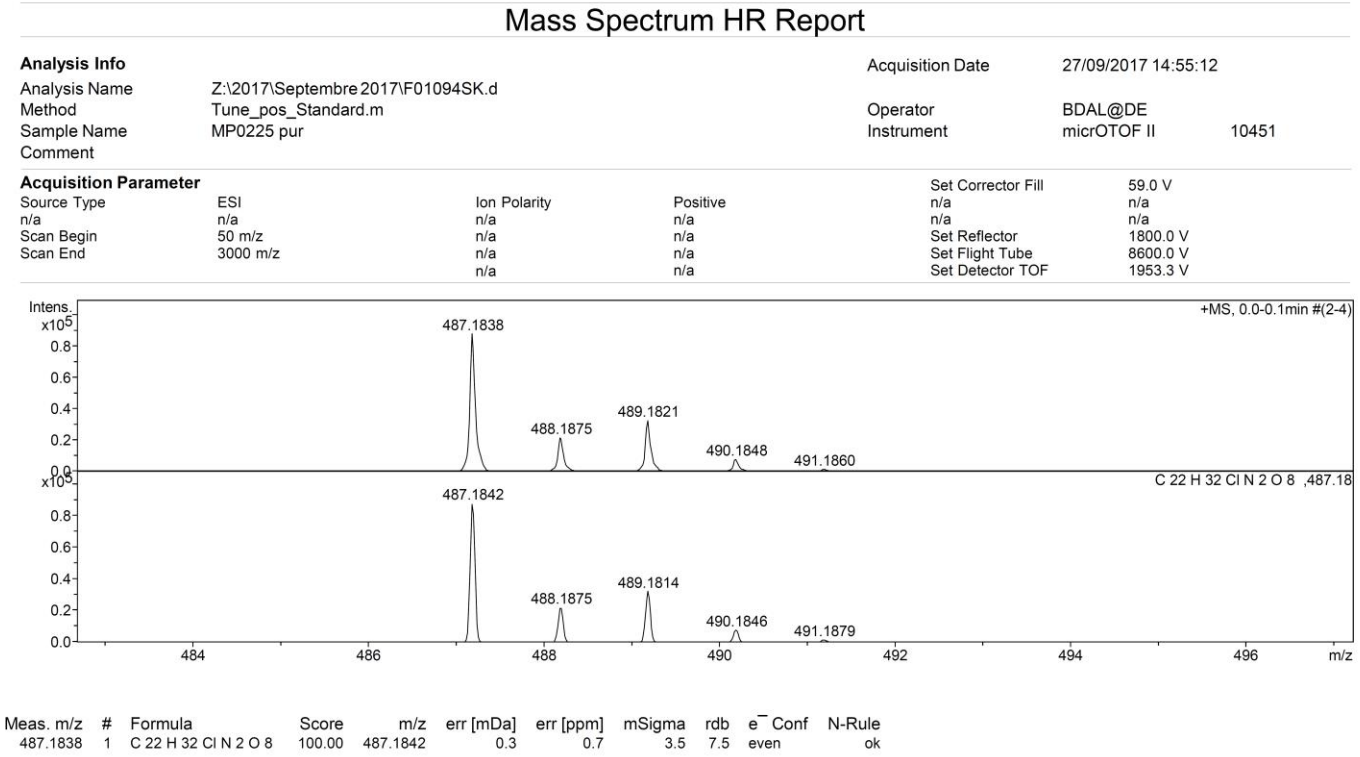


Fig S9. HRMS (ESI-MS) spectrum of compound **10a**

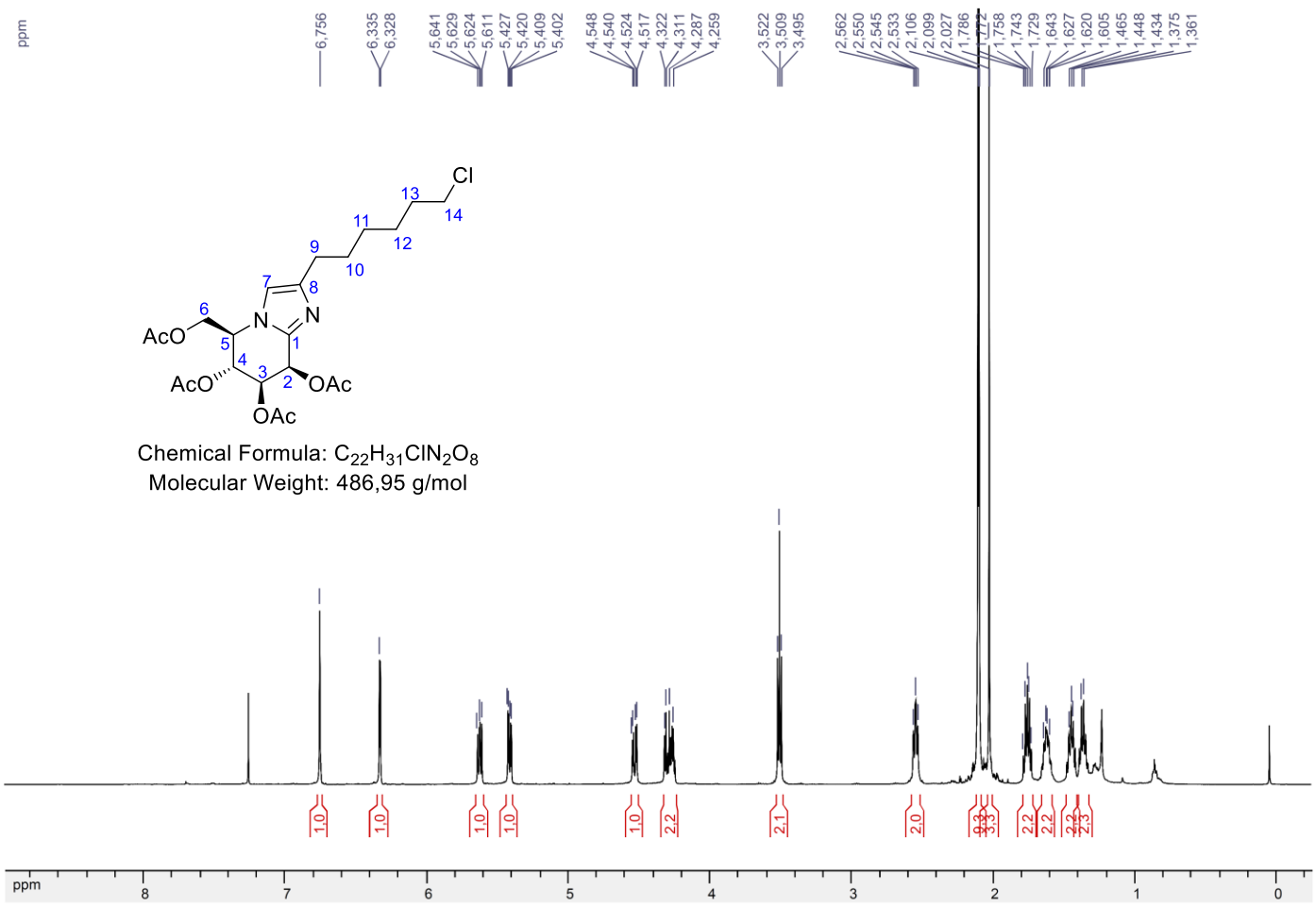


Fig S10. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **10b**

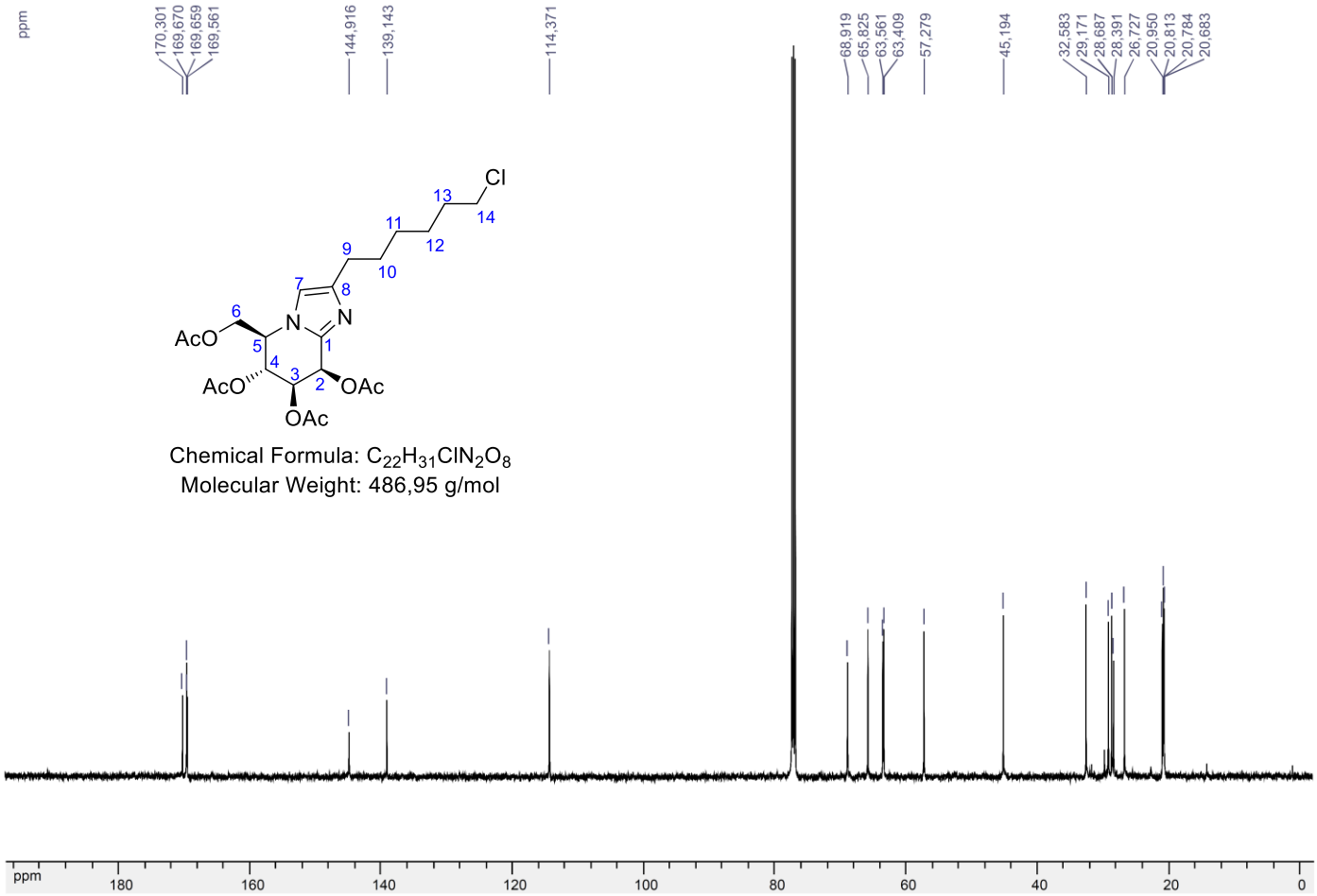


Fig S11. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **10b**

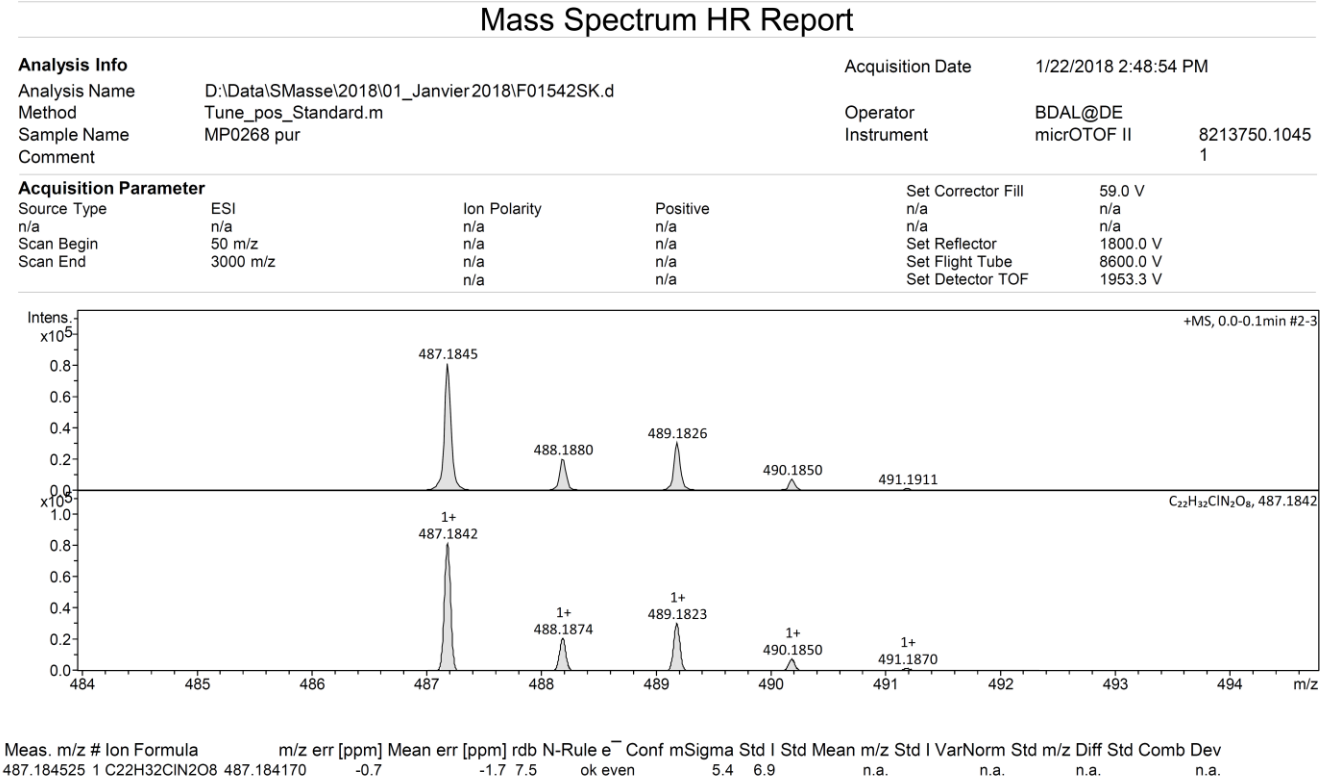


Fig S12. HRMS (ES-MS) spectrum of compound **10b**

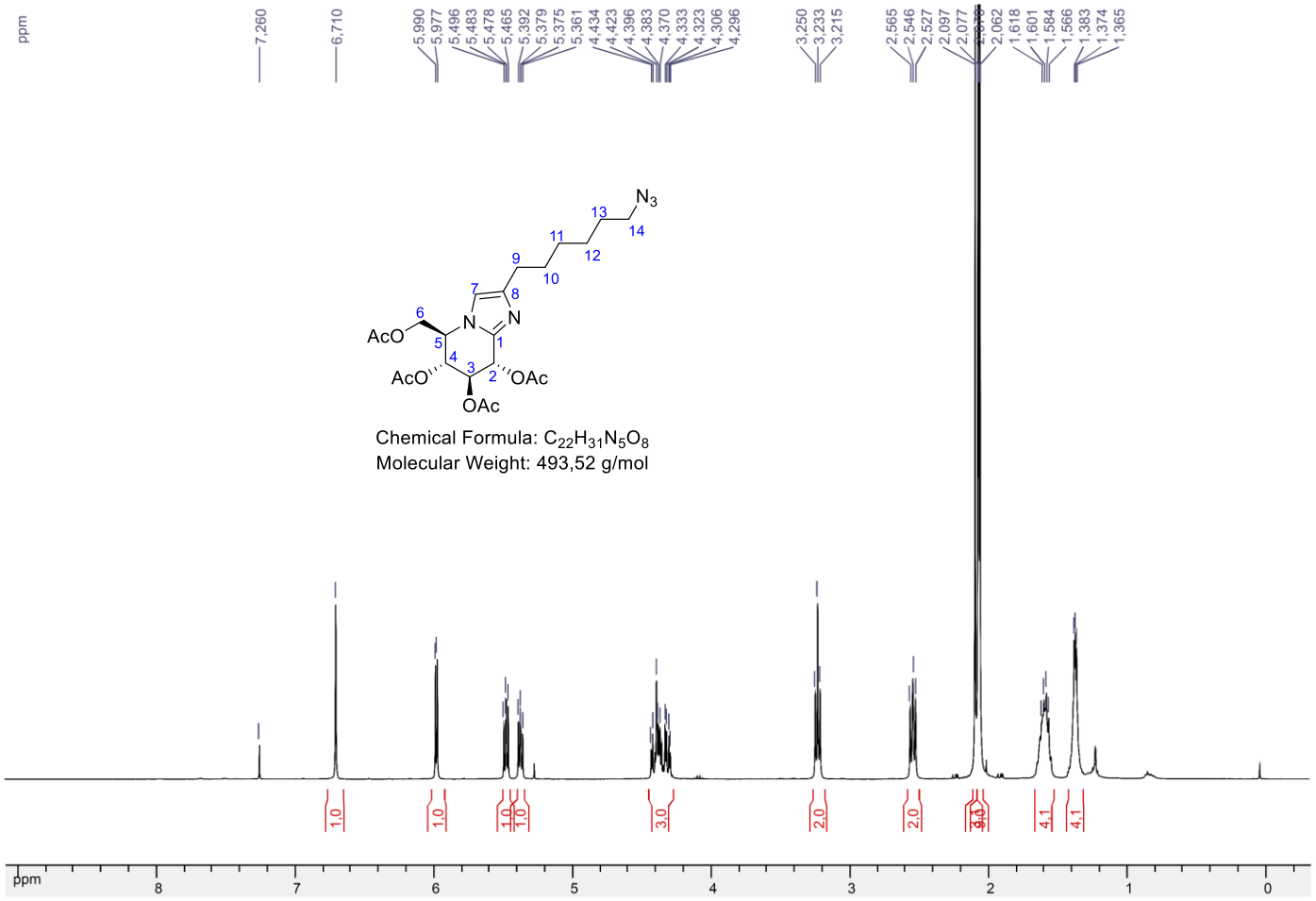


Fig S13. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **11a**

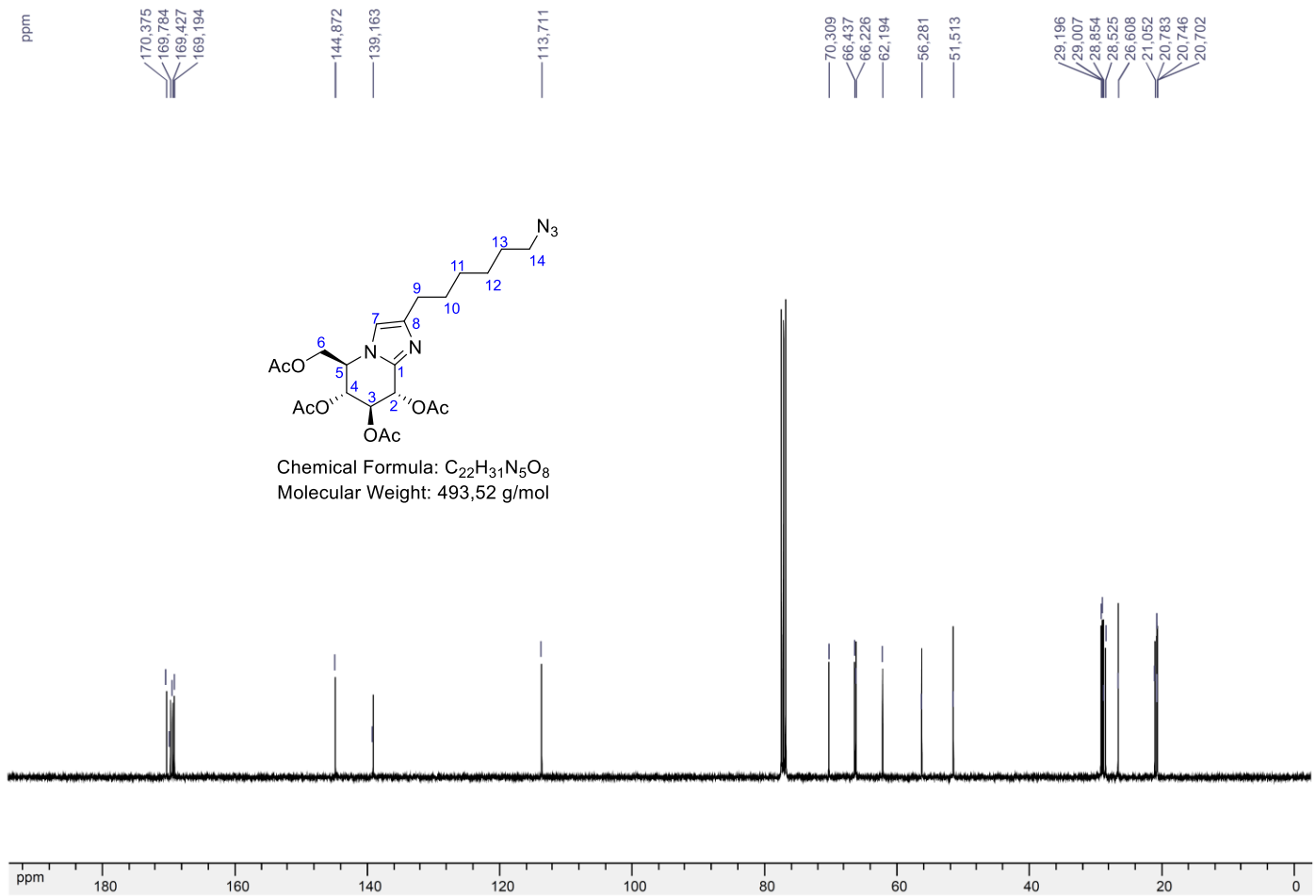


Fig S14. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **11a**

Mass Spectrum HR Report

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Comment			1

Acquisition Parameter

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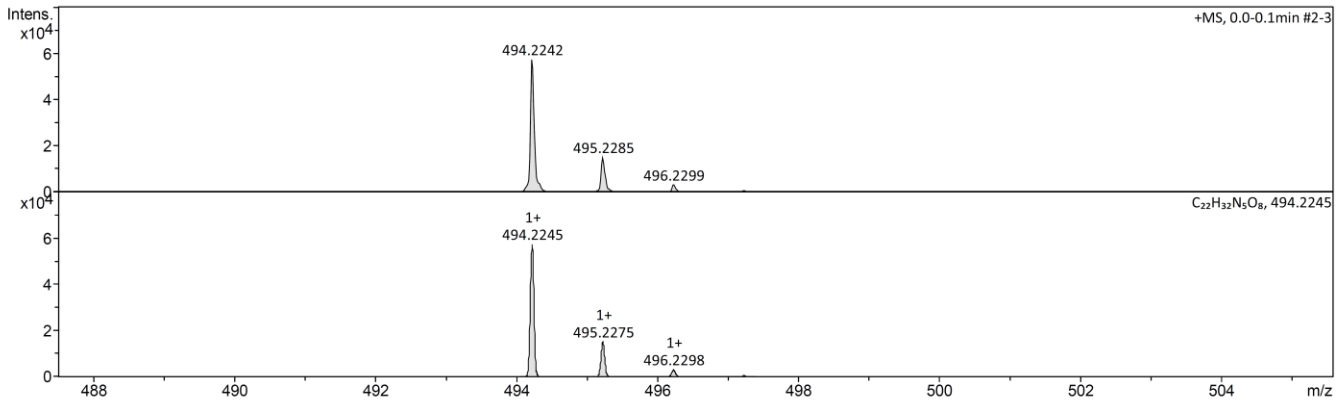
Scan End	3000 m/z	n/a	n/a	Set Reflector	1800.0 V
		n/a	n/a	Set Flight Tube	8600.0 V
				Set Detector TOF	1953.3 V



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494.224166	1	C22H32N5O8	494.224539	0.8	0.1	9.5	ok	even	1.4	2.2	n.a.	n.a.	n.a.	n.a.

Fig S15. HRMS (ESI-MS) spectrum of compound **11a**

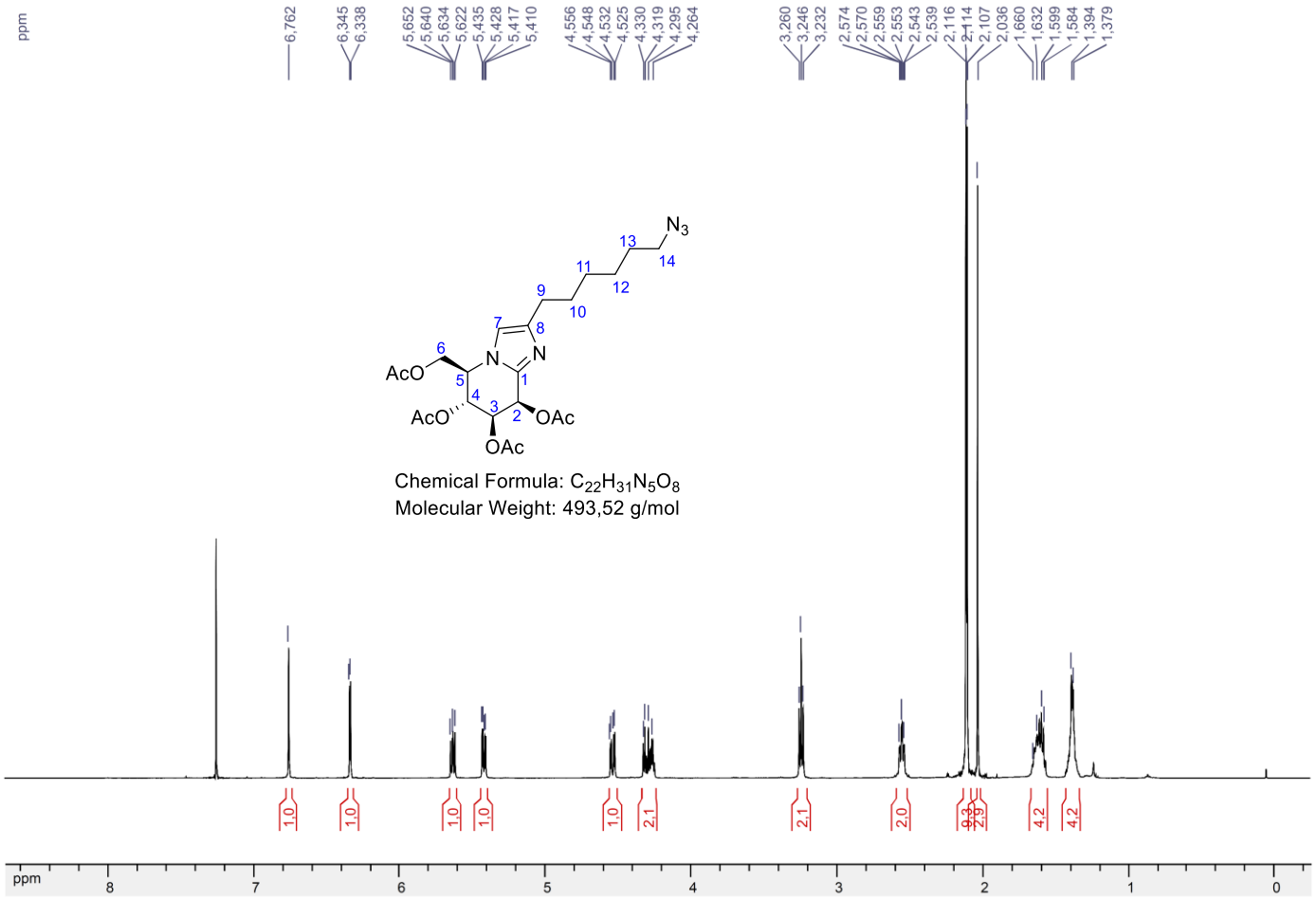


Fig S16. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **11b**

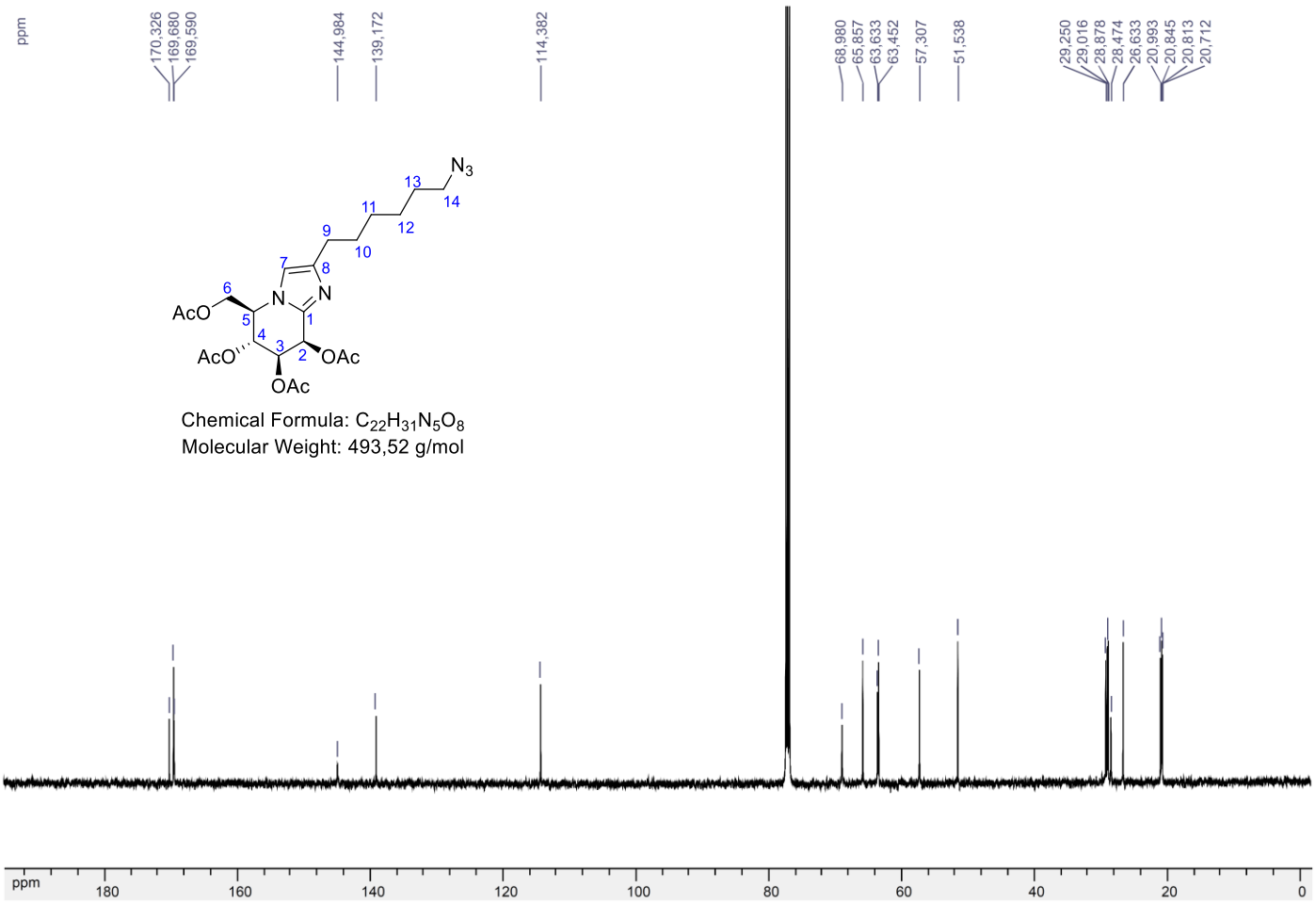
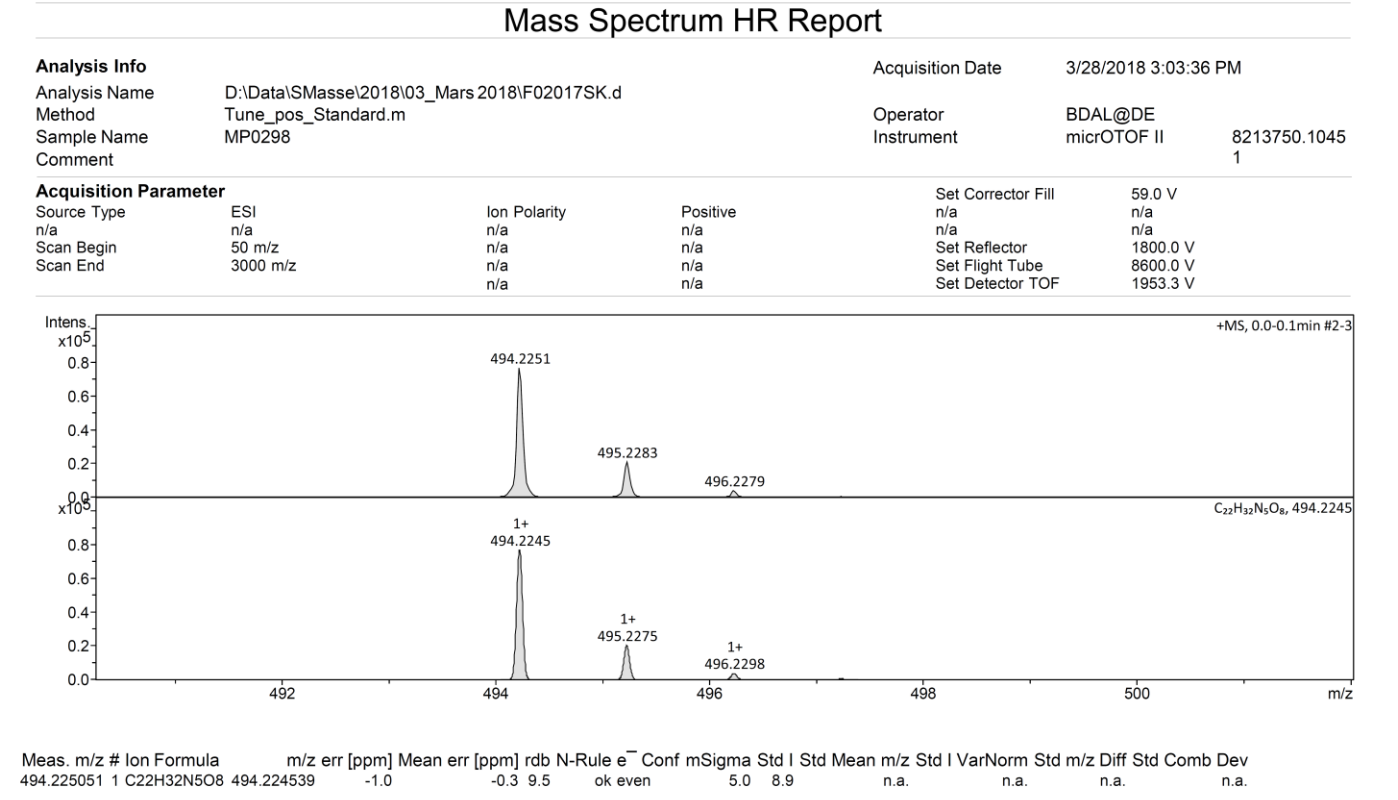


Fig S17. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **11b**



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494.225051	1	C22H32N5O8	494.224539	-1.0	-0.3	9.5	ok	even	5.0	8.9	n.a.	n.a.	n.a.	n.a.

Fig S18. HRMS (ESI-MS) spectrum of compound **11b**

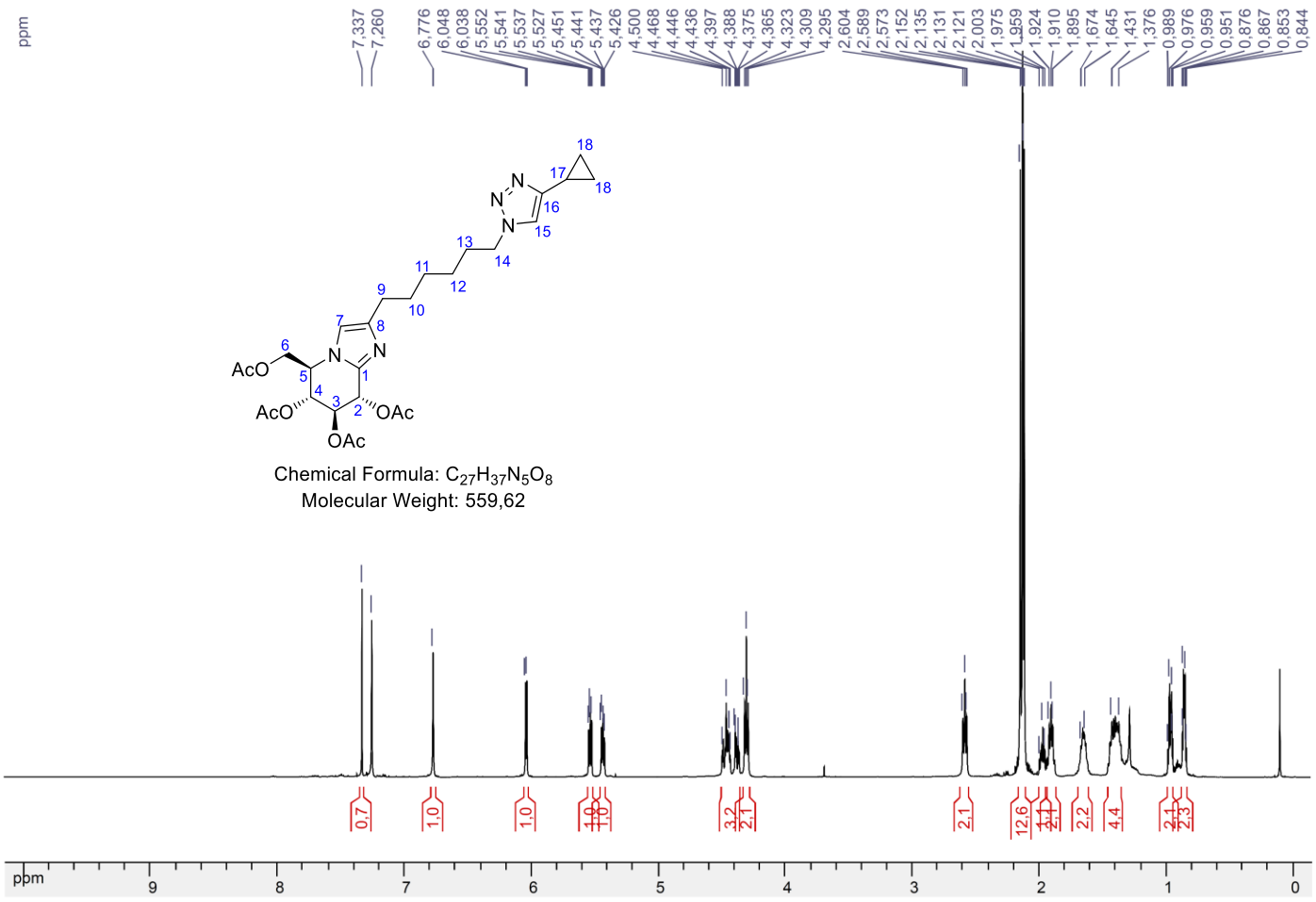


Fig S19. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **12a**

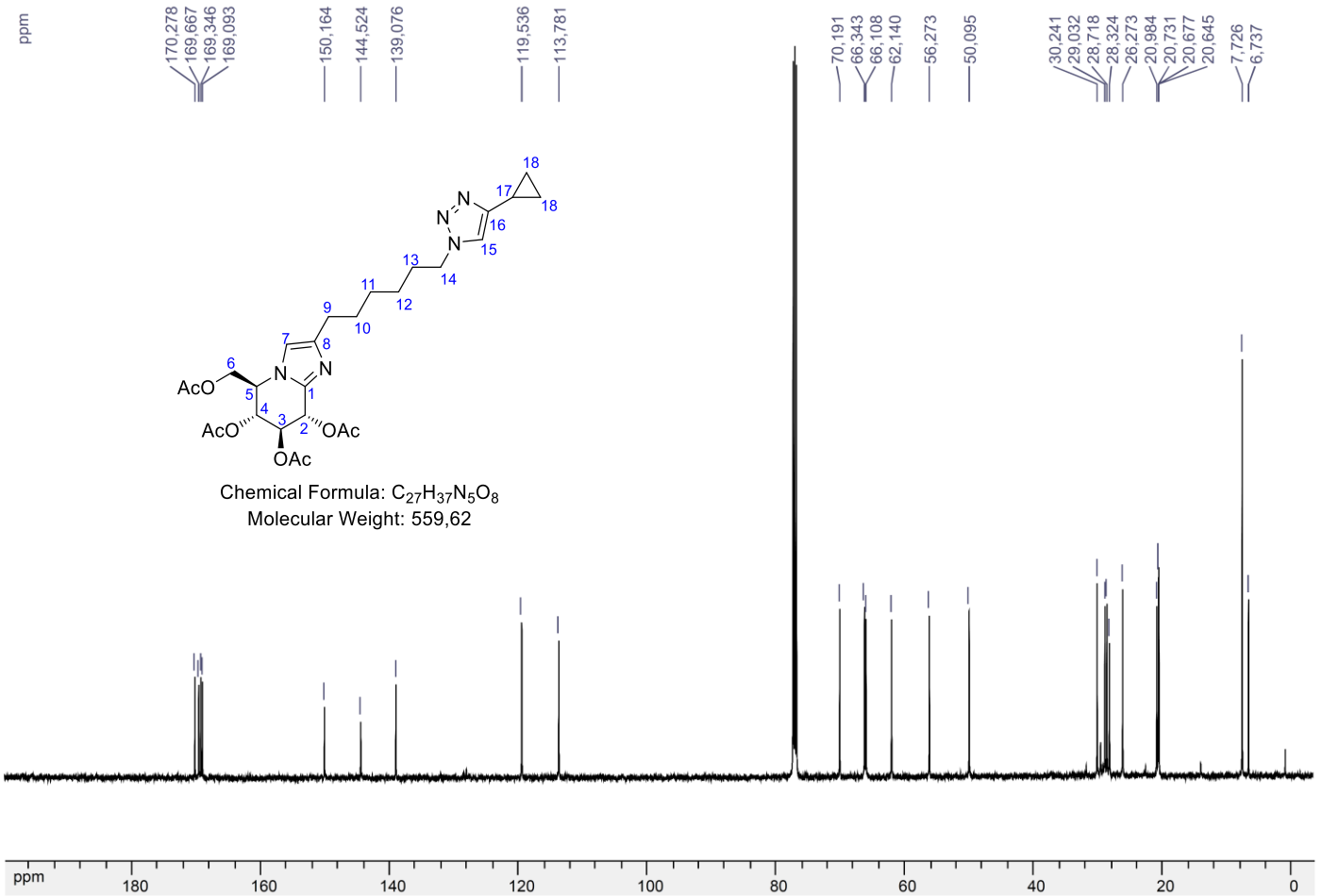


Fig S20. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **12a**

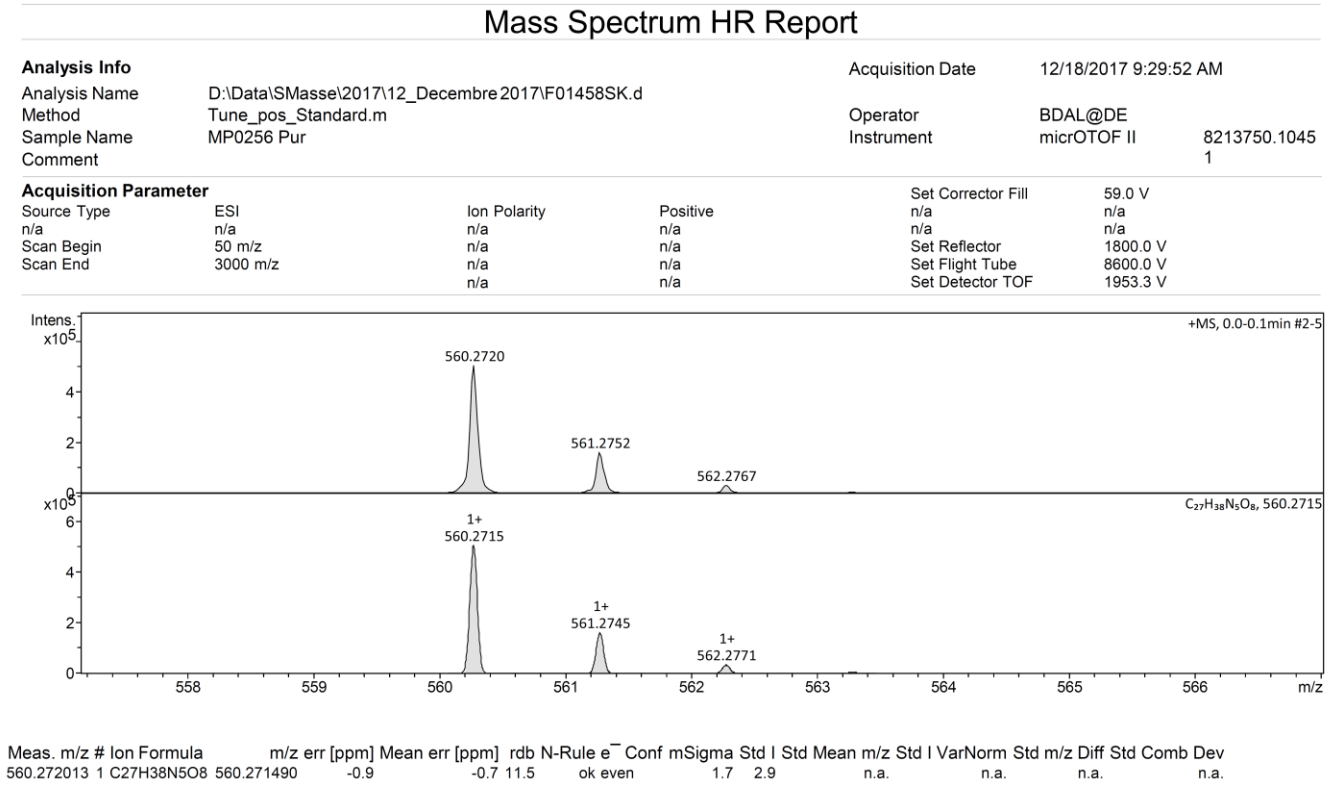


Fig S21. HRMS (ESI-MS) spectrum of compound **12a**

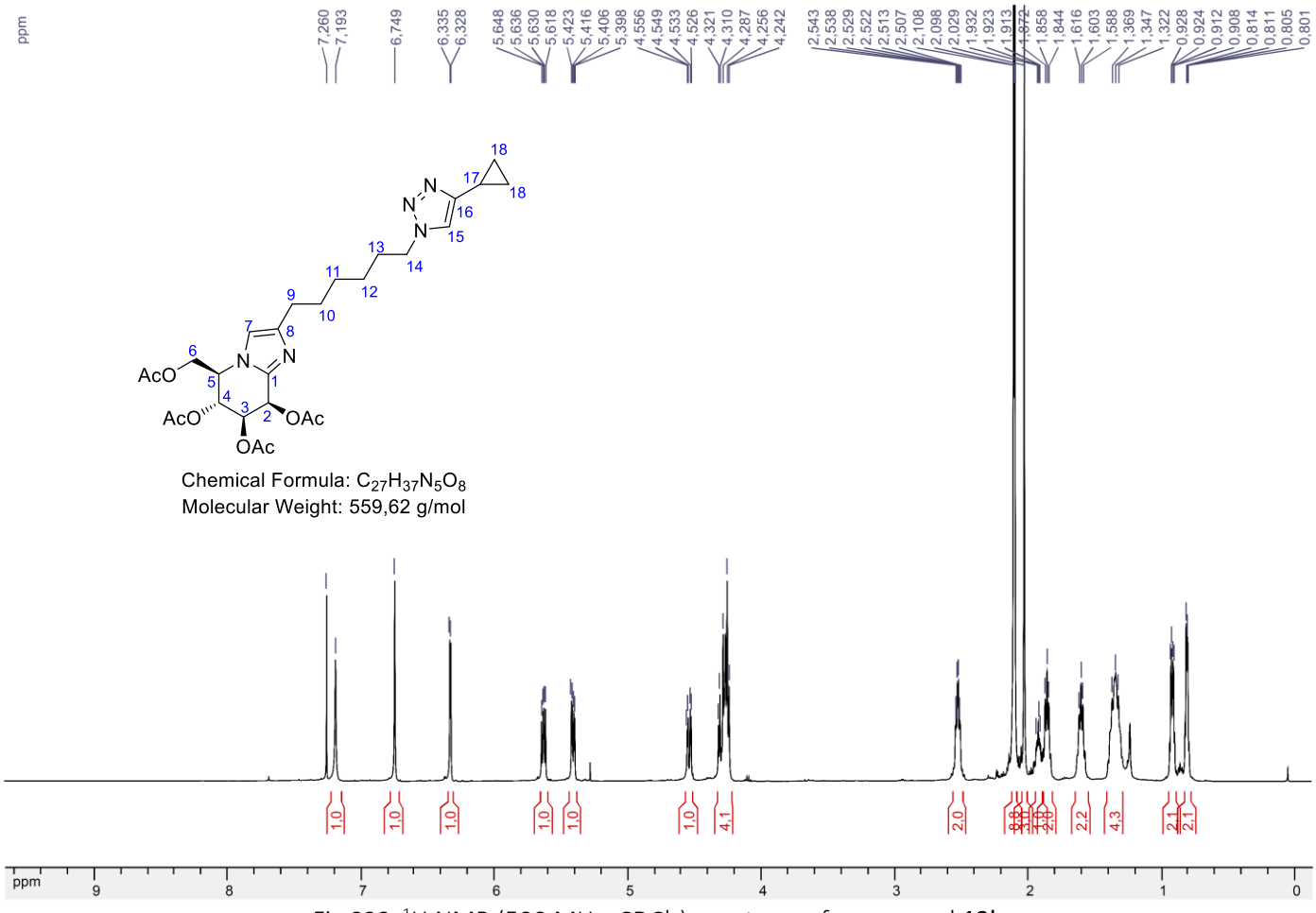


Fig S22. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **12b**

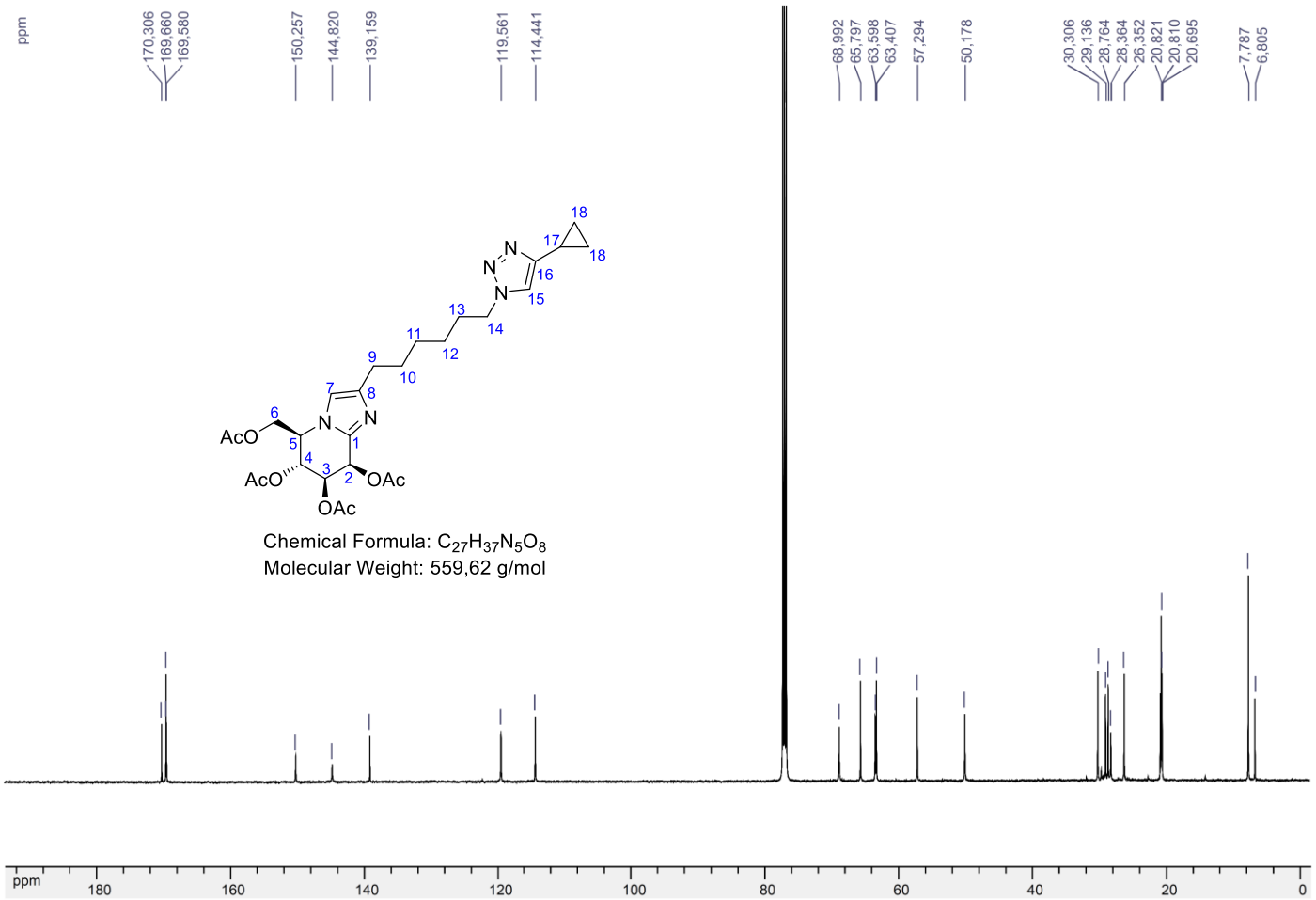
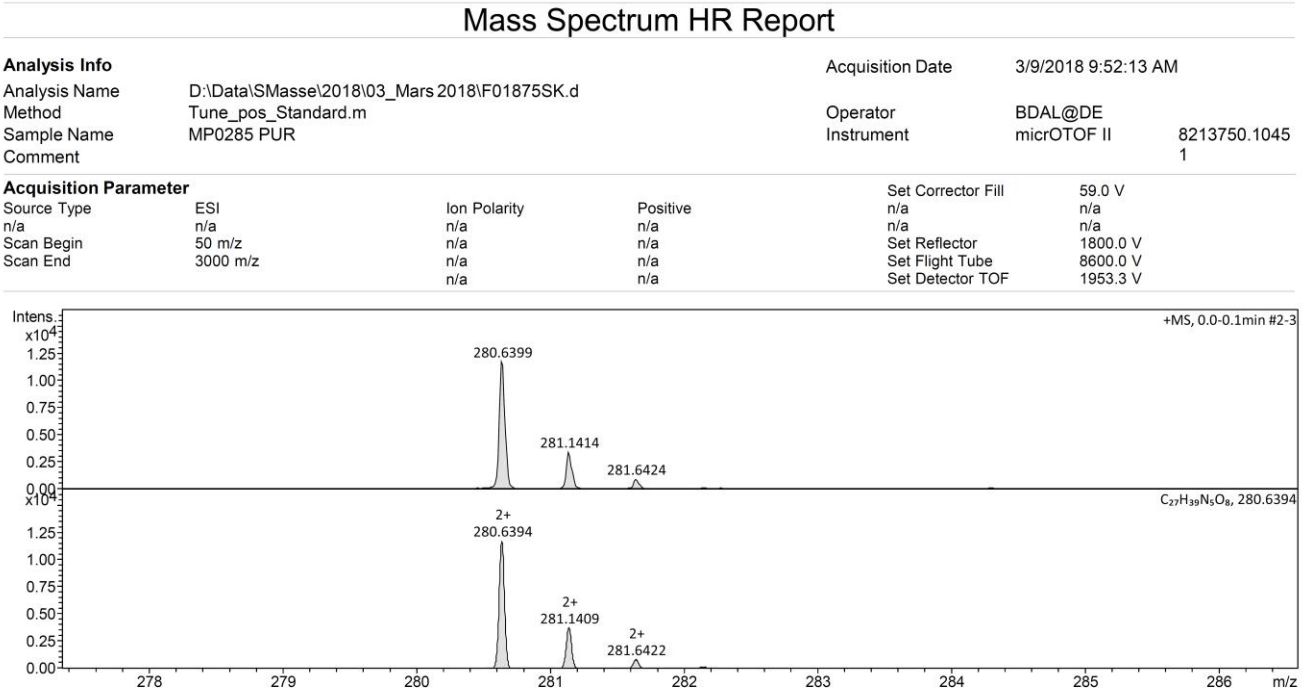


Fig S23. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **12b**



Mass Spectrum HR Report

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Comment			1

Acquisition Parameter

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Scan End	3000 m/z	n/a	n/a	Set Flight Tube	8600.0 V
		n/a	n/a	Set Detector TOF	1953.3 V

Meas. m/z	#	Ion Formula	m/z err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
280.639938	1	C27H39N5O8	280.639383	-2.0	1748.7	11.0	ok	even	16.0	24.2	n.a.	n.a.	n.a.	n.a.
560.268955	1	C27H38N5O8	560.271490	4.5	4.1	11.5	ok	even	5.4	9.4	n.a.	n.a.	n.a.	n.a.

Fig S24. HRMS (ESI-MS) spectrum of compound **12b**

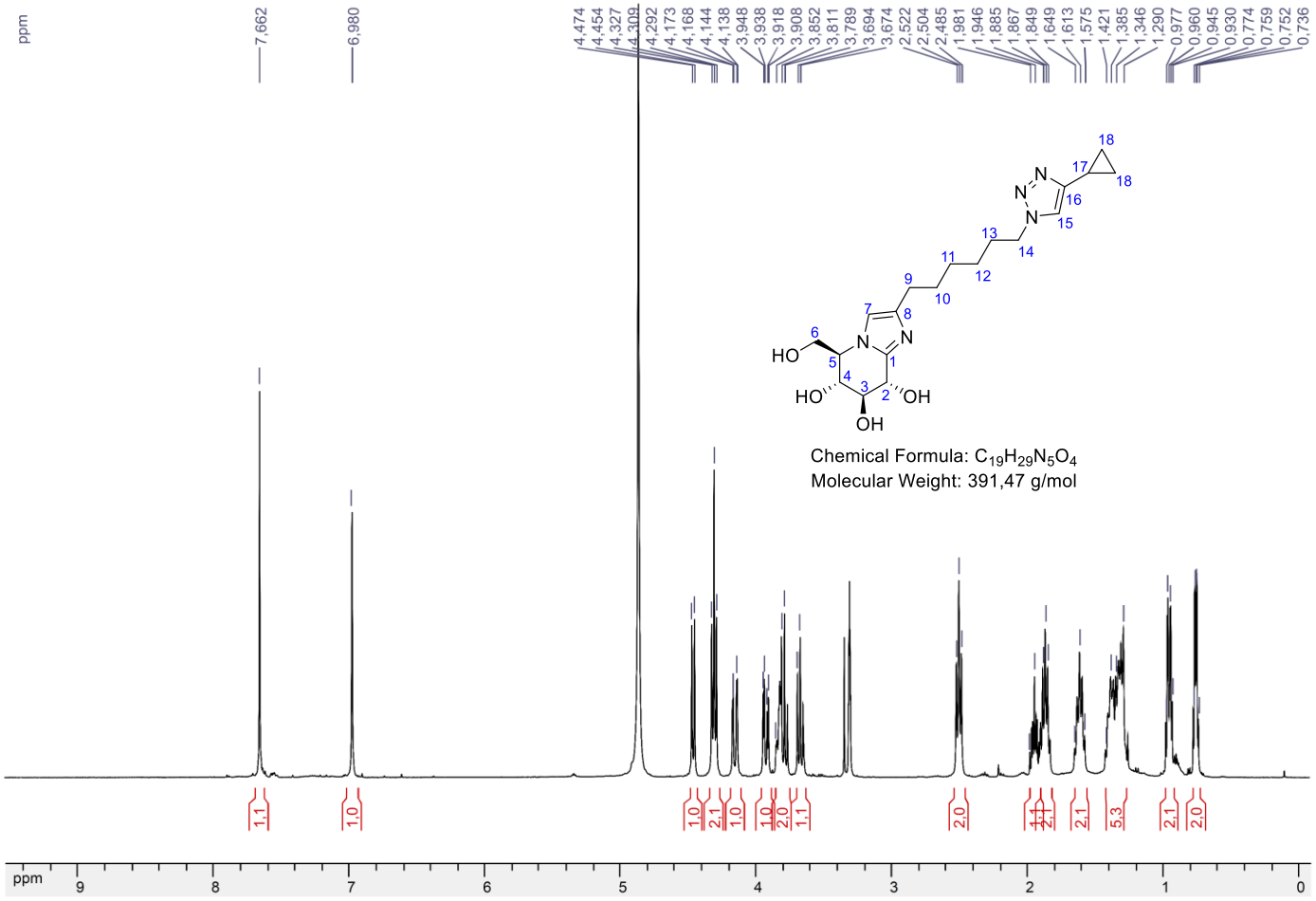


Fig S25. ^{1}H NMR (400 MHz, CD_3OD) spectrum of compound **13a**

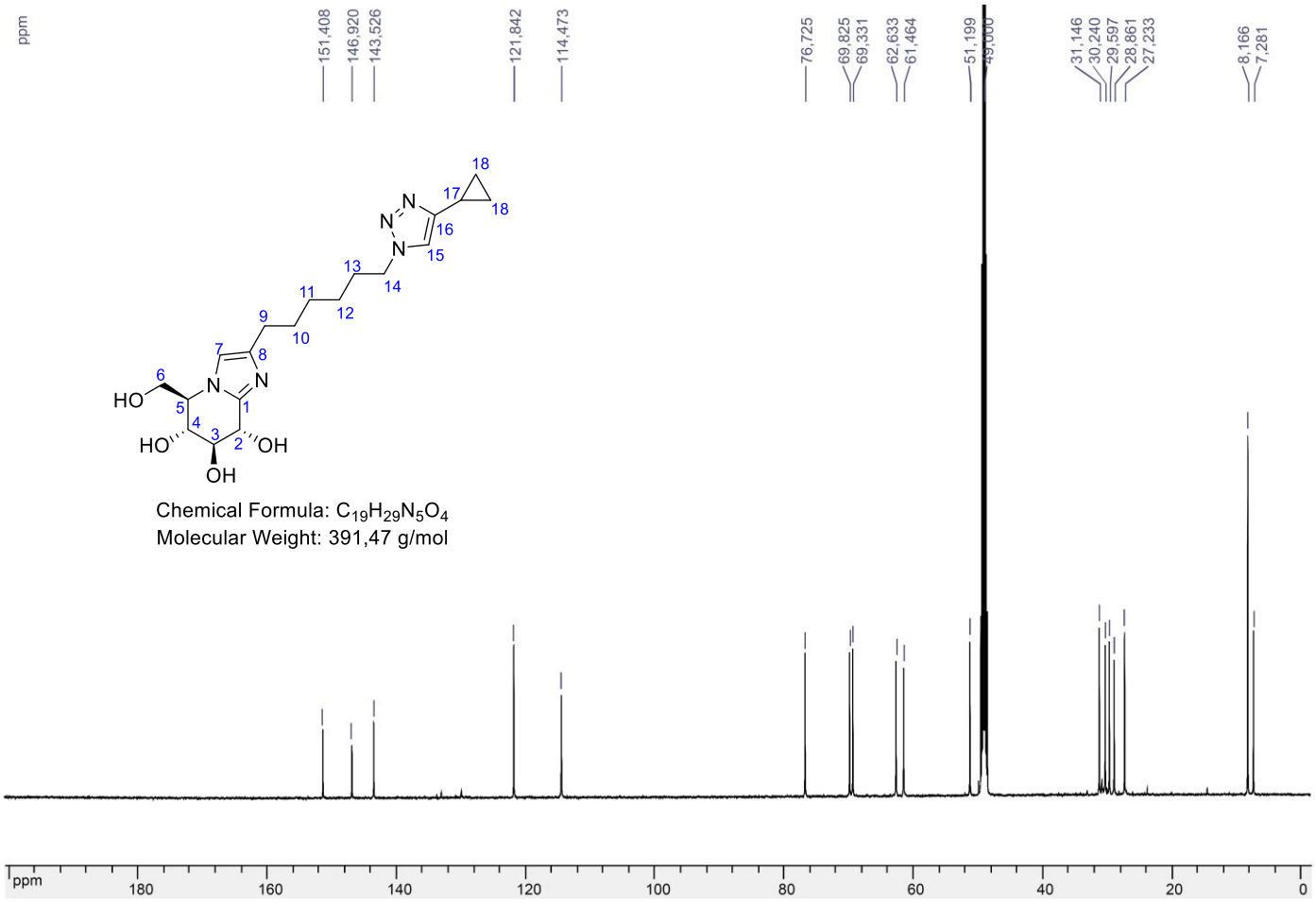


Fig S26. ^{13}C NMR (100 MHz, CD_3OD) spectrum of compound **13a**

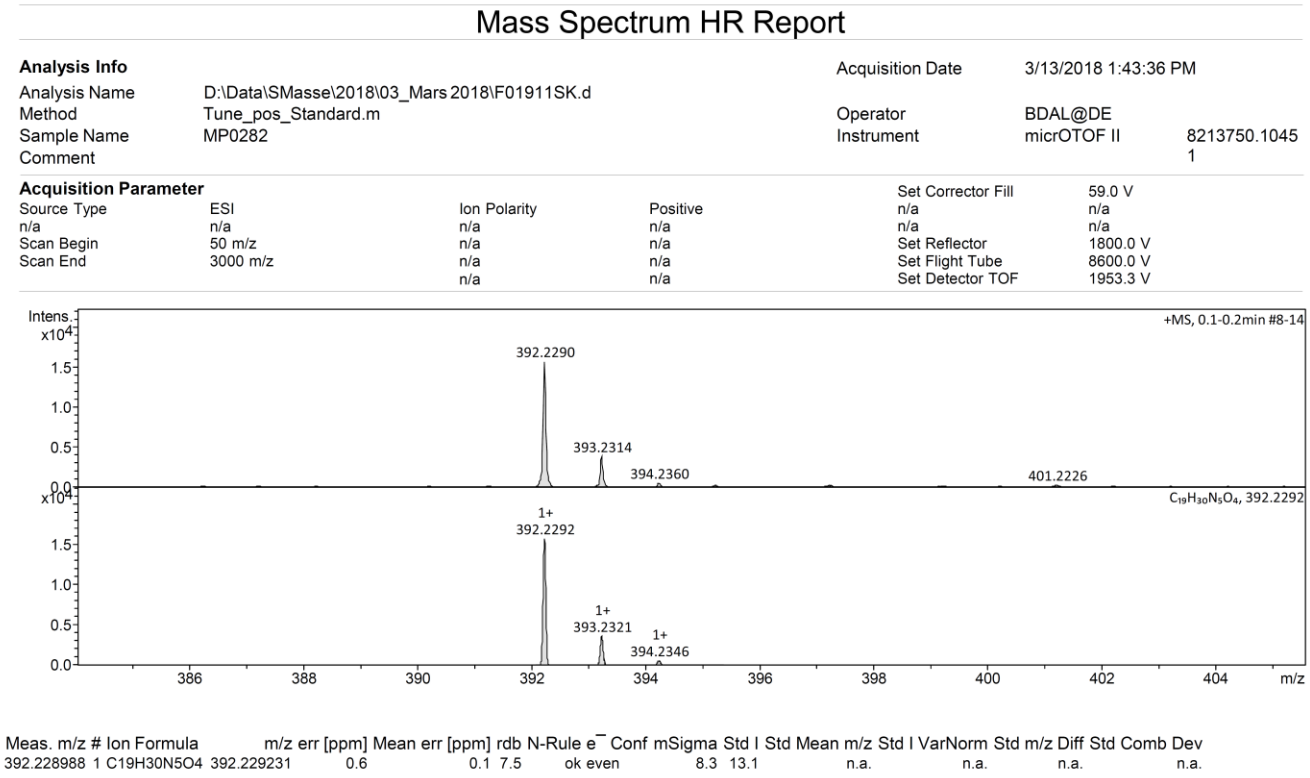


Fig S27. HRMS (ESI-MS) spectrum of compound **13a**

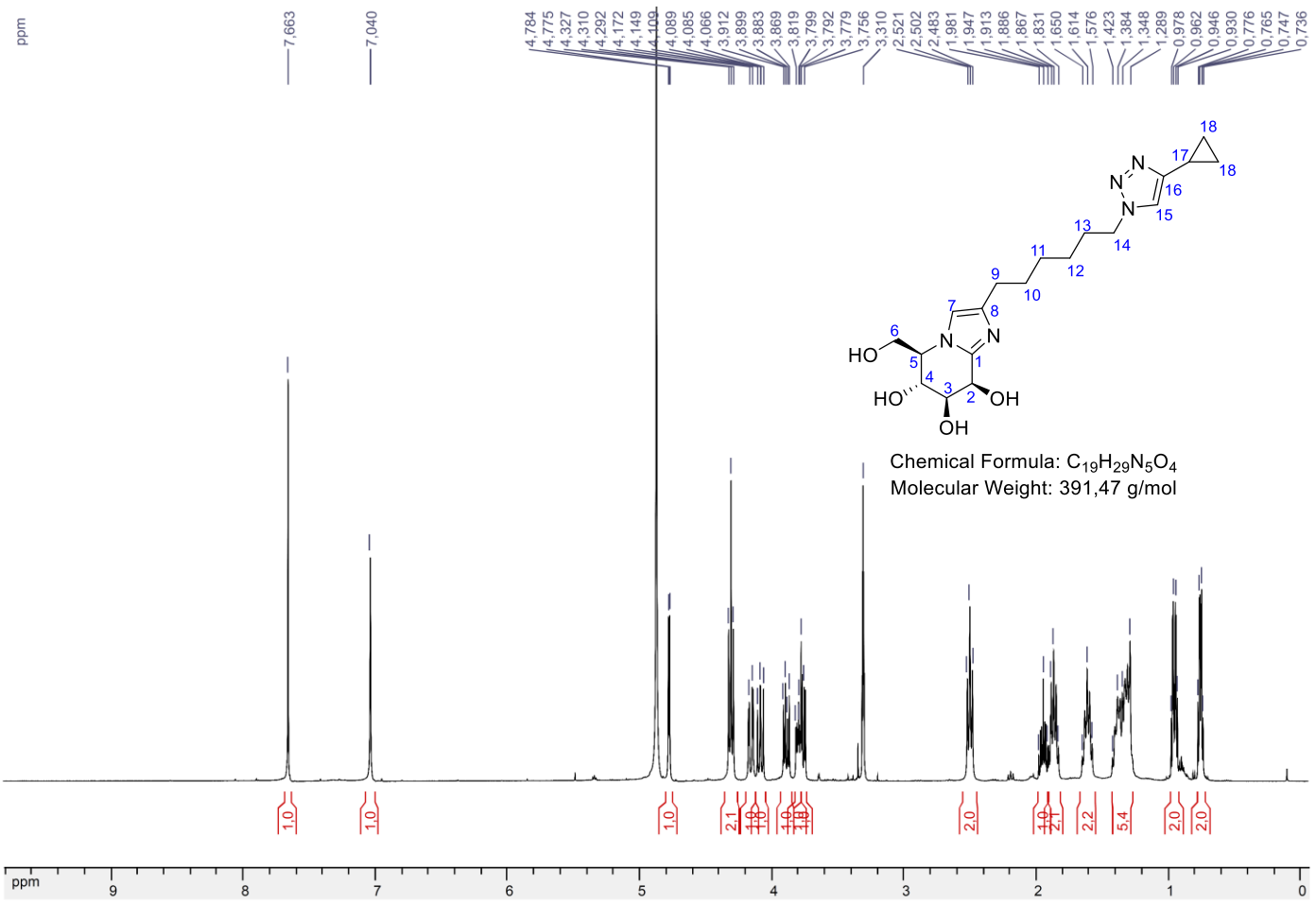


Fig S28. ^{1}H NMR (400 MHz, CD_3OD) spectrum of compound **13b**

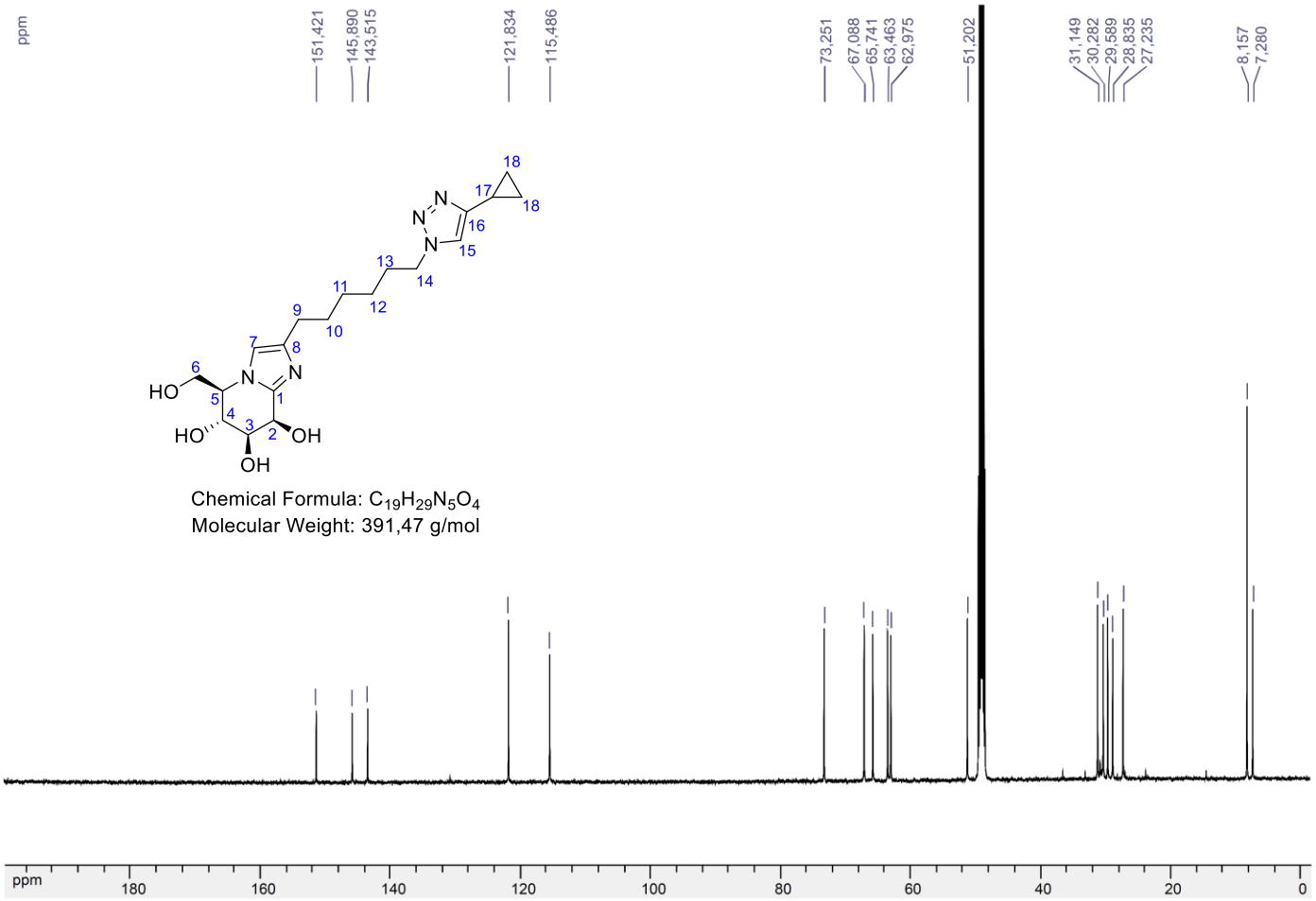
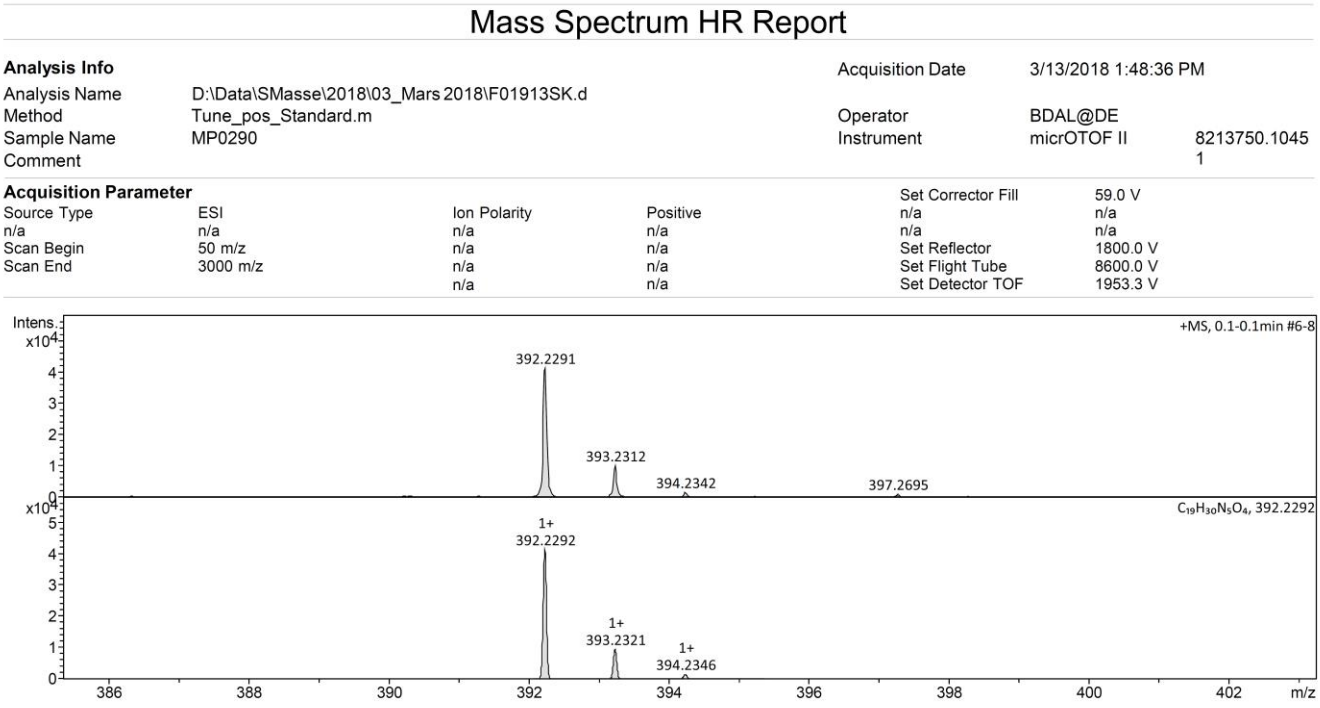


Fig S29. ^{13}C NMR (100 MHz, CD_3OD) spectrum of compound **13b**



Meas. m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I	VarNorm	Std m/z	Diff Std Comb	Dev
196.618868	1	C19H31N5O4	196.618254	-3.1	-2.7	7.0	ok	even	2.5	4.7	n.a.	n.a.	n.a.	n.a.		
392.229128	1	C19H30N5O4	392.229231	0.3	0.9	7.5	ok	even	9.3	15.9	n.a.	n.a.	n.a.	n.a.		

Fig S30. HRMS (ESI-MS) spectrum of compound **13b**

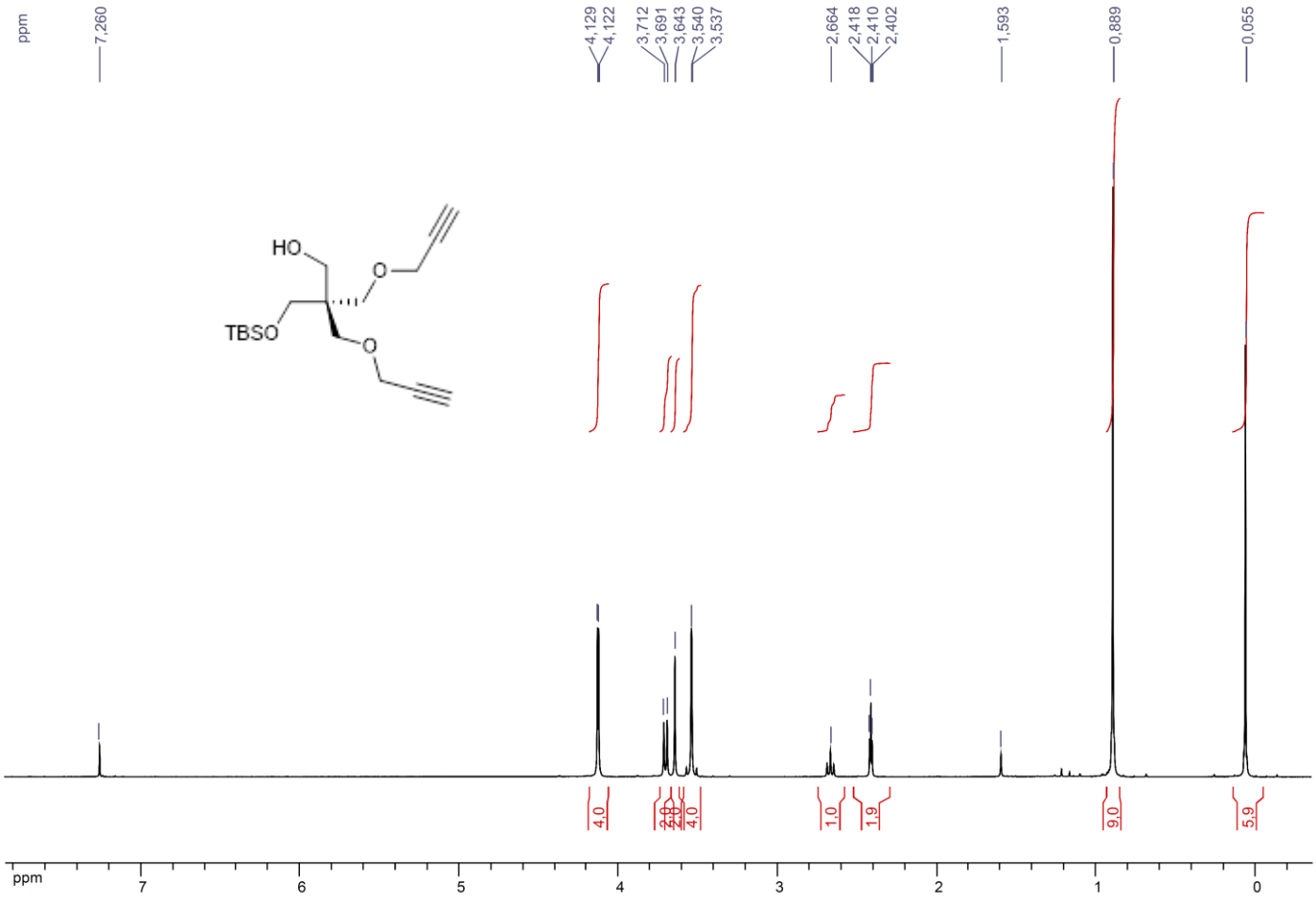


Fig S31. ^{1}H NMR (300 MHz, $CDCl_3$) spectrum of compound **16a**

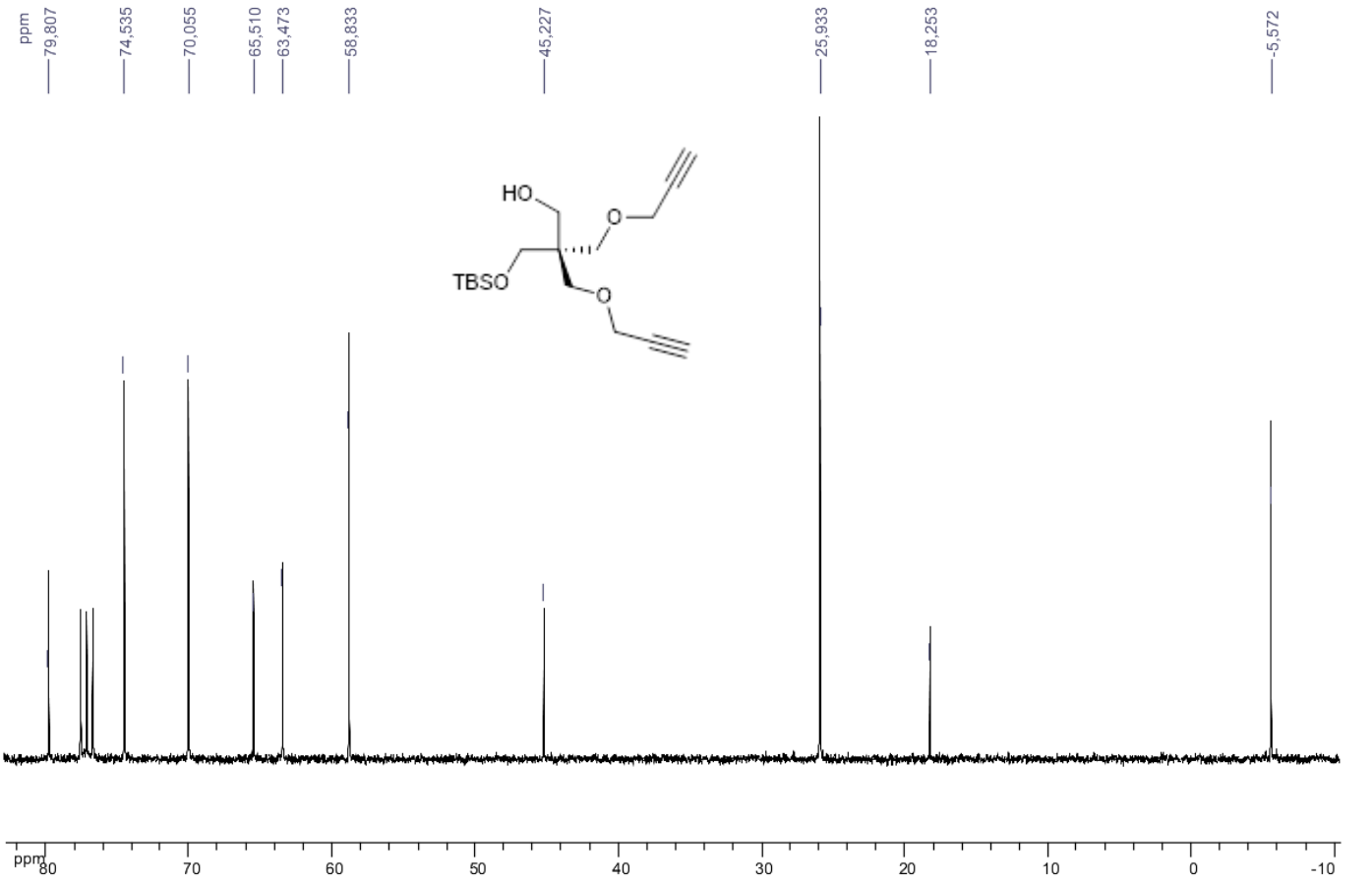


Fig S32. ^{13}C NMR (75 MHz, $CDCl_3$) spectrum of compound **16a**

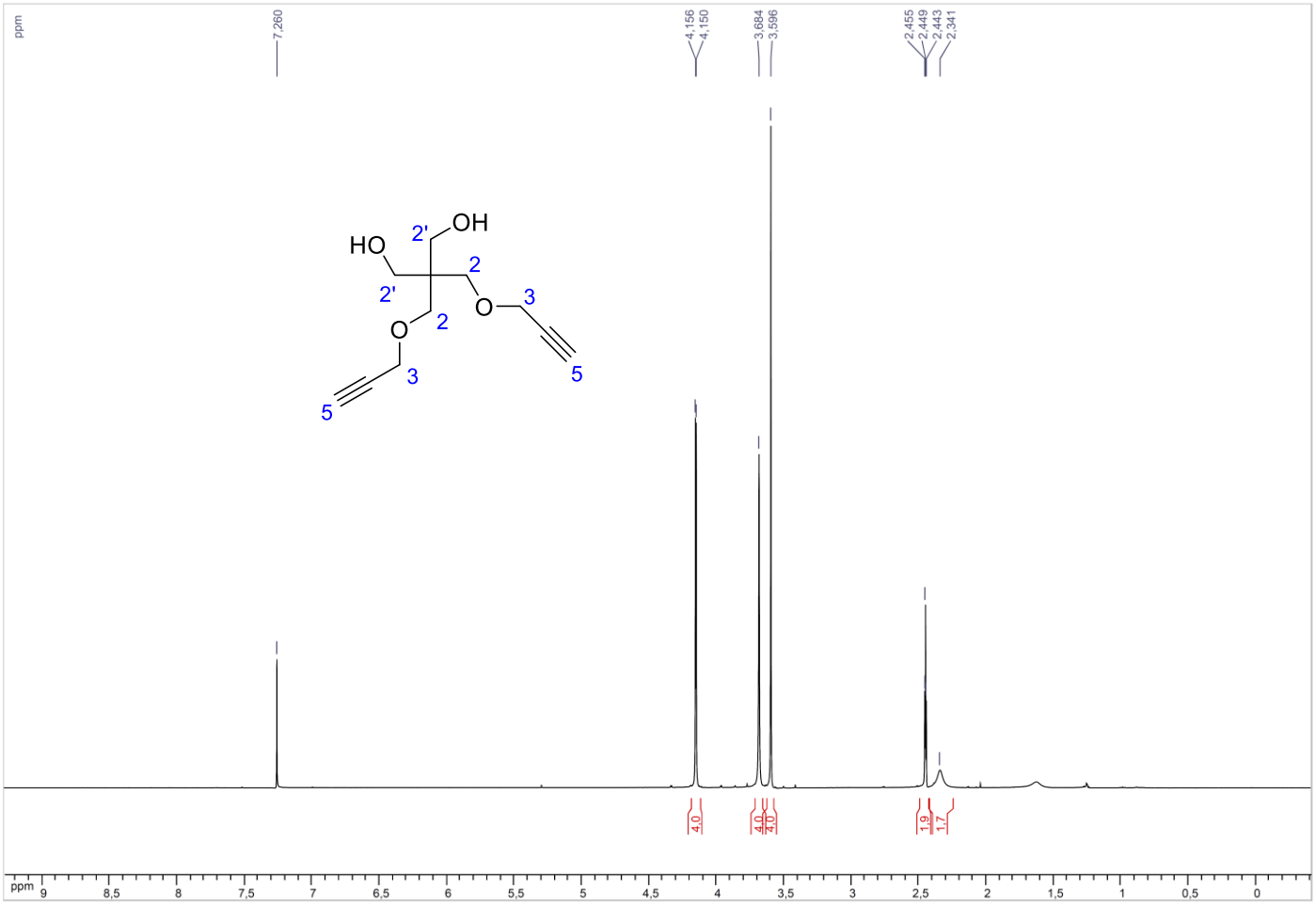


Fig S33. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **17a**

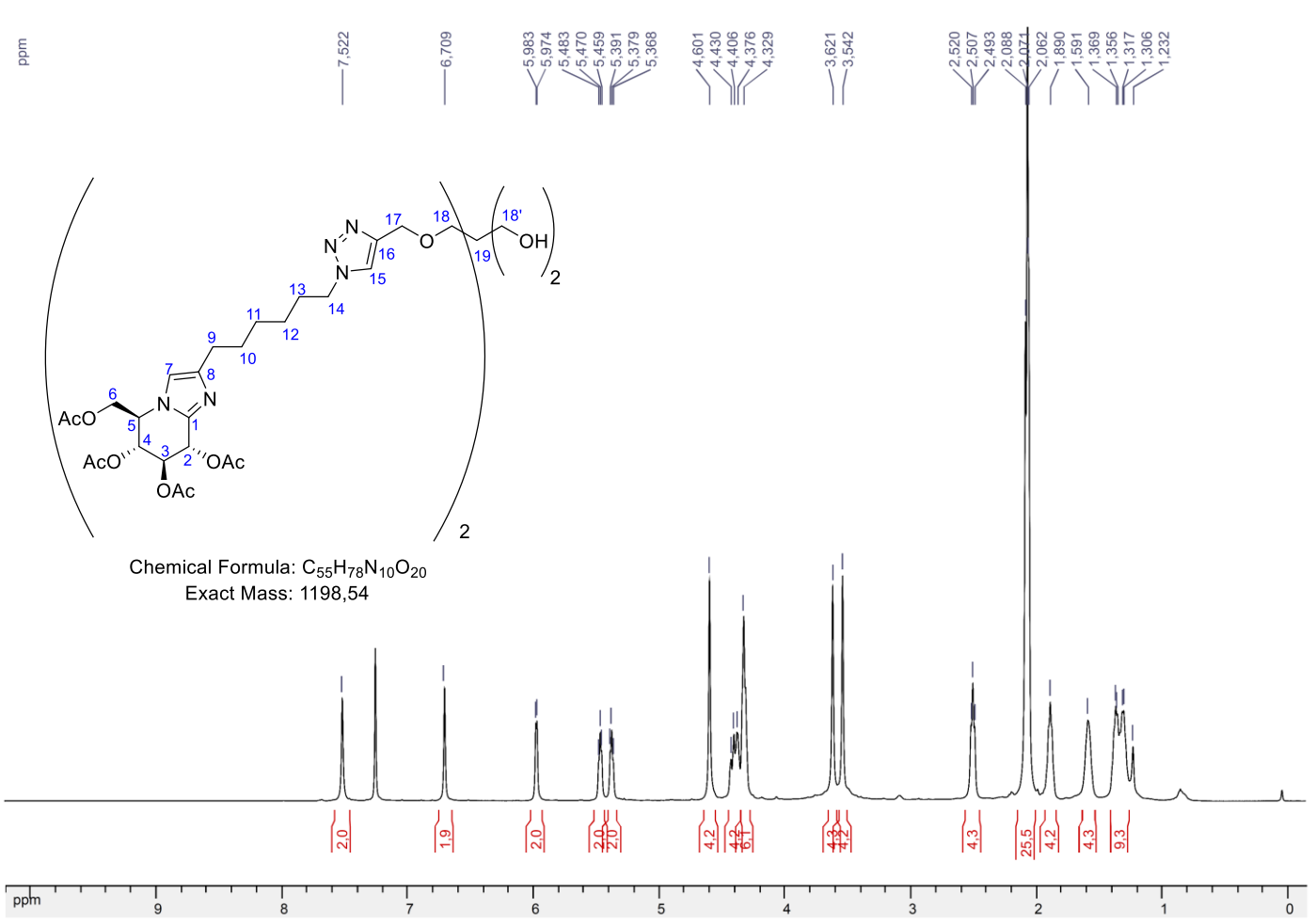


Fig S34. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **18a**

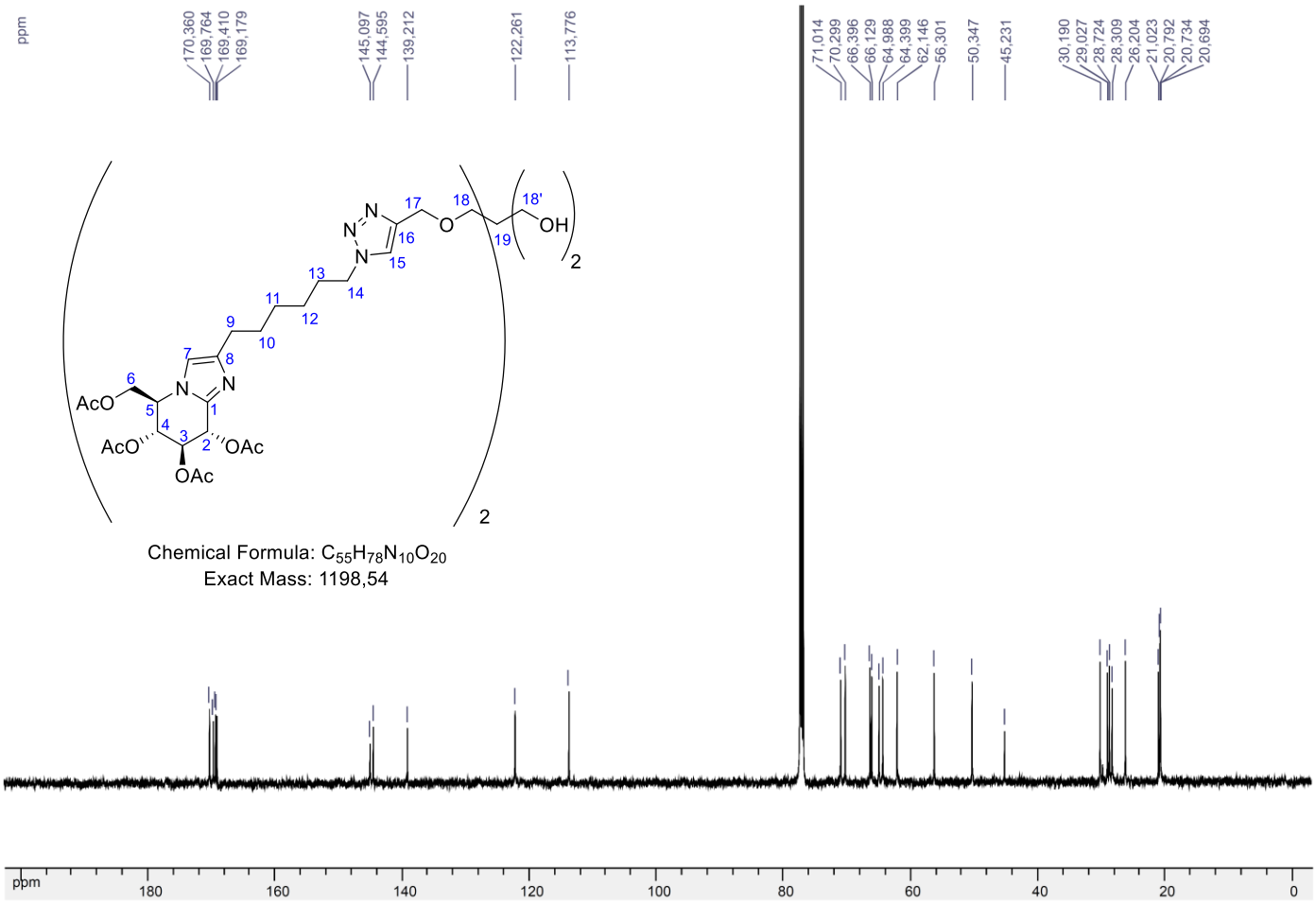


Fig S35. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **18a**

Mass Spectrum HR Report

Analysis Info

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Comment			

Acquisition Parameter

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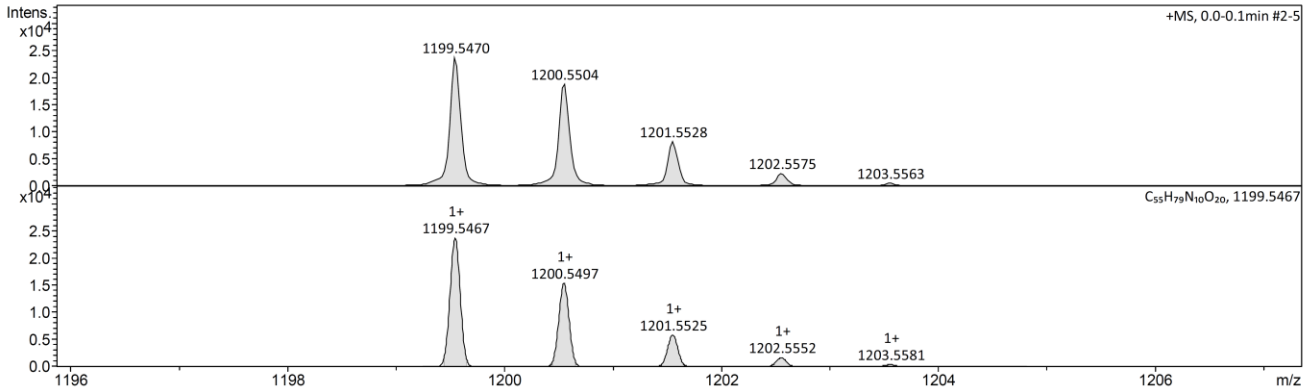
Scan End	3000 m/z	n/a	n/a	Set Flight Tube	8600.0 V
		n/a	n/a	Set Detector TOF	1953.3 V



Meas. m/z	#	Ion Formula	m/z err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I	VarNorm	Std m/z	Diff Std Comb	Dev
1199.546970	1	C55H79N10O20	1199.546661	-0.3	-0.4	21.5	ok	even	78.9	72.4	n.a.		n.a.		n.a.	

Fig S36. HRMS (ESI-MS) spectrum of compound **18a**

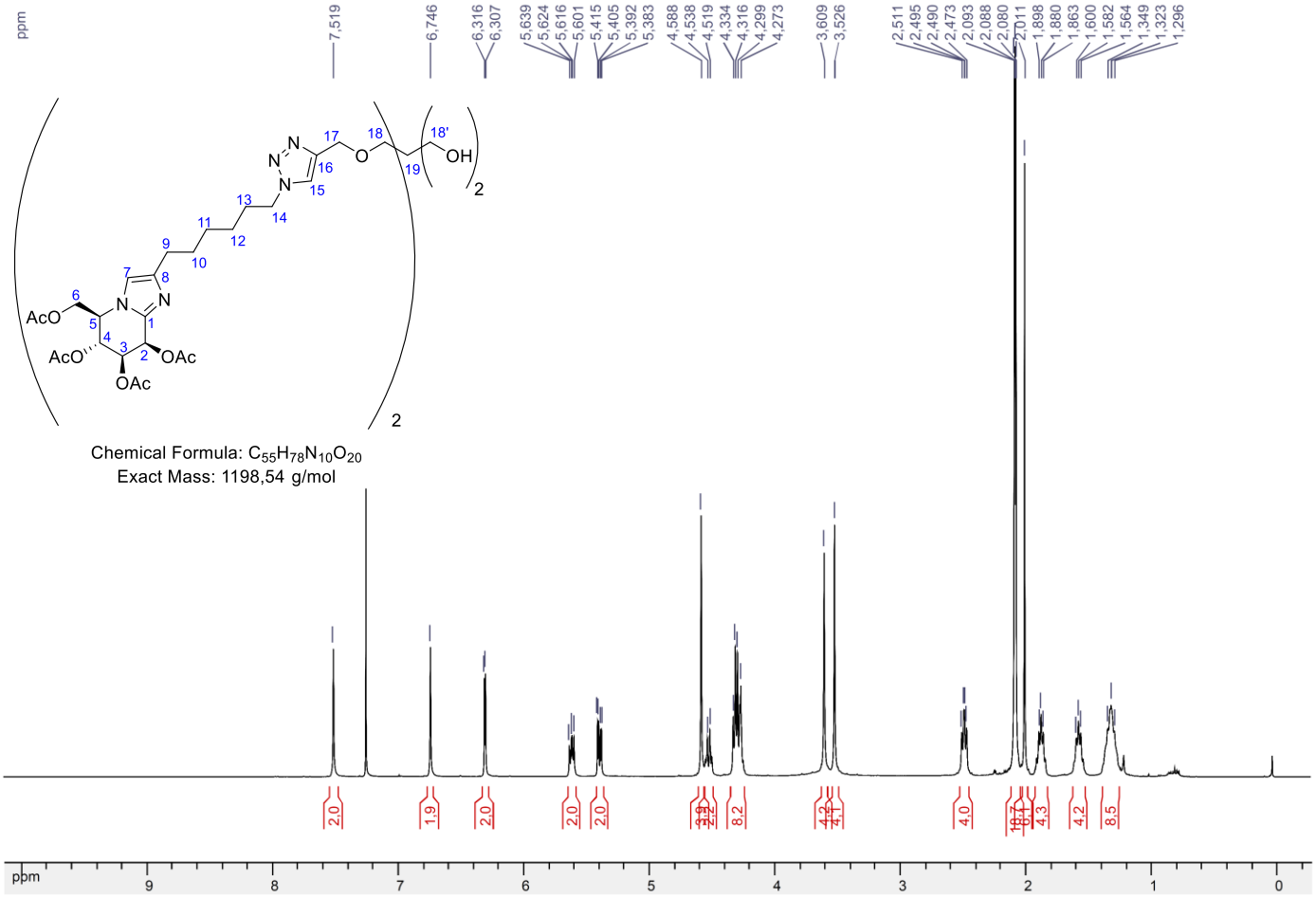


Fig S37. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **18b**

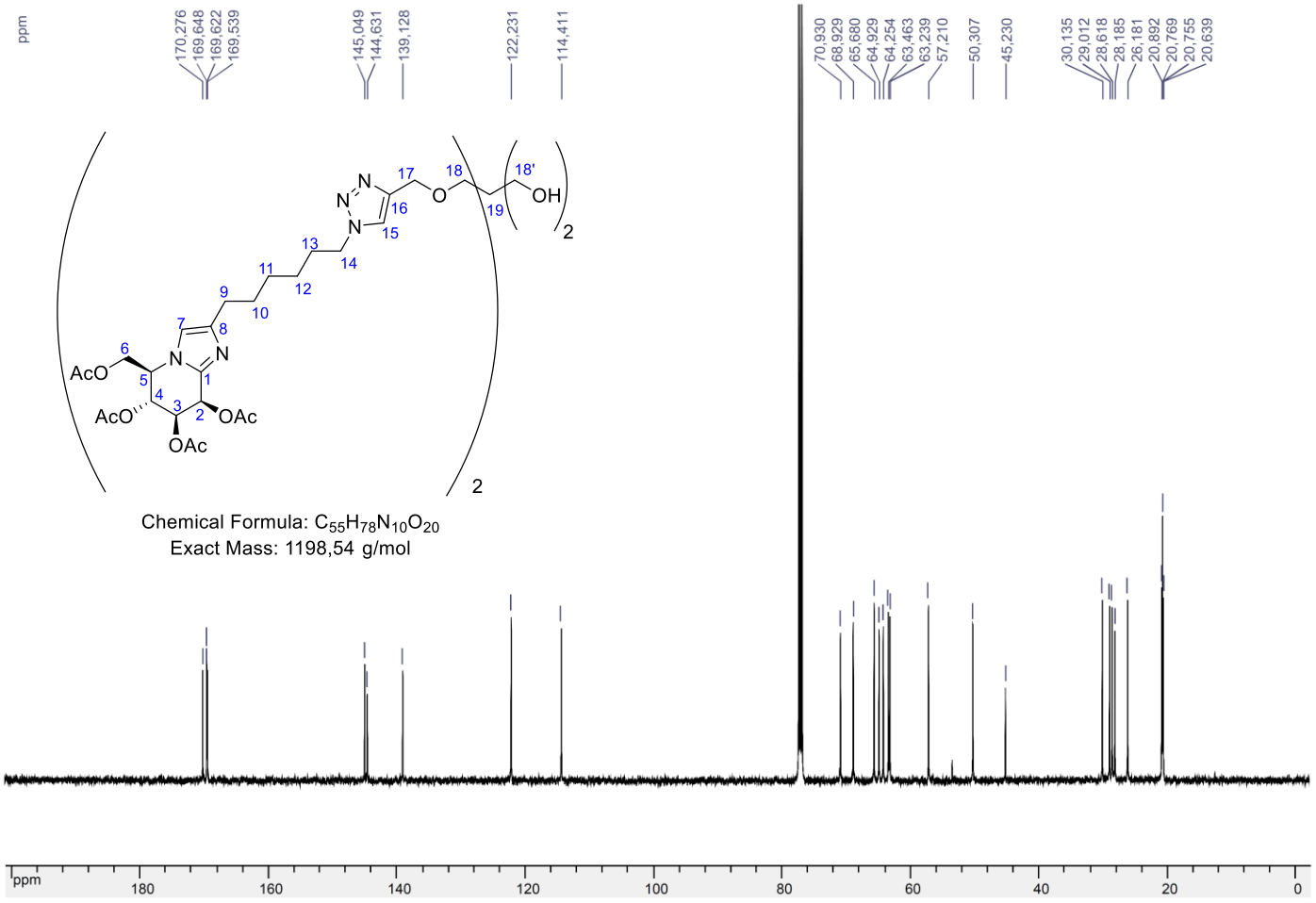


Fig S38. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **18b**

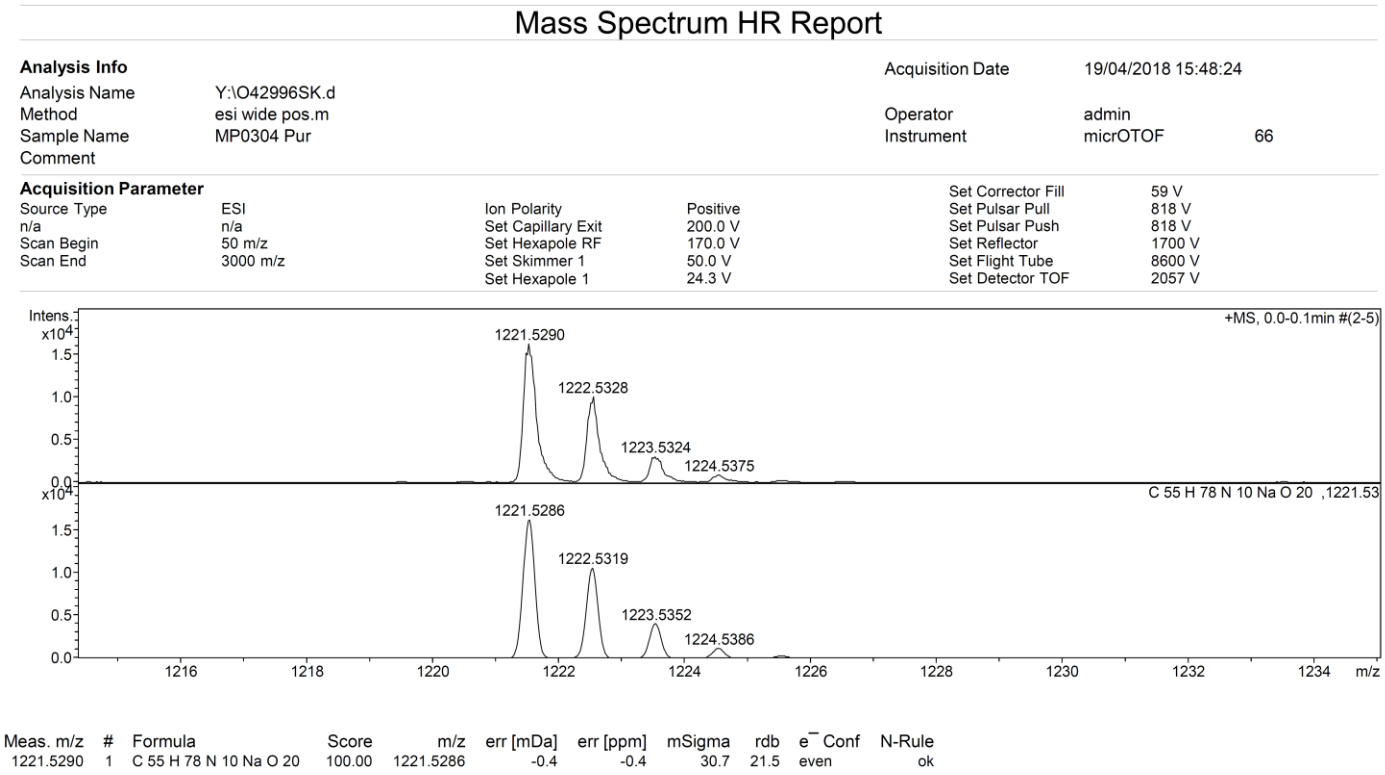


Fig S39. HRMS (ESI-MS) spectrum of compound **18b**

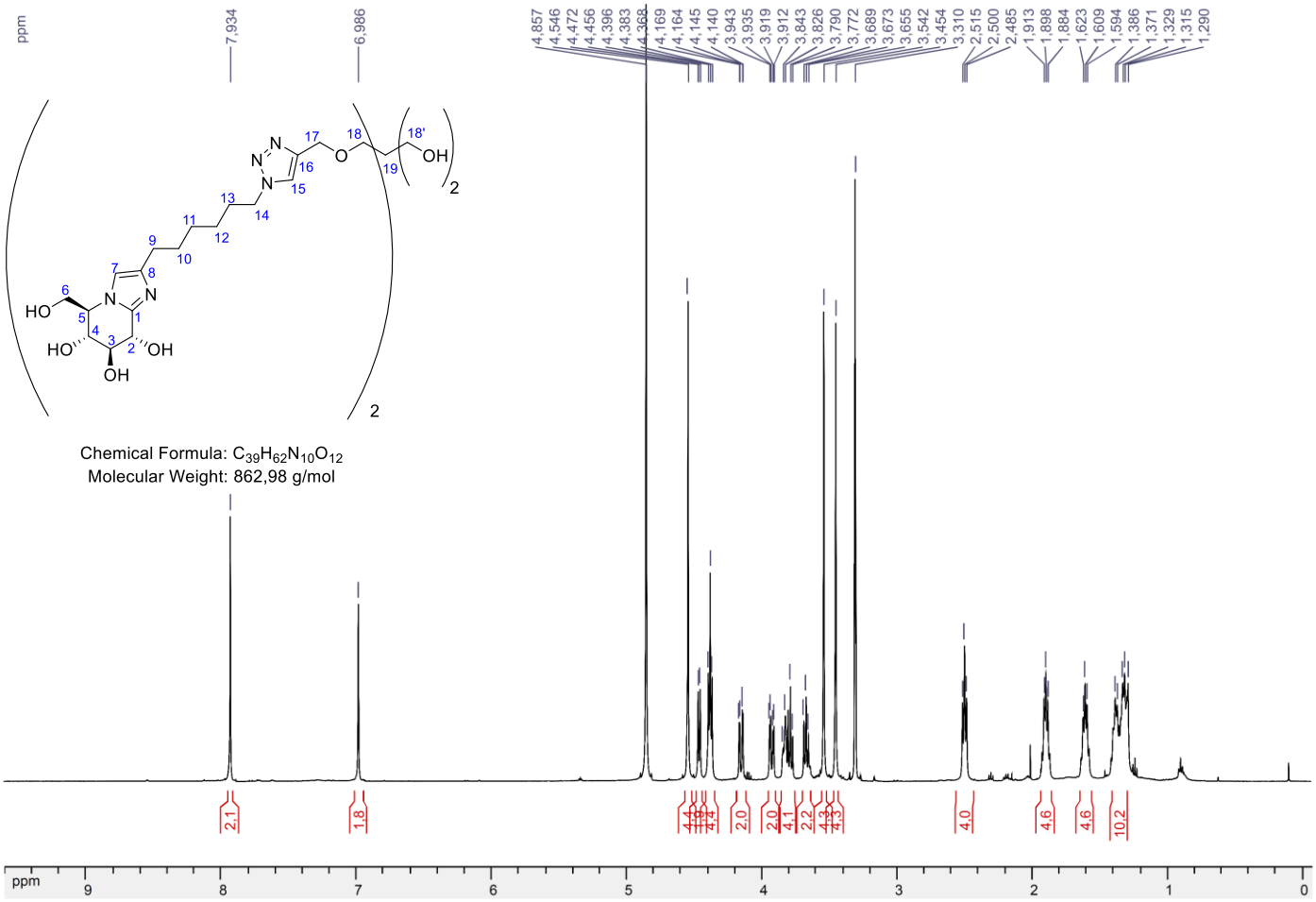


Fig S40. ^{1}H NMR (500 MHz, CD_3OD) spectrum of compound **19a**

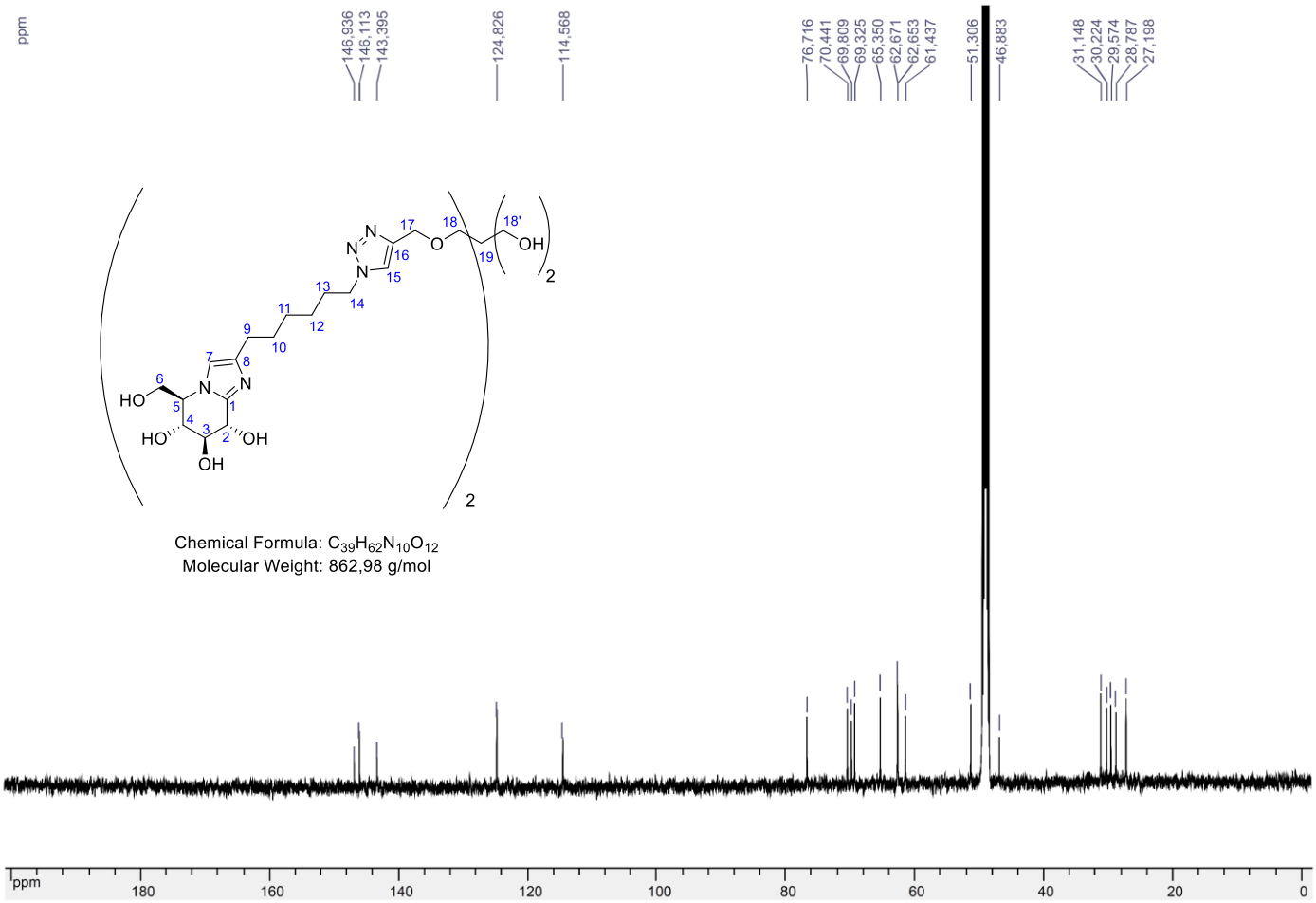
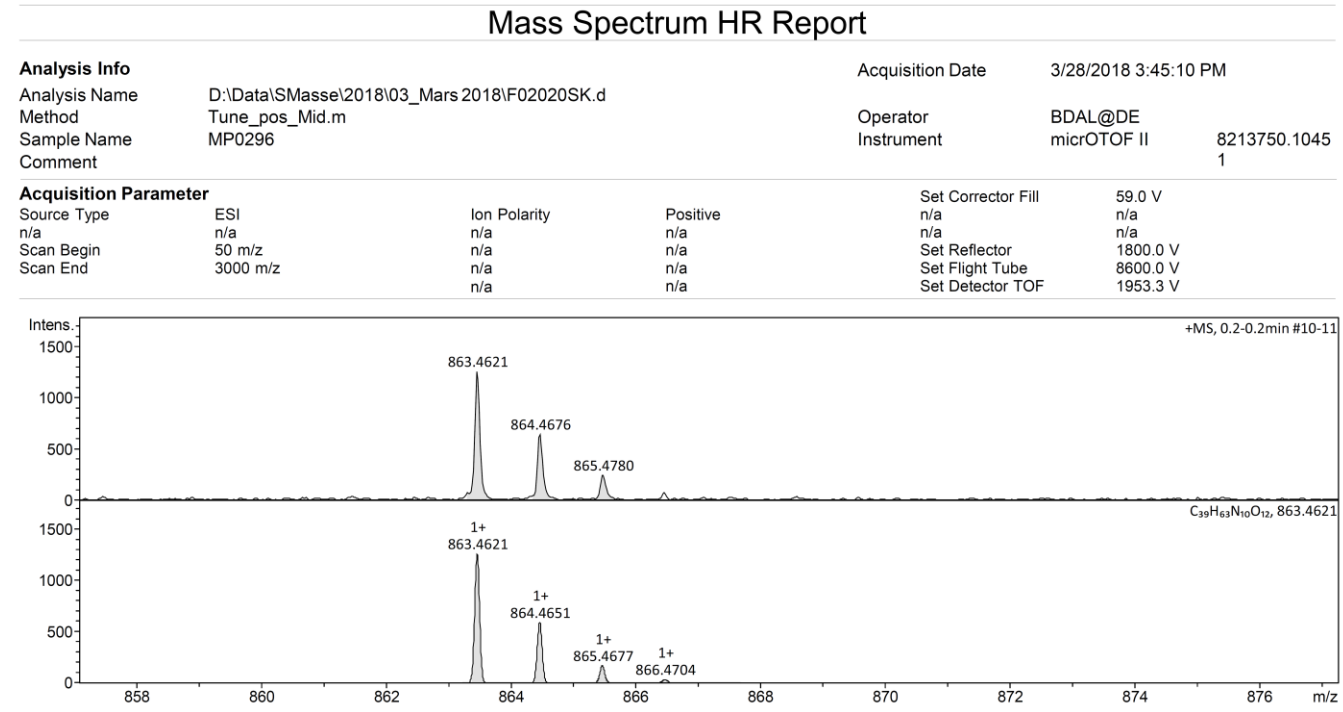


Fig S41. ^{13}C NMR (125 MHz, CD_3OD) spectrum of compound **19a**



Meas. m/z	#	Ion Formula	m/z err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I	VarNorm	Std m/z	Diff Std Comb	Dev
432.238217	1	C39H64N10O12	432.234710	-8.1	-7.4	13.0	ok	even	82.5	98.6	n.a.	n.a.	n.a.	n.a.	
863.462135	1	C39H63N10O12	863.462144	0.0	547.7	13.5	ok	even	40.7	48.2	n.a.	n.a.	n.a.	n.a.	

Fig S42. HRMS (ESI-MS) spectrum of compound **19a**

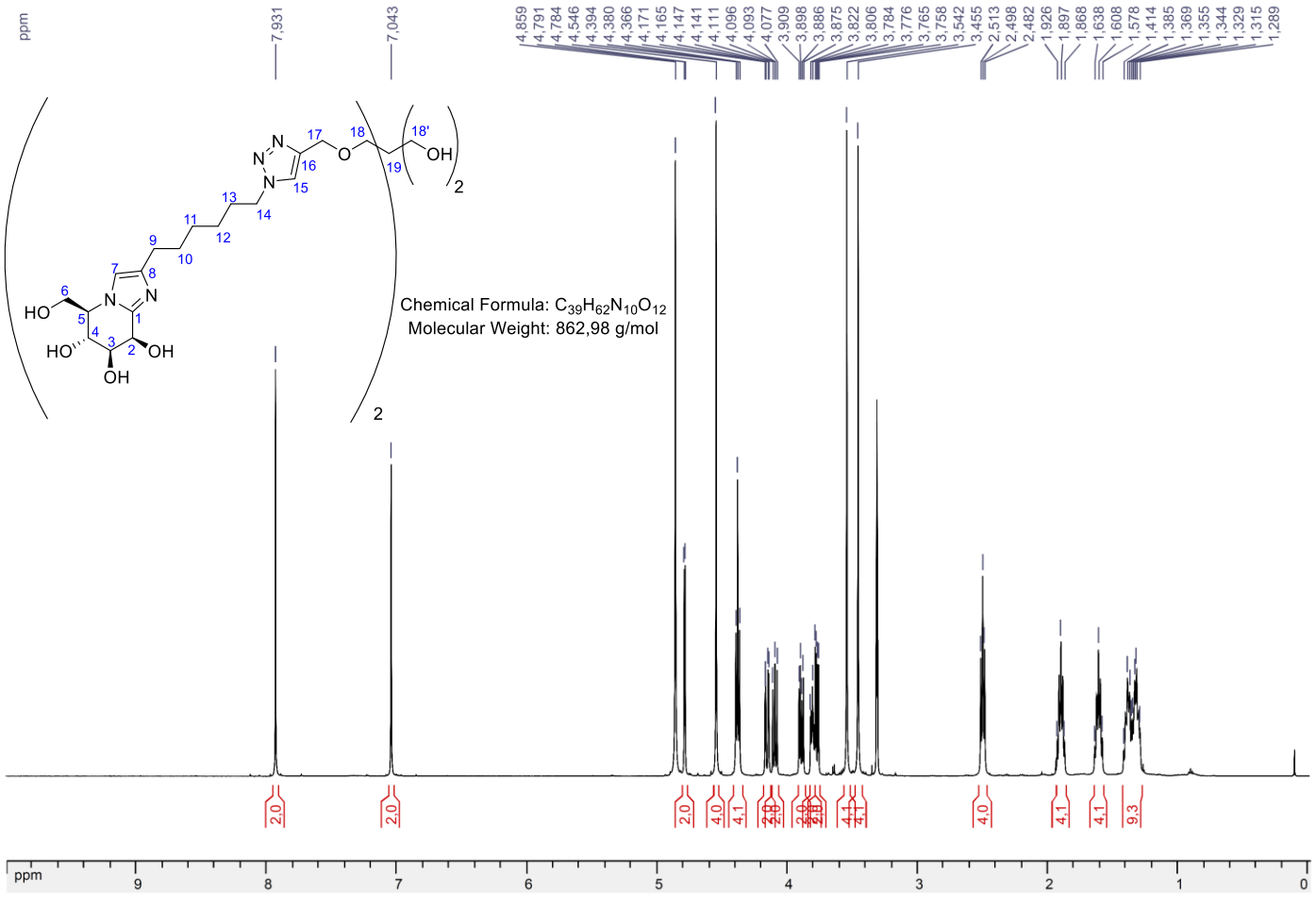


Fig S43. ^{1}H NMR (500 MHz, CD_3OD) spectrum of compound **19b**

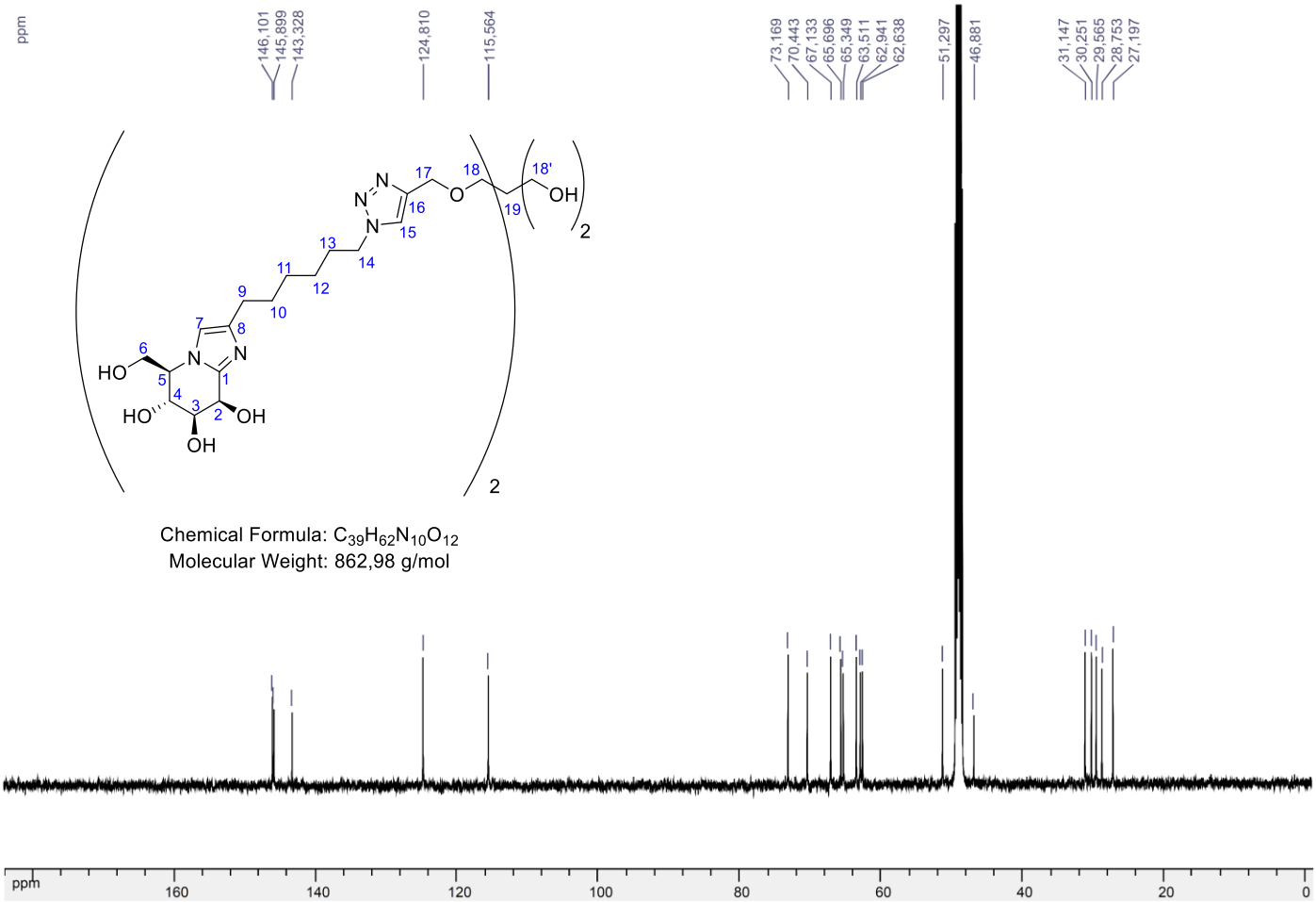


Fig S44. ^{13}C NMR (125 MHz, CD_3OD) spectrum of compound **19b**

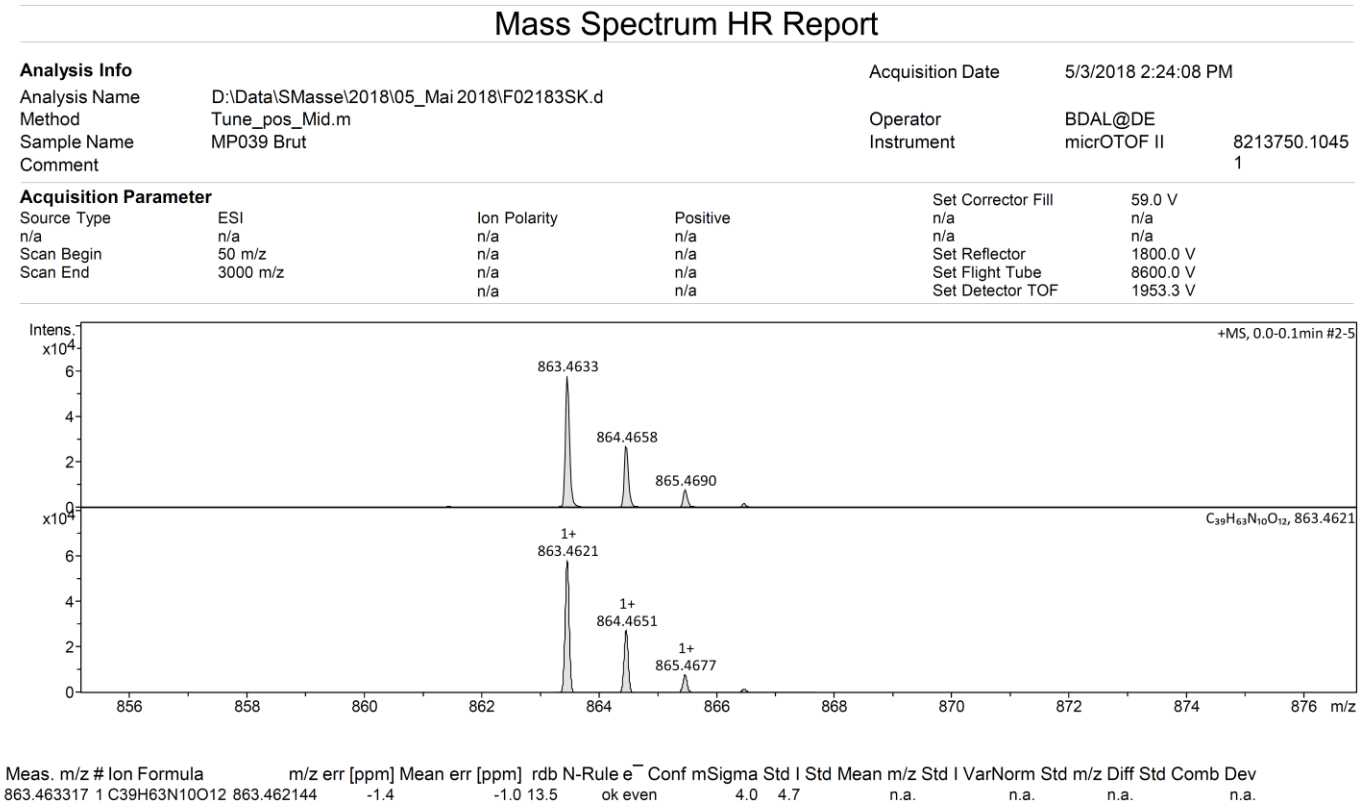


Fig S45. HRMS (ESI-MS) spectrum of compound **19b**

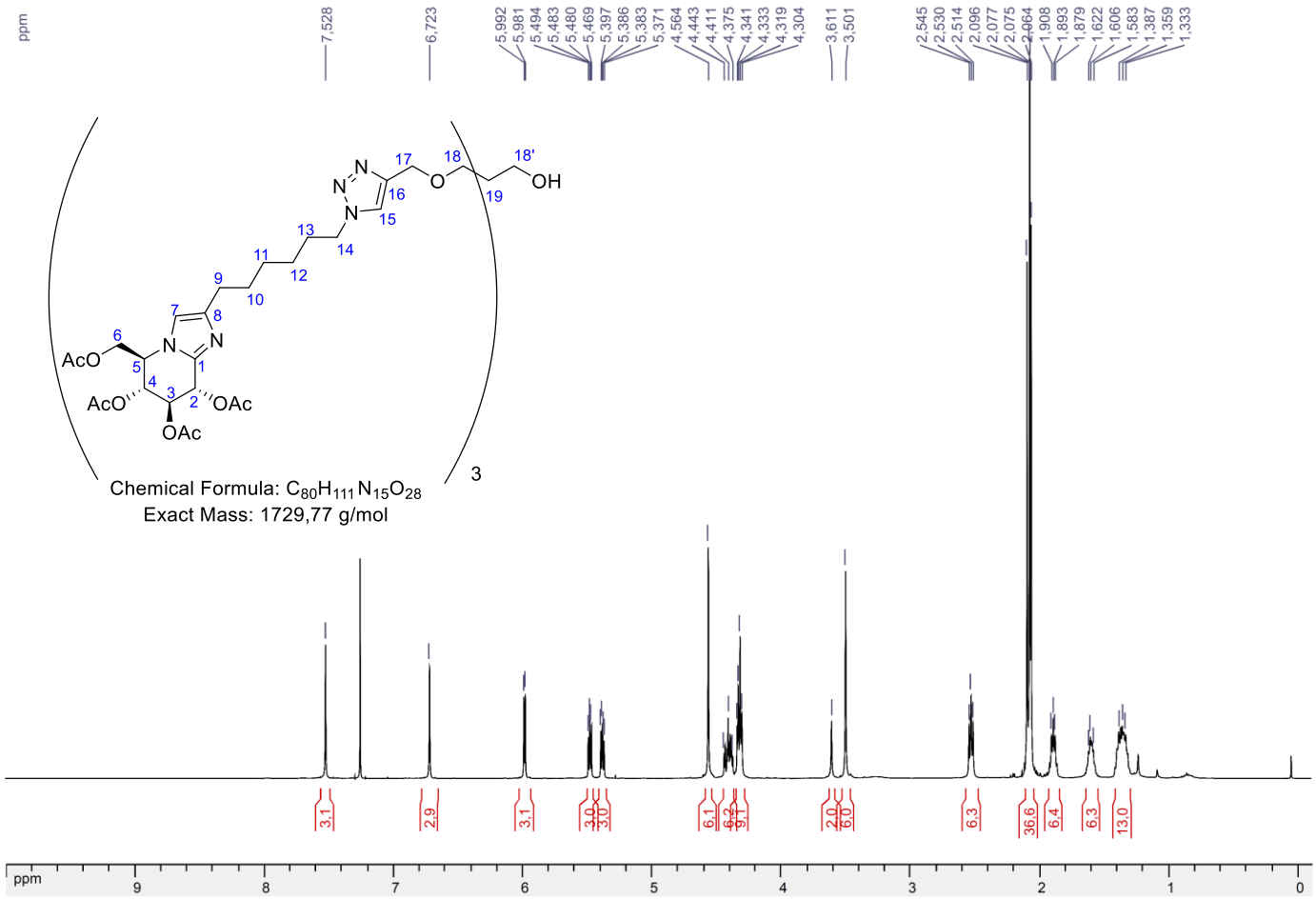


Fig S46. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **20a**

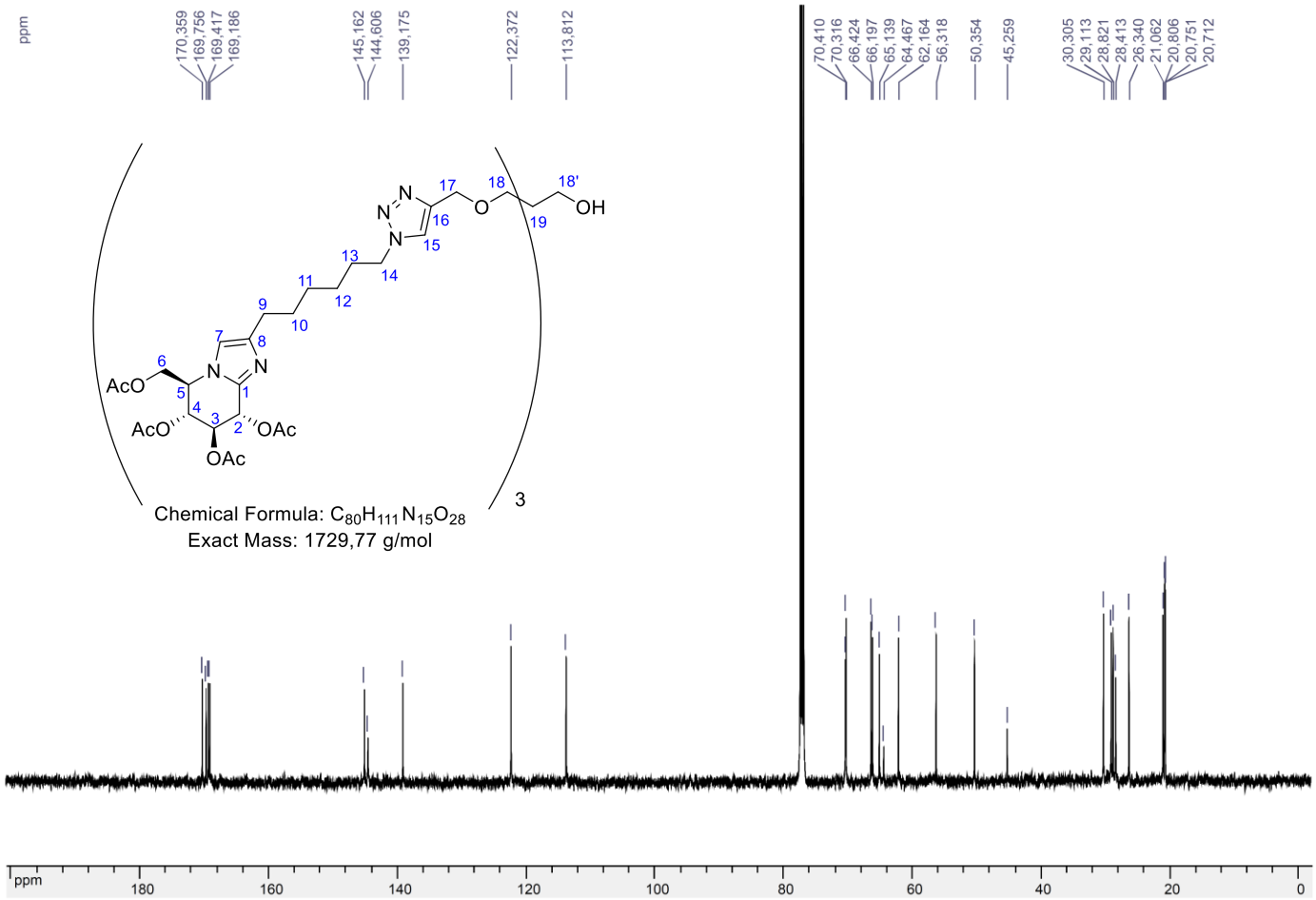
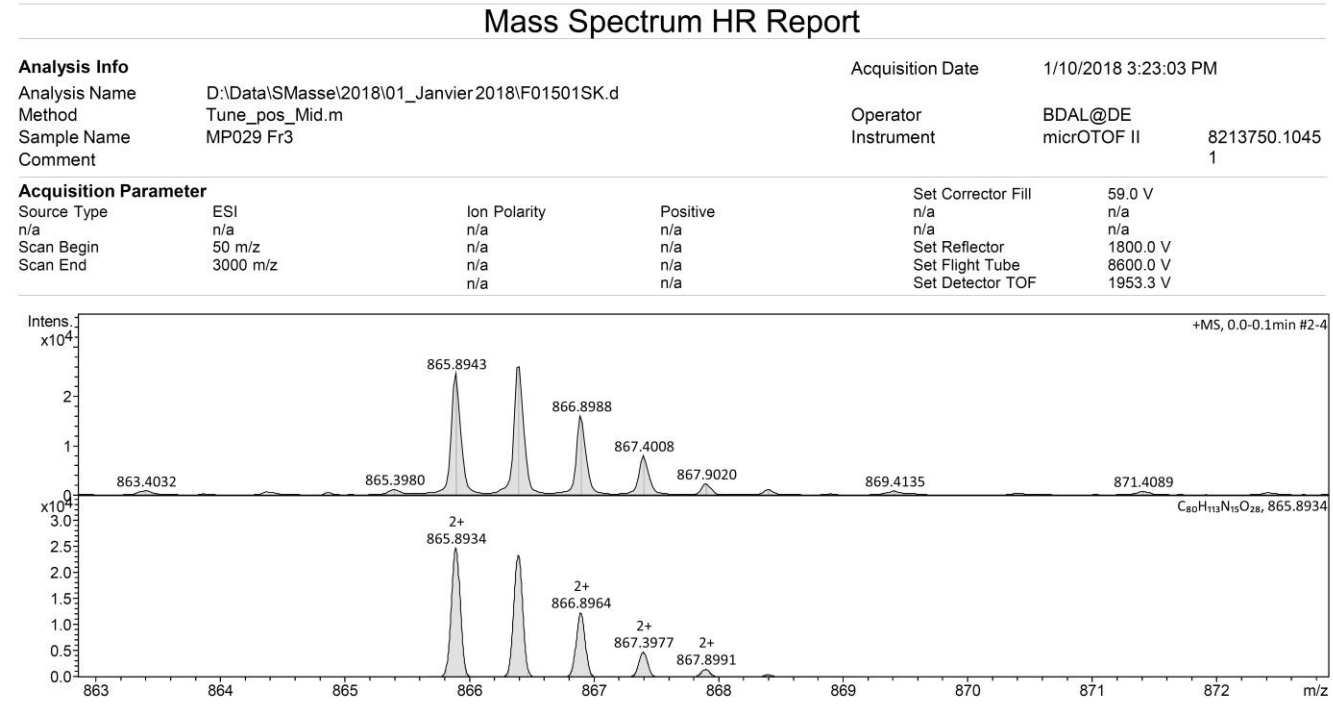


Fig S47. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **20a**



Meas. m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I	VarNorm	Std m/z Diff	Std Comb Dev
865.894263	1	C80H113N15O28	865.893425	-1.0	-2.4	32.0	ok	even	77.2	70.0	n.a.		n.a.	n.a.	n.a.
1730.777194	1	C80H112N15O28	1730.779574	1.4	526.9	32.5	ok	even	83.7	71.5	n.a.		n.a.	n.a.	n.a.

Fig S48. HRMS (ESI-MS) spectrum of compound **20a**

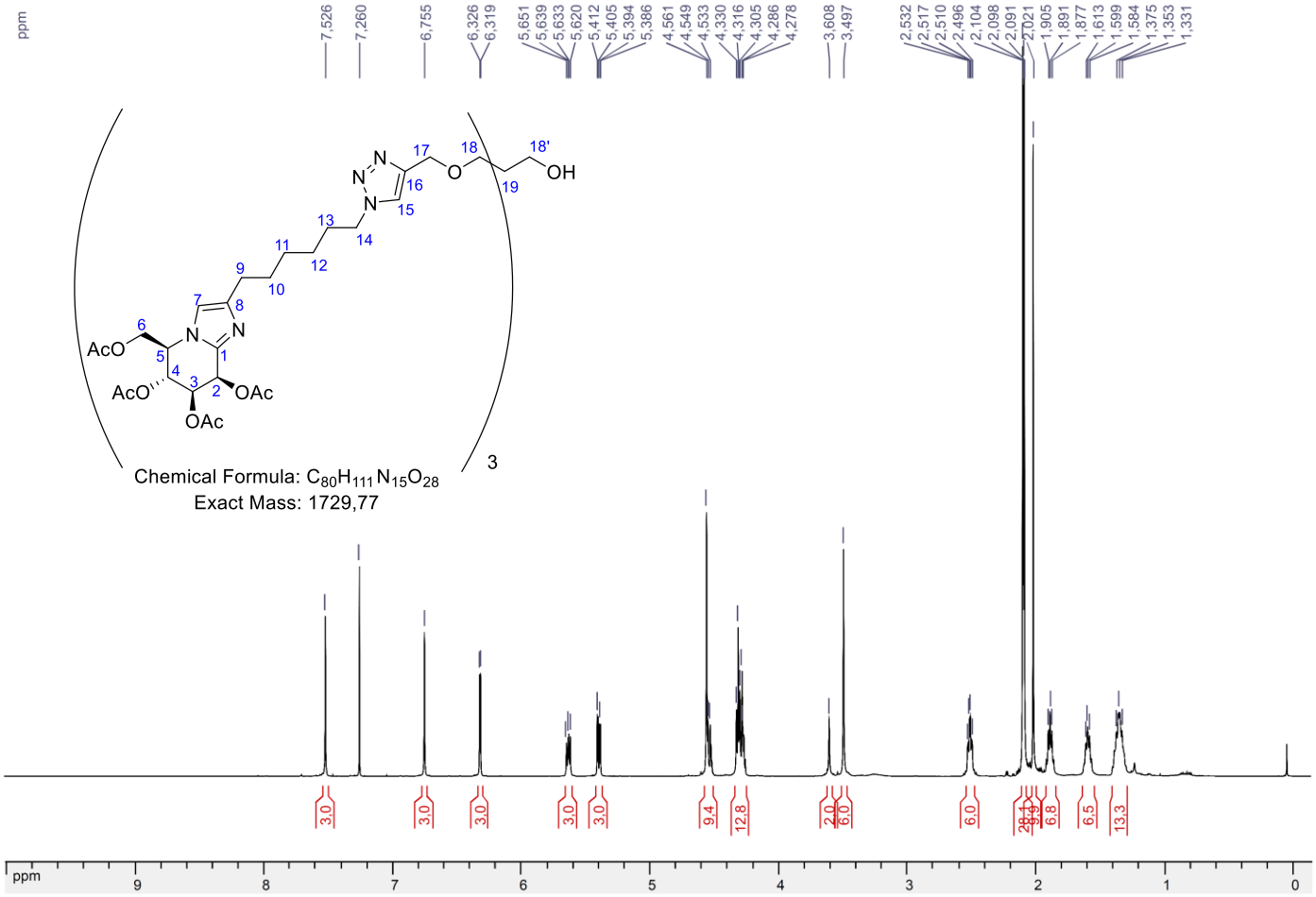


Fig S49. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **20b**

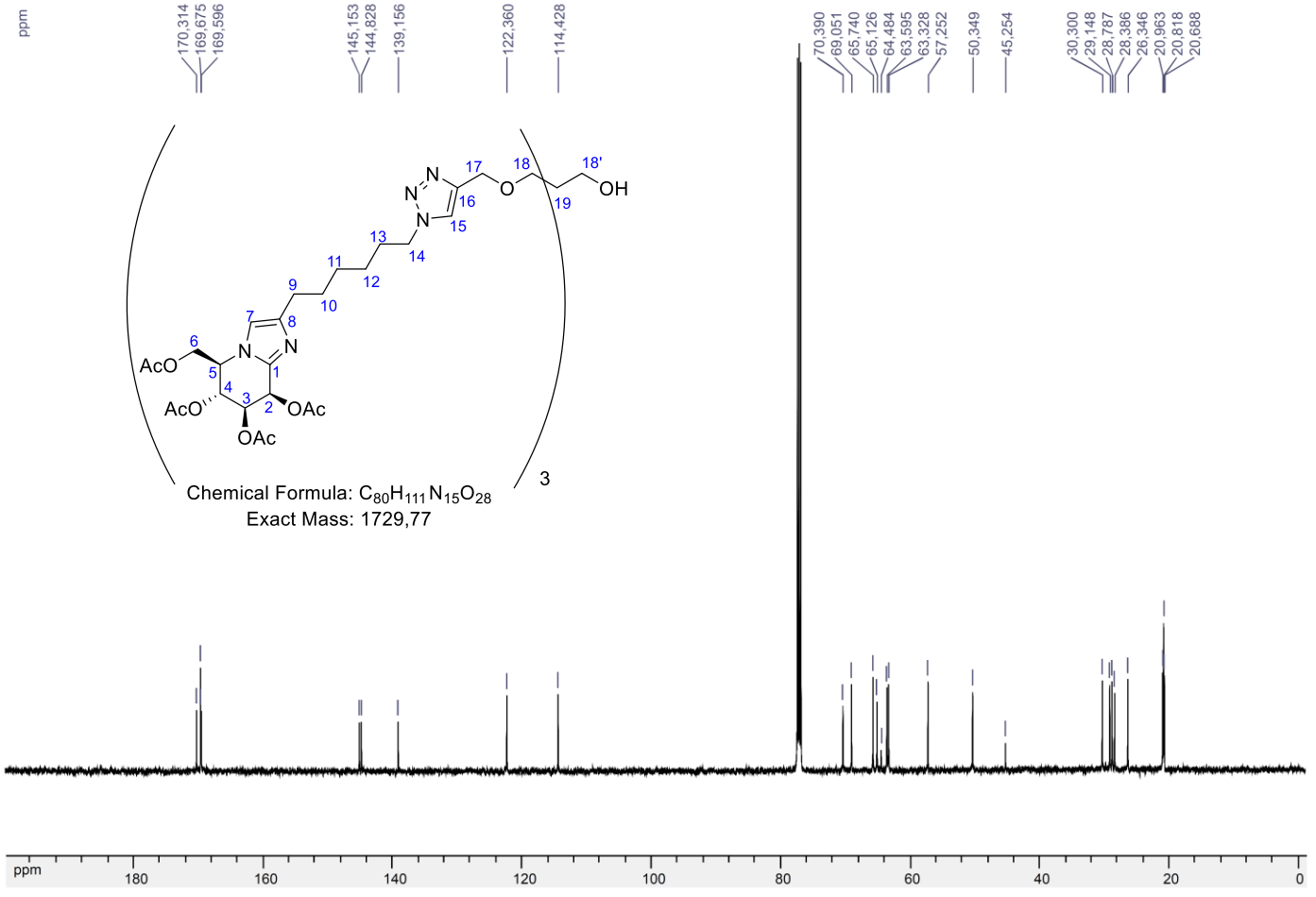
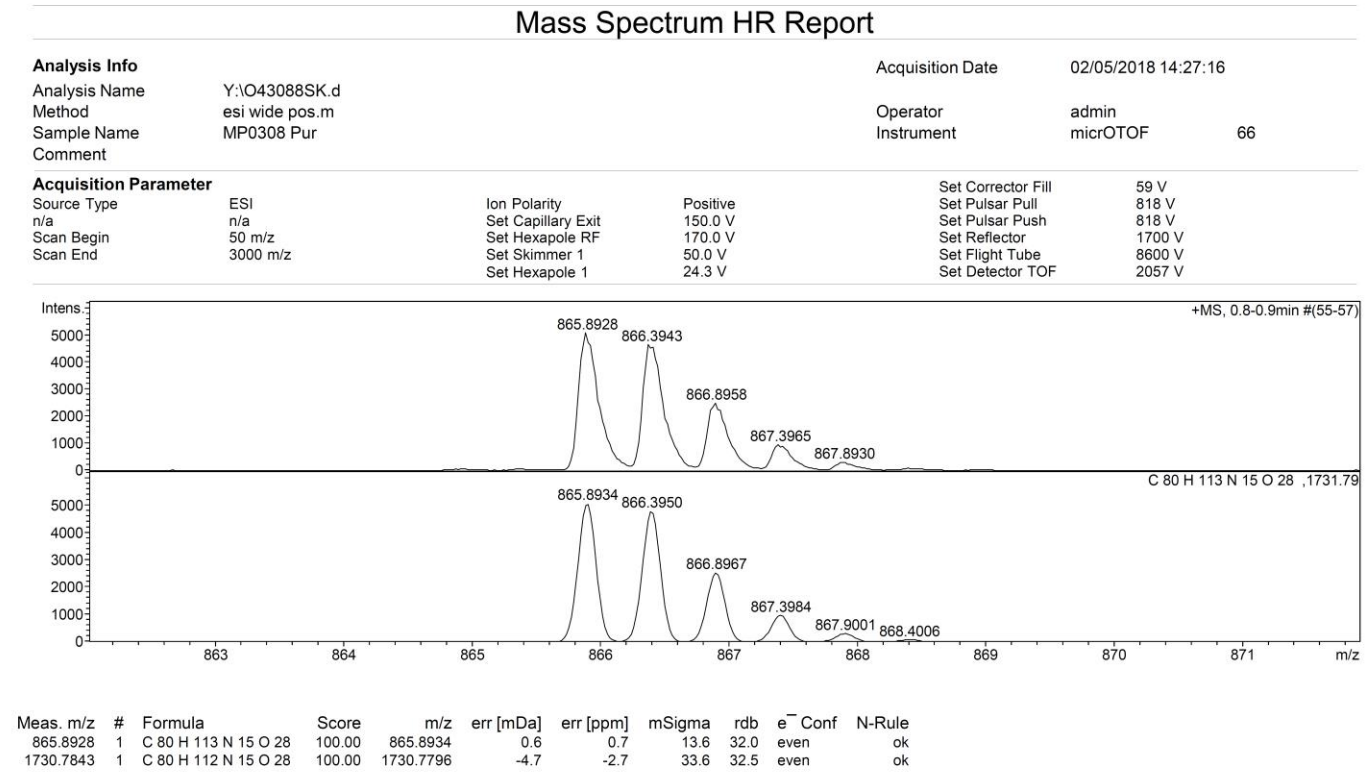


Fig S50. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **20b**



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
865.8928	1	C 80 H 113 N 15 O 28	100.00	865.8934	0.6	0.7	13.6	32.0	even	ok
1730.7843	1	C 80 H 112 N 15 O 28	100.00	1730.7796	-4.7	-2.7	33.6	32.5	even	ok

Fig S51. HRMS (ESI-MS) spectrum of compound **20b**

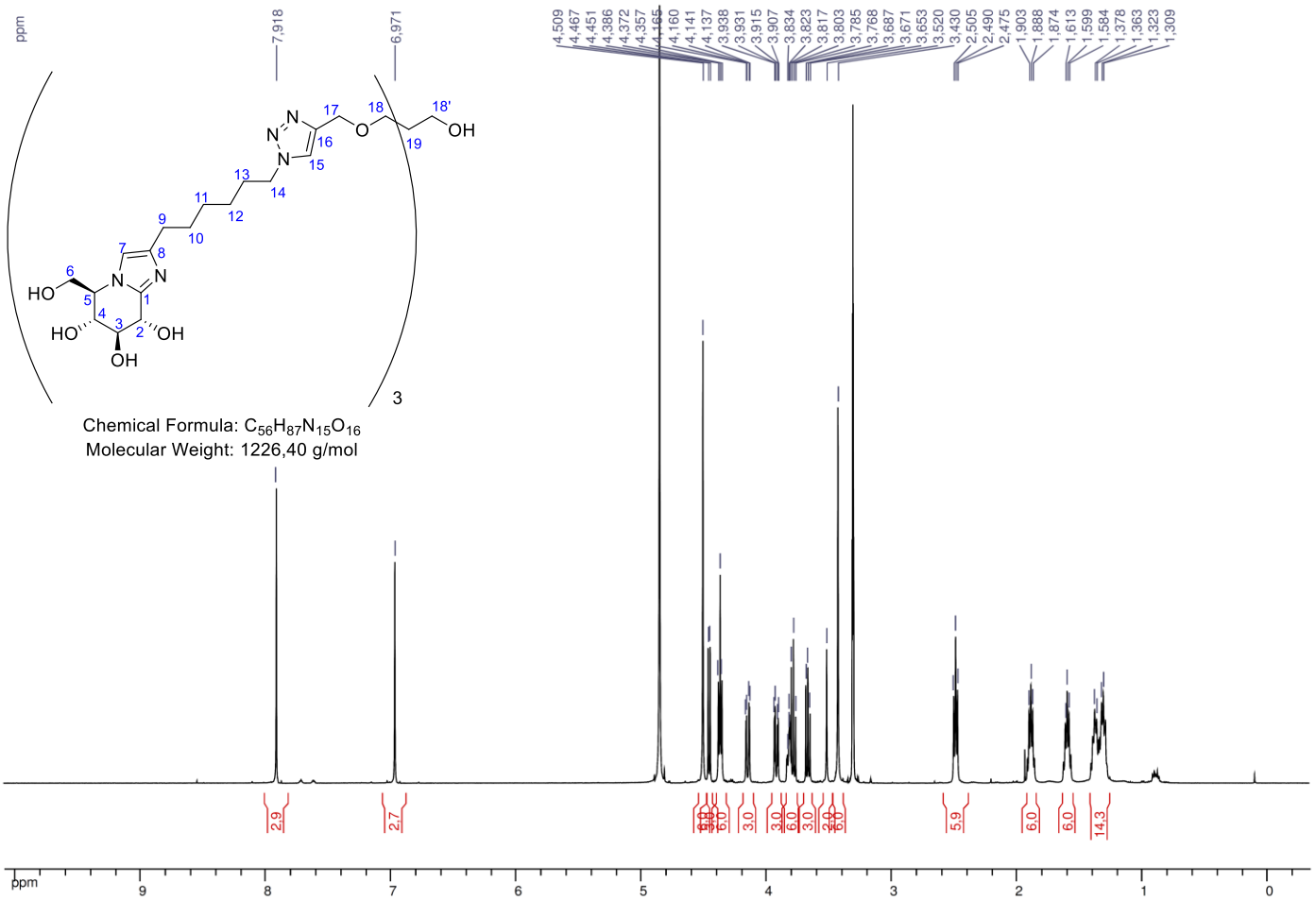


Fig S52. ^{1}H NMR (500 MHz, CD_3OD) spectrum of compound **21a**

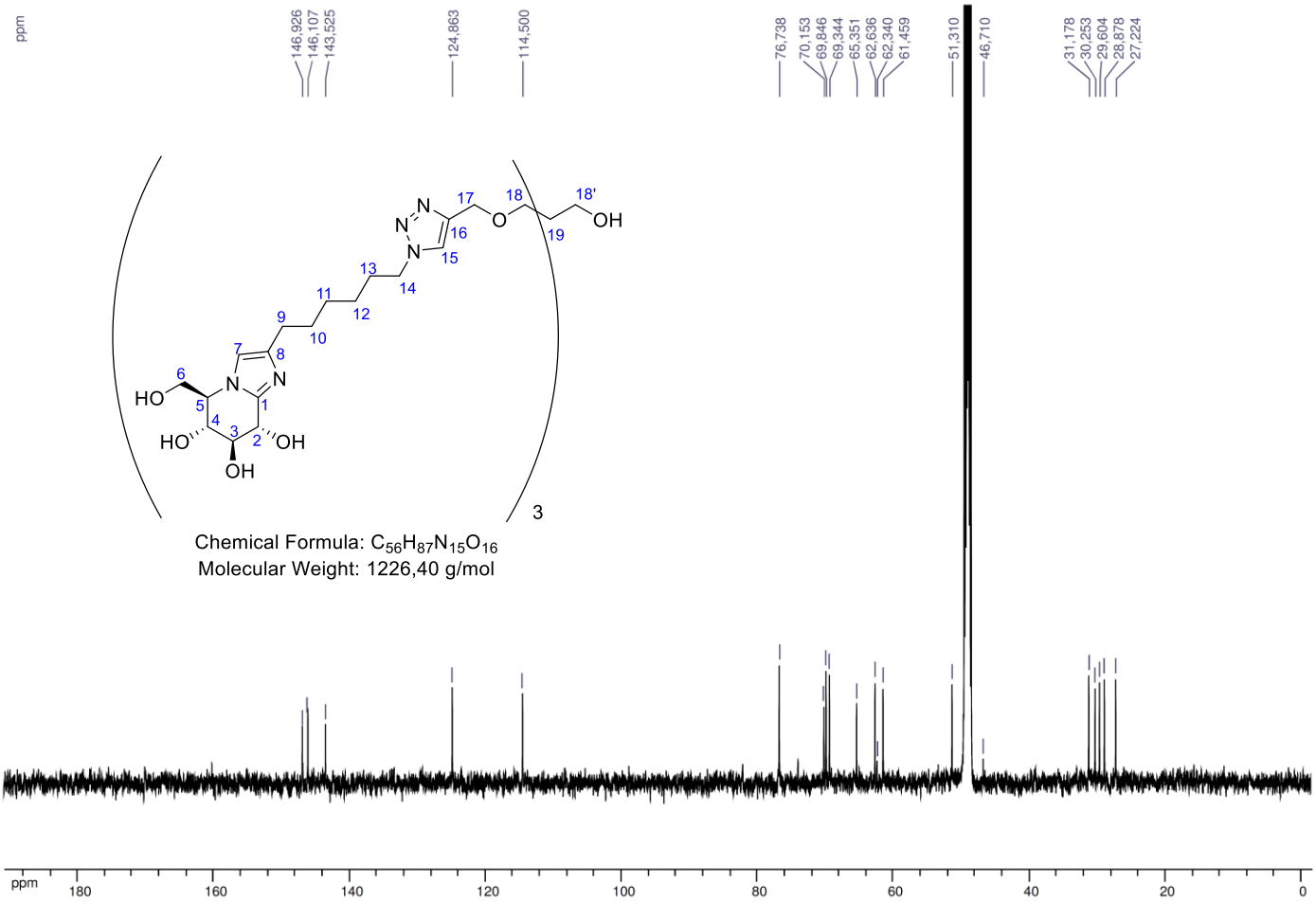
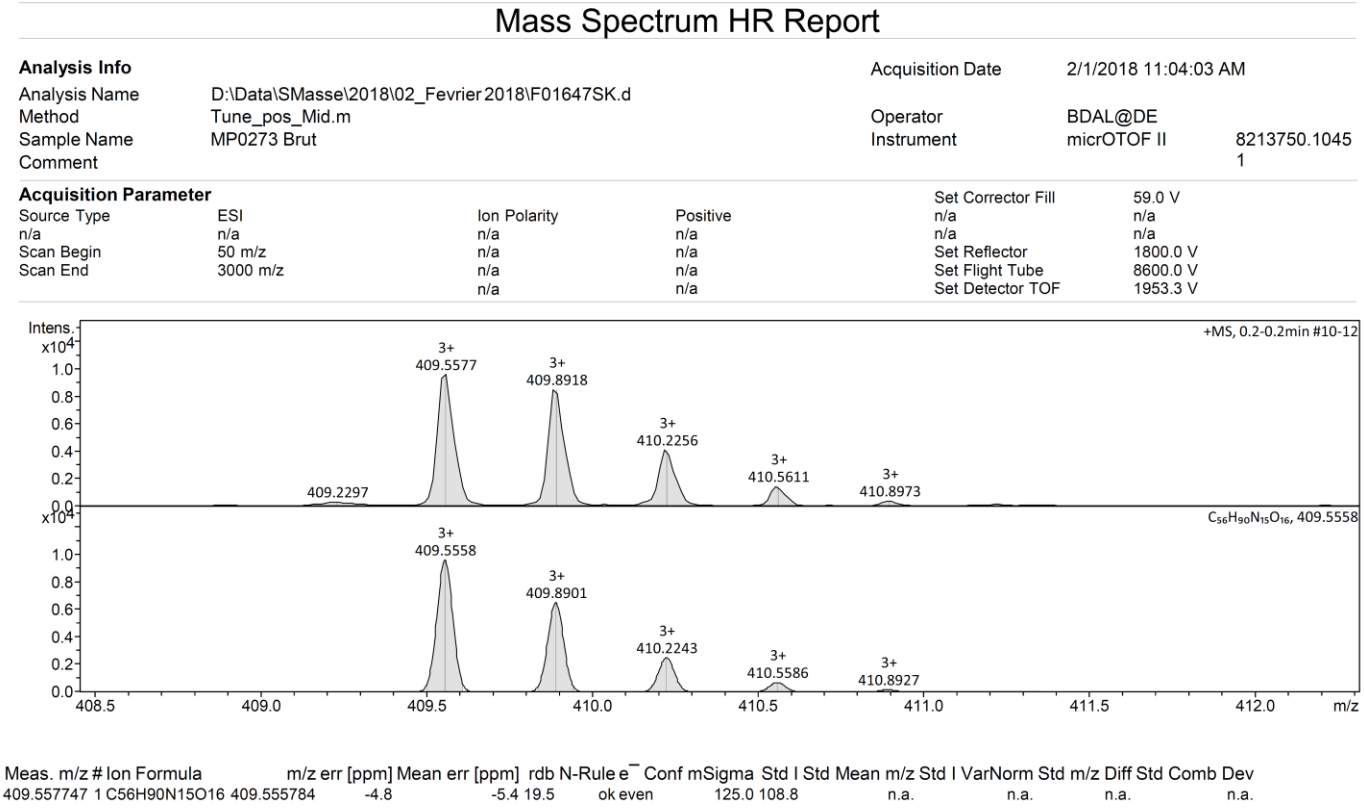


Fig S53. ^{13}C NMR (125 MHz, CD_3OD) spectrum of compound **21a**



Meas. m/z	#	Ion Formula	m/z err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I	VarNorm	Std m/z	Diff Std	Comb Dev
409.557747	1	C56H90N15O16	409.555784	-4.8	-5.4	19.5	ok	even	125.0	108.8	n.a.	n.a.	n.a.	n.a.	

Fig S54. HRMS (ESI-MS) spectrum of compound **21a**

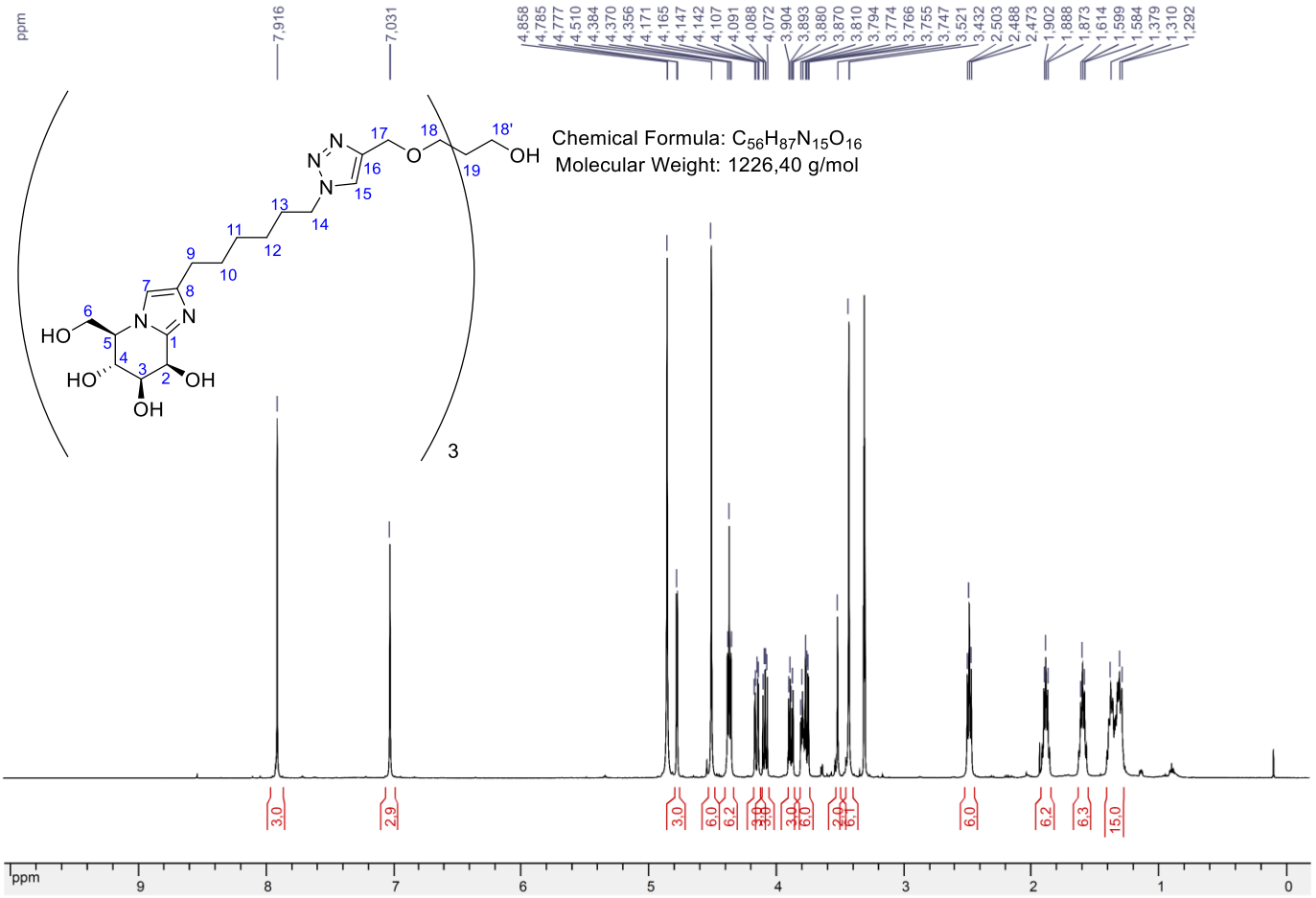


Fig S55. ^{1}H NMR (500 MHz, CD_3OD) spectrum of compound **21b**

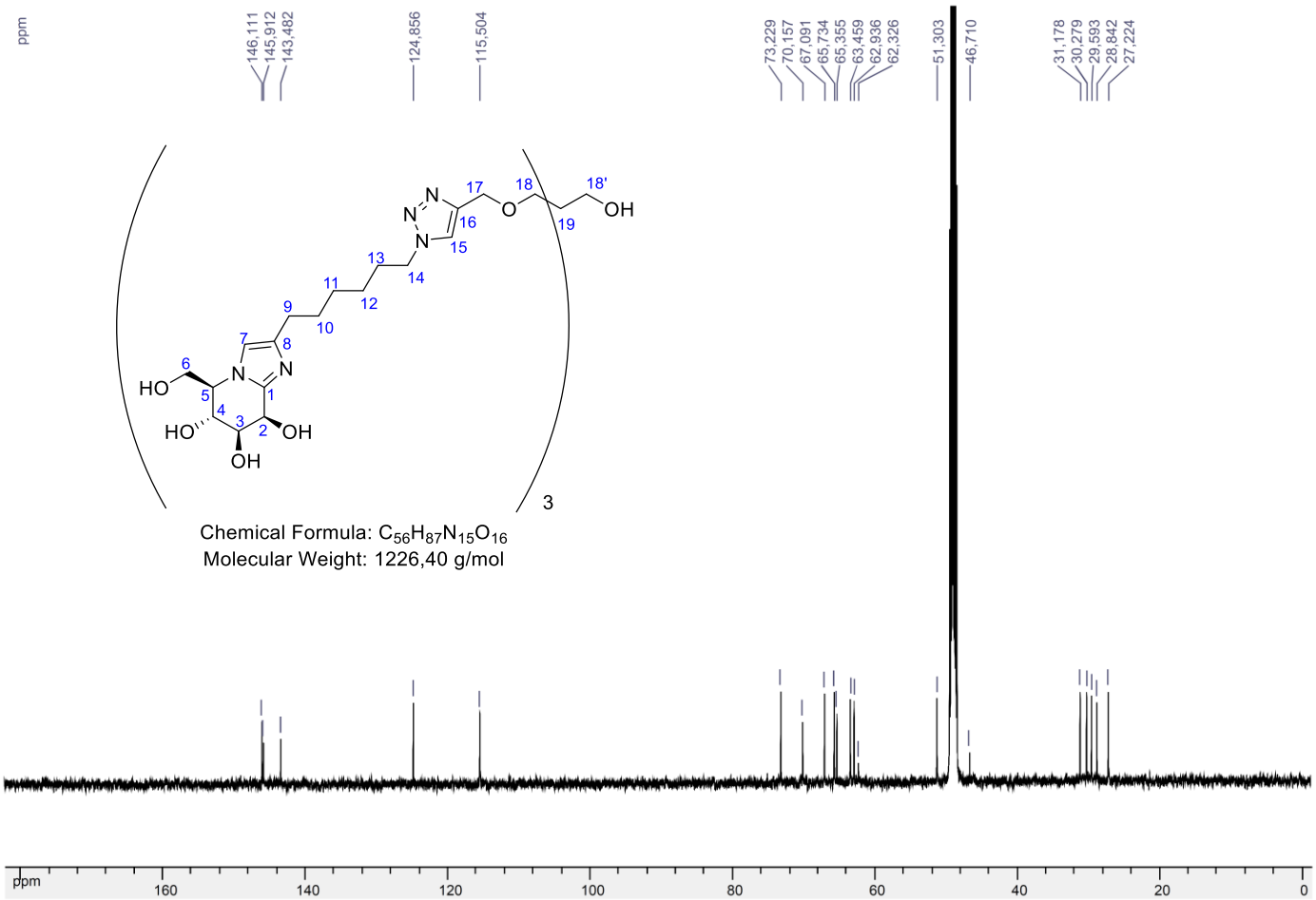


Fig S56 ^{13}C NMR (125 MHz, CD_3OD) spectrum of compound **21b**

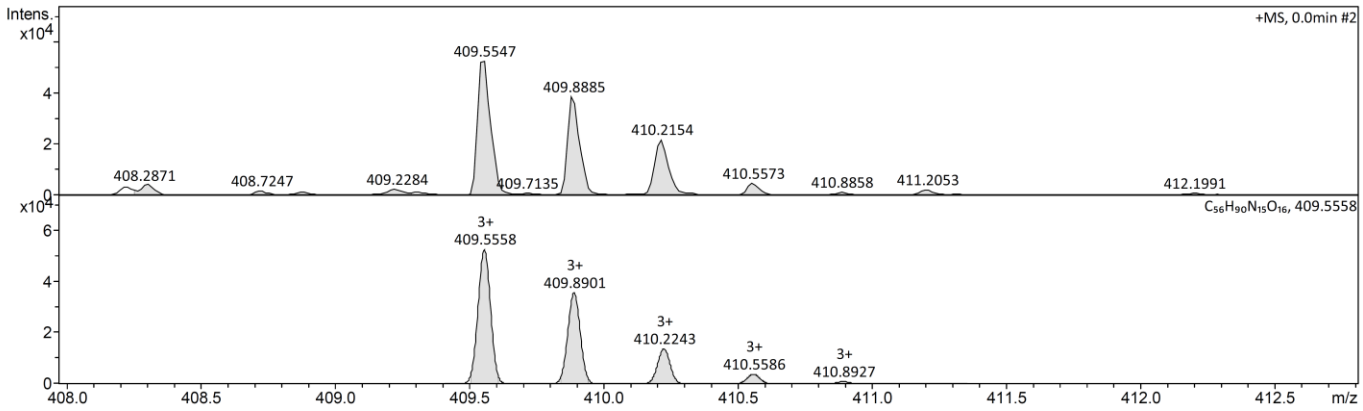
Mass Spectrum HR Report

Analysis Info

Analysis Name	D:\Data\SMasse\2018\05_Mai 2018\F02187SK.d	Acquisition Date	5/3/2018 3:06:45 PM
Method	Tune_pos_Mid.m		
Sample Name	MP0311 Brut	Operator	BDAL@DE
Comment		Instrument	micrOTOF II 8213750.1045 1

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Corrector Fill	59.0 V
n/a	n/a	n/a	n/a	n/a	n/a
Scan Begin	50 m/z	n/a	n/a	Set Reflector	1800.0 V
Scan End	3000 m/z	n/a	n/a	Set Flight Tube	8600.0 V
		n/a	n/a	Set Detector TOF	1953.3 V



Meas. m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I	VarNorm Std m/z	Diff Std Comb	Dev
409.5547	1	C56H90N15O16	409.5558	2.5	7.8	19.5	ok	even	73.9	75.9	n.a.	n.a.	n.a.	n.a.	
613.8288	1	C56H89N15O16	613.8300	2.1	822.2	20.0	ok	even	12.0	12.1	n.a.	n.a.	n.a.	n.a.	
1226.6504	1	C56H88N15O16	1226.6528	1.9	413.2	20.5	ok	even	34.1	31.5	n.a.	n.a.	n.a.	n.a.	

Fig S57. HRMS (ESI-MS) spectrum of compound **21b**

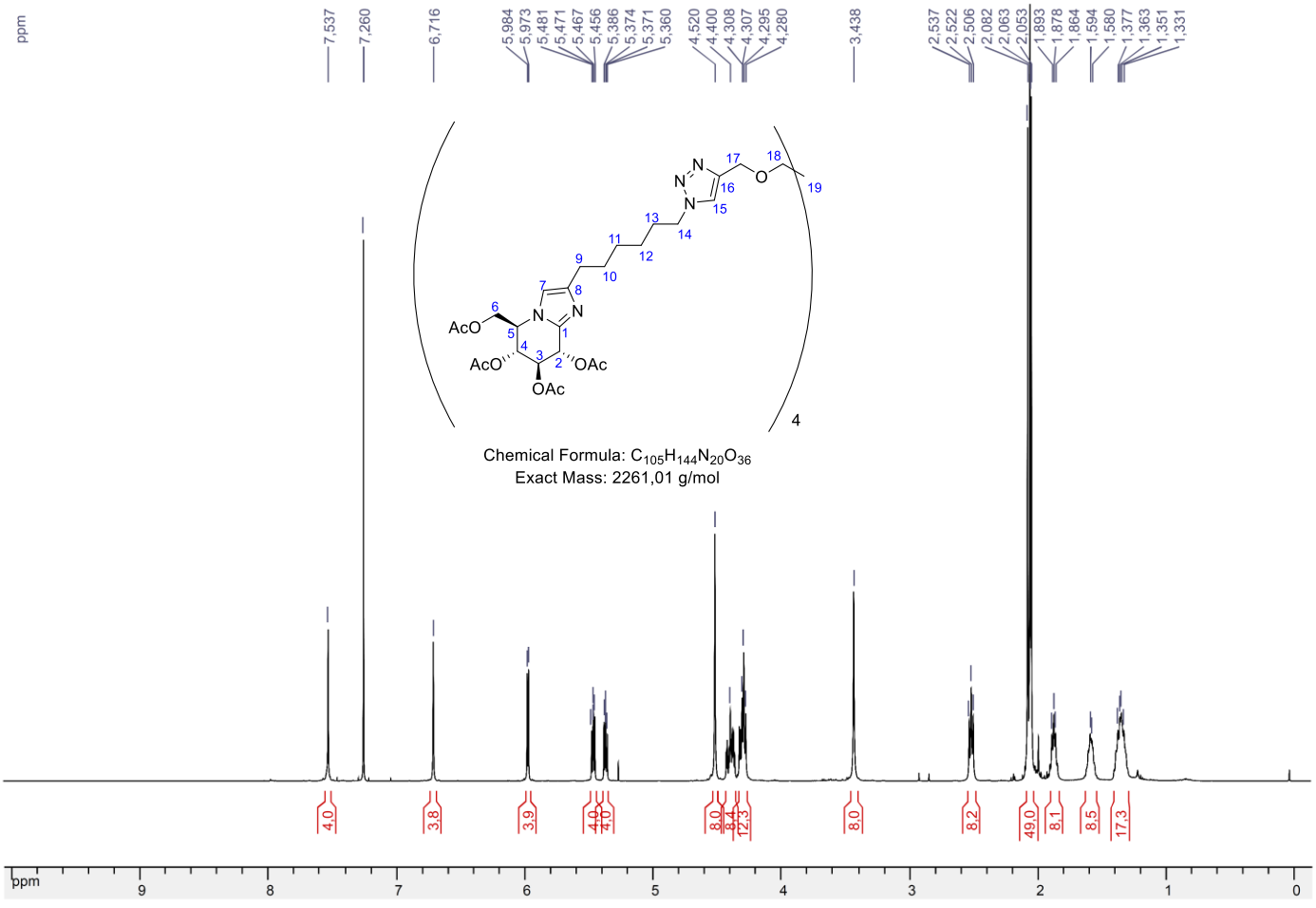


Fig S58. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **22a**

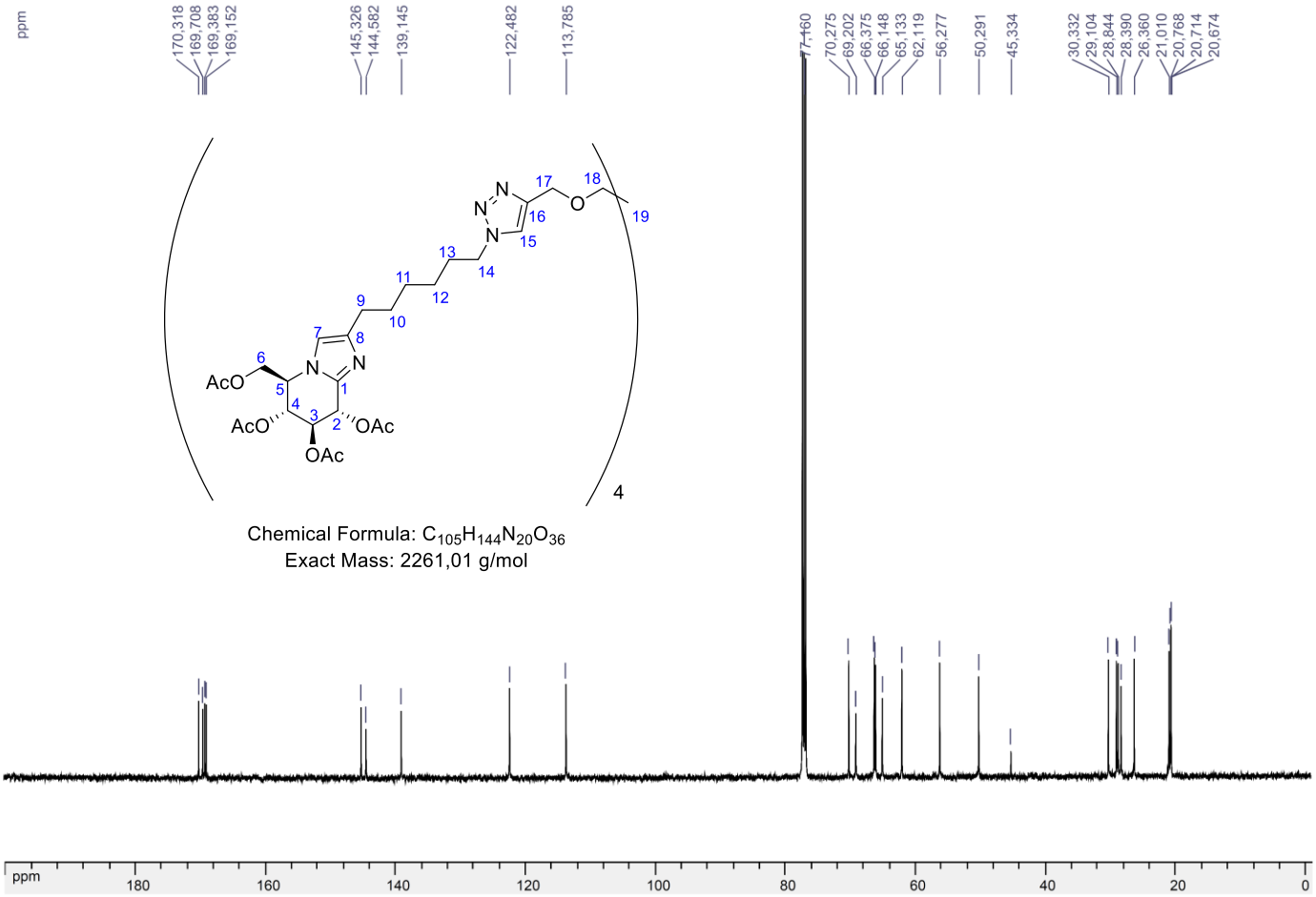
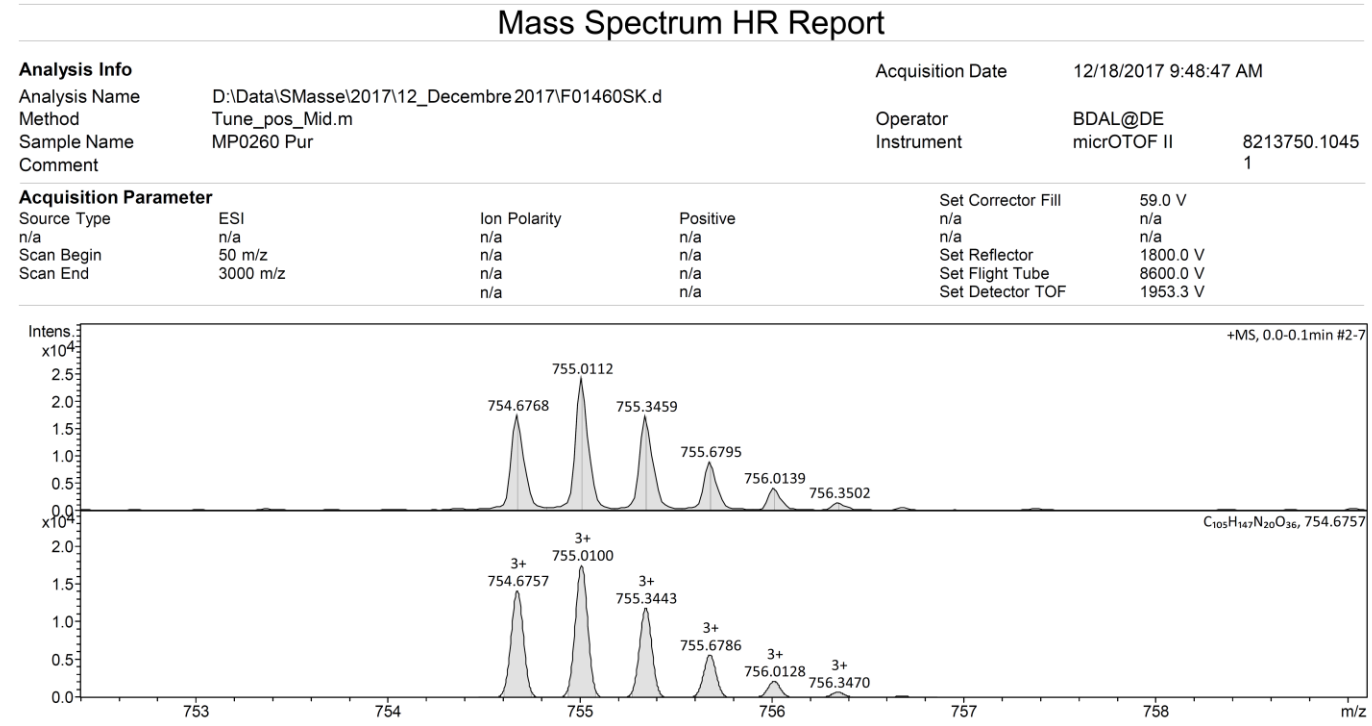


Fig S59. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **22a**



Meas. m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I	VarNorm	Std m/z	Diff Std	Comb Dev
754.676829	1	C105H147N20O36	754.675680	-1.5	-1.9	42.5	ok	even	47.9	41.7	n.a.		n.a.		n.a.	n.a.

Fig S60. HRMS (ESI-MS) spectrum of compound **22a**

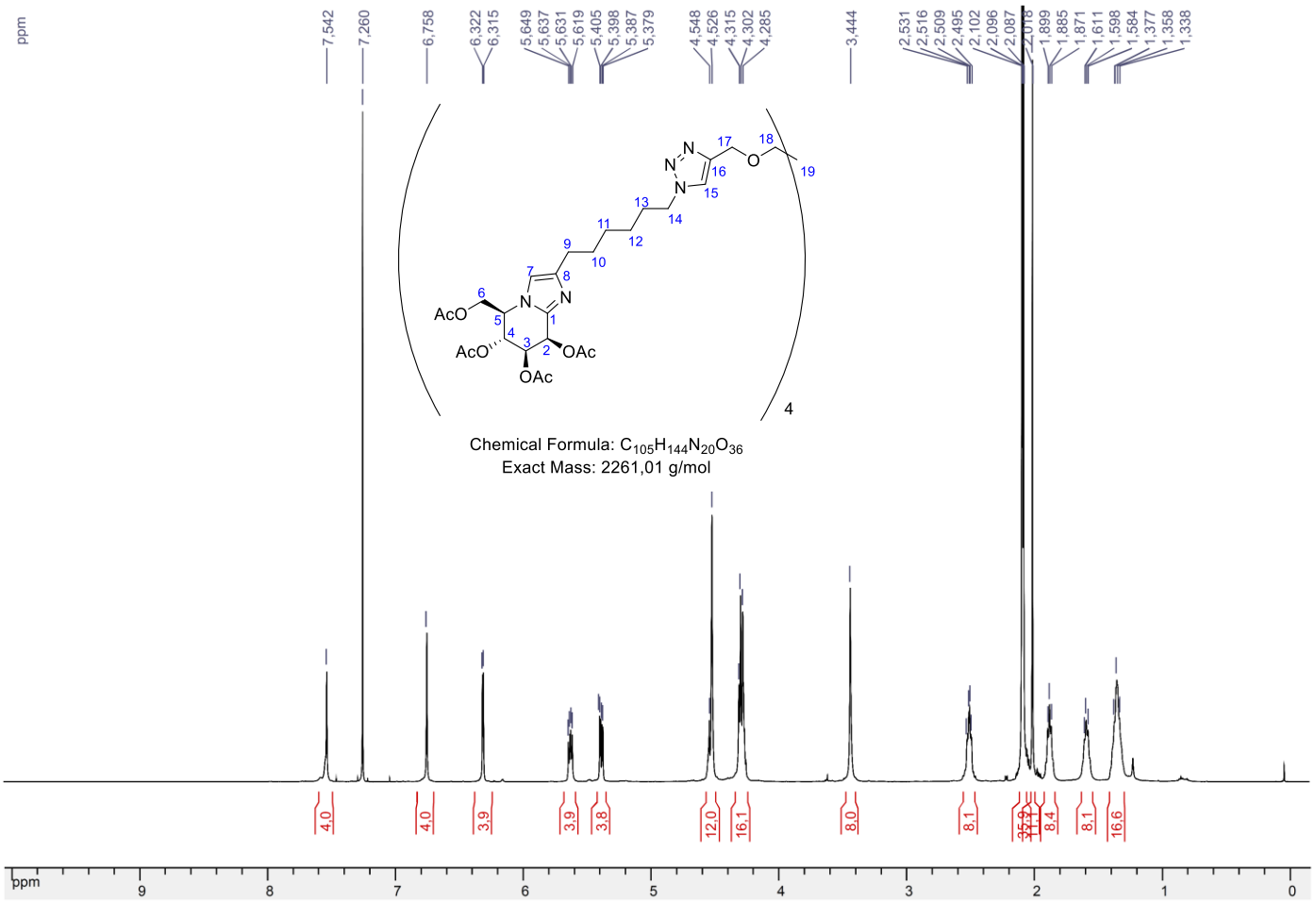


Fig S61. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **22b**

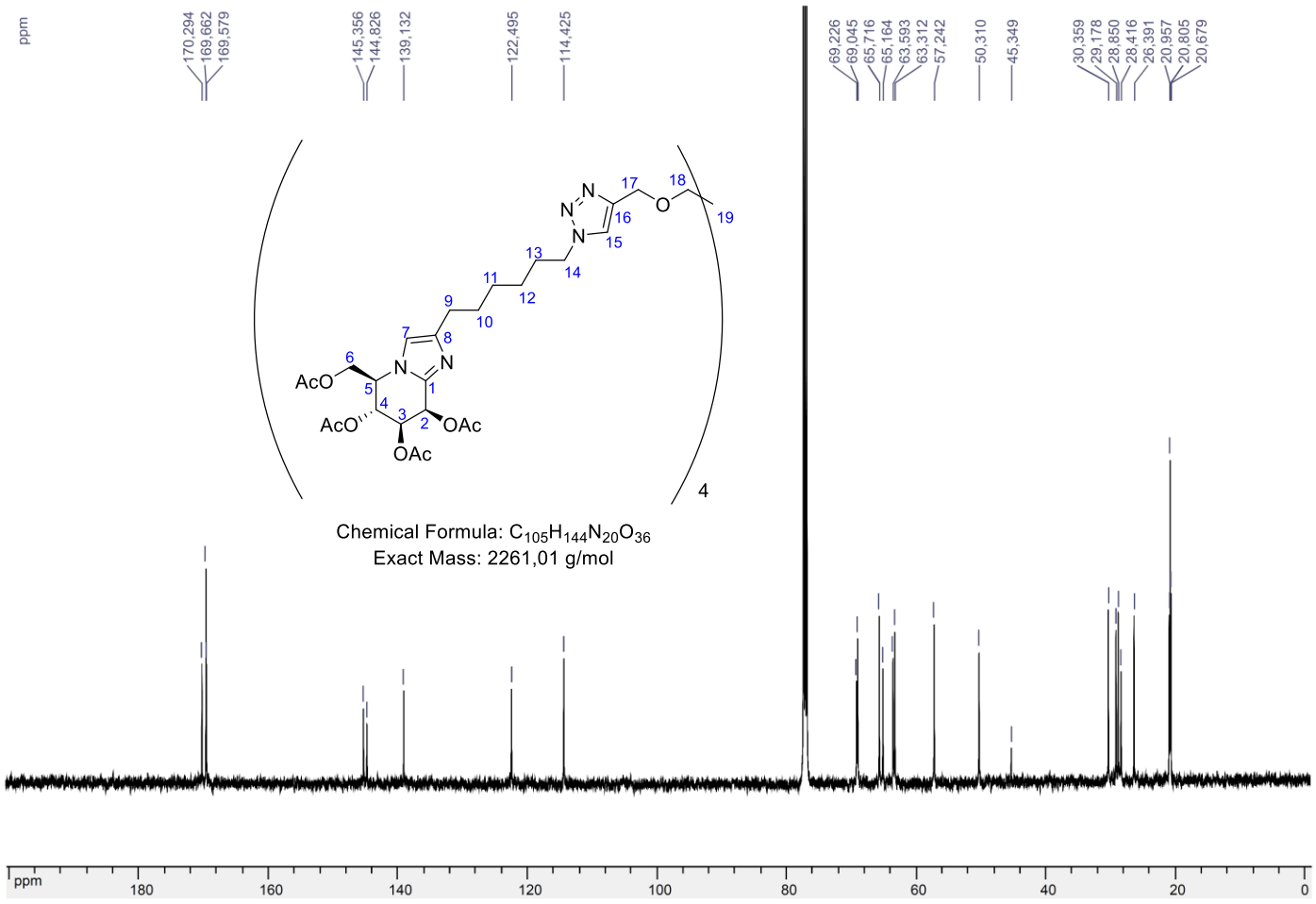


Fig S62. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **22**

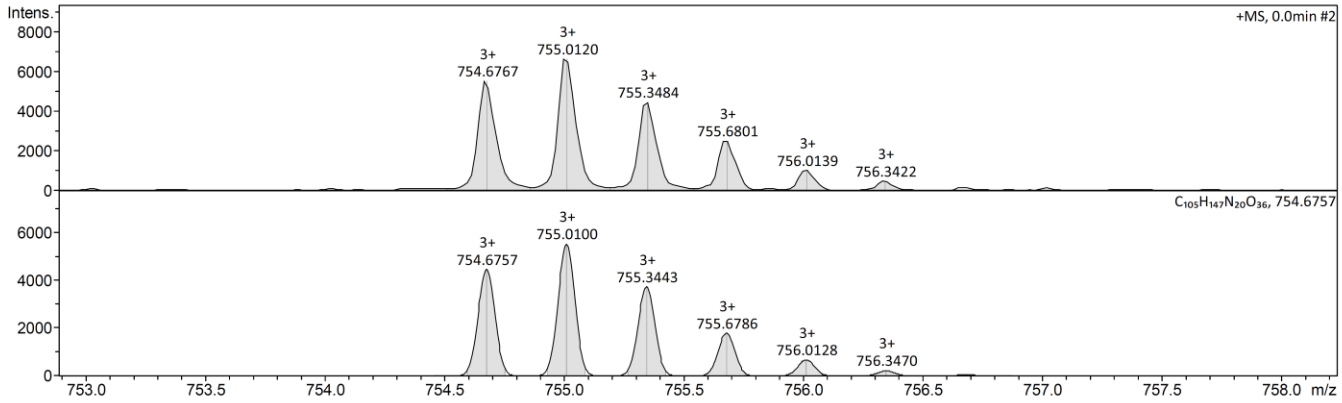
Mass Spectrum HR Report

Analysis Info

Analysis Name	D:\Data\SMasse\2018\03_Mars 2018\F02021SK.d	Acquisition Date	3/28/2018 3:50:59 PM
Method	Tune_pos_Mid.m	Operator	BDAL@DE
Sample Name	MP0300	Instrument	micrOTOF II 8213750.1045
Comment			1

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Corrector Fill	59.0 V
n/a	n/a	n/a	n/a	n/a	n/a
Scan Begin	50 m/z	n/a	n/a	n/a	n/a
Scan End	3000 m/z	n/a	n/a	Set Reflector	1800.0 V
		n/a	n/a	Set Flight Tube	8600.0 V
		n/a	n/a	Set Detector TOF	1953.3 V



Meas. m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I	VarNorm	Std m/z	Diff Std Comb	Dev
566.261420	1	C105H148N20O36	566.258579	-5.0	-4.0	42.0	ok	even	55.1	39.9	n.a.	n.a.	n.a.	n.a.		
	2	C104H160N20O36	566.282054	36.4	37.5	35.0	ok	even	56.6	41.7	n.a.	n.a.	n.a.	n.a.		
754.676697	1	C105H147N20O36	754.675680	-1.3	-1.8	42.5	ok	even	30.7	26.5	n.a.	n.a.	n.a.	n.a.		

Fig S63. HRMS (ESI-MS) spectrum of compound **22b**

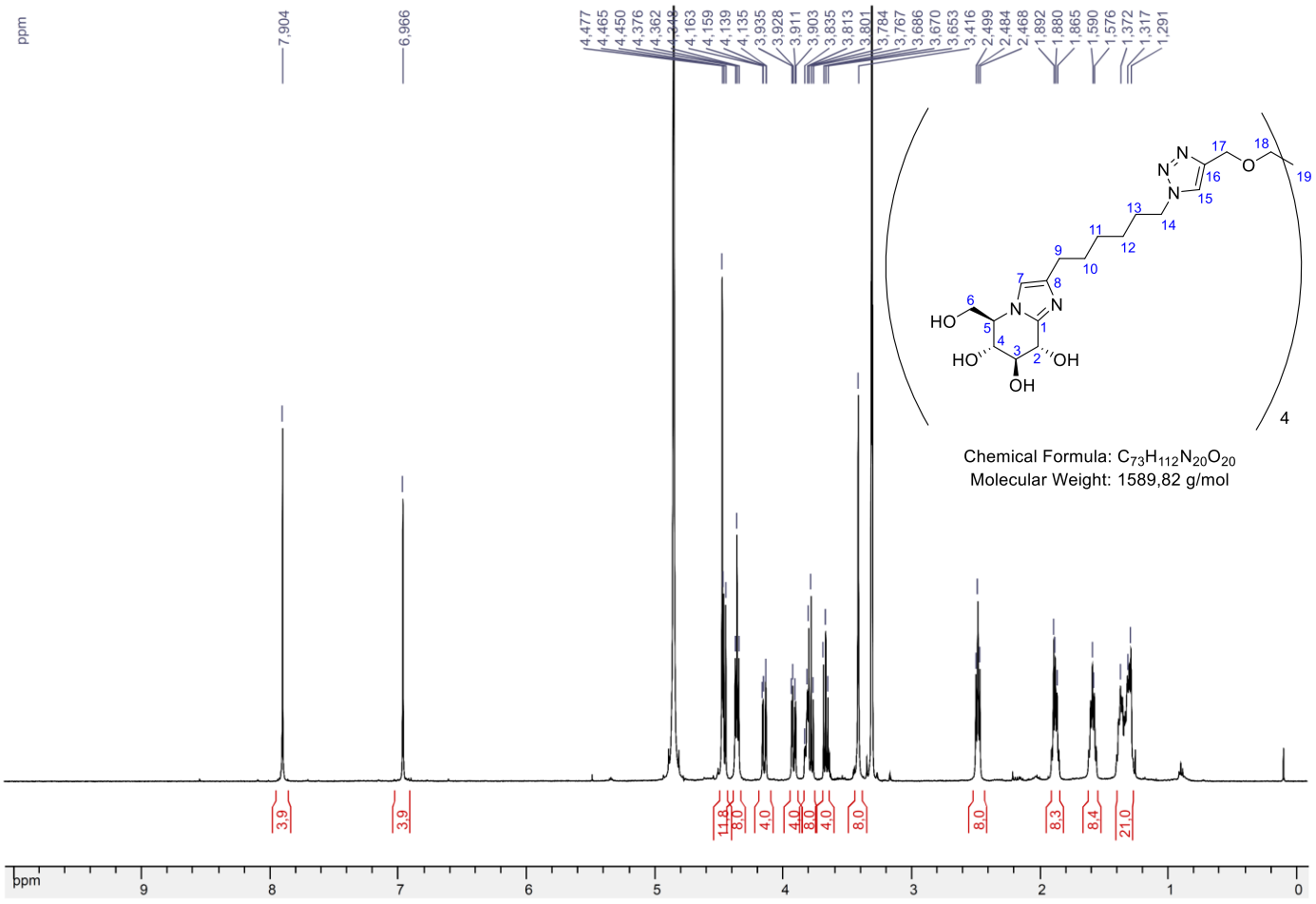


Fig S64. ^{1}H NMR (500 MHz, CD_3OD) spectrum of compound **23a**

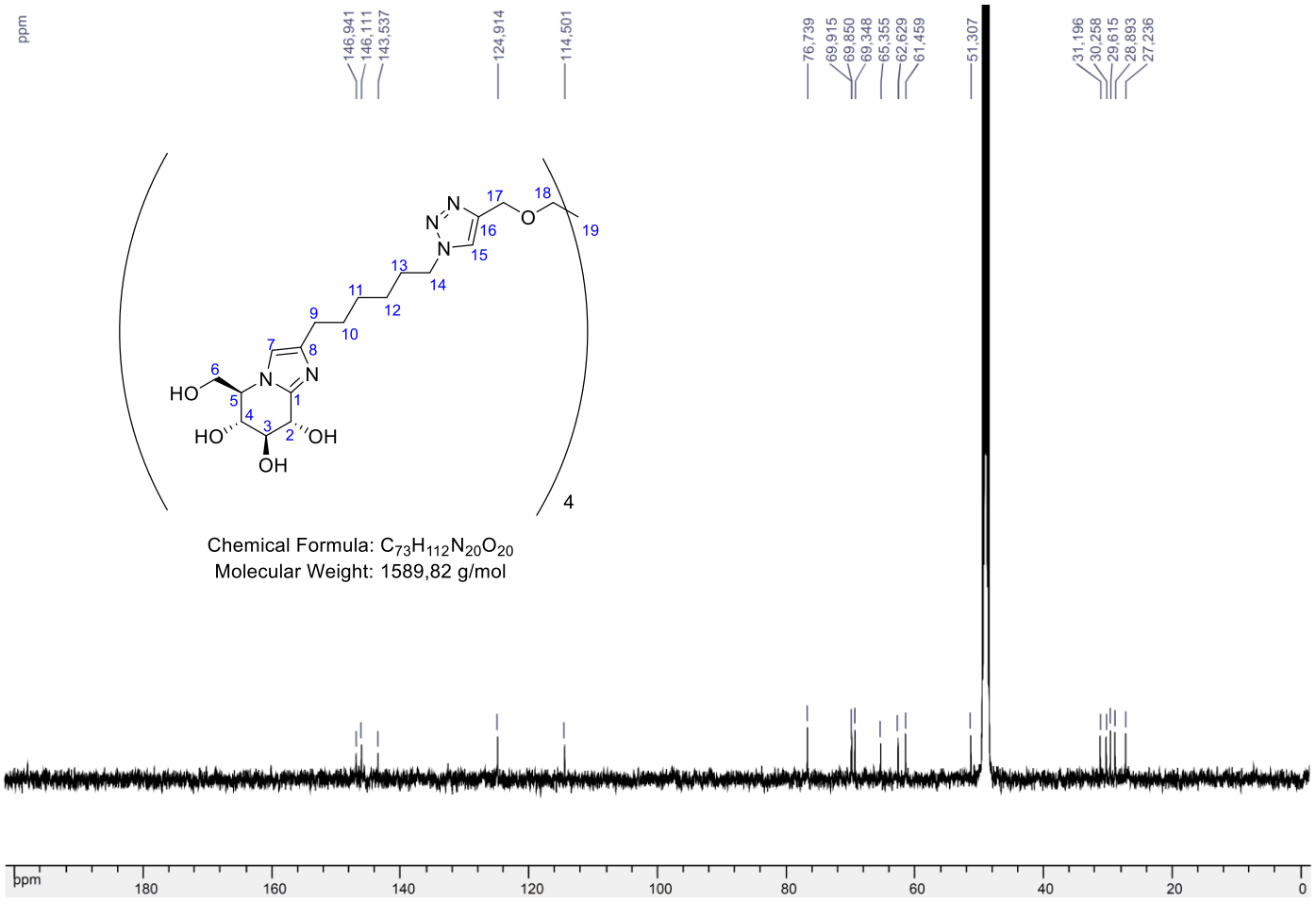


Fig S65. ^{13}C NMR (125 MHz, CD_3OD) spectrum of compound **23a**

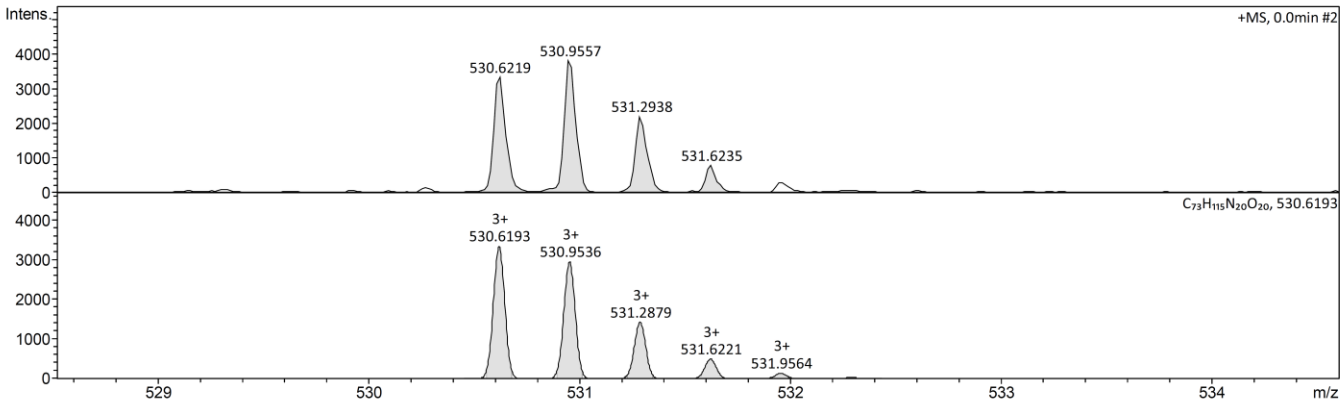
Mass Spectrum HR Report

Analysis Info

Analysis Name	D:\Data\SMasse\2018\01_Janvier 2018\F01540SK.d	Acquisition Date	1/22/2018 11:57:22 AM
Method	Tune_pos_Mid.m	Operator	BDAL@DE
Sample Name	MP0270	Instrument	micrOTOF II 8213750.1045
Comment			1

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Corrector Fill	59.0 V
n/a	n/a	n/a	n/a	n/a	n/a
Scan Begin	50 m/z	n/a	n/a	Set Reflector	1800.0 V
Scan End	3000 m/z	n/a	n/a	Set Flight Tube	8600.0 V
		n/a	n/a	Set Detector TOF	1953.3 V



Meas. m/z	#	Ion Formula	m/z err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I	VarNorm Std m/z	Diff Std Comb	Dev
530.621901	1	C73H115N20O20	530.619335	-4.8	880.0	26.5	ok	even	106.1	90.8	n.a.	n.a.	n.a.	n.a.

Fig S66. HRMS (ESI-MS) spectrum of compound **23a**

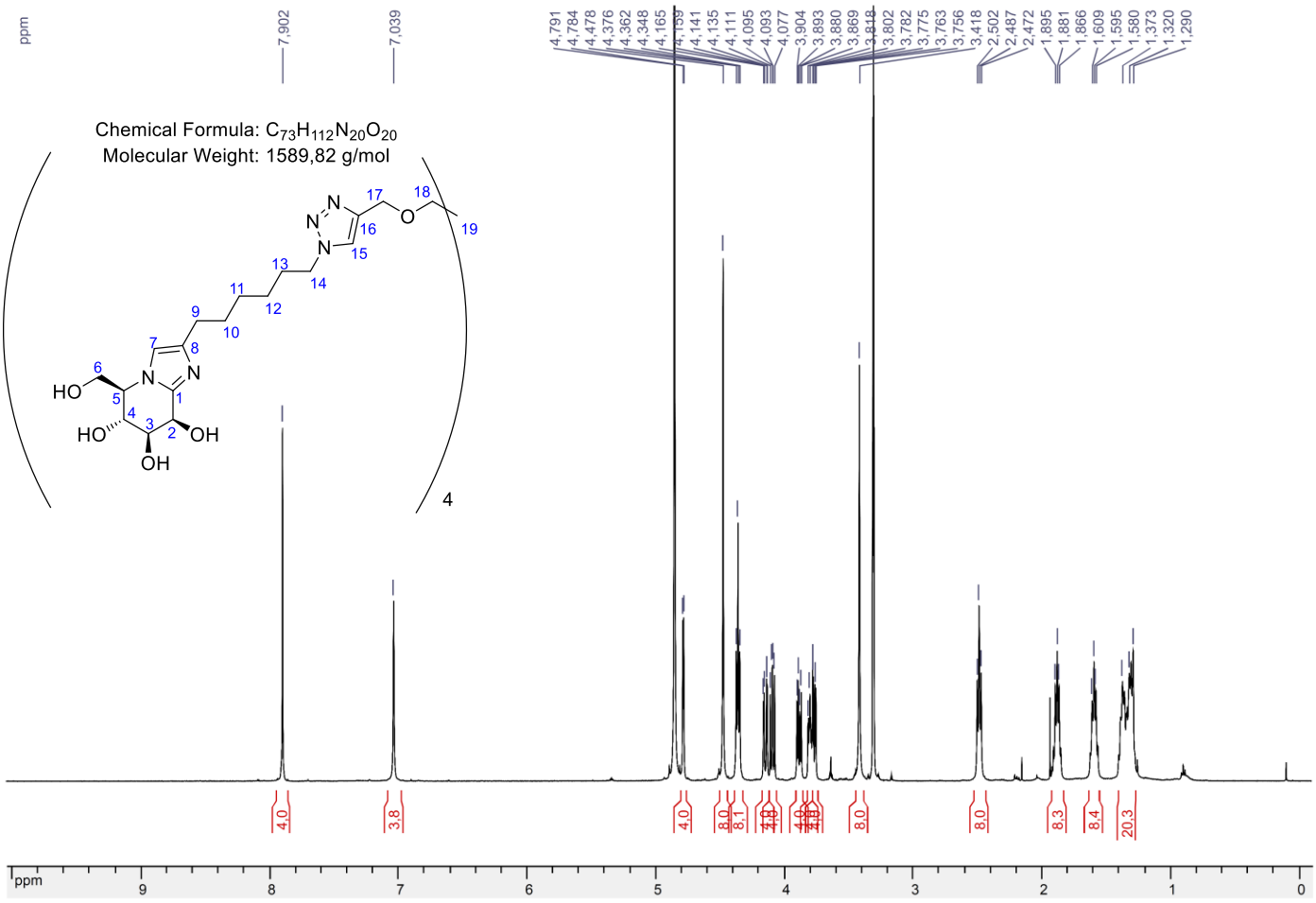


Fig S67. ^{1}H NMR (500 MHz, CD_3OD) spectrum of compound **23b**

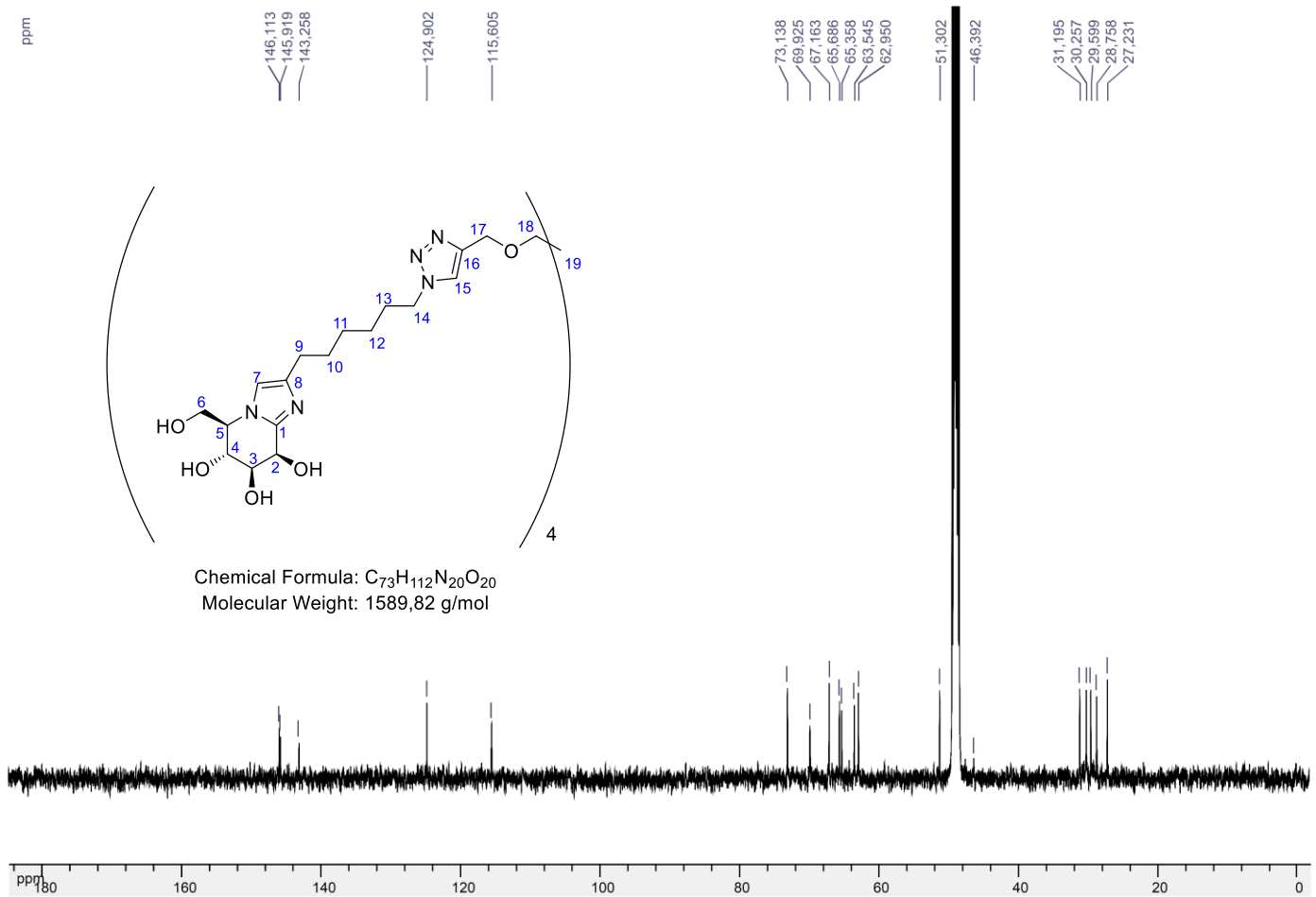


Fig S68. ^{13}C NMR (125 MHz, CD_3OD) spectrum of compound **23b**

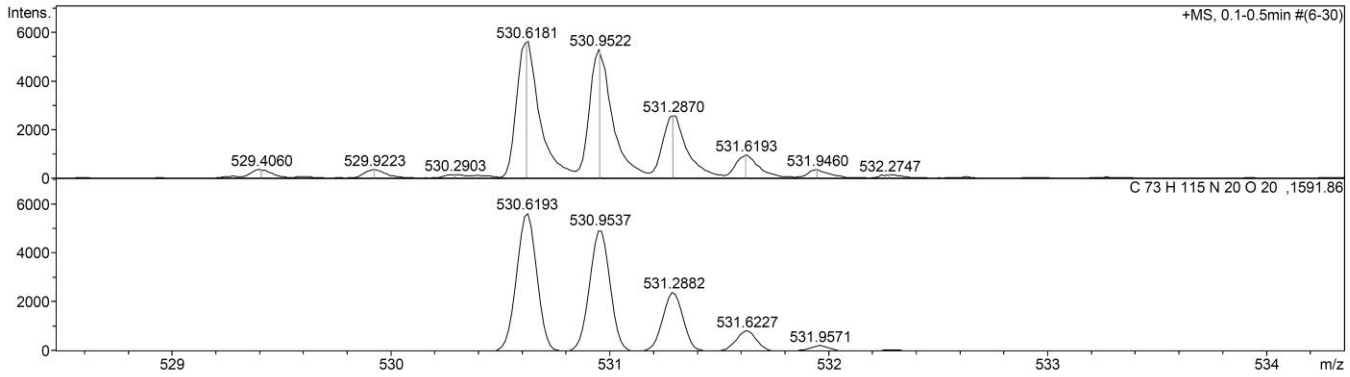
Mass Spectrum HR Report

Analysis Info

Analysis Name	Y:\O42997SK.d	Acquisition Date	19/04/2018 15:58:33
Method	esi wide pos.m		
Sample Name	MP0306	Operator	admin
Comment	MeOH	Instrument	micrOTOF 66

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Corrector Fill	59 V
n/a	n/a	Set Capillary Exit	200.0 V	Set Pulsar Pull	818 V
Scan Begin	50 m/z	Set Hexapole RF	170.0 V	Set Pulsar Push	818 V
Scan End	3000 m/z	Set Skimmer 1	50.0 V	Set Reflector	1700 V
		Set Hexapole 1	24.3 V	Set Flight Tube	8600 V
				Set Detector TOF	2057 V



Meas. m/z	#	Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I VarNorm	Std m/z Diff	Std Comb Dev
530.6181	1	C 73 H 115 N 20 O 20	530.6193	2.2	3.2	26.5	ok	even	35.5	26.3	2.4	10.3	1.0	842.7
795.4306	1	C 73 H 114 N 20 O 20	795.4254	-6.6	-7.2	27.0	ok	even	19.5	17.0	5.8	8.1	1.9	842.7

Fig S69. HRMS (ESI-MS) spectrum of compound **23b**

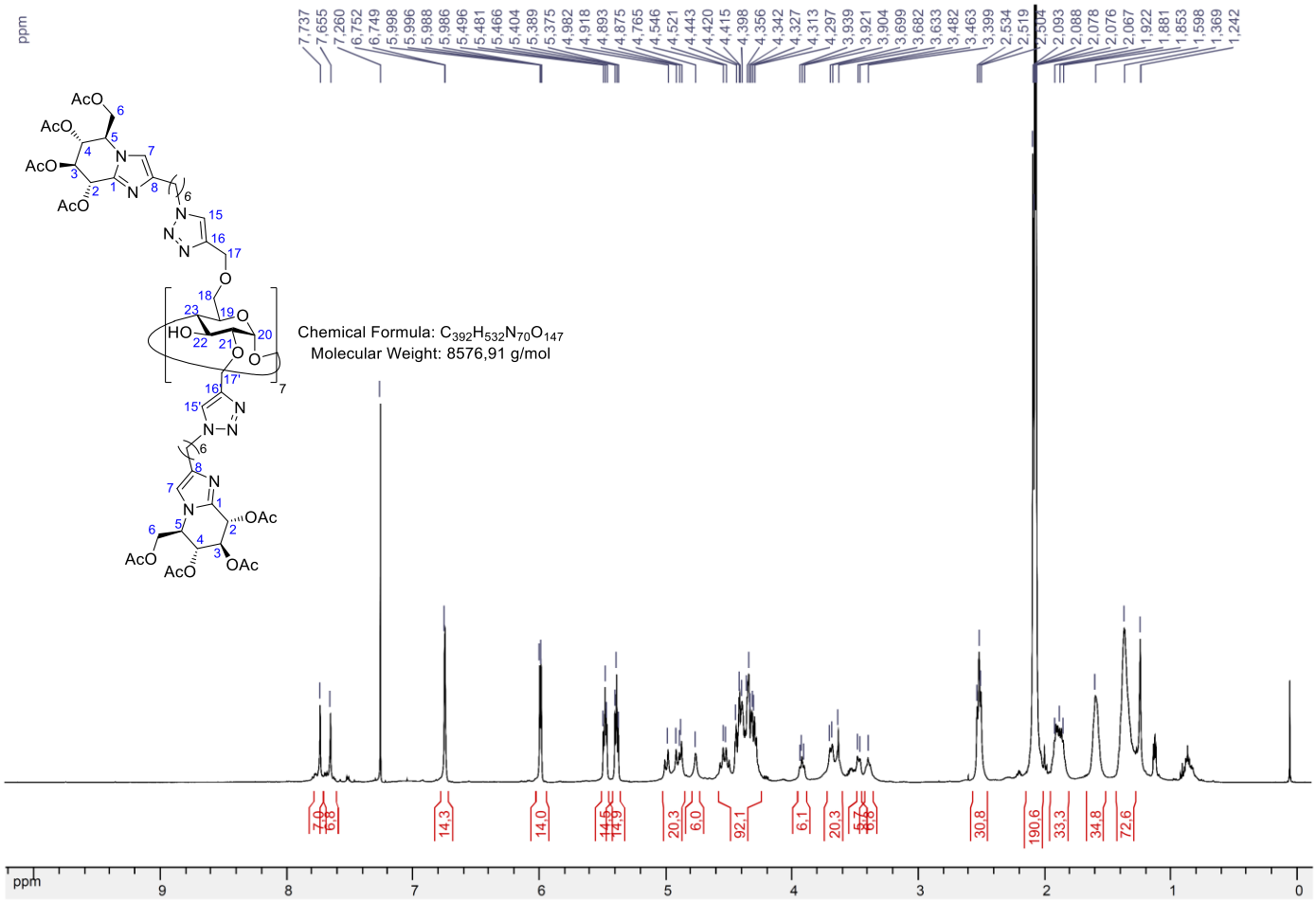


Fig S70. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **25a**

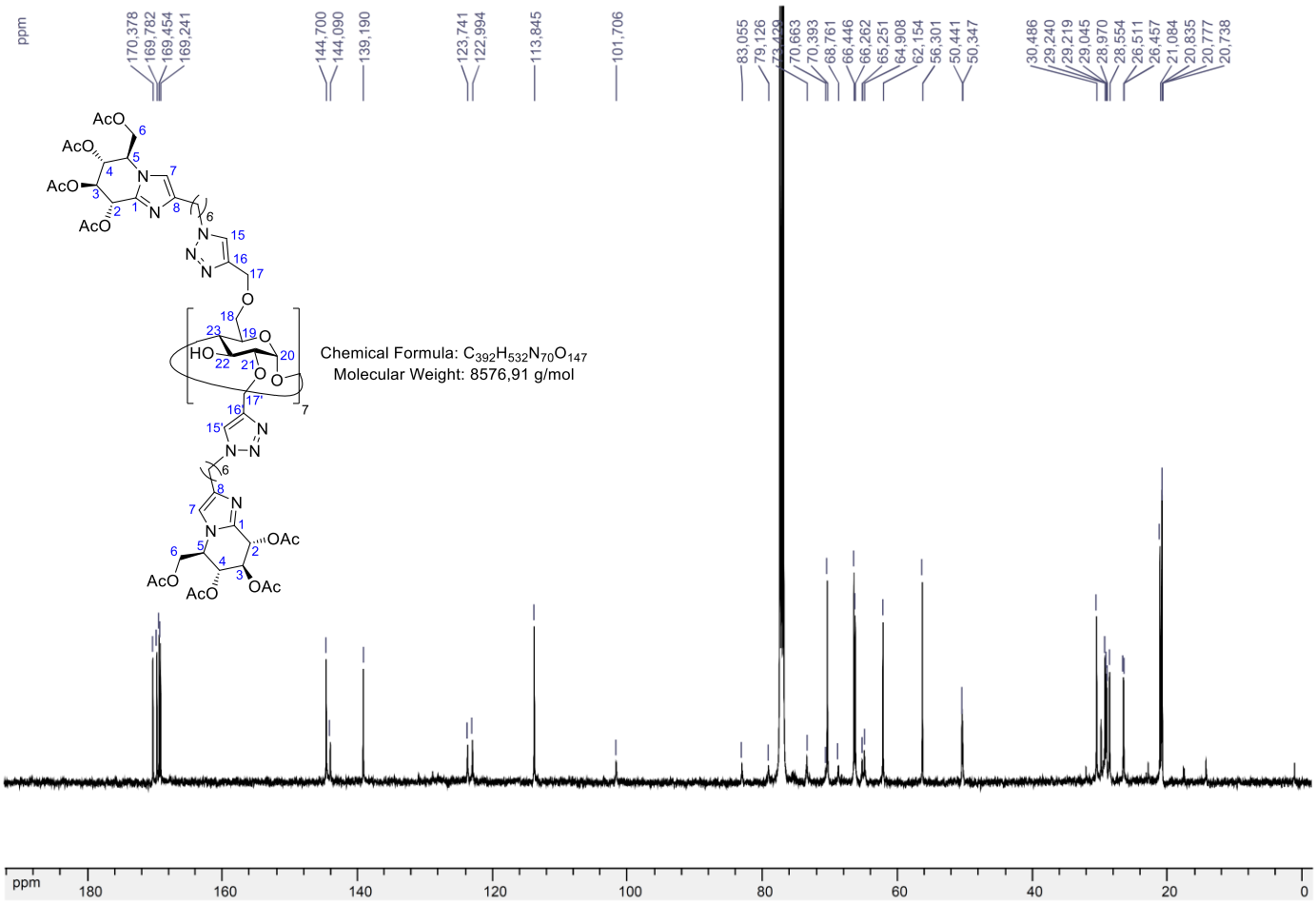


Fig S71. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **25a**

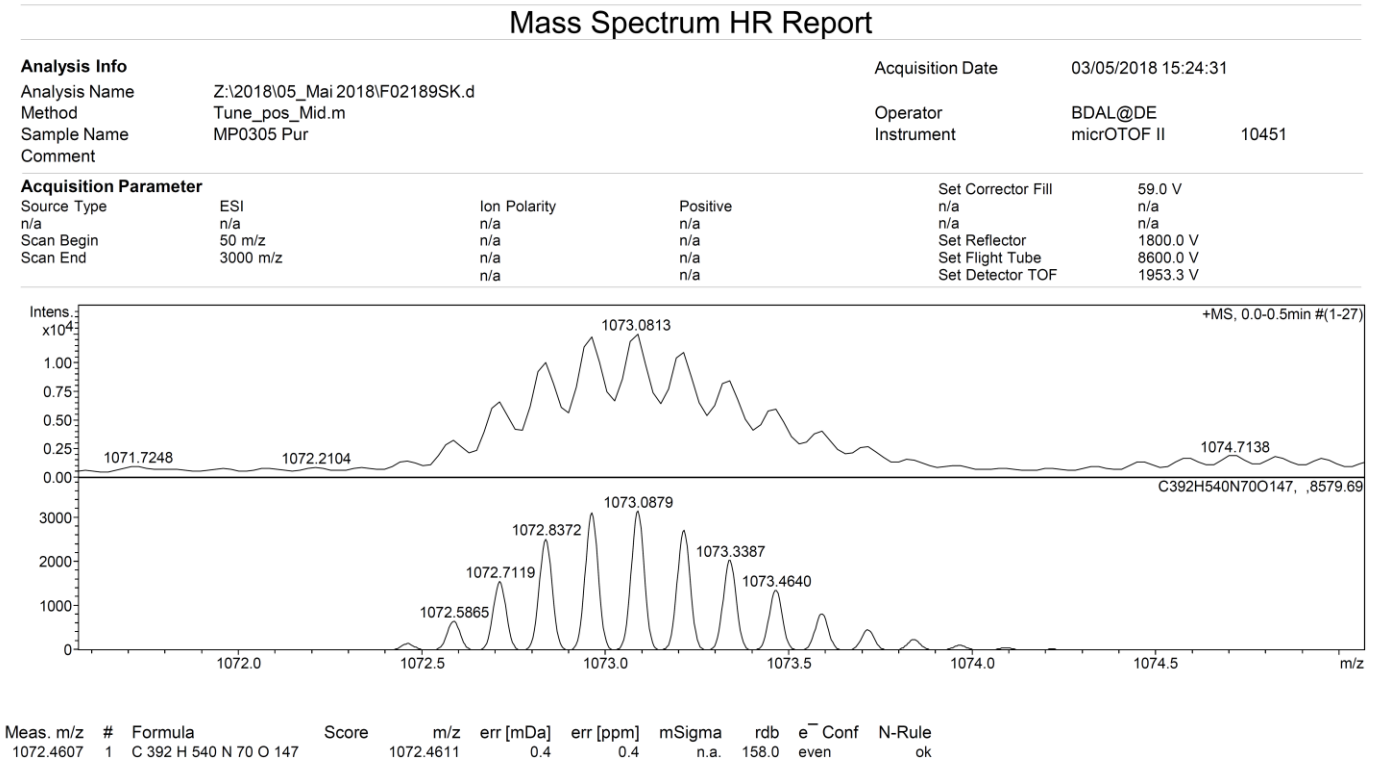


Fig S72. HRMS (ESI-MS) spectrum of compound **25a**

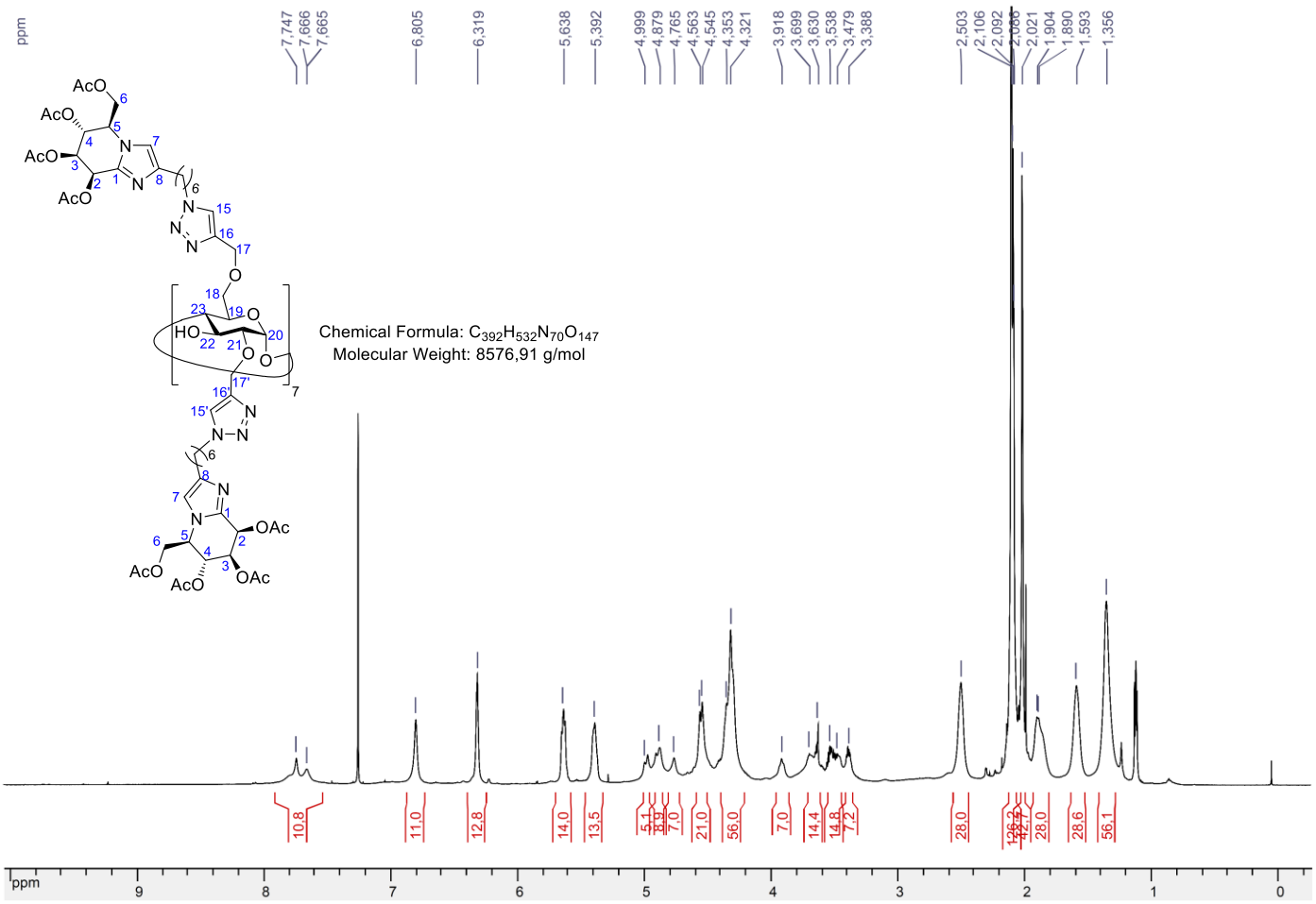


Fig S73. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **25b**

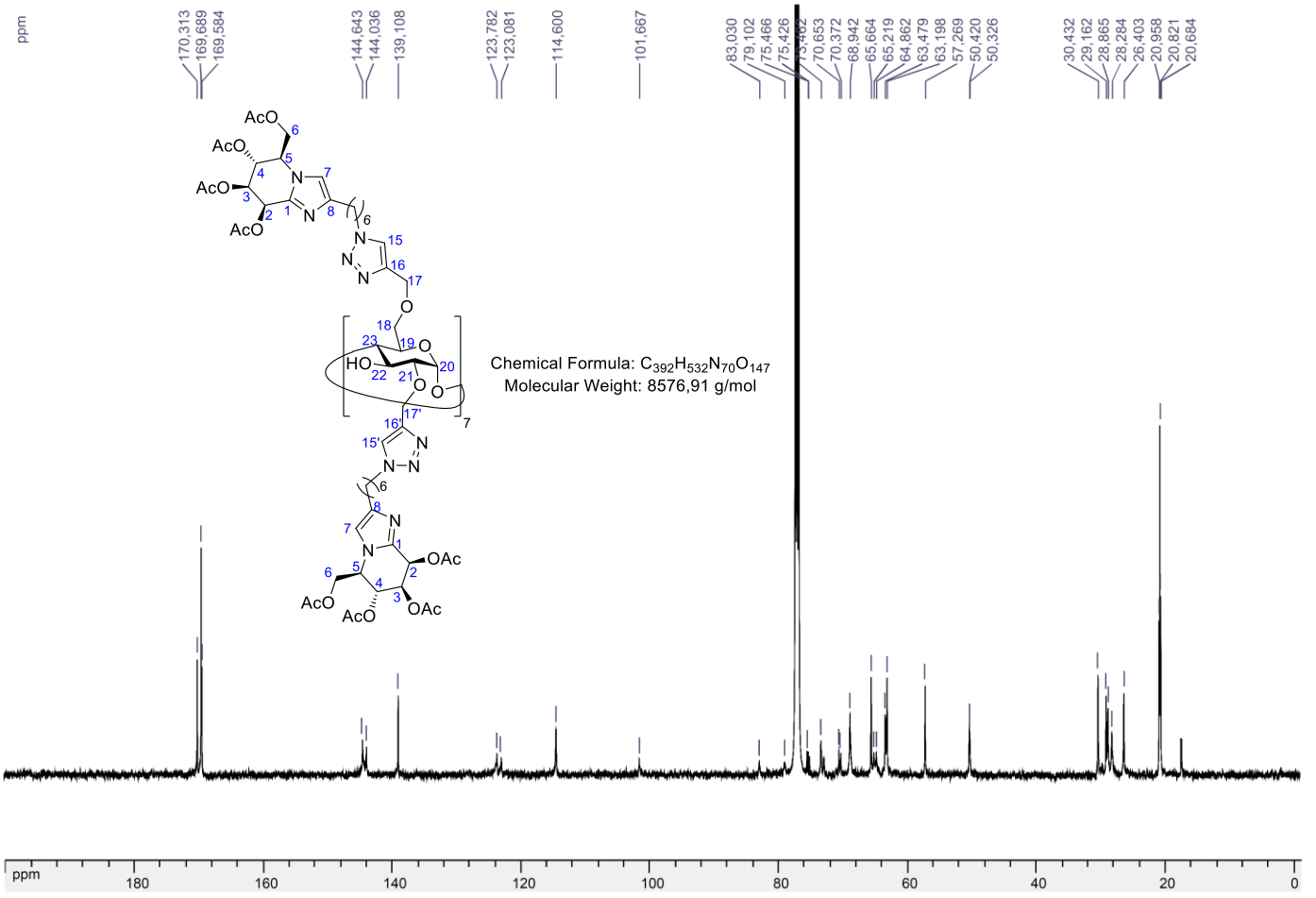


Fig S74. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound **25b**

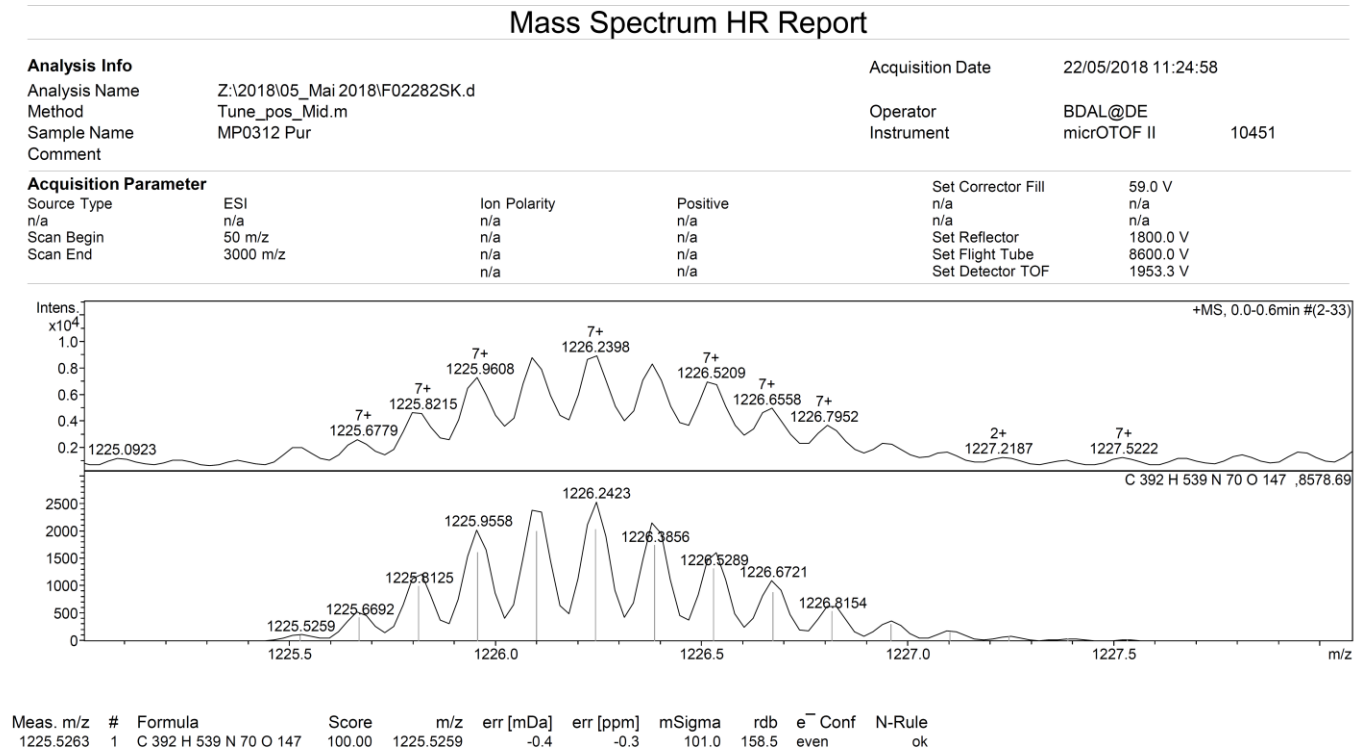


Fig S75. HRMS (ESI-MS) spectrum of compound **25b**

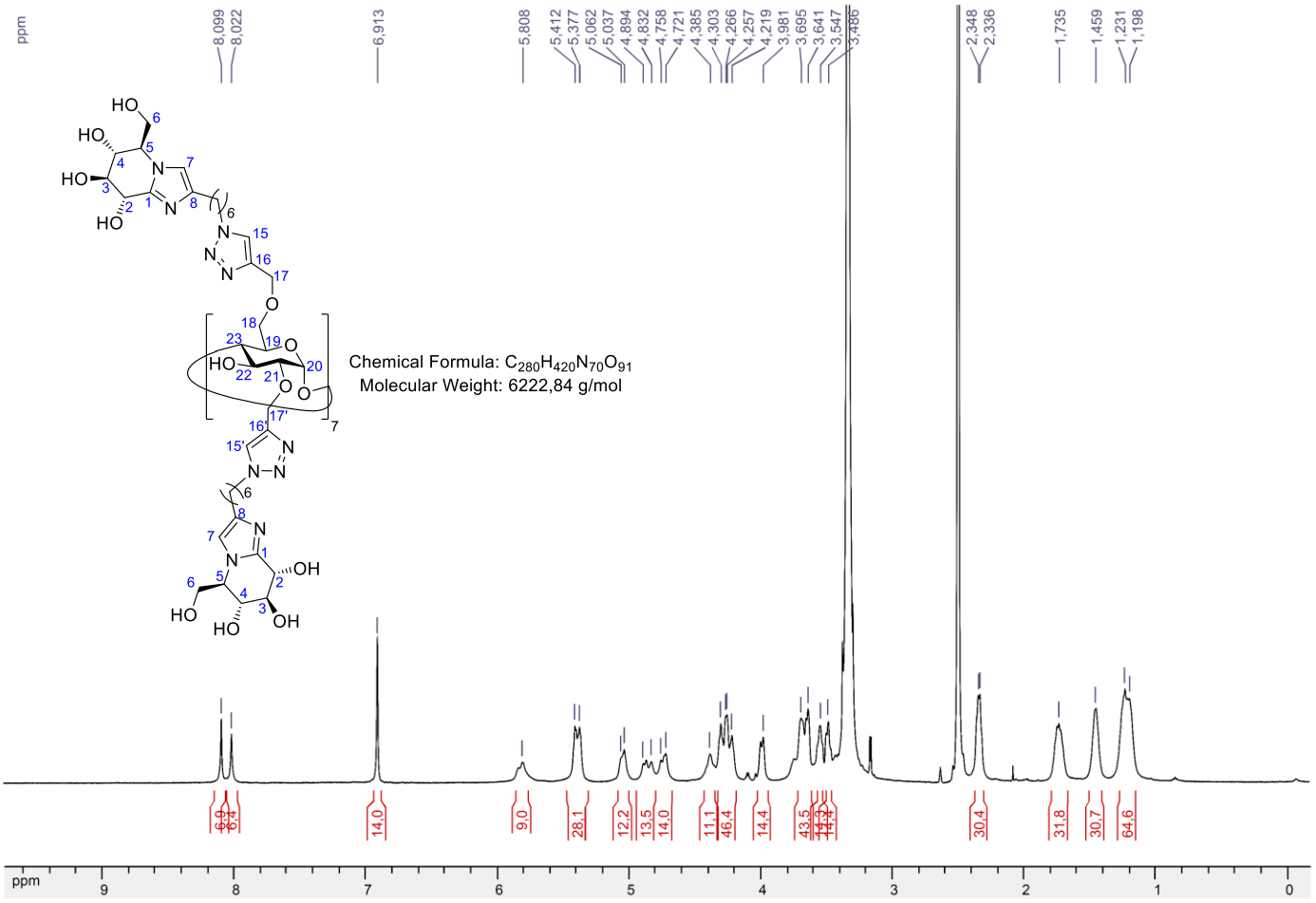


Fig S76. ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **26a**

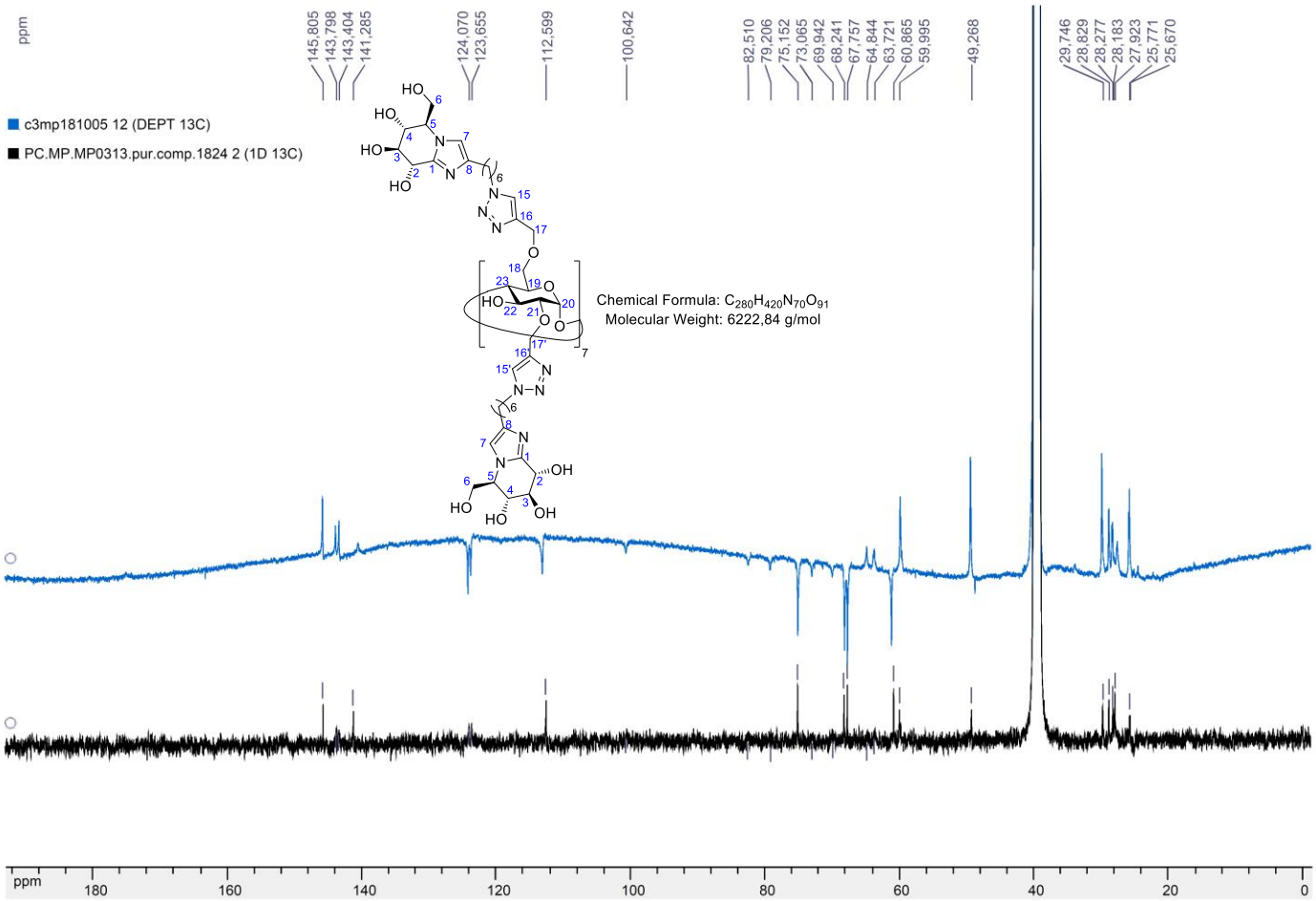


Fig S77. ^{13}C (125 MHz, DMSO-d_6) and DEPT spectra of compound **26a**

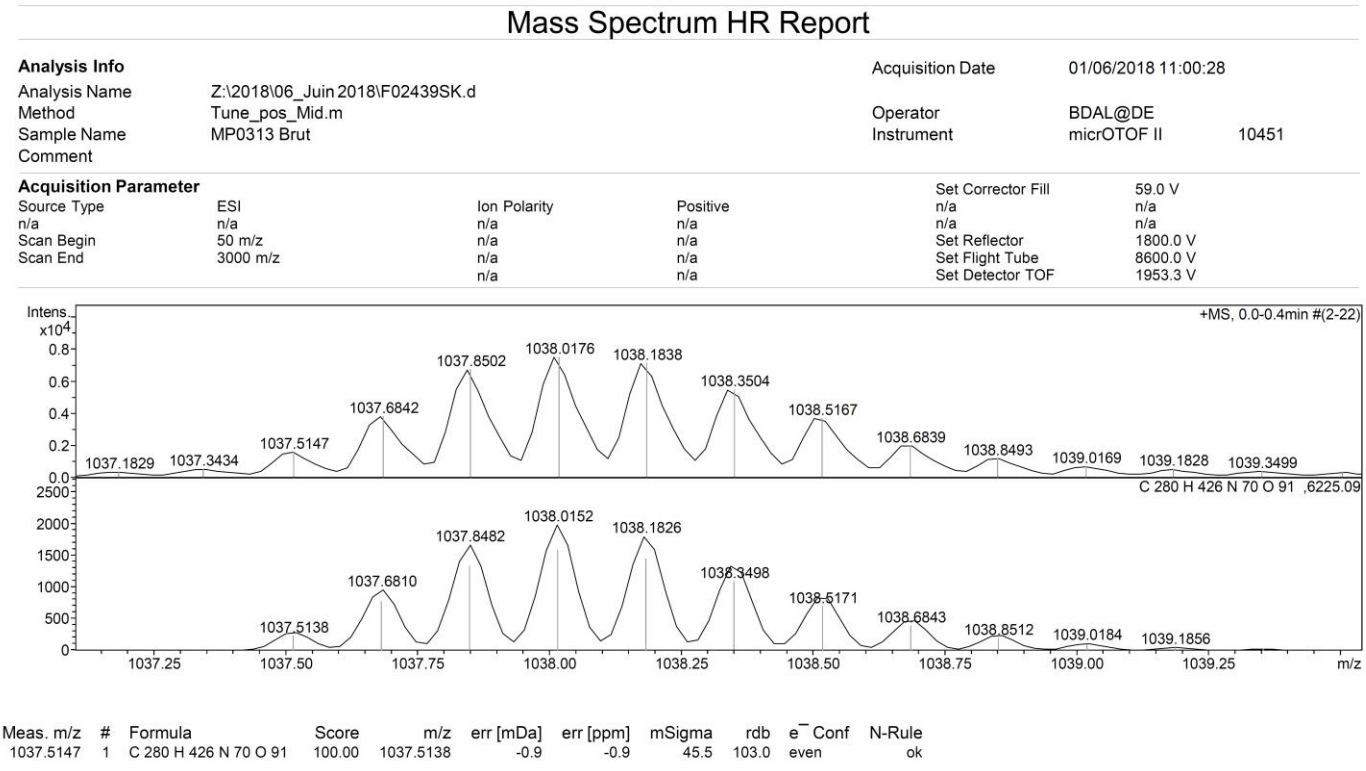


Fig S78. HRMS (ESI-MS) spectrum of compound **26a**

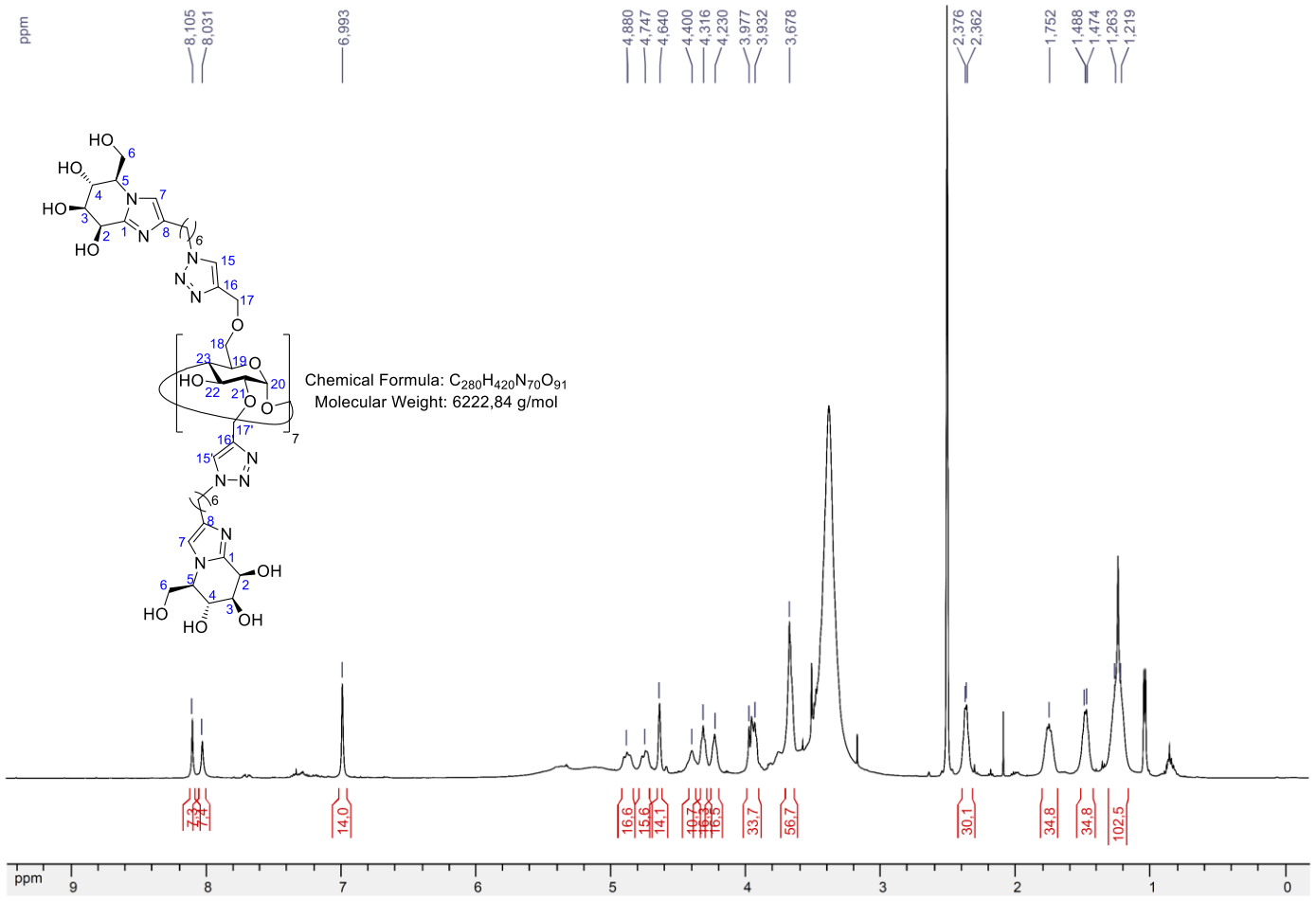


Fig S79. ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **26b**

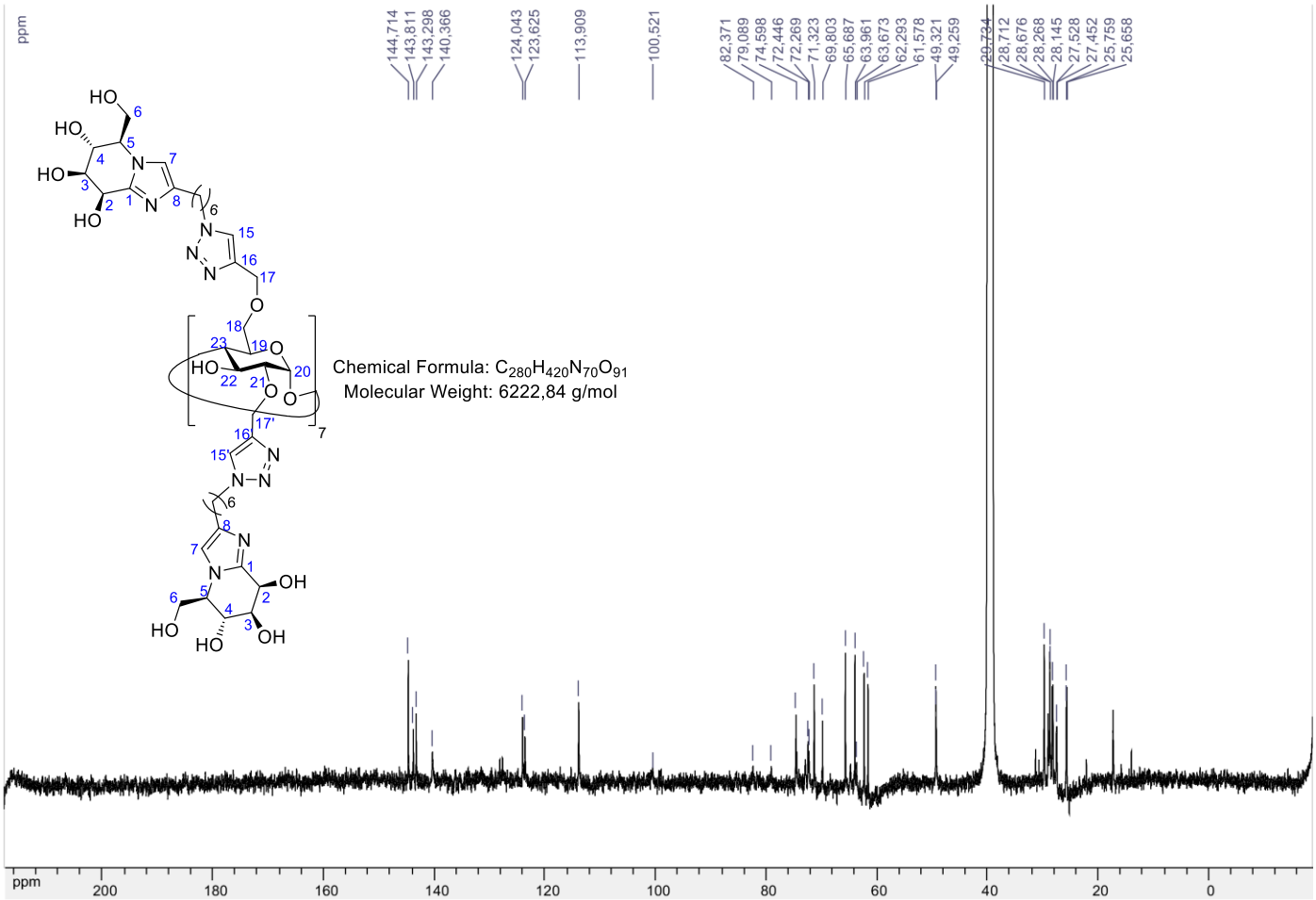


Fig S80. ^{13}C NMR (125 MHz, DMSO-d_6) spectrum of compound **26b**

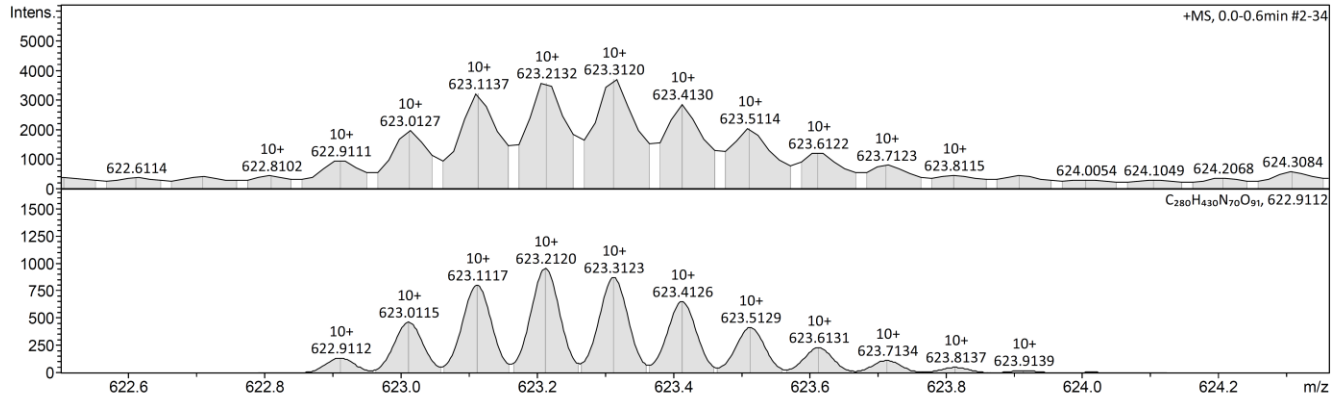
Mass Spectrum HR Report

Analysis Info

Analysis Name	D:\Data\SMasse\2018\10_Octobre 2018\F03021SK.d	Acquisition Date	10/5/2018 2:58:58 PM
Method	Tune_pos_Mid.m	Operator	BDAL@DE
Sample Name	MP0315 BIS	Instrument	micrOTOF II 8213750.1045 1
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Corrector Fill	55.7 V
n/a	n/a	n/a	n/a	n/a	n/a
Scan Begin	50 m/z	n/a	n/a	Set Reflector	1800.0 V
Scan End	3000 m/z	n/a	n/a	Set Flight Tube	8600.0 V
		n/a	n/a	Set Detector TOF	1961.2 V



Meas. m/z	#	Ion Formula	m/z	err [ppm]	Mean err [ppm]	rdb	N-Rule	e⁻ Conf	mSigma	Std I	Std Mean m/z	Std I	VarNorm	Std m/z Diff	Std Comb Dev
622.911096	1	C280H430N70O91	622.911169	0.1	0.3	101.0	ok	even	85.5	51.9	n.a.	n.a.	n.a.	n.a.	n.a.
778.387515	1	C280H428N70O91	778.387142	-0.5	1.1	102.0	ok	even	141.7	84.9	n.a.	n.a.	n.a.	n.a.	n.a.

Fig S81. HRMS (ESI-MS) spectrum of compound **26b**

Inhibition assays against Jack Bean α-mannosidase

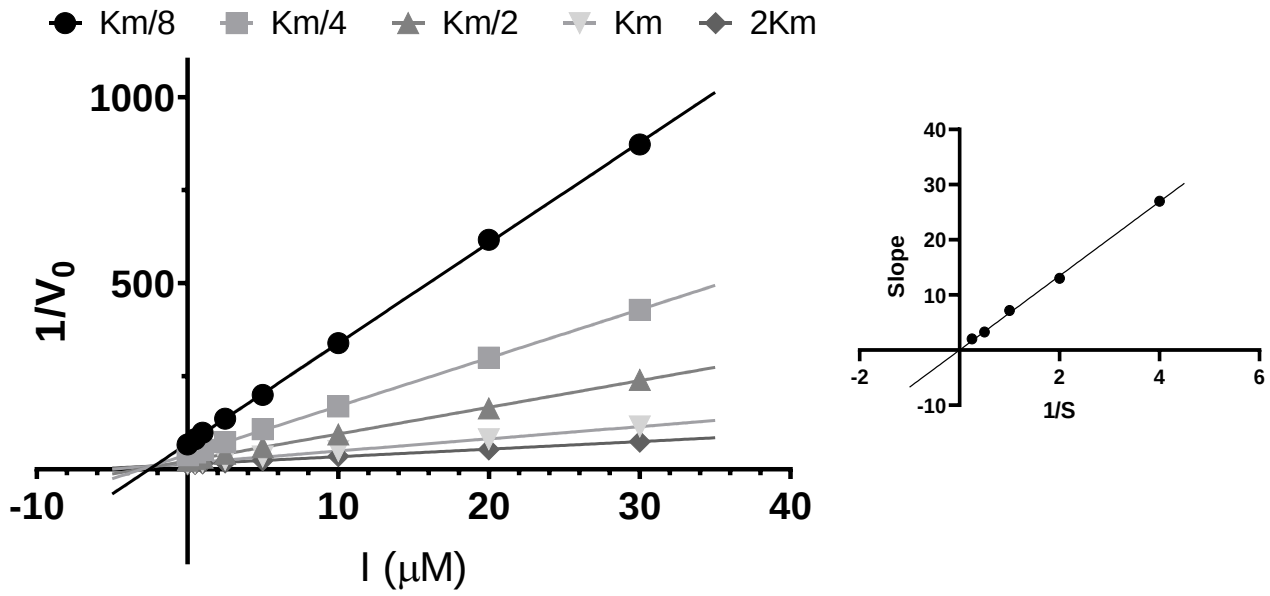


Fig S82. Dixon plot and replot of compound **13a**

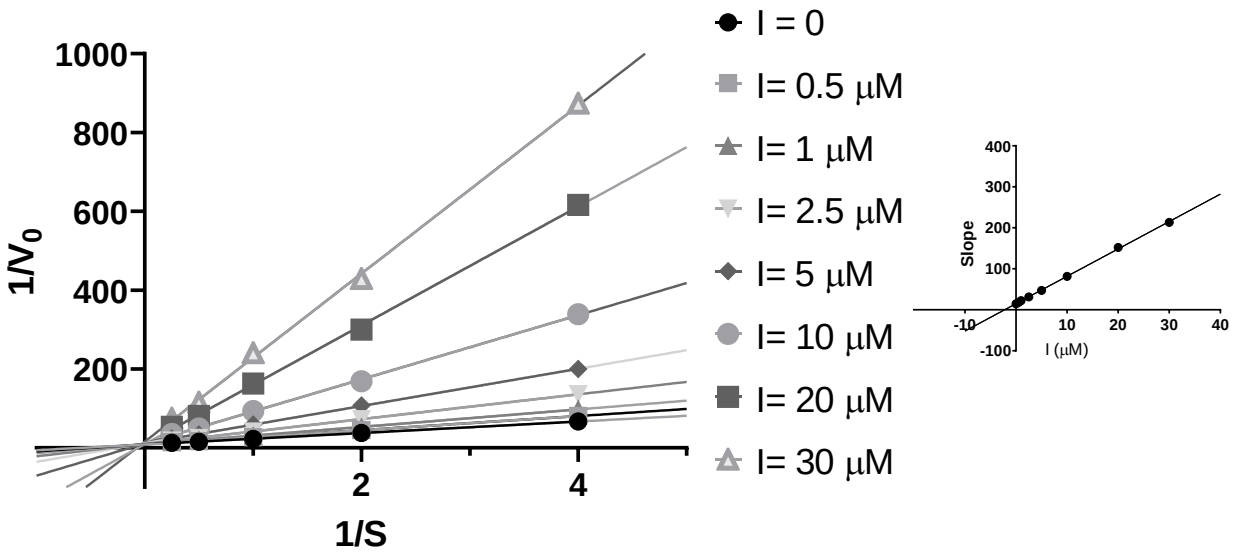


Fig S83. Lineweaver Burk plot and replot for K_i determination (2.23±0.13 μM) of compound **13a**

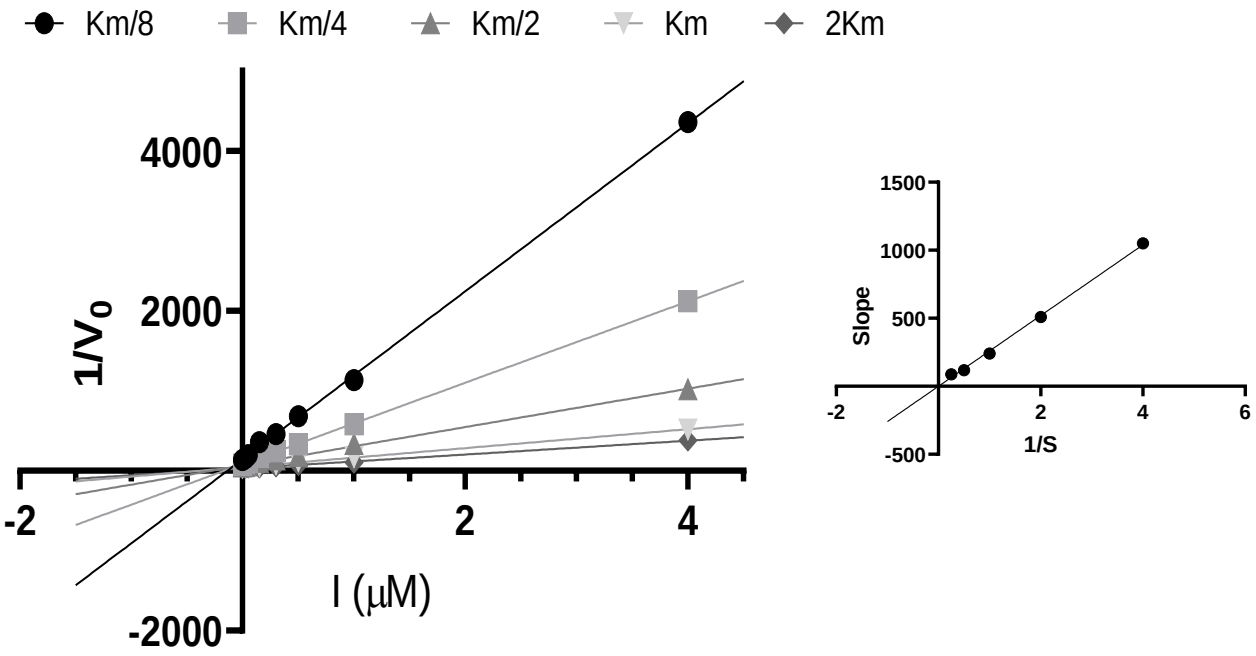


Fig S84. Dixon plot and replot of compound **13b**

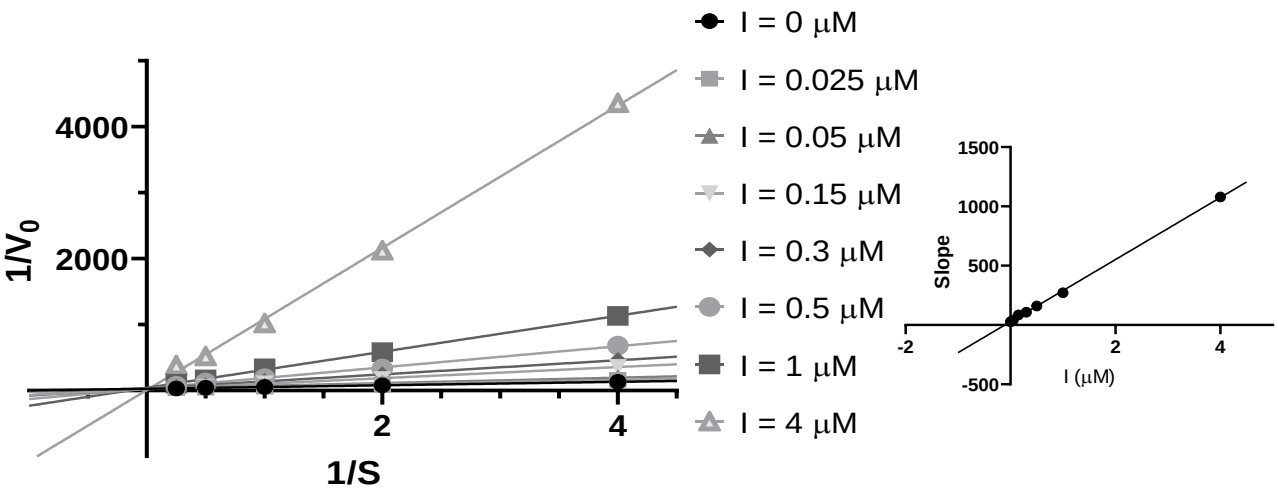


Fig S85. Lineweaver Burk plot and replot for K_i determination (0.11±0.02 μM) of compound **13b**

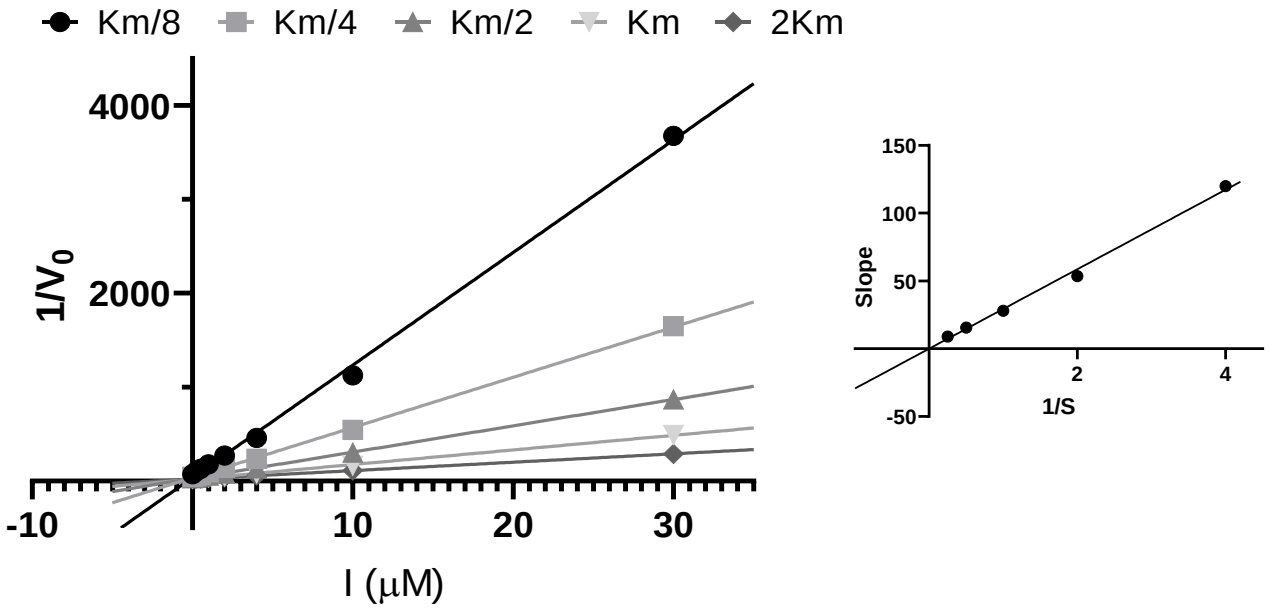


Fig S86. Dixon plot and replot of compound **19a**

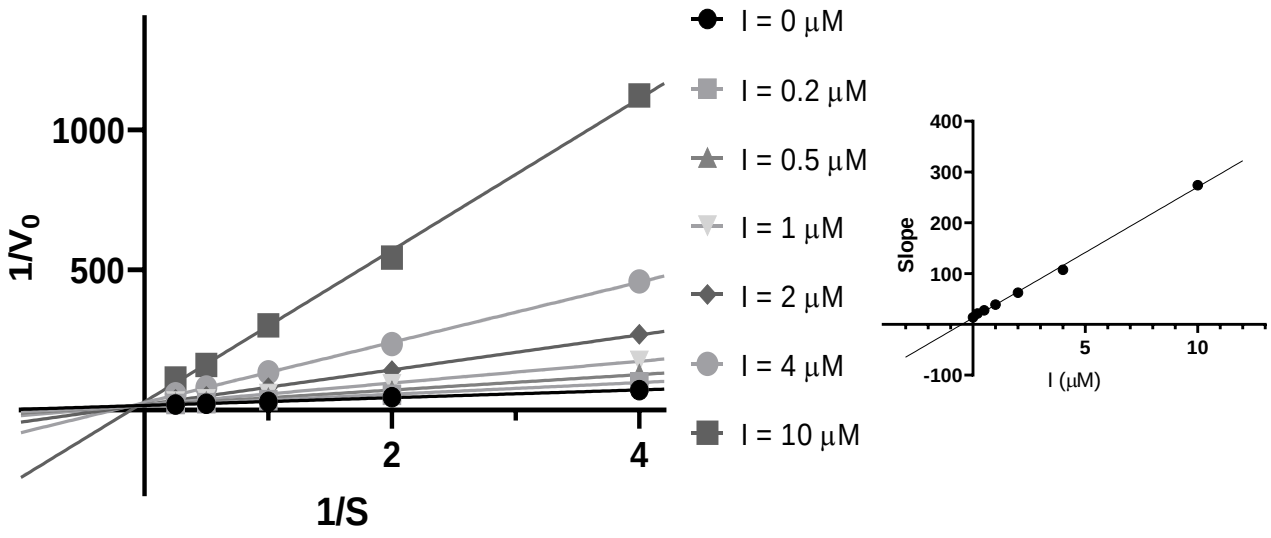


Fig S87. Lineweaver Burk plot and replot for K_i determination (0.49±0.64 μM) of compound **19a**

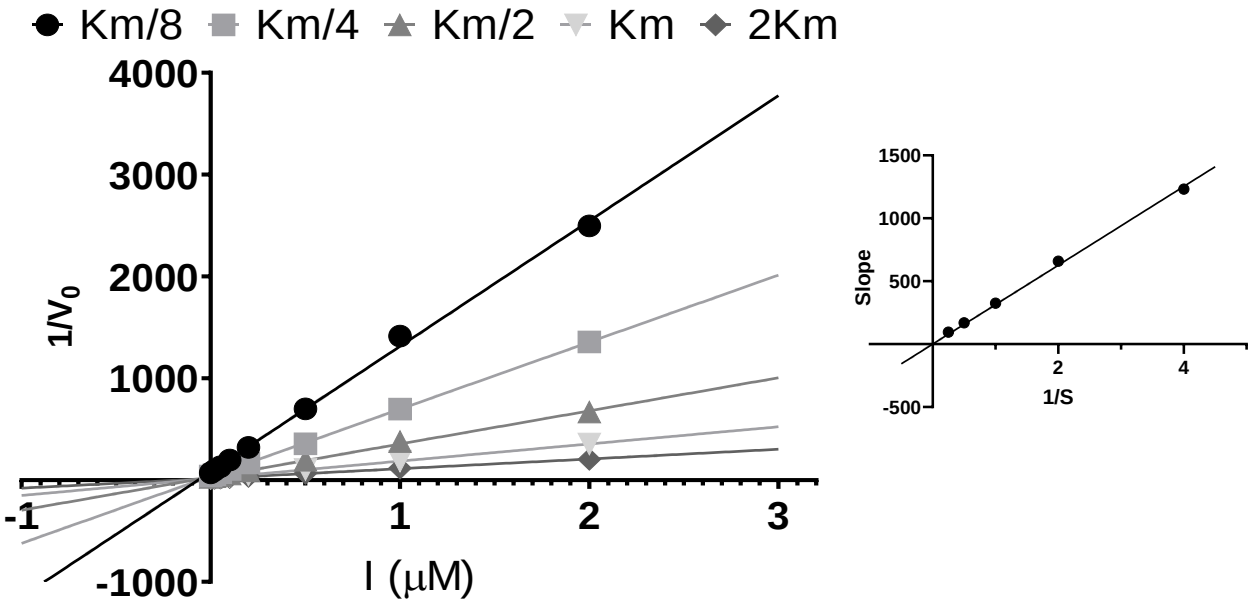


Fig S88. Dixon plot and replot of compound **19b**

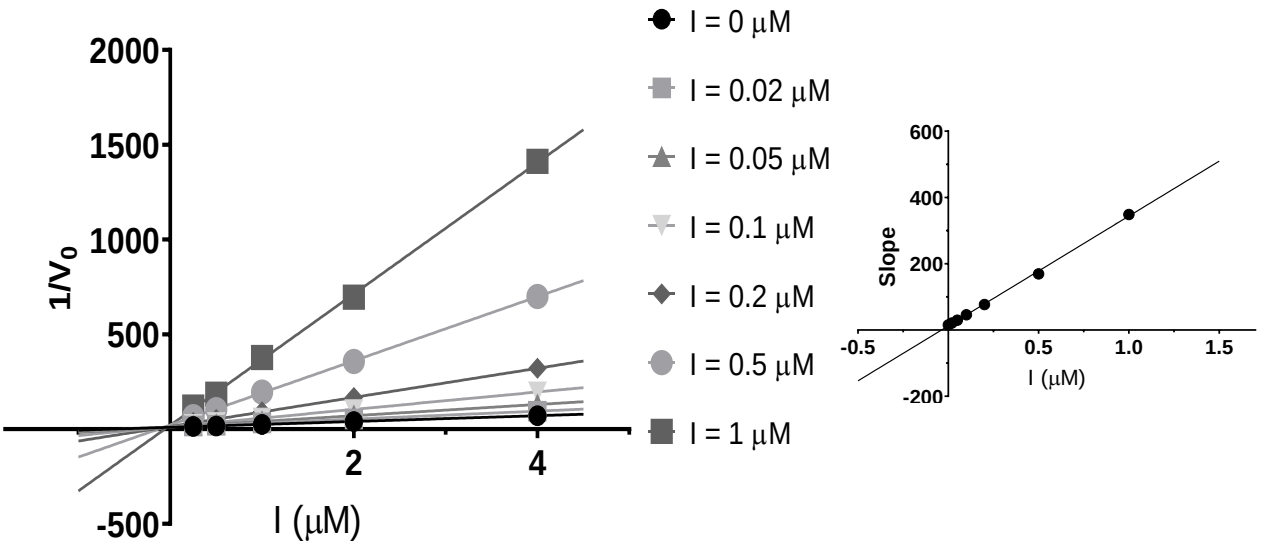


Fig S89. Lineweaver Burk plot and replot for K_i determination (0.037±0.007 μM) of compound **19b**

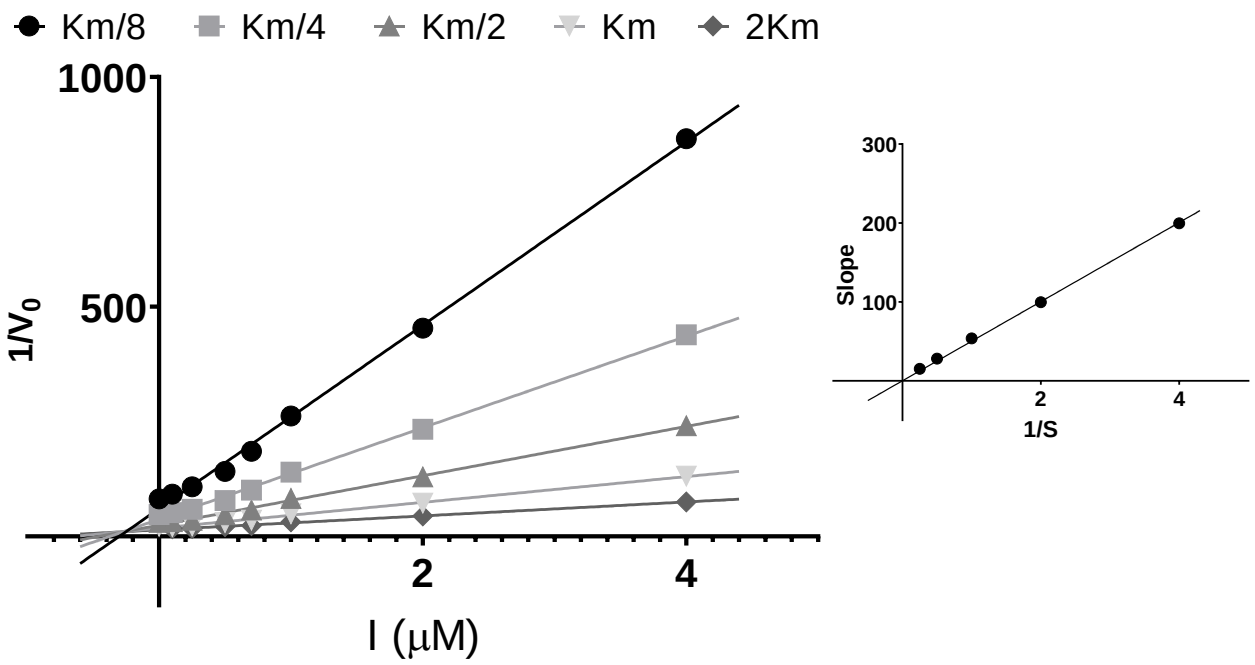


Fig S90. Dixon plot and replot of compound **21a**

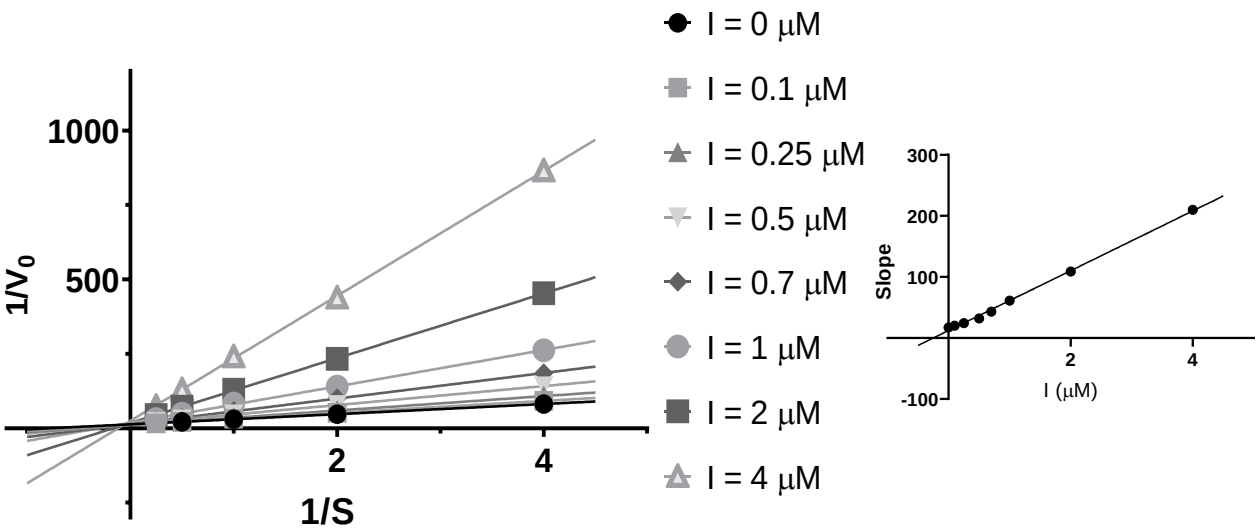


Fig S91. Lineweaver Burk plot and replot for K_i determination (0.25±0.03 μM) of compound **21a**

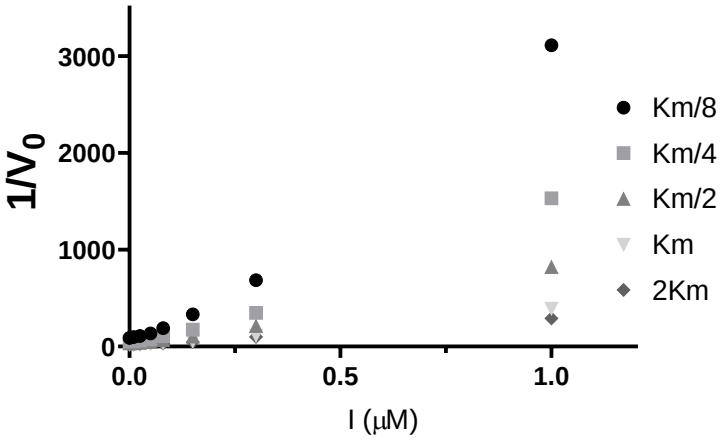


Fig S92. Dixon plot of compound **21b**

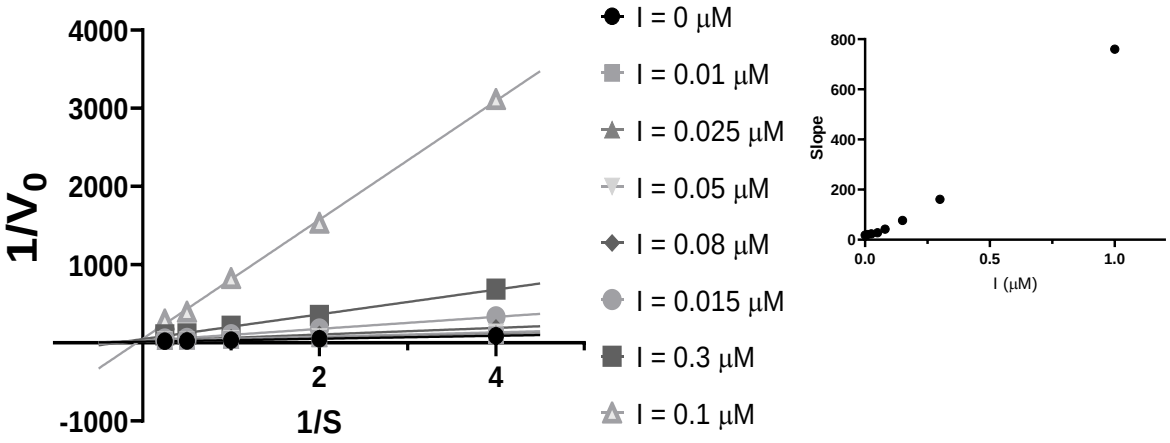


Fig S93. Lineweaver Burk plot and replot of compound **21b**

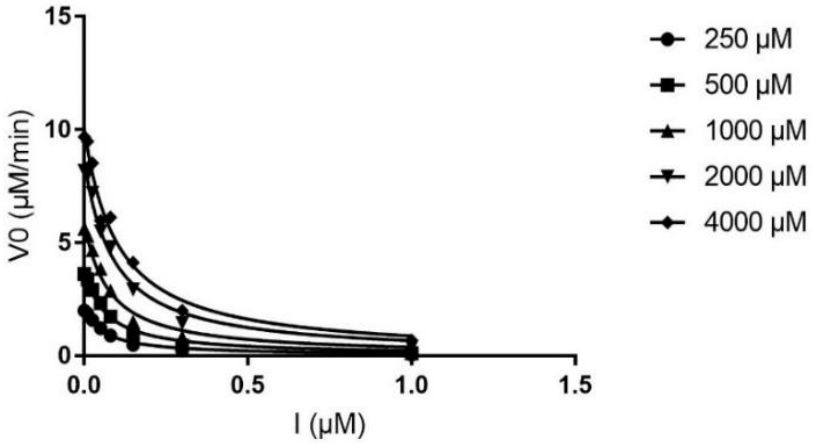


Fig S94. Plot of enzyme velocity as a function of inhibitor **21b** concentration.
The solid curves drawn through the data points represent the best fit to the Morrison equation used to obtain K_i value (0.037±0.010 μM) for the tight binding inhibitor **21b**

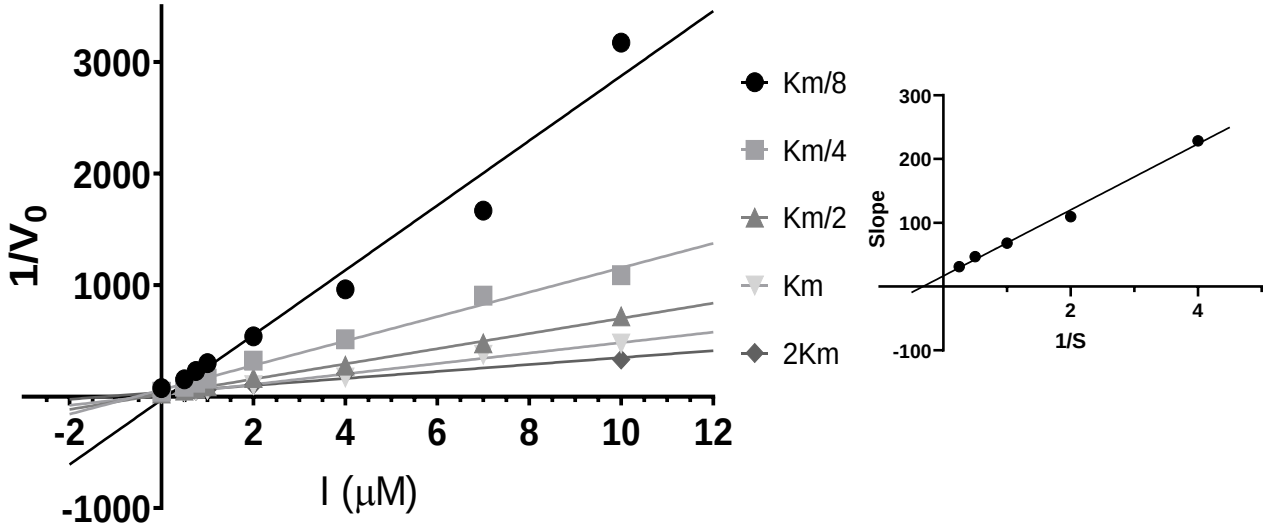


Fig S95. Dixon plot and replot of compound **23a**

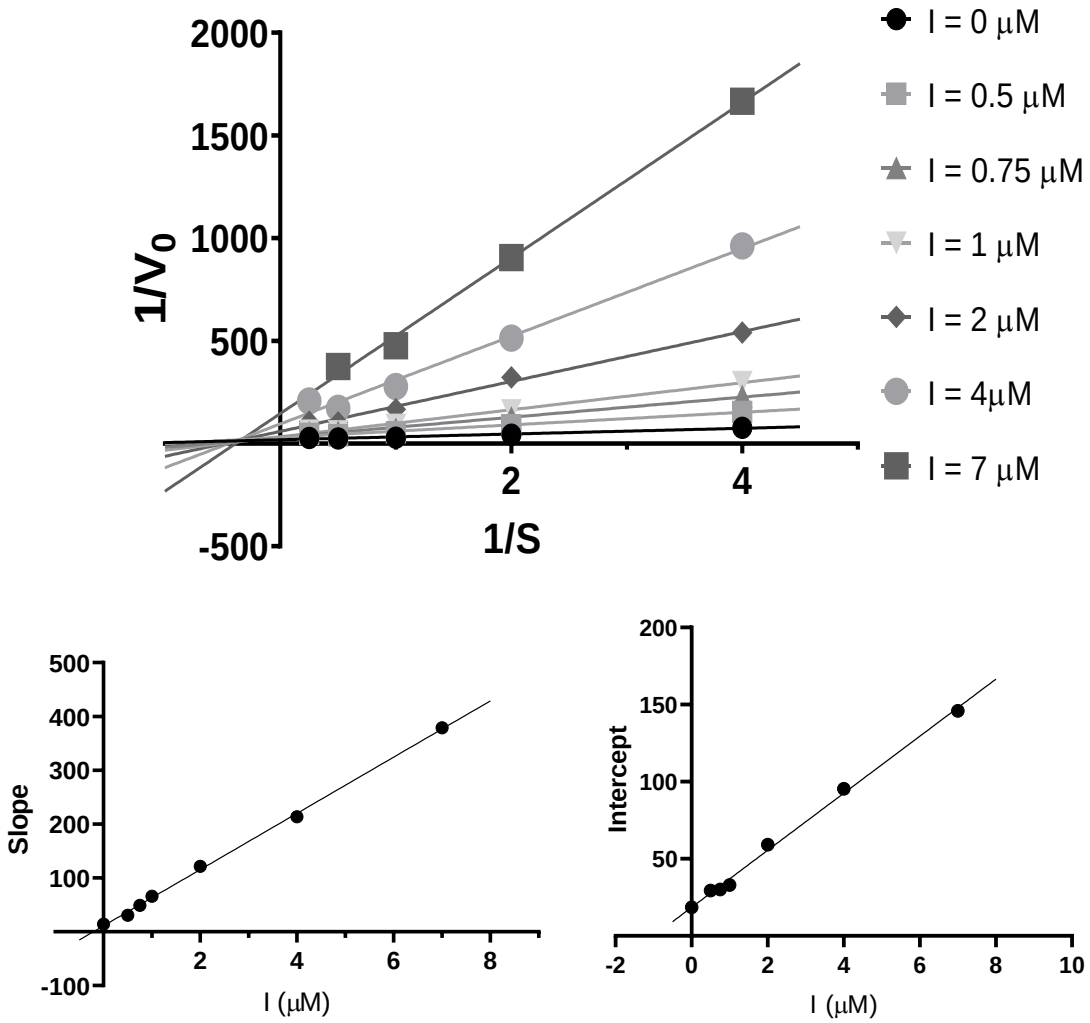


Fig S96. Lineweaver Burk plot, slope and intercept replots of reciprocal plot data for K_i determination (K_i = 0.21±0.05 μM; K_i' = 1.00±0.096 μM) of compound **23a**

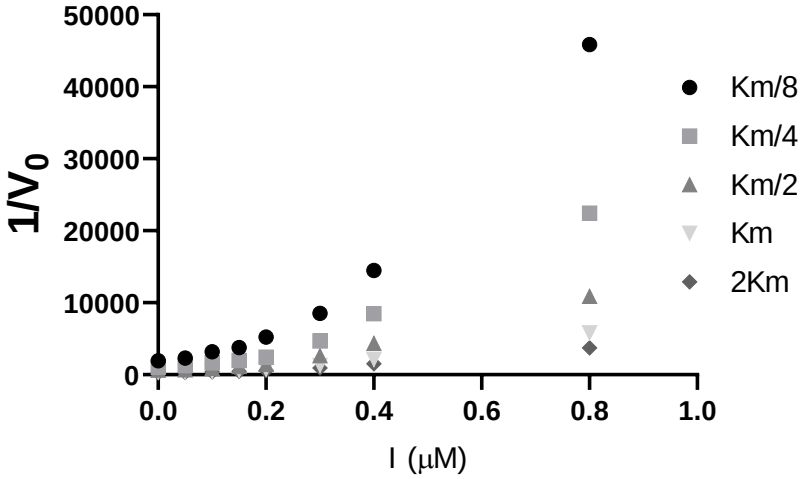


Fig S97. Dixon plot of compound **23b**

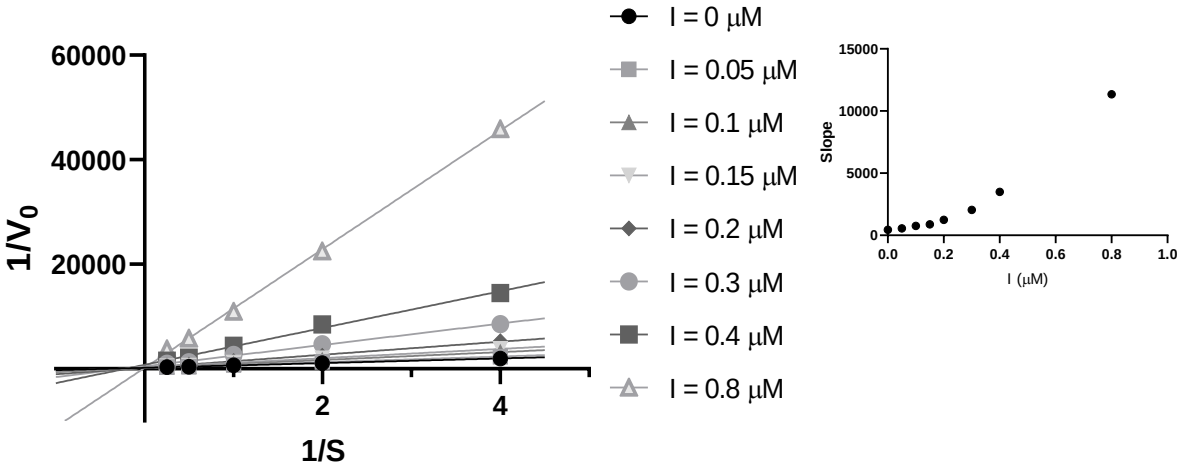


Fig S98. Lineweaver Burk plot and replot of compound **23b**

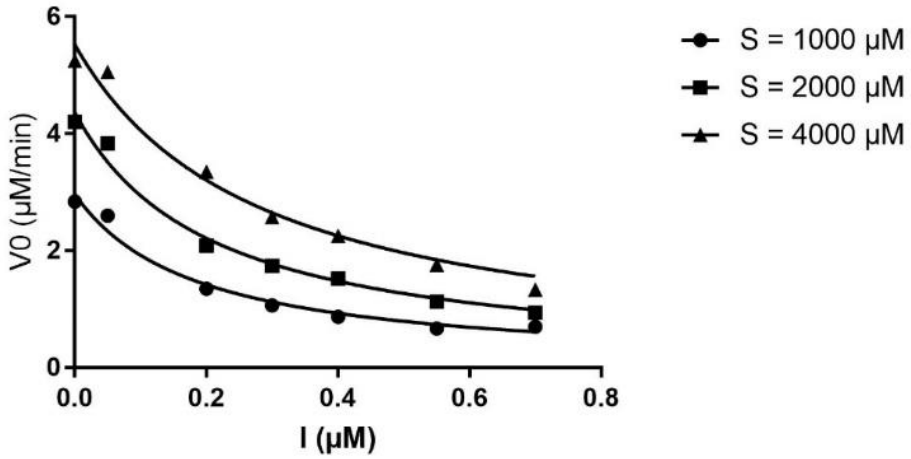


Fig S99. Plot of enzyme velocity as a function of inhibitor **23b** concentration.
The solid curves drawn through the data points represent the best fit to the Morrison equation used to obtain K_i value (0.091±0.017 μM) for the tight binding inhibitor **23b**

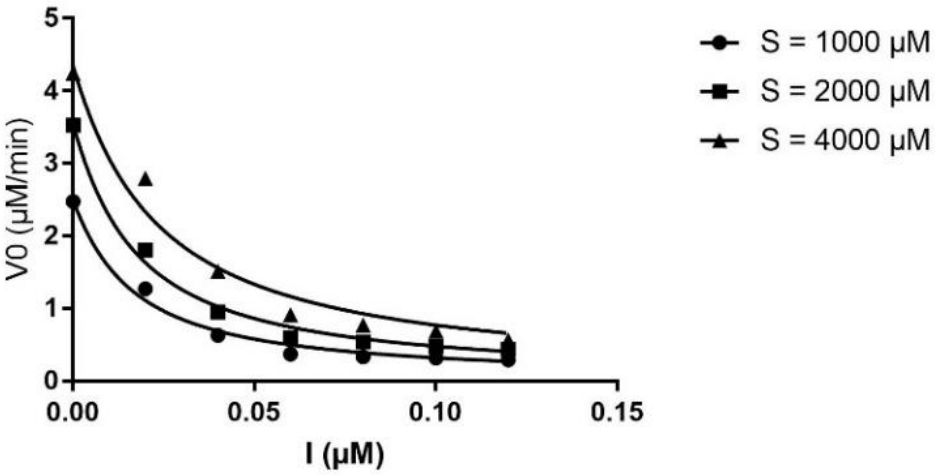


Fig S100. Plot of enzyme velocity as a function of inhibitor **26a** concentration.
The solid curves drawn through the data points represent the best fit to the Morrison equation used to obtain K_i value (0.006±0.001 µM) for the tight binding inhibitor **26a**

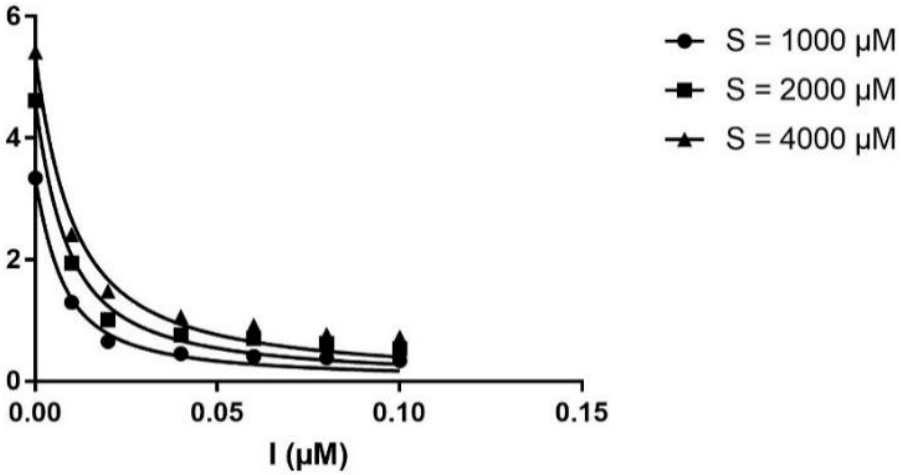


Fig S101. Plot of enzyme velocity as a function of inhibitor **26b** concentration.
The solid curves drawn through the data points represent the best fit to the Morrison equation used to obtain K_i value (0.002±0.0005 µM) for the tight binding inhibitor **26b**