
SUPPORTING INFORMATION

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

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

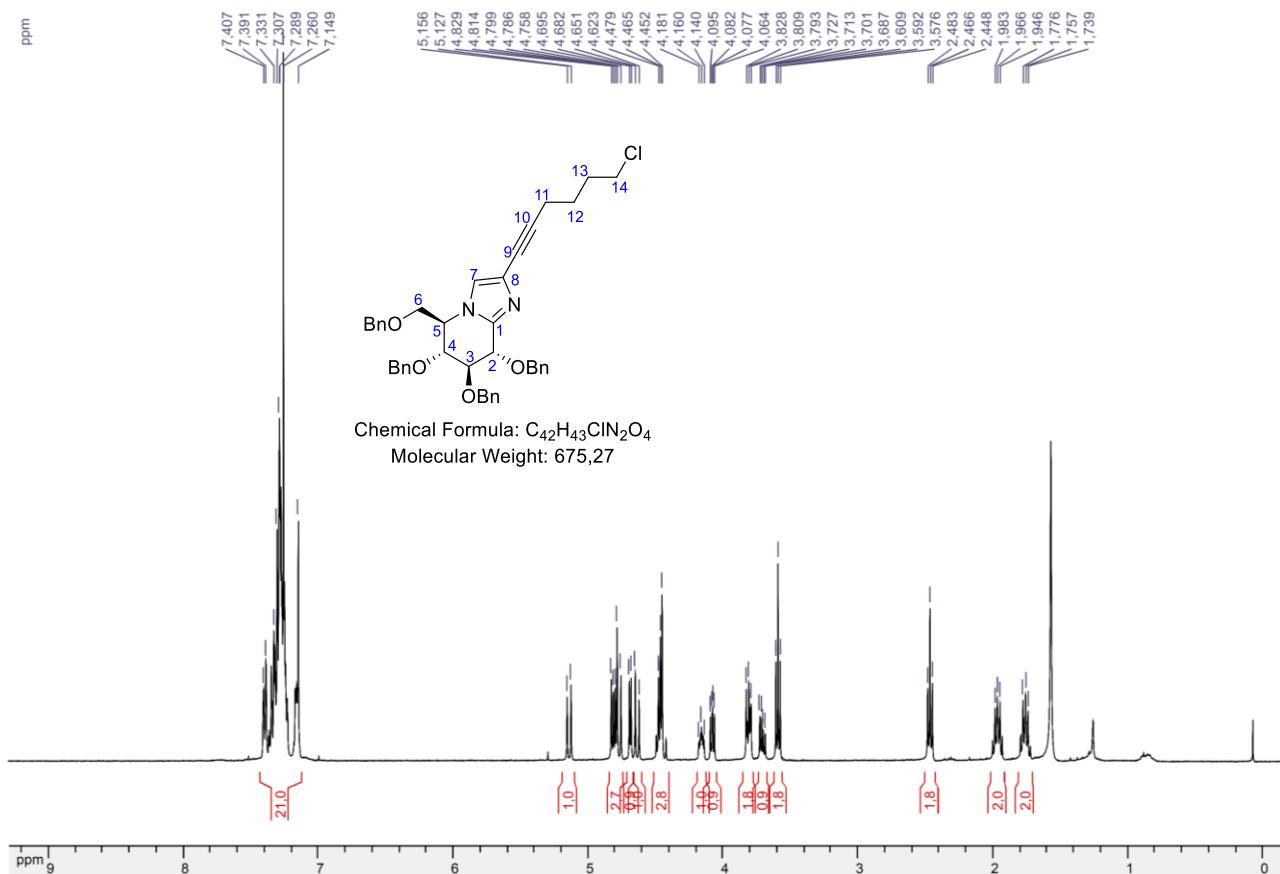


Fig S1. ^1H NMR (400 MHz, CDCl_3) spectrum of compound 9a

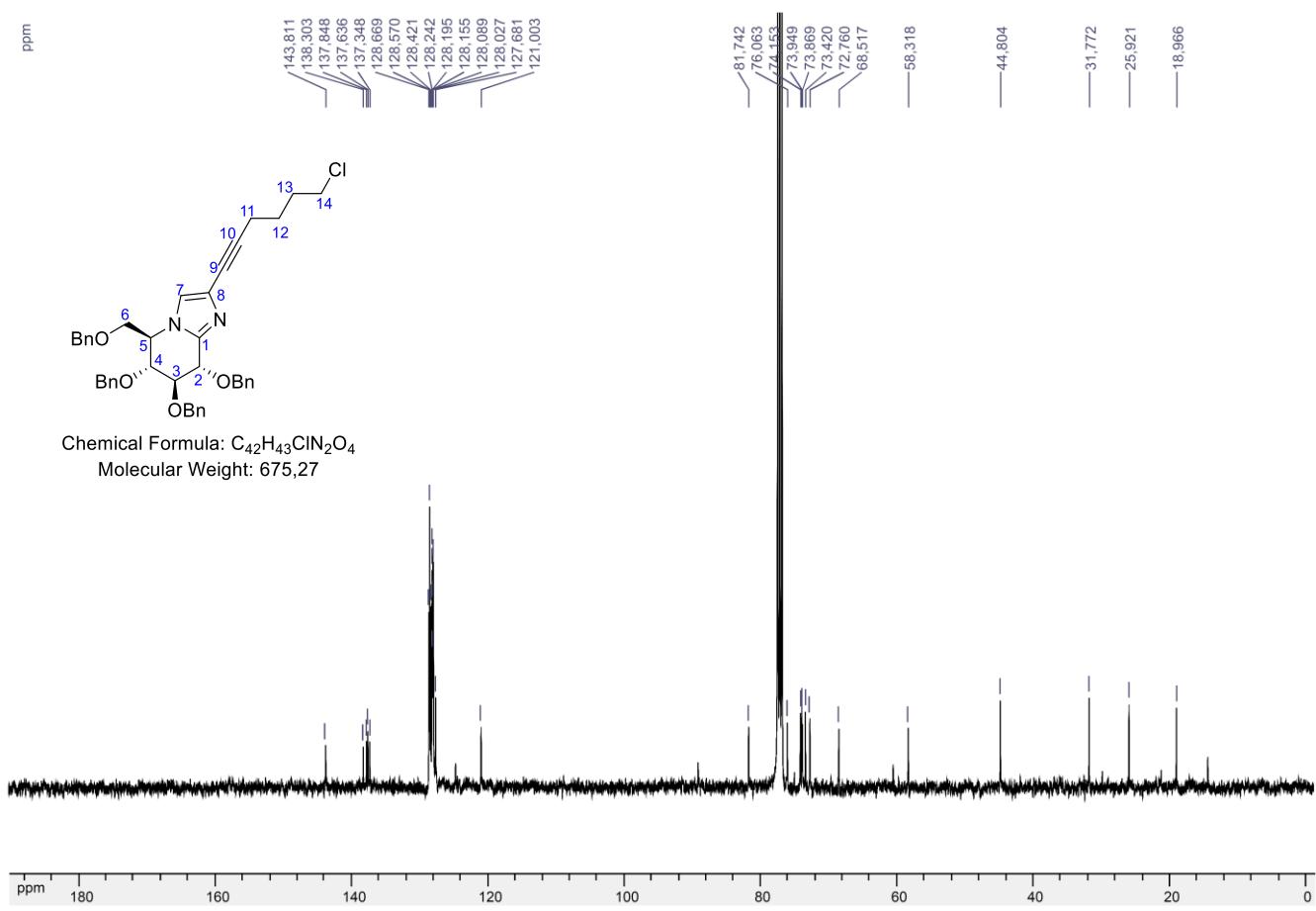


Fig S2. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound 9a

Mass Spectrum HR Report

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 Comment

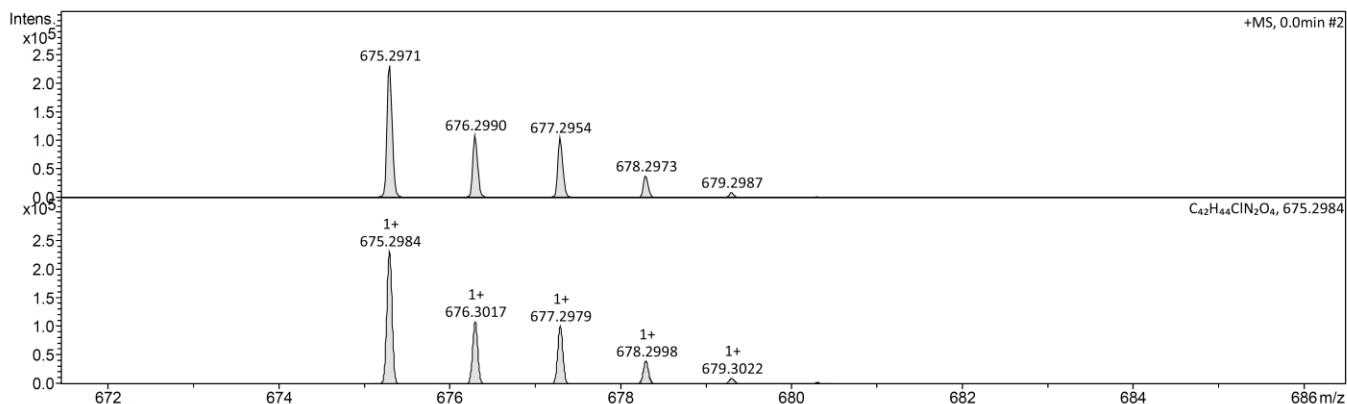
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 Instrument micrOTOF II

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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

675.29701 1 C42H44ClN2O4 675.298412 2.0 3.4 21.5 ok even 8.1 7.8 n.a. n.a. n.a. n.a. n.a.

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

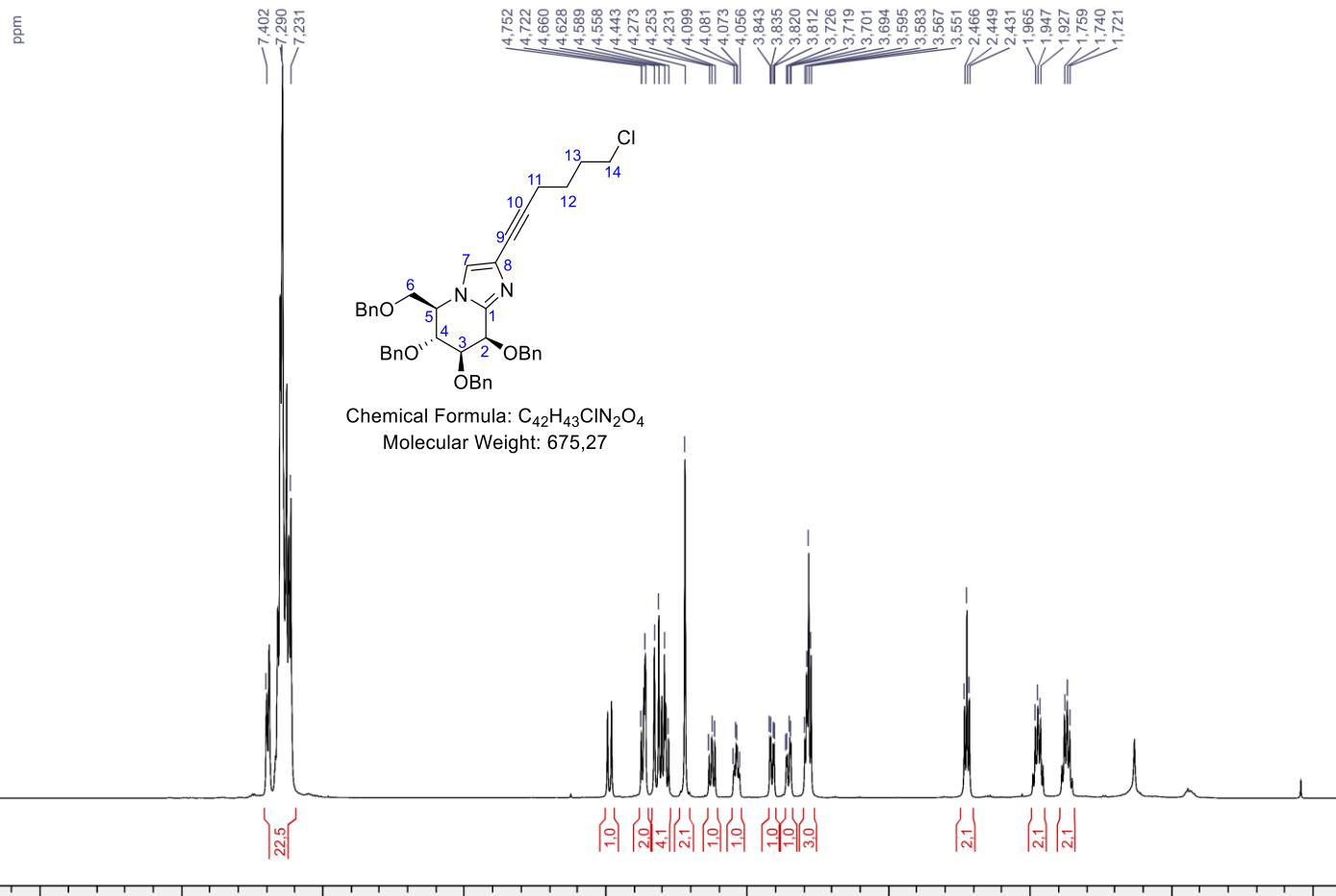


Fig S4. ¹H NMR (400 MHz, CDCl₃) spectrum of compound 9b

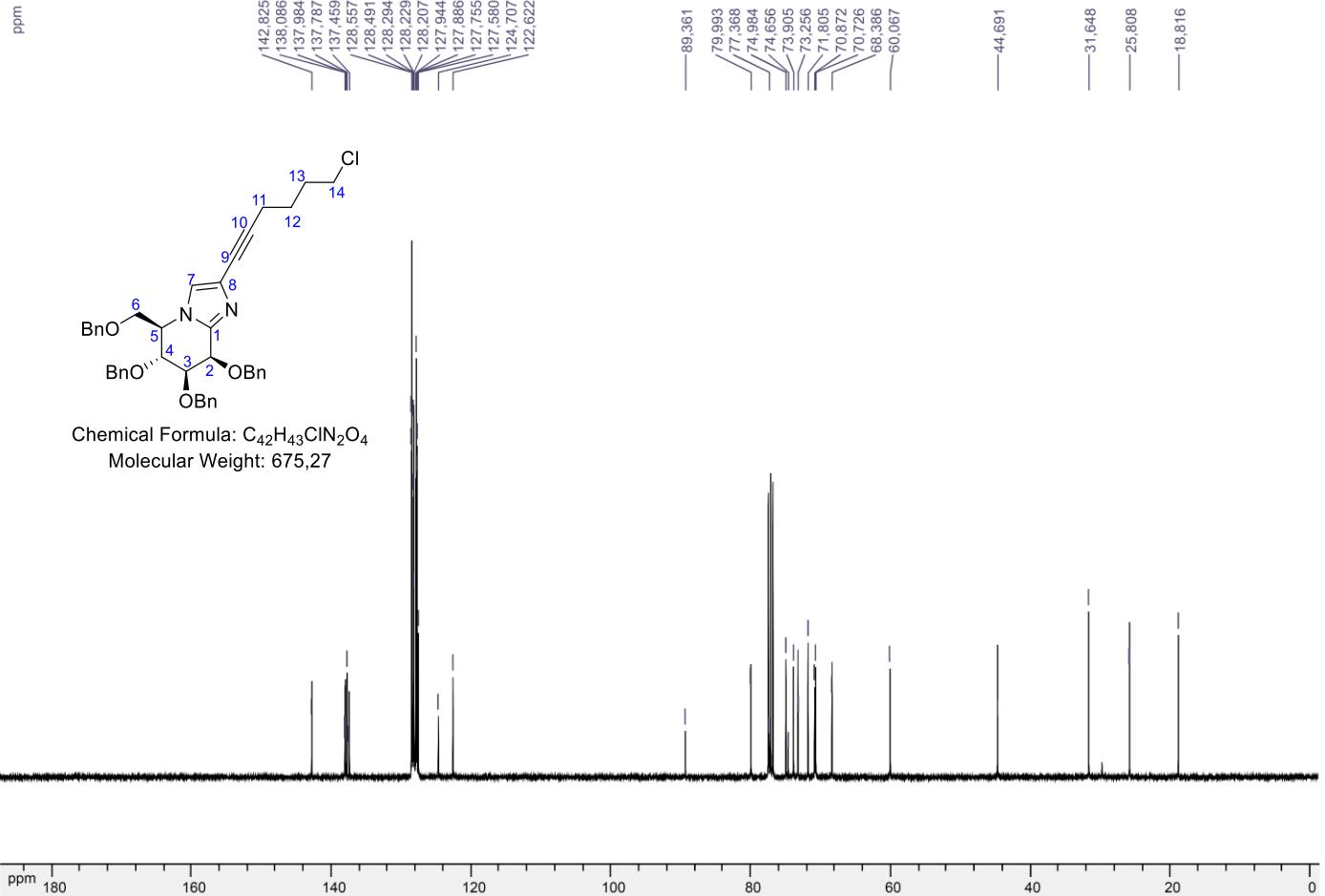
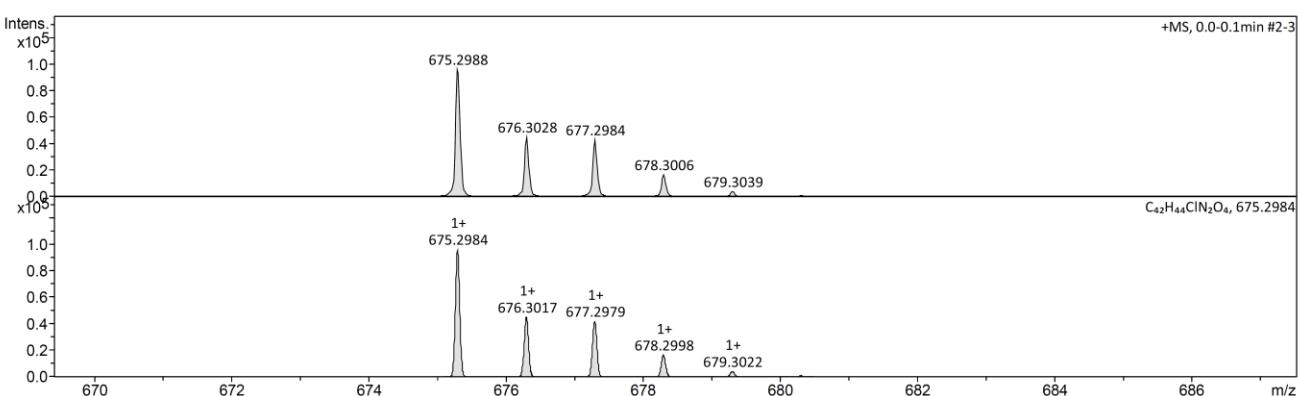


Fig S5. ¹³C NMR (100 MHz, CDCl₃) spectrum of compound 9b

Mass Spectrum HR Report

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Scan End	3000 m/z	n/a	Set Flight Tube
		n/a	Set Detector TOF
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			n/a
			n/a
			1800.0 V
			8600.0 V
			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
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Fig S6. HRMS (ESI-MS) spectrum of compound 9b

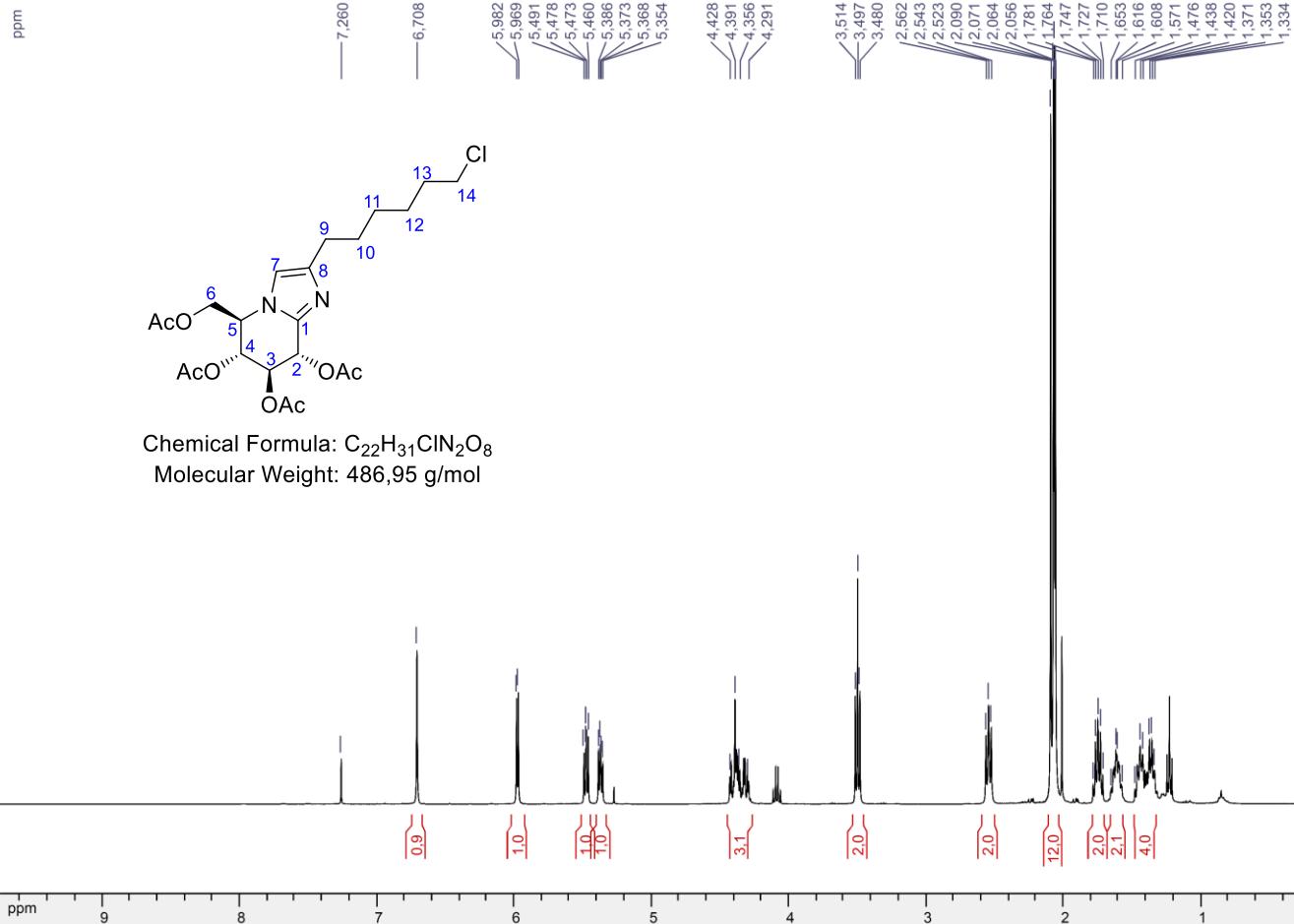


Fig S7. ^1H NMR (400 MHz, CDCl_3) spectrum of compound 10a

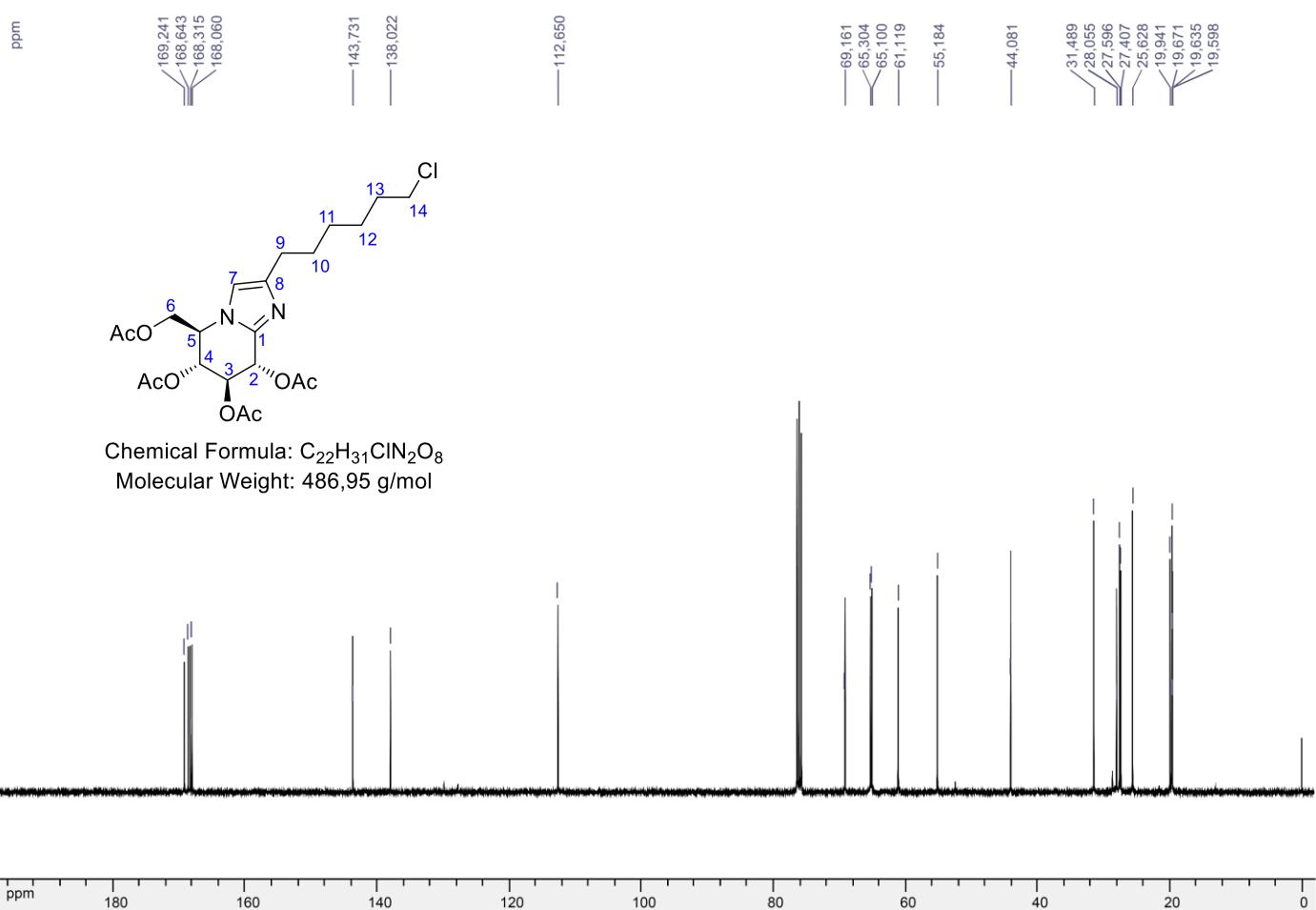


Fig S8. ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound 10a

Mass Spectrum HR Report

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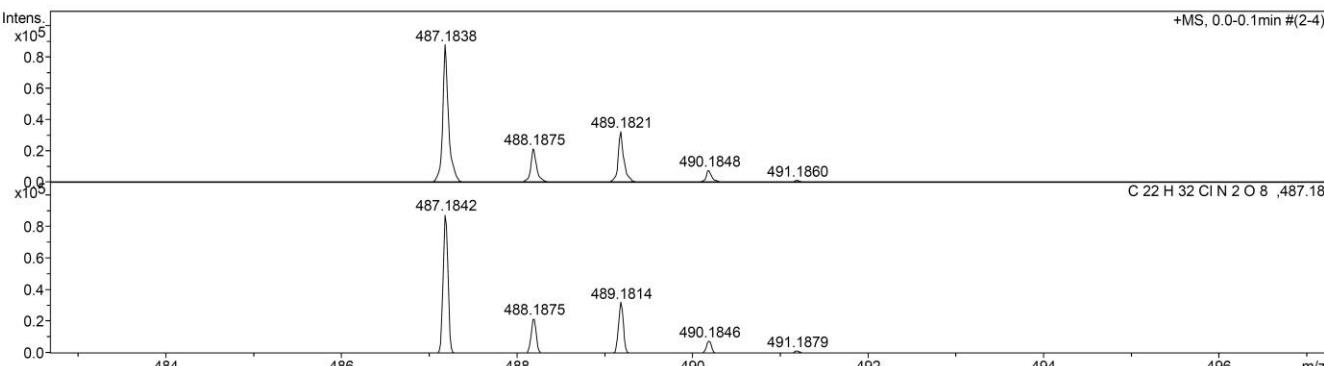
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 Instrument

 BDAL@DE
 micrOTOF II
 10451

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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



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

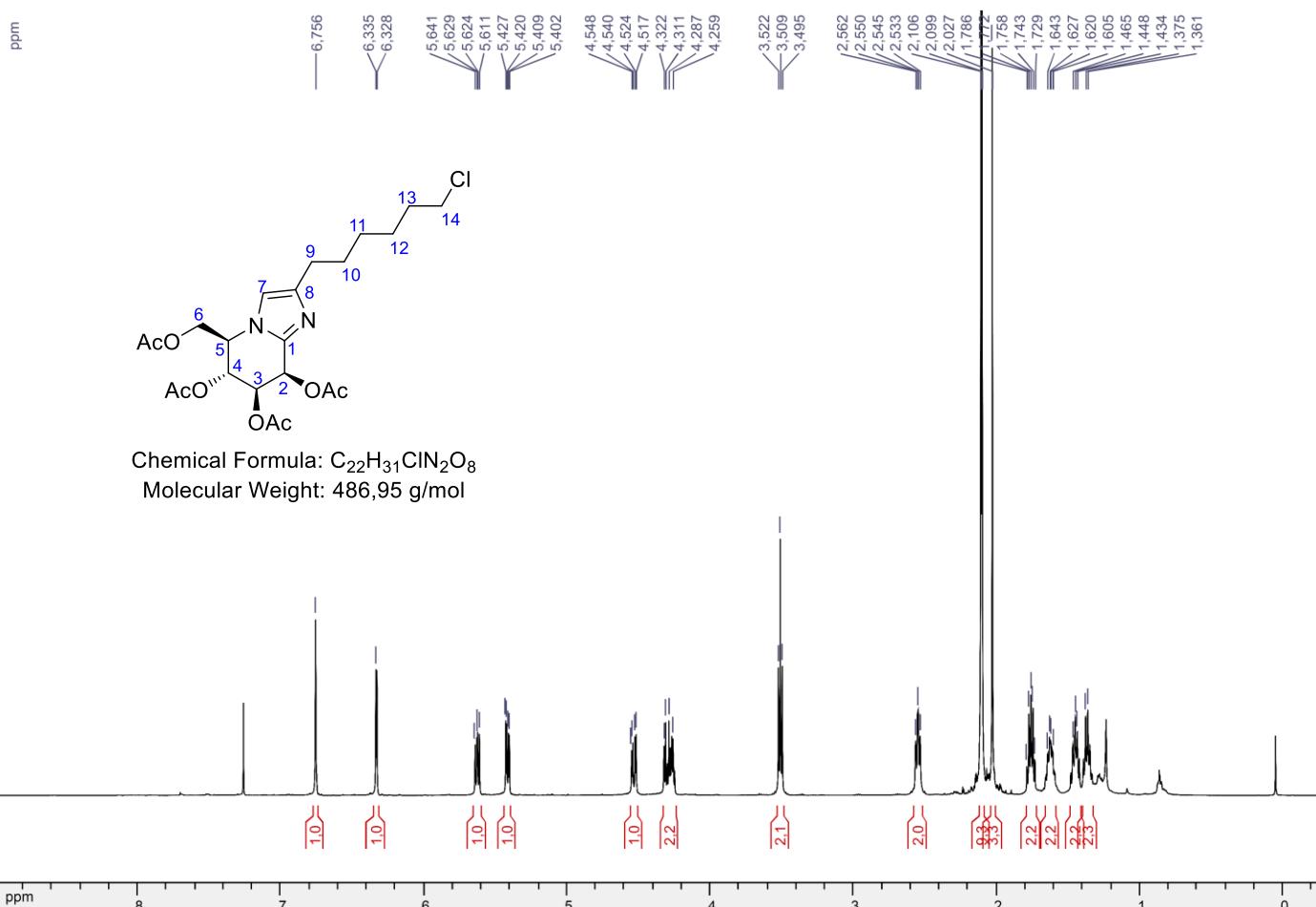
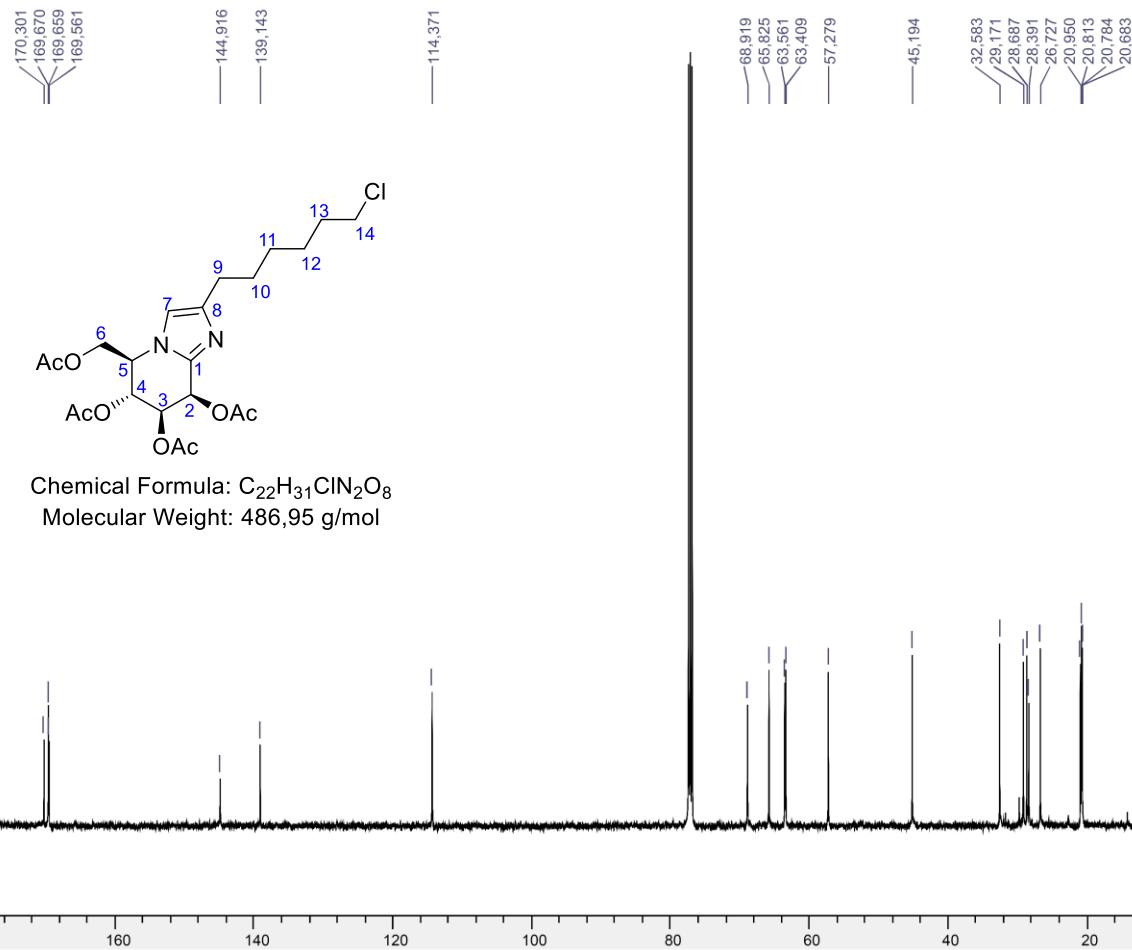


Fig S10. ¹H NMR (500 MHz, CDCl₃) spectrum of compound **10b**

ppm

Fig S11. ¹³C NMR (125 MHz, CDCl₃) spectrum of compound 10b

Mass Spectrum HR Report

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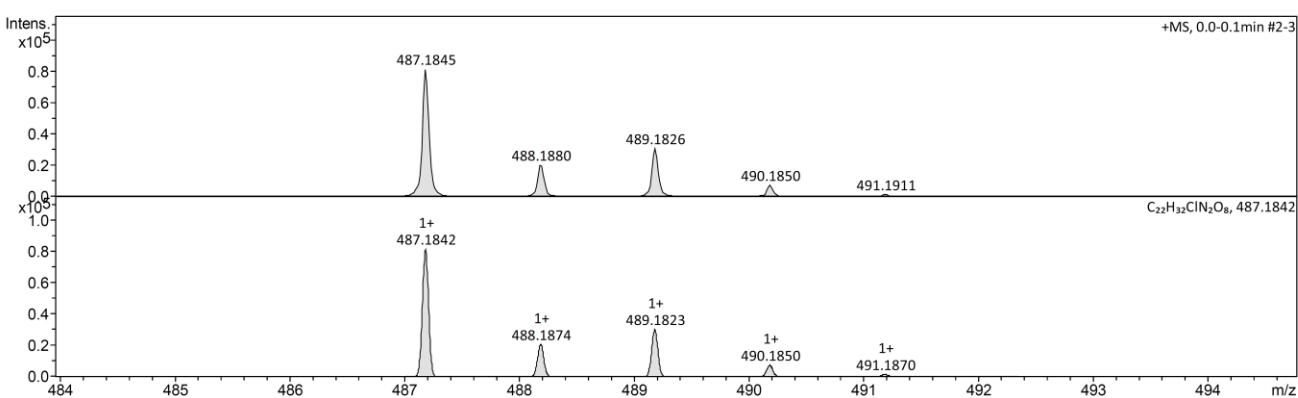
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micrOTOF II
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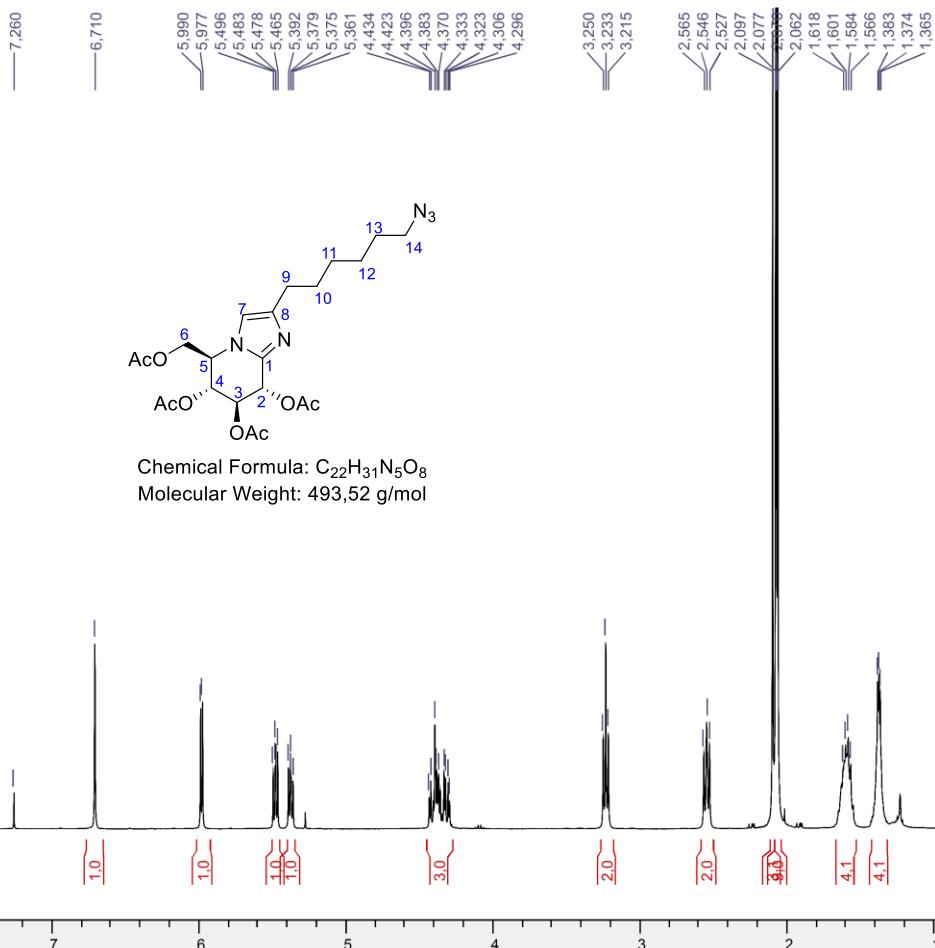
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	n/a	n/a	n/a	Set Detector TOF	1953.3 V



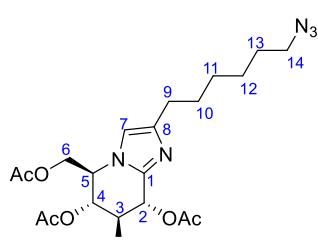
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487.184525 1 C22H32CIN2O8	487.184170	-0.7	-1.7	7.5	ok even	5.4	6.9	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	

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

ppm

Fig S13. ¹H NMR (500 MHz, CDCl₃) spectrum of compound 11a

ppm



Chemical Formula: C₂₂H₃₁N₅O₈
Molecular Weight: 493,52 g/mol

ppm

Fig S14. ¹³C NMR (125 MHz, CDCl₃) spectrum of compound 11a

Mass Spectrum HR Report

Analysis Info

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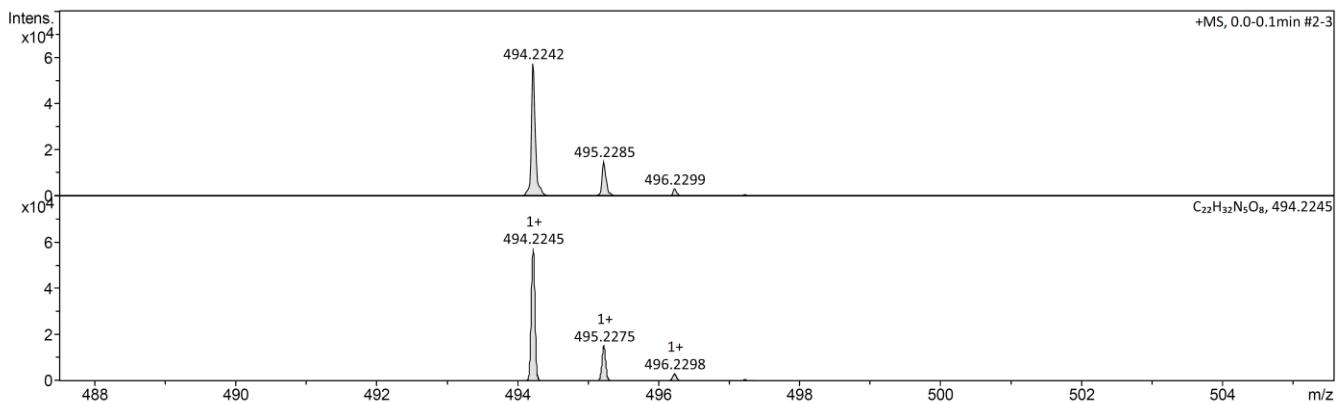
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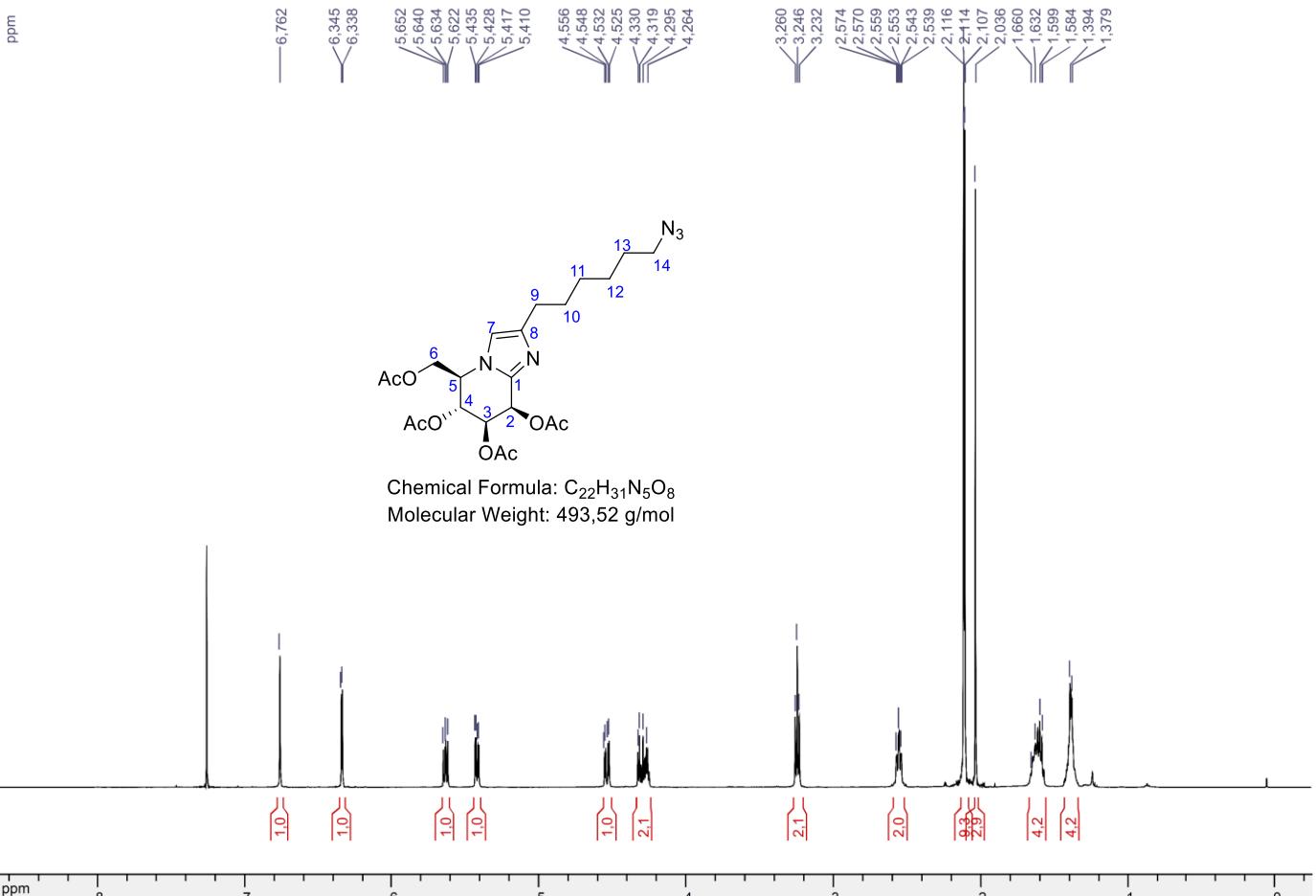
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		n/a	n/a	Set Detector TOF	1953.3 V



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



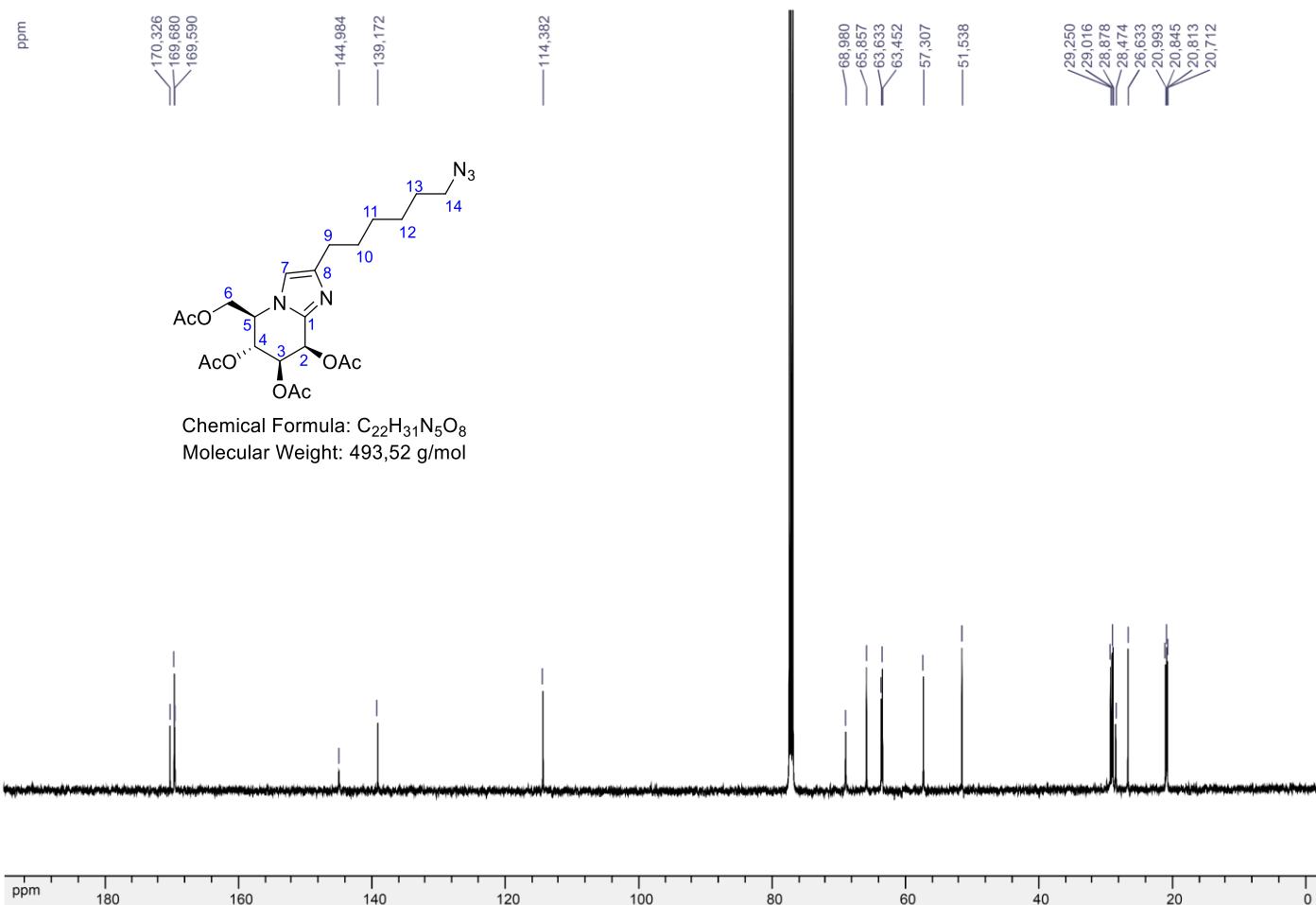
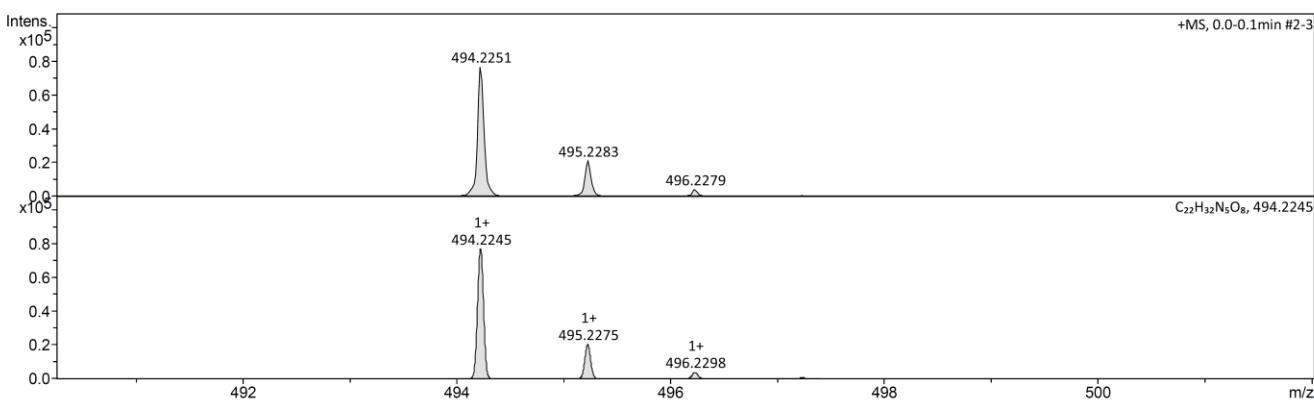


Fig S17. ¹³C NMR (125 MHz, CDCl₃) spectrum of compound 11b

Mass Spectrum HR Report

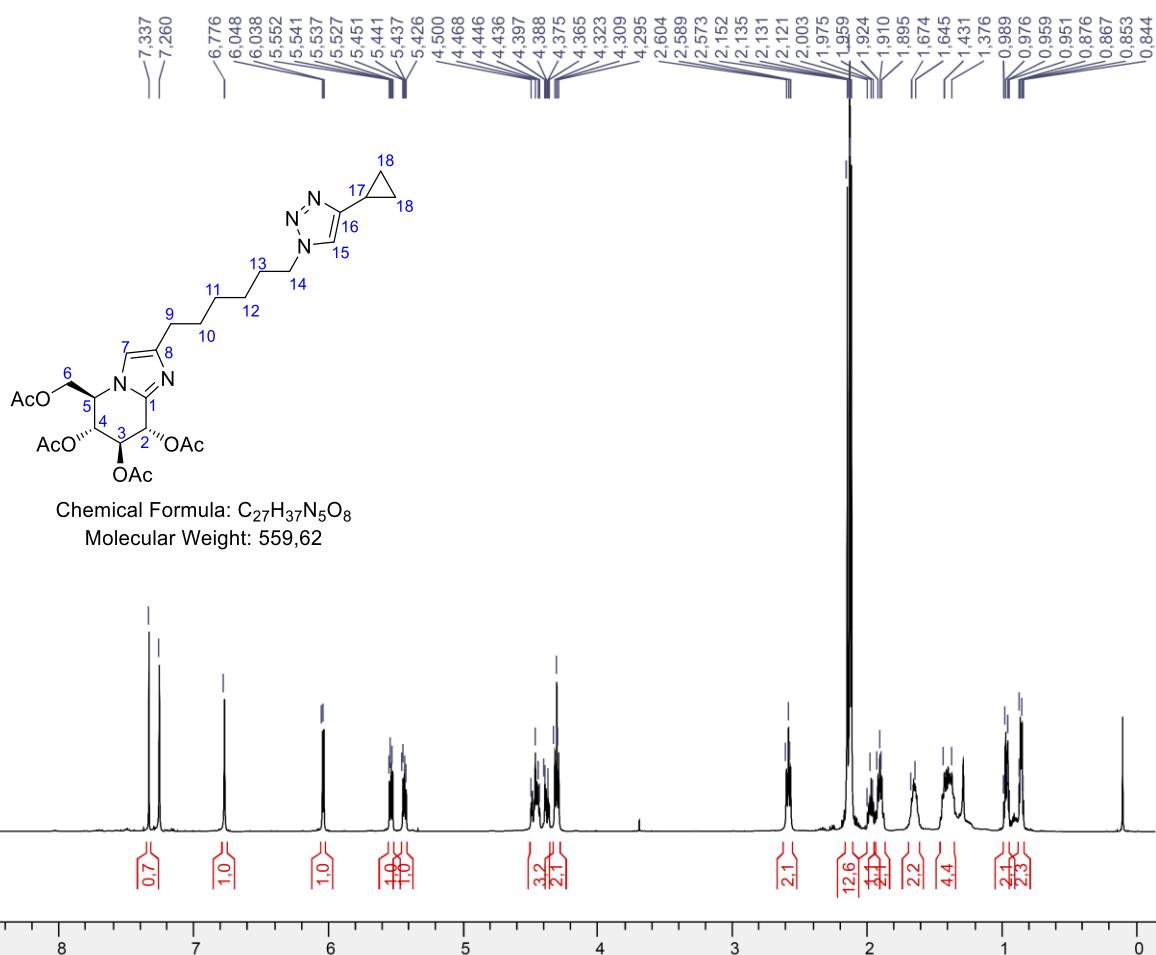
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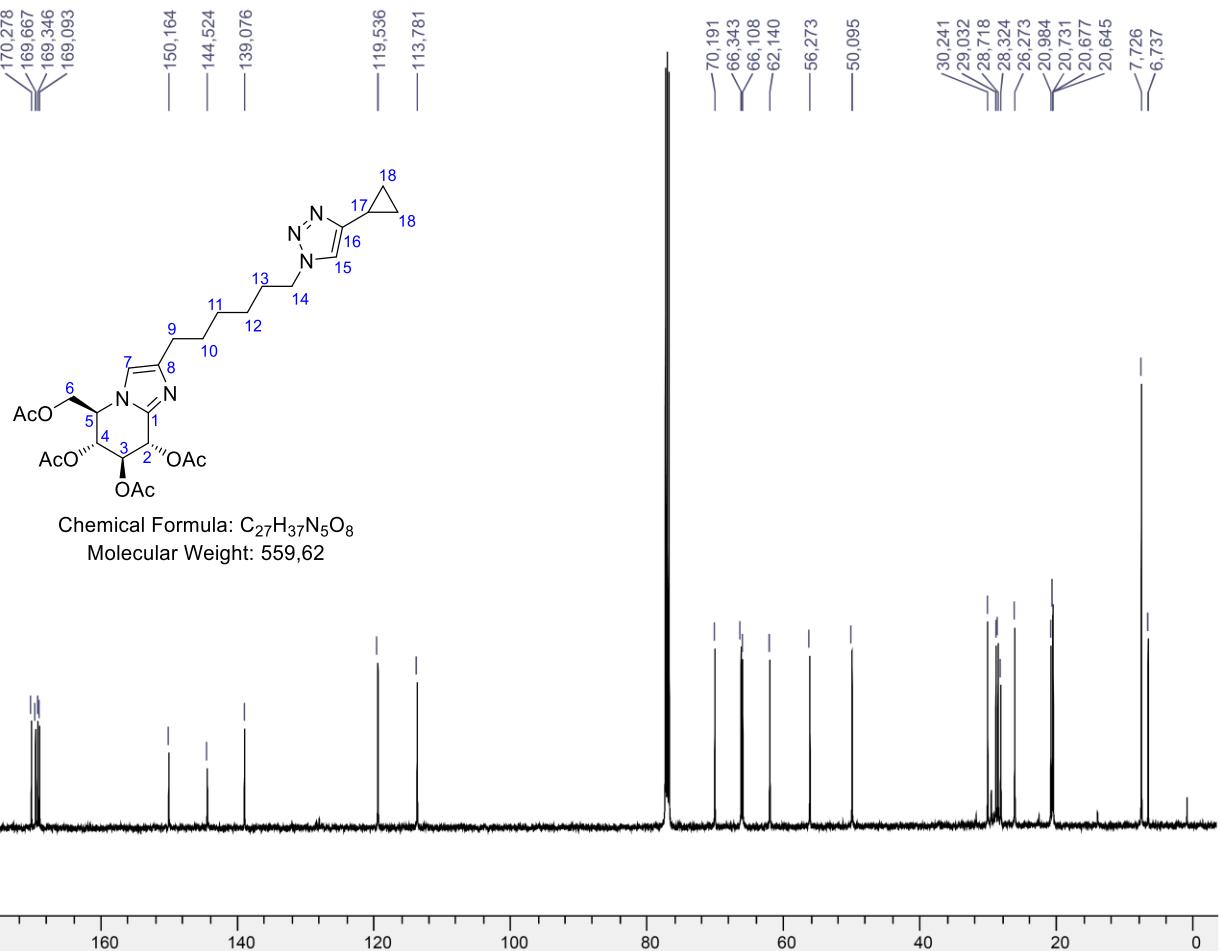
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Fig S18. HRMS (ESI-MS) spectrum of compound 11b

ppm

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

ppm

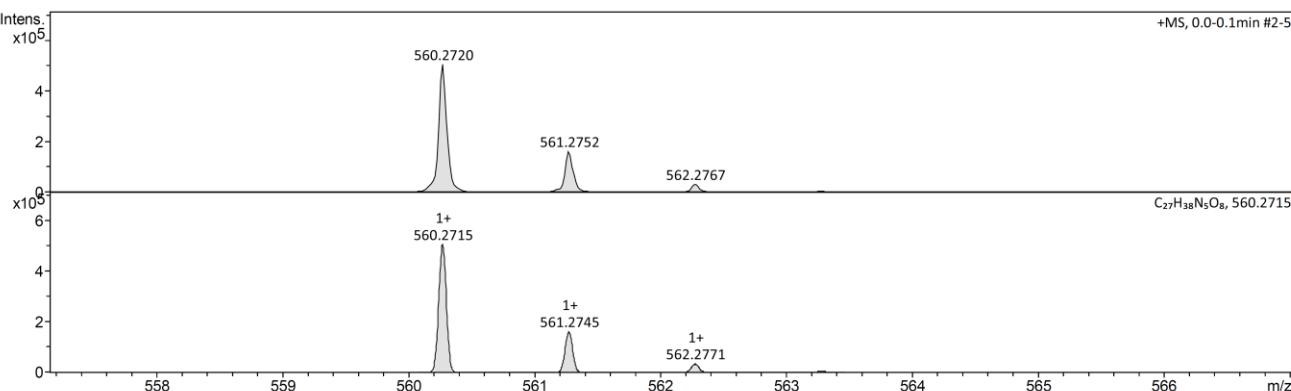
Fig S20. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound 12a

Mass Spectrum HR Report

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Comment			1

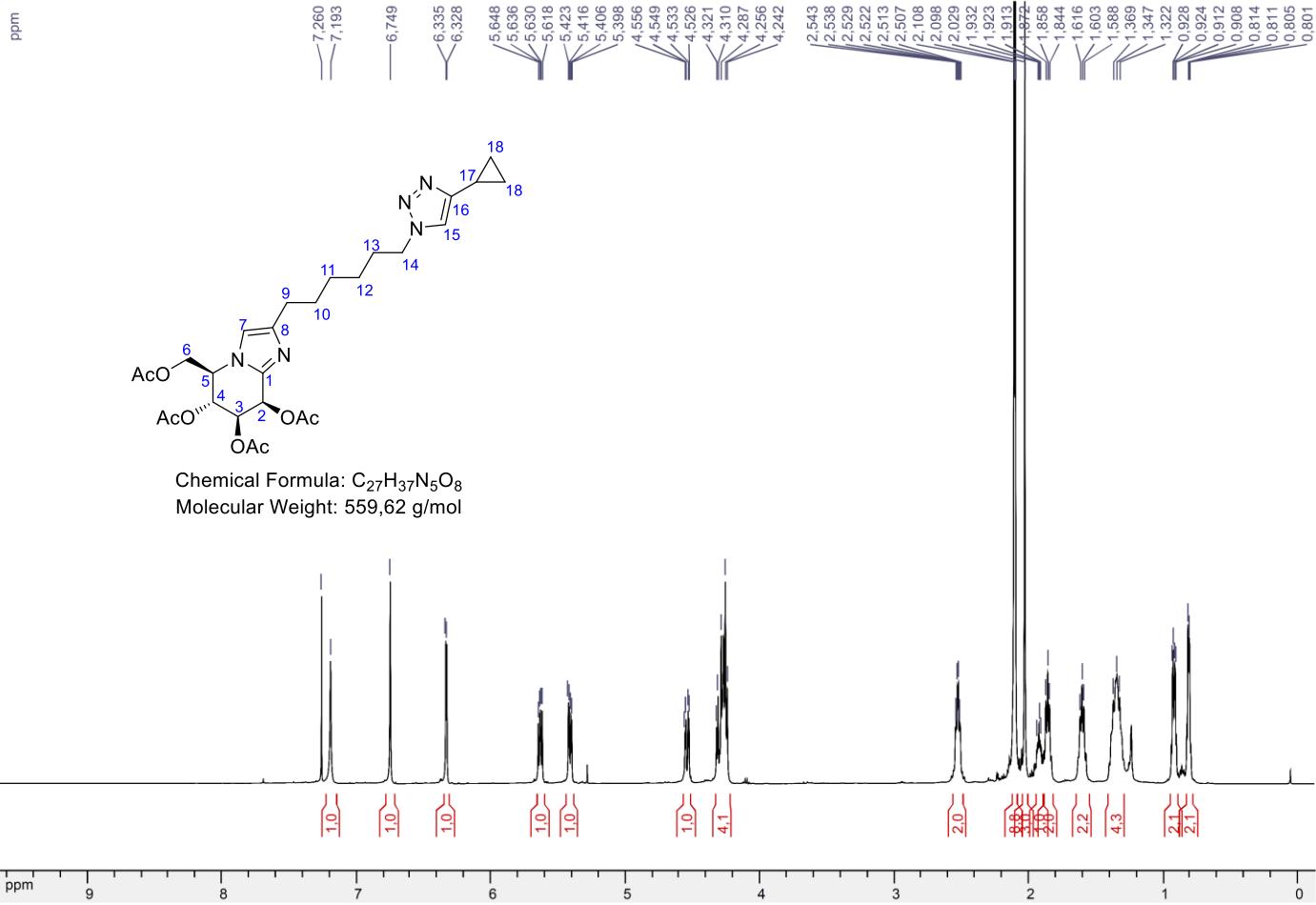
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Scan End	3000 m/z	n/a	n/a	Set Flight Tube	8600.0 V
		n/a	n/a	Set Detector TOF	1953.3 V



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560.272013	1	C ₂₇ H ₃₈ N ₅ O ₈	560.271490	-0.9	-0.7	11.5	ok even	1.7	2.9	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	

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



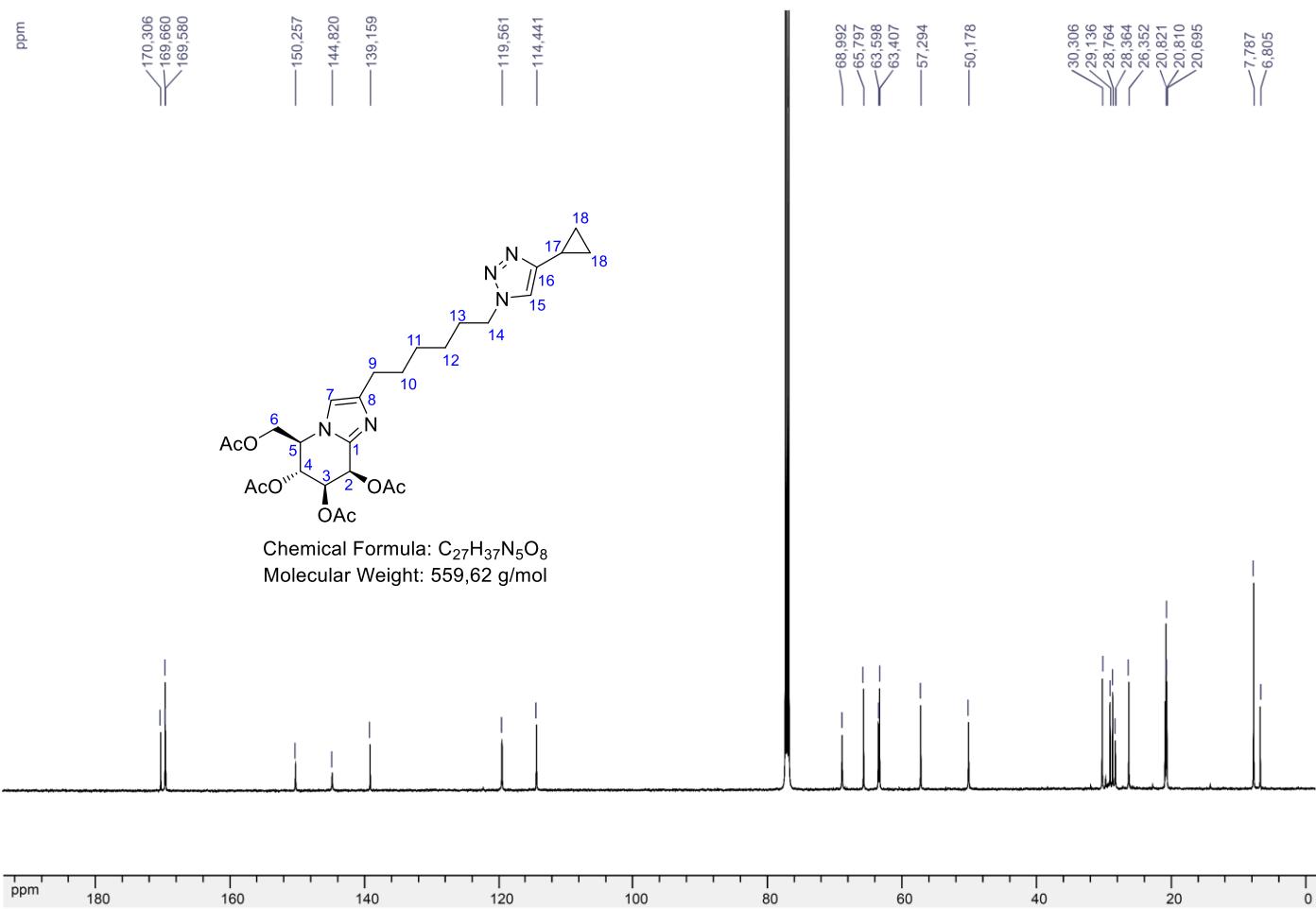
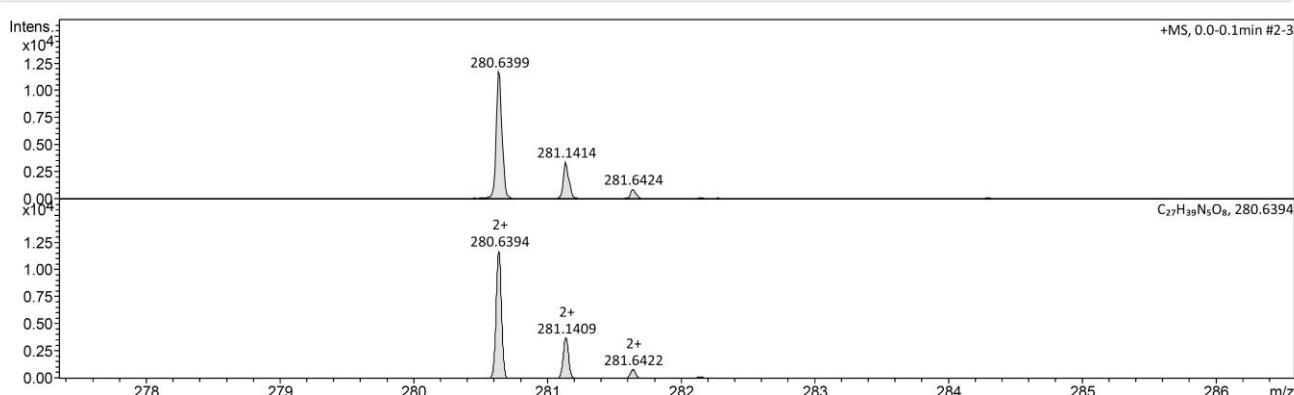


Fig S23. ¹³C NMR (125 MHz, CDCl₃) spectrum of compound 12b

Mass Spectrum HR Report

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Comment			8213750.1045 1
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Scan End	3000 m/z	Set Flight Tube	8600.0 V
	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	C ₂₇ H ₃₉ N ₅ O ₈	280.639383	-2.0	1748.7	11.0	ok	even	16.0	24.2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	
560.268955	1	C ₂₇ H ₃₈ N ₅ O ₈	560.271490	4.5	4.1	11.5	ok	even	5.4	9.4	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	

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

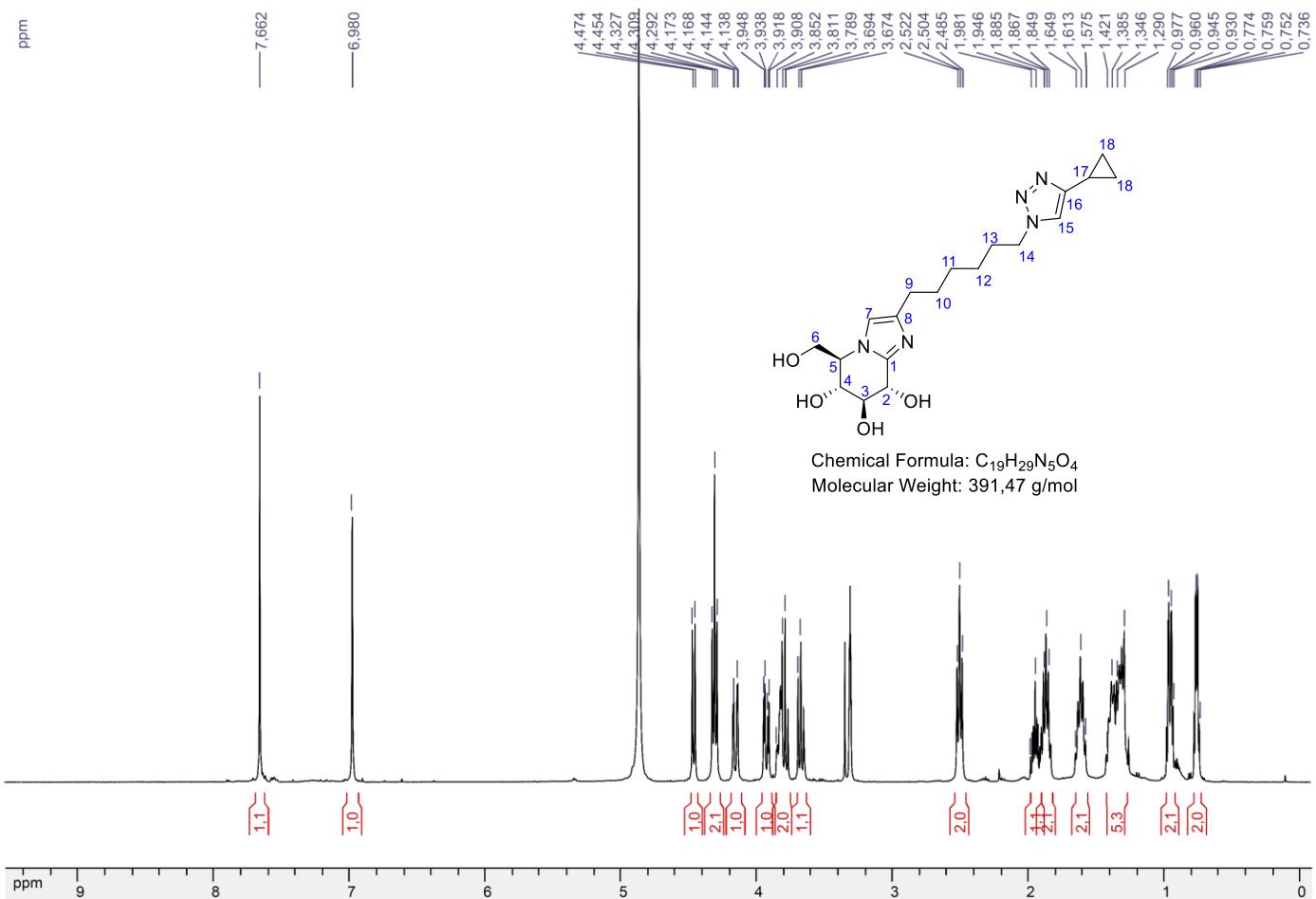


Fig S25. ¹H NMR (400 MHz, CD₃OD) spectrum of compound 13a

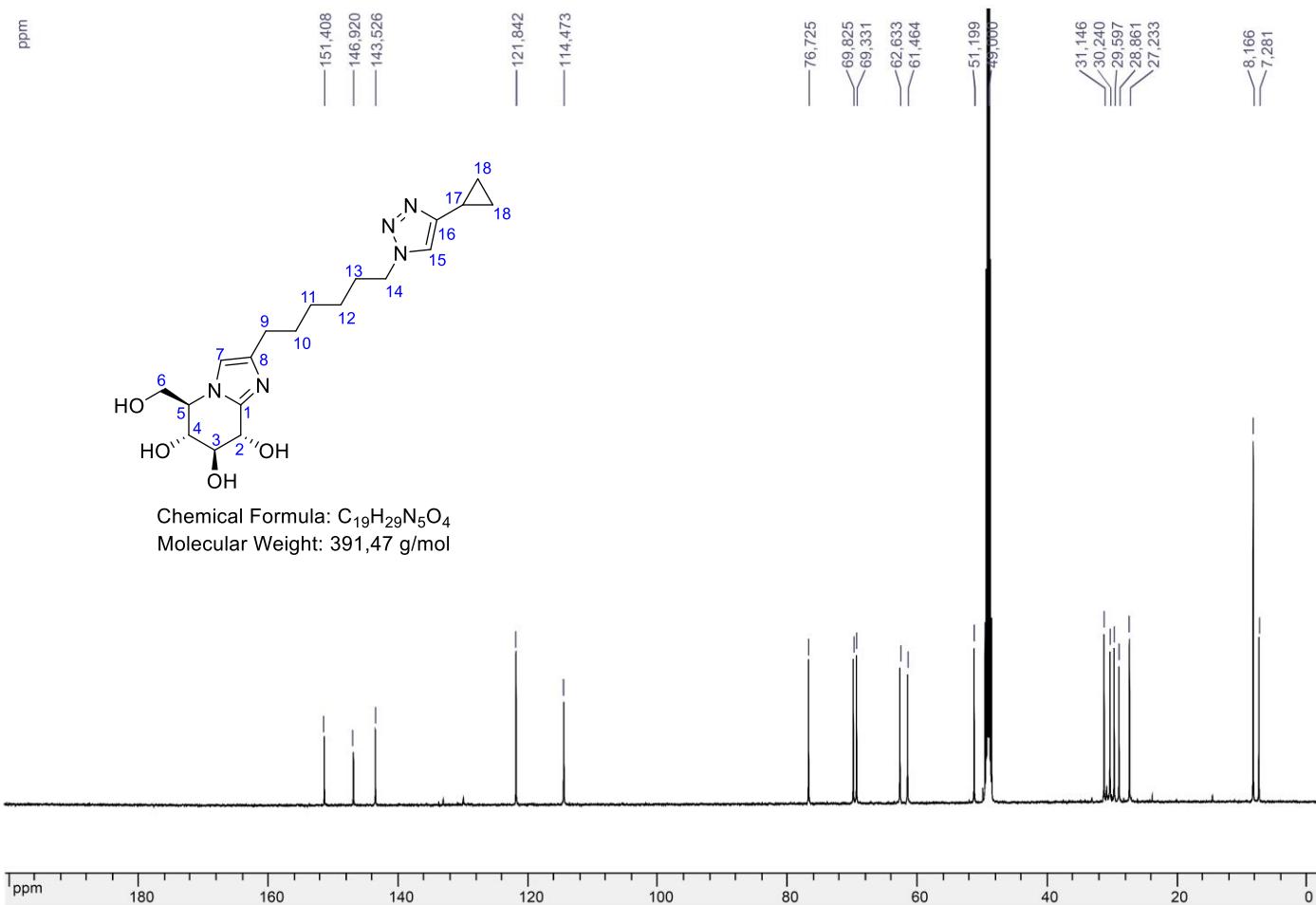


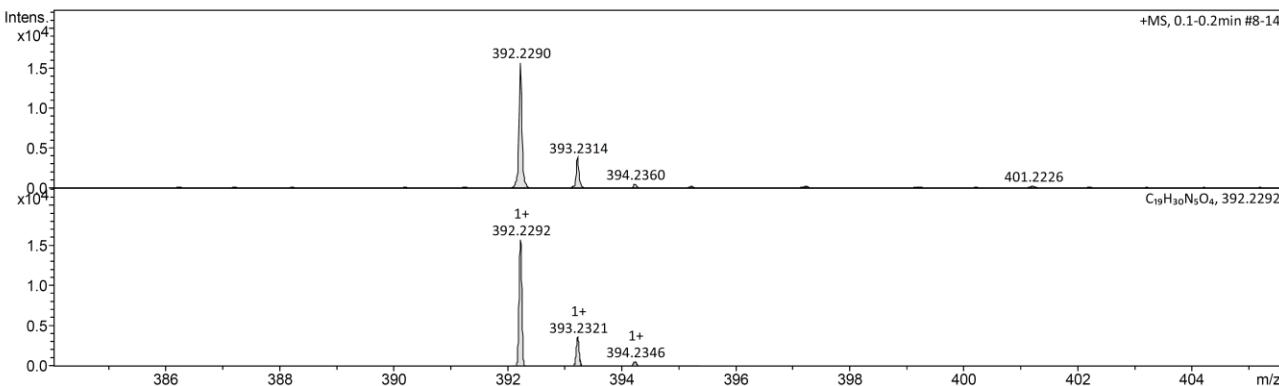
Fig S26. ¹³C NMR (100 MHz, CD₃OD) spectrum of compound 13a

Mass Spectrum HR Report

Analysis Info		Acquisition Date		3/13/2018 1:43:36 PM	
Analysis Name	D:\Data\SMasse\2018\03_Mars 2018\F01911SK.d				
Method	Tune_pos_Standard.m				
Sample Name	MP0282				
Comment		Operator	Instrument	BDAL@DE	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	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 I	Mean m/z	Std I	VarNorm	Std I	Diff Std	Comb Dev
392.228988	1	C ₁₉ H ₃₀ N ₅ O ₄	392.229231	0.6	0.1	7.5	ok even	8.3	13.1	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.

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

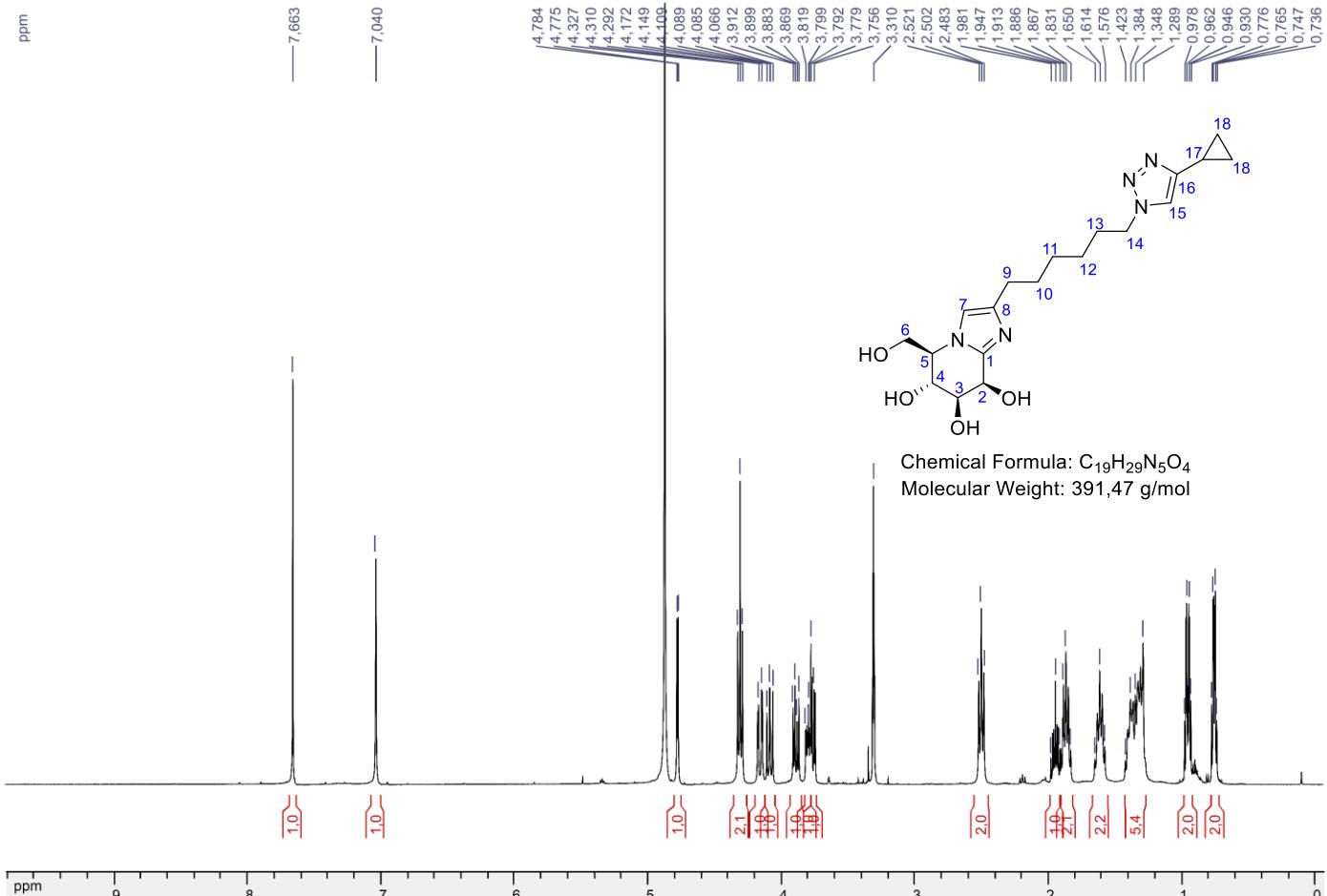


Fig S28. ¹H NMR (400 MHz, CD₃OD) spectrum of compound 13b

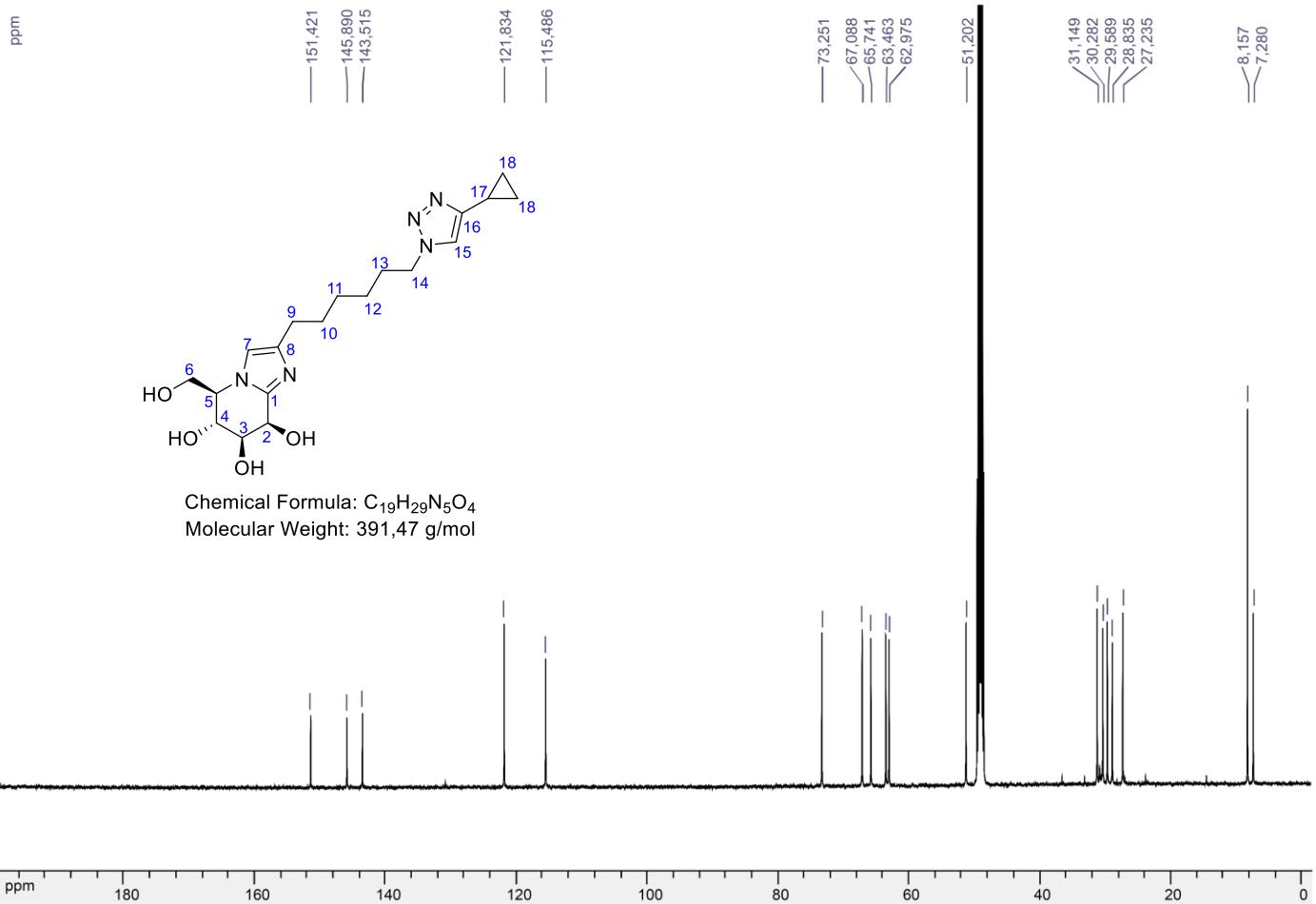
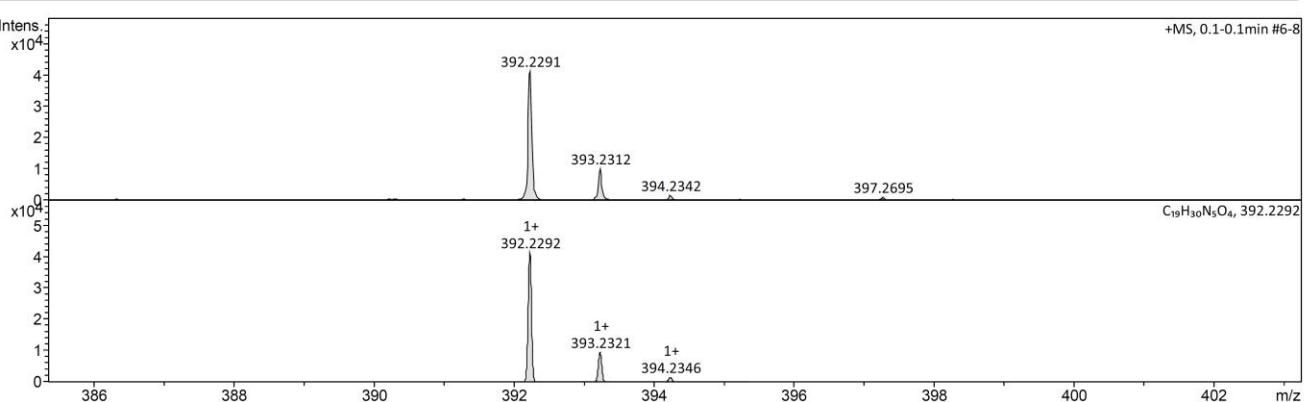


Fig S29. ¹³C NMR (100 MHz, CD₃OD) spectrum of compound 13b

Mass Spectrum HR Report

Analysis Info		Acquisition Date	
Analysis Name	D:\Data\SMasse\2018\03_Mars 2018\F01913SK.d		3/13/2018 1:48:36 PM
Method	Tune_pos_Standard.m		
Sample Name	MP0290	Operator Instrument	BDAL@DE micrOTOF II
Comment			8213750.1045 1

Acquisition Parameter			
Source Type	ESI	Ion Polarity	Positive
n/a	n/a	n/a	n/a
Scan Begin	50 m/z	n/a	Set Corrector Fill
Scan End	3000 m/z	n/a	59.0 V
	n/a	n/a	n/a
	n/a	n/a	Set Reflector
	n/a	n/a	1800.0 V
	n/a	n/a	Set Flight Tube
	n/a	n/a	8600.0 V
	n/a	n/a	Set Detector TOF
	n/a	n/a	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
196.618868	1	C ₁₉ H ₃₁ N ₅ O ₄	196.618254	-3.1	-2.7	7.0	ok even	2.5	4.7	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	
392.229128	1	C ₁₉ H ₃₀ N ₅ O ₄	392.229231	0.3	0.9	7.5	ok even	9.3	15.9	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	

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

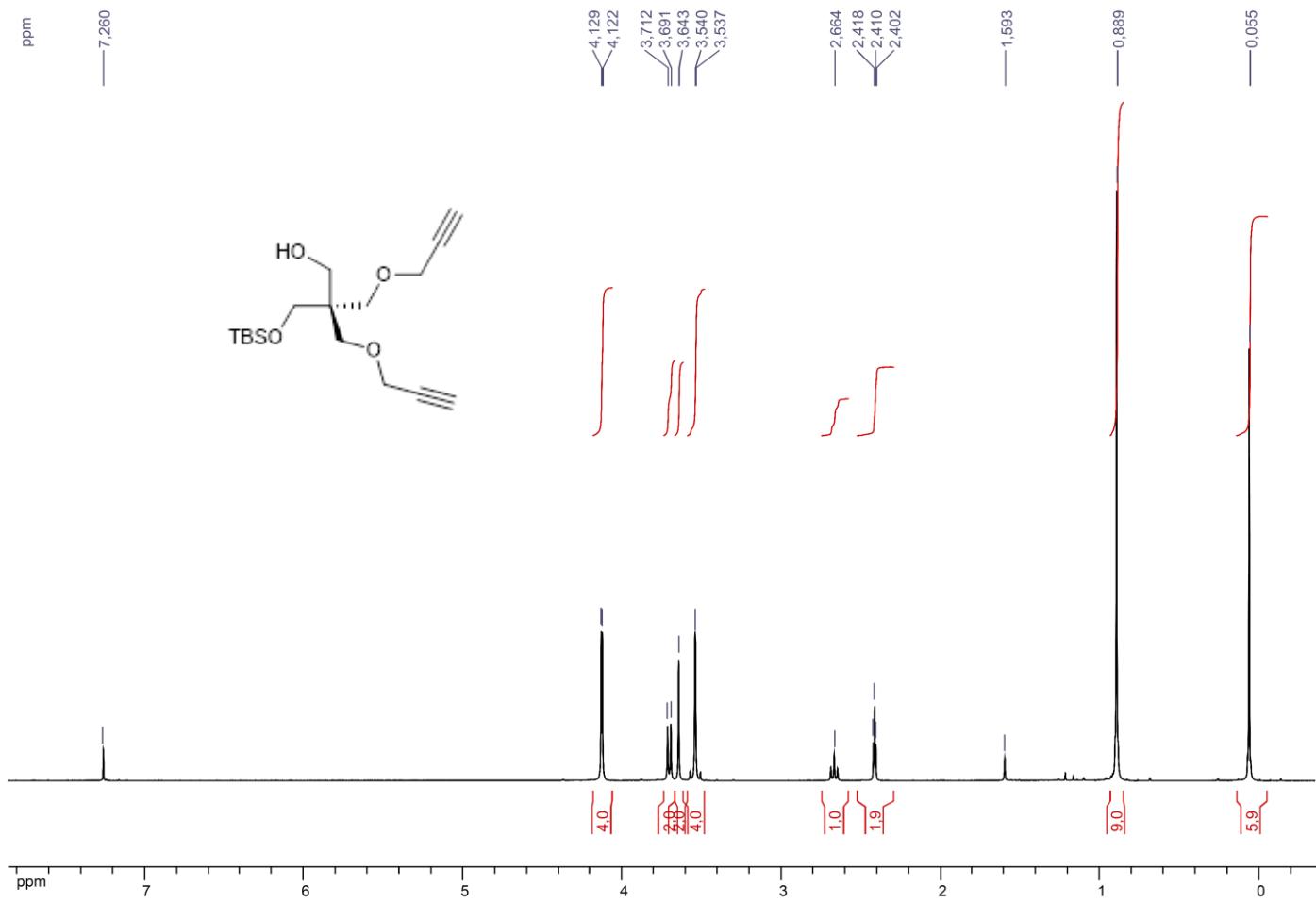


Fig S31. ¹H NMR (300 MHz, CDCl₃) spectrum of compound 16a

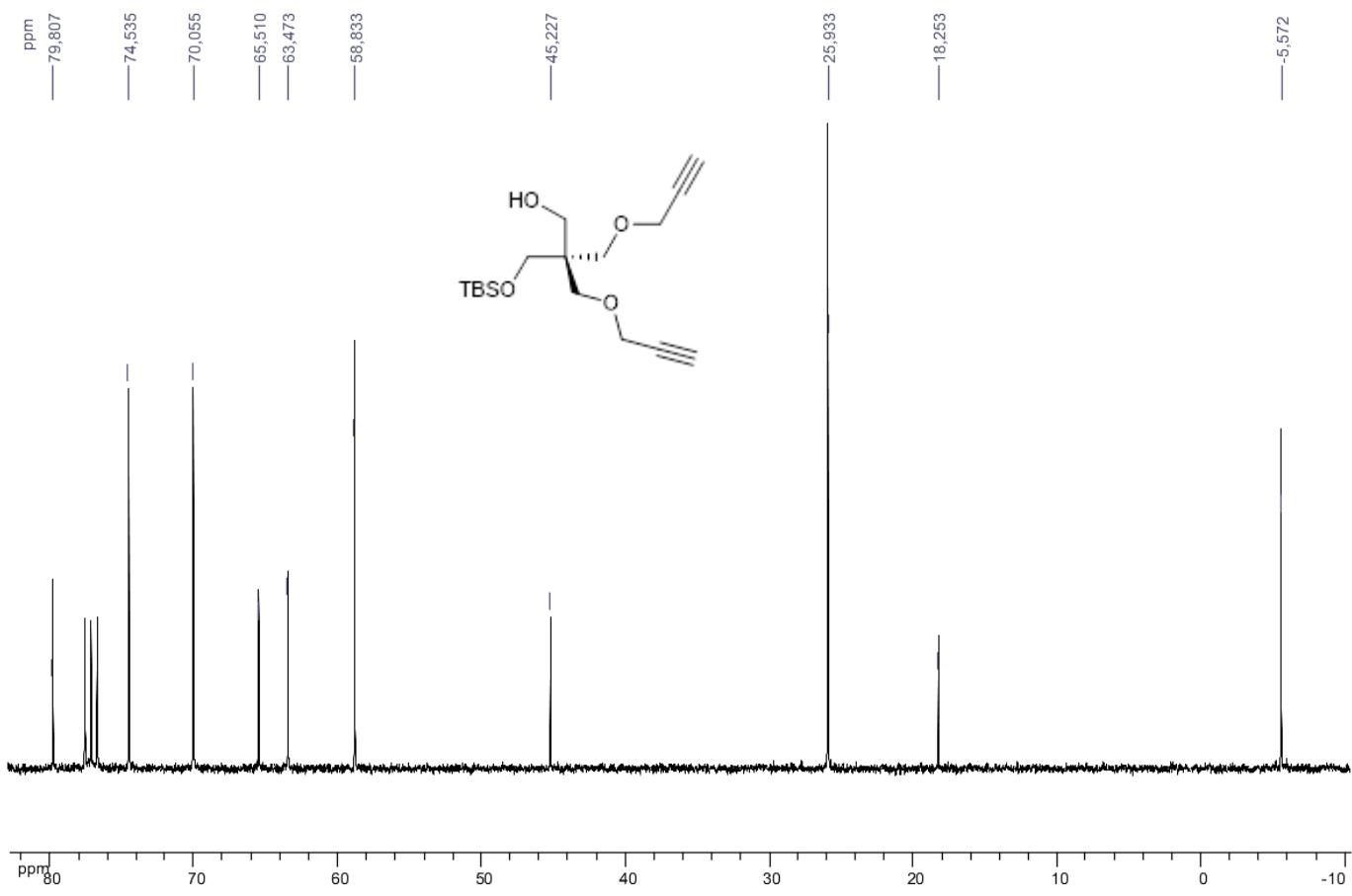


Fig S32. ¹³C NMR (75 MHz, CDCl₃) spectrum of compound 16a

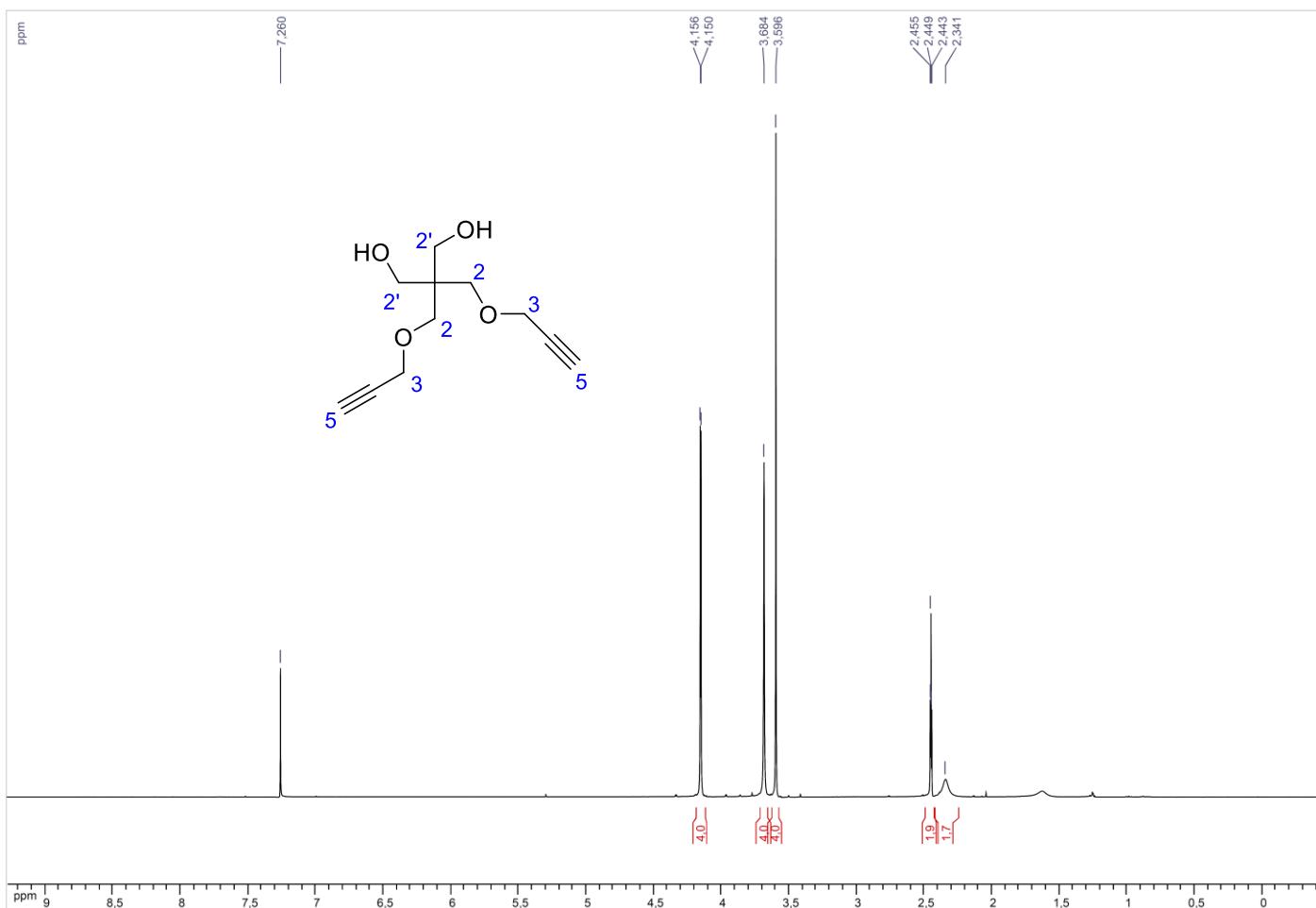


Fig S33. ^1H NMR (400 MHz, CDCl_3) spectrum of compound 17a

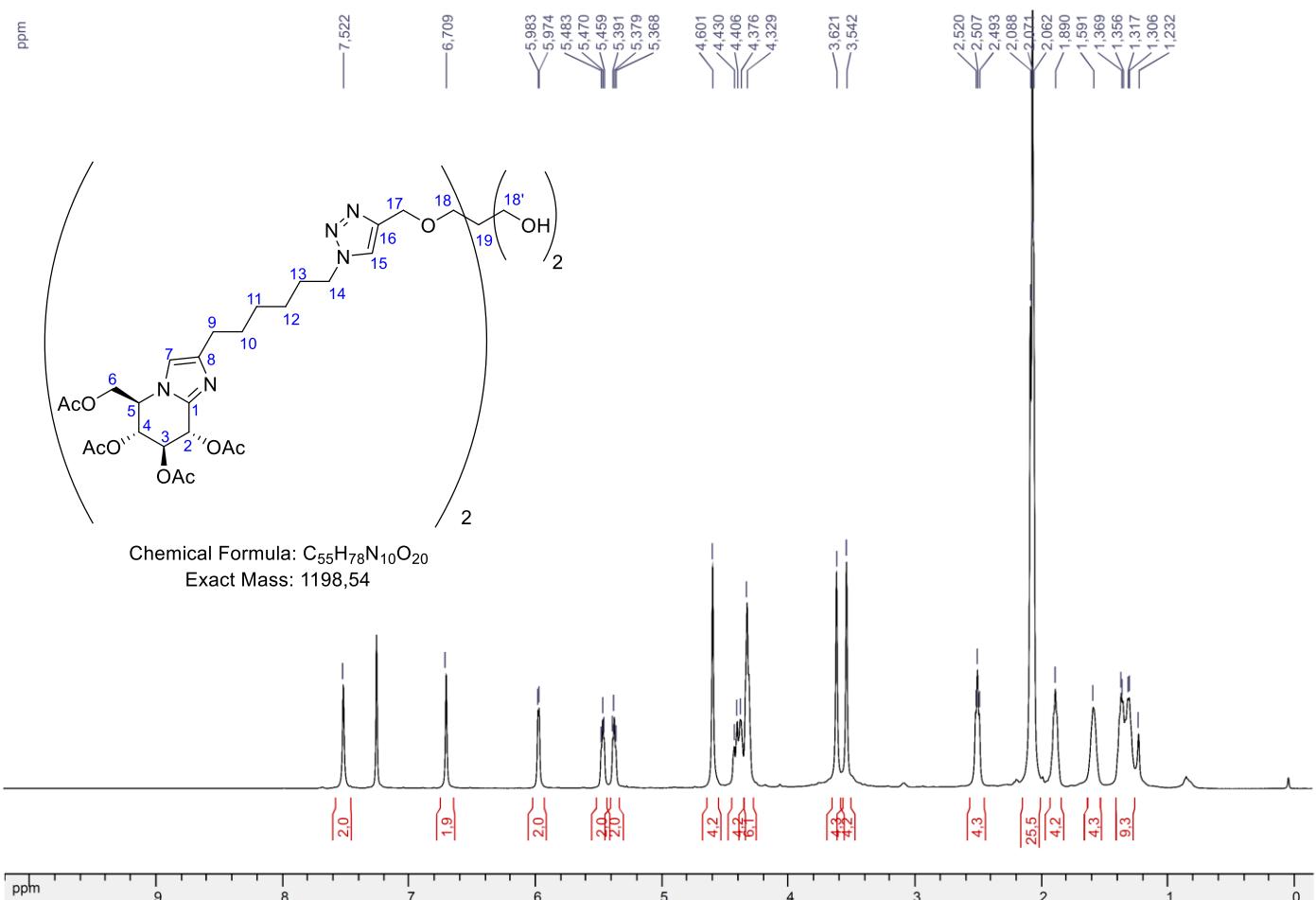


Fig S34. ^1H NMR (500 MHz, CDCl_3) spectrum of compound 18a

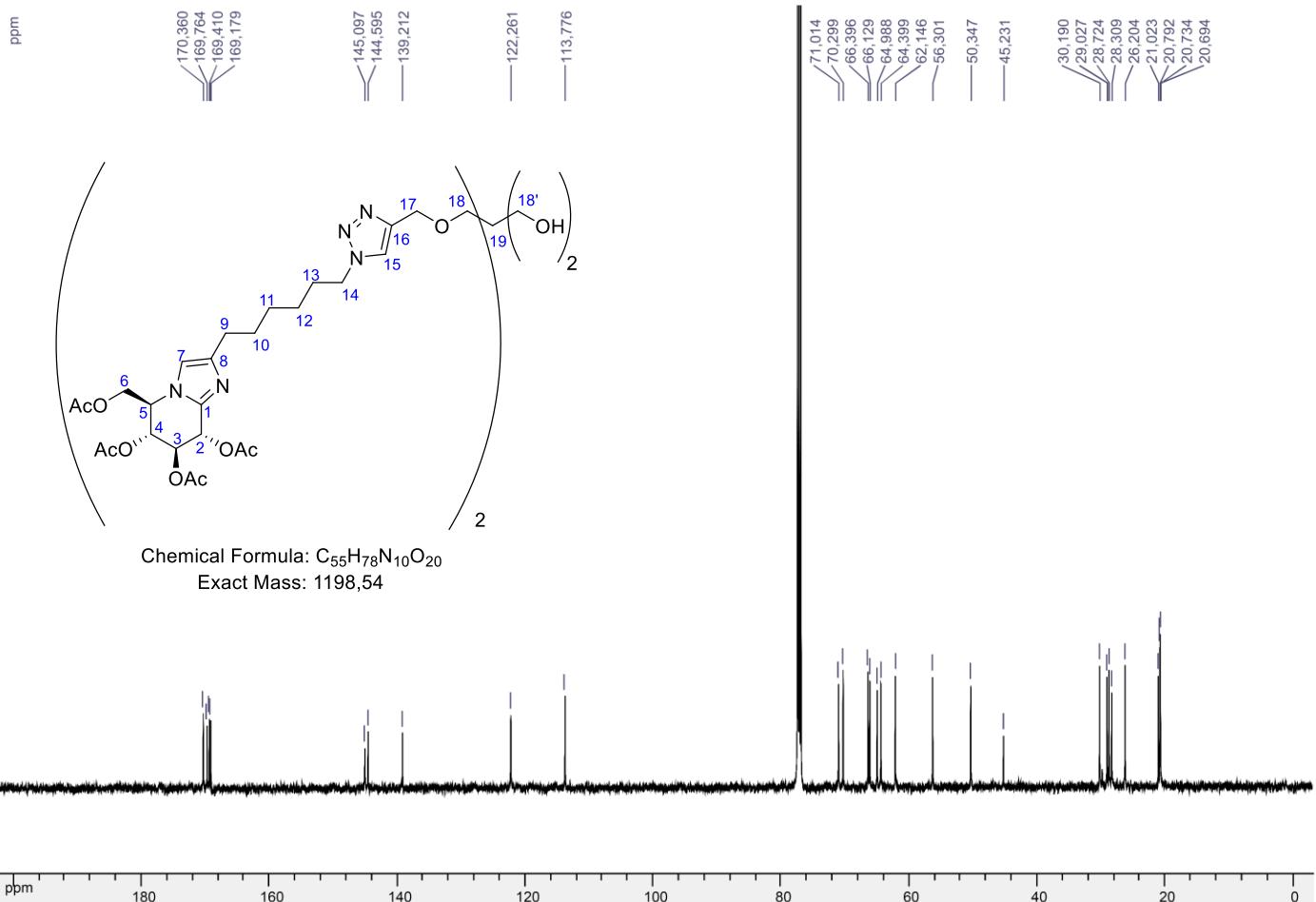
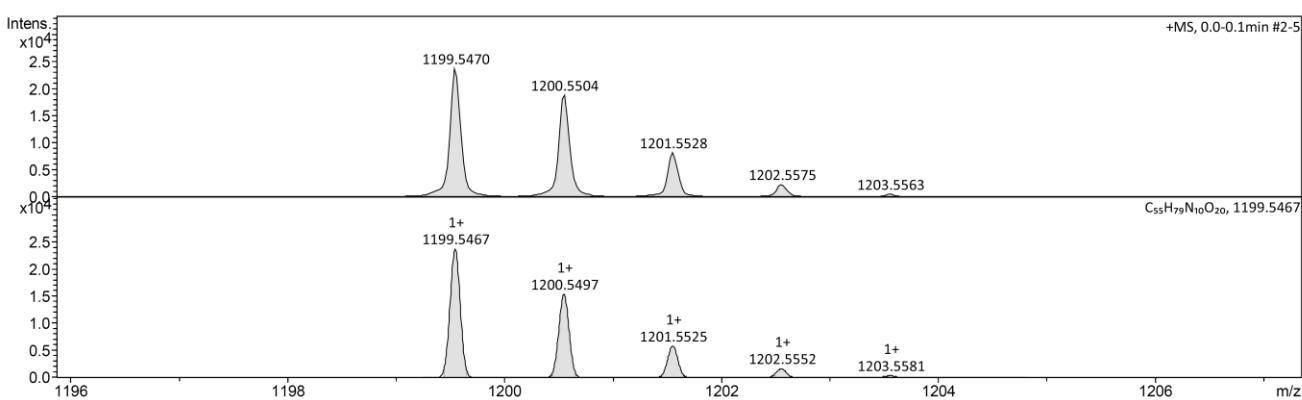


Fig S35. ^{13}C NMR (125 MHz, $CDCl_3$) spectrum of compound 18a

Mass Spectrum HR Report

Analysis Info		Acquisition Date	2/1/2018 11:11:33 AM
Analysis Name	D:\Data\SMasse\2018\02_Fevrier 2018\F01648SK.d		
Method	Tune_pos_Mid.m	Operator	BDAL@DE
Sample Name	MP0272 Pur	Instrument	micrOTOF II
Comment			8213750.1045 1
Acquisition Parameter		Set Corrector Fill	59.0 V
Source Type	ESI	n/a	n/a
n/a	n/a	n/a	n/a
Scan Begin	50 m/z	n/a	1800.0 V
Scan End	3000 m/z	n/a	8600.0 V
		n/a	1953.3 V



Meas. m/z # Ion Formula	m/z err [ppm]	Mean err 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 $C_{55}H_{78}N_{10}O_{20}$ 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

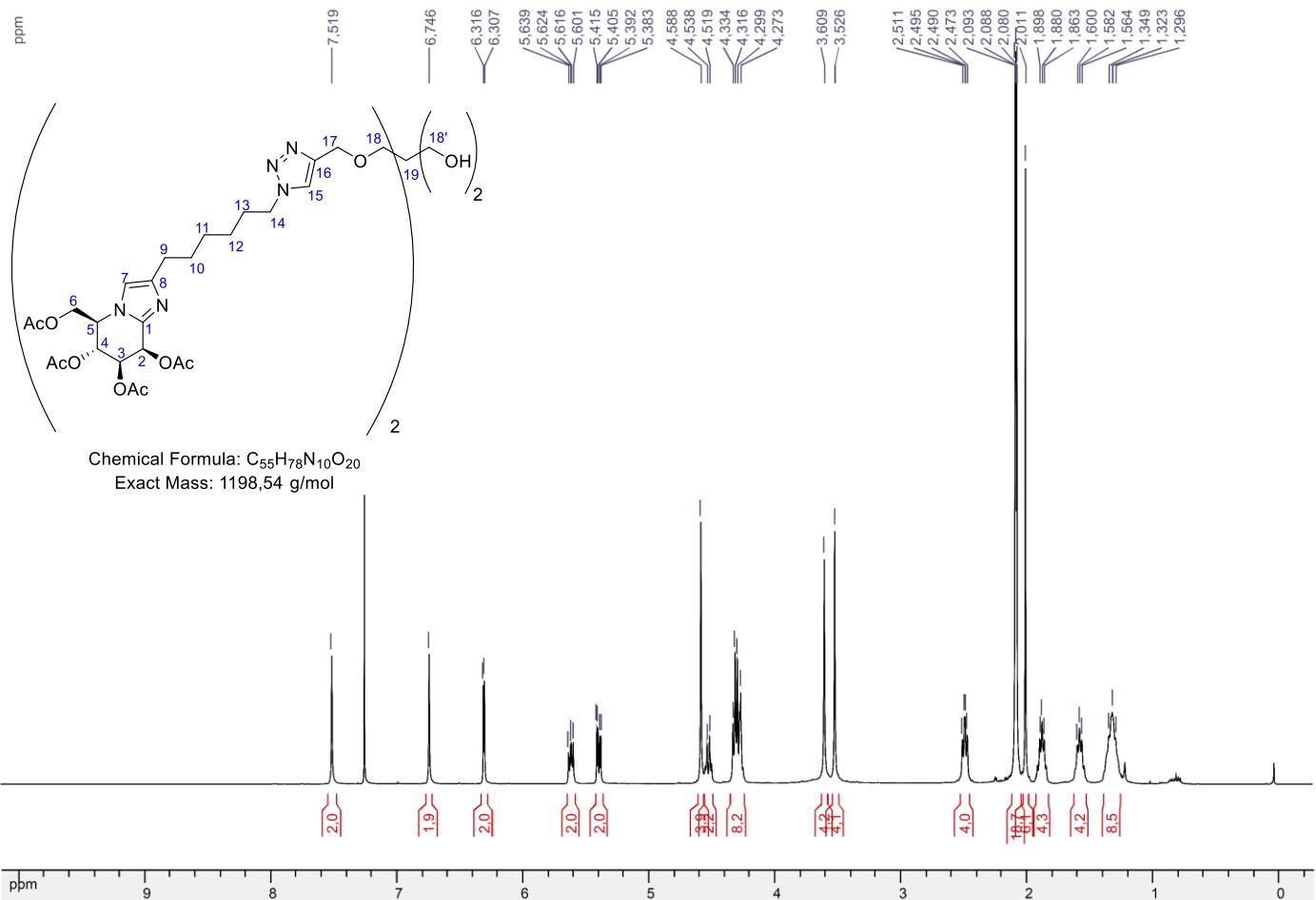


Fig S37. ¹H NMR (400 MHz, CDCl₃) spectrum of compound 18b

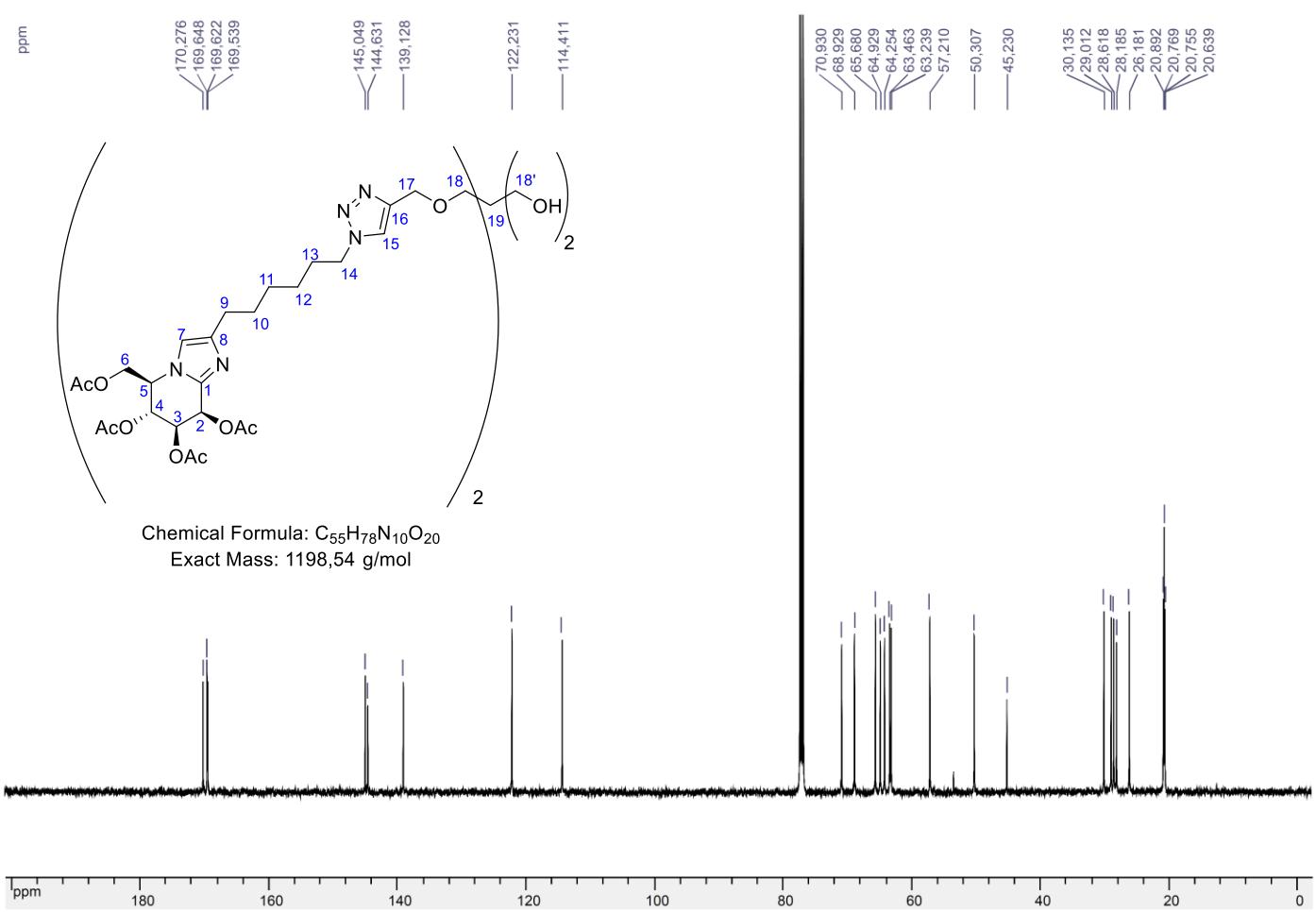
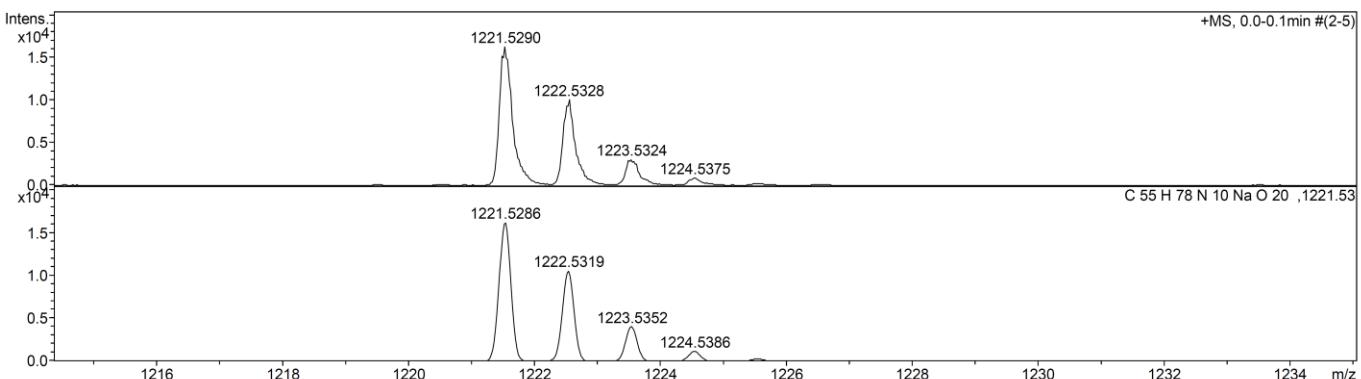


Fig S38. ¹³C NMR (100 MHz, CDCl₃) spectrum of compound 18b

Mass Spectrum HR Report

Analysis Info		Acquisition Date		19/04/2018 15:48:24	
Analysis Name	Y:\O42996SK.d <th>Operator</th> <td><th>Instrument</th><td></td></td>	Operator	<th>Instrument</th> <td></td>	Instrument	
Method	esi wide pos.m				
Sample Name	MP0304 Pur				
Comment					
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	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
1221.5290	1	C 55 H 78 N 10 Na O 20	100.00	1221.5286	-0.4	-0.4	30.7	21.5	even	ok

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

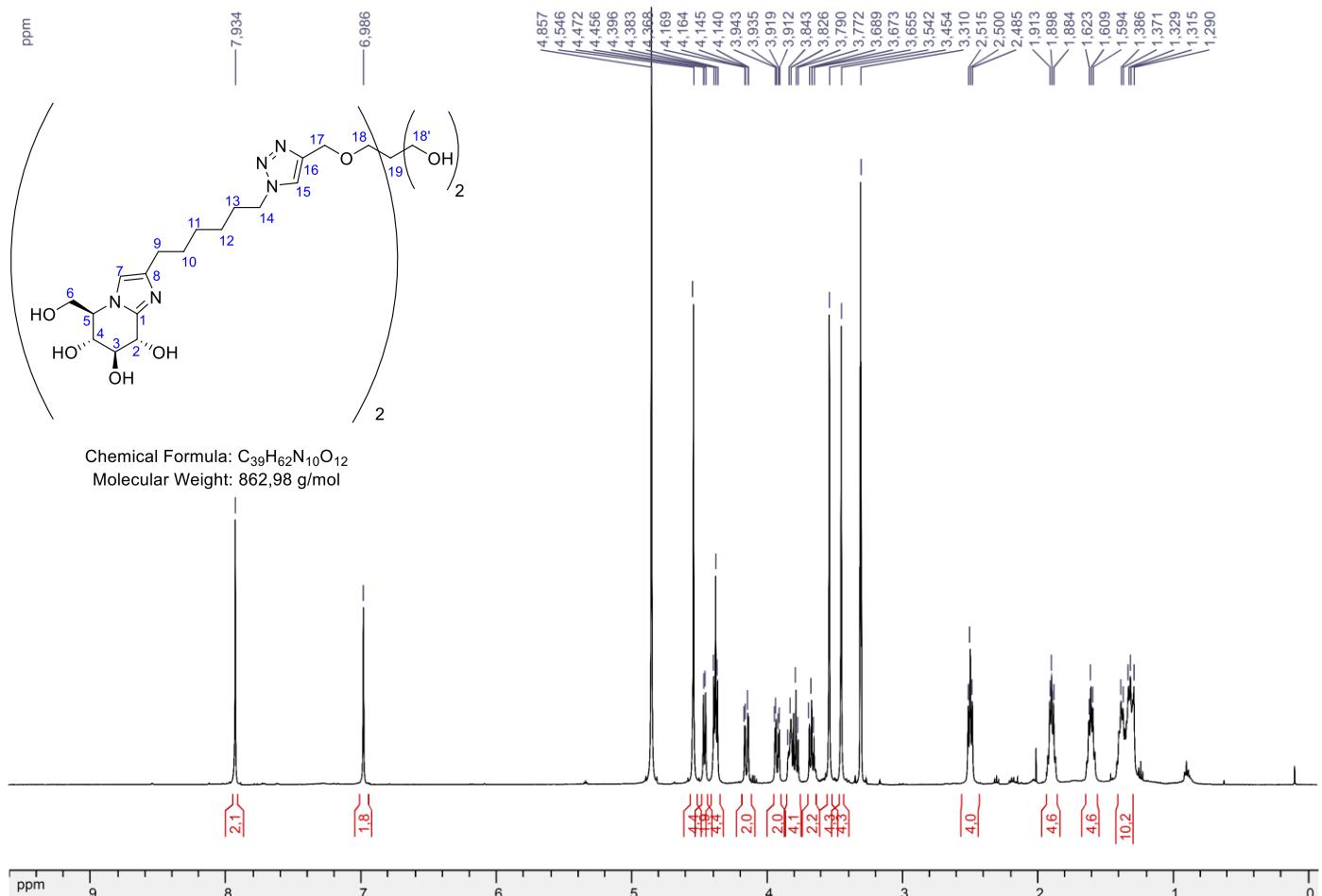


Fig S40. ¹H NMR (500 MHz, CD₃OD) spectrum of compound **19a**

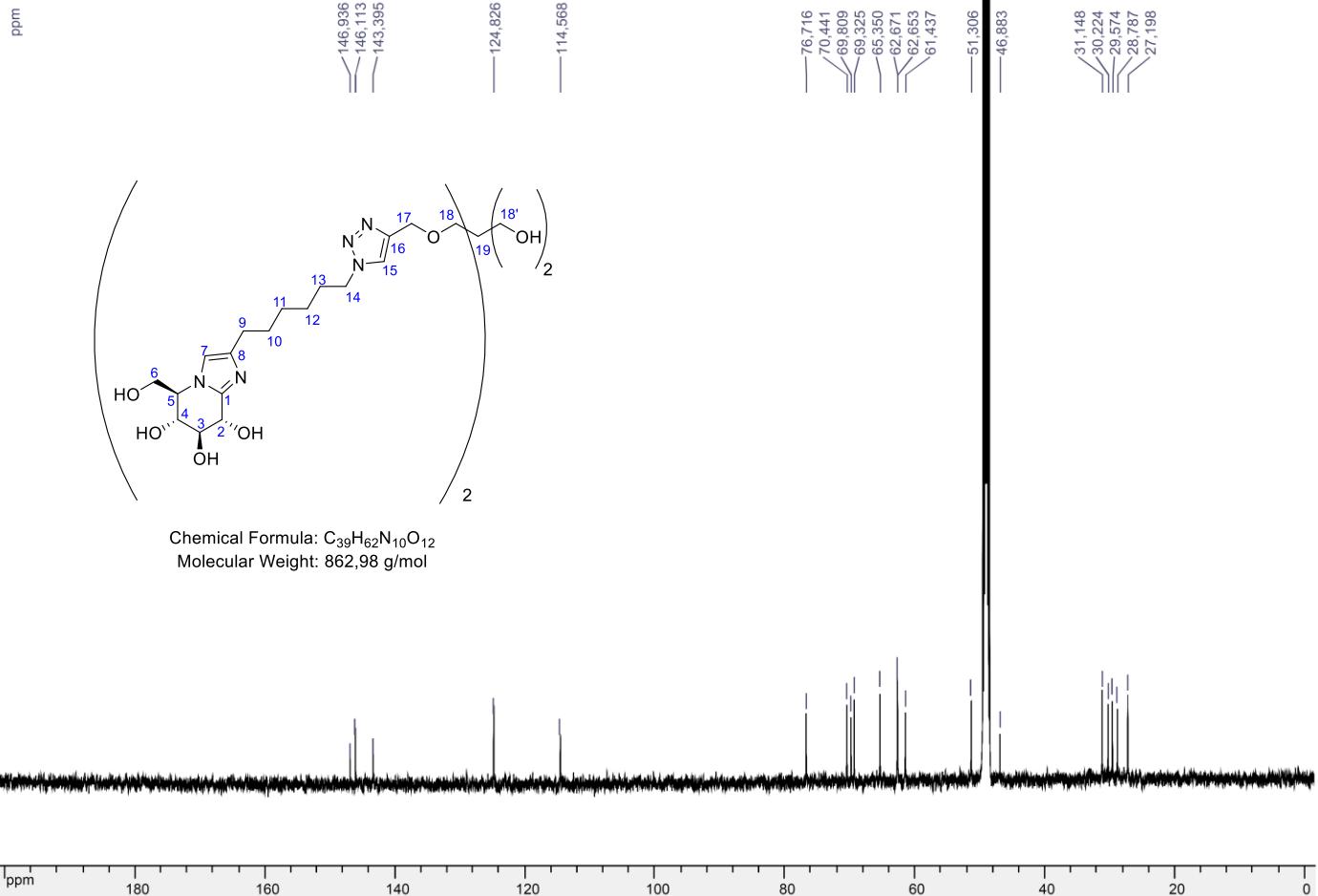
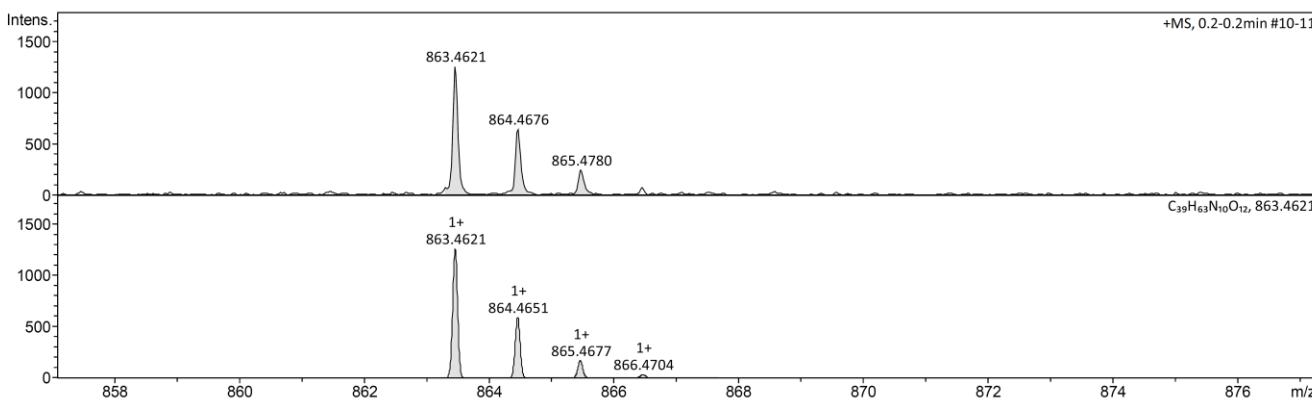


Fig S41. ^{13}C NMR (125 MHz, CD_3OD) spectrum of compound 19a

Mass Spectrum HR Report

Analysis Info		Acquisition Date	3/28/2018 3:45:10 PM
Analysis Name	D:\Data\SMasse\2018\03_Mars 2018\F02020SK.d		
Method	Tune_pos_Mid.m	Operator	BDAL@DE
Sample Name	MP0296	Instrument	micrOTOF II
Comment			8213750.1045 1

Acquisition Parameter				
Source Type	ESI	Ion Polarity	Positive	Set Corrector Fill
n/a	n/a	n/a	n/a	59.0 V
Scan Begin	50 m/z	n/a	n/a	n/a
Scan End	3000 m/z	n/a	n/a	Set Reflector
		n/a	n/a	1800.0 V
		n/a	n/a	Set Flight Tube
		n/a	n/a	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	VarNorm	Std	m/z Diff	Comb	Dev
432.238217	1	$C_{39}H_{64}N_{10}O_{12}$	432.234710	-8.1	-7.4	13.0	ok even	82.5	98.6	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
863.462135	1	$C_{39}H_{63}N_{10}O_{12}$	863.462144	0.0	547.7	13.5	ok even	40.7	48.2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.

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

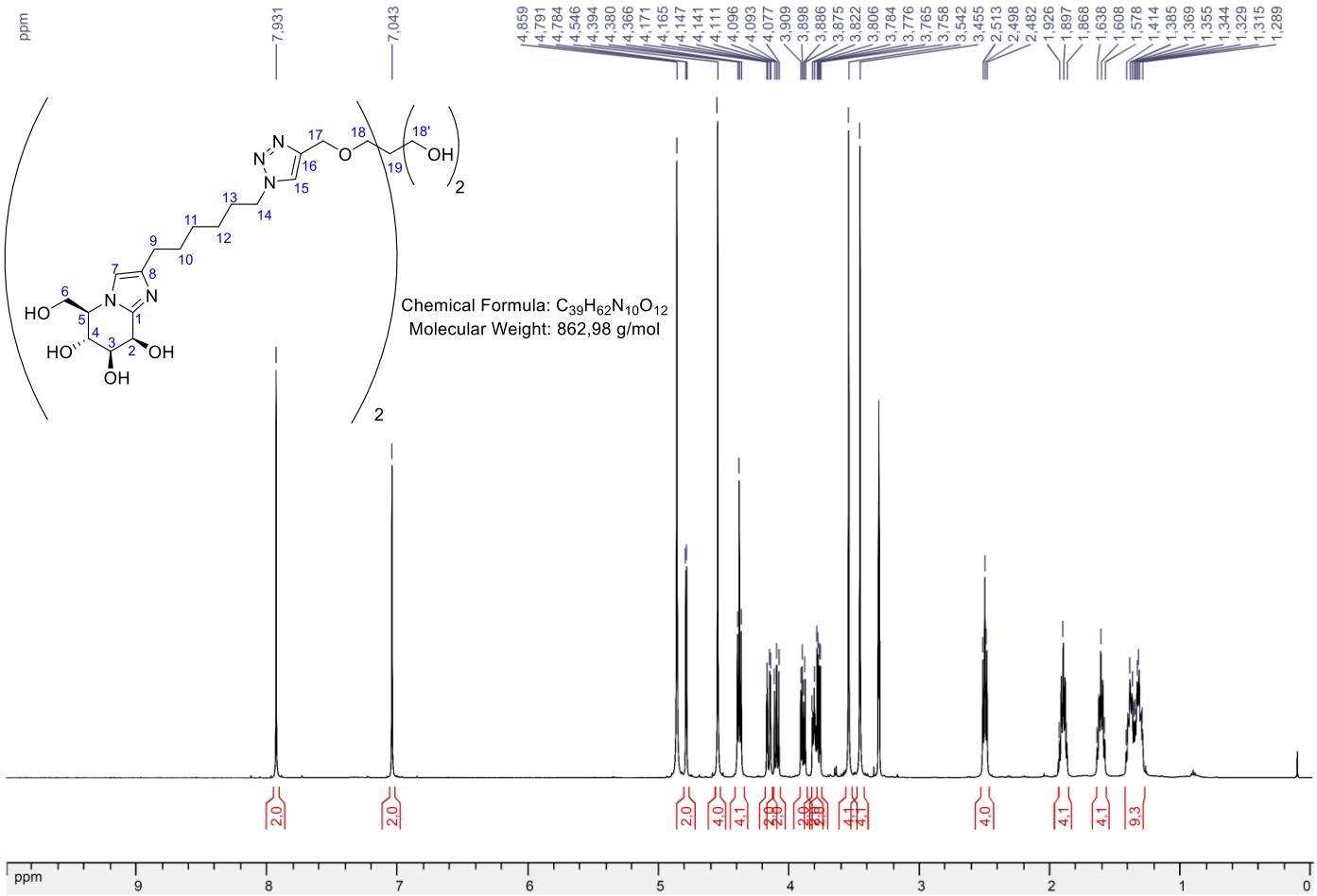


Fig S43. ¹H NMR (500 MHz, CD₃OD) spectrum of compound 19b

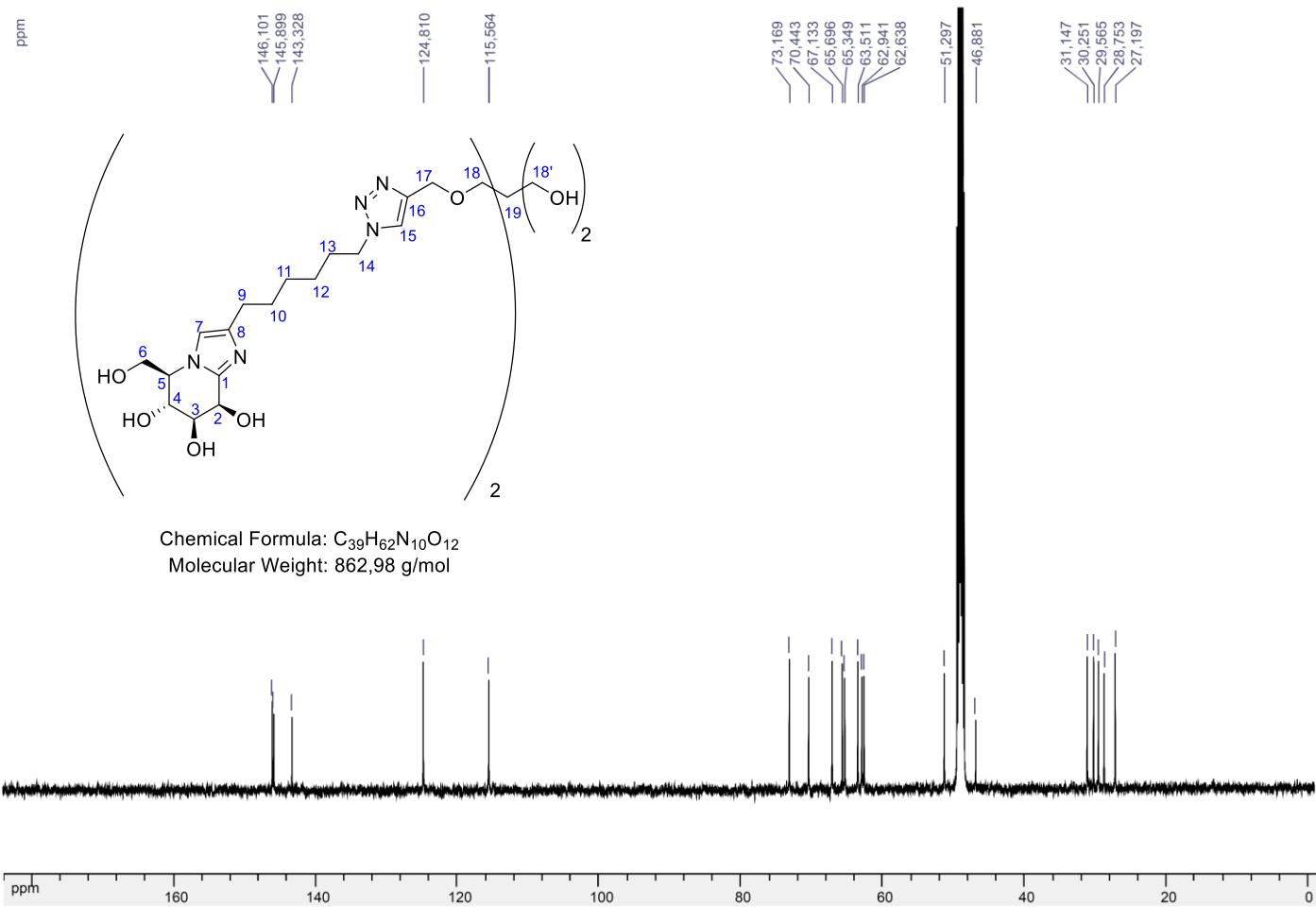


Fig S44. ¹³C NMR (125 MHz, CD₃OD) spectrum of compound 19b

Mass Spectrum HR Report

Analysis Info

Analysis Name D:\Data\SMassel\2018\05_Mai 2018\F02183SK.d
 Method Tune_pos_Mid.m
 Sample Name MP039 Brut
 Comment

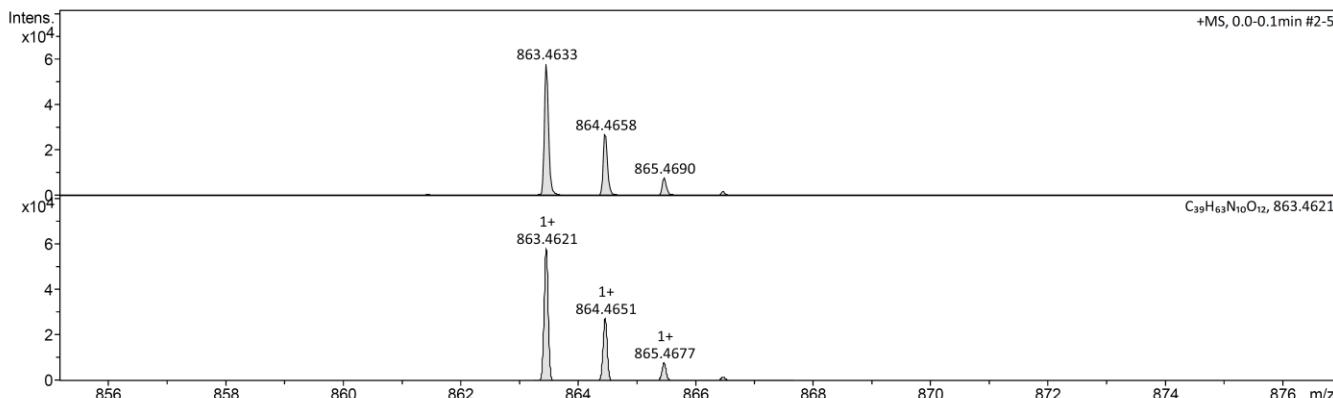
Acquisition Date 5/3/2018 2:24:08 PM

 Operator BDAL@DE
 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
Scan Begin 50 m/z	n/a	Set Reflector 1800.0 V
Scan End 3000 m/z	n/a	Set Flight Tube 8600.0 V
	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
 863.463317 1 C39H63N10O12 863.462144 -1.4 -1.0 13.5 ok even 4.0 4.7 n.a. n.a. n.a. n.a.

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

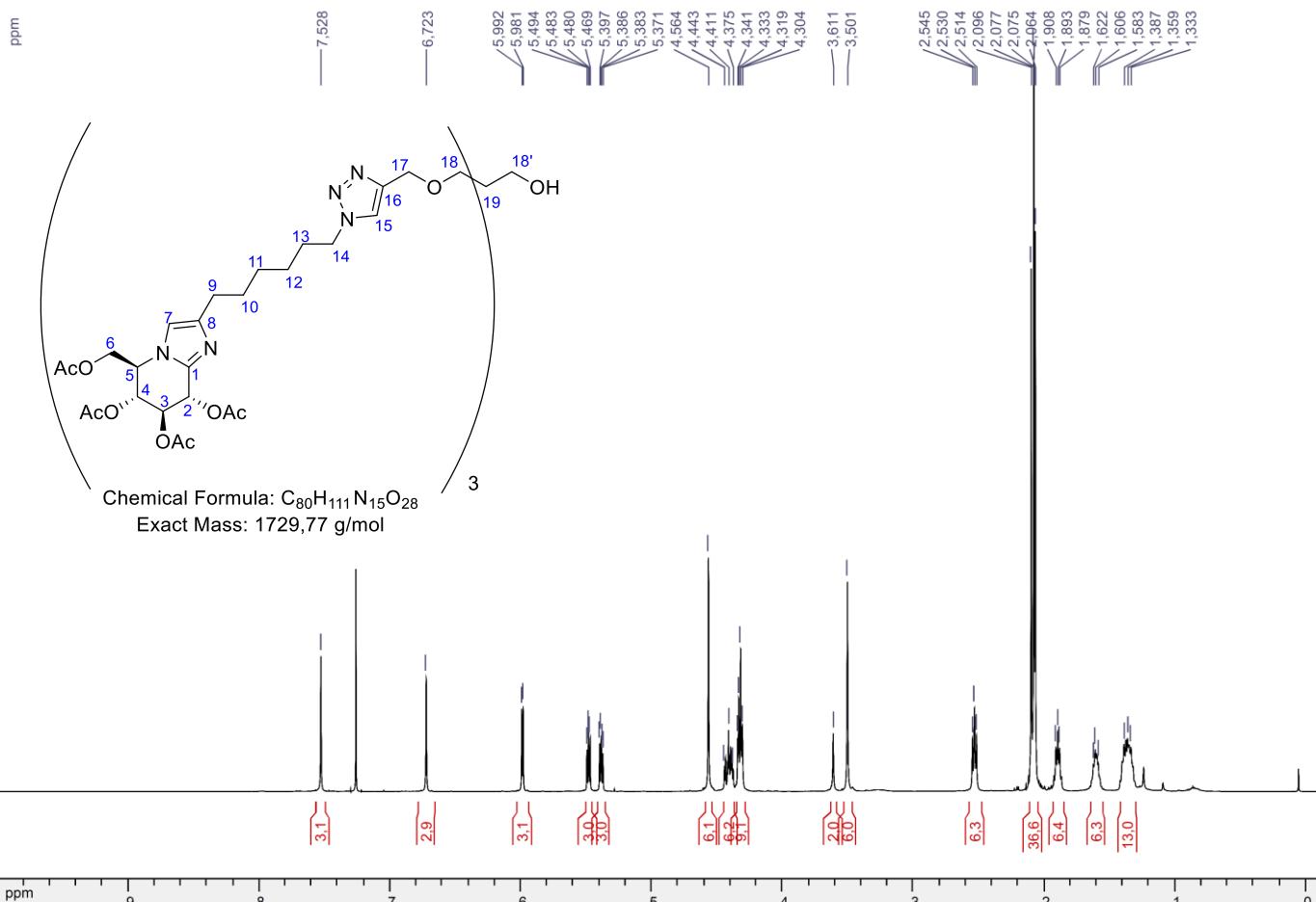


Fig S46. ¹H NMR (500 MHz, CDCl₃) spectrum of compound **20a**

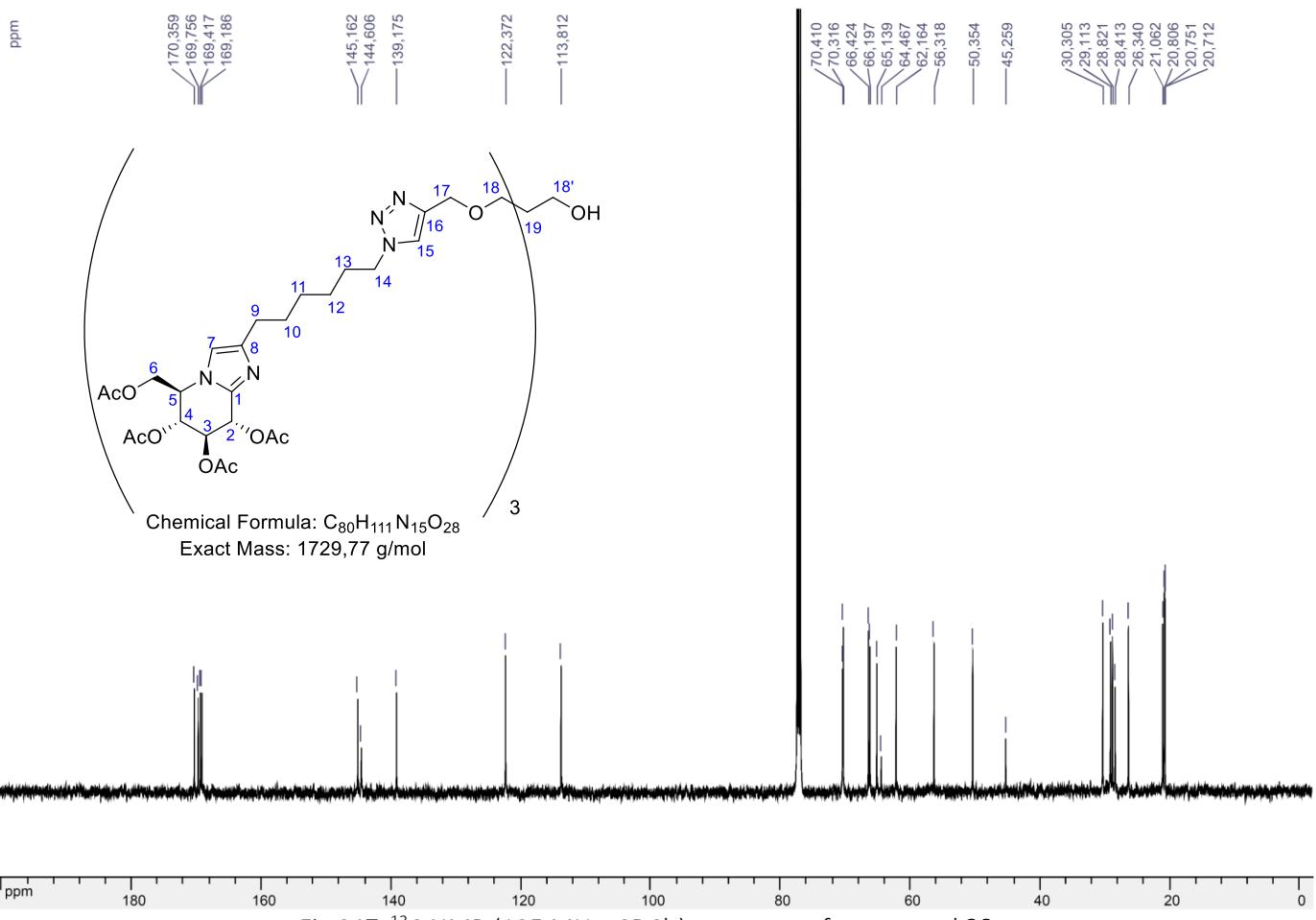
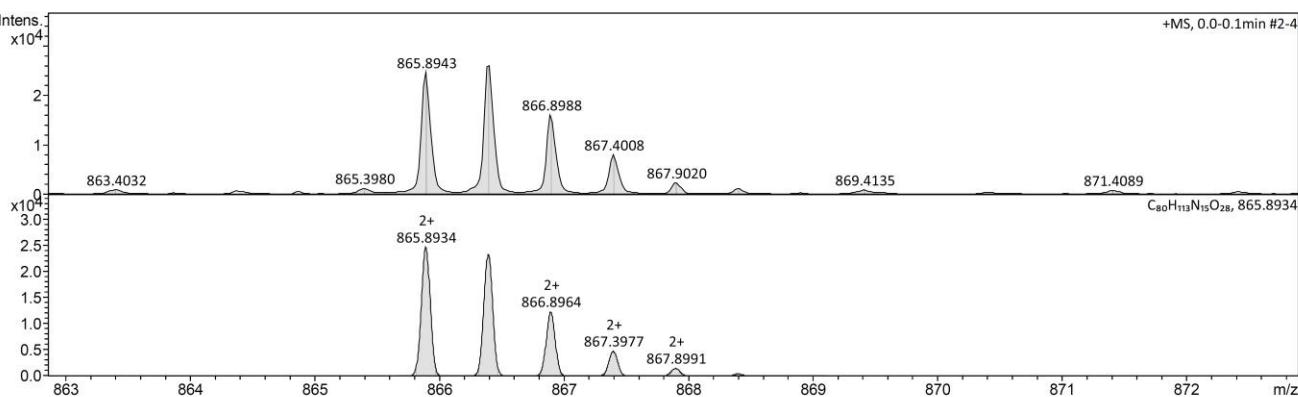


Fig S47. ^{13}C NMR (125 MHz, CDCl_3) spectrum of compound 20a

Mass Spectrum HR Report

Analysis Info		Acquisition Date	1/10/2018 3:23:03 PM	
Analysis Name	D:\Data\SMasse\2018\01_Janvier 2018\F01501SK.d			
Method	Tune_pos_Mid.m	Operator	BDAL@DE	
Sample Name	MP029 Fr3	Instrument	micrOTOF II	
Comment			8213750.1045 1	
Acquisition Parameter		Set Corrector Fill	59.0 V	
Source Type	ESI	Ion Polarity	n/a	
n/a	n/a	Positive	n/a	
Scan Begin	50 m/z	n/a	Set Reflector	1800.0 V
Scan End	3000 m/z	n/a	Set Flight Tube	8600.0 V
		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	VarNorm	Std m/z	Diff	Std Comb Dev
865.894263 1 $C_{80}H_{113}N_{15}O_{28}$	865.893425 -1.0	-2.4 32.0	ok even		77.2	70.0	n.a.	n.a.	n.a.	n.a.	n.a.	
1730.777194 1 $C_{80}H_{112}N_{15}O_{28}$	1730.779574 1.4	526.9 32.5	ok even		83.7	71.5	n.a.	n.a.	n.a.	n.a.	n.a.	

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

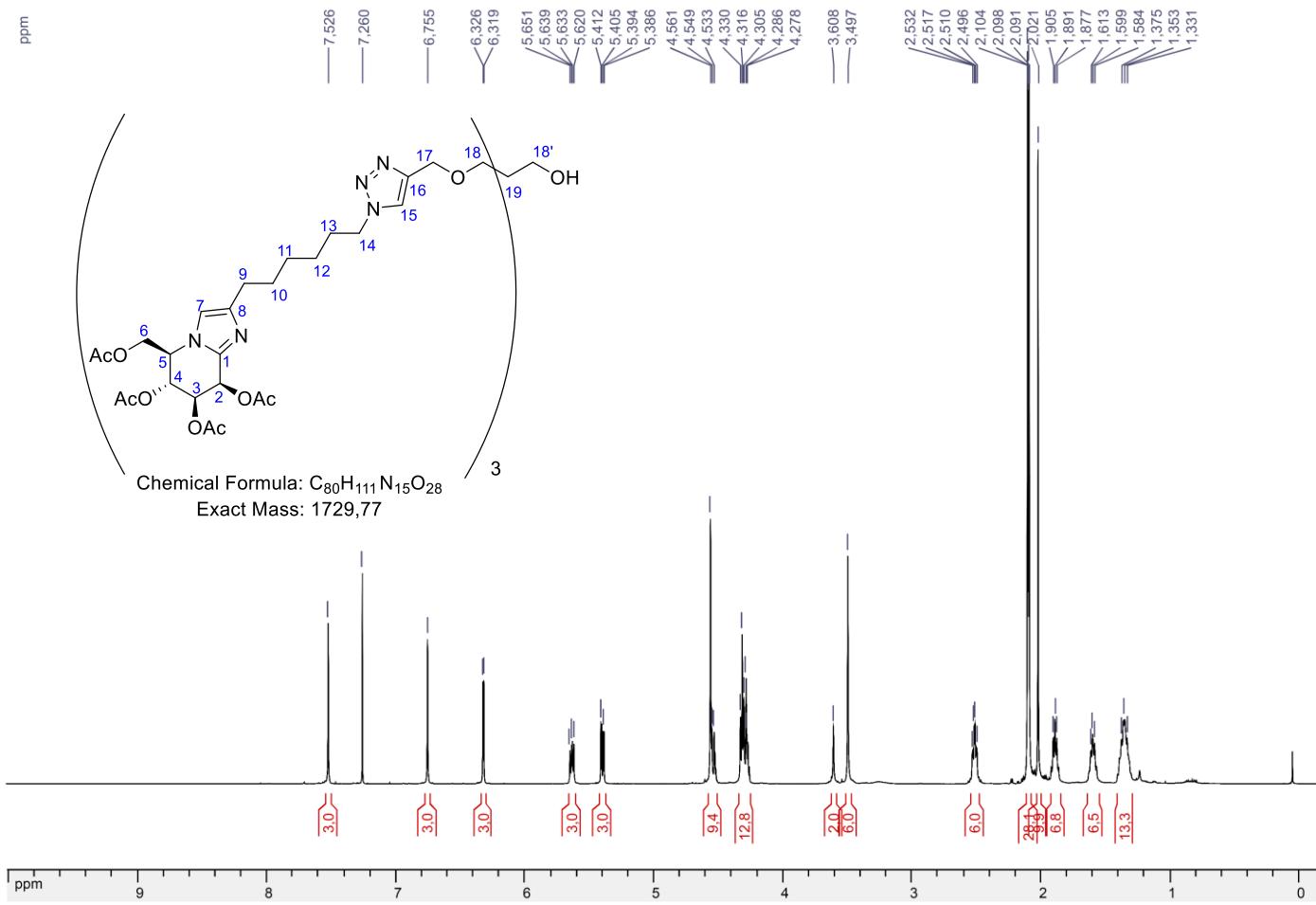


Fig S49. ¹H NMR (500 MHz, CDCl₃) spectrum of compound 20b

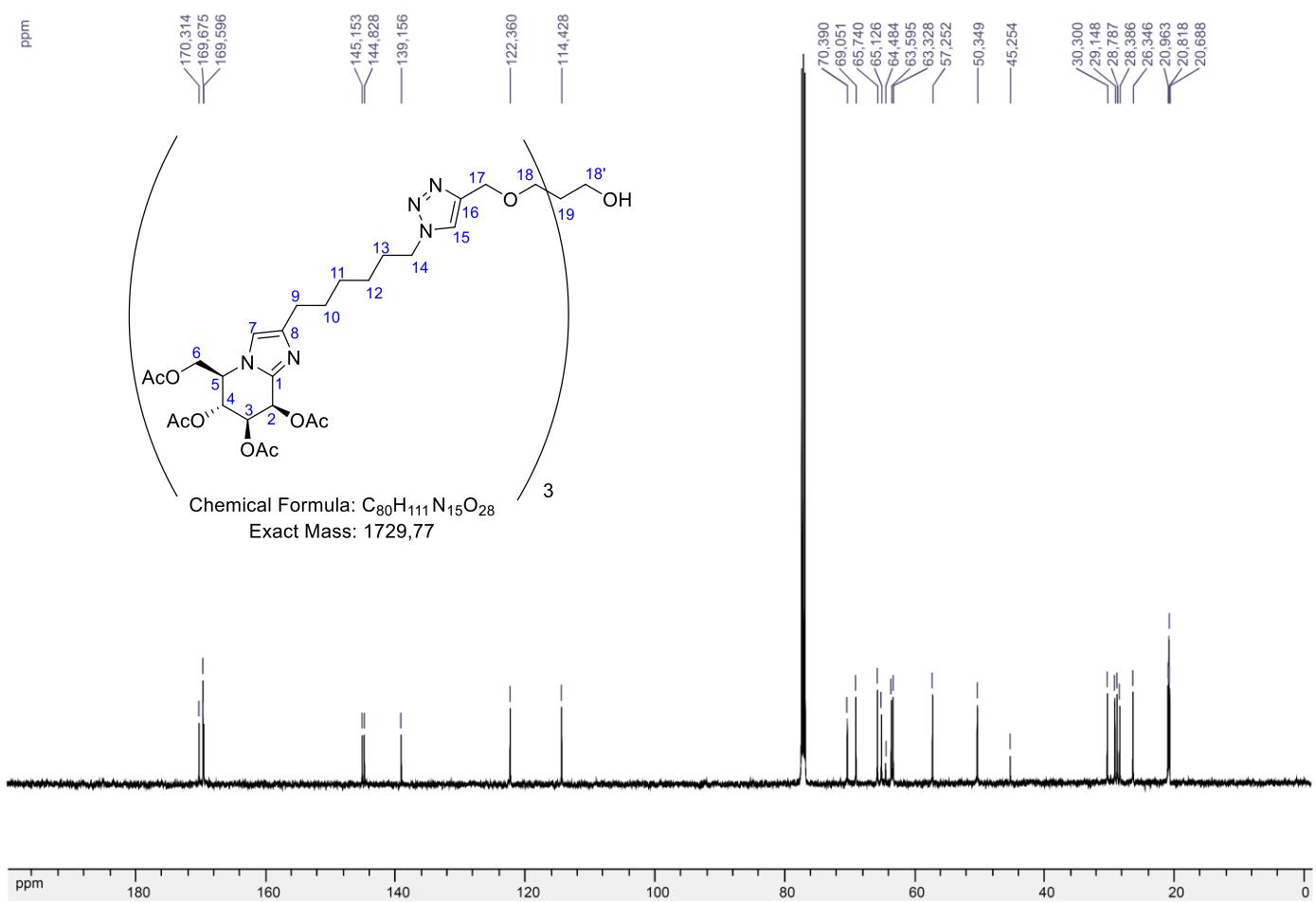
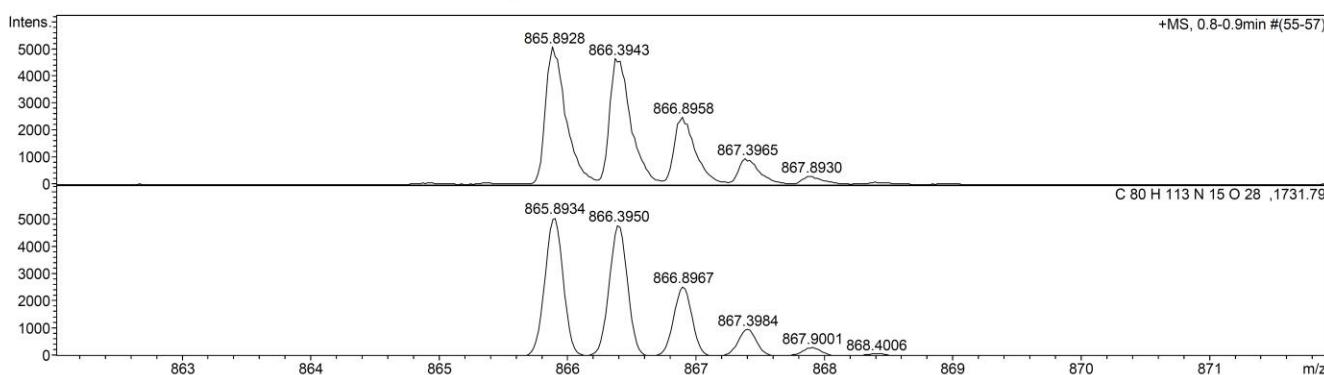


Fig S50. ¹³C NMR (125 MHz, CDCl₃) spectrum of compound 20b

Mass Spectrum HR Report

Analysis Info				Acquisition Date	02/05/2018 14:27:16
Analysis Name	Y:\O43088SK.d	Method	esi wide pos.m	Operator	admin
Sample Name	MP0308 Pur	Comment		Instrument	micrOTOF
Acquisition Parameter			<th>Set Corrector Fill</th> <td>59 V</td>	Set Corrector Fill	59 V
Source Type	ESI	Ion Polarity	Positive	Set Pulsar Pull	818 V
n/a	n/a	Set Capillary Exit	150.0 V	Set Pulsar Push	818 V
Scan Begin	50 m/z	Set Hexapole RF	170.0 V	Set Reflector	1700 V
Scan End	3000 m/z	Set Skimmer 1	50.0 V	Set Flight Tube	8600 V
		Set Hexapole 1	24.3 V	Set Detector TOF	2057 V



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**

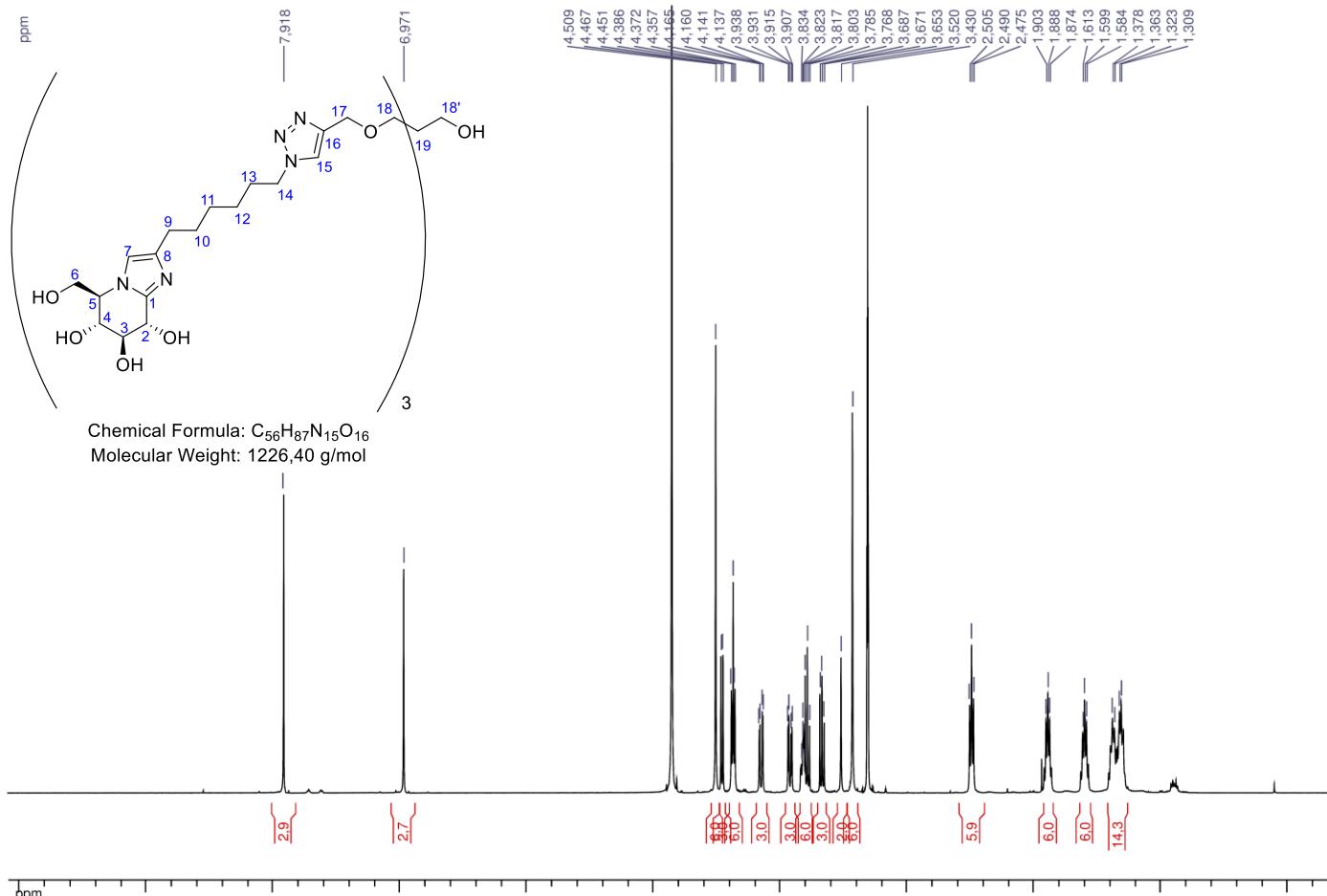


Fig S52. ¹H NMR (500 MHz, CD₃OD) spectrum of compound **21a**

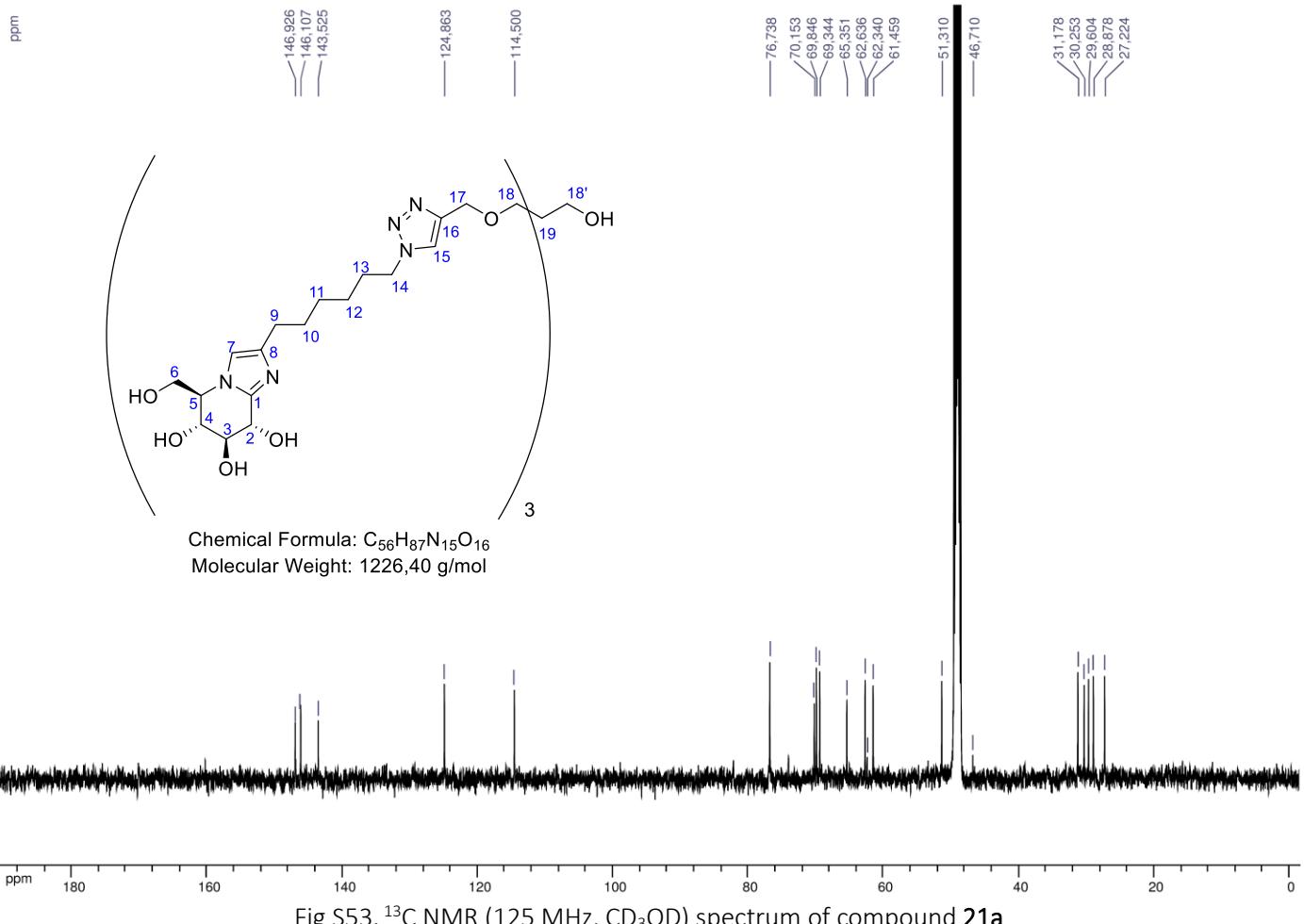
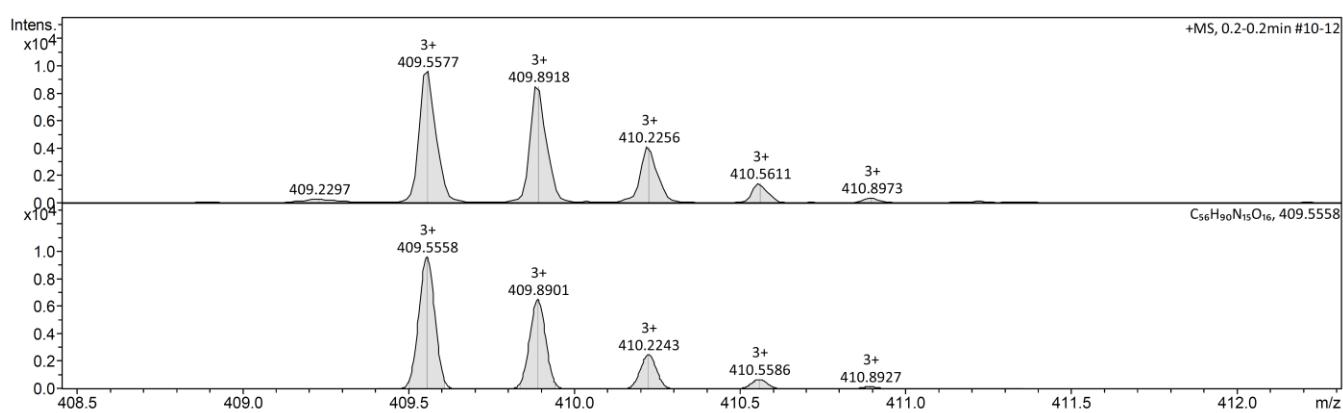


Fig S53. ^{13}C NMR (125 MHz, CD_3OD) spectrum of compound 21a

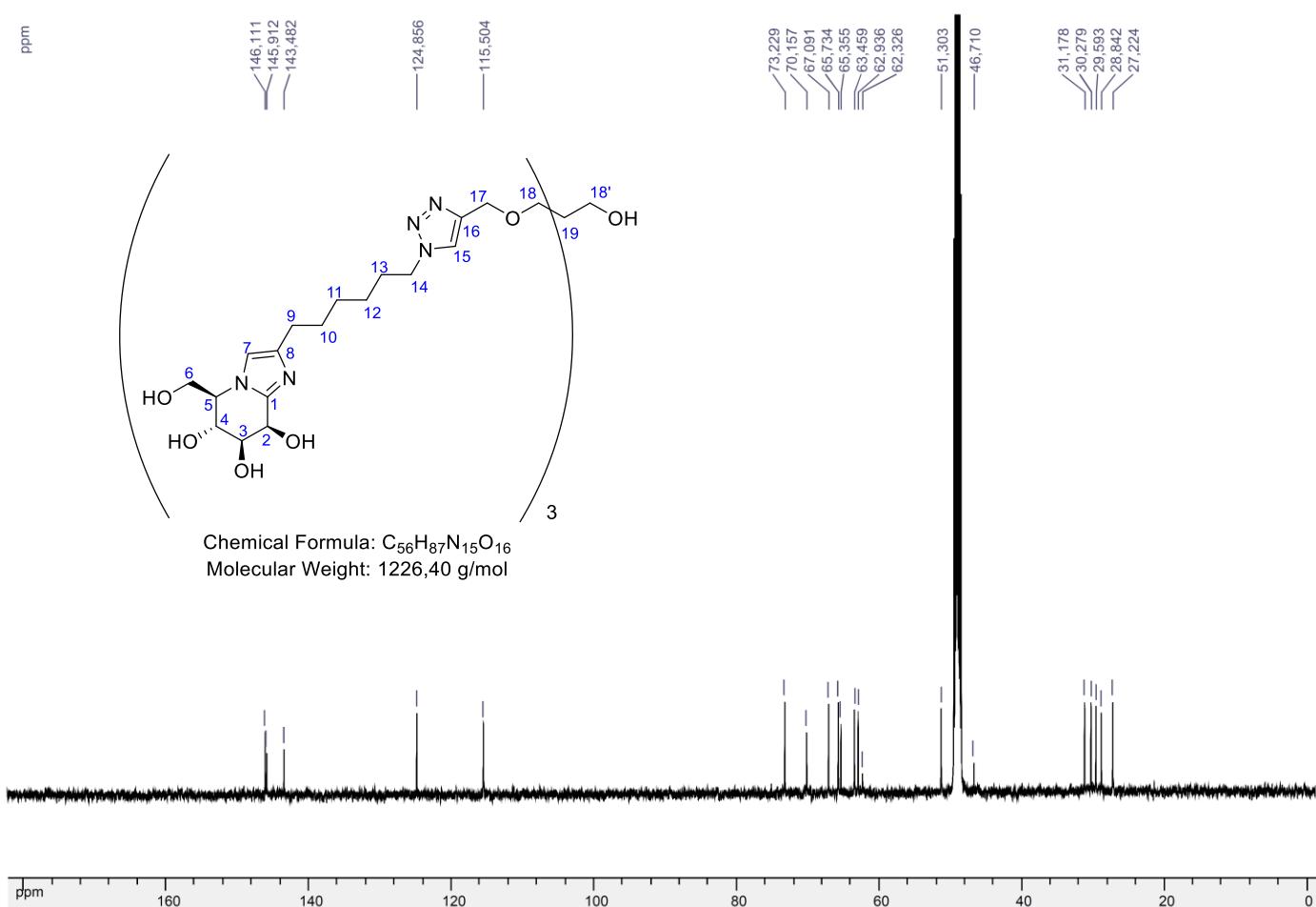
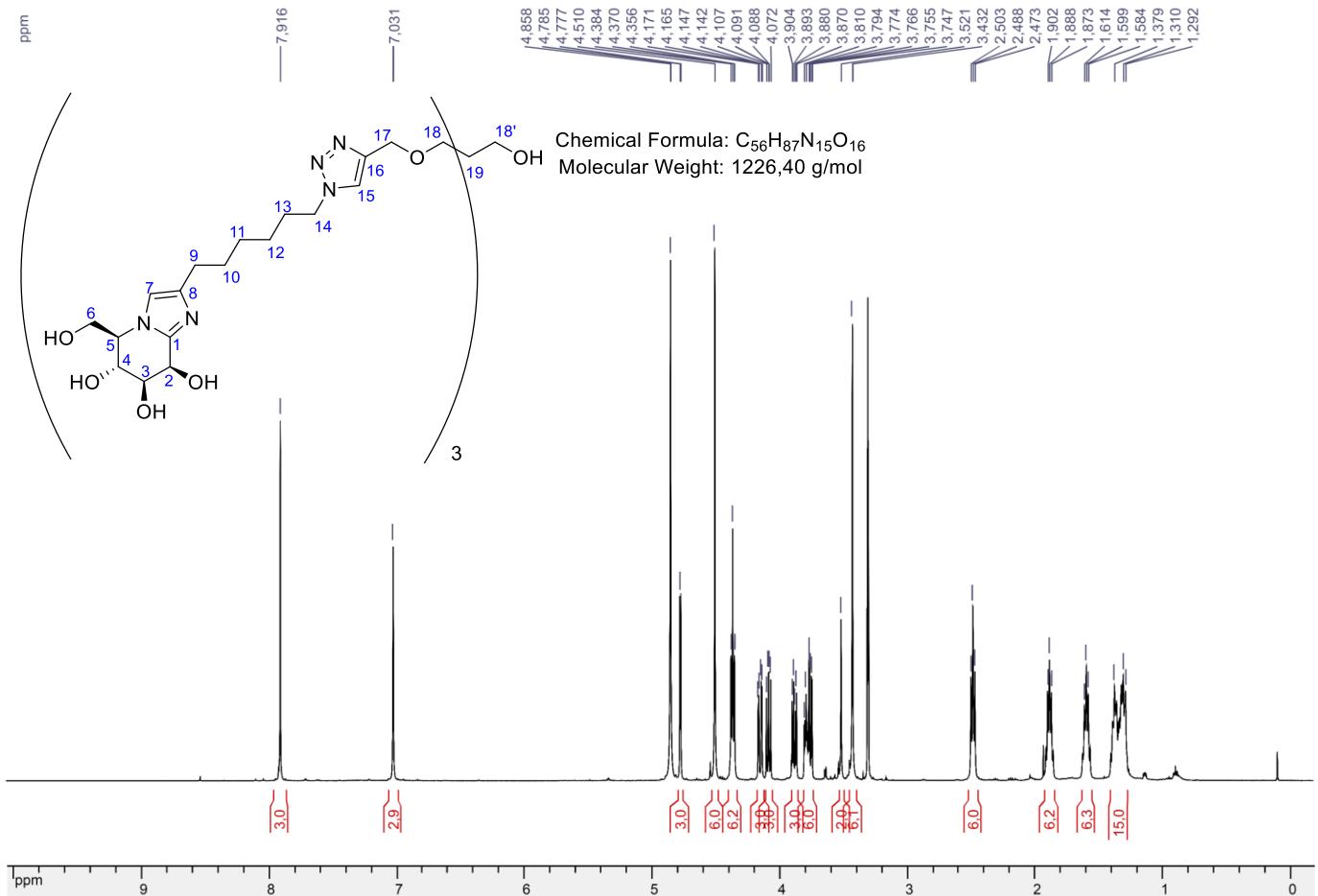
Mass Spectrum HR Report

Analysis Info		Acquisition Date		
Analysis Name	D:\Data\SMasse\2018\02_Fevrier 2018\F01647SK.d	2/1/2018 11:04:03 AM		
Method	Tune_pos_Mid.m		Operator	BDAL@DE
Sample Name	MP0273 Brut		Instrument	micrOTOF II
Comment				8213750.1045 1
Acquisition Parameter		Set Corrector Fill		
Source Type	ESI	n/a	59.0 V	
n/a	n/a	n/a	n/a	n/a
Scan Begin	50 m/z	n/a	Set Reflector	1800.0 V
Scan End	3000 m/z	n/a	Set Flight Tube	8600.0 V
		n/a	Set Detector TOF	1953.3 V



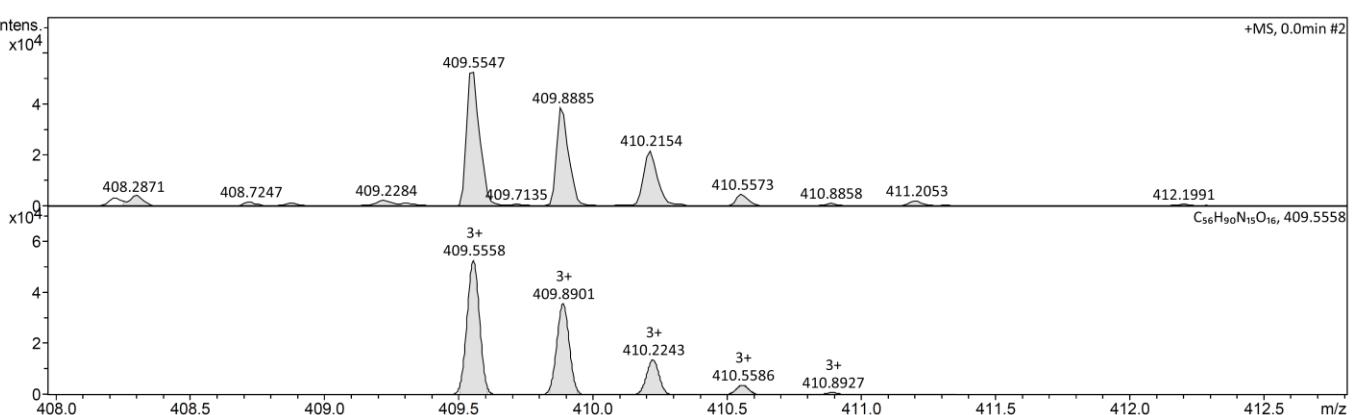
Meas. m/z	# Ion	Formula	m/z err [ppm]	Mean err [ppm]	rdb N-Rule e ⁻	Conf	mSigma	Std I	Std Mean	m/z Std I	VarNorm	Std m/z	Diff	Std Comb	Dev
409.557747	1	$\text{C}_{56}\text{H}_{90}\text{N}_{15}\text{O}_{16}$	409.555784	-4.8	-5.4 19.5	ok even	125.0	108.8	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.

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



Mass Spectrum HR Report

Analysis Info				Acquisition Date	5/3/2018 3:06:45 PM
Analysis Name	D:\Data\SMasse\2018\05_Mai 2018\F02187SK.d			Operator	BDAL@DE
Method	Tune_pos_Mid.m			Instrument	micrOTOF II
Sample Name	MP0311 Brut				8213750.1045
Comment					1
Acquisition Parameter				Set Corrector Fill	59.0 V
Source Type	ESI	Ion Polarity	Positive	n/a	n/a
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 I	Diff	Std I	Comb Dev
409.5547	1	$C_{56}H_{90}N_{15}O_{16}$	409.5558	2.5	7.8	19.5	ok even	73.9	75.9	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
613.8288	1	$C_{56}H_{89}N_{15}O_{16}$	613.8300	2.1	822.2	20.0	ok even	12.0	12.1	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1226.6504	1	$C_{56}H_{88}N_{15}O_{16}$	1226.6528	1.9	413.2	20.5	ok even	34.1	31.5	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.

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

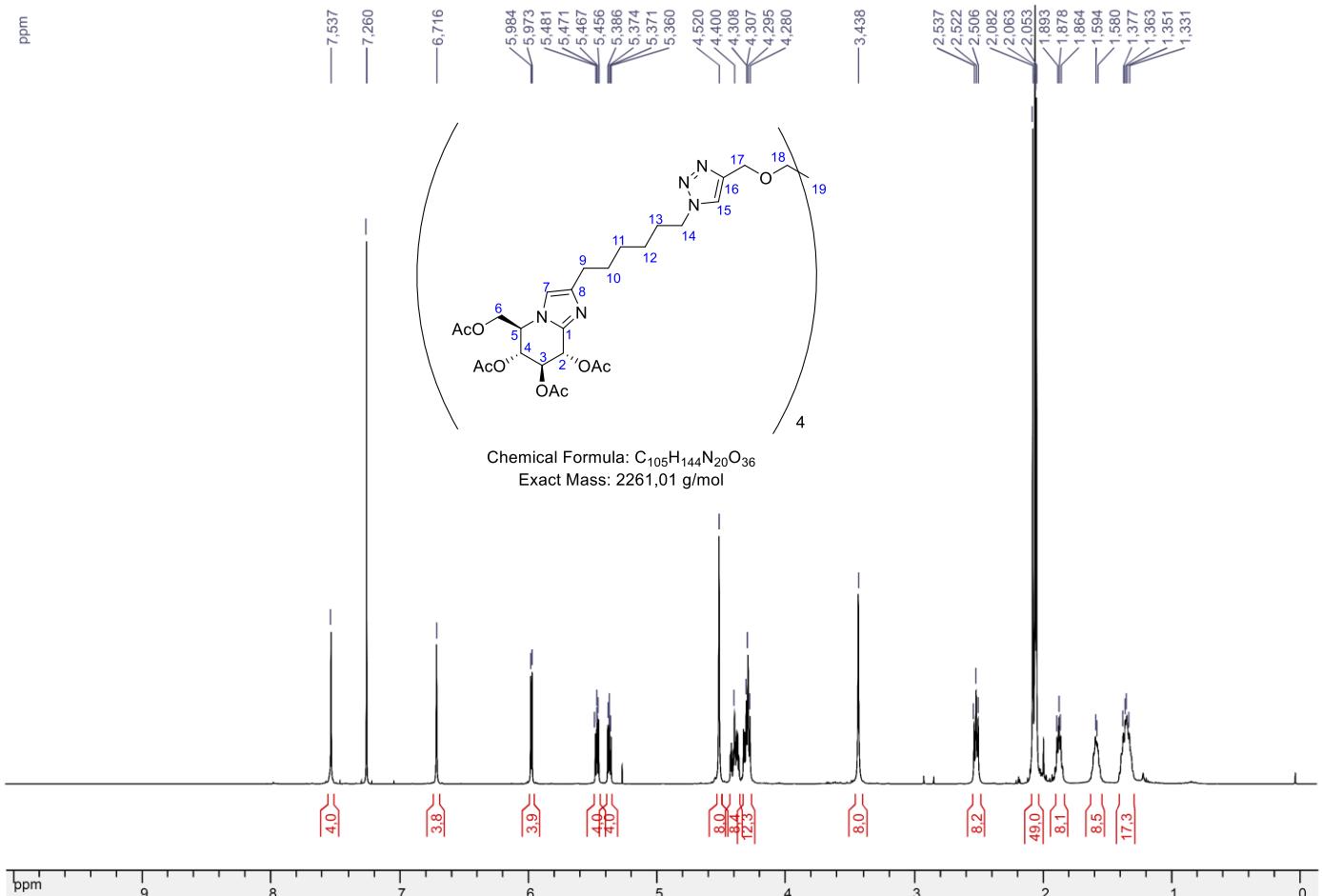


Fig S58. 1H NMR (500 MHz, $CDCl_3$) spectrum of compound 22a

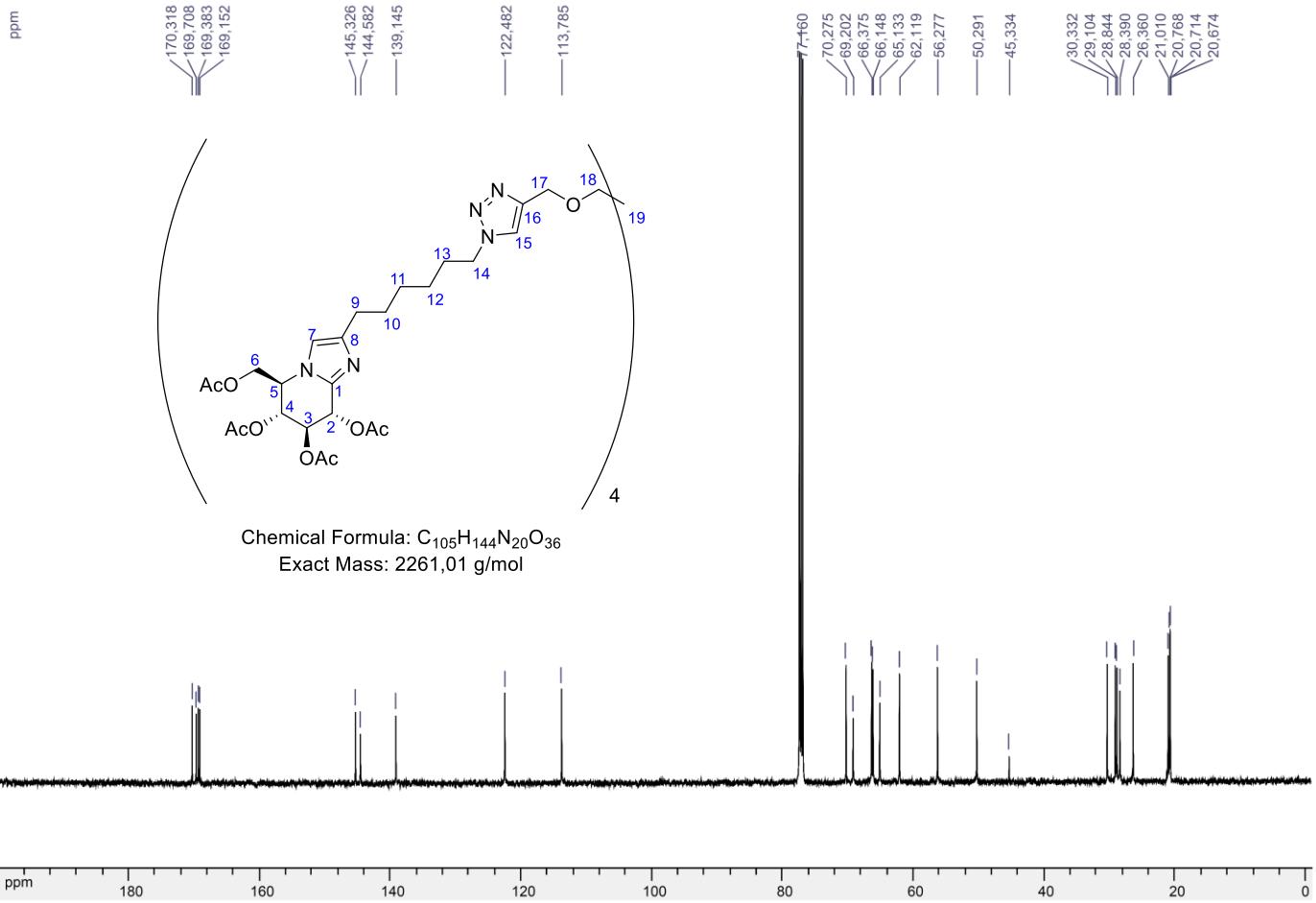
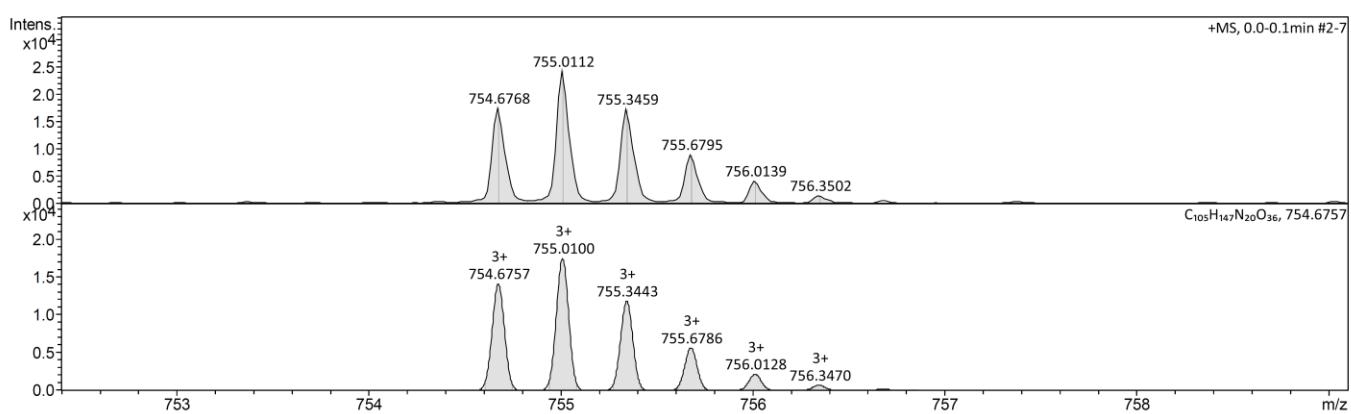


Fig S59. ^{13}C NMR (125 MHz, CDCl_3) spectrum of compound 22a

Mass Spectrum HR Report

Analysis Info		Acquisition Date	12/18/2017 9:48:47 AM
Analysis Name	D:\Data\SMasse\2017\12_Decembre 2017\F01460SK.d		
Method	Tune_pos_Mid.m	Operator	BDAL@DE
Sample Name	MP0260 Pur	Instrument	micrOTOF II
Comment			8213750.1045 1
Acquisition Parameter		Set Corrector Fill	59.0 V
Source Type	ESI	n/a	n/a
n/a	n/a	n/a	n/a
Scan Begin	50 m/z	Set Reflector	1800.0 V
Scan End	3000 m/z	Set Flight Tube	8600.0 V
		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
754.676829 1 $C_{105}H_{147}N_{20}O_{36}$ 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

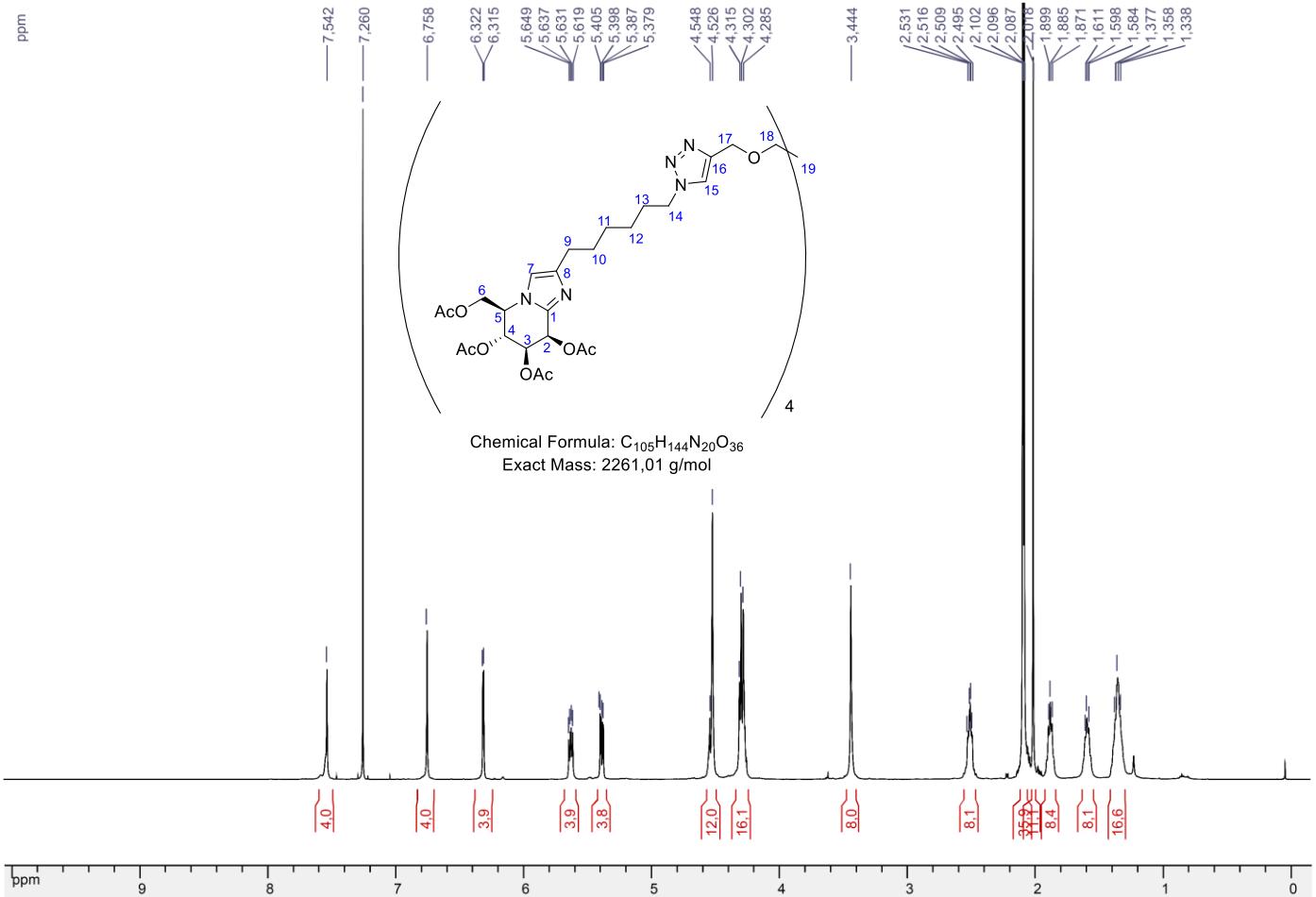


Fig S61. ¹H NMR (500 MHz, CDCl₃) spectrum of compound 22b

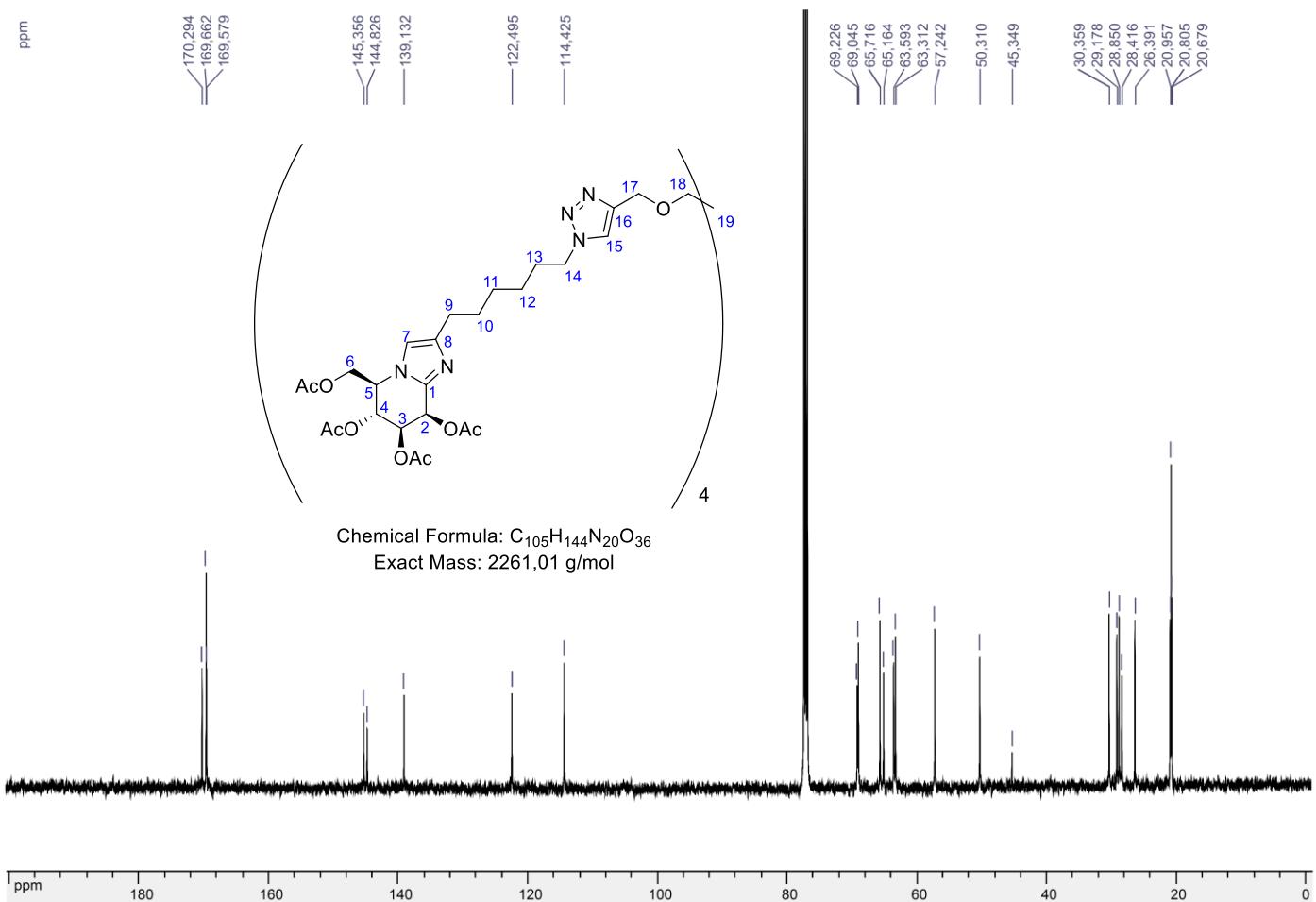


Fig S62. ¹³C NMR (125 MHz, CDCl₃) spectrum of compound 22

Mass Spectrum HR Report

Analysis Info

Analysis Name D:\Data\SMasse\2018\03_Mars 2018\F02021SK.d
 Method Tune_pos_Mid.m
 Sample Name MP0300
 Comment

Acquisition Date

3/28/2018 3:50:59 PM

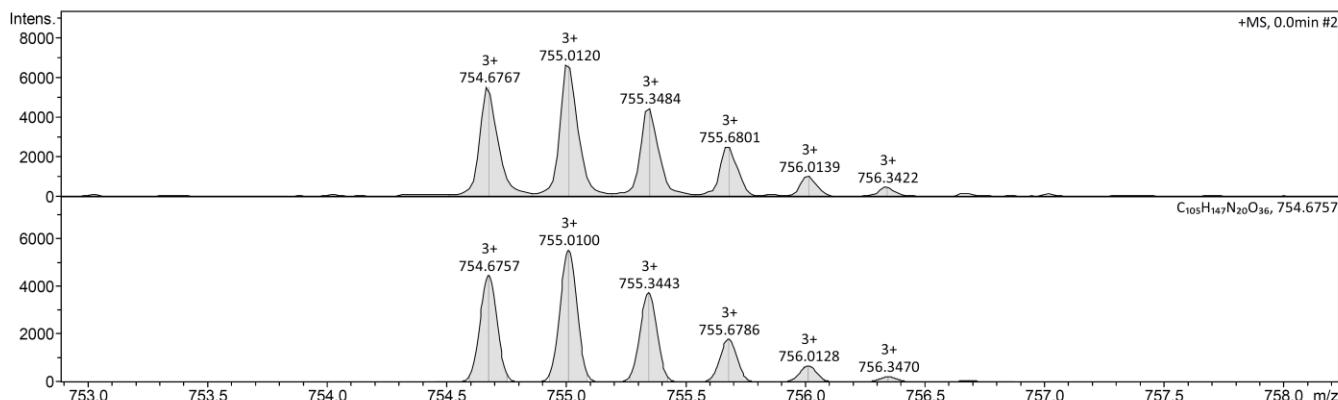
 Operator
Instrument

 BDAL@DE
micrOTOF II

 8213750.1045
1

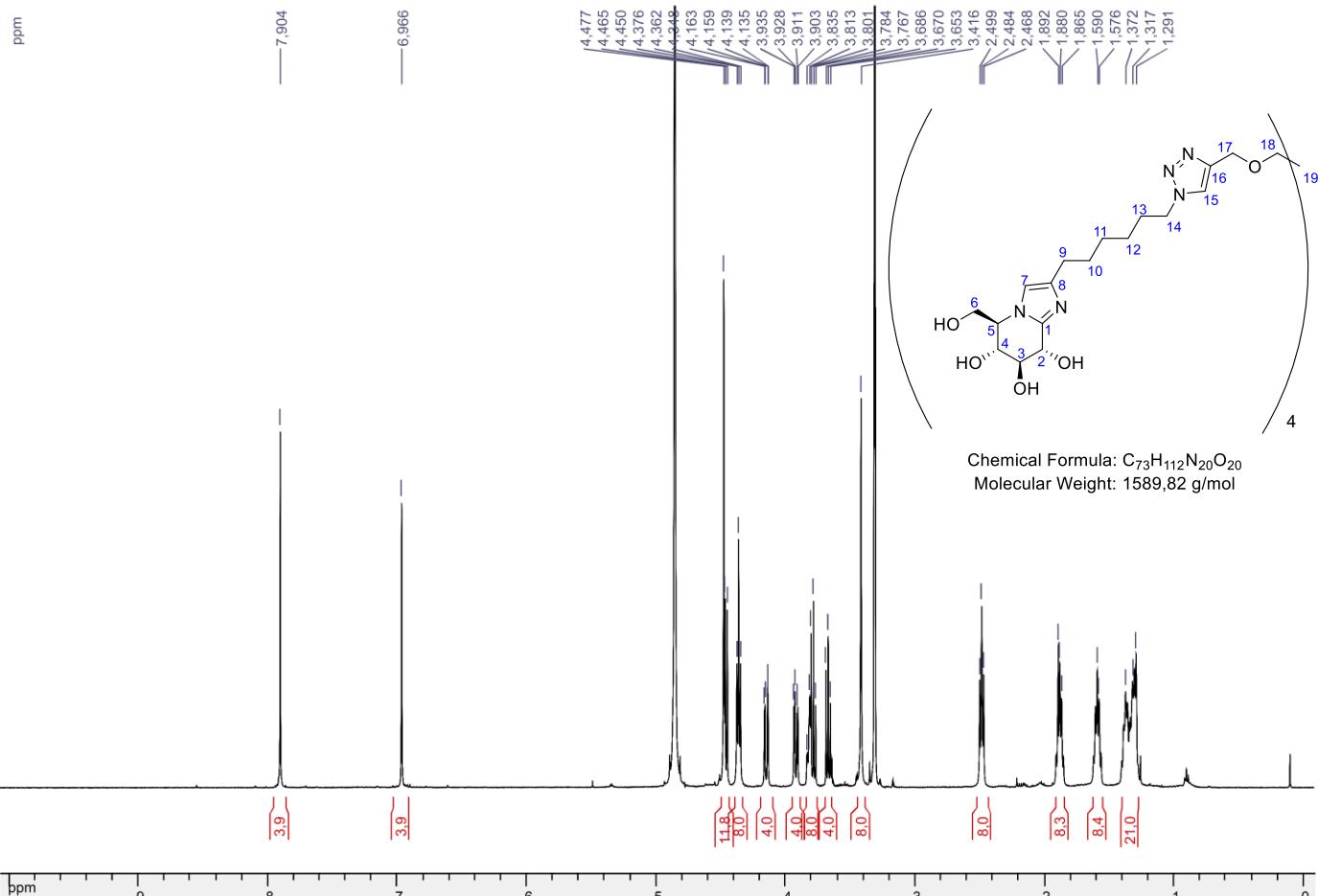
Acquisition Parameter

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 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.	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.	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.	n.a.

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


 Fig S64. ¹H NMR (500 MHz, CD₃OD) spectrum of compound 23a

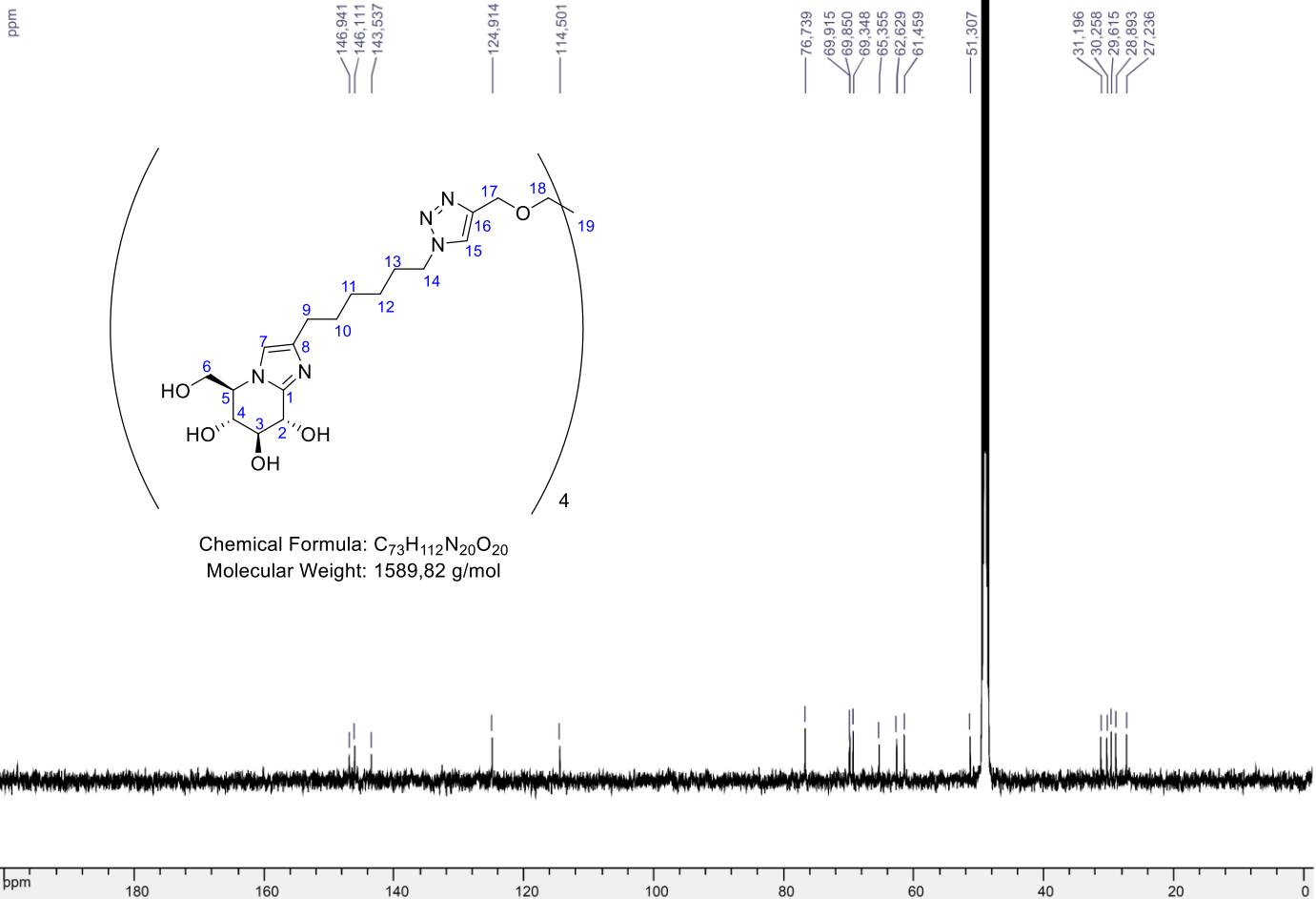


Fig S65. ^{13}C NMR (125 MHz, CD_3OD) spectrum of compound 23a

Mass Spectrum HR Report

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

Acquisition Parameter		Set Corrector Fill	59.0 V
Source Type	ESI	n/a	n/a
n/a	n/a	n/a	n/a
Scan Begin	50 m/z	n/a	1800.0 V
Scan End	3000 m/z	n/a	8600.0 V
		n/a	1953.3 V

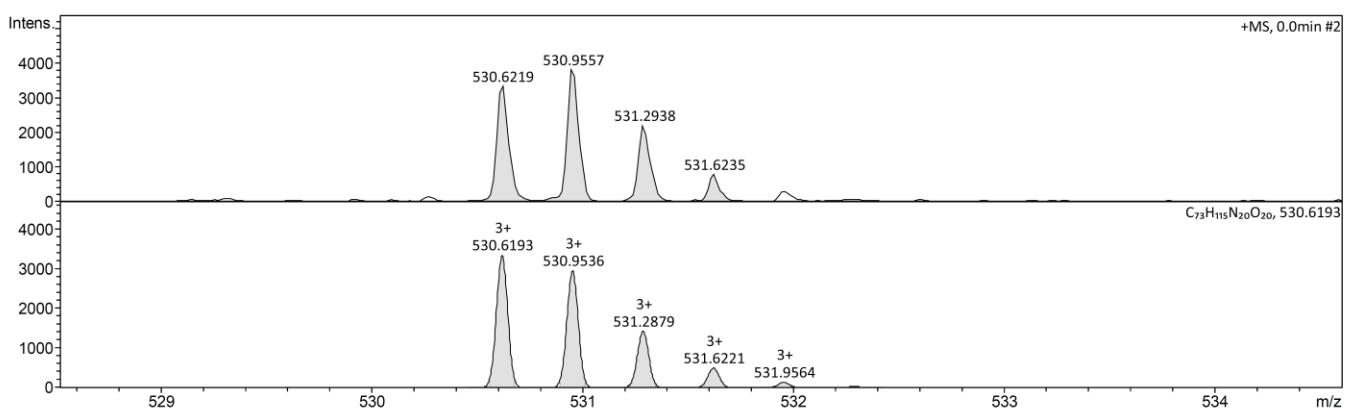


Fig S66. HRMS (ESI-MS) spectrum of compound 23a

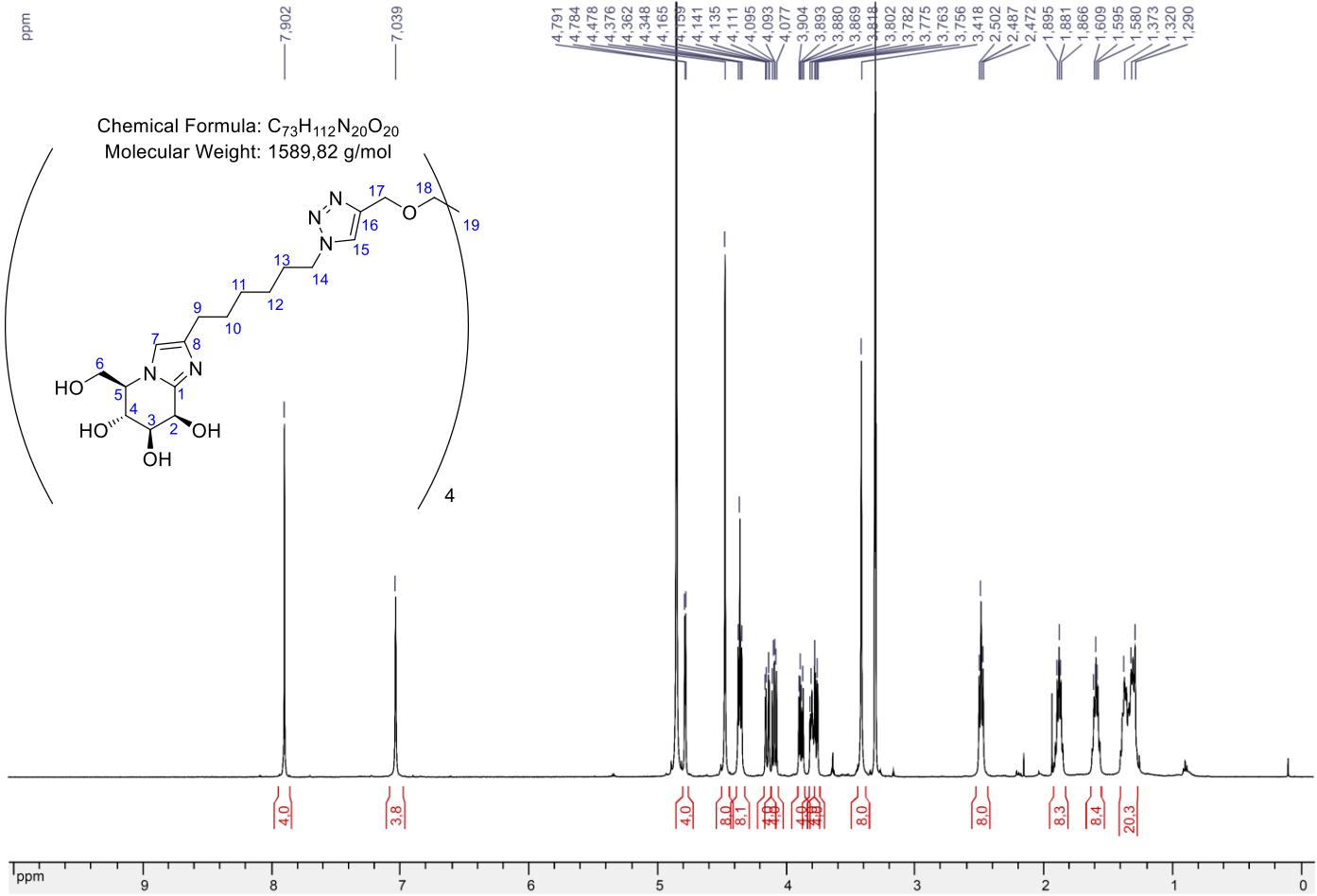


Fig S67. ¹H NMR (500 MHz, CD₃OD) spectrum of compound 23b

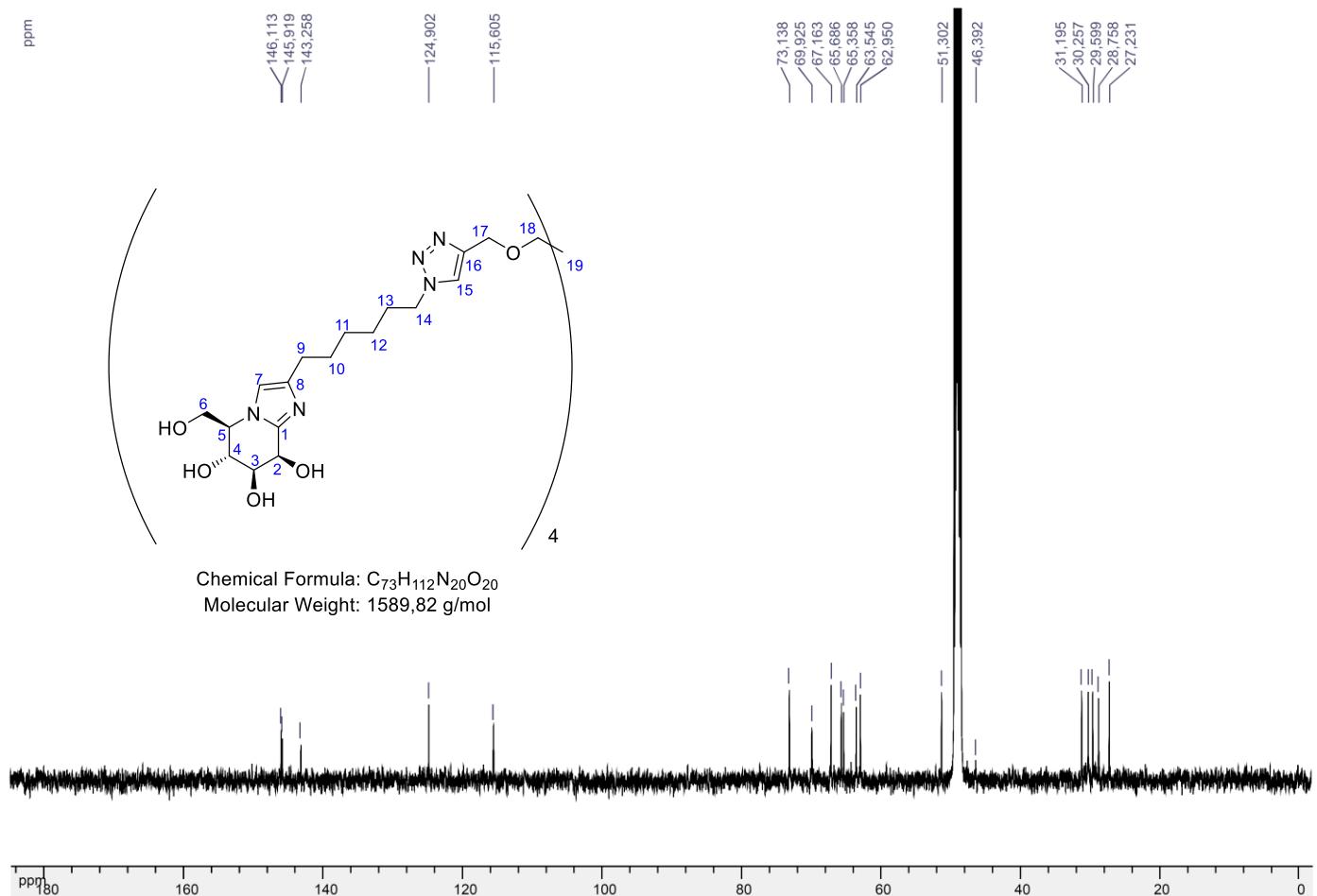
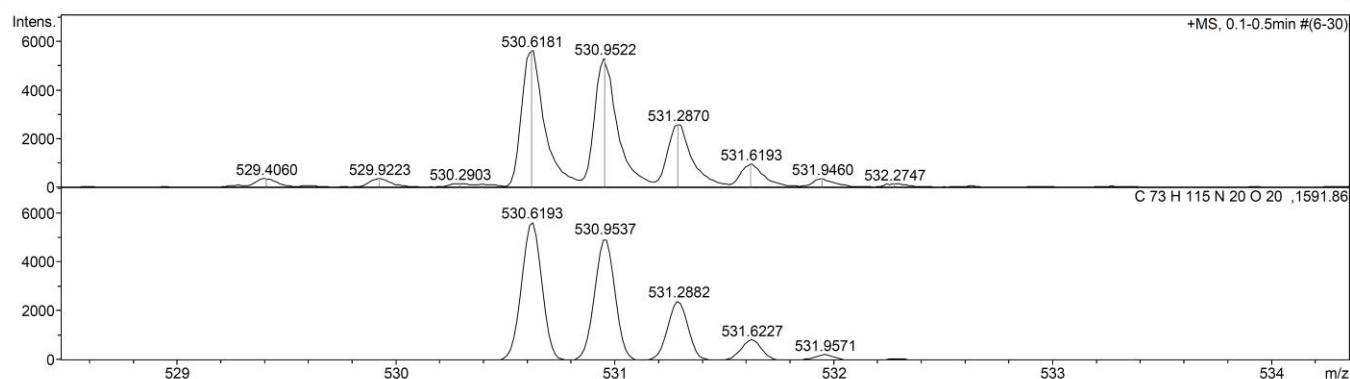


Fig S68. ¹³C NMR (125 MHz, CD₃OD) spectrum of compound 23b

Mass Spectrum HR Report

Analysis Info				Acquisition Date	19/04/2018 15:58:33
Analysis Name	Y:\O42997SK.d	Method	esi wide pos.m	Operator	admin
Sample Name	MP0306	Comment	MeOH	Instrument	micrOTOF
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-Ru le	e ⁻ Conf	mSigma a	Std I	Std I Mean m/z	Std I VarNor m	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

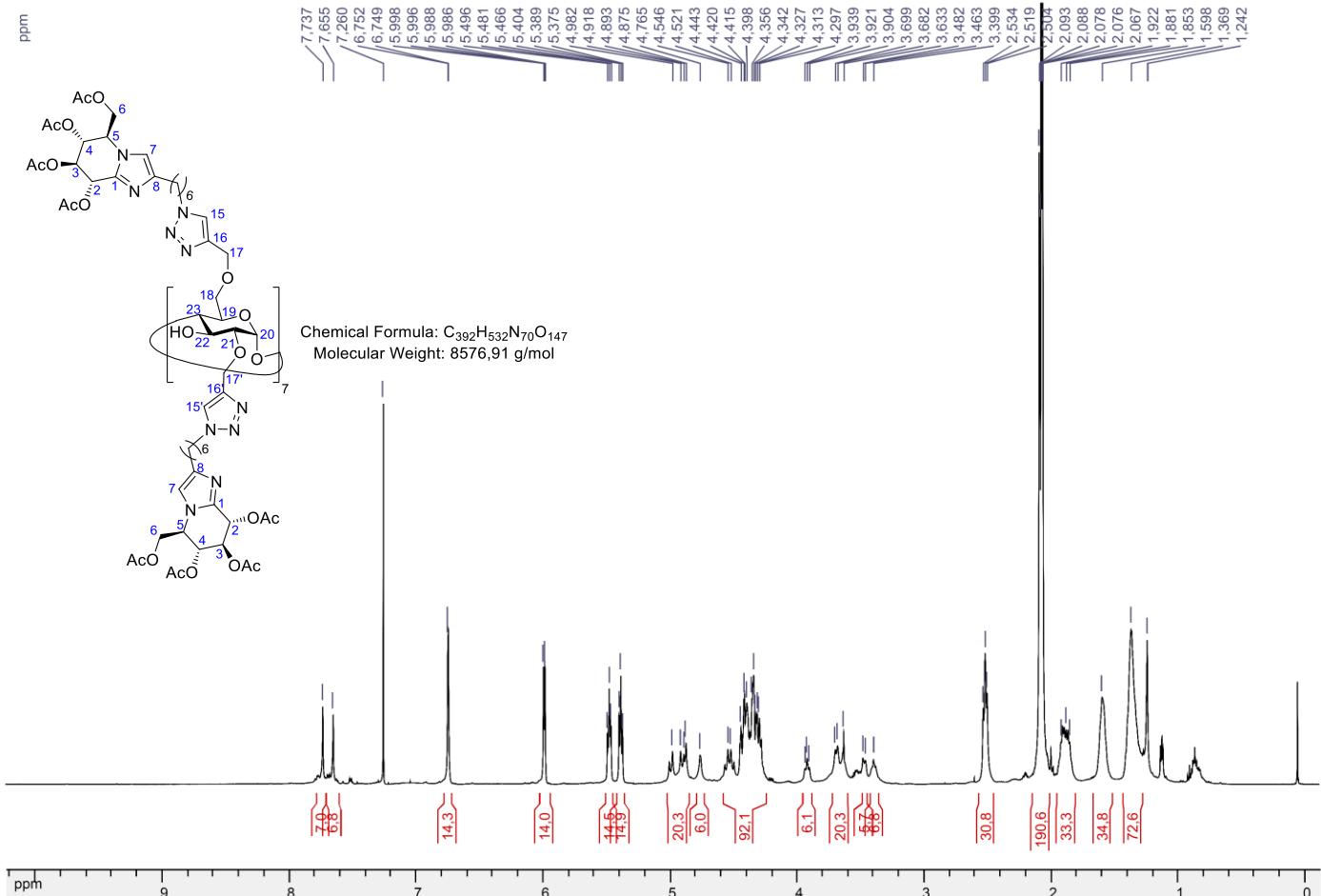


Fig S70. ¹H NMR (500 MHz, CDCl₃) spectrum of compound 25a

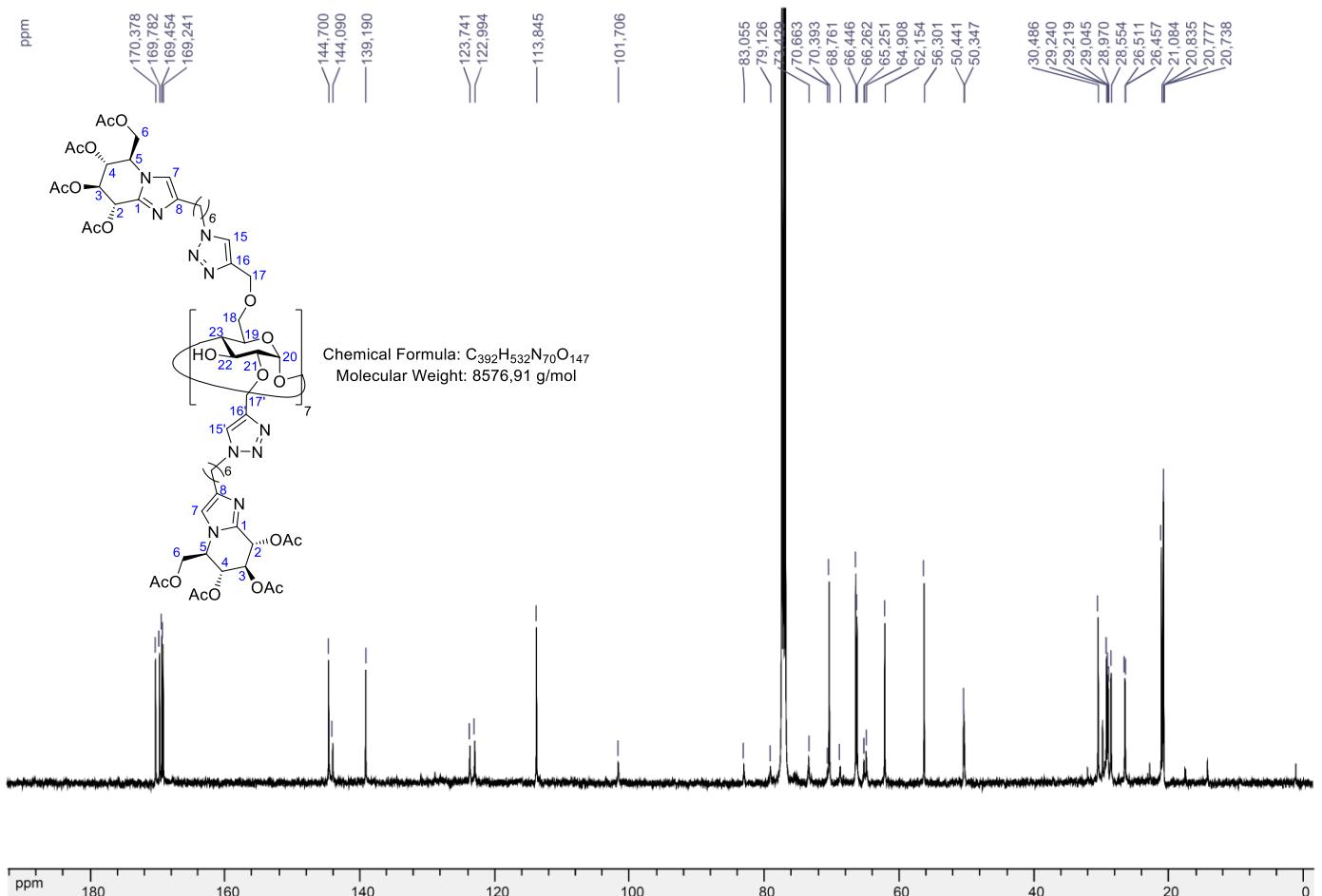


Fig S71. ^{13}C NMR (125 MHz, CDCl_3) spectrum of compound 25a

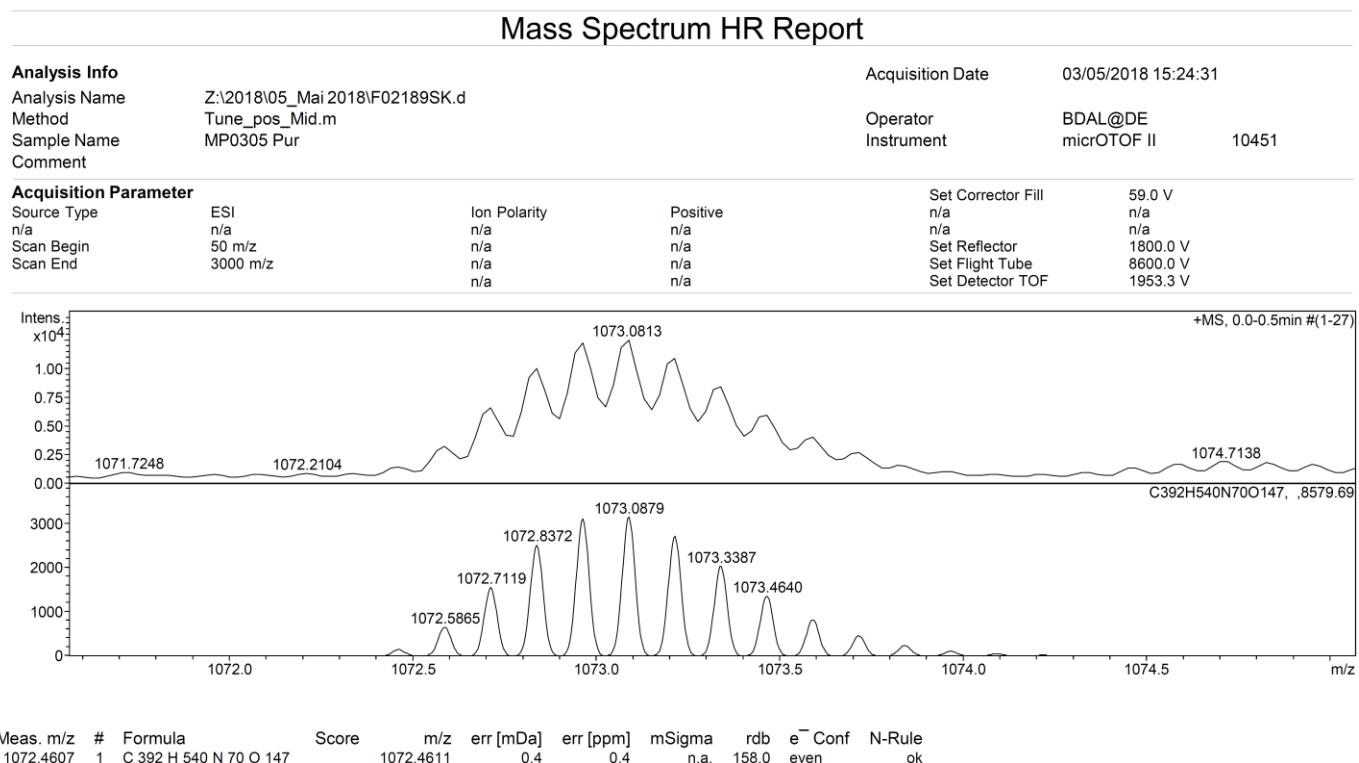
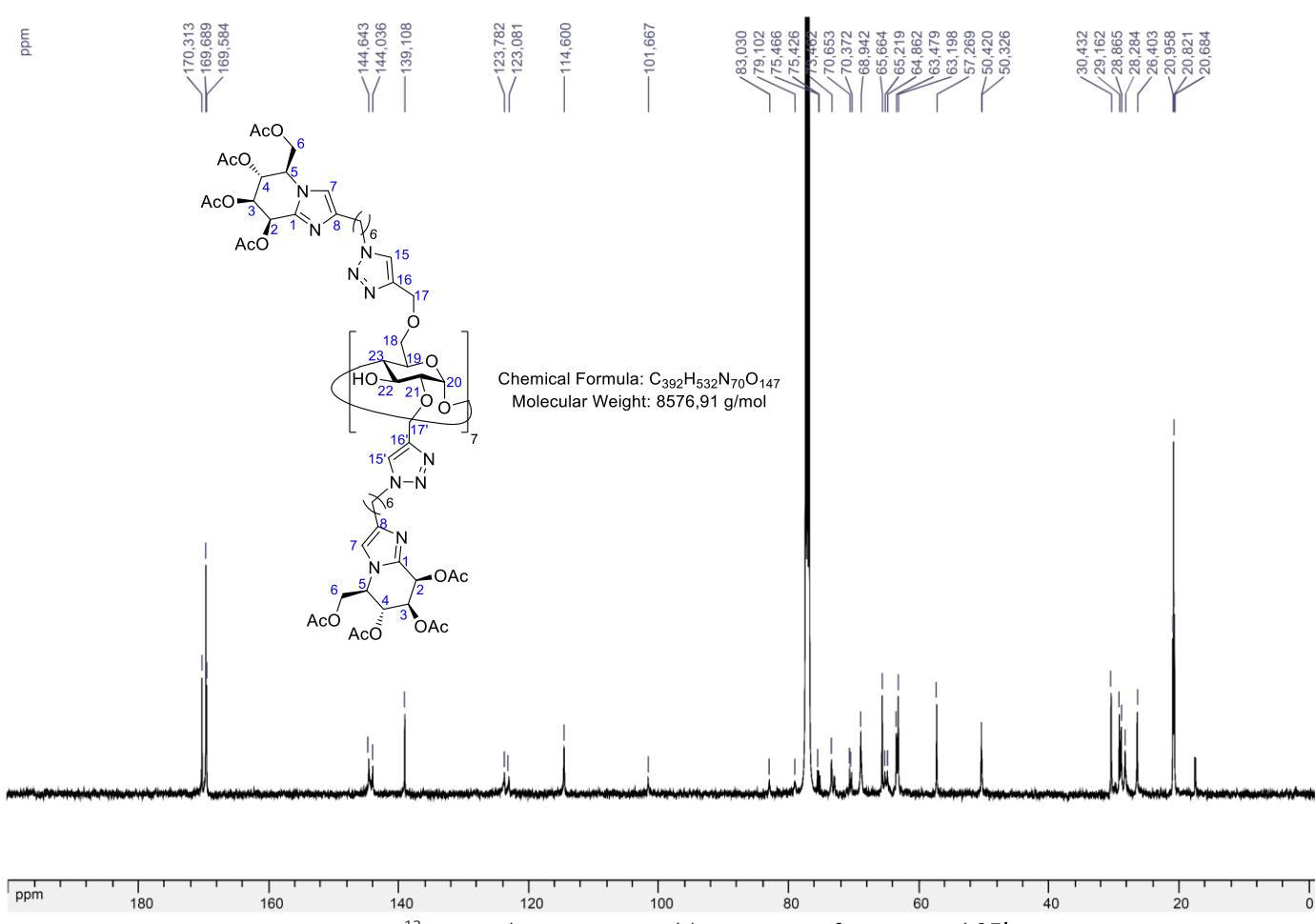
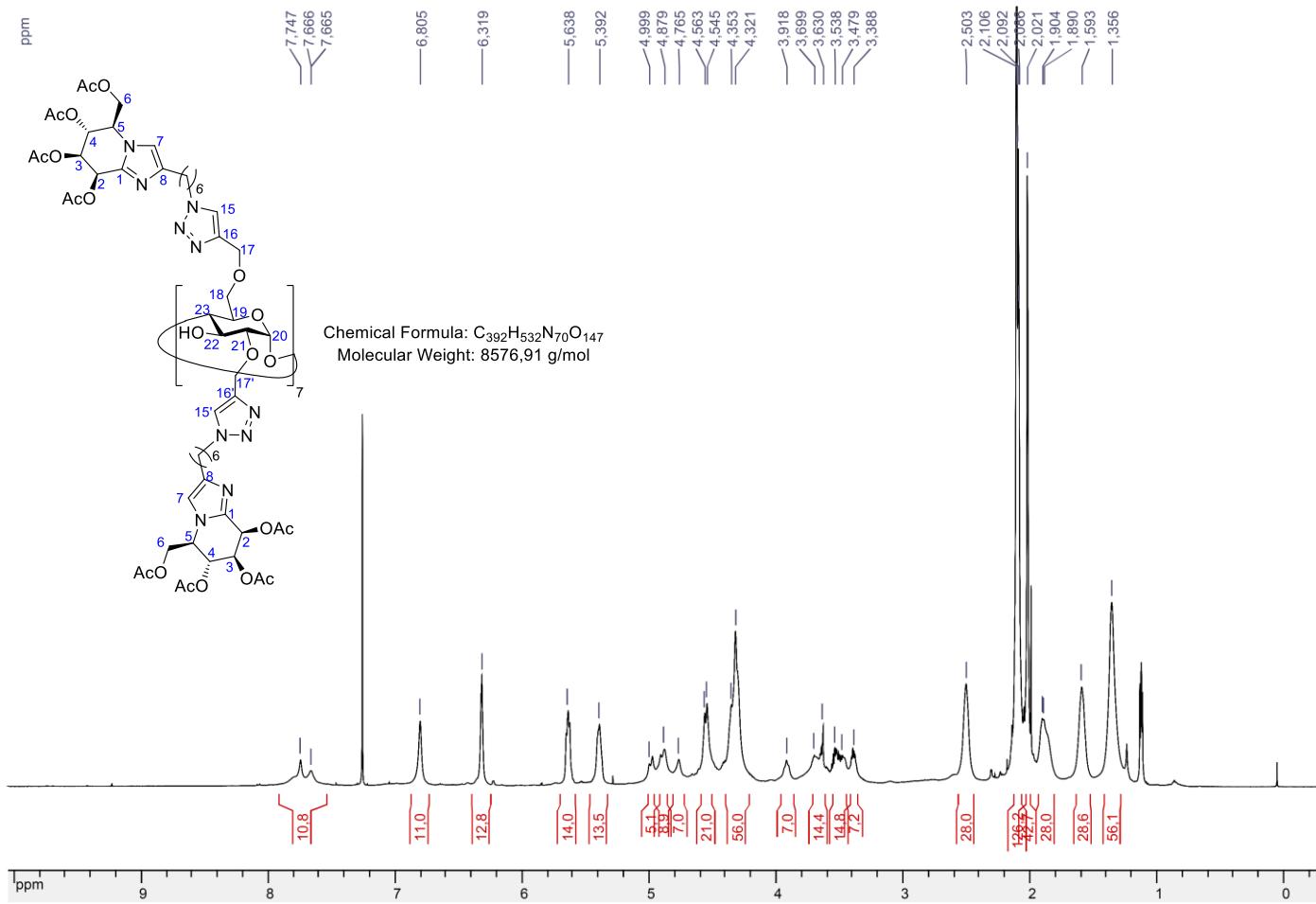


Fig S72. HRMS (ESI-MS) spectrum of compound 25a



Mass Spectrum HR Report

Analysis Info

Analysis Name Z:\2018\05_Mai 2018\F02282SK.d
 Method Tune_pos_Mid.m
 Sample Name MP0312 Pur
 Comment

Acquisition Date

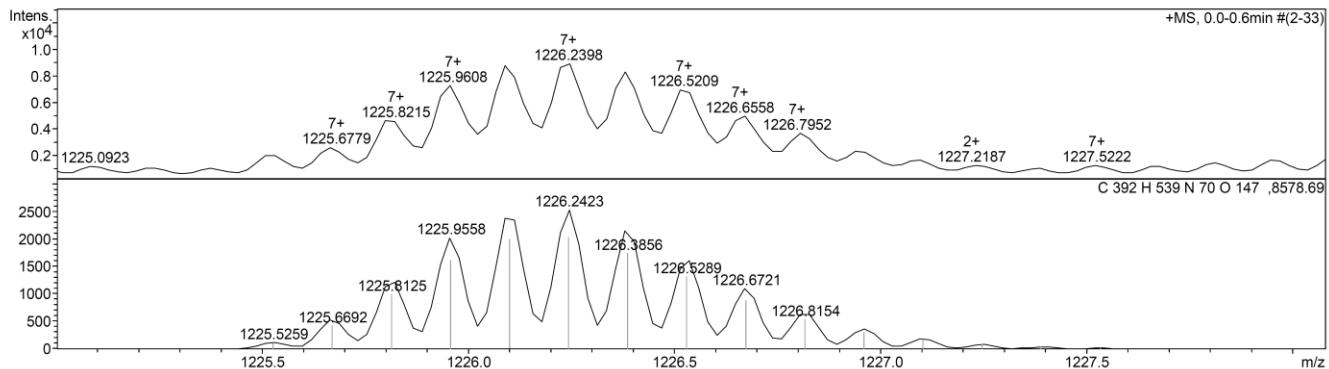
22/05/2018 11:24:58

 Operator
 Instrument

 BDAL@DE
 micrOTOF II
 10451

Acquisition Parameter

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



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule
1225.5263	1	C 392 H 539 N 70 O 147	100.00	1225.5259	-0.4	-0.3	101.0	158.5	even	ok

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

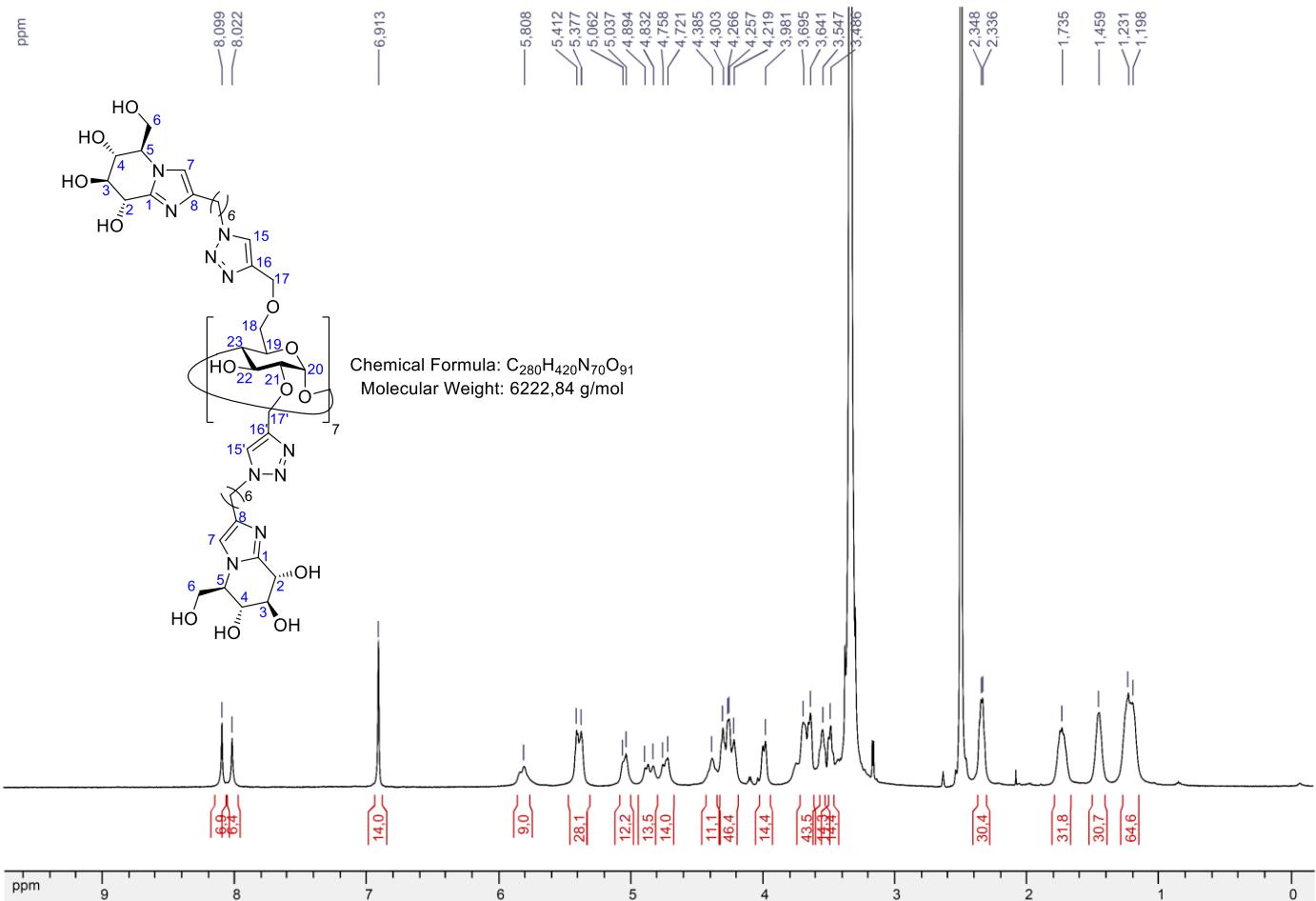


Fig S76. ¹H NMR (500 MHz, DMSO-d₆) spectrum of compound 26a

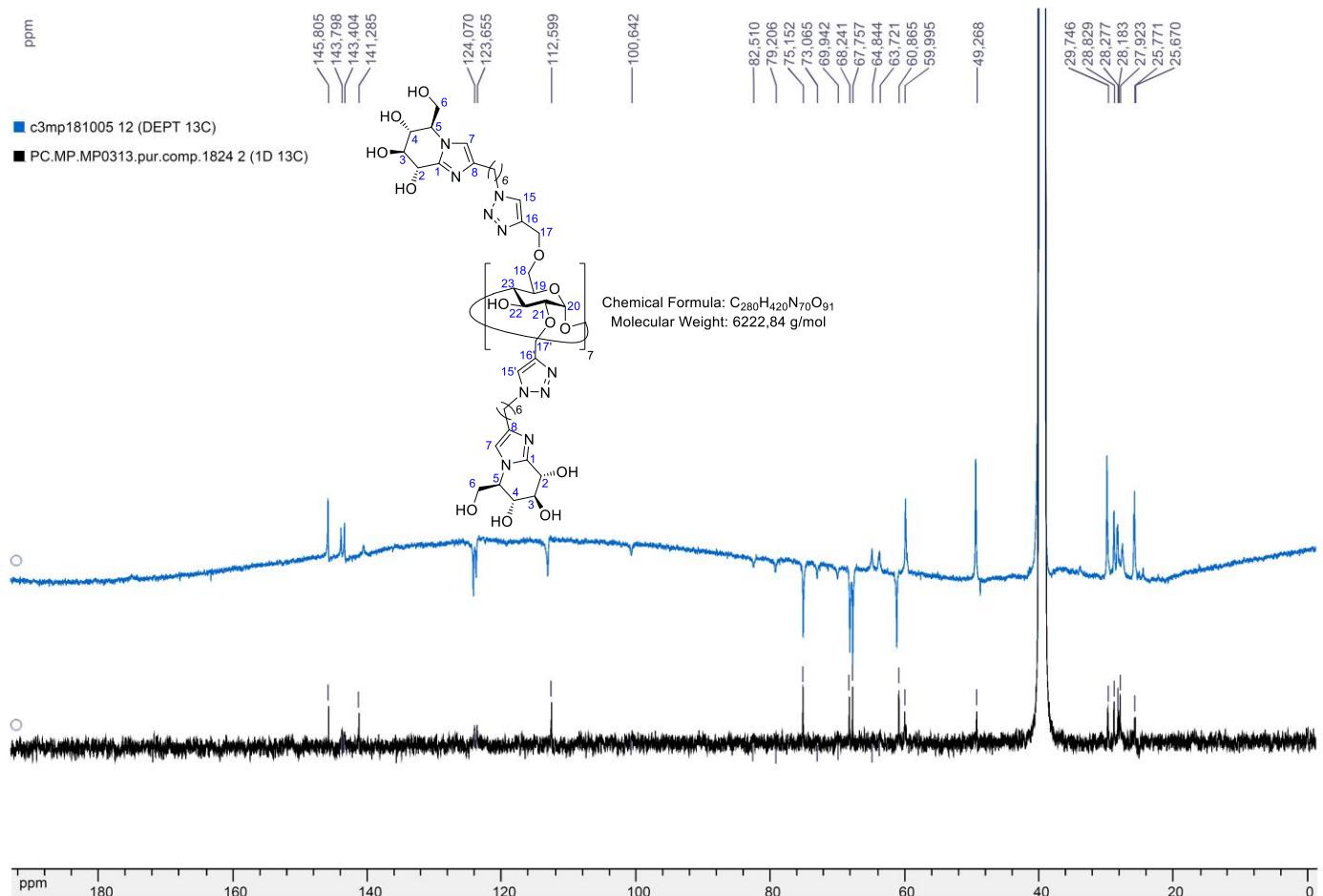


Fig S77. ^{13}C (125 MHz, DMSO-d₆) and DEPT spectra of compound 26a

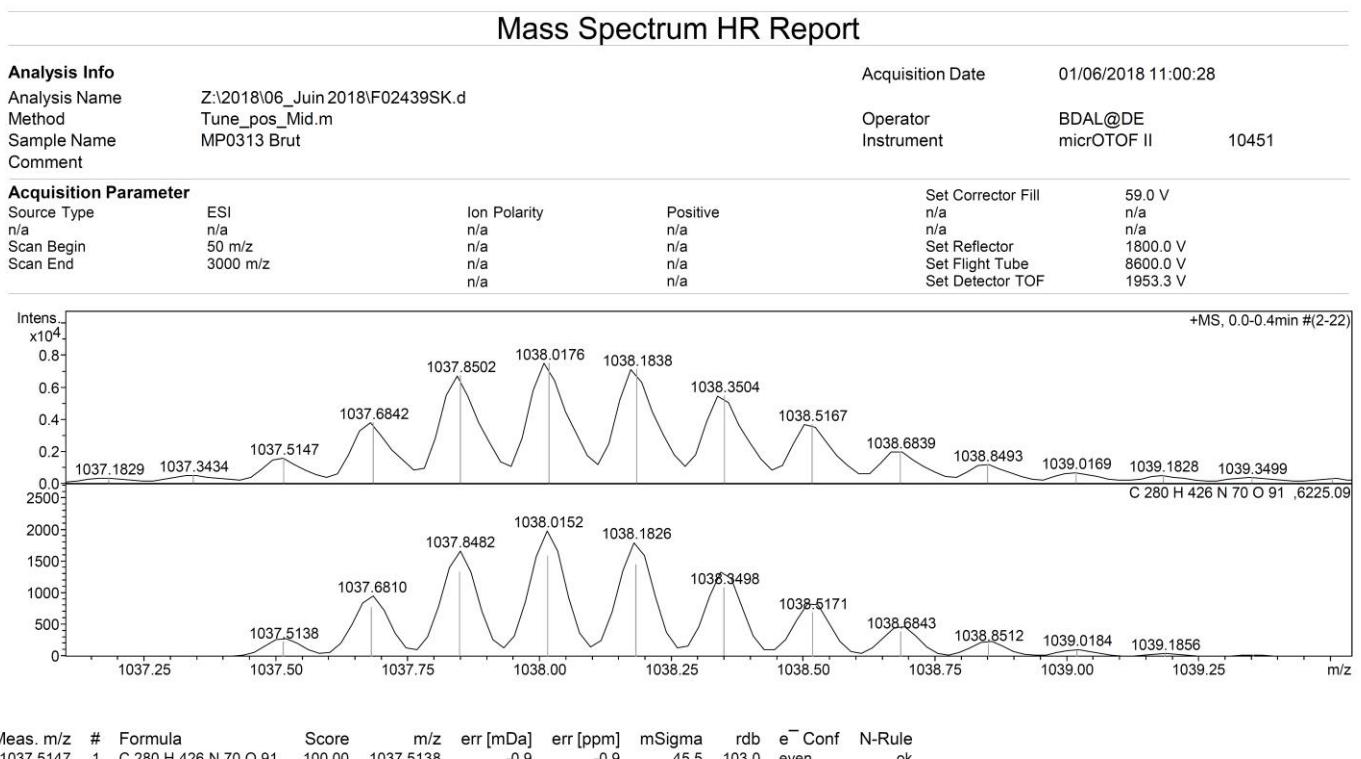


Fig S78. HRMS (ESI-MS) spectrum of compound 26a

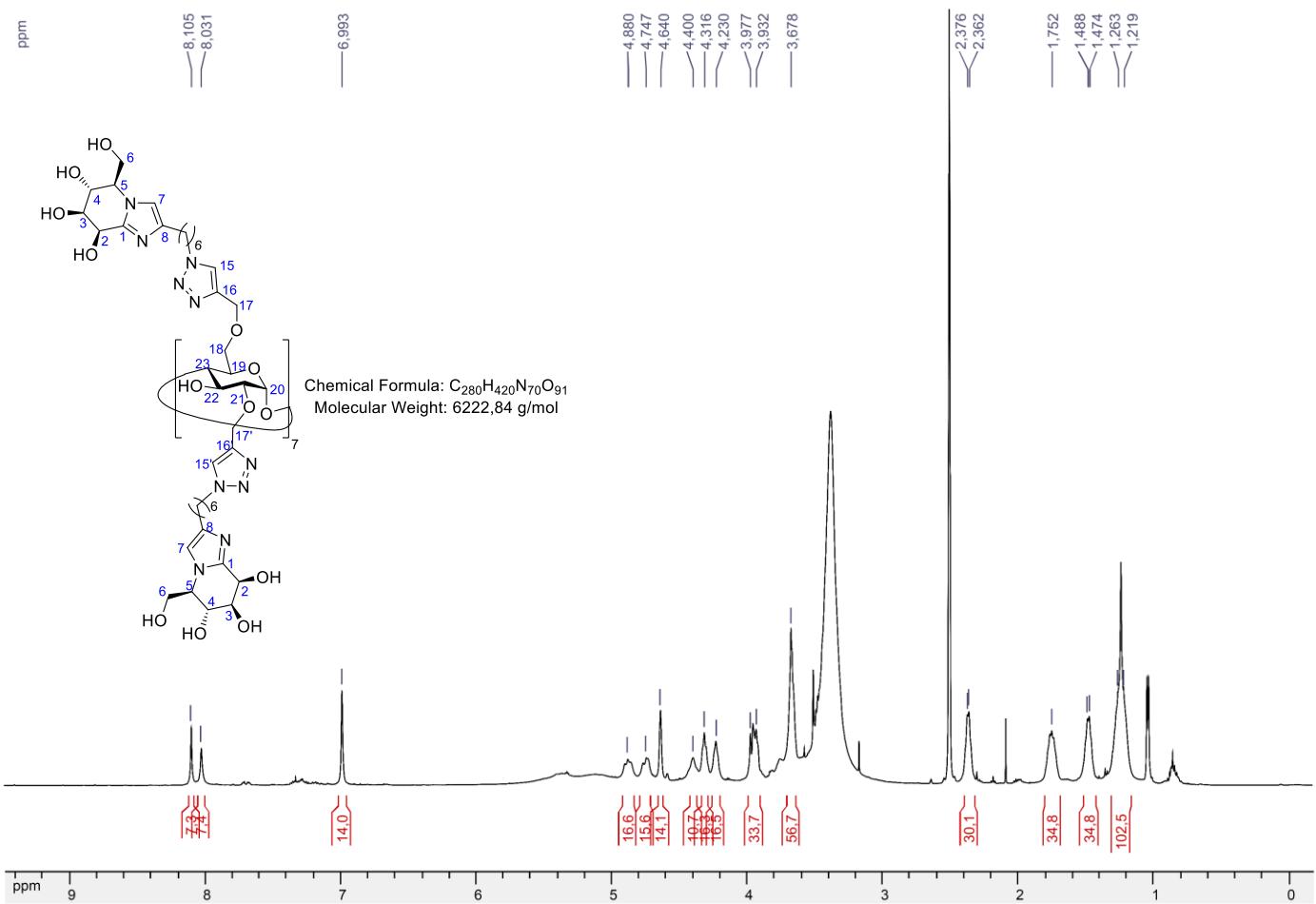


Fig S79. ^1H NMR (500 MHz, DMSO-d₆) spectrum of compound 26b

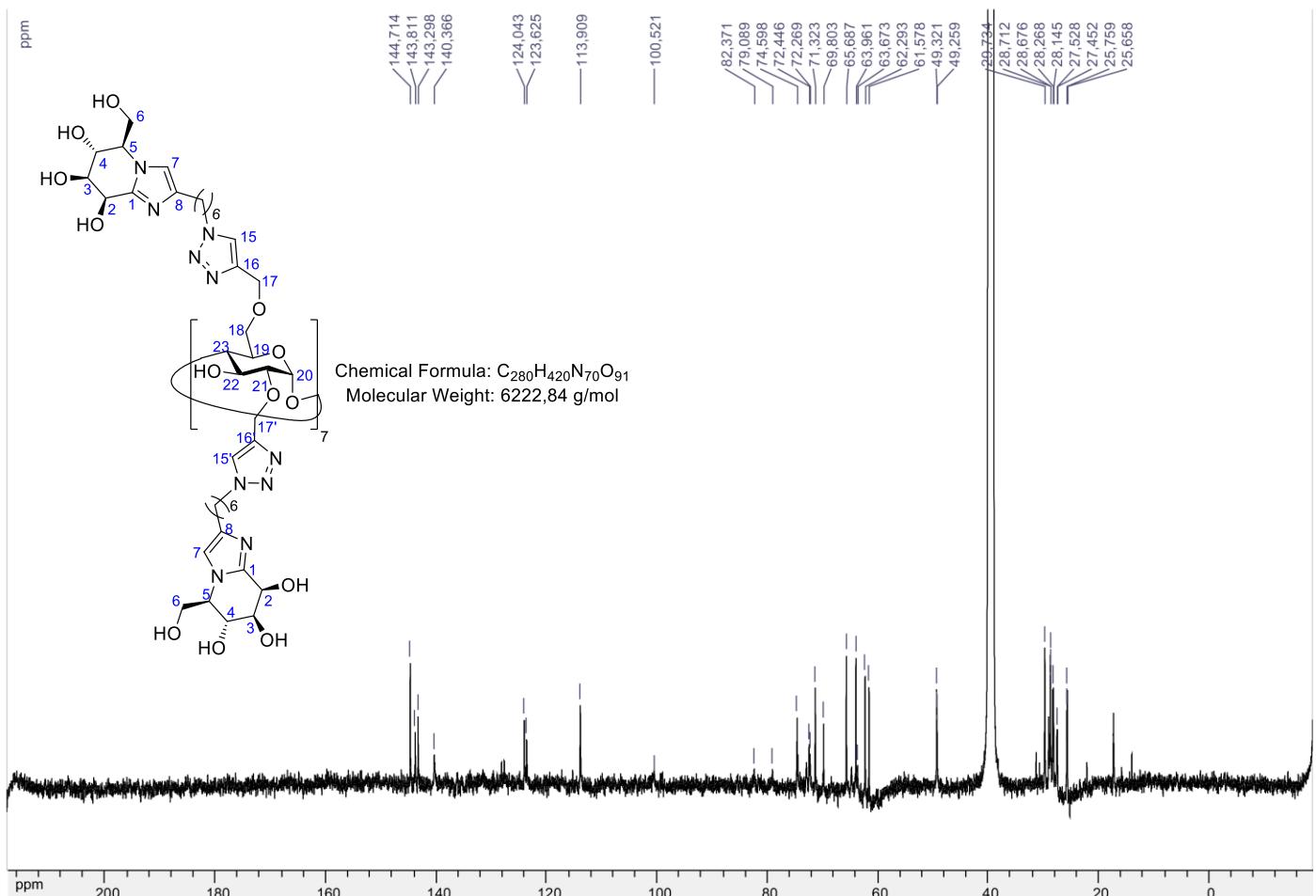


Fig S80. ^{13}C NMR (125 MHz, DMSO-d₆) spectrum of compound 26b

Mass Spectrum HR Report

Analysis Info

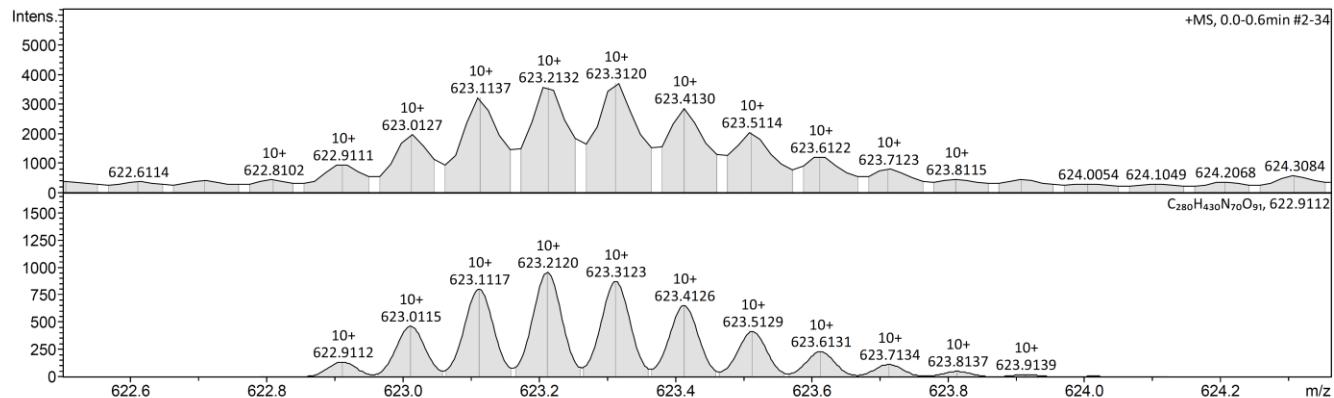
Analysis Name D:\Data\SMasse\2018\10_Octobre 2018\F03021SK.d
 Method Tune_pos_Mid.m
 Sample Name MP0315 BIS
 Comment

Acquisition Date 10/5/2018 2:58:58 PM

Operator BDAL@DE
 Instrument micrOTOF II
 8213750.1045
 1

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 C ₂₈₀ H ₄₃₀ N ₇₀ O ₉₁ 622.911169	0.1	0.3 101.0	ok even	85.5	51.9	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
778.387515 1 C ₂₈₀ H ₄₂₈ N ₇₀ O ₉₁ 778.387142	-0.5	1.1 102.0	ok even	141.7	84.9	n.a.	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

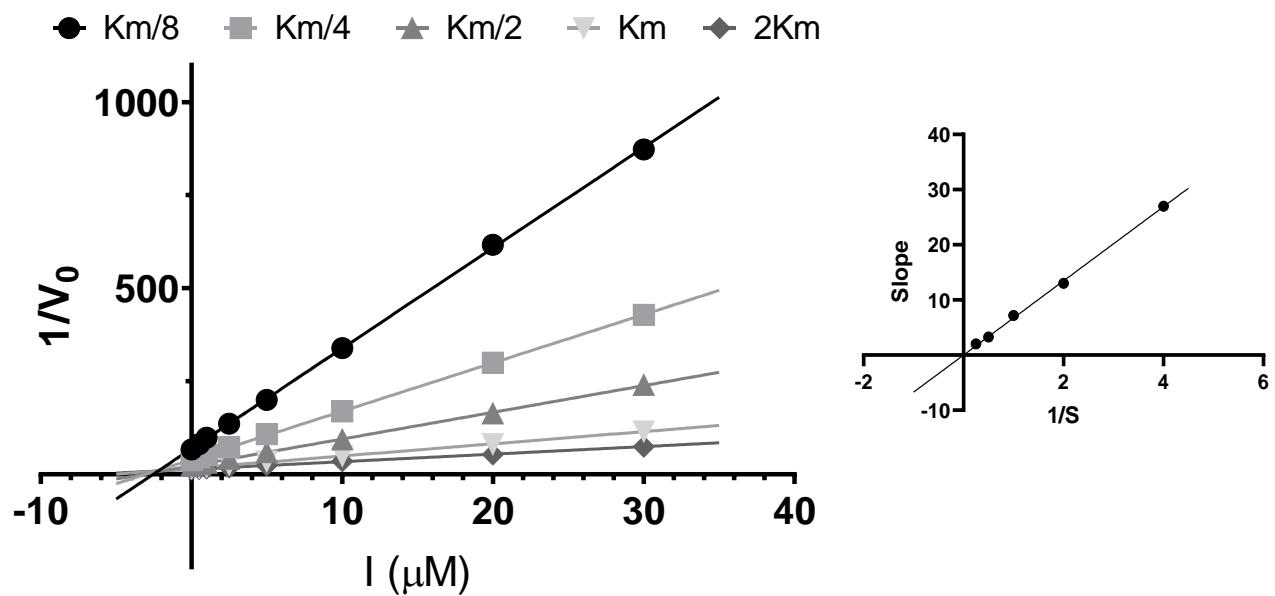


Fig S82. Dixon plot and replot of compound **13a**

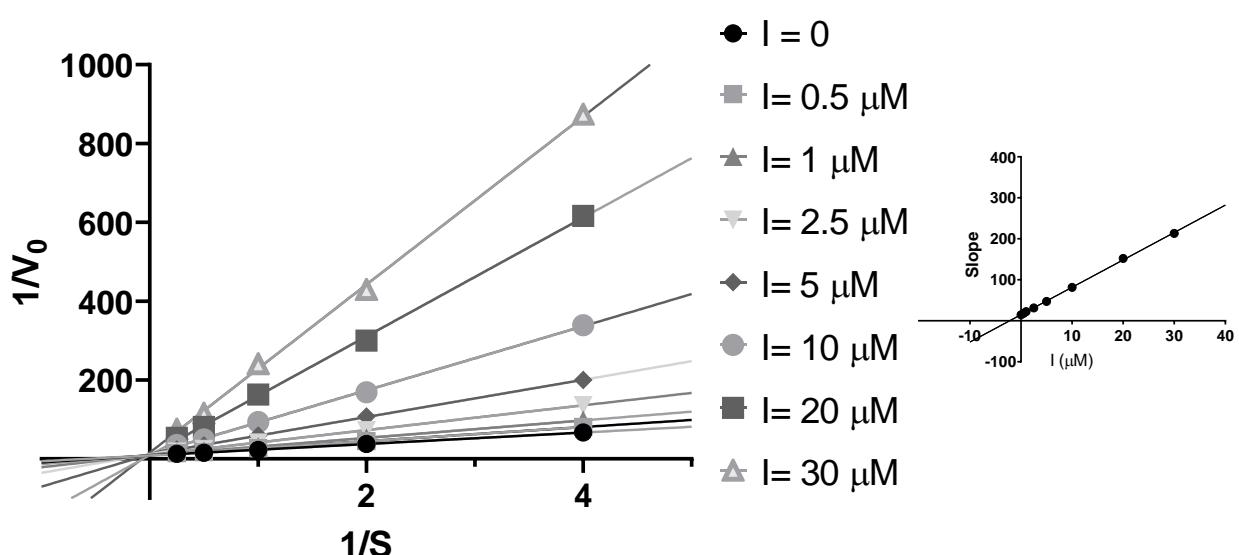


Fig S83. Lineweaver Burk plot and replot for K_i determination
 $(2.23 \pm 0.13 \mu\text{M})$ of compound **13a**

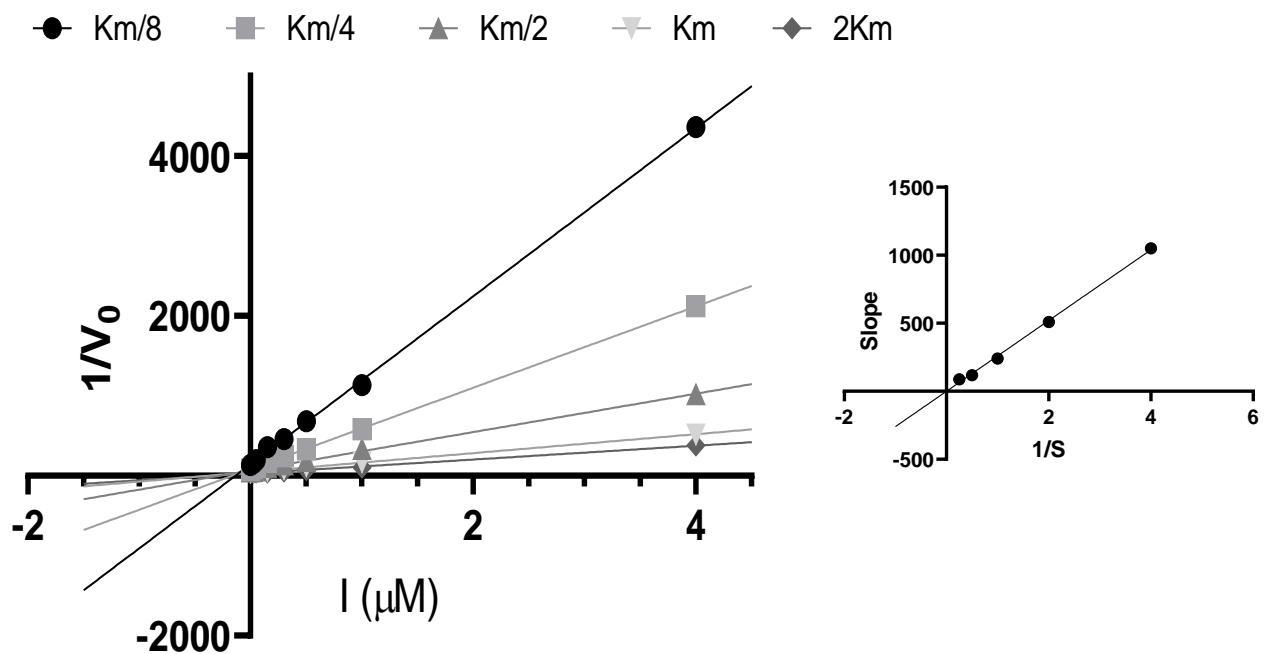


Fig S84. Dixon plot and replot of compound **13b**

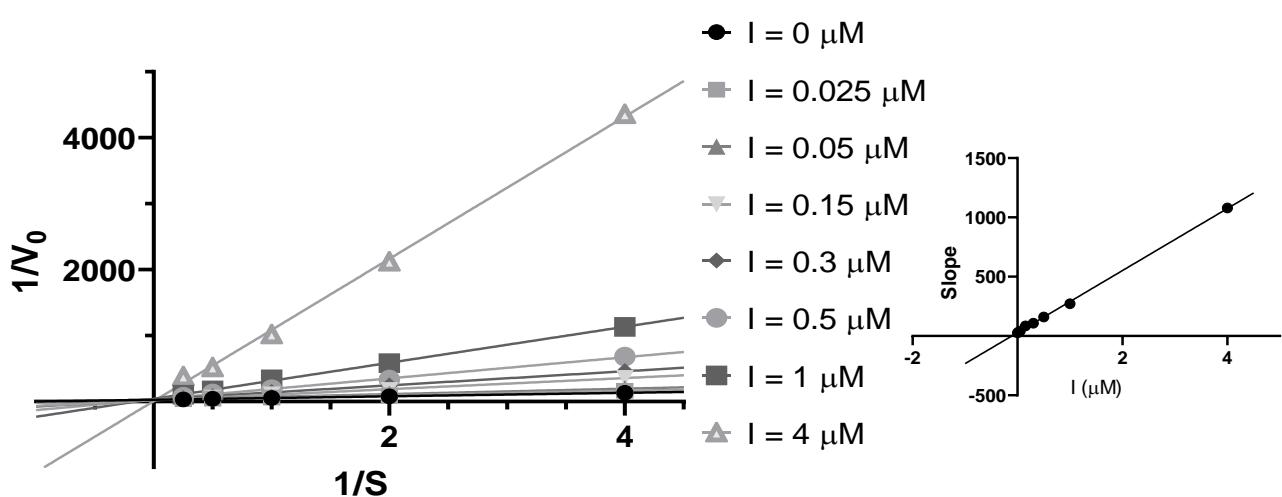


Fig S85. Lineweaver Burk plot and replot for K_i determination
 $(0.11 \pm 0.02 \mu\text{M})$ of compound **13b**

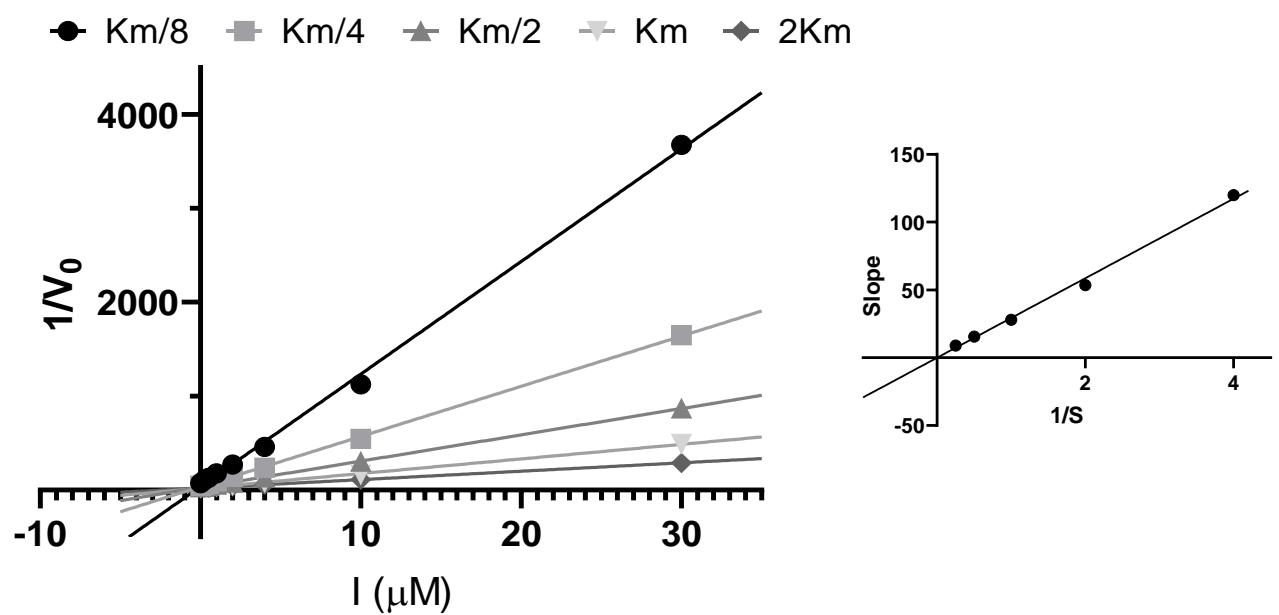


Fig S86. Dixon plot and replot of compound **19a**

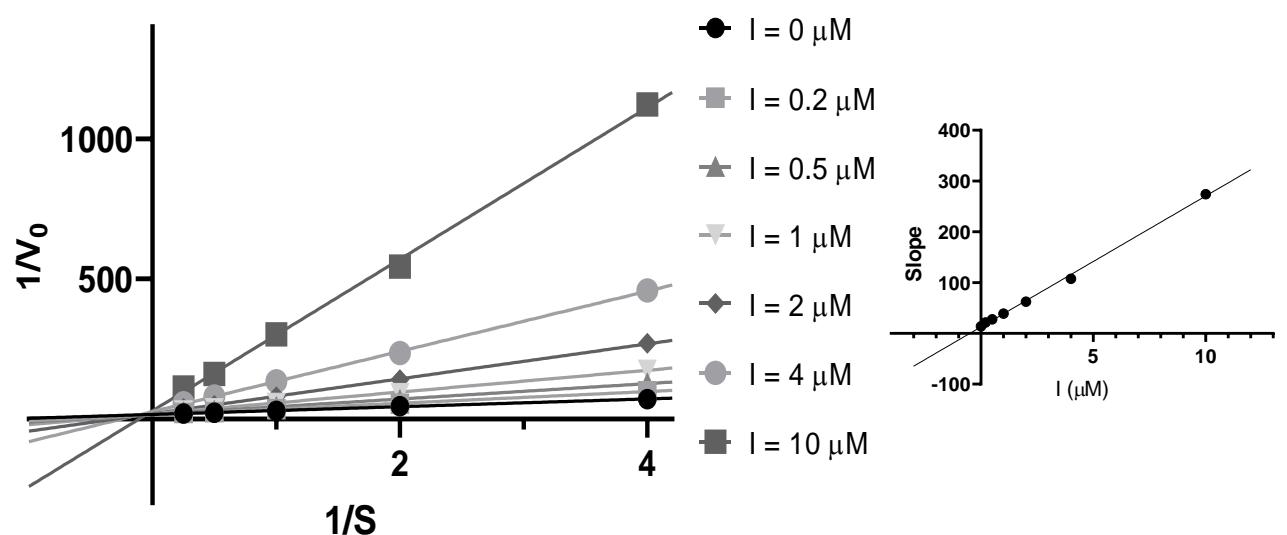


Fig S87. Lineweaver Burk plot and replot for K_i determination ($0.49 \pm 0.64 \mu\text{M}$) of compound **19a**

● Km/8 ■ Km/4 ▲ Km/2 ▽ Km ◆ 2Km

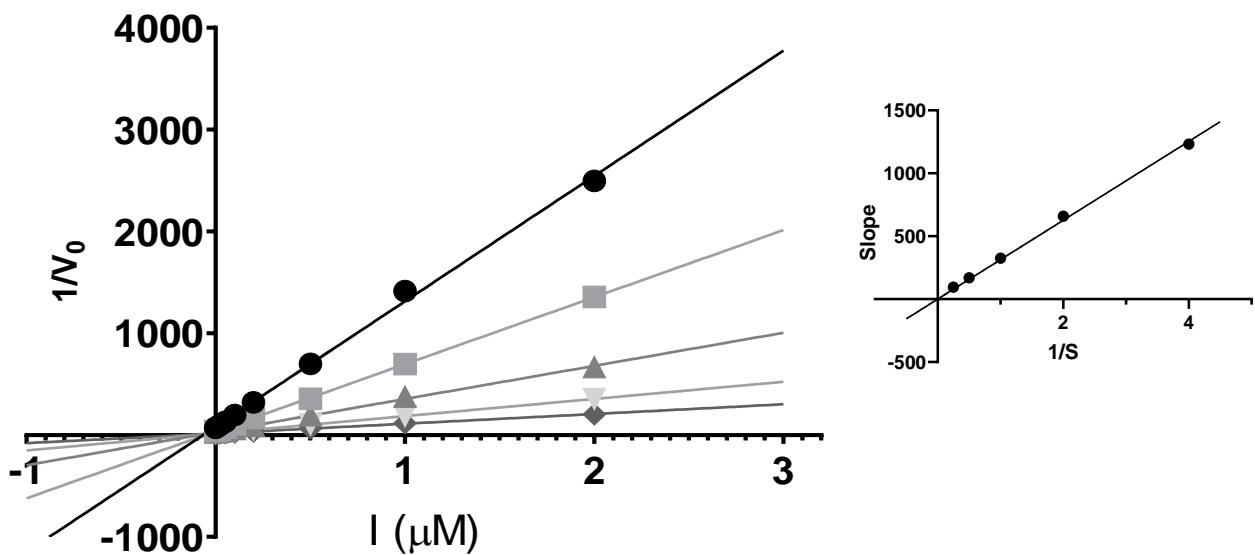


Fig S88. Dixon plot and replot of compound **19b**

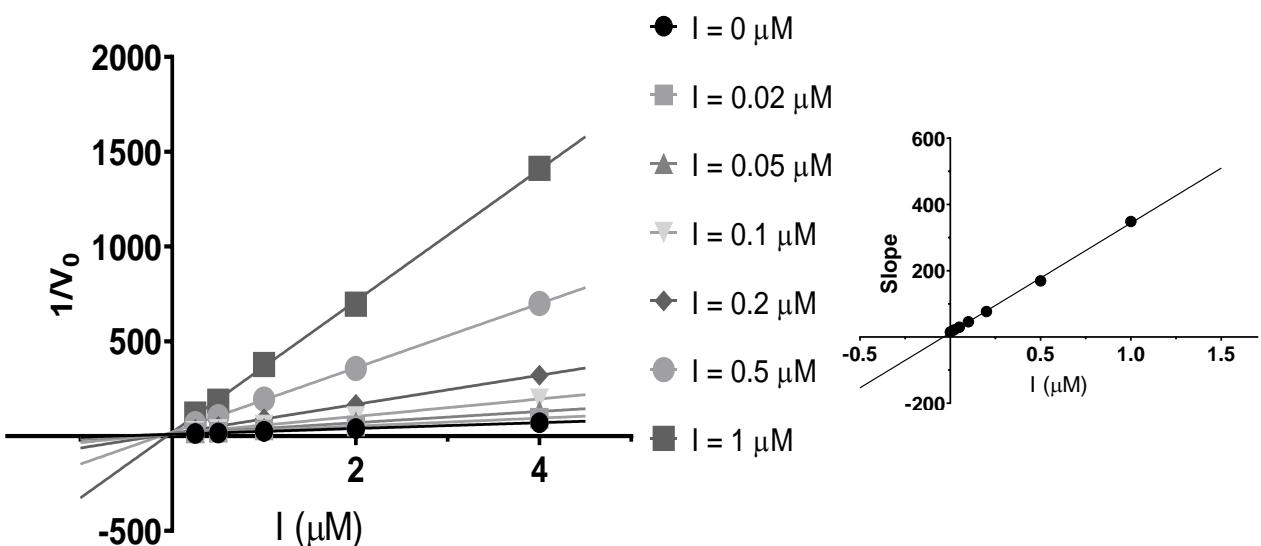


Fig S89. Lineweaver Burk plot and replot for K_i determination
($0.037 \pm 0.007 \mu\text{M}$) of compound **19b**

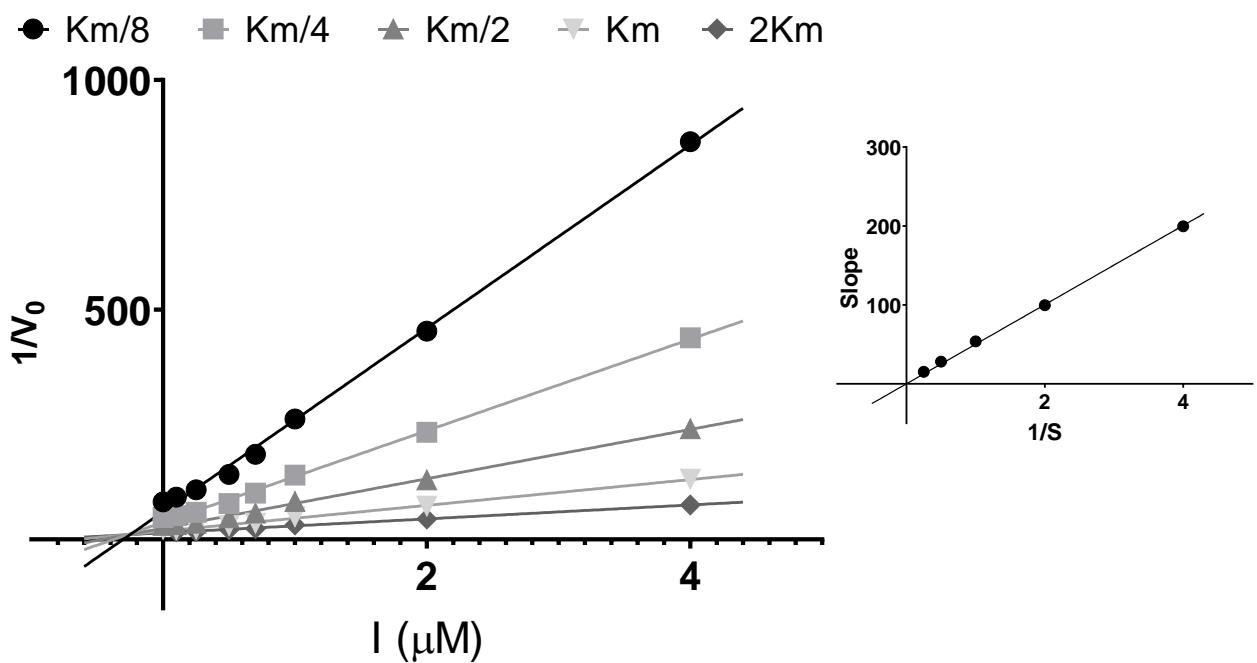


Fig S90. Dixon plot and replot of compound **21a**

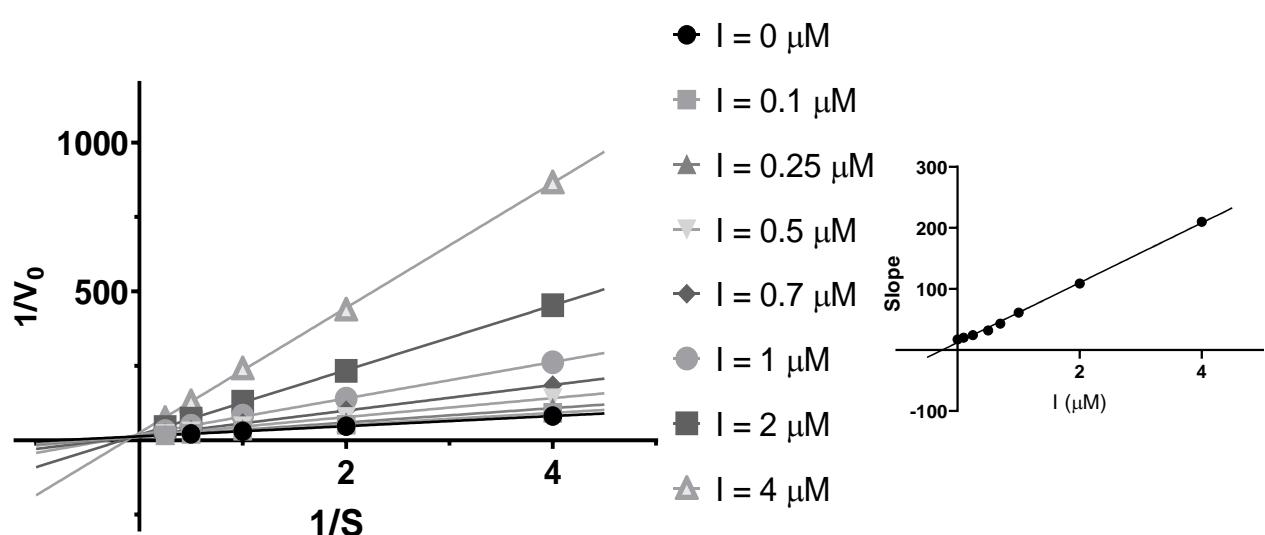


Fig S91. Lineweaver Burk plot and replot for K_i determination ($0.25 \pm 0.03 \mu\text{M}$) of compound **21a**

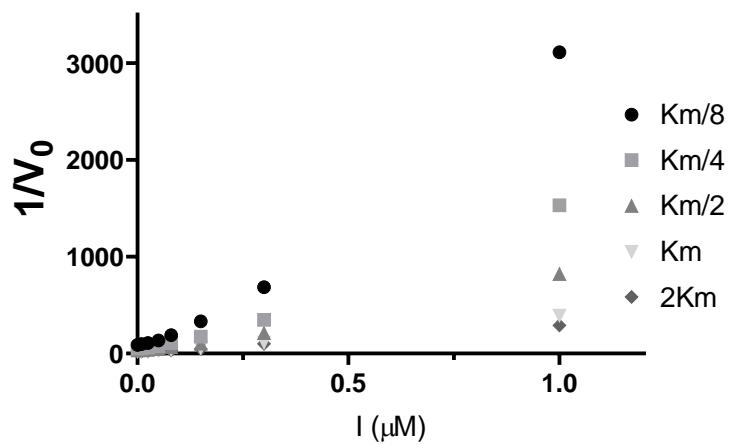


Fig S92. Dixon plot of compound **21b**

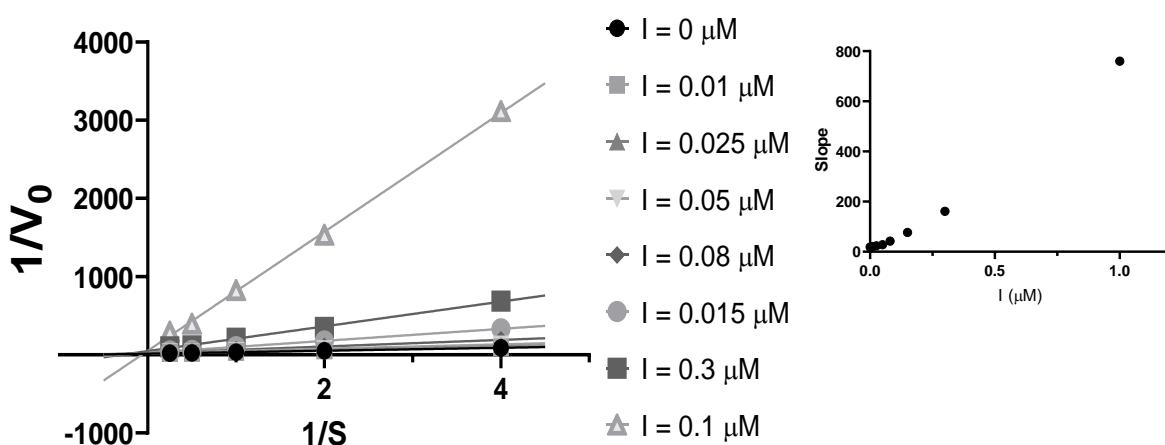


Fig S93. Lineweaver Burk plot and replot of compound **21b**

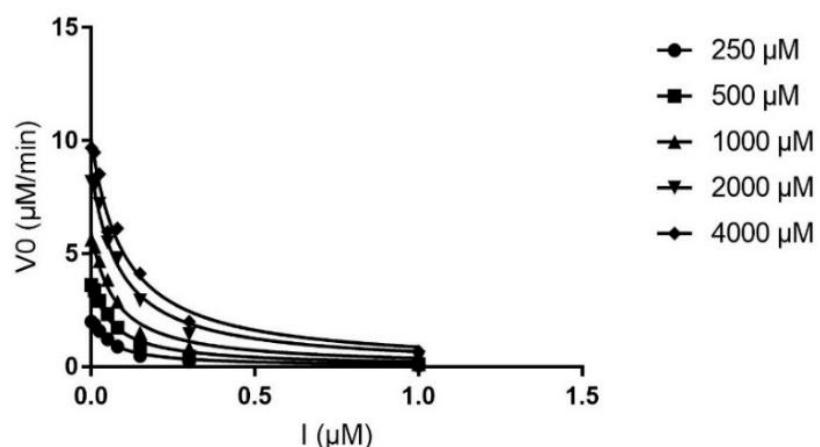


Fig S94. Plot of enzyme velocity as a function of inhibitor **21b** concentration.

The solid curves drawn through the data points represent the best fit to the Morrison equation used to obtain K_i value ($0.037 \pm 0.010 \mu\text{M}$) for the tight binding inhibitor **21b**

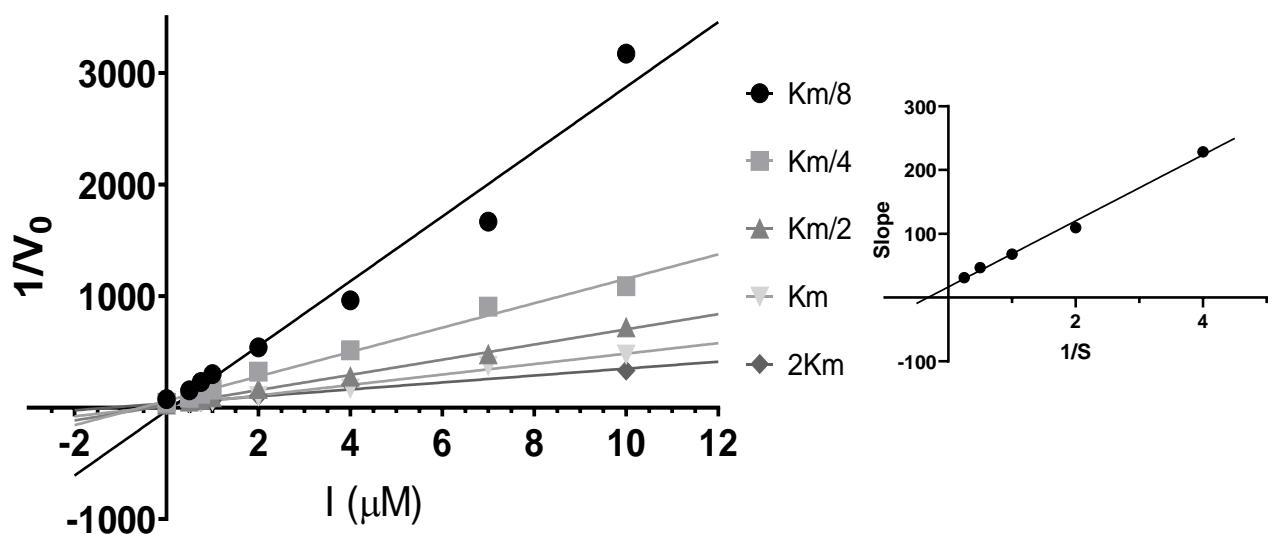


Fig S95. Dixon plot and replot of compound 23a

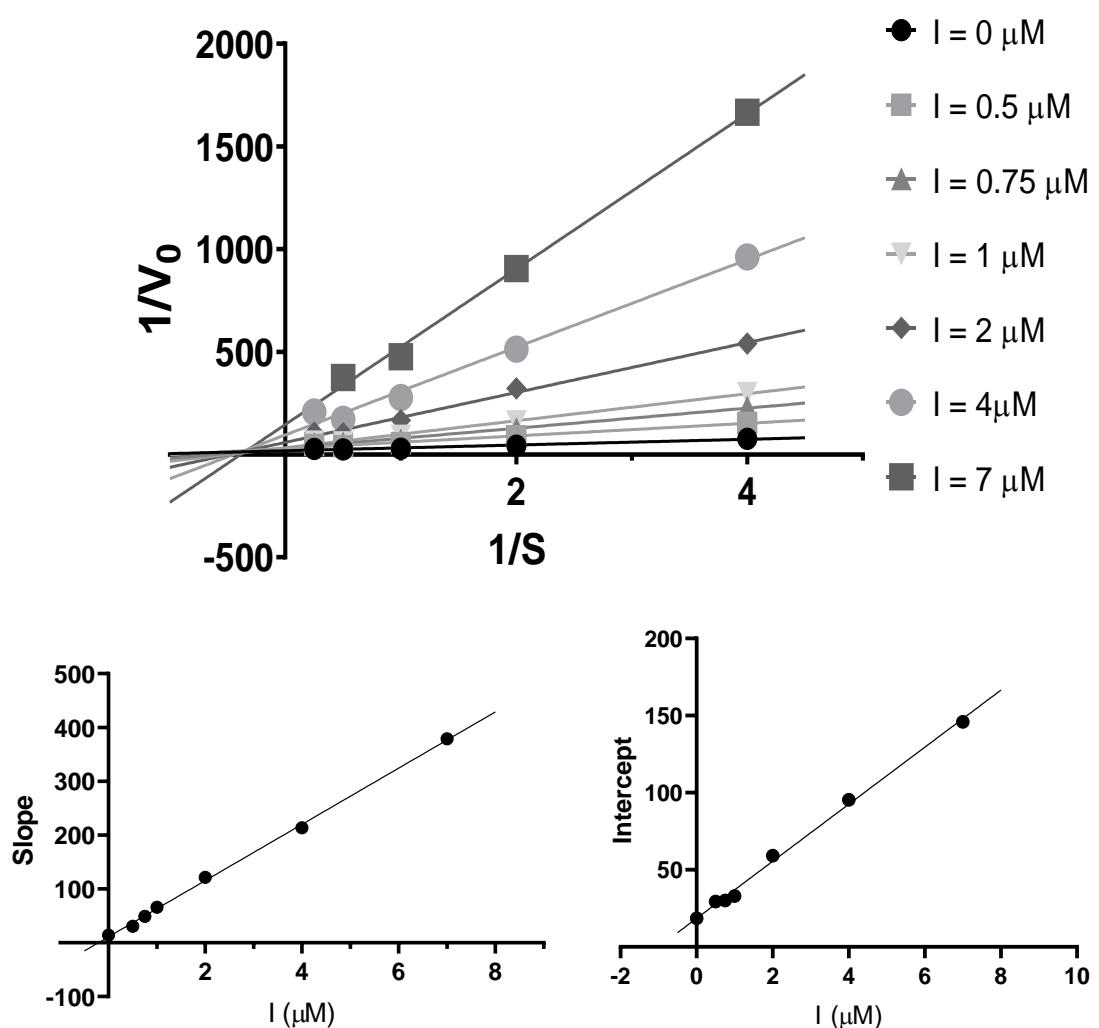


Fig S96. Lineweaver Burk plot, slope and intercept replots of reciprocal plot data for K_i determination ($K_i = 0.21 \pm 0.05 \mu\text{M}$; $K'_i = 1.00 \pm 0.096 \mu\text{M}$) of compound 23a

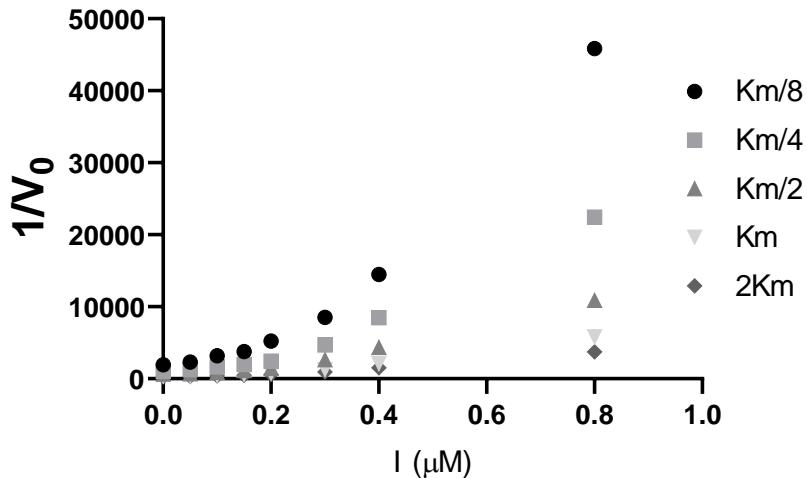


Fig S97. Dixon plot of compound **23b**

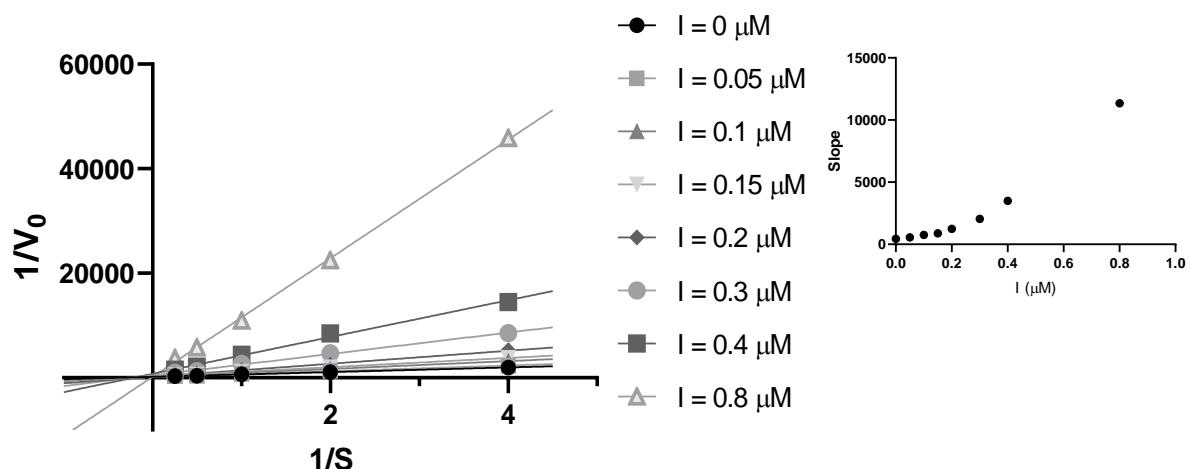


Fig S98. Lineweaver Burk plot and replot of compound **23b**

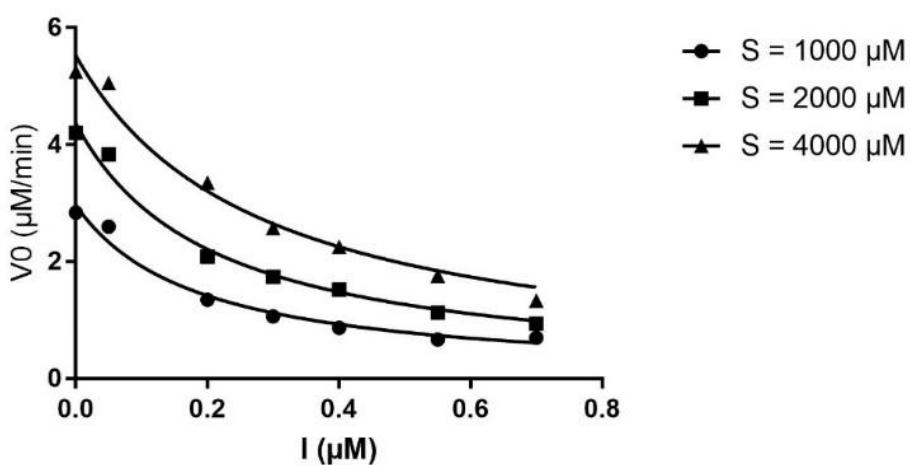


Fig S99. Plot of enzyme velocity as a function of inhibitor **23b** concentration.

The solid curves drawn through the data points represent the best fit to the Morrison equation used to obtain K_i value ($0.091 \pm 0.017 \mu\text{M}$) for the tight binding inhibitor **23b**

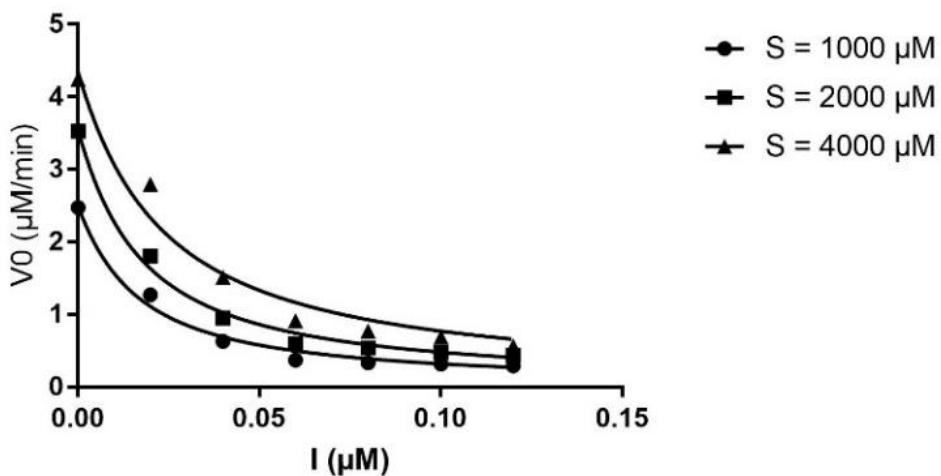


Fig S100. Plot of enzyme velocity as a function of inhibitor **26a** concentration.
The solid curves drawn through the data points represent the best fit to the Morrison equation used to obtain K_i value
($0.006 \pm 0.001 \mu\text{M}$) for the tight binding inhibitor **26a**

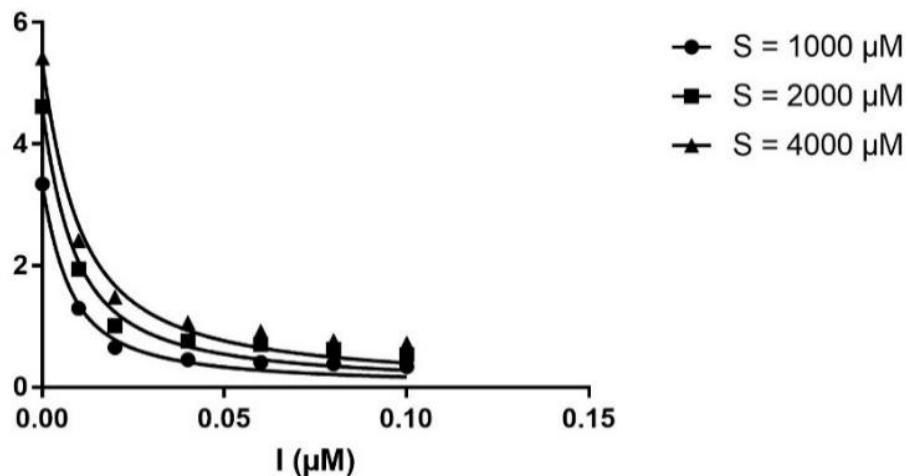


Fig S101. Plot of enzyme velocity as a function of inhibitor **26b** concentration.
The solid curves drawn through the data points represent the best fit to the Morrison equation used to obtain K_i value
($0.002 \pm 0.0005 \mu\text{M}$) for the tight binding inhibitor **26b**