

Supporting Information

Scalable synthesis of the unusual amino acid segment (ADMOA unit) of marine anti-inflammatory peptide: solomonamide A

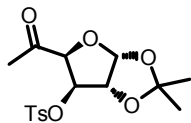
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E-mail: srivaric@iict.res.in

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^1H NMR, 300 MHz, CDCl_3

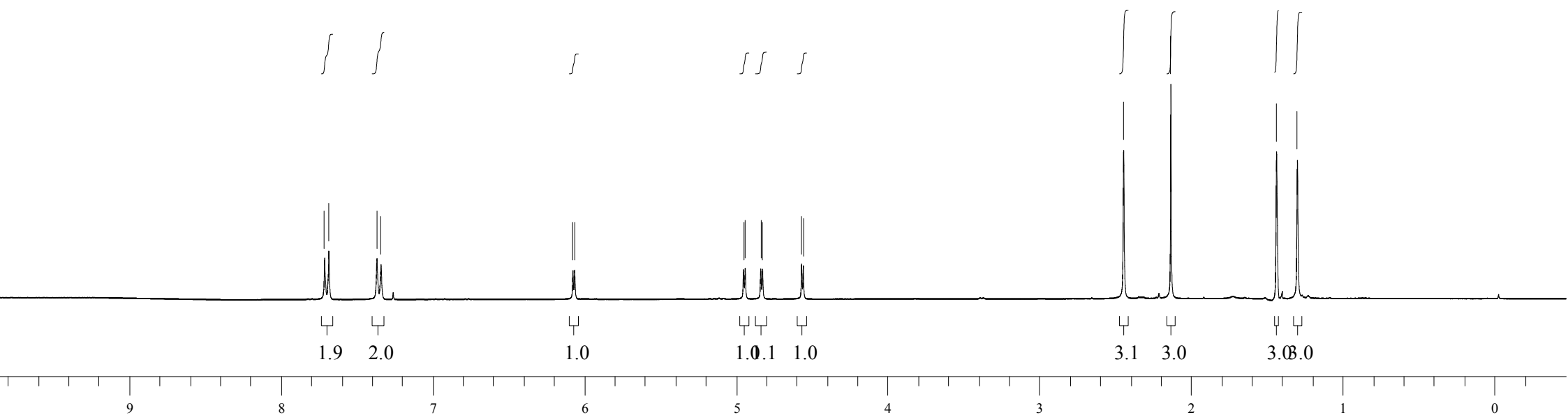
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7.339

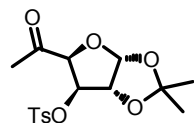
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4.824
4.567
4.556

2.444
2.133

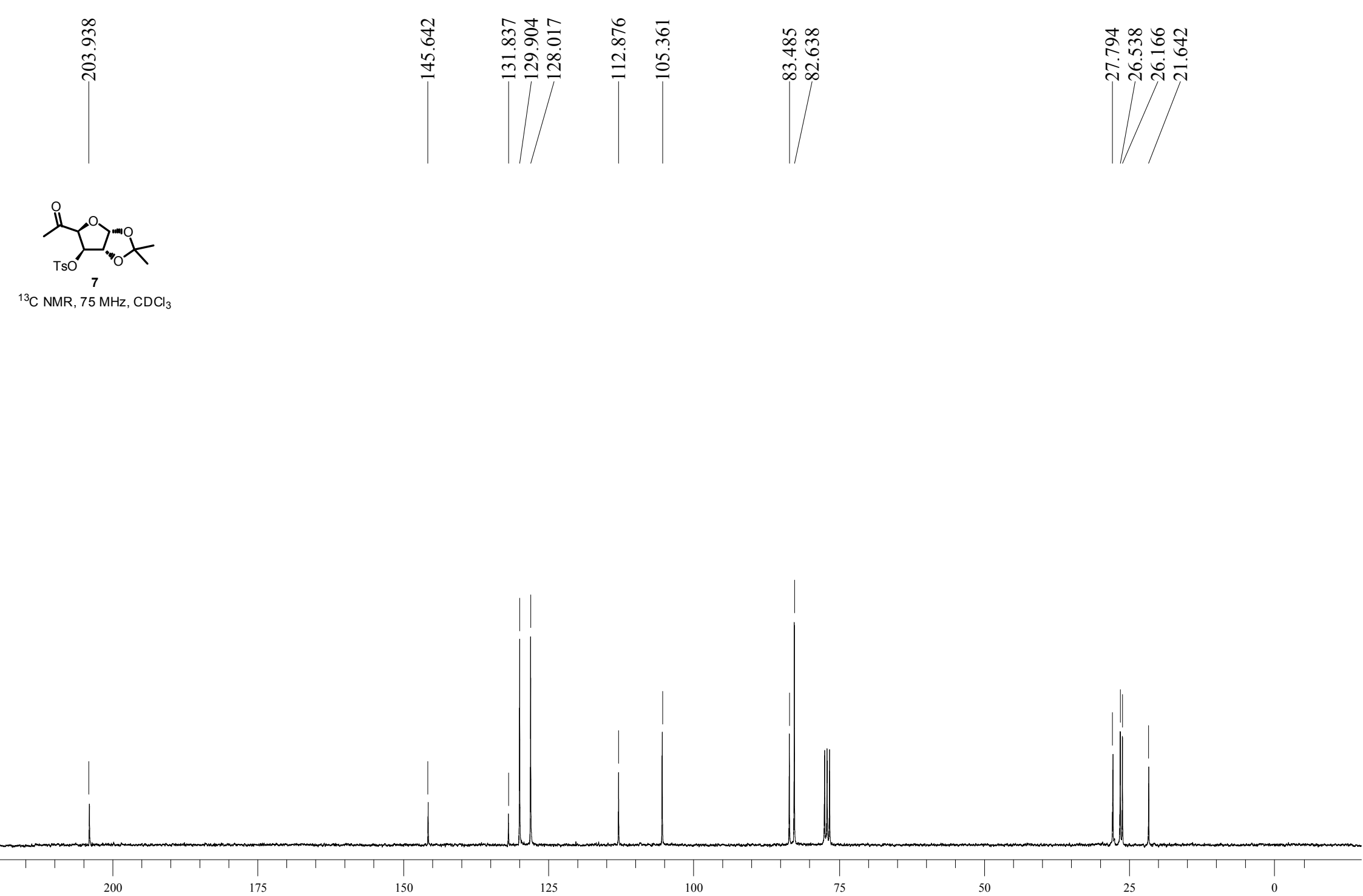
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1.299





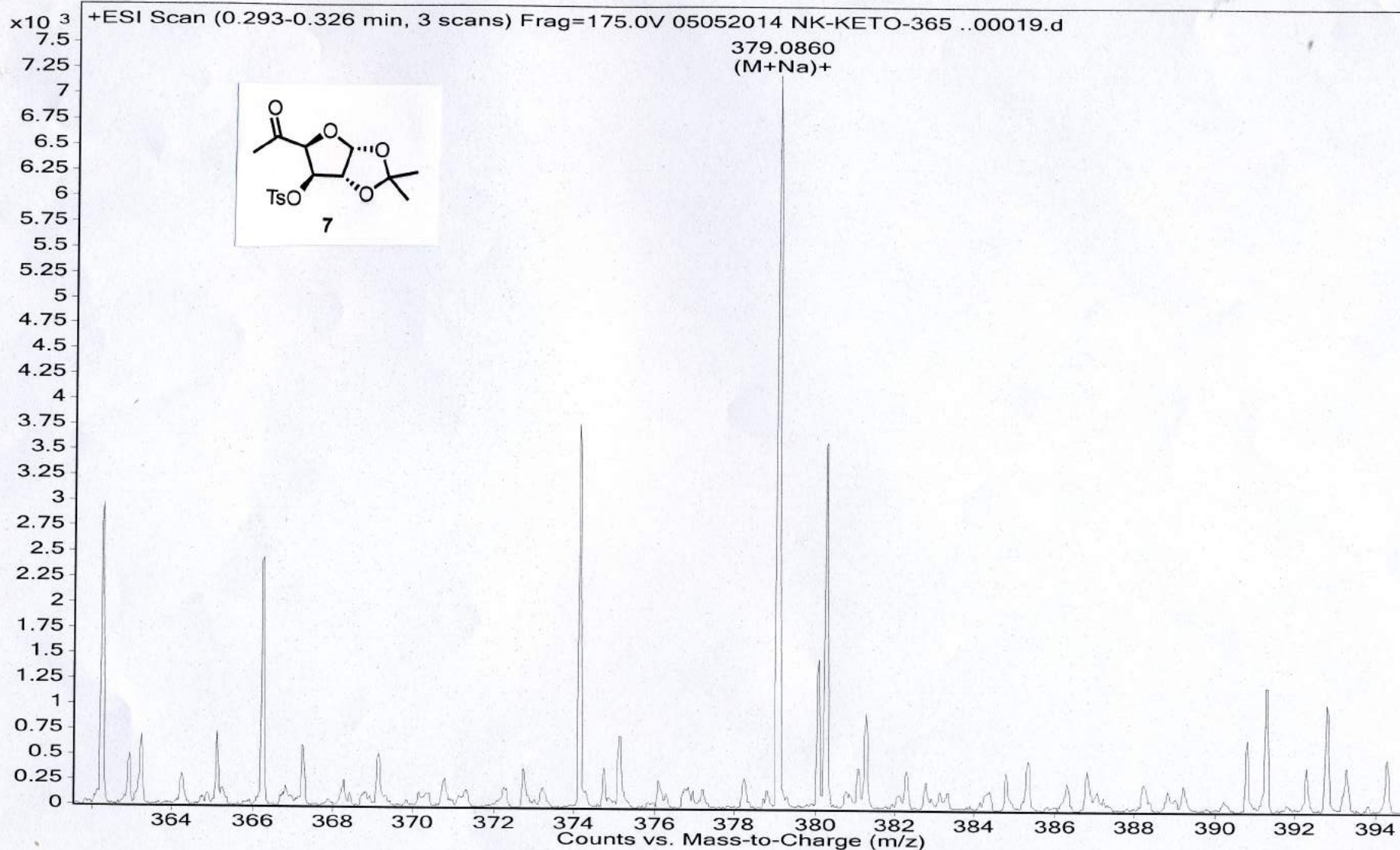
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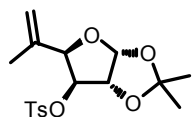
^{13}C NMR, 75 MHz, CDCl_3



m/z	Ion	Formula	Abundance
379.086	(M+Na)+	C ₁₆ H ₂₀ NaO ₇ S	7288.7

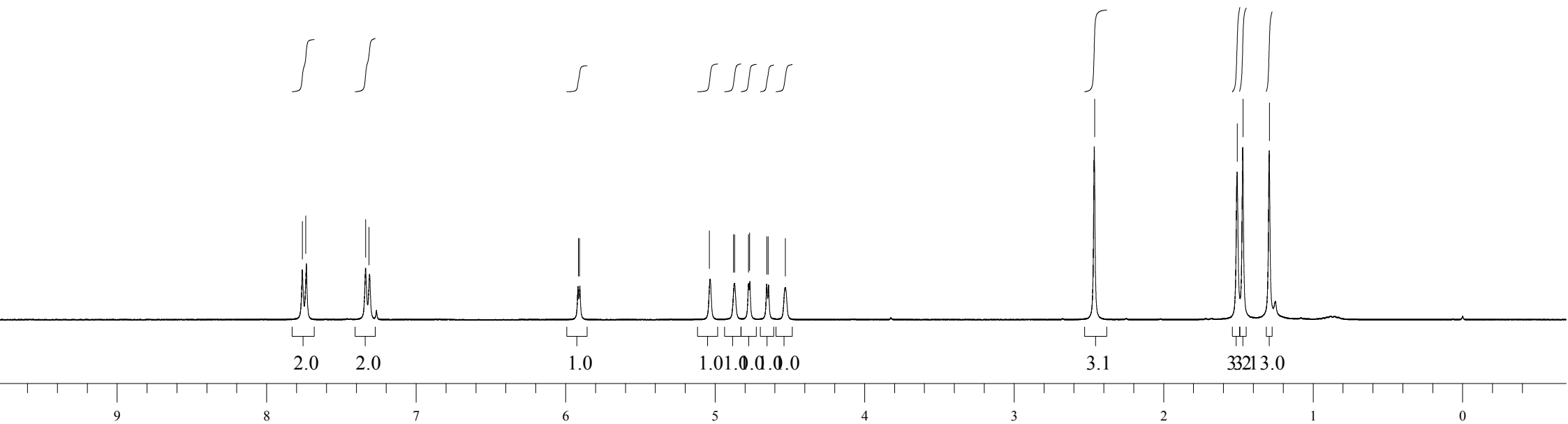
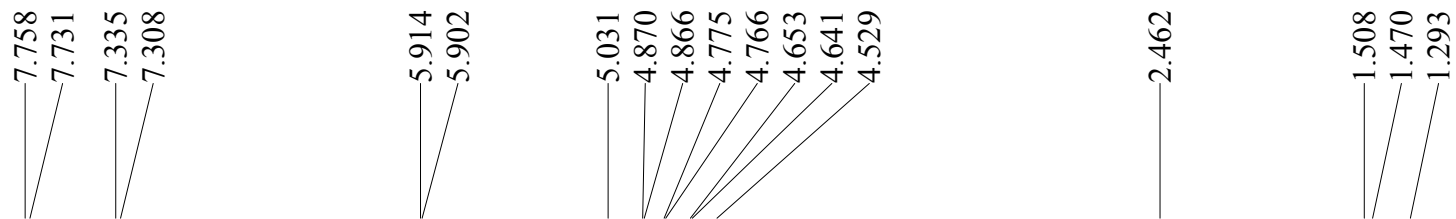
Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross Score	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DBE
✓	C ₁₆ H ₂₀ O ₇ S	C ₁₆ H ₂₀ NaO ₇ S	379.0822	64.55		356.0968	356.093	-10.67	10.67	91.47	75.78	42.79	379.086	7

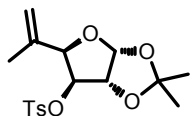




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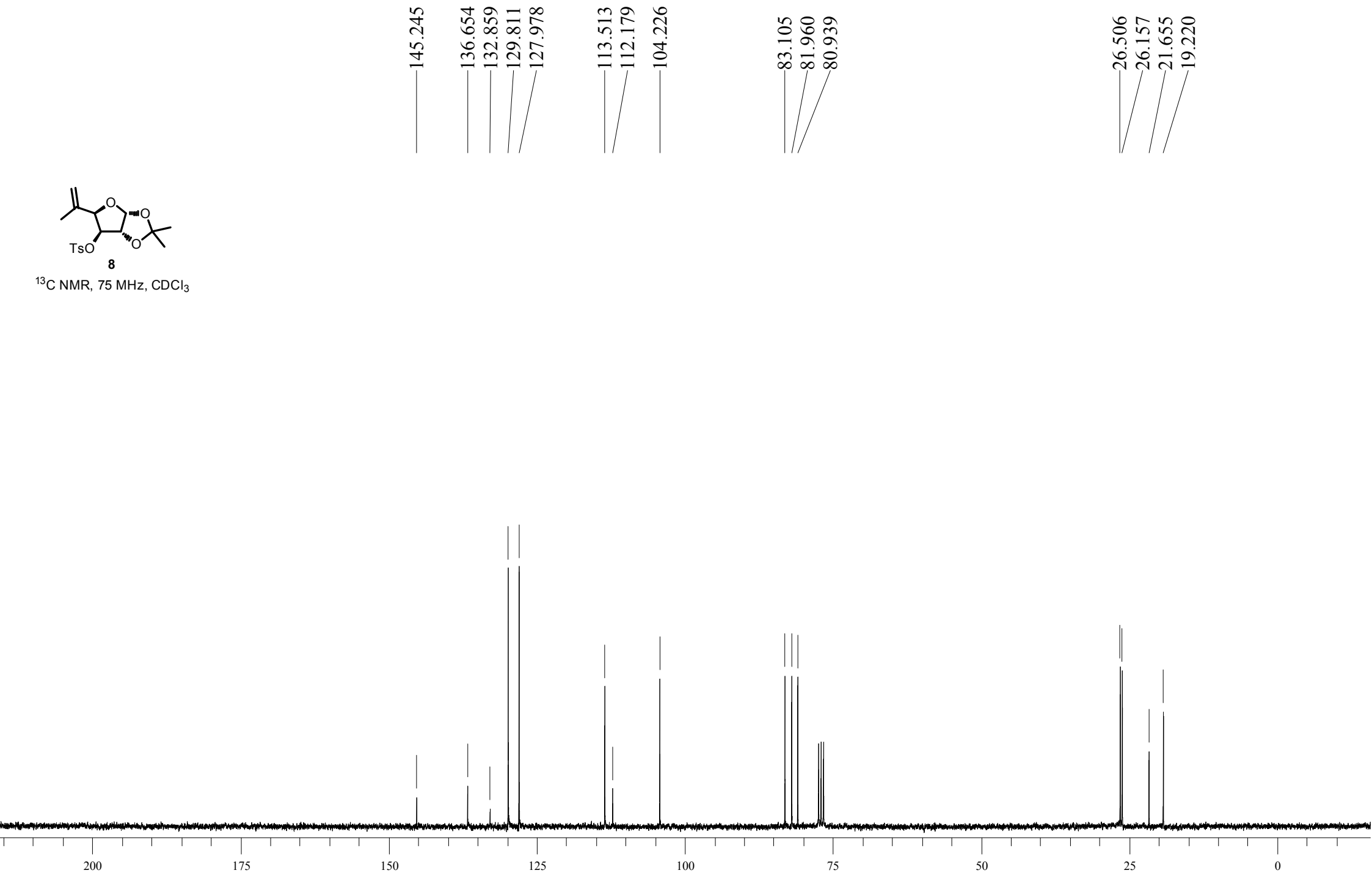
^1H NMR, 300 MHz, CDCl_3



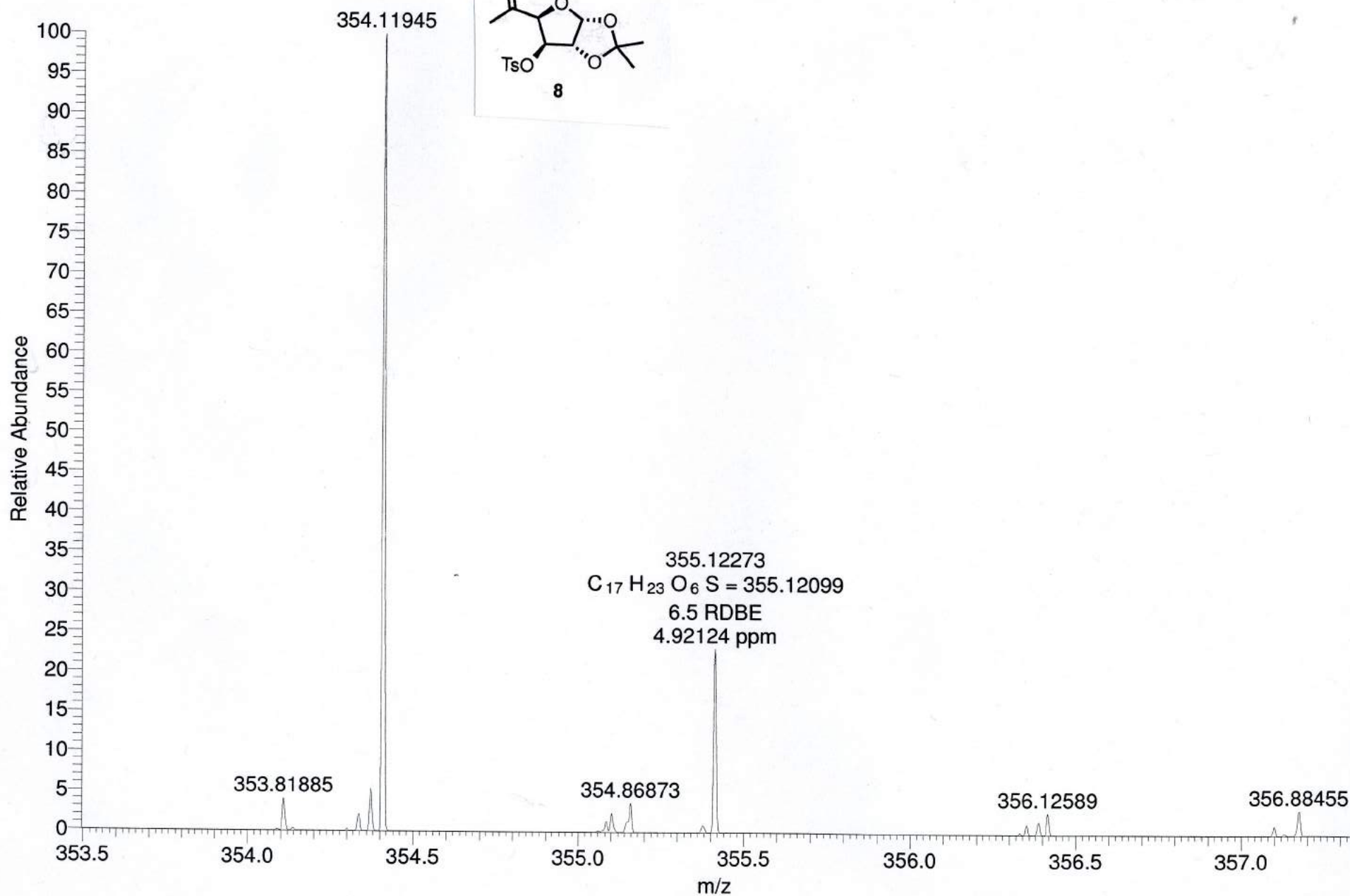


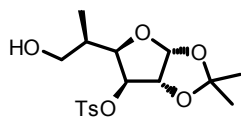
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^{13}C NMR, 75 MHz, CDCl_3



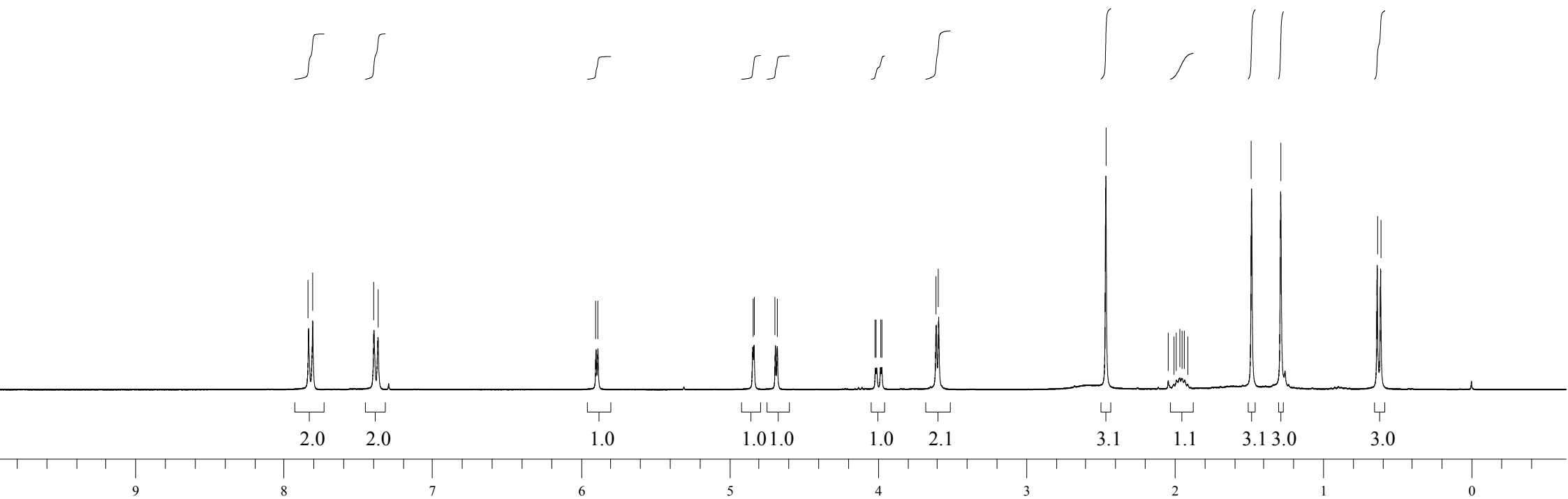
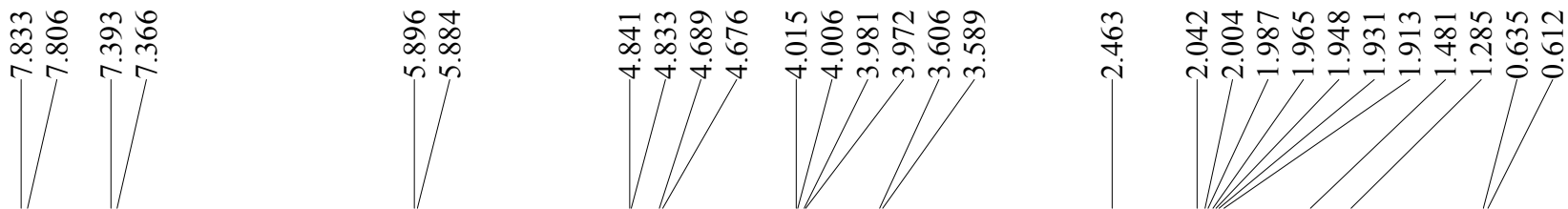
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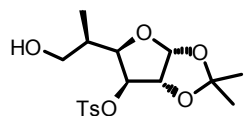




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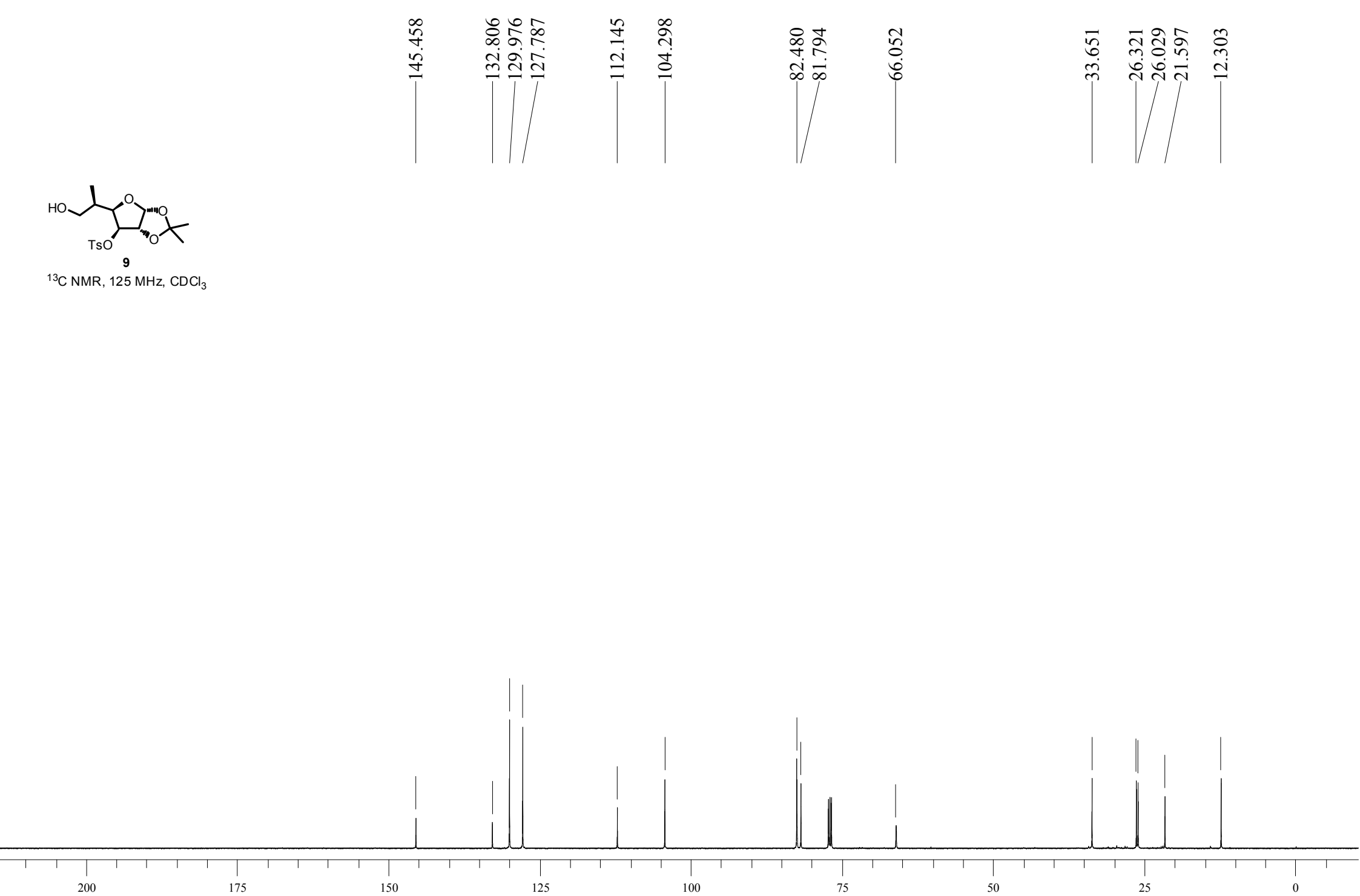
^1H NMR, 300 MHz, CDCl_3





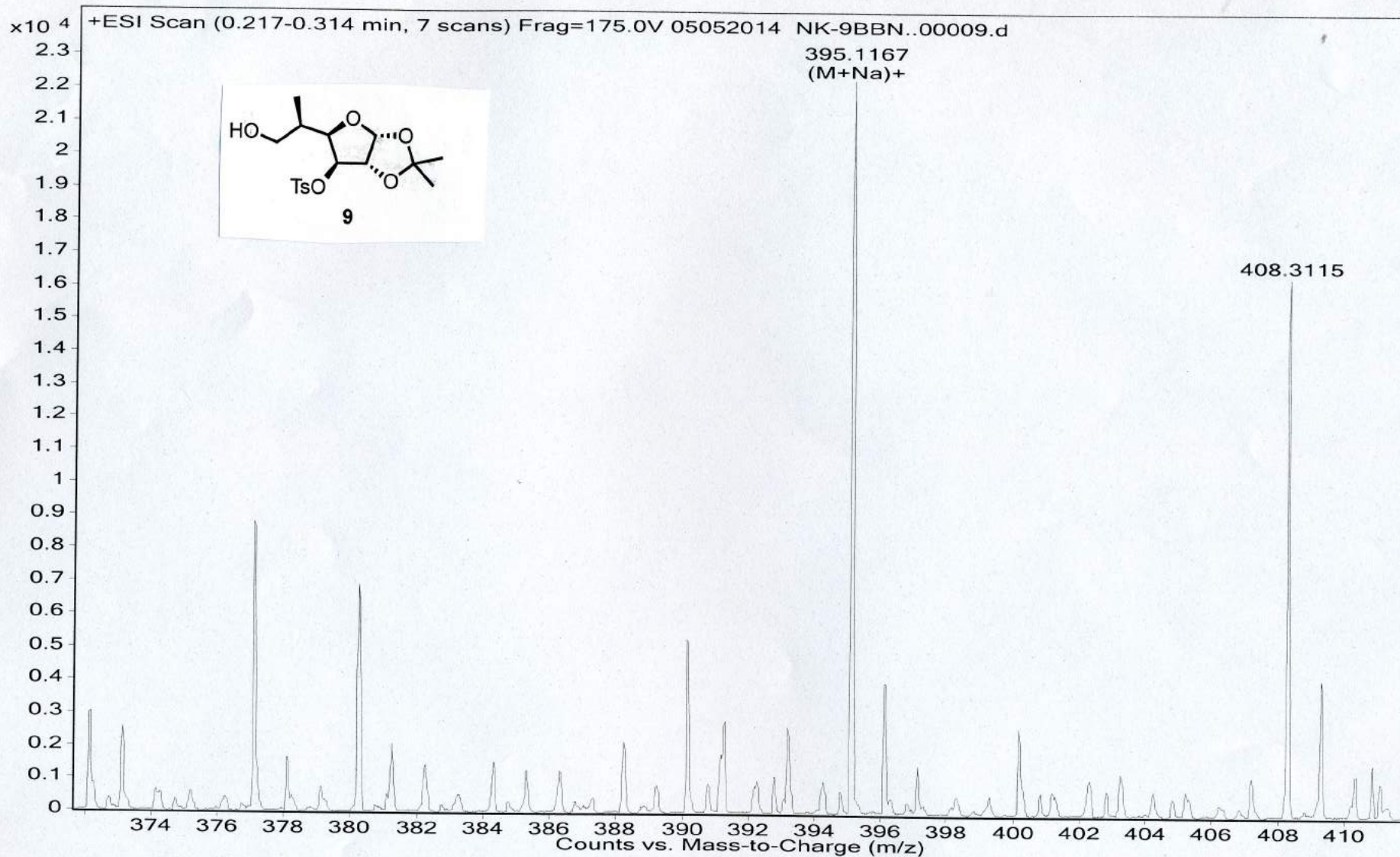
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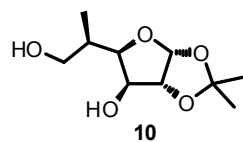
^{13}C NMR, 125 MHz, CDCl_3



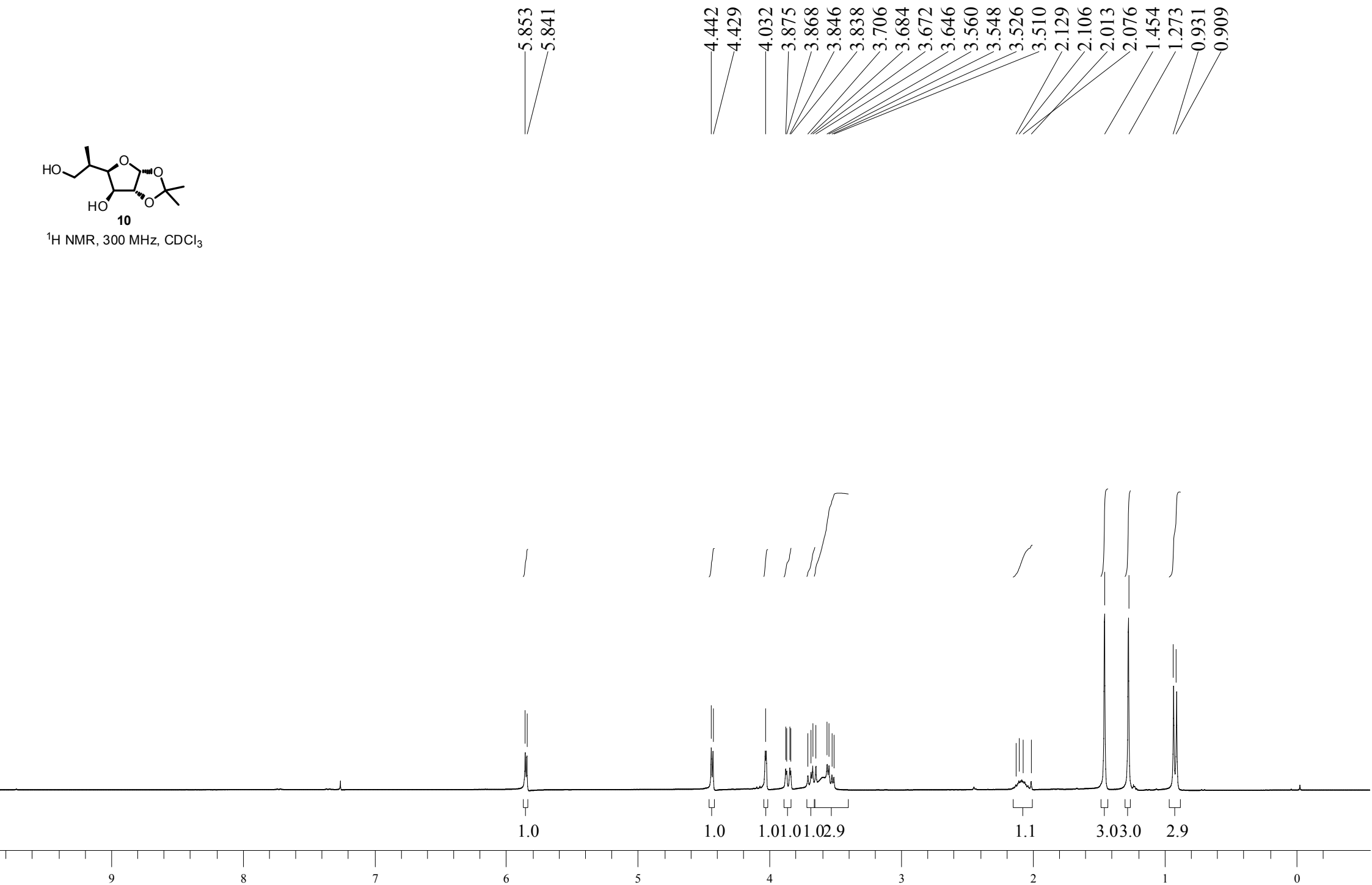
m/z	Ion	Formula	Abundance
395.1167	(M+Na) ⁺	C ₁₇ H ₂₄ NaO ₇ S	22536.3

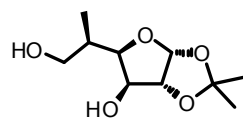
Best	Formula (M)	Ion Formula	Calc. m/z	Score	Cross Score	Mass	Calc. Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DBE
✓	C ₁₇ H ₂₄ O ₇ S	C ₁₇ H ₂₄ NaO ₇ S	395.1135	75.07		372.1275	372.1243	-8.73	8.73	96.96	88.57	55.17	395.1167	6





^1H NMR, 300 MHz, CDCl_3





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^{13}C NMR, 125 MHz, CDCl_3

111.388

104.347

84.667

84.242

74.559

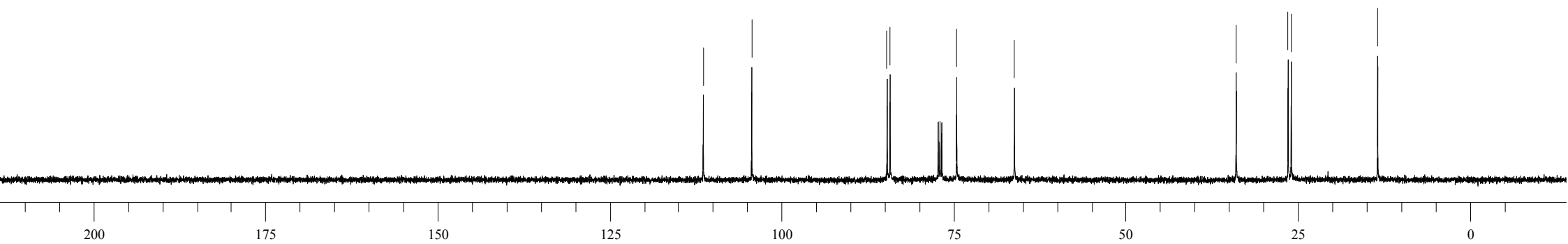
66.176

33.948

26.400

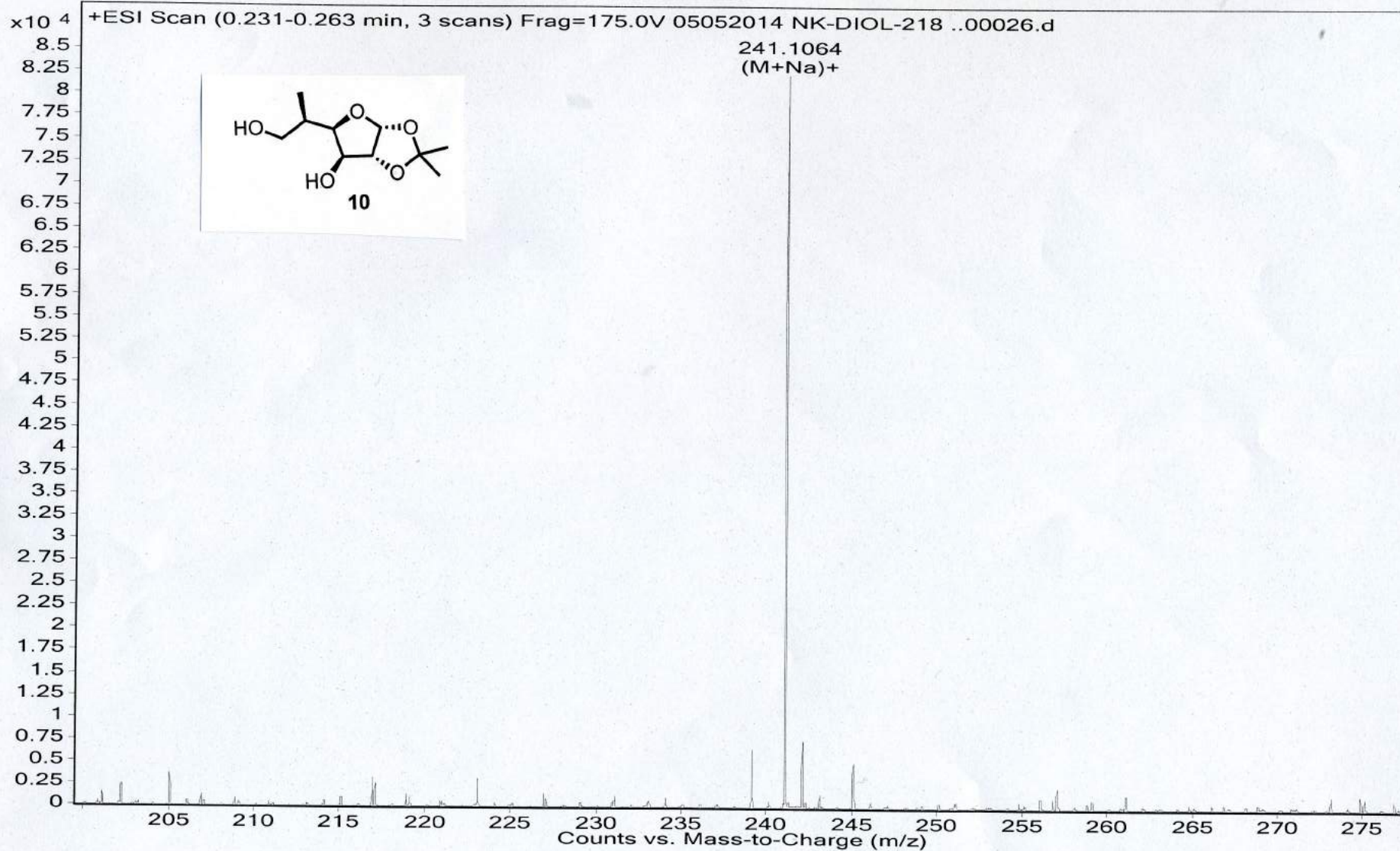
25.938

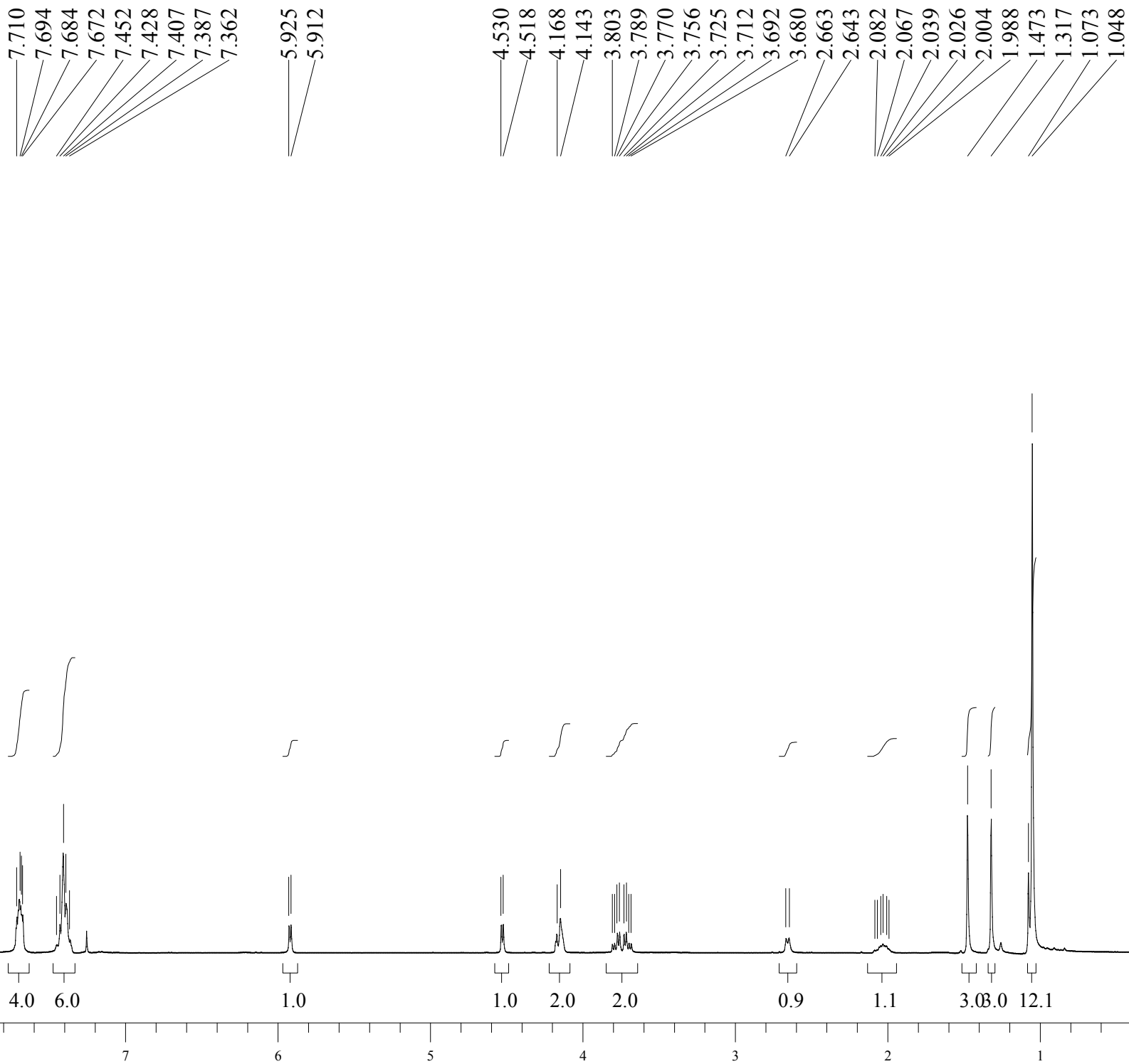
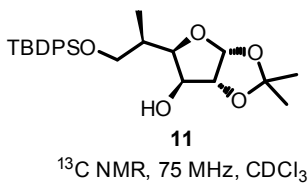
13.387

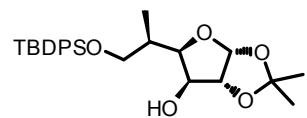


m/z	Ion	Formula	Abundance
241.1064	(M+Na)+	C ₁₀ H ₁₈ NaO ₅	82937.3

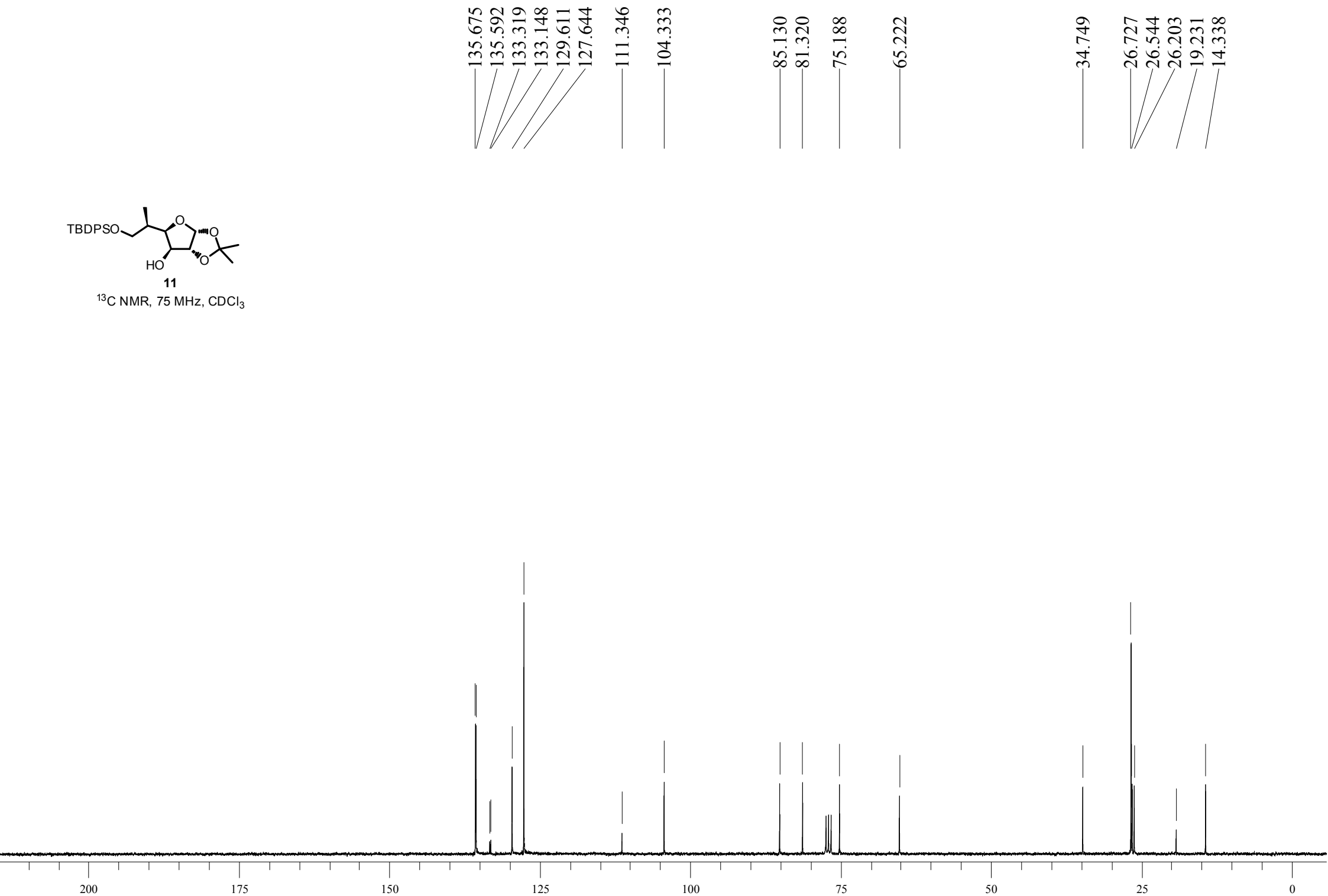
Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross Score	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DBE
☒	C ₁₀ H ₁₈ O ₅	C ₁₀ H ₁₈ NaO ₅	241.1046	83.42		218.1172	218.1154	-7.95	7.95	97.08	80.85	76.51	241.1064	2





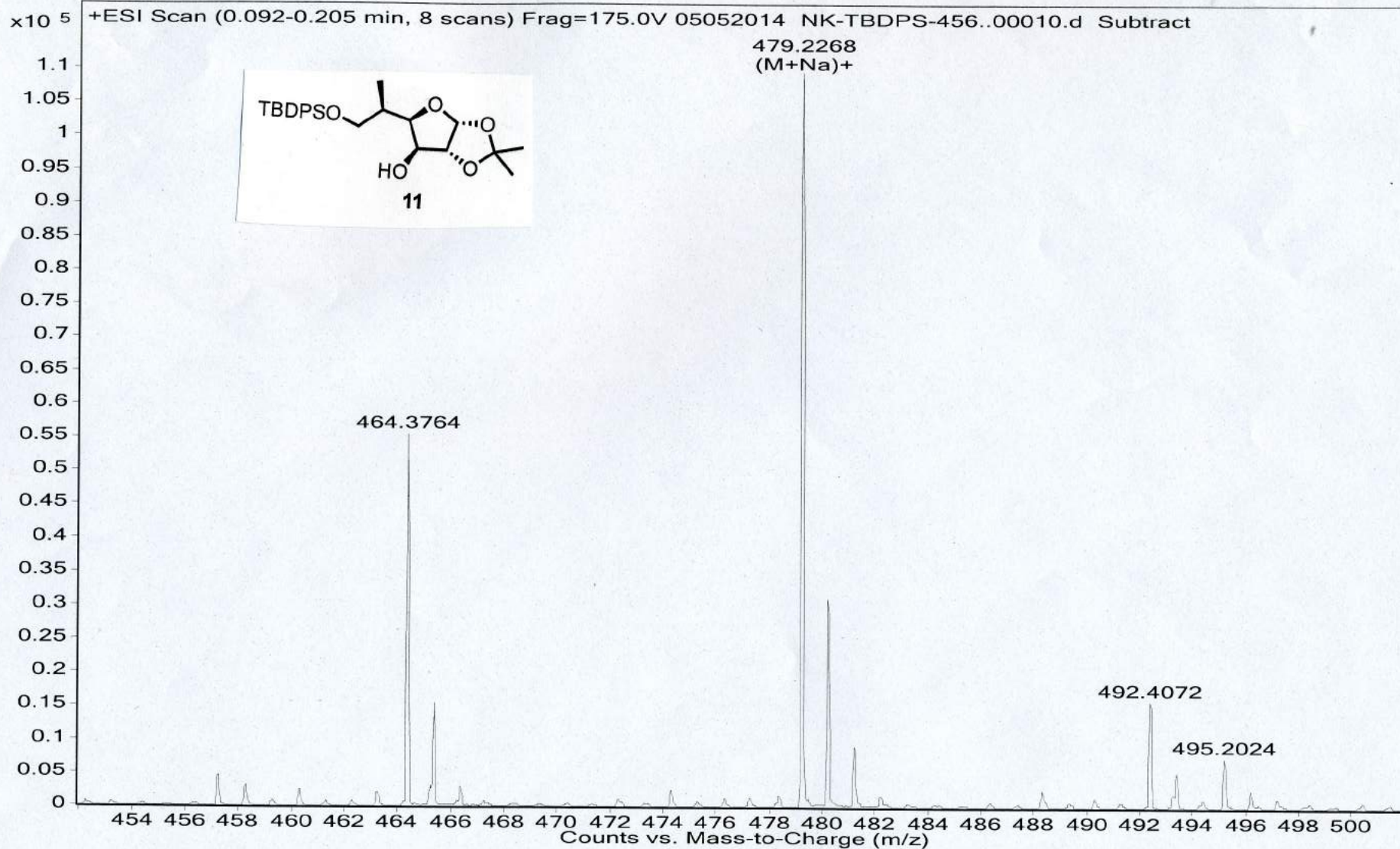


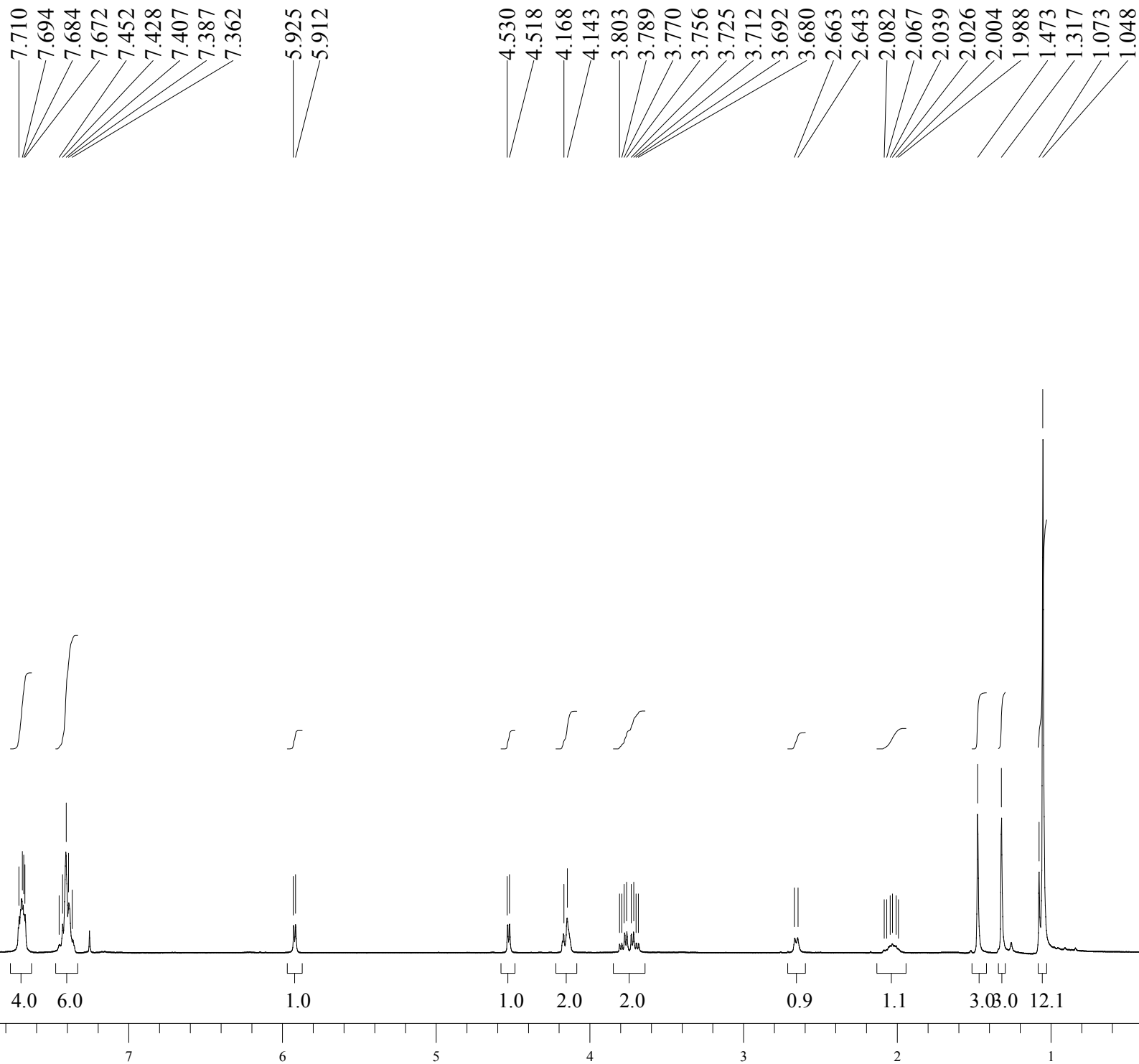
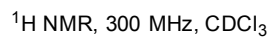
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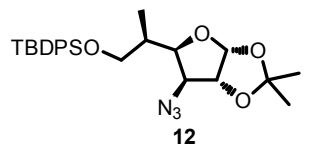
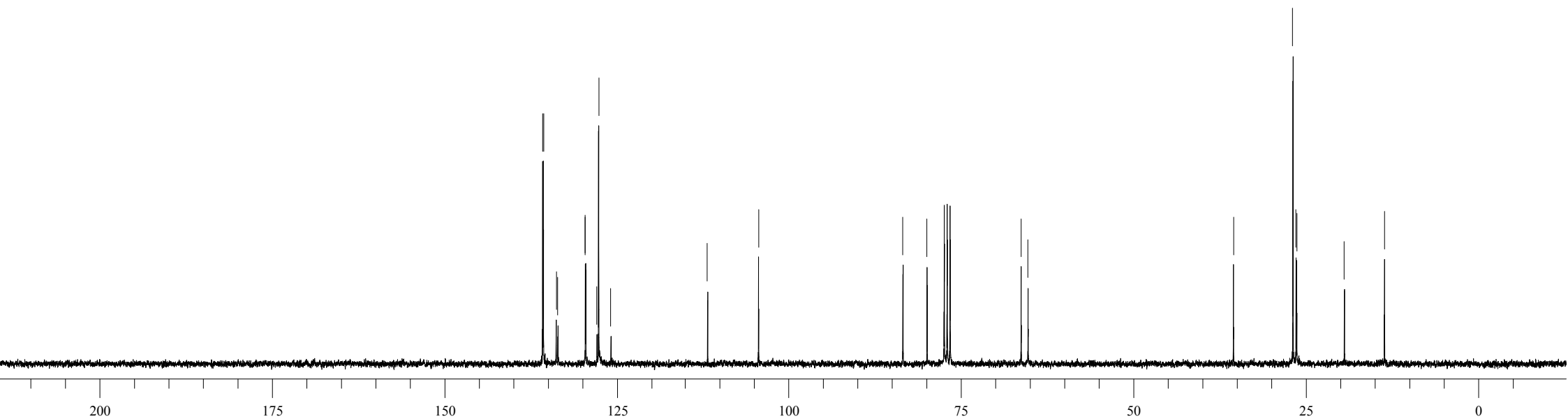
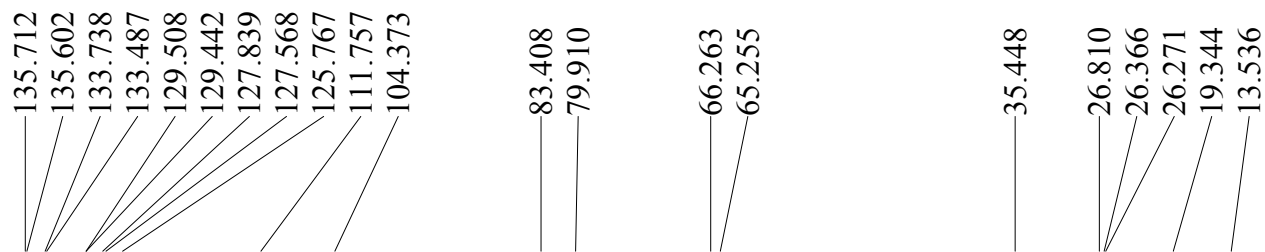
 ^{13}C NMR, 75 MHz, CDCl_3 

m/z	Ion	Formula	Abundance
479.2268	(M+Na)+	C ₂₆ H ₃₆ NaO ₅ Si	110454.1

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross Score	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DBE
✓	C ₂₆ H ₃₆ O ₅ Si	C ₂₆ H ₃₆ NaO ₅ Si	479.2224	66.65		456.2376	456.2332	-9.54	9.54	86.85	91.41	42.15	479.2268	10

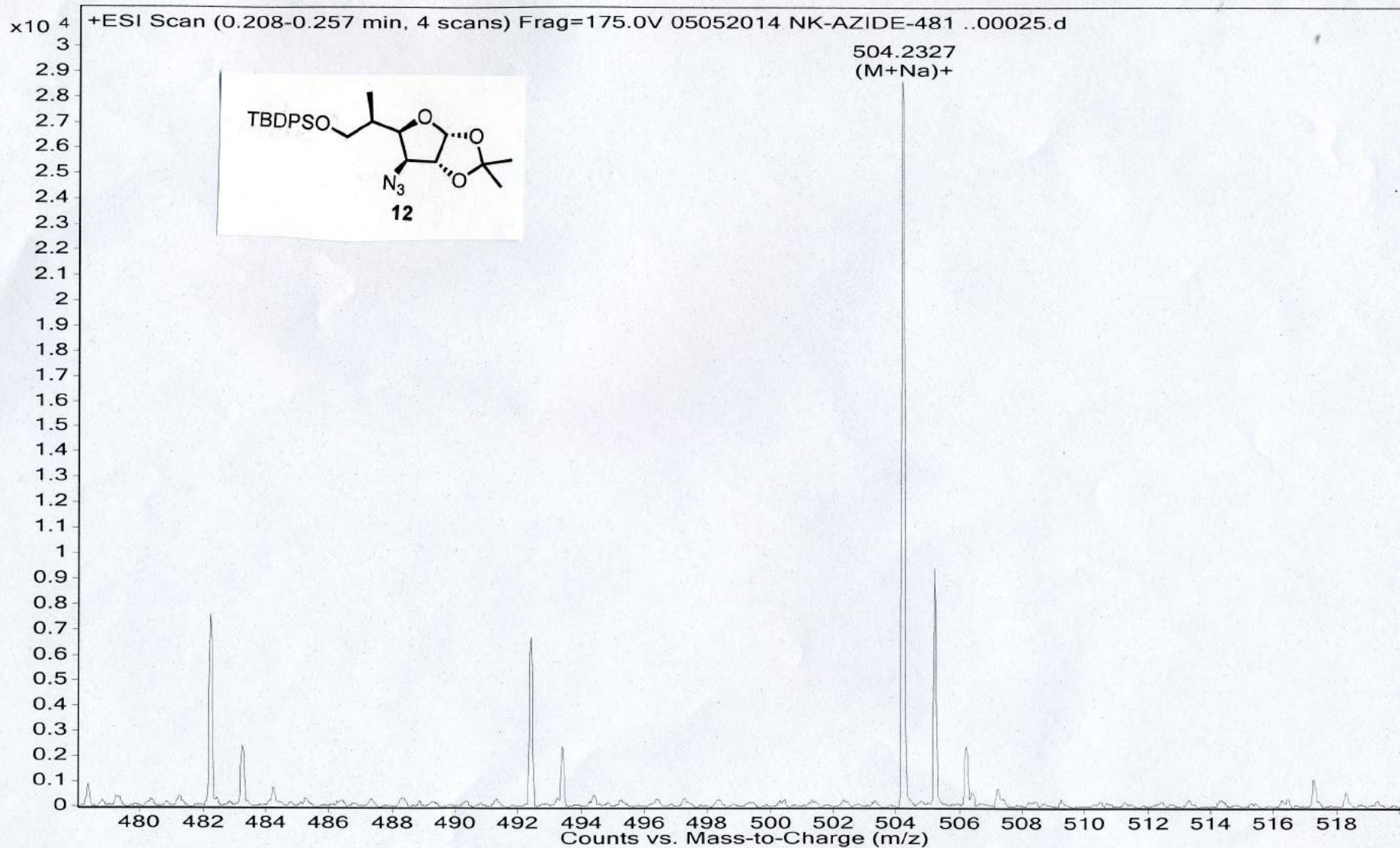


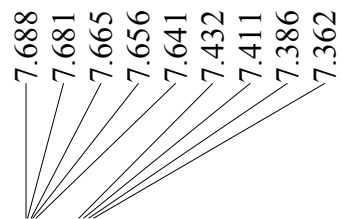
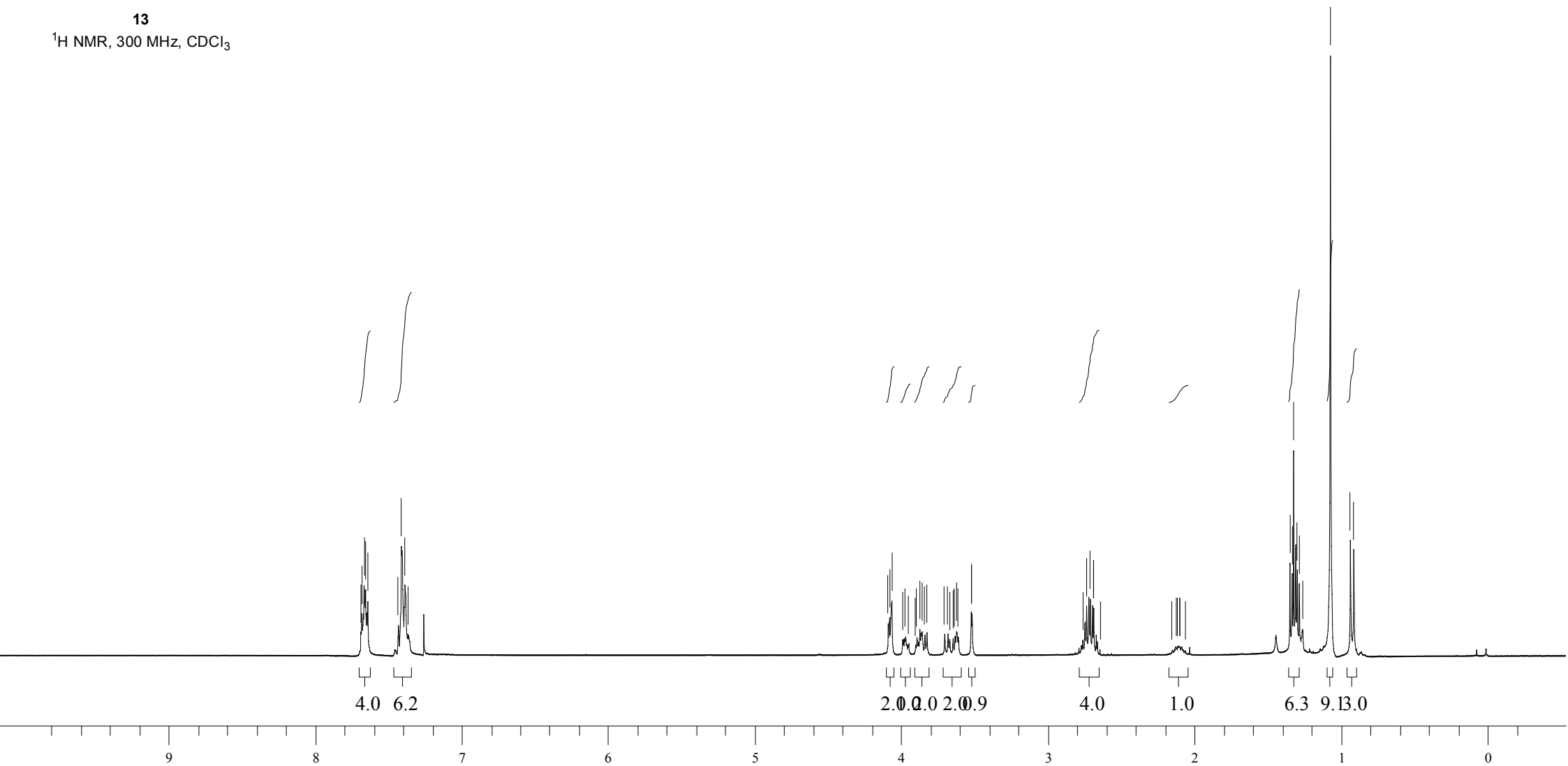
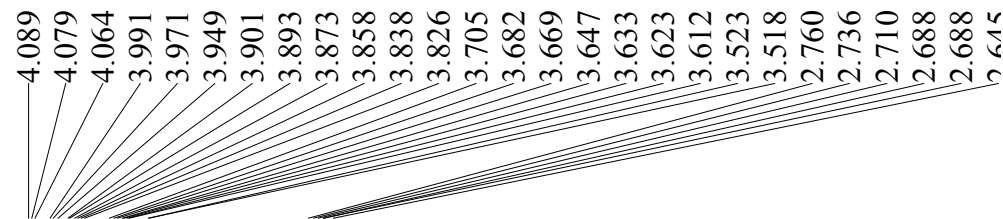


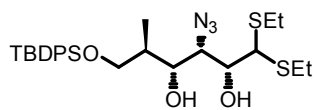
 ^{13}C NMR, 75 MHz, CDCl_3 

m/z	Ion	Formula	Abundance
504.2327	(M+Na)+	C ₂₆ H ₃₅ N ₃ NaO ₄ Si	29113.9

Best	Formula (M)	Ion Formula	Calc m/z	Score	Cross Score	Mass	Calc Mass	Diff (ppm)	Abs Diff (ppm)	Abund Match	Spacing Match	Mass Match	m/z	DBE
✓	C ₂₆ H ₃₅ N ₃ O ₄ Si	C ₂₆ H ₃₅ N ₃ NaO ₄ Si	504.2289	73.44		481.2435	481.2397	-7.83	7.83	95.71	84.96	54.32	504.2327	12

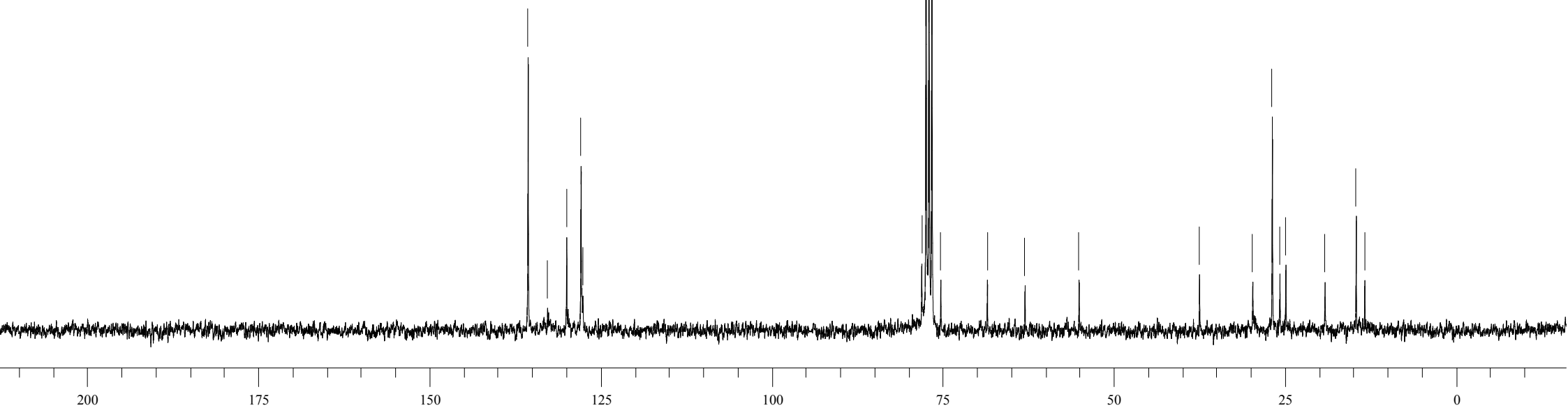
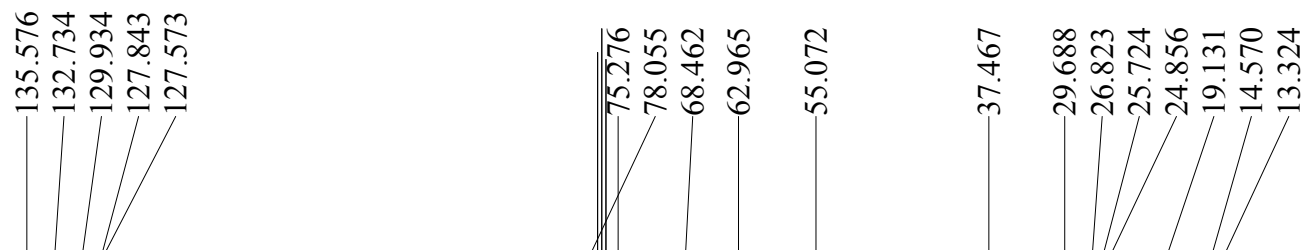


 ^1H NMR, 300 MHz, CDCl_3 



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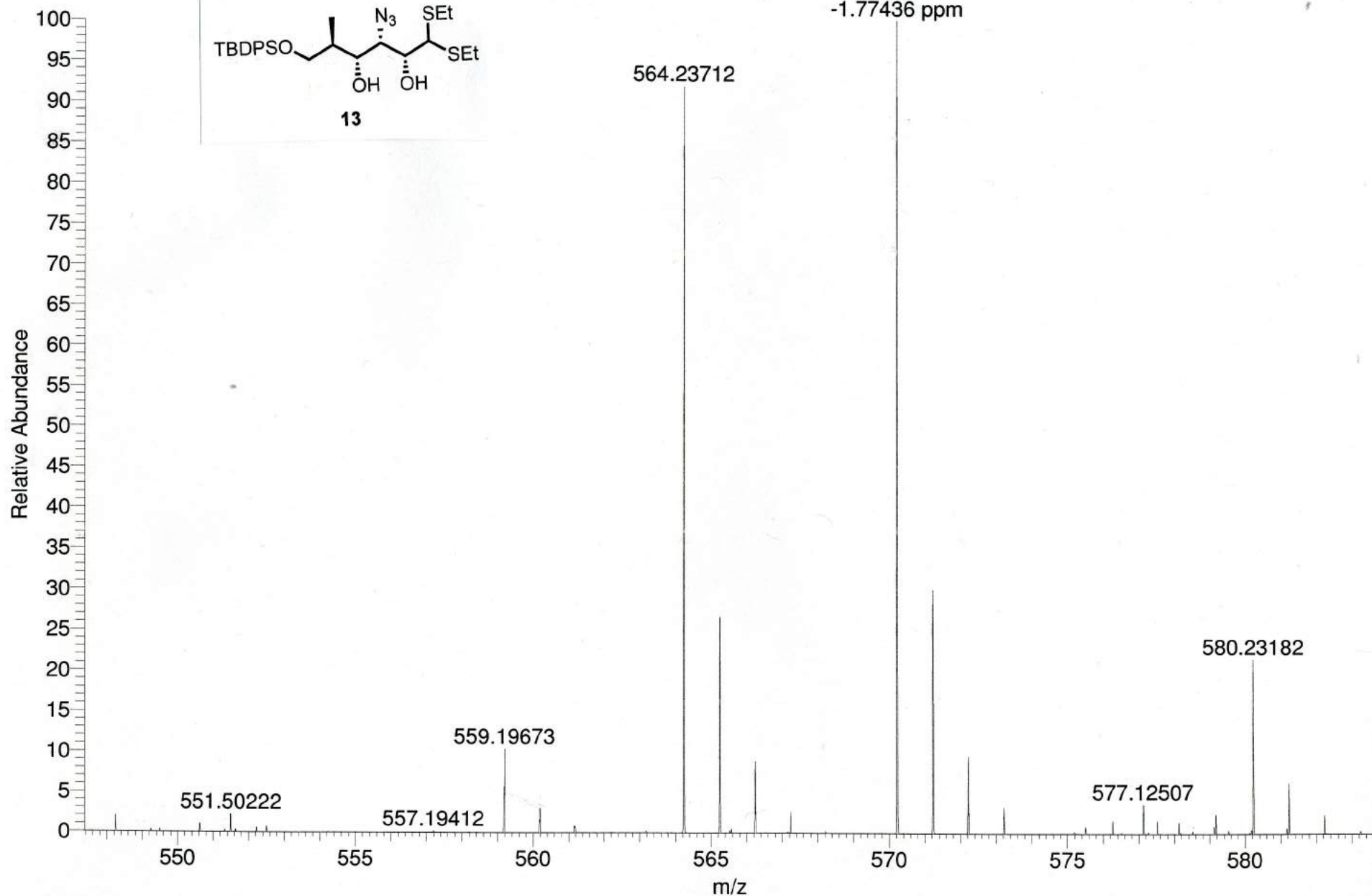
^{13}C NMR, 75 MHz, CDCl_3

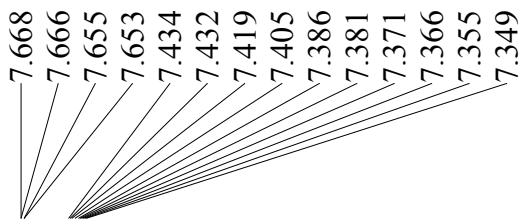
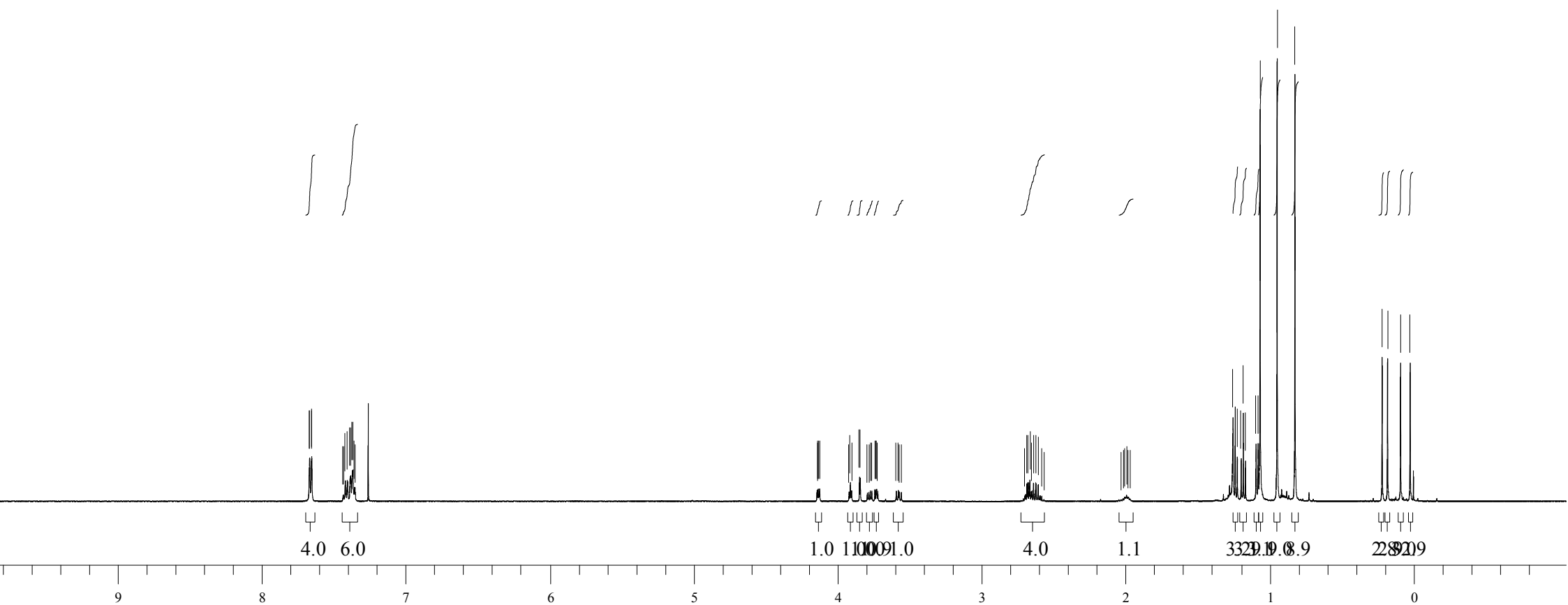
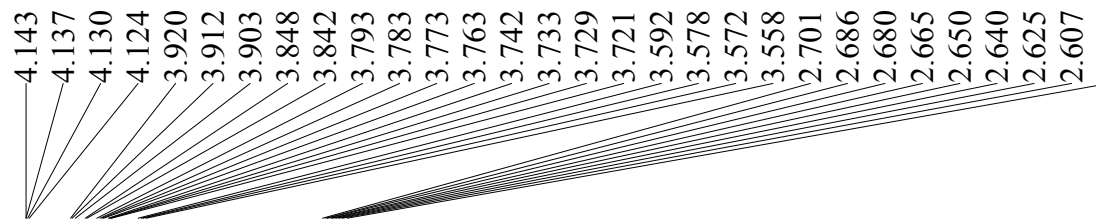


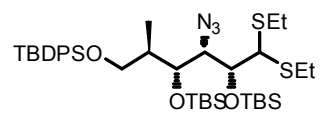
DITHANE-1 #7-18 RT: 0.05-0.13 AV: 12 NL: 9.91E5

T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

570.22407
 $C_{27}H_{41}O_3N_3NaS_2Si = 570.22508$
9.5 RDBE
-1.77436 ppm

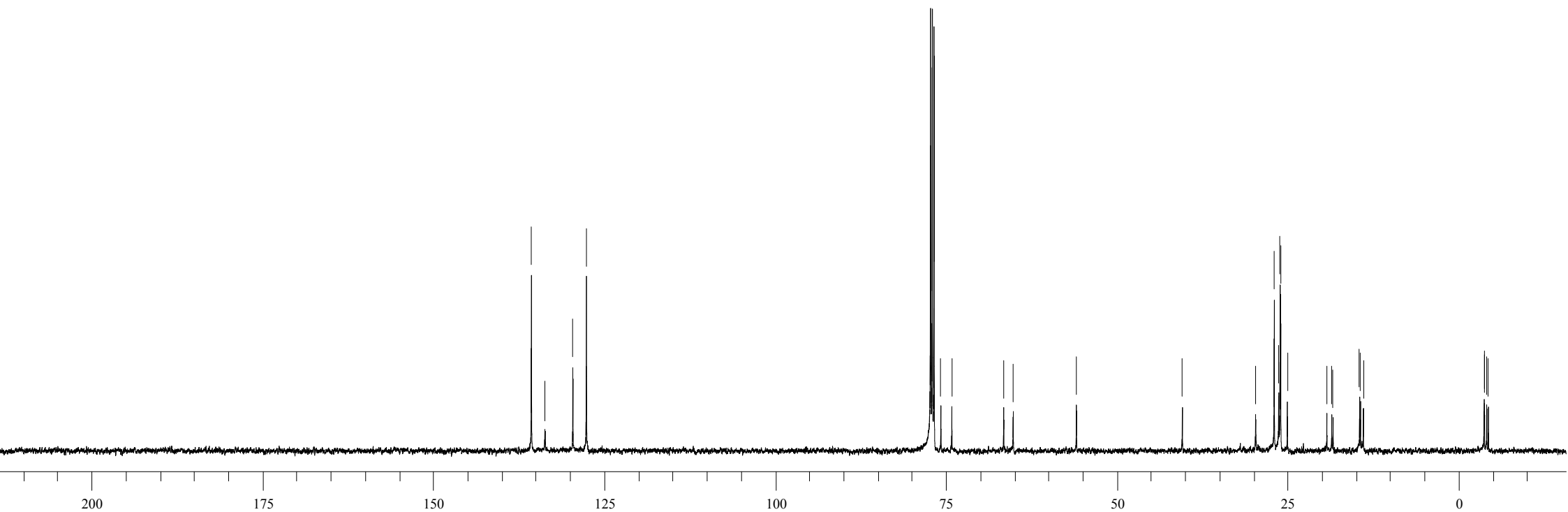


¹H NMR, 500 MHz, CDCl₃



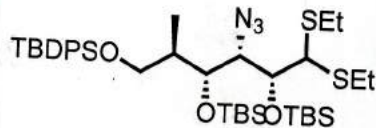
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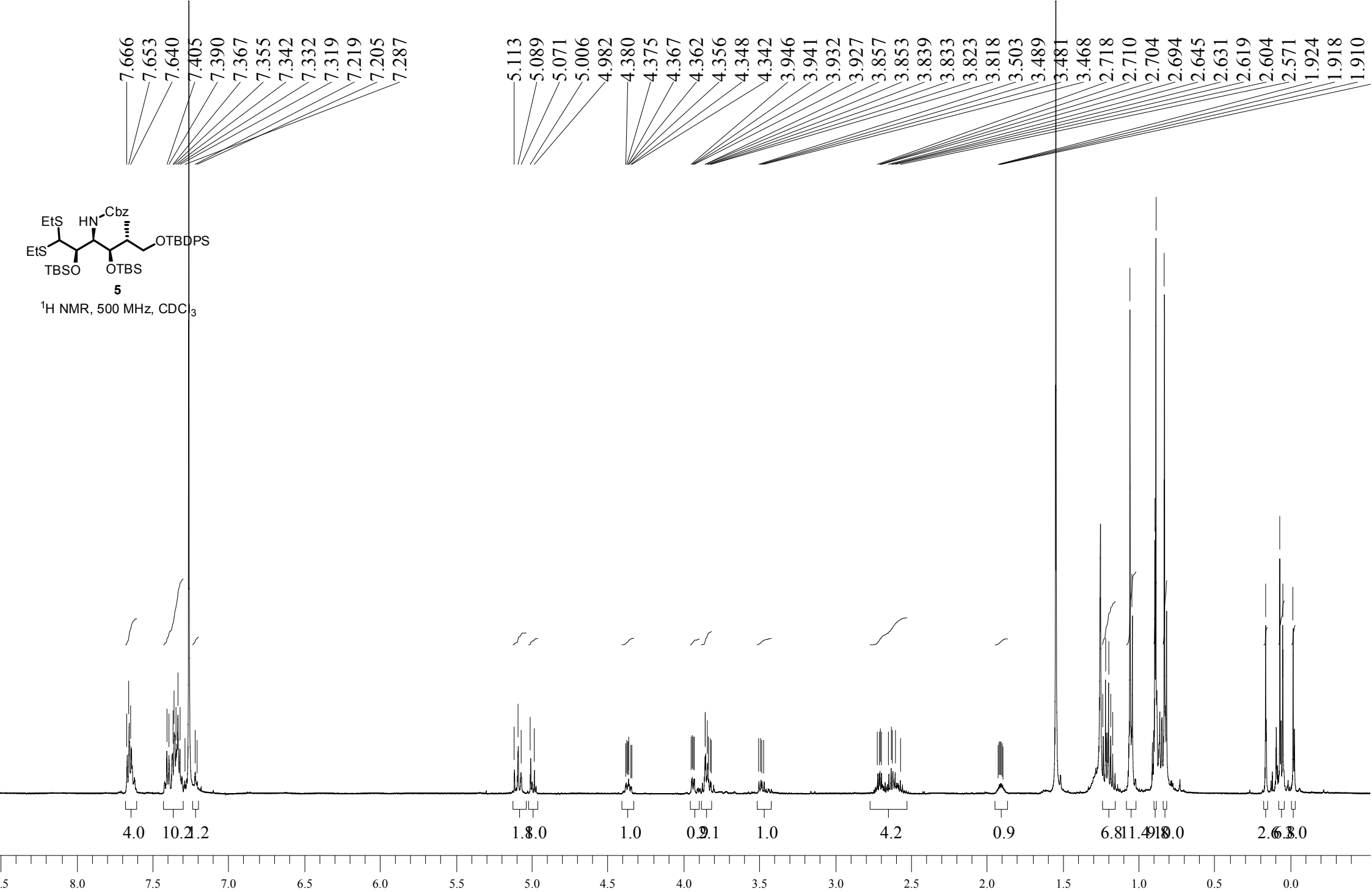
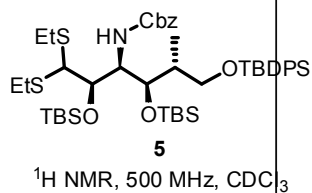
¹³C NMR, 125 MHz, CDCl₃

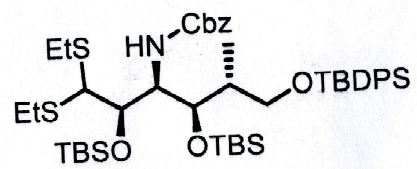


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T: FTMS {1,1} + p ESI Full ms [75.00-1500.00]

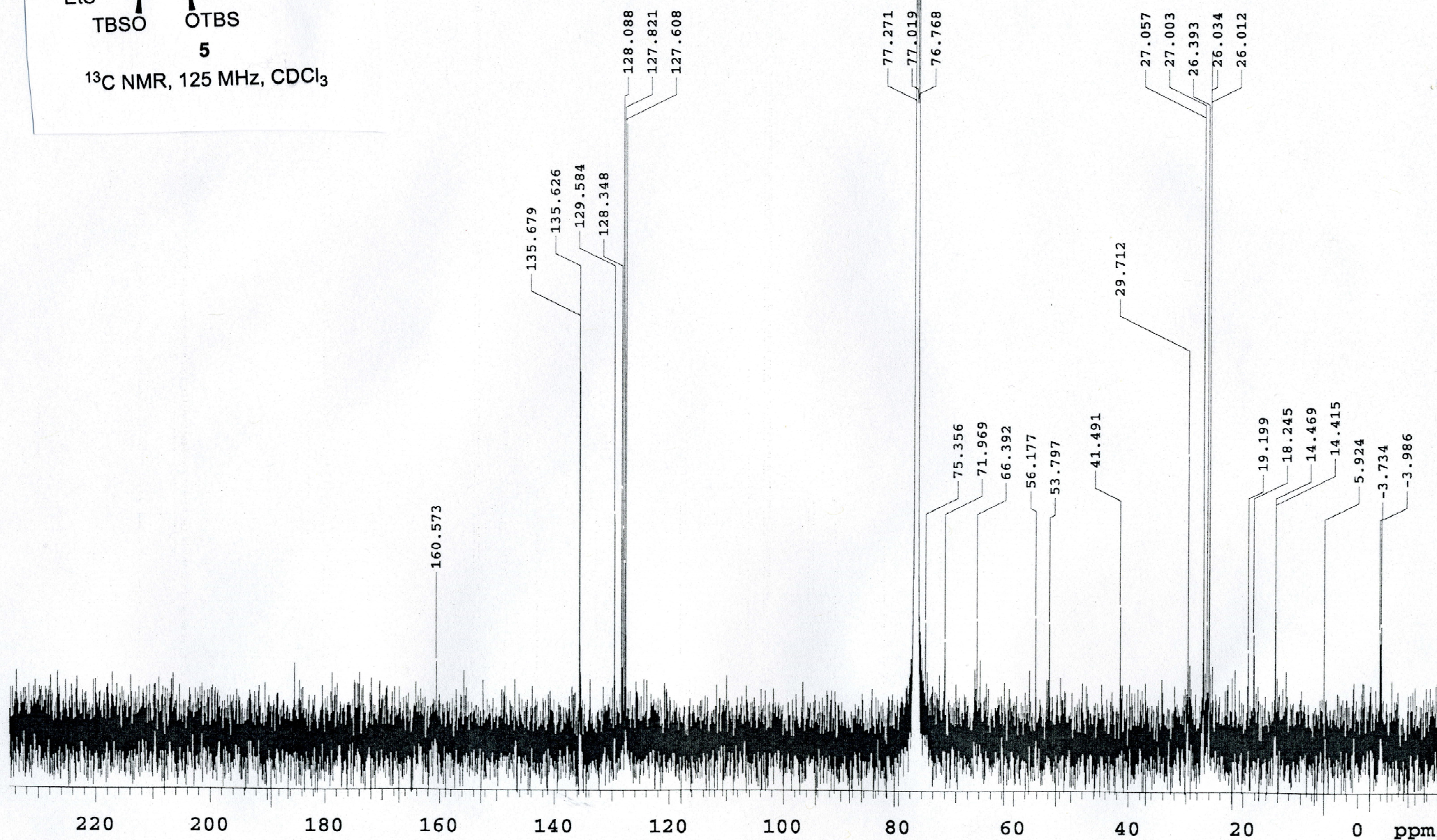






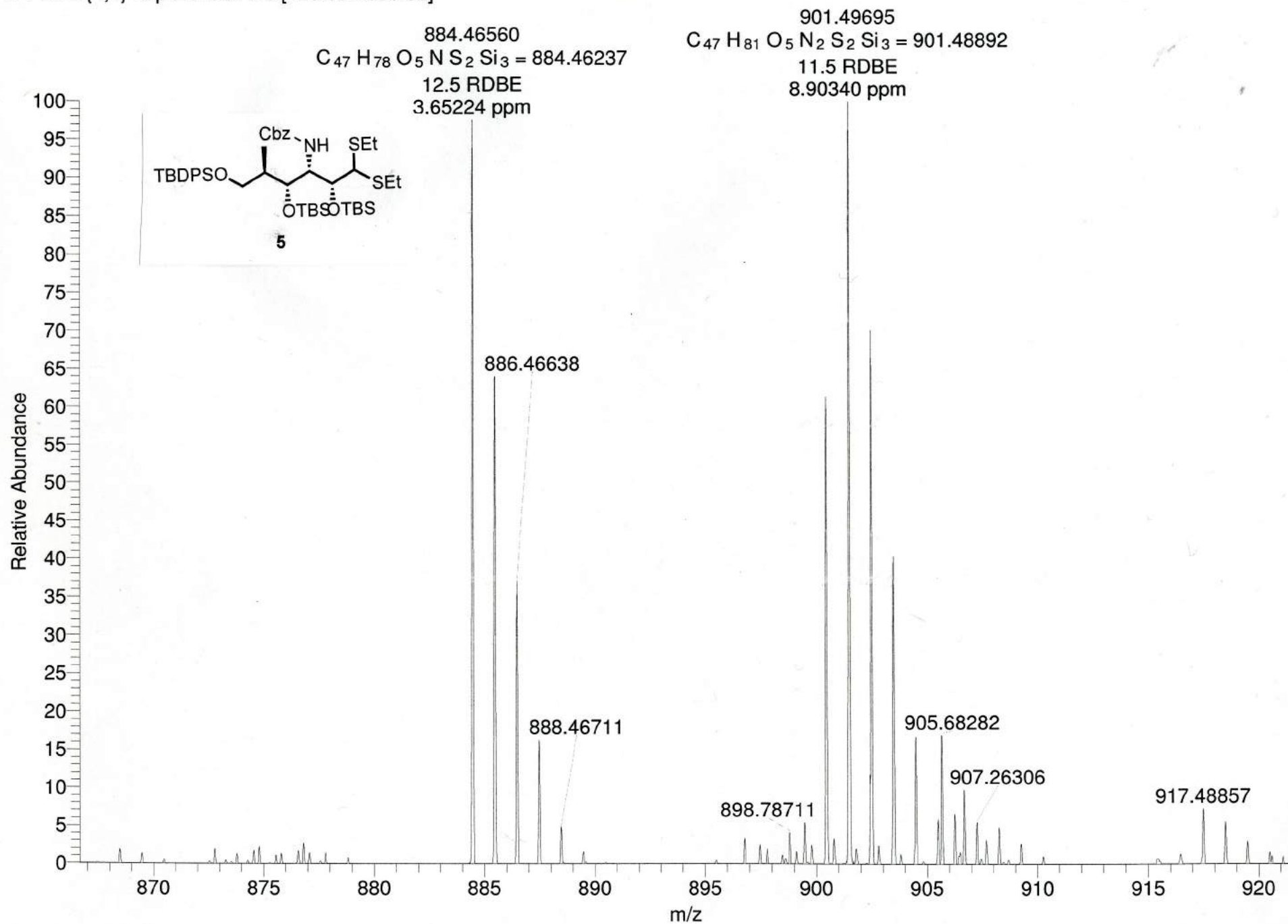
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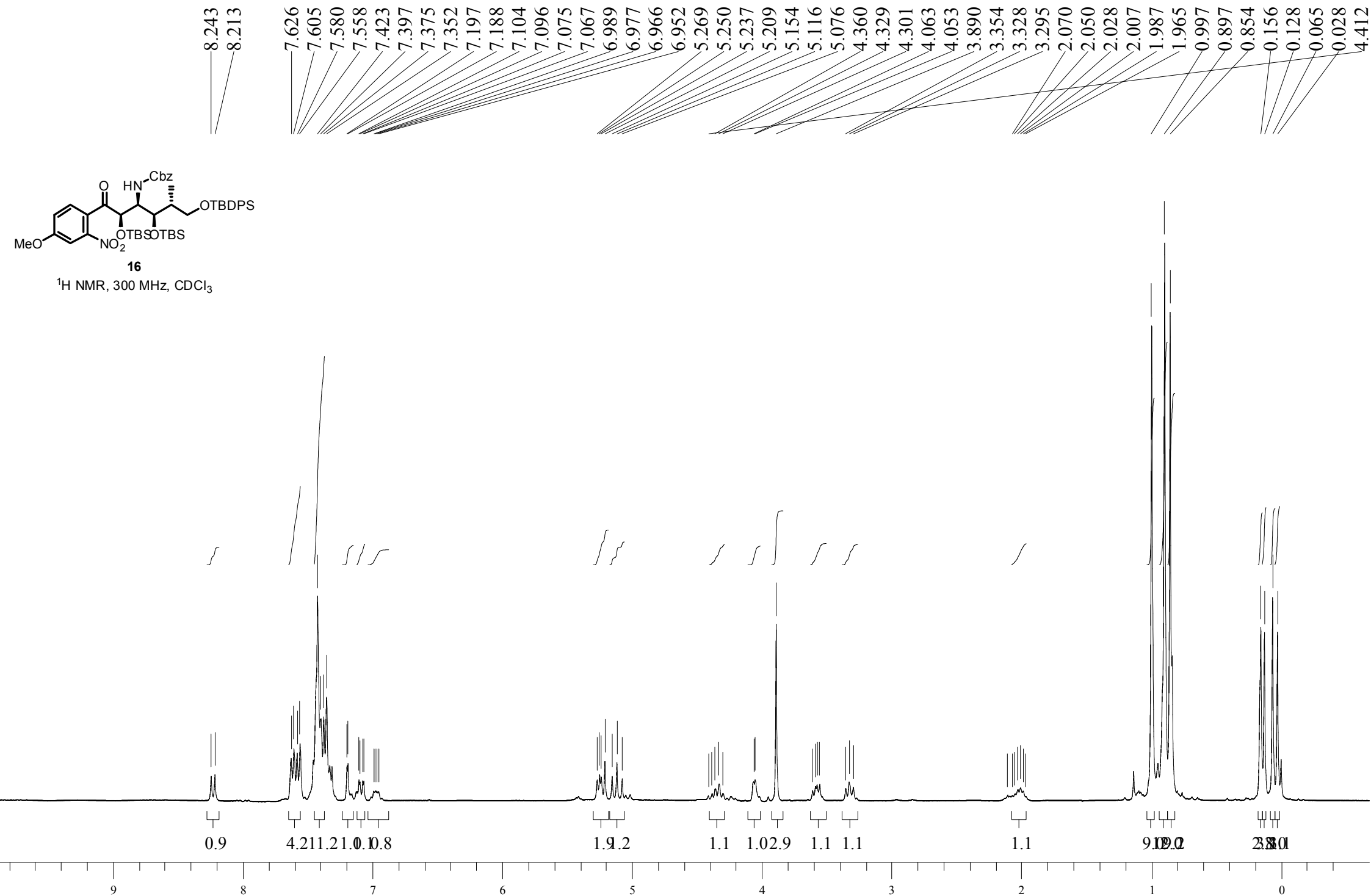
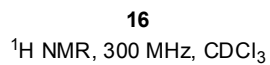
^{13}C NMR, 125 MHz, CDCl_3

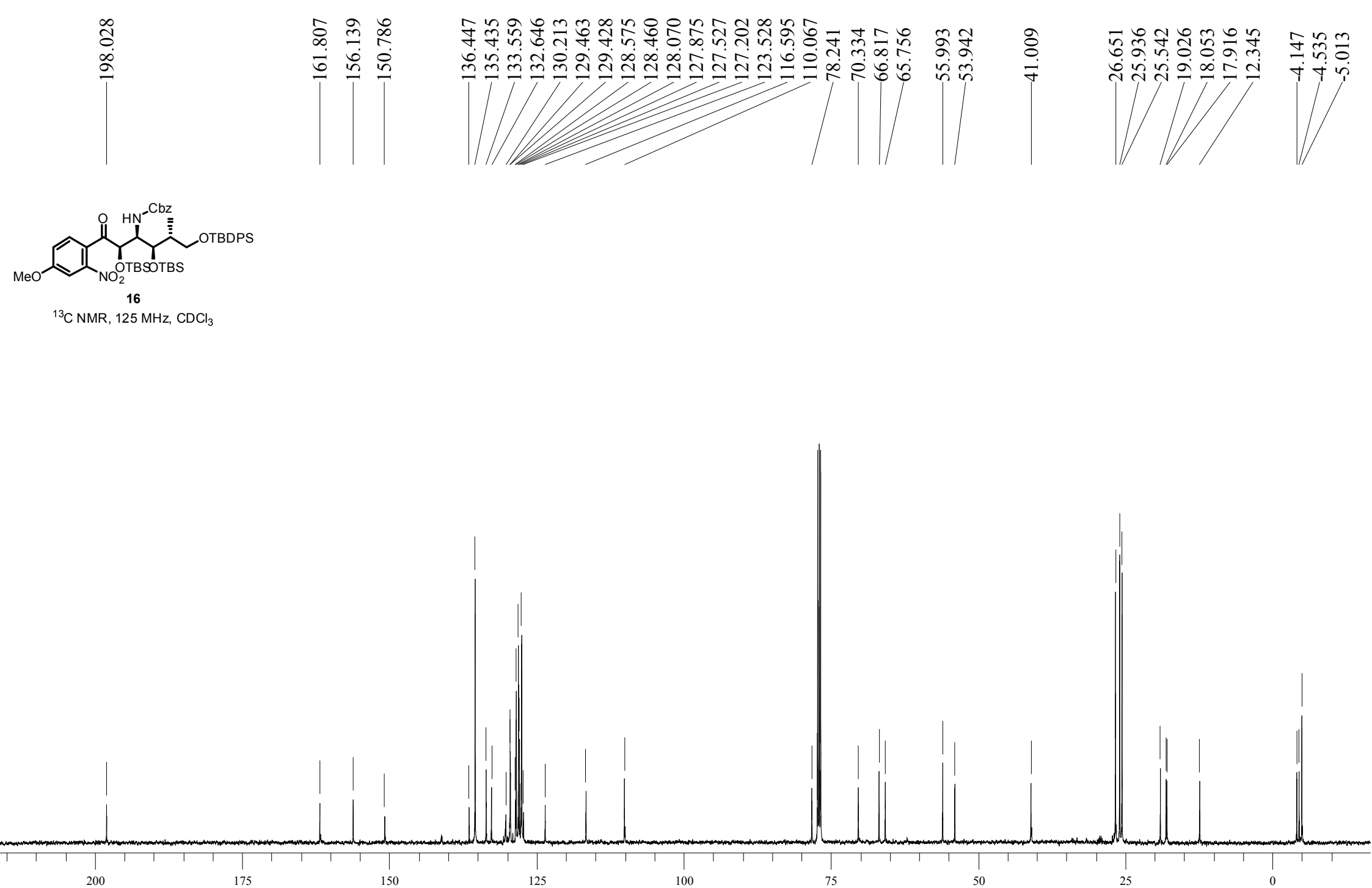
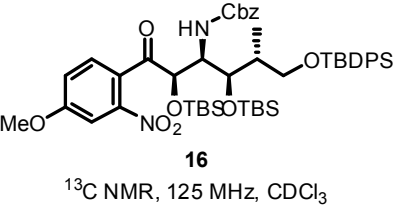


NK-883 #20-25 RT: 0.10-0.12 AV: 6 NL: 5.26E4

T: FTMS {1,1} + p ESI Full ms [110.00-2000.00]

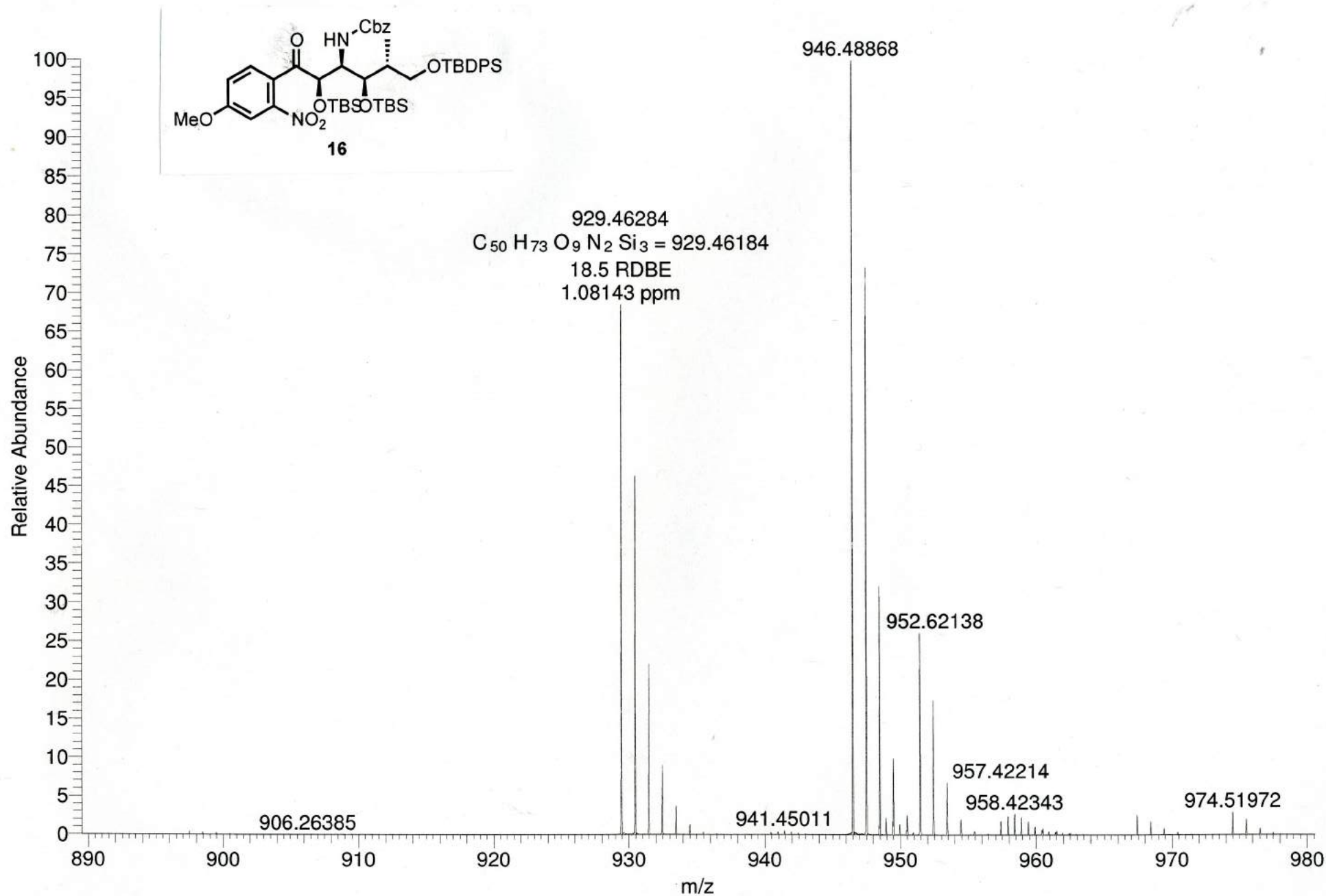


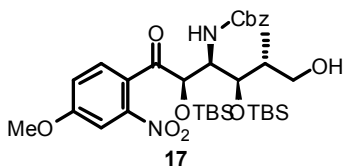




NK-145B #2-23 RT: 0.02-0.17 AV: 22 NL: 1.16E7

T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

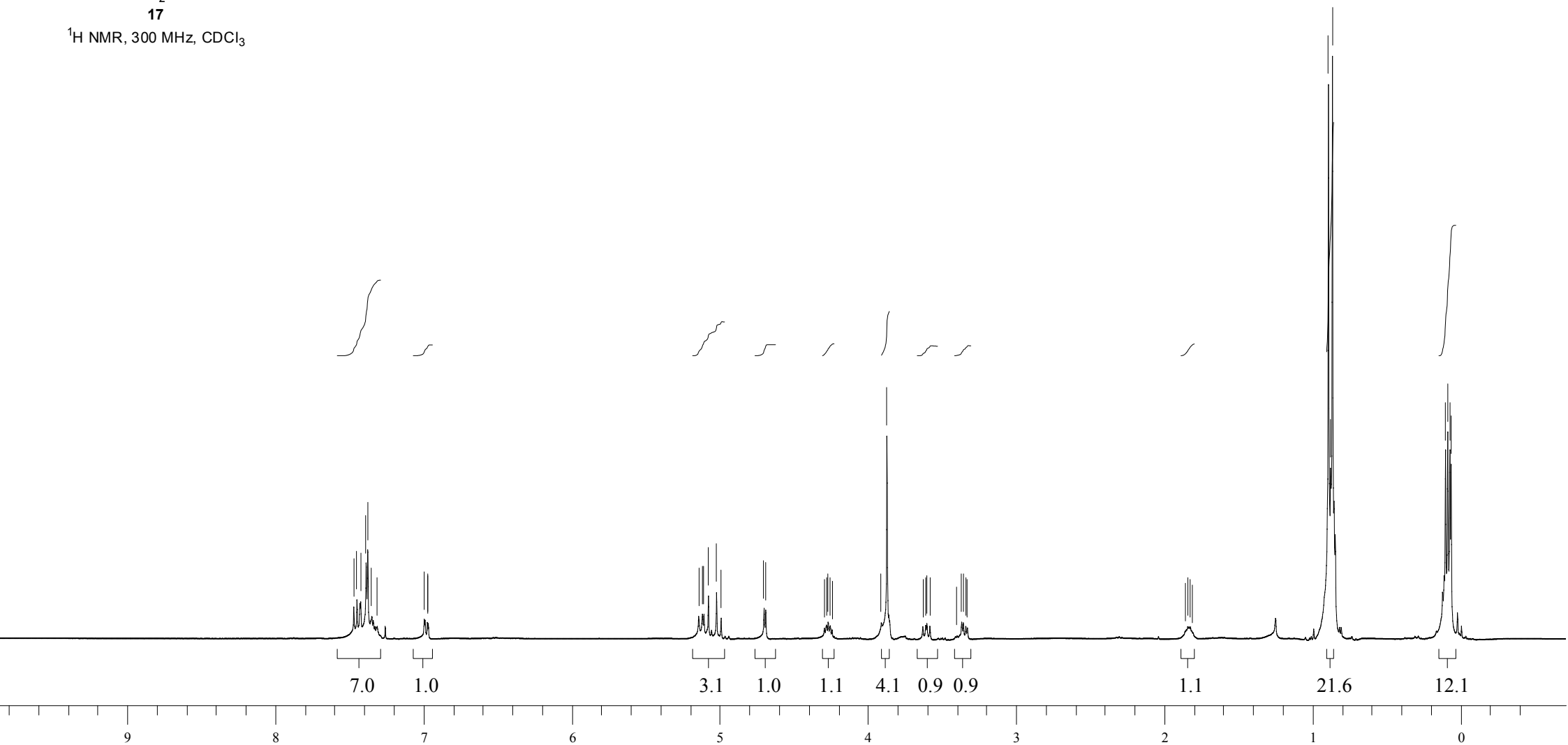


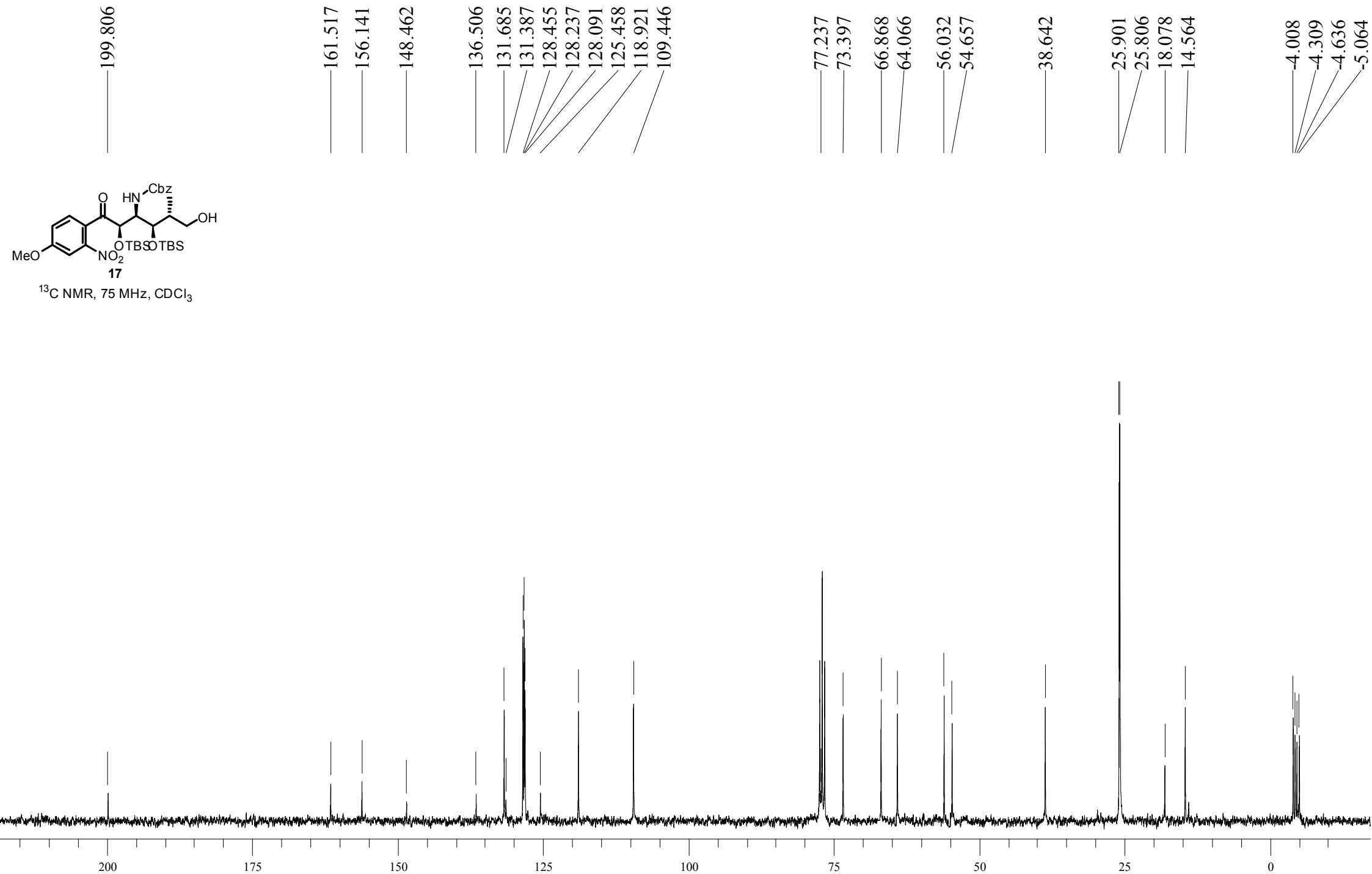
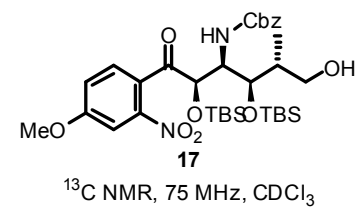


^1H NMR, 300 MHz, CDCl_3

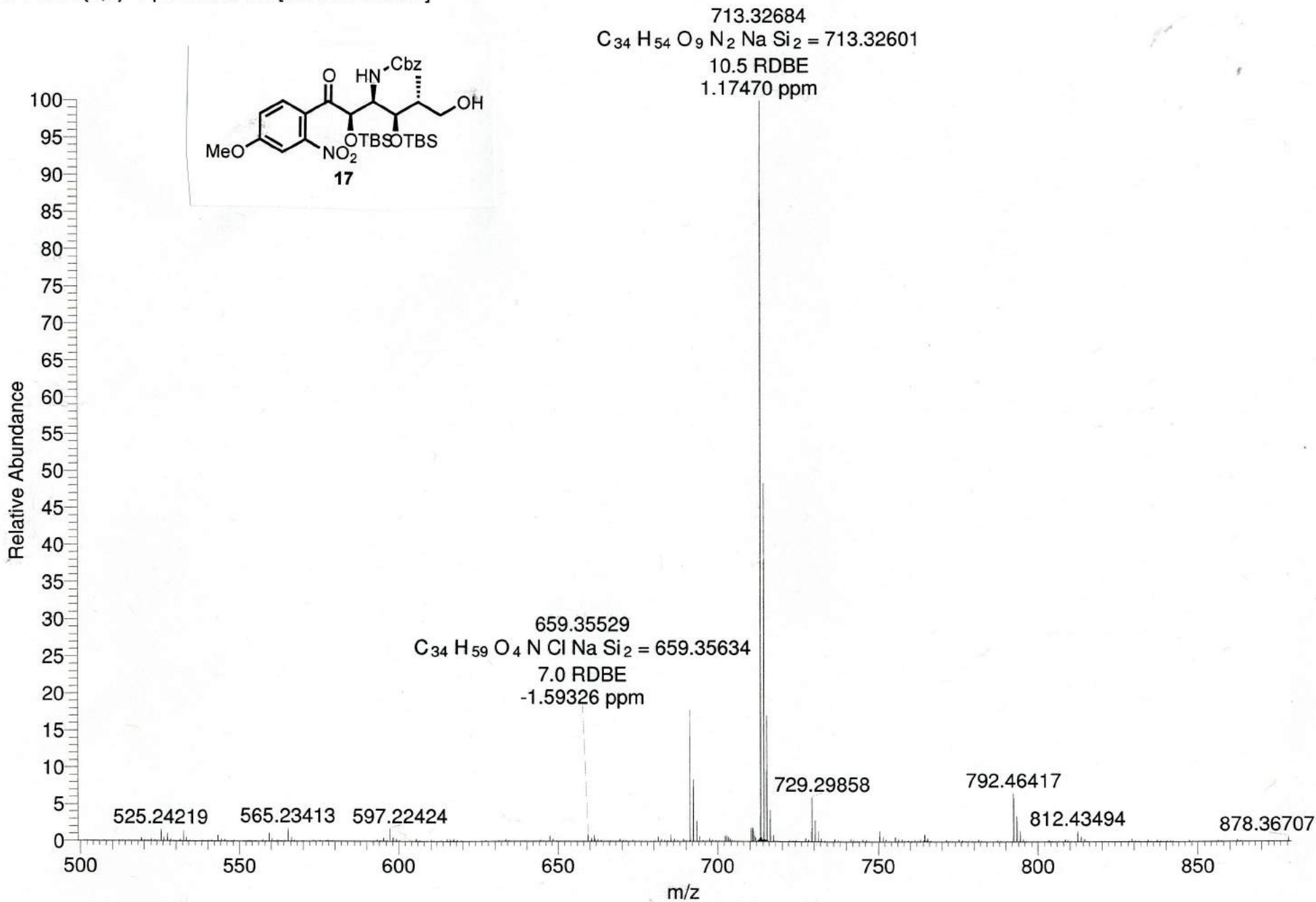
7.470
 7.449
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 7.376
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 7.311
 6.995
 6.974
 6.968

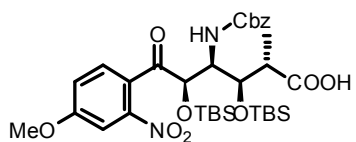
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 3.610
 3.602
 3.582
 3.397
 3.367
 3.357
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 0.062



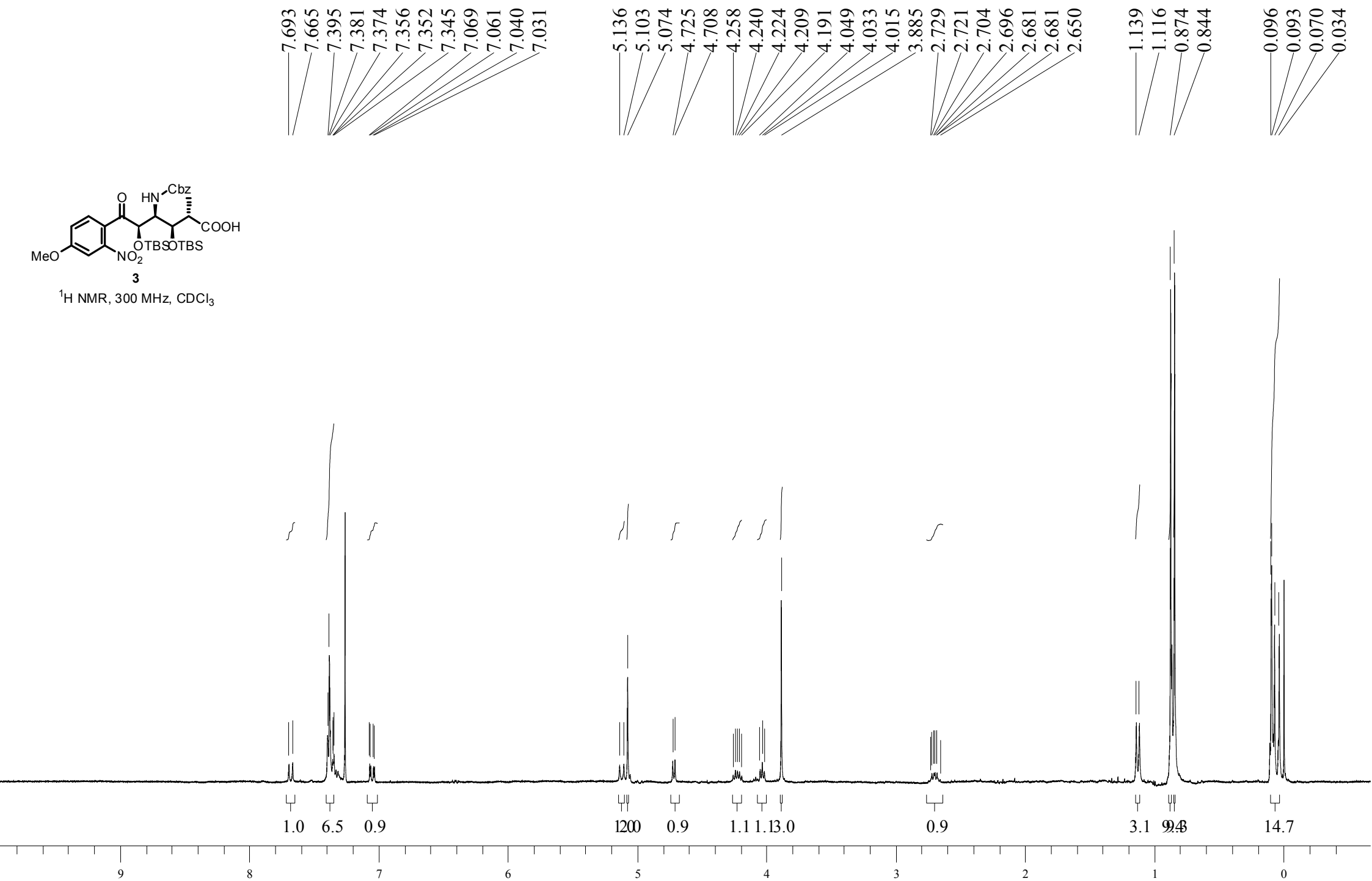


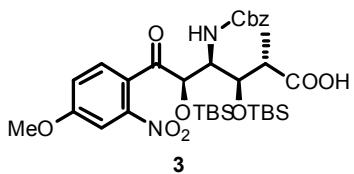
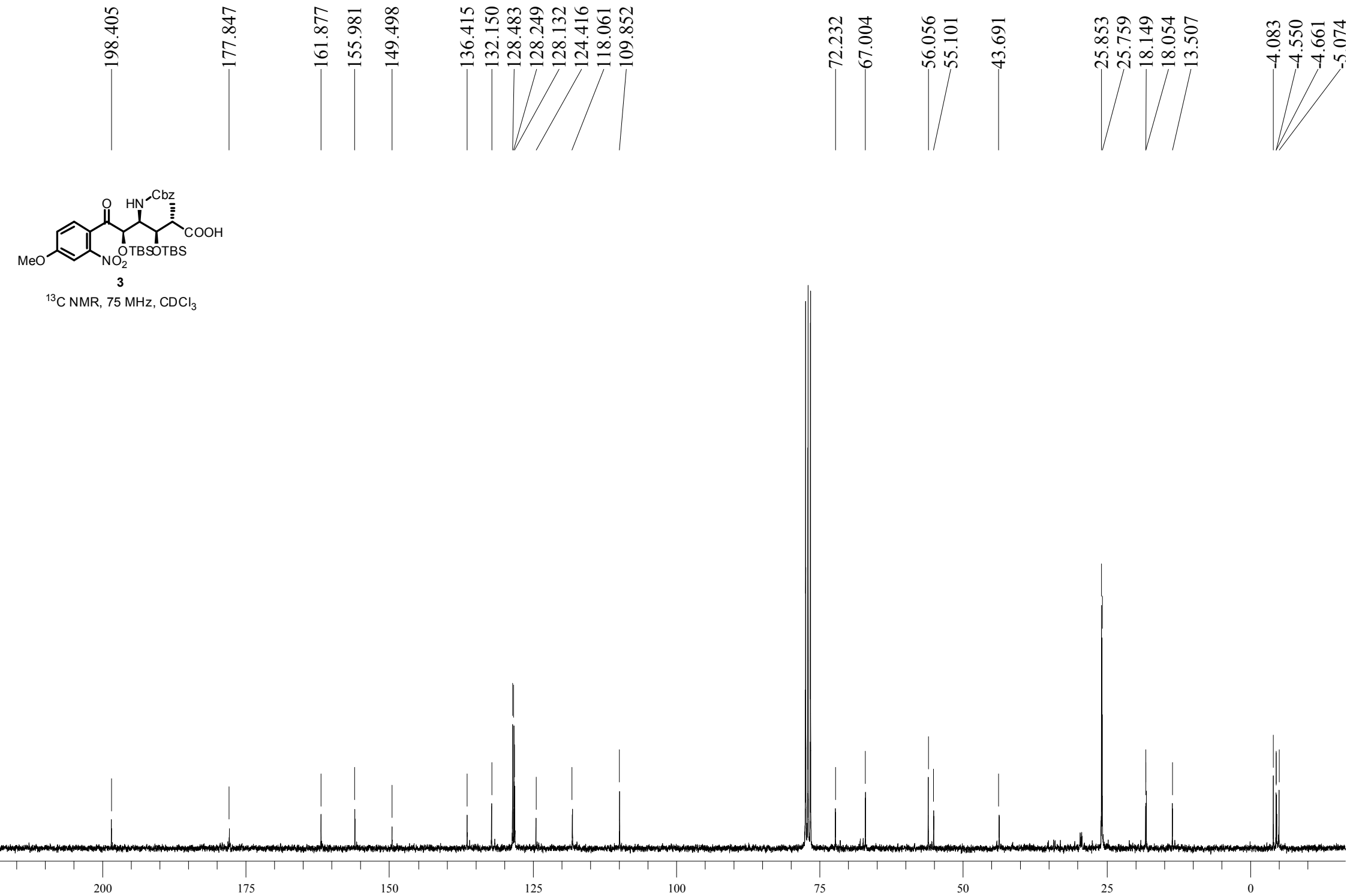
NK-29B #9 RT: 0.09 AV: 1 NL: 6.46E7
T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]





3
 ^1H NMR, 300 MHz, CDCl_3



 ^{13}C NMR, 75 MHz, CDCl_3 

KAVITHATO4-3_121116170223 #7 RT: 0.07 AV: 1 NL: 1.55E7

T: FTMS {1,1} + p ESI Full ms [100.00-2000.00]

