

Supporting Information

Glucopyranosylidene-spiro-thiazolinones: synthetic studies and determination of absolute configuration by TDDFT-ECD calculations

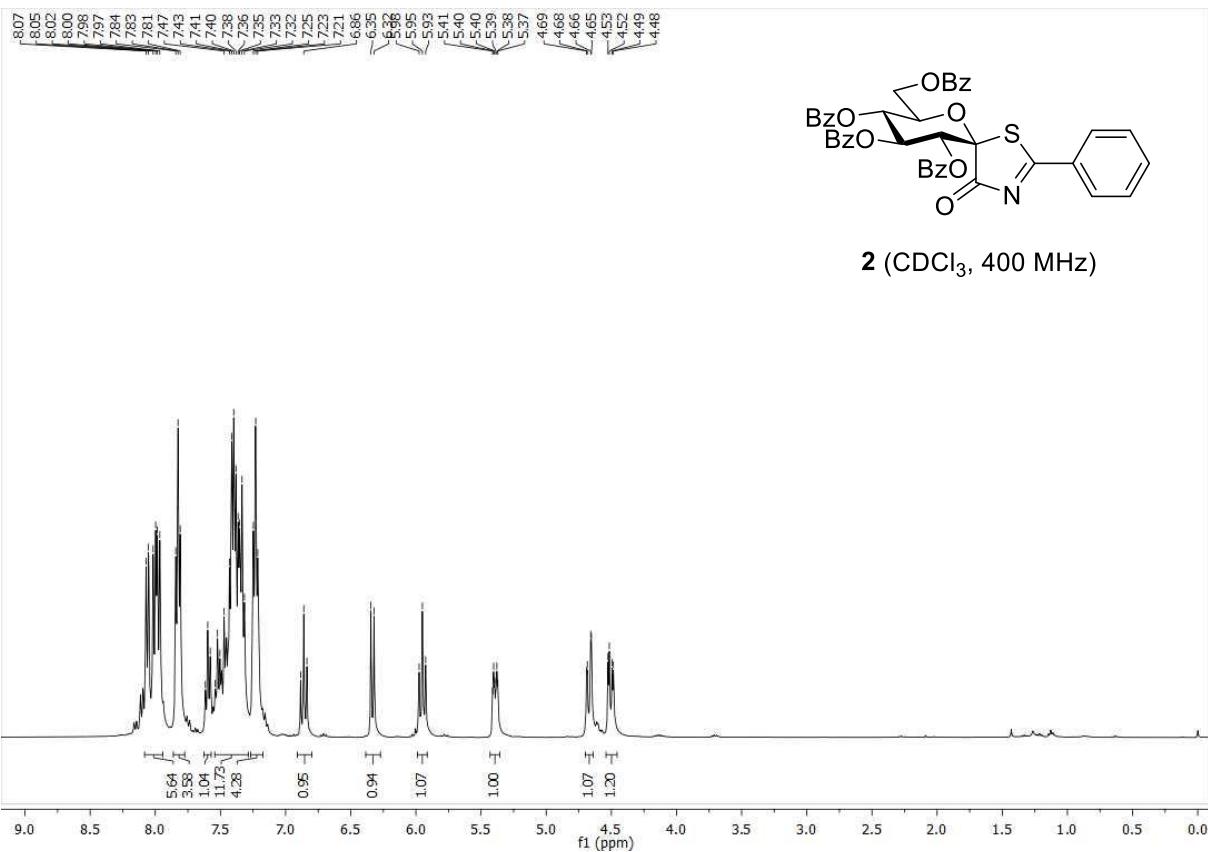
Katalin E. Szabó, Sándor Kun, Attila Mándi, Tibor Kurtán, László Somsák*

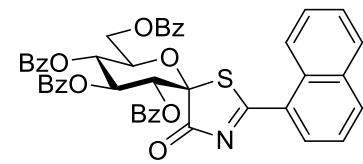
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Hungary*

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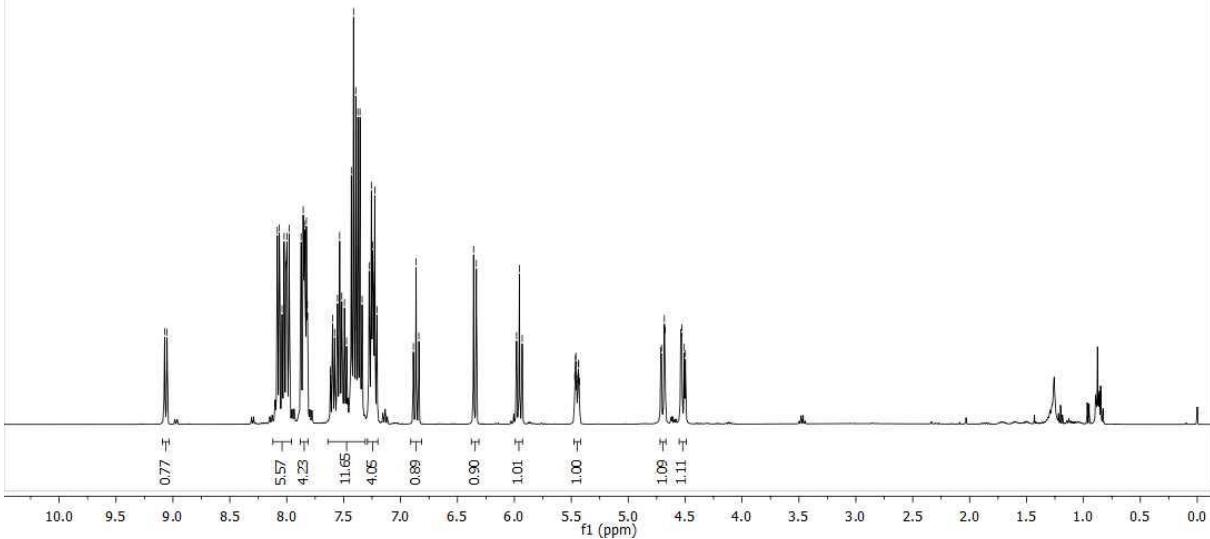
Copies of NMR spectra of the prepared compounds	S2
Low energy conformers of (1'R)- 15 , (1'S)- 15 , (2R,1'R)- 21 , (2S,1'R)- 21	S16

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somsak.laszlo@science.unideb.hu





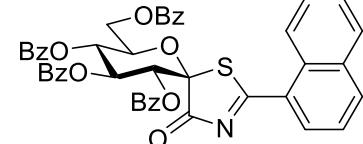
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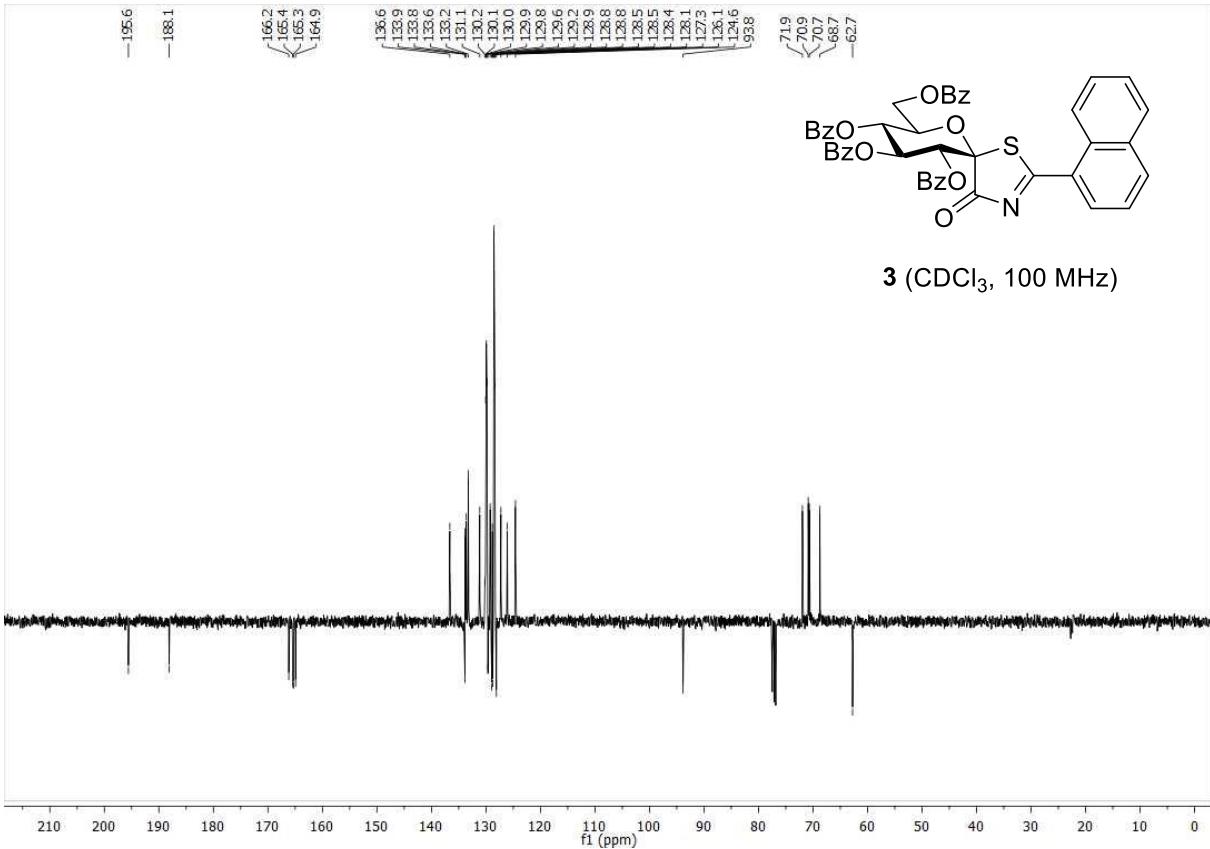
166.2
165.4
165.3
164.9

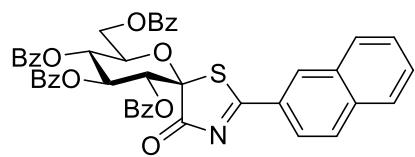
136.6
133.9
133.8
133.6
133.2
131.1
130.2
130.1
130.0
129.9
129.8
129.6
129.2
129.1
128.9
128.8
128.5
128.5
128.4
128.1
127.3
126.1
126.1
93.8

71.9
70.9
70.7
68.7
-62.7

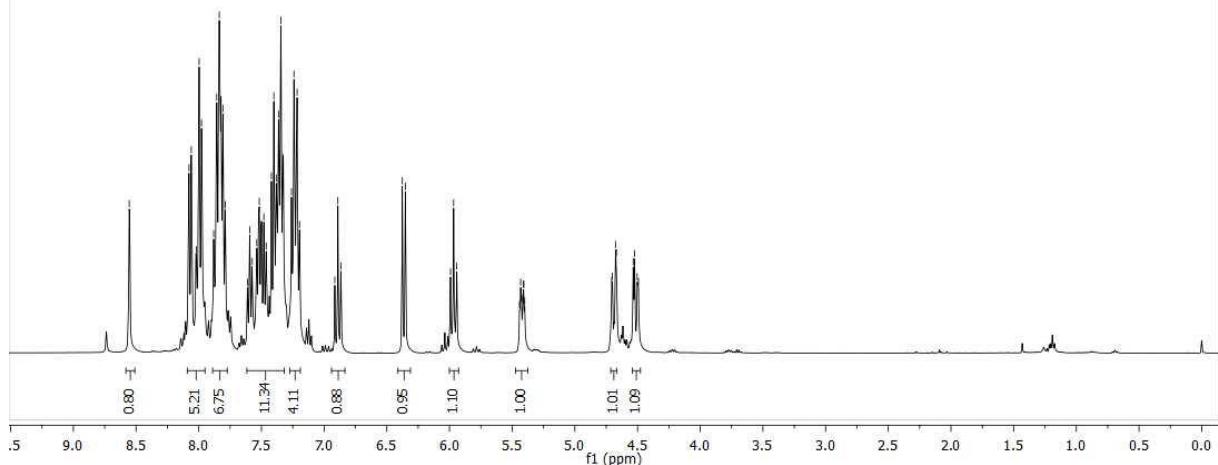


3 (CDCl_3 , 100 MHz)





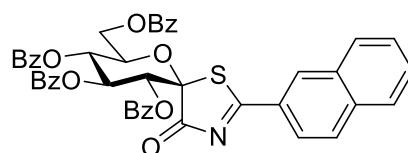
4 (CDCl_3 , 400 MHz)



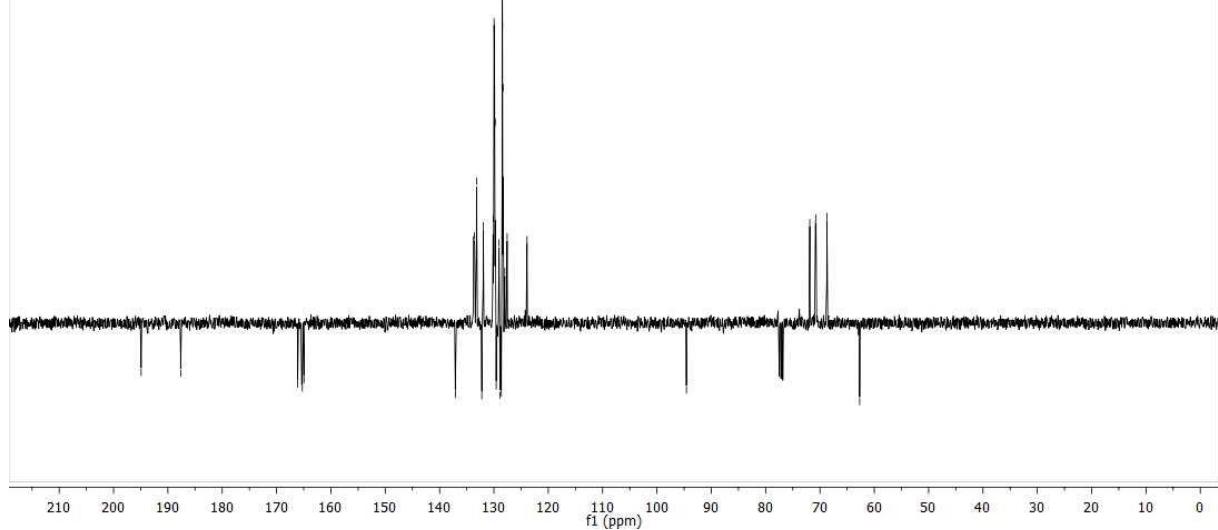
-199.9
-187.6

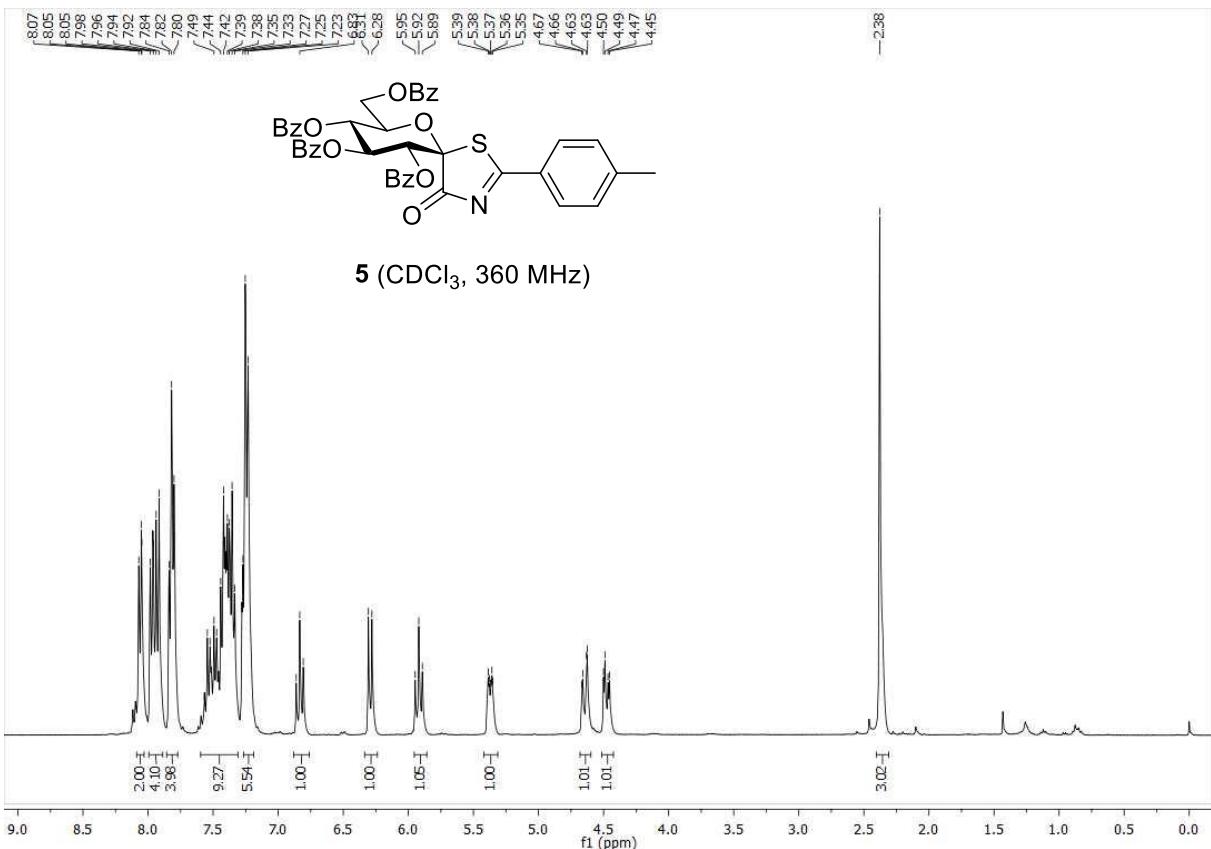
-166.1
<-165.4
<-165.3
<-165.0
137.1
133.8
133.6
133.2
132.2
132.0
130.1
130.0
129.9
129.8
129.6
129.1
128.9
128.7
128.6
128.5
128.4
128.3
128.0
127.6
123.9
-94.6

71.9
<70.8
<70.7
68.7
-62.7

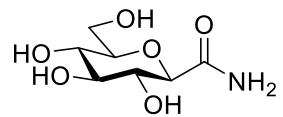


4 (CDCl_3 , 100 MHz)

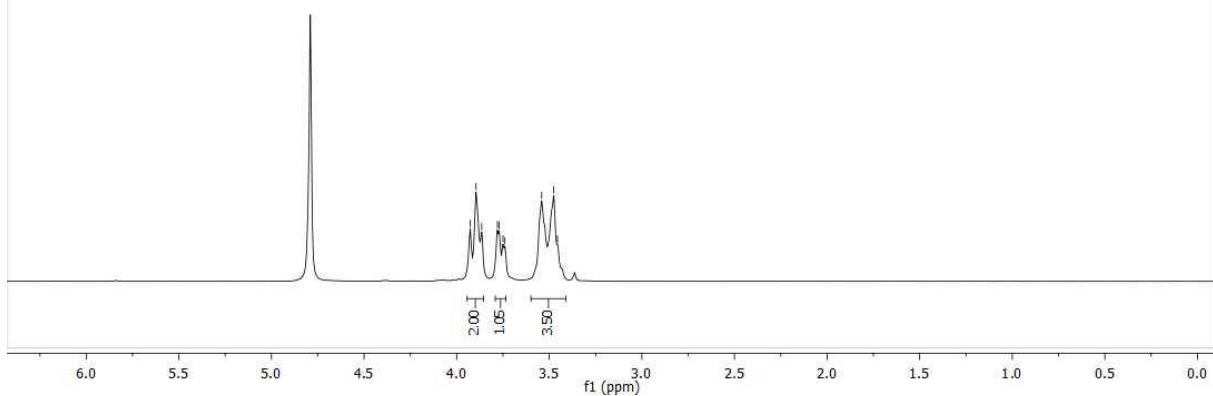




3.93
3.90
3.86
3.78
3.77
3.75
3.74
3.54
3.48
3.46

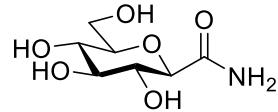


11 (D_2O , 400 MHz)

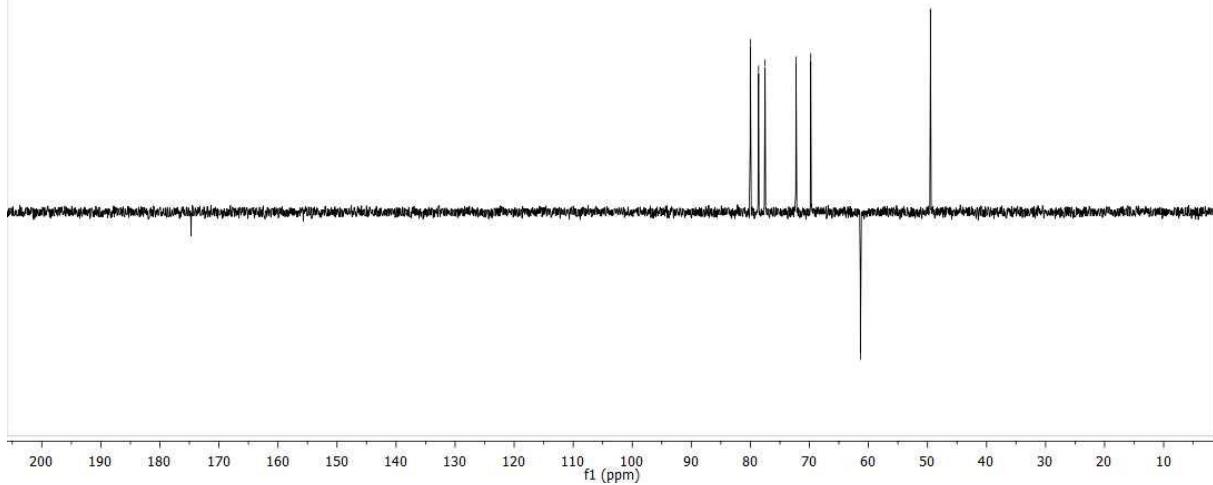


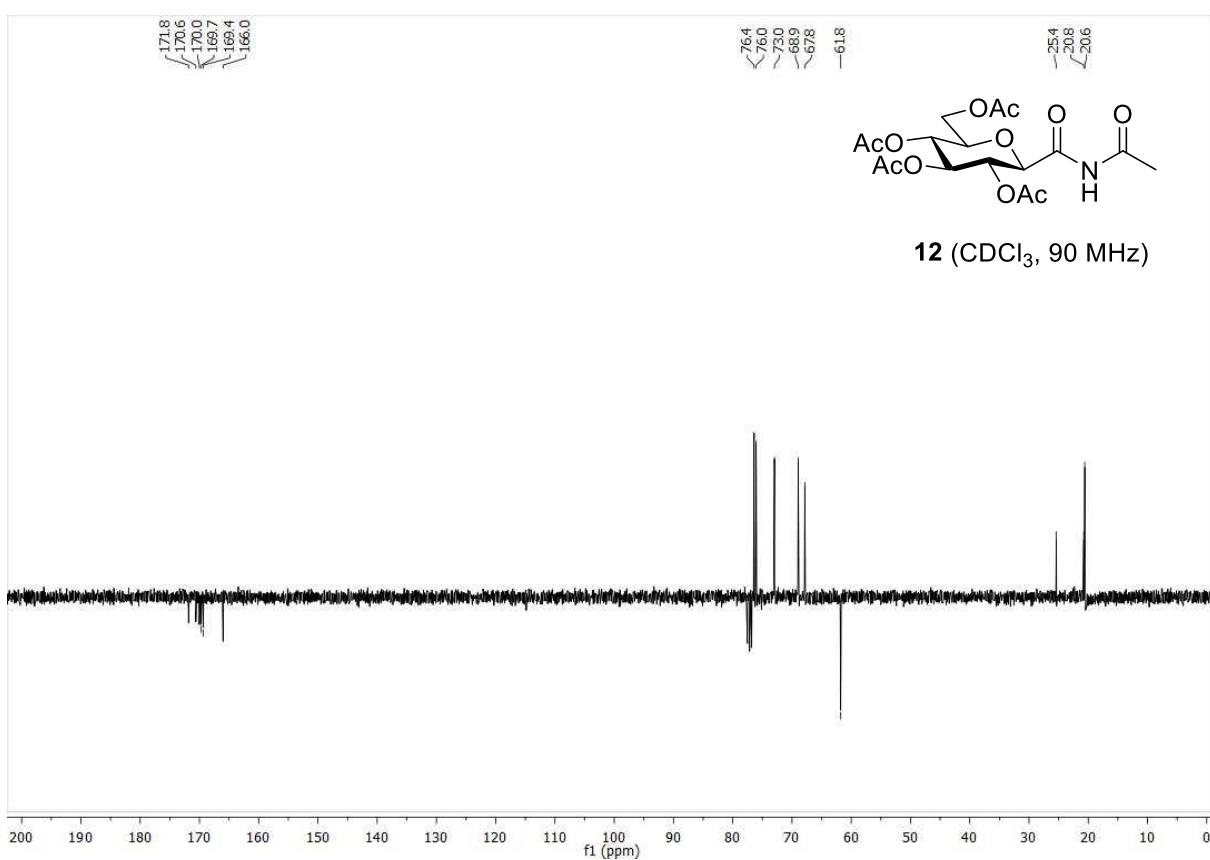
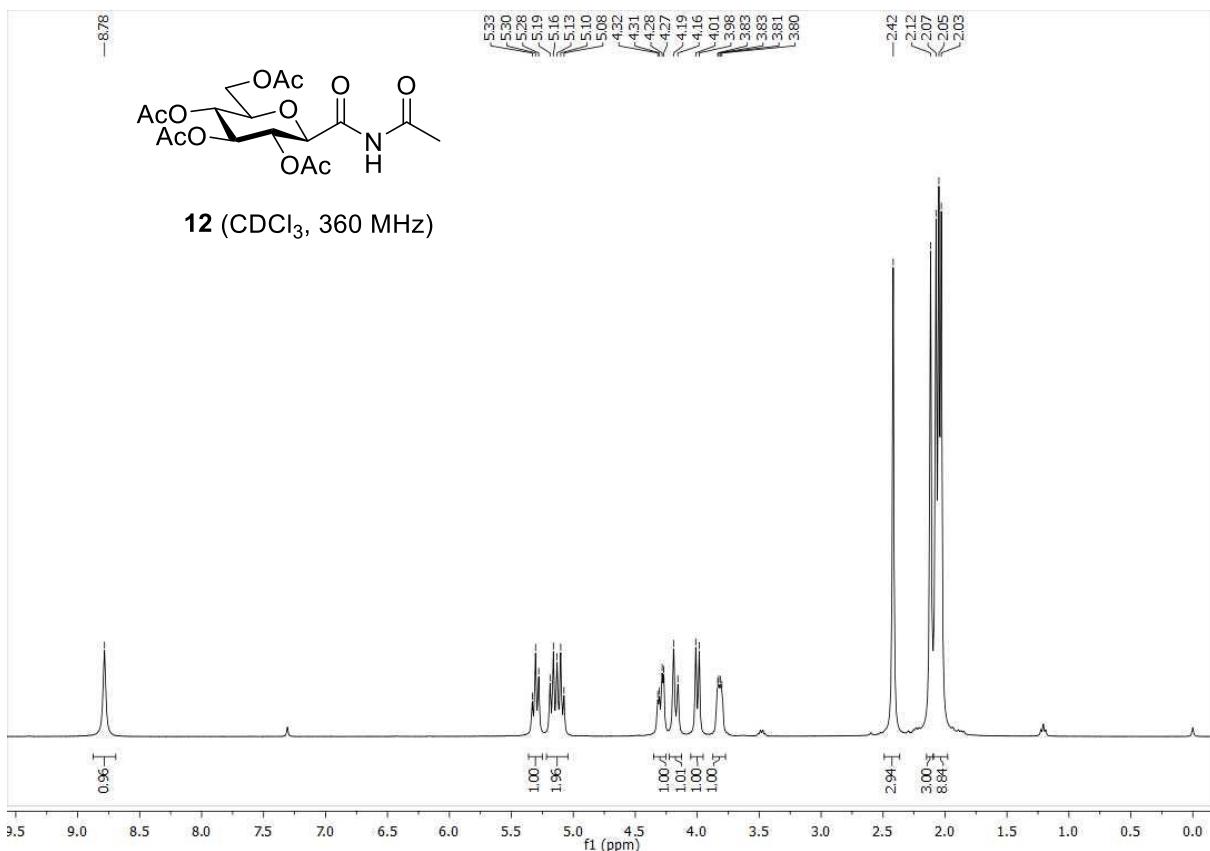
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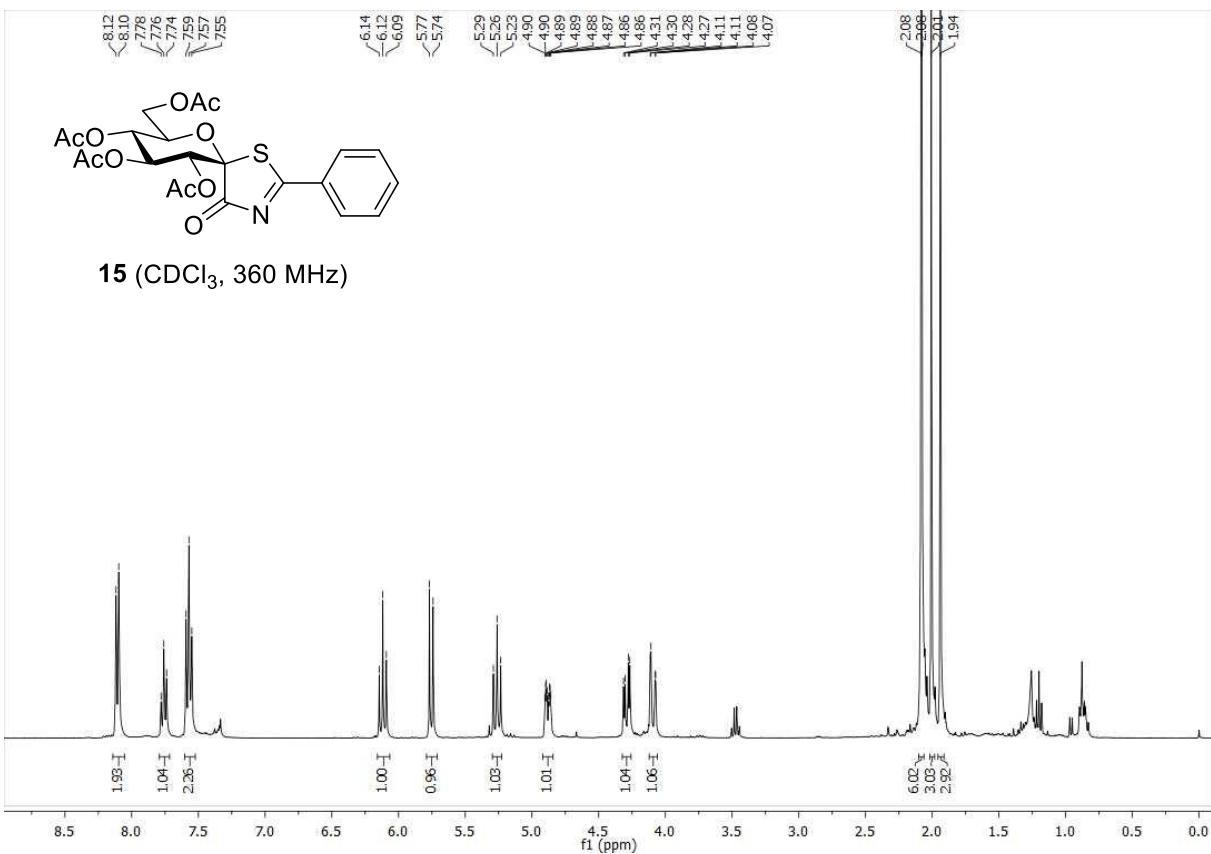
800
786
775
723
698

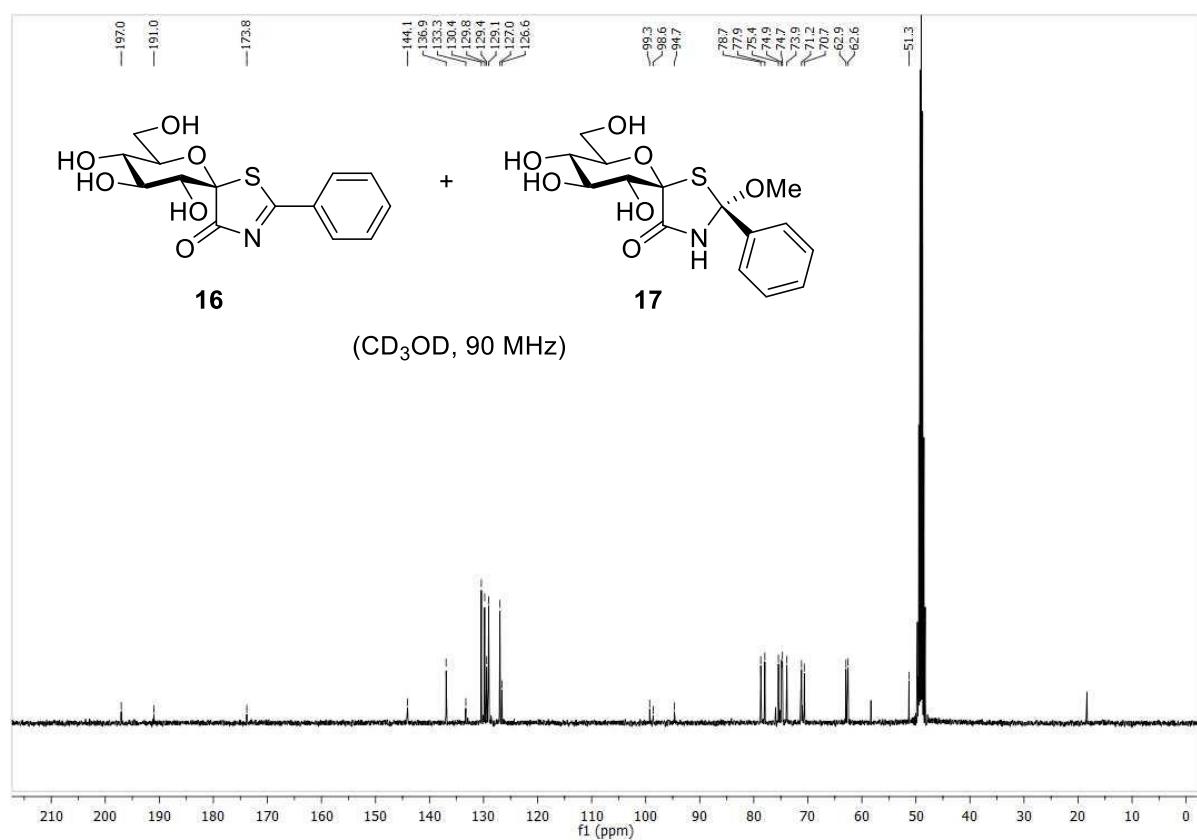
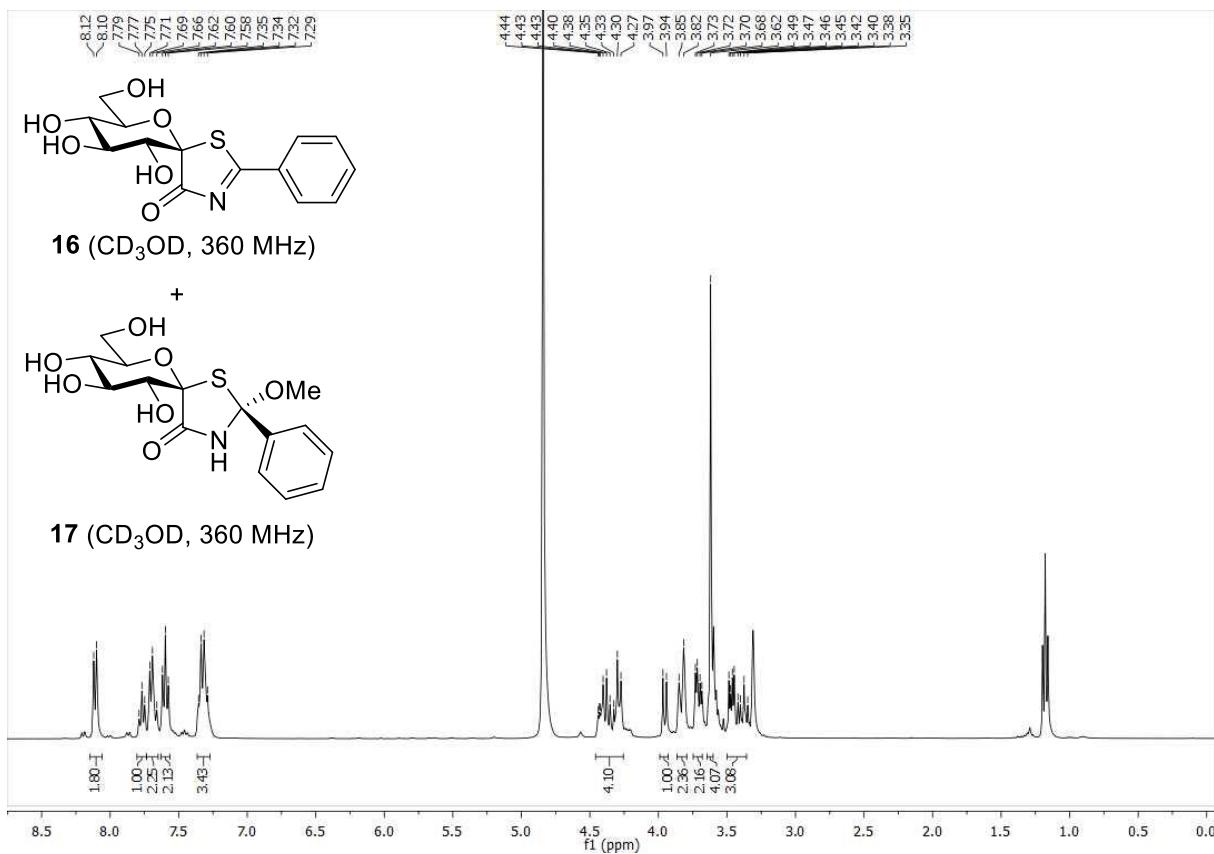


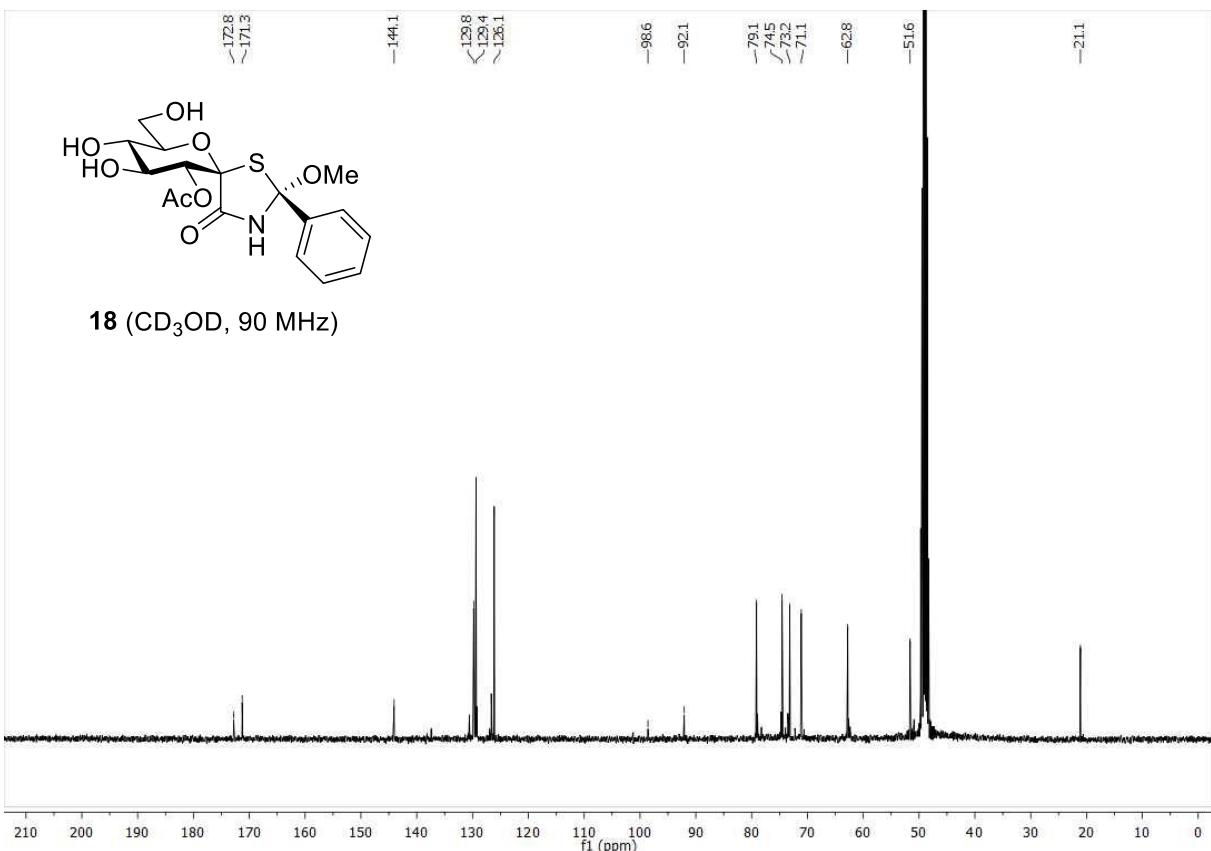
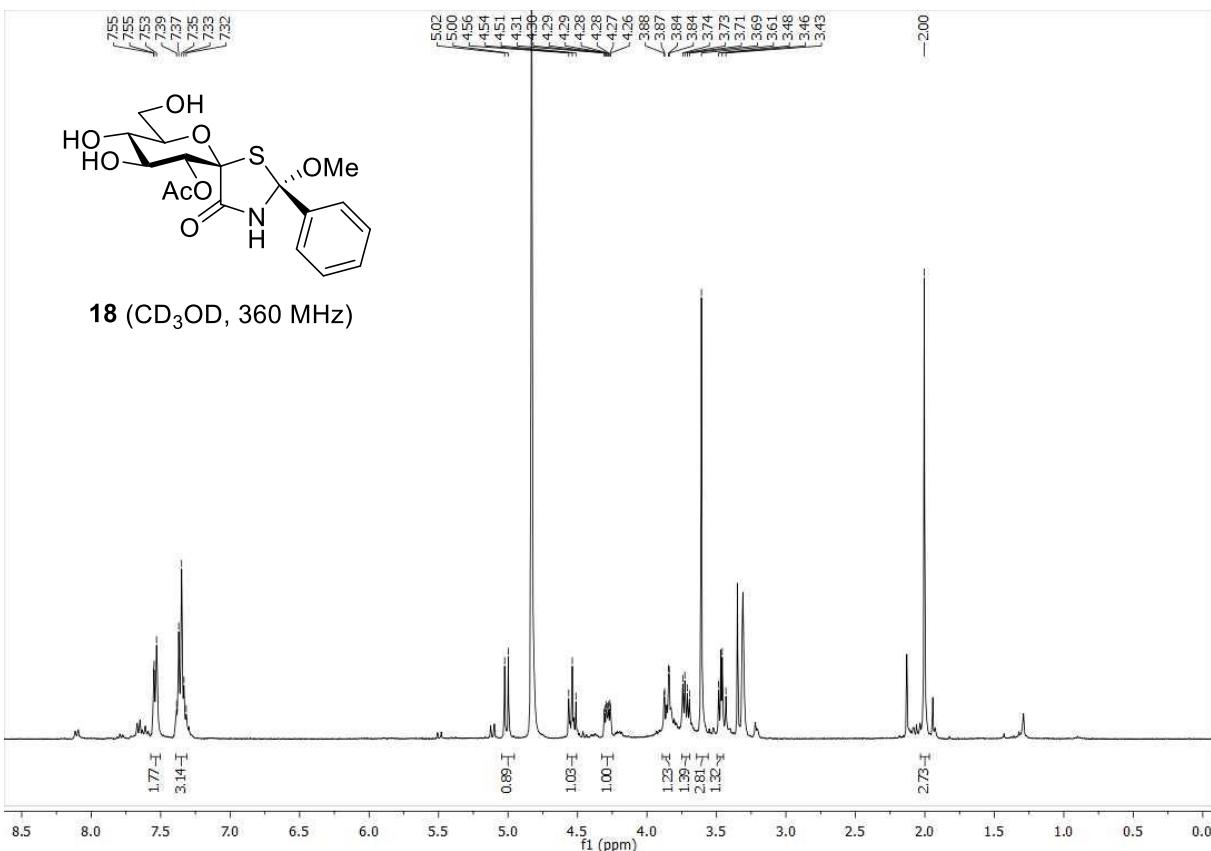
11 (D_2O , 100 MHz)

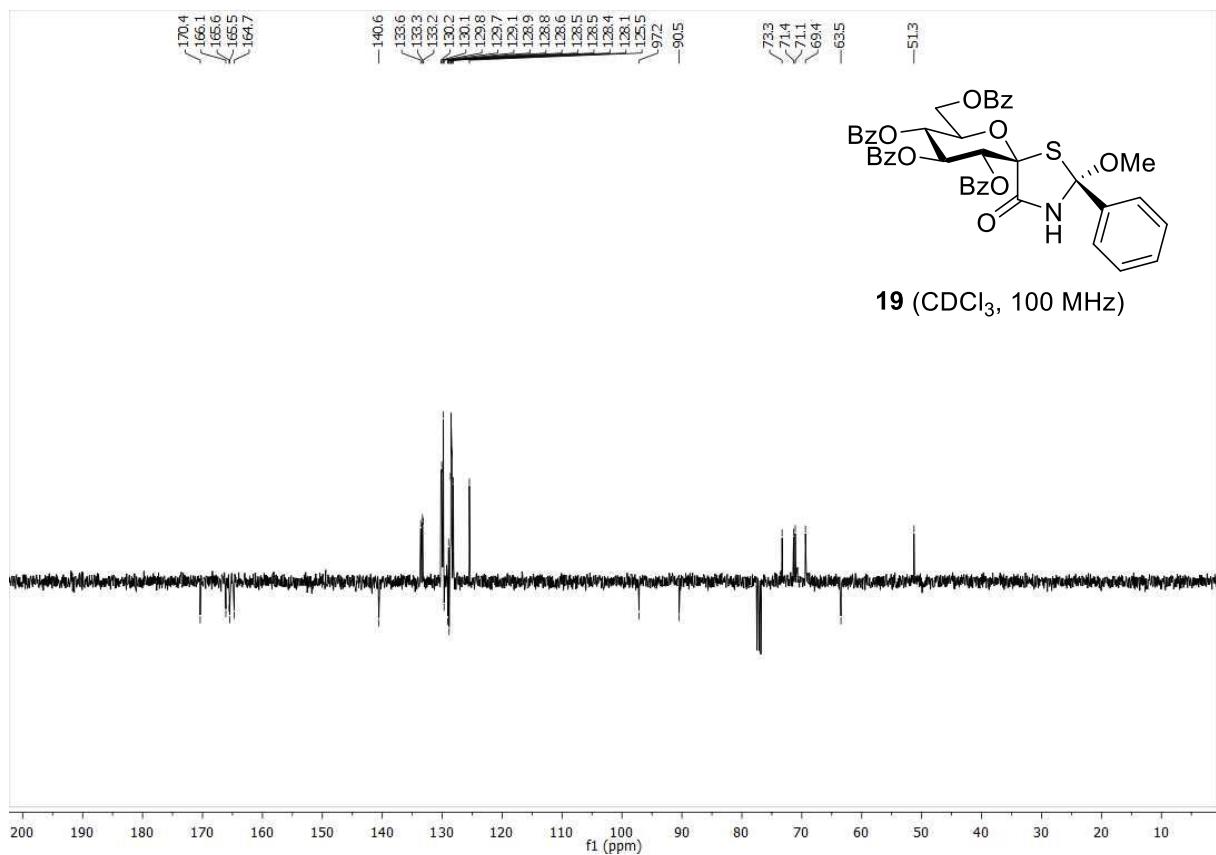
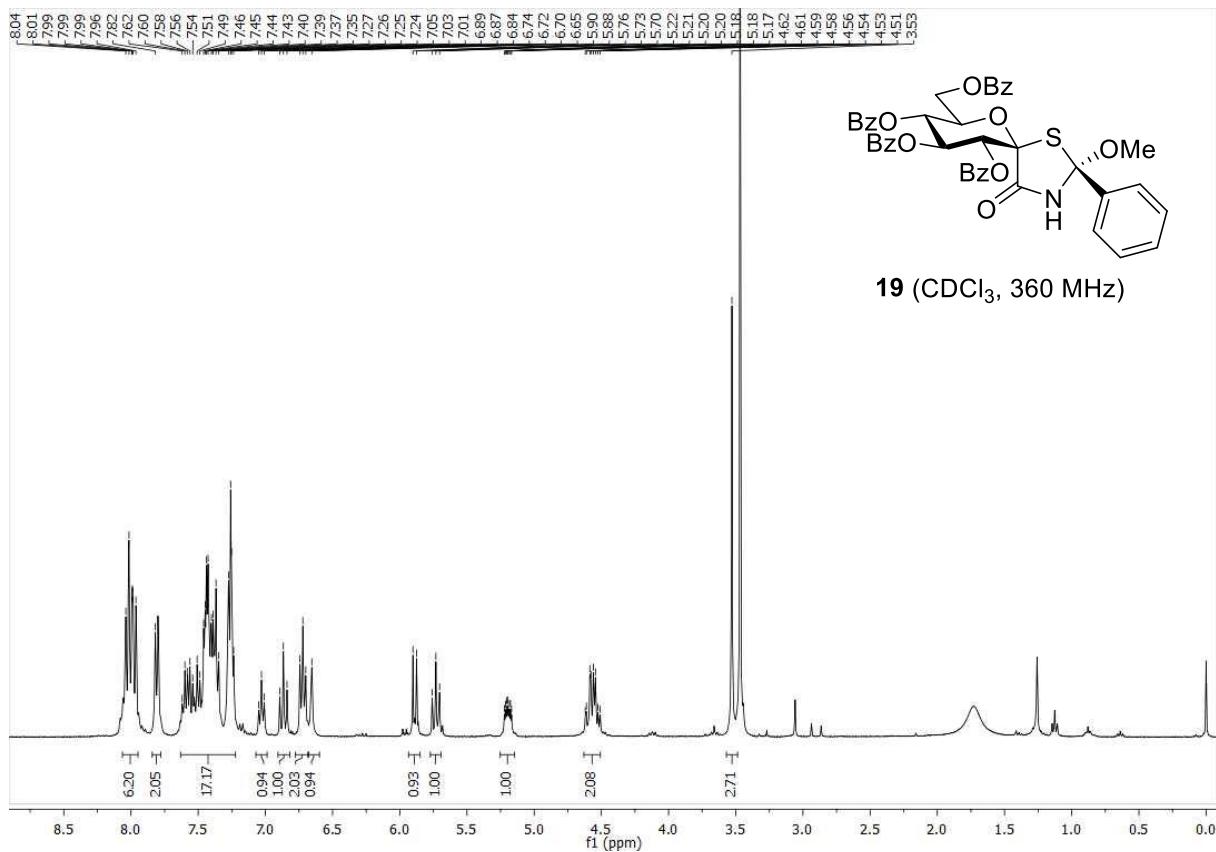


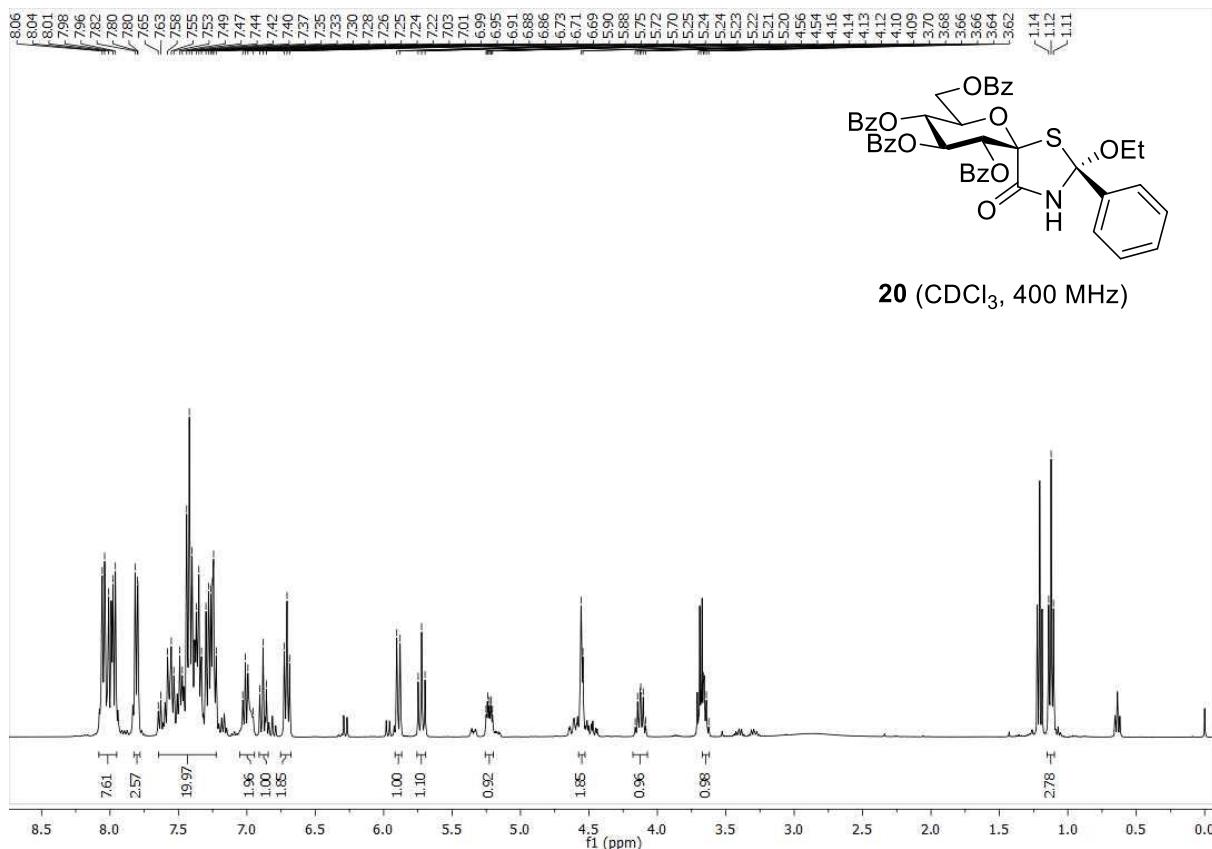


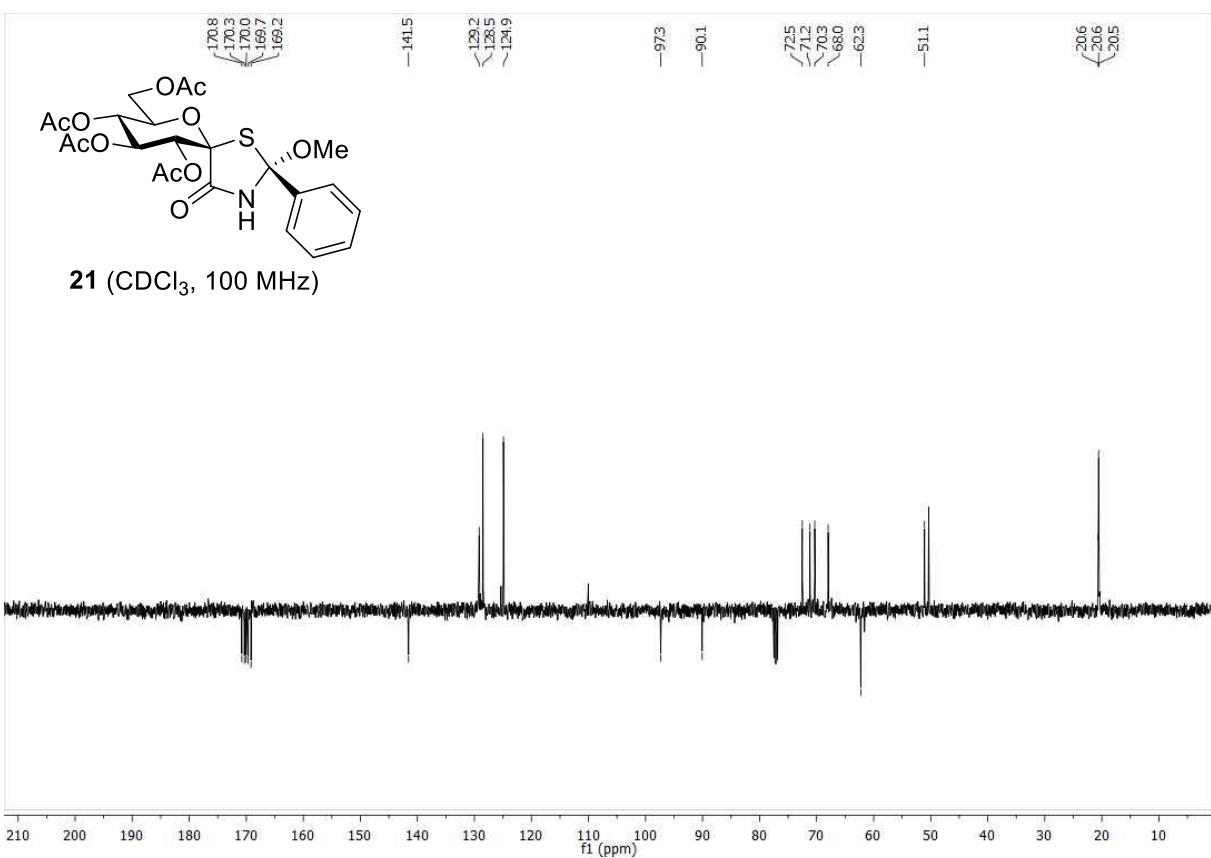
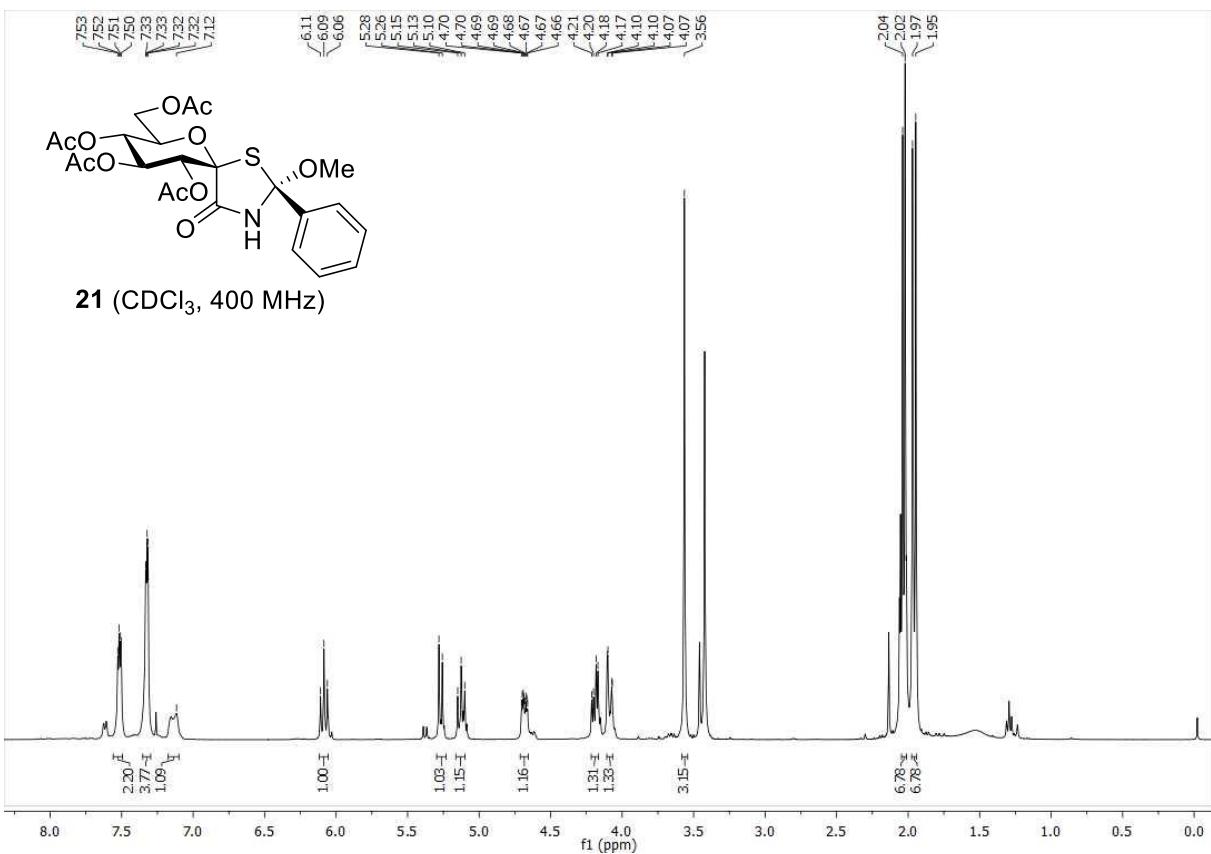


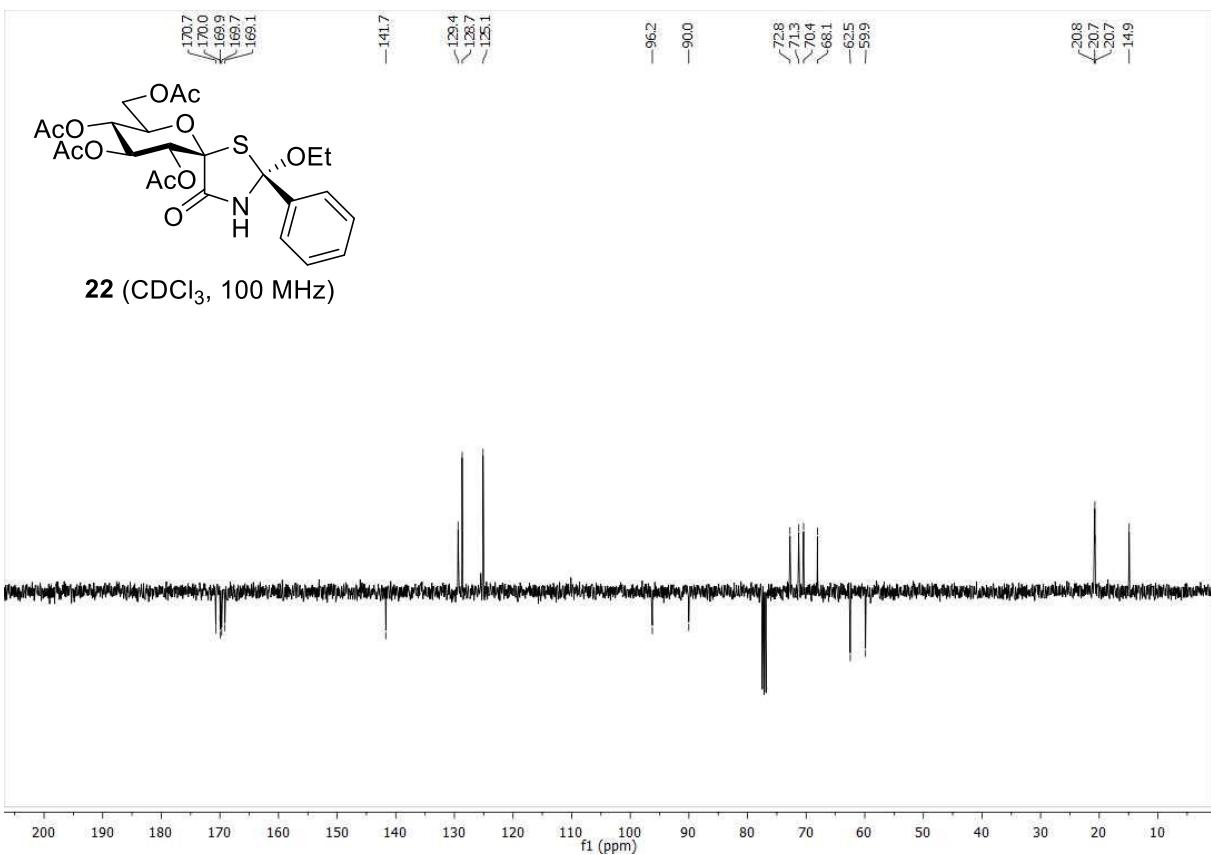
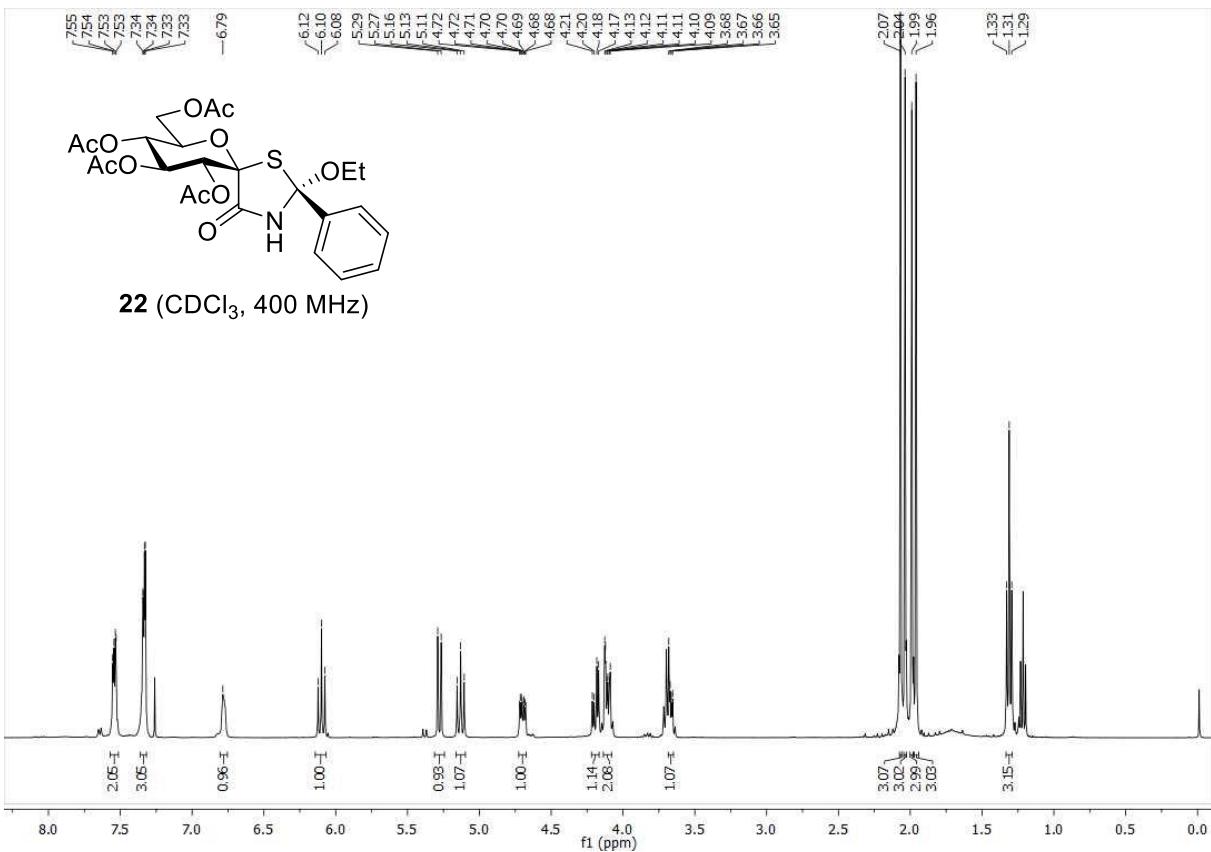


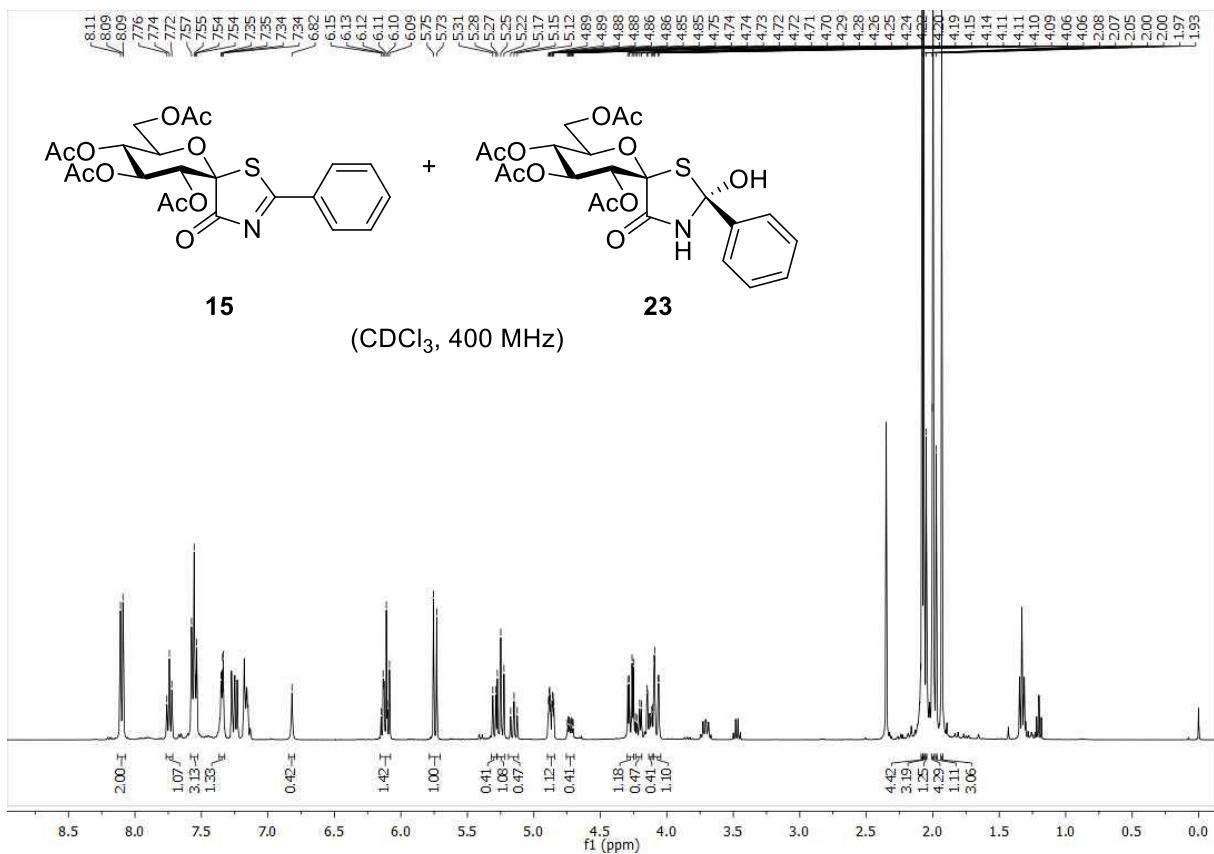


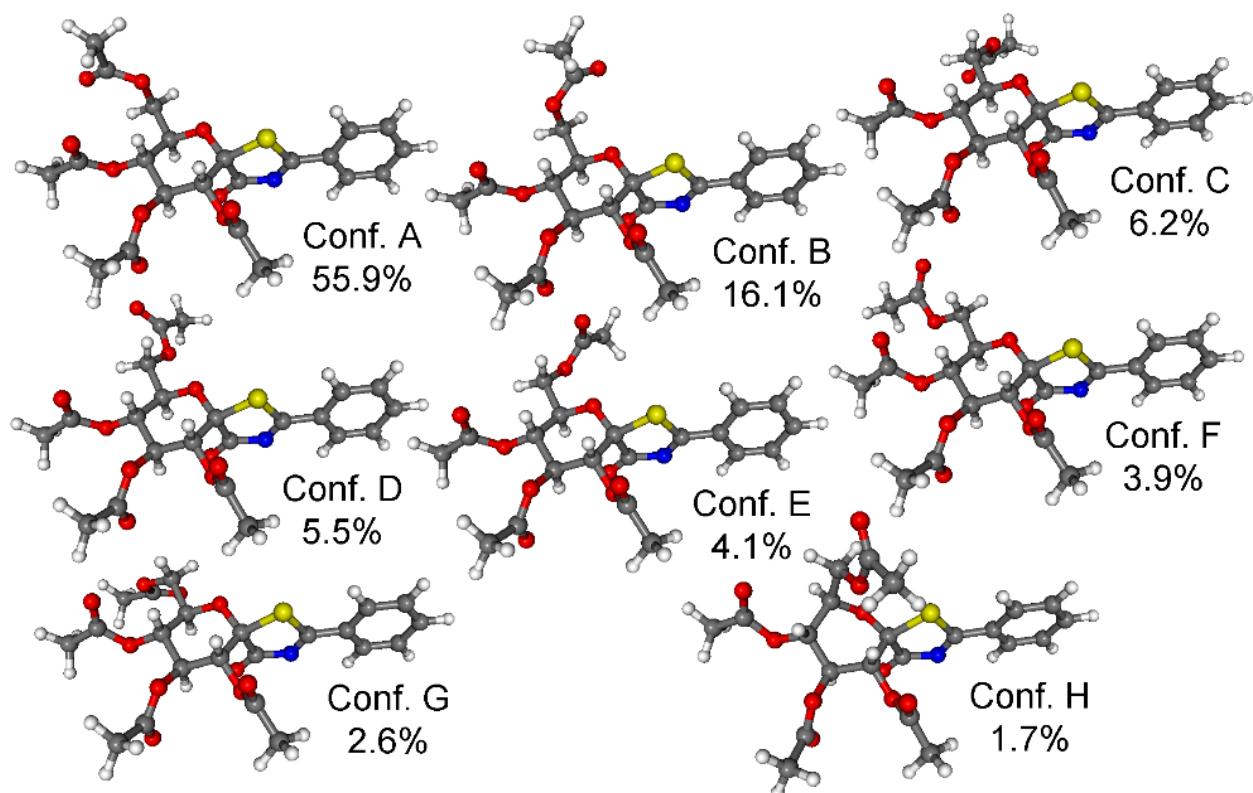




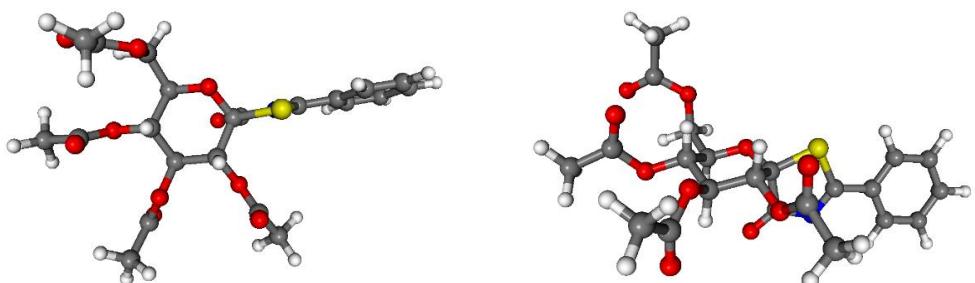








(a)



(b)

Figure S1. (a) Structures and populations of the low-energy ($\geq 1\%$) ω B97XD/TZVP PCM/MeCN conformers of (1'R)-15; (b) different views of conformer A to show steric hindrance of the C-2 carbon by the 2'-OAc substituent.

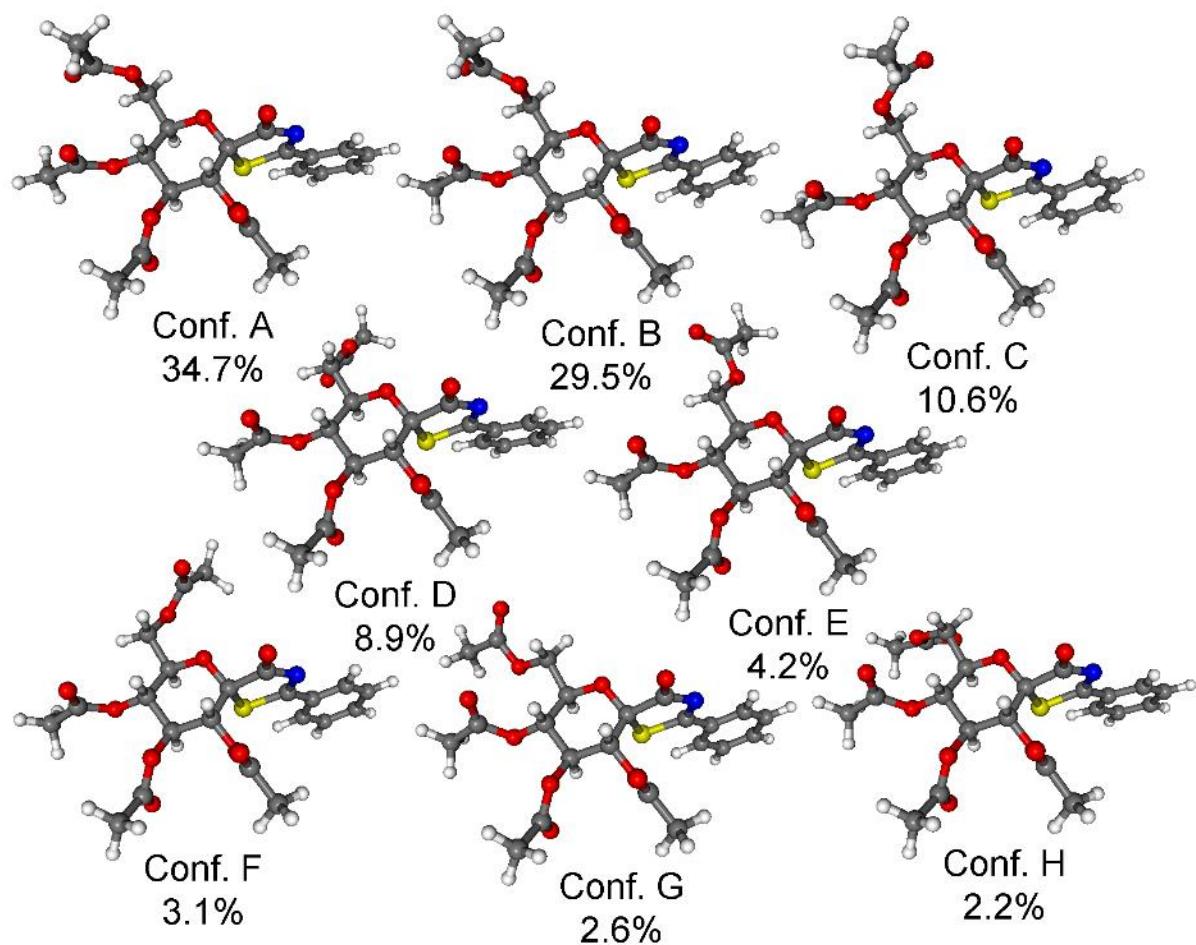


Figure S2. Structures and populations of the low-energy ($\geq 1\%$) ω B97XD/TZVP PCM/MeCN conformers of (1'S)-15.

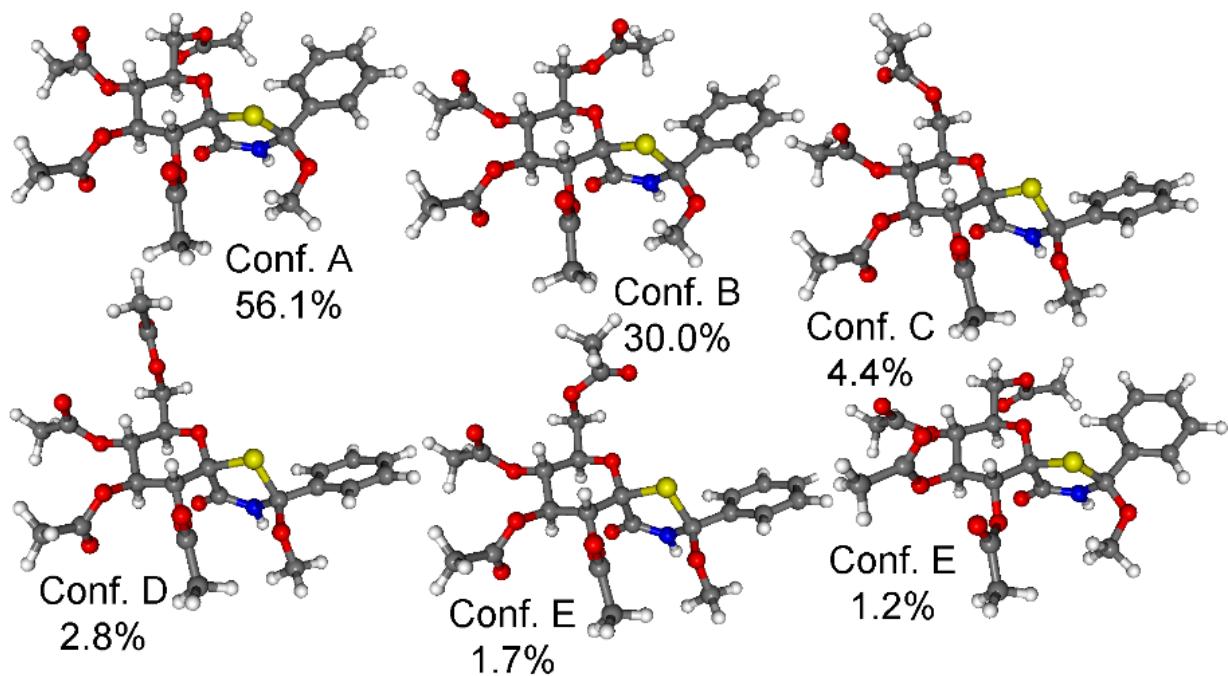


Figure S3. Structures and populations of the low-energy ($\geq 1\%$) ω B97XD/TZVP PCM/MeCN conformers of (2*R*,1'*R*)-**21**.

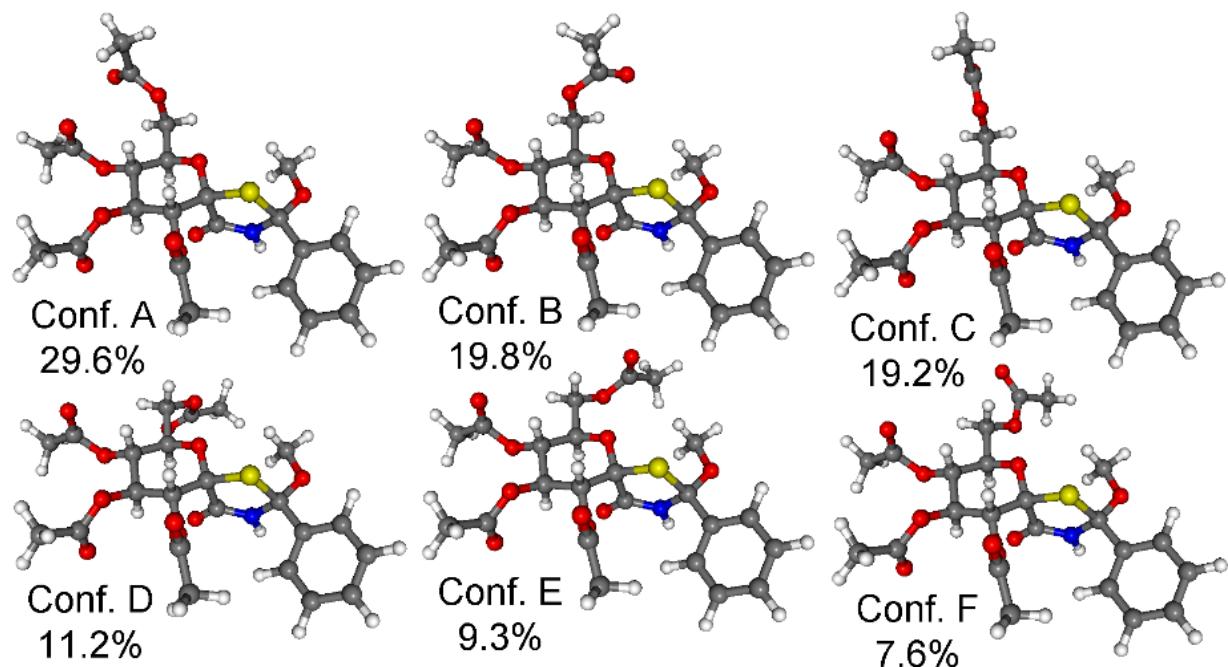


Figure S4. Structures and populations of the low-energy ($\geq 1\%$) ω B97XD/TZVP PCM/MeCN conformers of (2*S*,1'*R*)-**21**.