

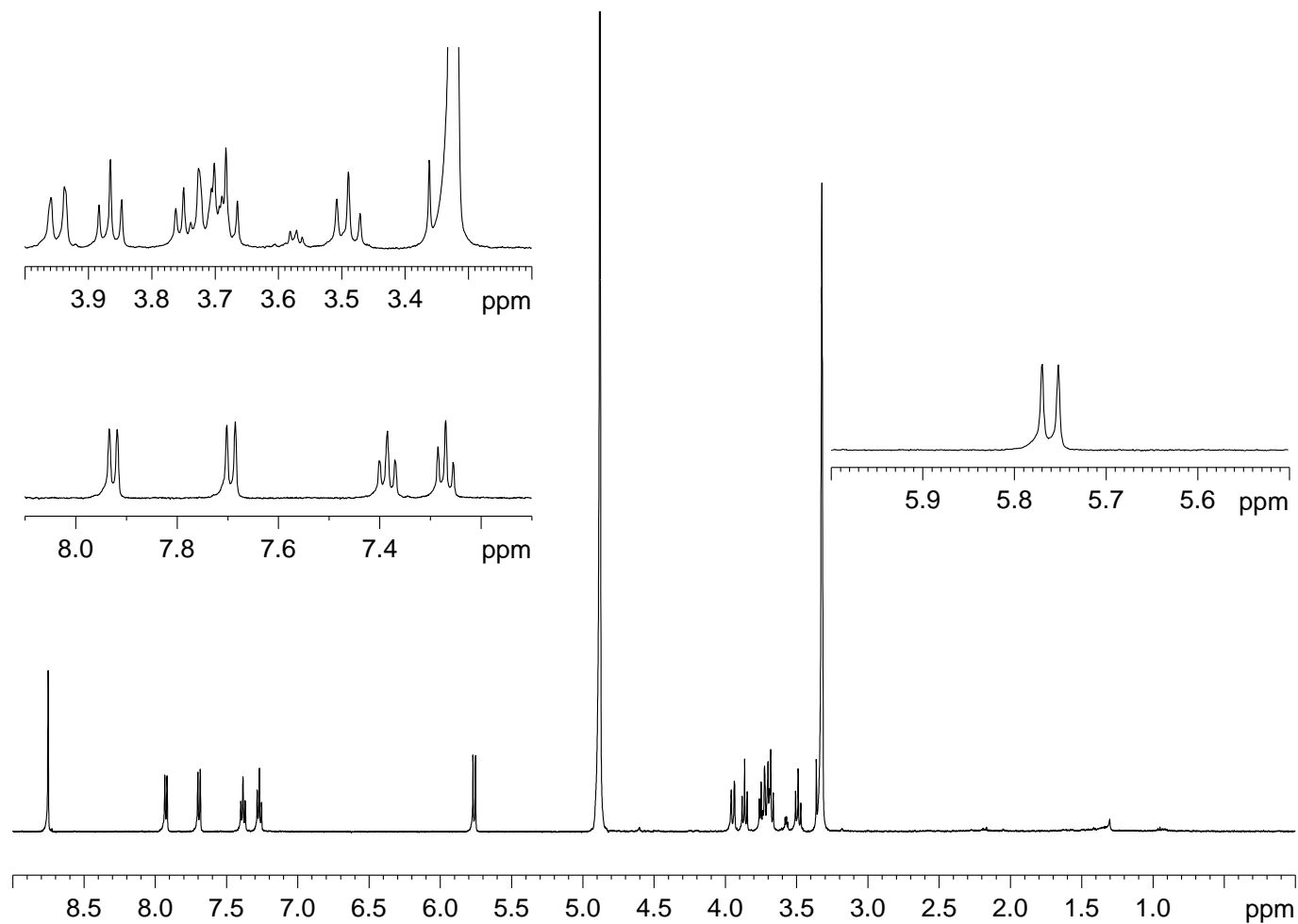
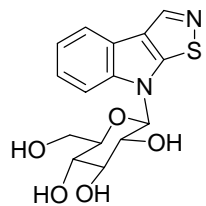
Supplementary Information for Manuscript

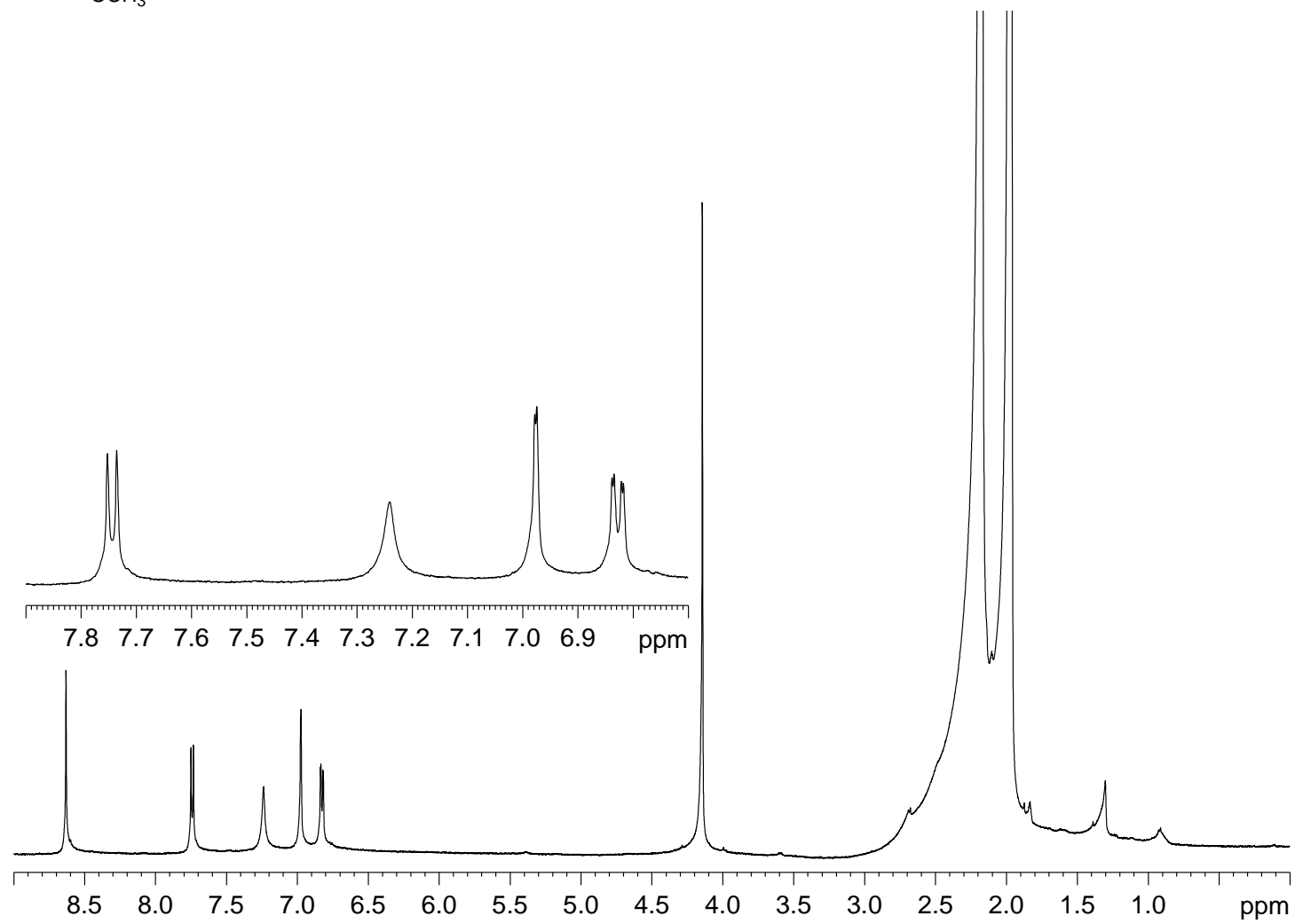
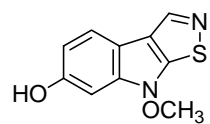
Metabolism of Crucifer Phytoalexins in *Sclerotinia sclerotiorum*: detoxification of strongly antifungal compounds involves glucosylation

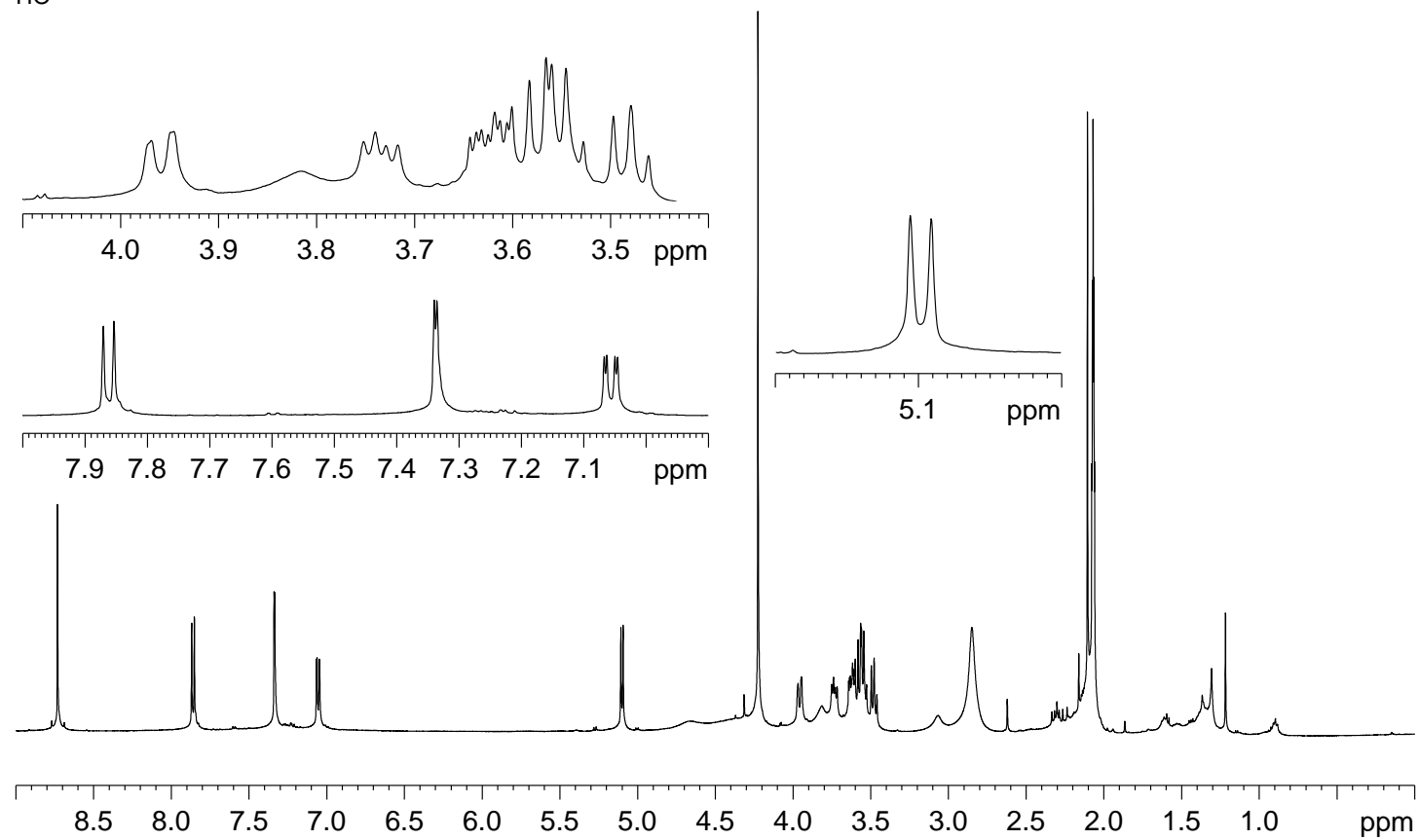
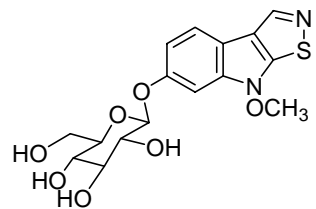
M. Soledade C. Pedras\* and Mohammad Hossain

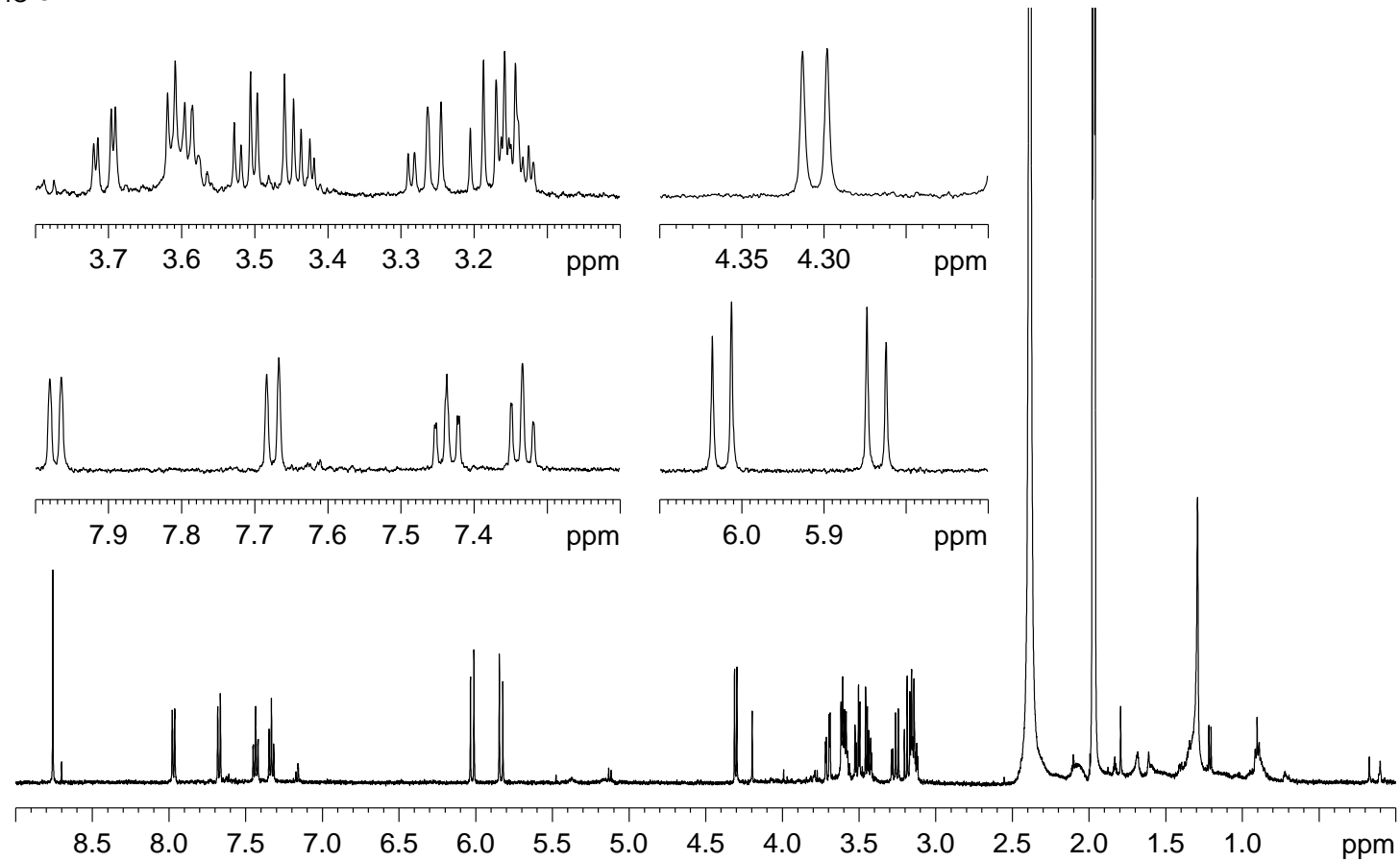
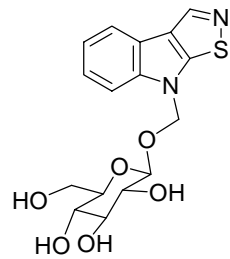
Department of Chemistry, University of Saskatchewan, 110 Science Place,  
Saskatoon, SK S7N 5C9, Canada

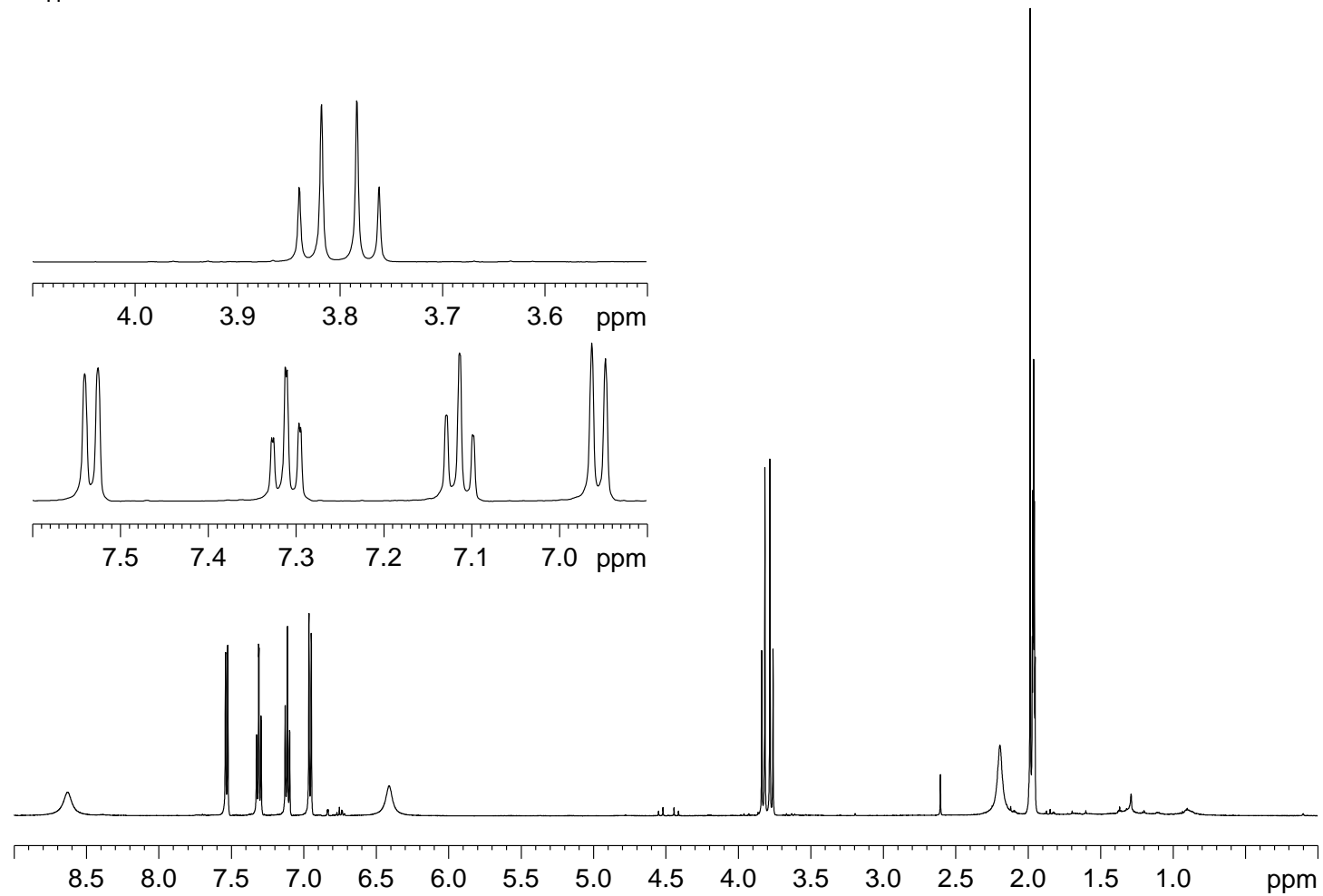
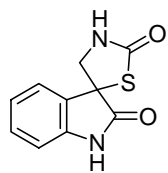
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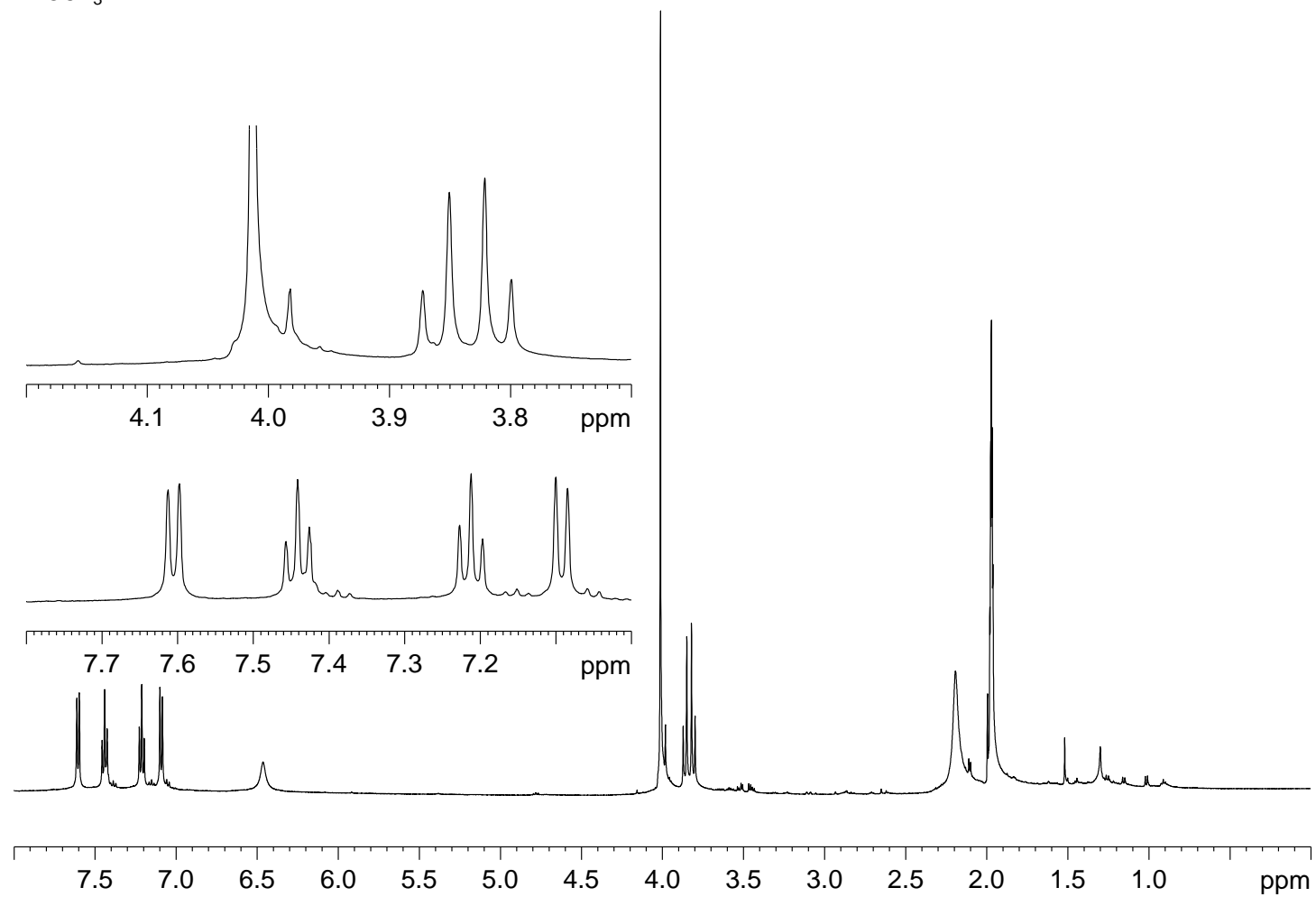
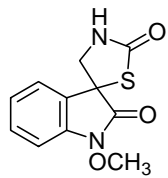
1- $\beta$ -D-Glucopyranosylbrassilexin (**12**, CD<sub>3</sub>OD)

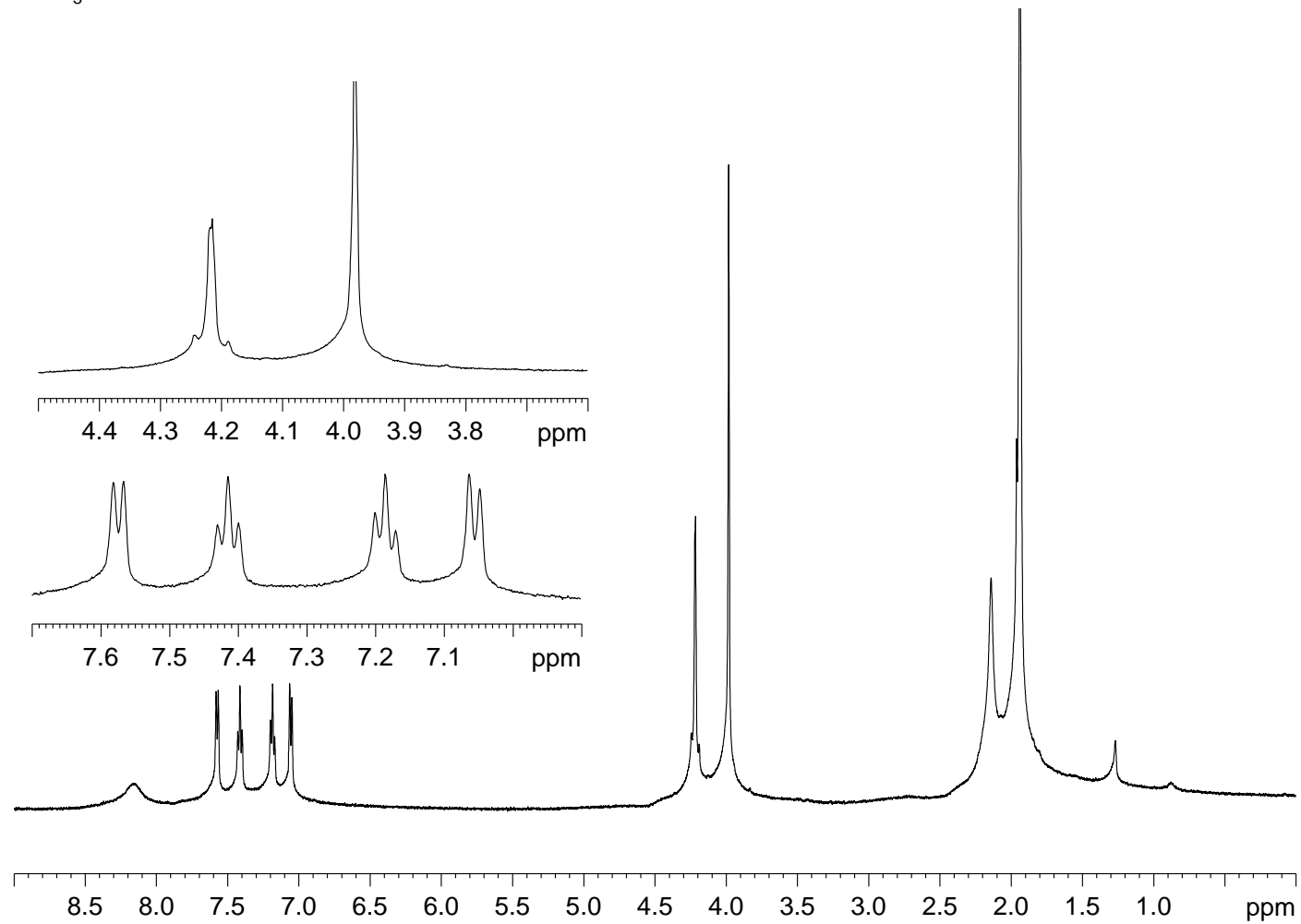
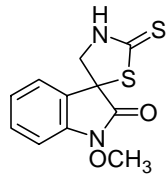
6-Hydroxysinalexin (**16**, CD<sub>3</sub>CN)

6-*O*- $\beta$ -D-Glucopyranosylsinalexin [17, (CD<sub>3</sub>)<sub>2</sub>CO]

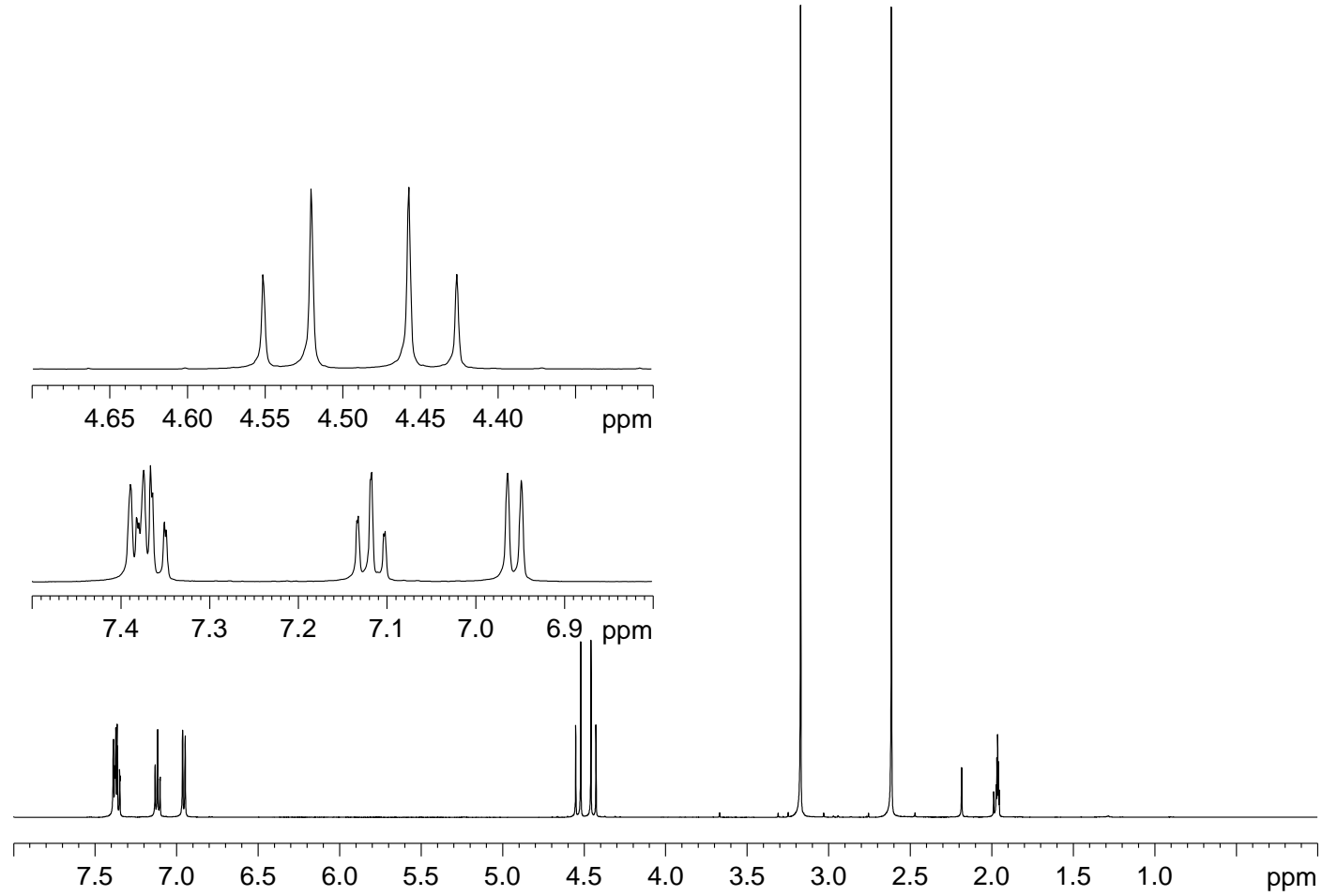
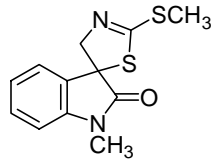
1-(*O*- $\beta$ -D-Glucopyranosyl)methylbrassicalexin [**19**, (CD<sub>3</sub>)<sub>2</sub>CO]

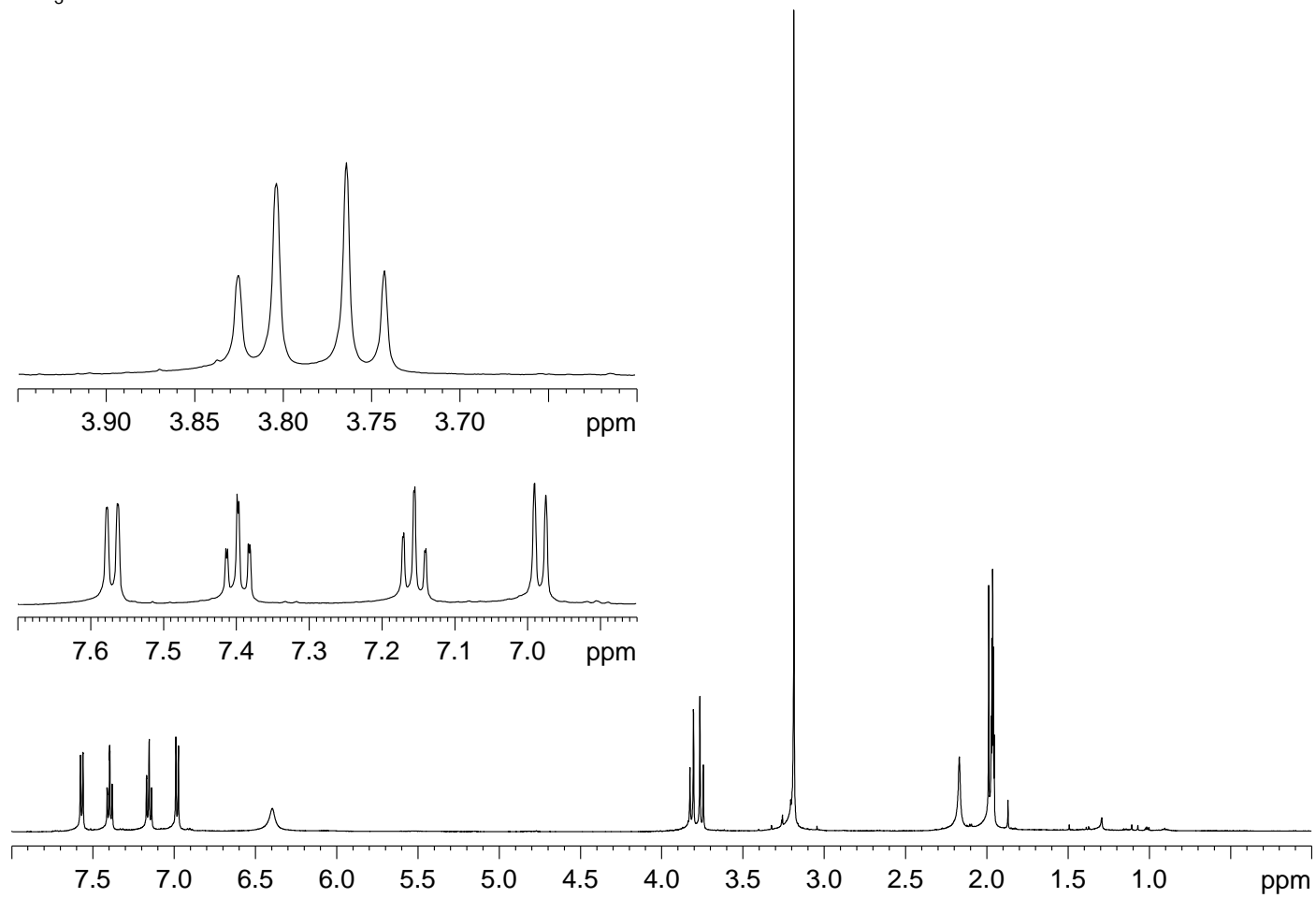
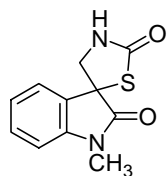
Spiro[3H-indole-3,5'-thiazolidin]-2(1H),2'-dione (**23**, CD<sub>3</sub>CN)

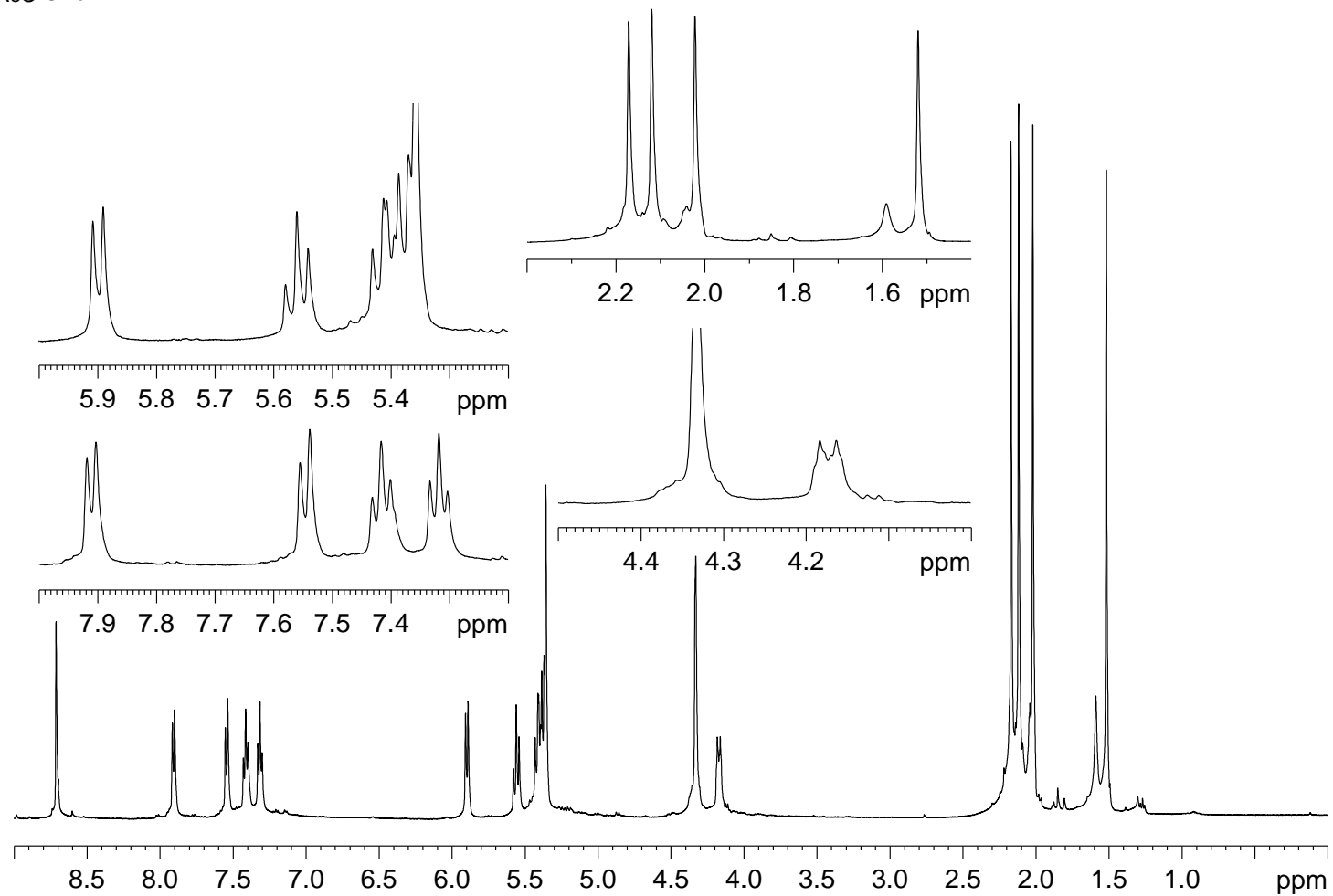
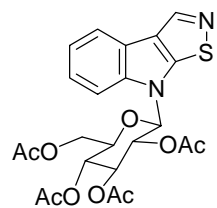
1-Methoxyspiro[3H-indole-3,5'-thiazolidin]-2(1H),2'-dione (**25**, CD<sub>3</sub>CN)

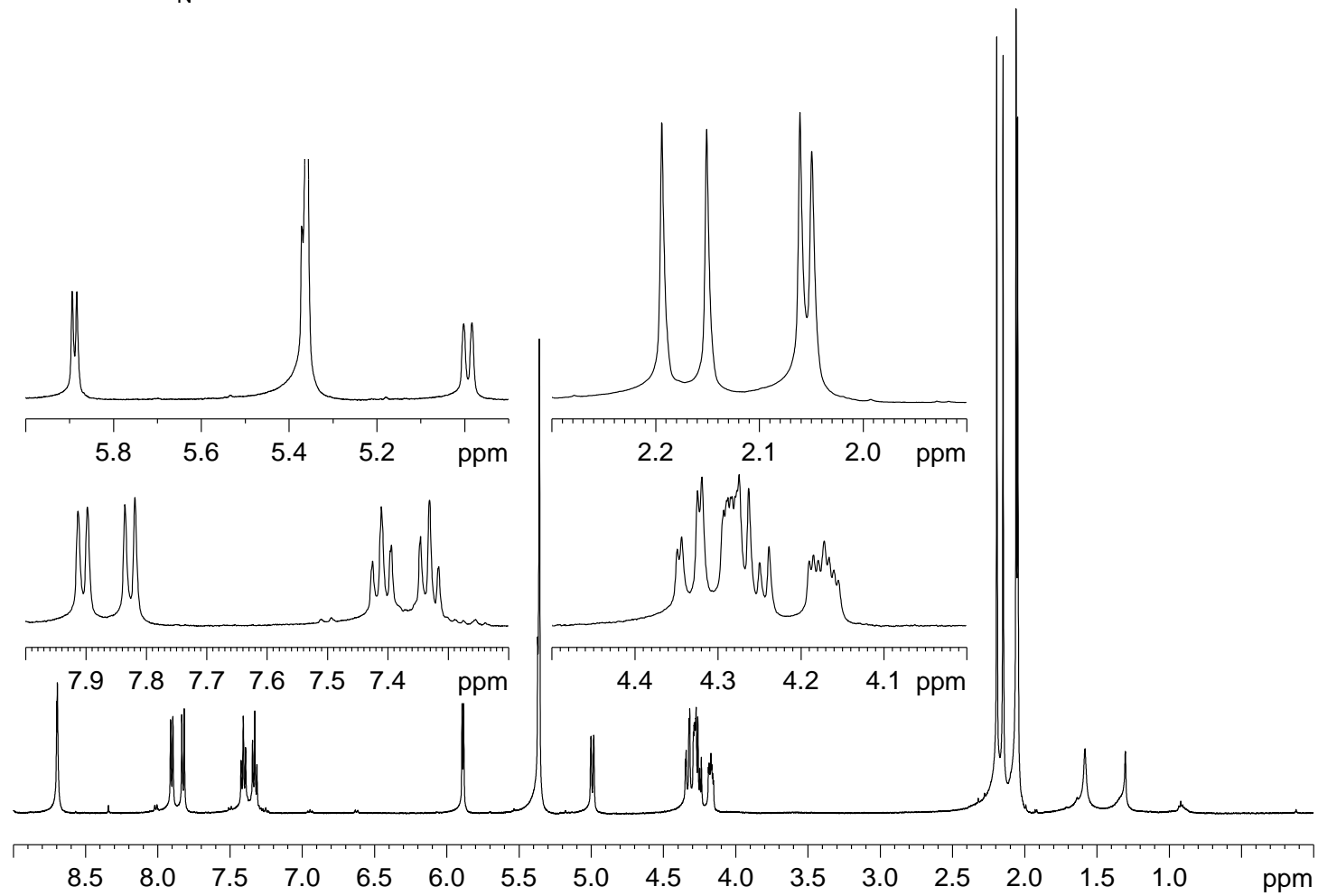
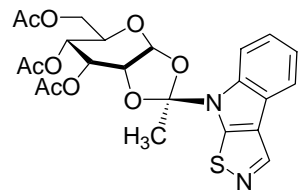
1-Methoxy-2'-thioxospiro[3H-indole-3,5'-thiazolidin]-2(1H)-one (**26**, CD<sub>3</sub>CN)

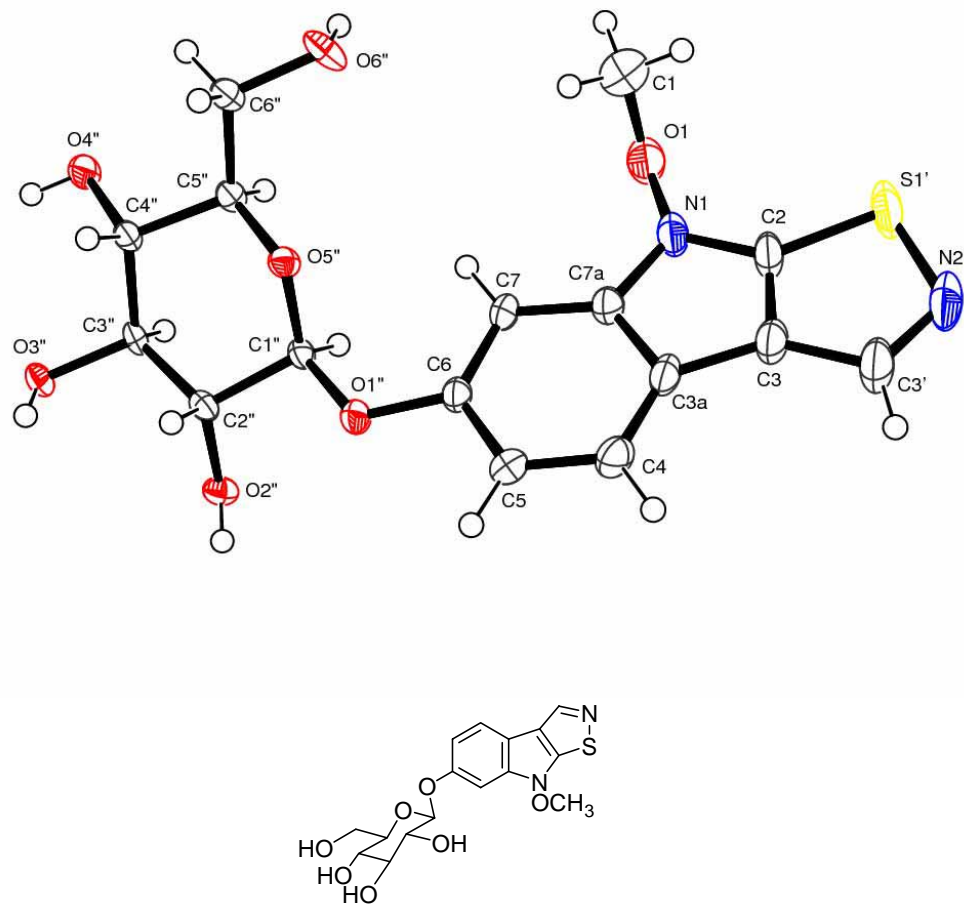


1-Methylspirobrassinin (**27**, CD<sub>3</sub>CN)

1-Methylspiro[3H-indole-3,5'-thiazolidin]-2(1H),2'-dione (**28**, CD<sub>3</sub>CN)

2,3,4,6-Tetra-*O*-acetyl-1- $\beta$ -D-glucopyranosyl brassilexin (**31**, CD<sub>2</sub>Cl<sub>2</sub>)

1-[1-(3,4,6-Tri-*O*-acetyl-1,2-*O*- $\alpha$ -D-glucopyranosyl)ethylidene]brassilexin (**32**, CD<sub>2</sub>Cl<sub>2</sub>)



**Fig. 3** X-ray structure of 6-oxy-(*O*- $\beta$ -D-glucopyranosyl)sinalexin (**17**): general ORTEP-3 view with non-H atom displacement ellipsoids drawn at the 50% probability level. The H atoms are drawn as small spheres of arbitrary size.

Empirical formula	C <sub>16</sub> H <sub>18</sub> N <sub>2</sub> O <sub>7</sub> S	
Formula weight	382.38	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21	
Unit cell dimensions	a = 13.8821(3) Å	$\alpha = 90^\circ$ .
	b = 4.5502(2) Å	$\beta = 109.8086(17)^\circ$ .
	c = 14.6589(4) Å	$\gamma = 90^\circ$ .
Volume	871.16(5) Å <sup>3</sup>	
Z	2	
Density (calculated)	1.458 Mg/m <sup>3</sup>	
Absorption coefficient	0.228 mm <sup>-1</sup>	
F(000)	400	
Crystal size	0.20 x 0.05 x 0.05 mm <sup>3</sup>	
Theta range for data collection	1.75 to 27.48°.	
Index ranges	-18<=h<=17, -4<=k<=5, -19<=l<=18	
Reflections collected	10196	
Independent reflections	3438 [R(int) = 0.0632]	
Completeness to theta = 27.48°	99.7 %	
Absorption correction	Psi-scan	
Max. and min. transmission	0.989 and 0.925	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	3438 / 1 / 239	
Goodness-of-fit on F <sup>2</sup>	1.058	
Final R indices [I>2sigma(I)]	R1 = 0.0471, wR2 = 0.1037	
R indices (all data)	R1 = 0.0559, wR2 = 0.1090	
Absolute structure parameter	0.10(12)	
Largest diff. peak and hole	0.324 and -0.320 e.Å <sup>-3</sup>	