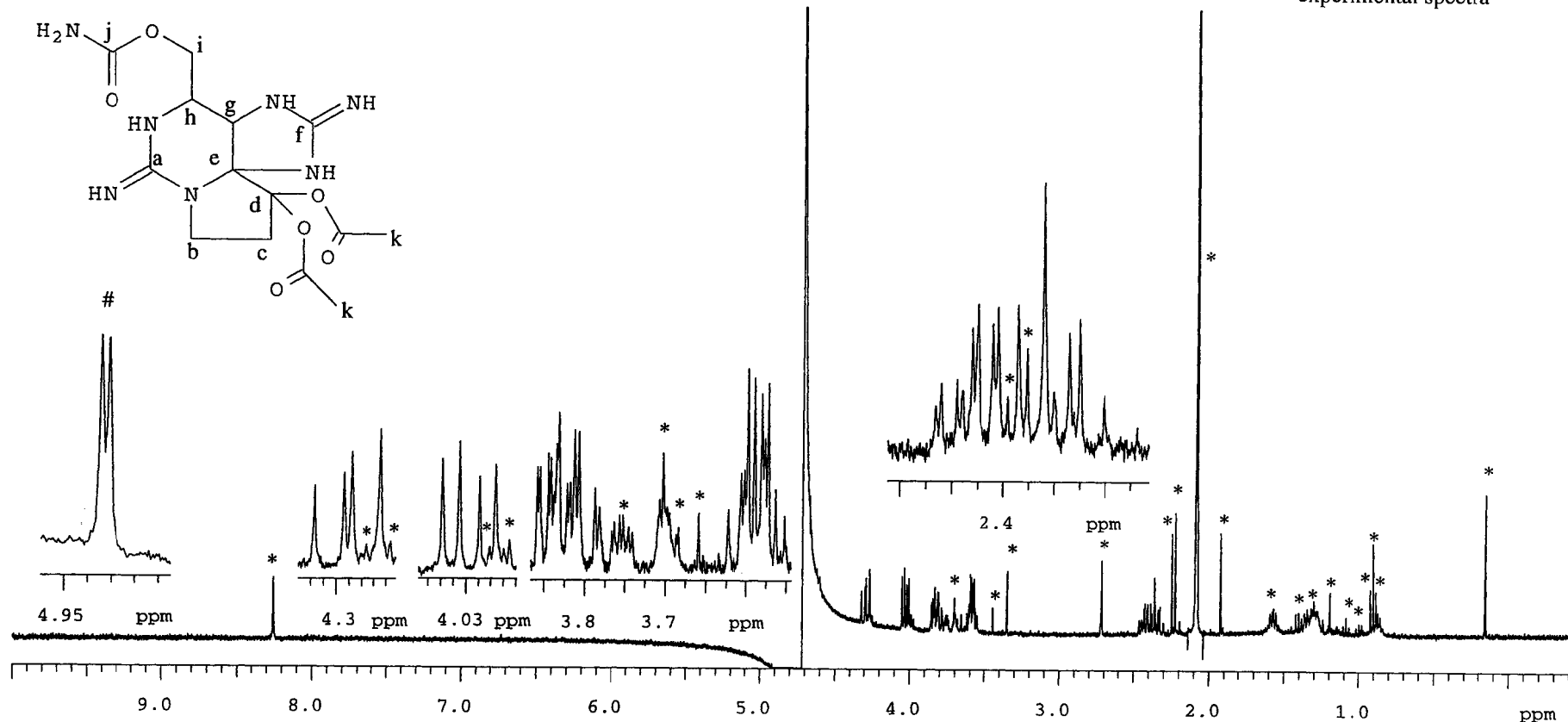


Saxitoxin (Saxitoxin diacetate)

[35523-89-8]

¹H NMRNext page: Simulated (top) and
experimental spectra

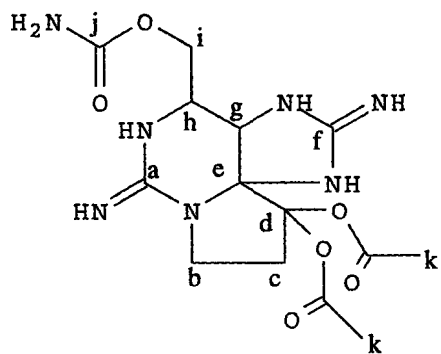
Solvent: D₂O; pH 2.5
 Concentration: 10 µg/ 0.8 ml
 Reference substance: ext. TSP-d₄
 Sample temperature: 30.0 °C
 Resonance frequency: 400.132 MHz
 Spectral width: 5102.0 Hz
 Data points (FID; spec.): 64 k; 64 k

Flip angle; Pulse width: 90 °; 5.5 µs
 No. of scans; Rep. time: 4096; 16.4 s
 Weighting; Line broad.: exp.; 0.1 Hz
 Spectral resolution: 0.5 Hz (0.16 ppm)
 Instrument: Bruker AMX-400
 Source reference: 990216-4956
 Signature: *Markku Mesilaakso*
 Markku Mesilaakso

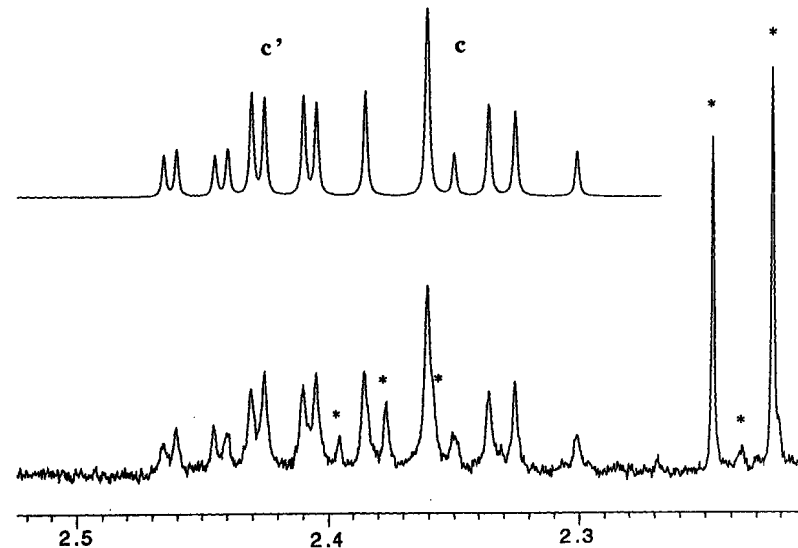
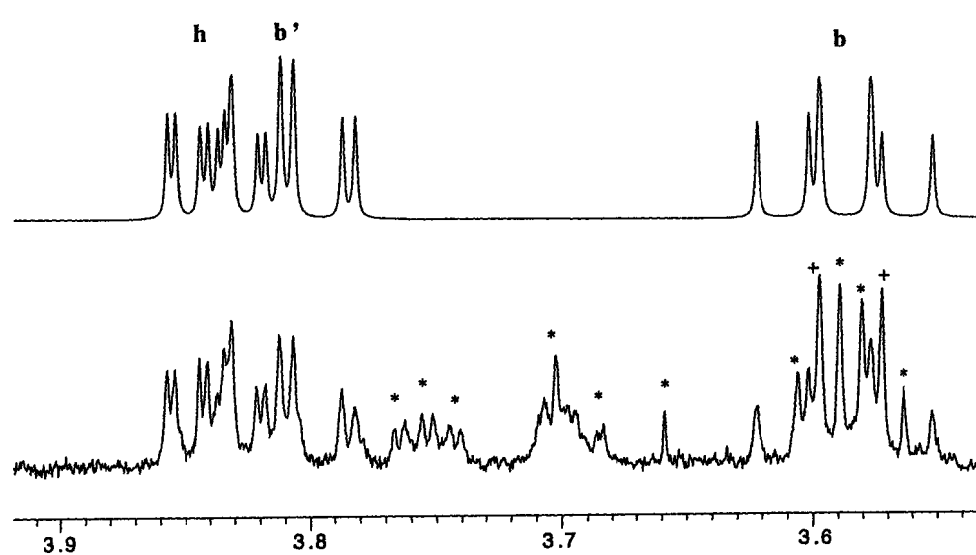
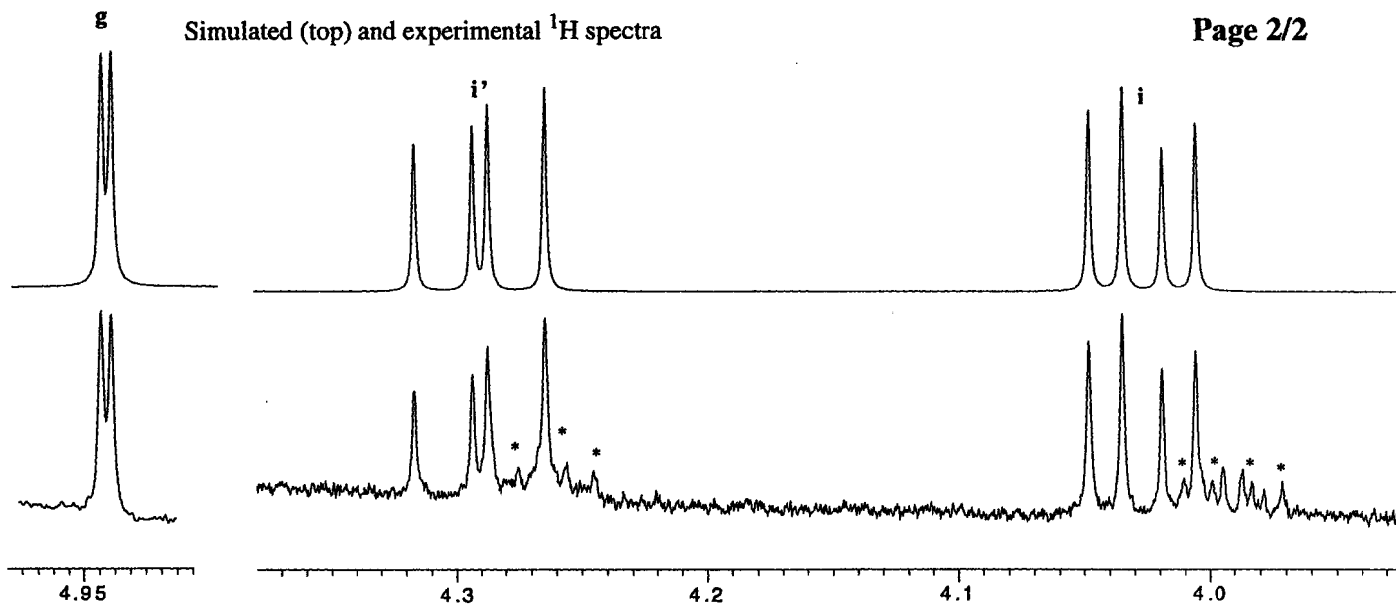
nuc.	δ [ppm]	J [Hz]	nuc.	δ [ppm]	J [Hz]
b	3.588	-10.2 (b'); 9.8 (c); 8.2 (c')	h	3.839	5.3 (i); 9.2 (i')
b'	3.809	10.2 (c); 1.7 (c')	i	4.028	-11.7 (i')
c	2.347	-14.0 (c')	i'	4.290	
c'	2.432		k	2.09	tentative assignment
g	4.93	1.3 (h)			

k probably overlaps with resonance of acetic acid
 # expansion of g from spectrum recorded at 50 °C

Saxitoxin (Saxitoxin diacetate)
[35523-89-8]



Simulated (top) and experimental ¹H spectra



+ resonance line overlapping with an impurity