SUPPORTING INFORMATION

Discovery and characterization of a sulfoquinovose mutarotase using kinetic analysis at equilibrium by exchange spectroscopy

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Contents

*Hs*SQM plasmid and sequence data

plasmid	resistance	details
pET29-HsSQM	Kan	C-terminal His_6-tagged *Herbaspirillum seropedicae* strain AU14040 sulfoquinovose mutarotase (WP_069374721.1)

pET29-HsSQM

CDS:

ATGTCGGCAGCTCTTGCGTCCCTGACACTTGCCCAAGGACCGTGGCAAGTGCGCGTGCTGCCTGCACTGGGCGGTGCGATTGC
AAGCGCCAGCTGGCGTGGTCAGCCGGTGCTGCGCCCGAGCGTCGAGGCACAGCTGCAGCAGGGCCTGGTTAGACGCTCTGCGT
GCTATCCGCTGCTGCCGTTTAGTAACCGTATCGGAAACGCGCAATTCGCCTTTGATGGCCAGACATACGCGCTGATTGCCAAC
TTTGACAACGAACCGCACGCTATCCACGGGCTGGGCTTTCAGCGCGCGTGGCAGGTTCAGTCTAGCTCGGCGGAAAGTCTTAC
TATGCAGCTCACCCACGCCTCGCCGAGCCCGGGTCAGTGGCCGTTTGCCTTGCGTGCCACCCAGGTGATTGCCATCGAAGGCG
ACGATCTGGTGCTGCGCCTGGAAGTGGAAAATACCGATCATCGCCGCGCCCCATGCGGCCTGGGCTGGCATCCGTTTTTTCCG
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CAGCACGGCCCCTCCGGATACGACCCAACTGGATACCTTAGTGATTGATAATTGCTTTACCGGCTGGAGCGGCCAGGCCGTCG
TTACCGGCCCCGCATCATCGTATTACCCTGACAGCGAGCCCGACCCTGCGTTGCGCGGTGCTGTTTCGCCCGCCGGGGCAGCCG
TTCTTCGCGTTTGAACCGGTGAGCCATCCGAACAATGCCCTGCACGGCGTTGCGCCGGCGATGCACATCCTGGAACCCGGTCA
GTGCCTGGCGGGCGAAATGCGCCTGAGCCTGTCGACCGCTCCGAGCATTCTGGCGGCCGCACTCGAGCACCACCACCACCACC
ACTGA

Translation:

MSAALASLTLAQGPWQVRVLPALGGAIASASWRGQPVLRPSVEAQLQQGLVRRSACYPLL
PFSNRIGNAQFAFDGQTYALIANFDNEPHAIHGLGFQRAWQVQSSSAESLTMQLTHASPS
PGQWPFALRATQVIAIEGDDLVLRLEVENTDHRRAPCGLGWHPFFPLDSAAQPTQLQTHW
QAMLVNGPDKLPCGSTAPPDTTQLDTLVIDNCFTGWSGQAVVTGPHHRITLTASPTLRCA
VLFRPPGQPFFAFEPVSHPNNALHGVAPAMHILEPGQCLAGEMRLSLSTAPSILAAALEH
HHHHH*

Table S1. Pairwise sequence comparisons of HsSQM with various hexose mutarotases.[*]

H. seropediaceae	***P. putida***	***E. coli***	***L. lactis***	***S. cerevisiae***	
***Hs*SQM** WP_069374721.1	**PpSQ_00415** KHL76357.1	**YihQ** NP_418315.3	**GalM** WP_039116219.1	**YMR099C** DAA09996.1	**% identity (%similarity)**
	35 (49)	19 (38)	13 (26)	13 (28)	**HsSQM**
		19 (37)	12 (24)	15 (29)	**PpSQ_00415**
			12 (29)	11 (23)	**YihQ**
				14 (23)	**GalM**
					YMR099C

[*] Calculated using the "Sequence Manipulation Suite" and the following groupings of similar amino acids: GAVLI, FYW, CM, ST, KRH, DENQ, P.

See: http://www.bioinformatics.org/sms2/ident_sim.html, Stothard, P. *Biotechniques*, 2000, 28, 1102–1104.

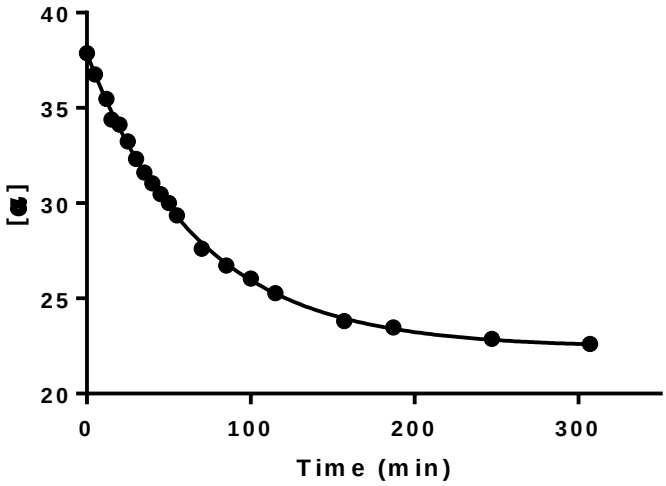
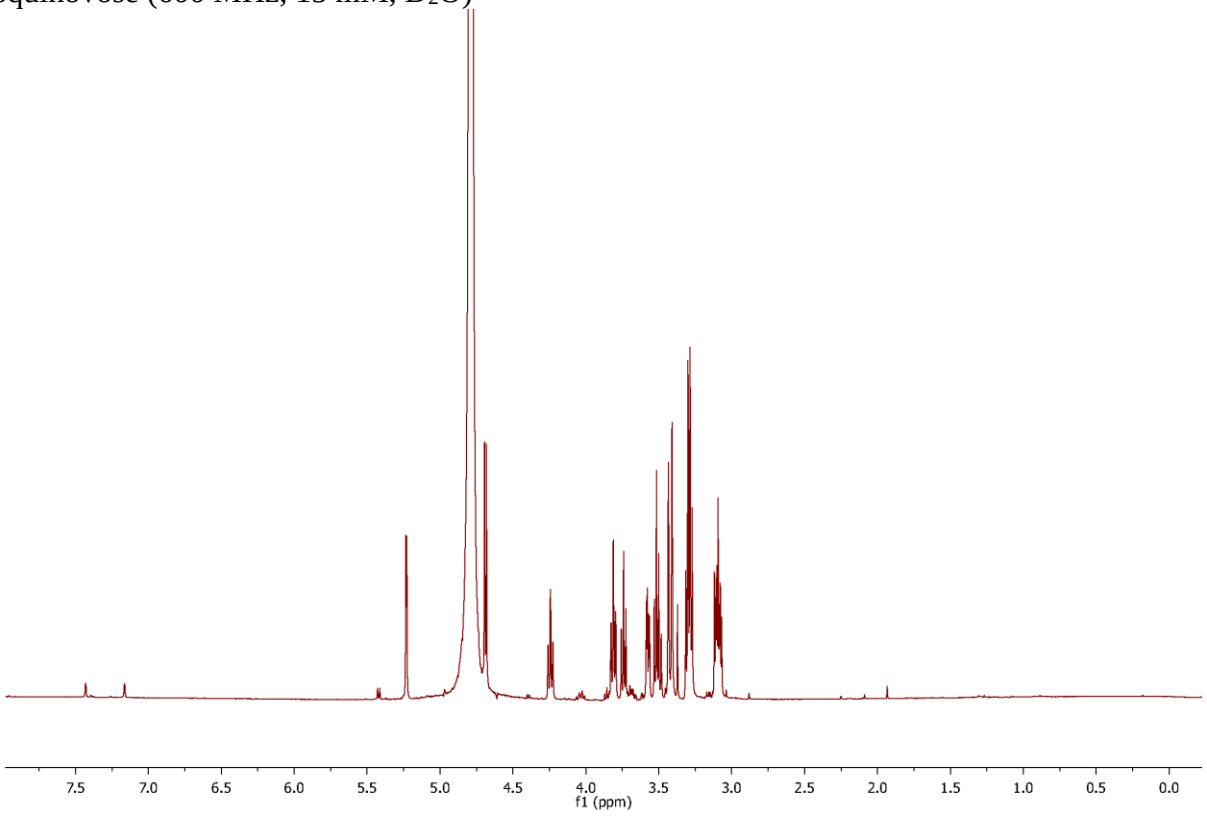


Figure S1. Mutarotation of SQ monitored by polarimetry.

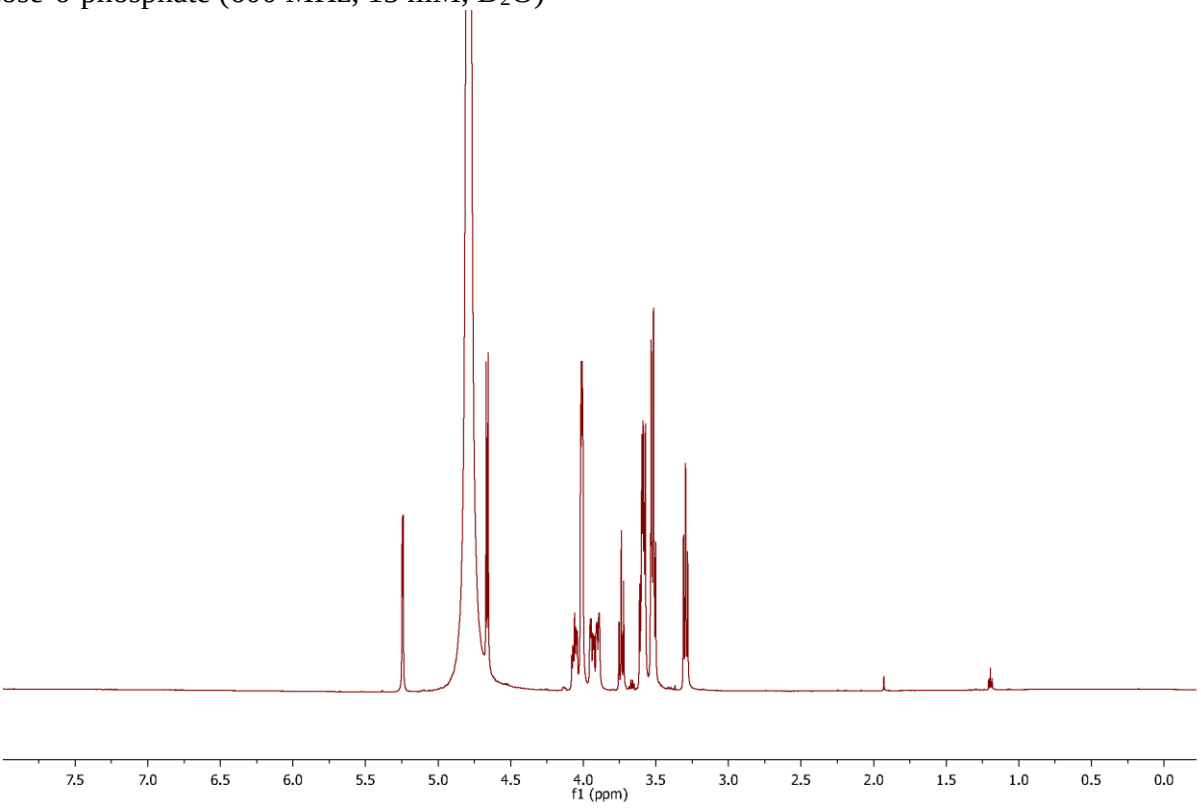
4-Nitrophenyl α-D-sulfoquinovoside in 50 mM sodium phosphate, 150 mM NaCl in H_2O (pH 7.1) was treated with sulfoquinovosidase, and after 5 min, the specific rotation was monitored as a function of time. pH 7.1, 26±1 °C.

1D ^{1}H NMR spectra

Sulfoquinovose (600 MHz, 15 mM, D_2O)

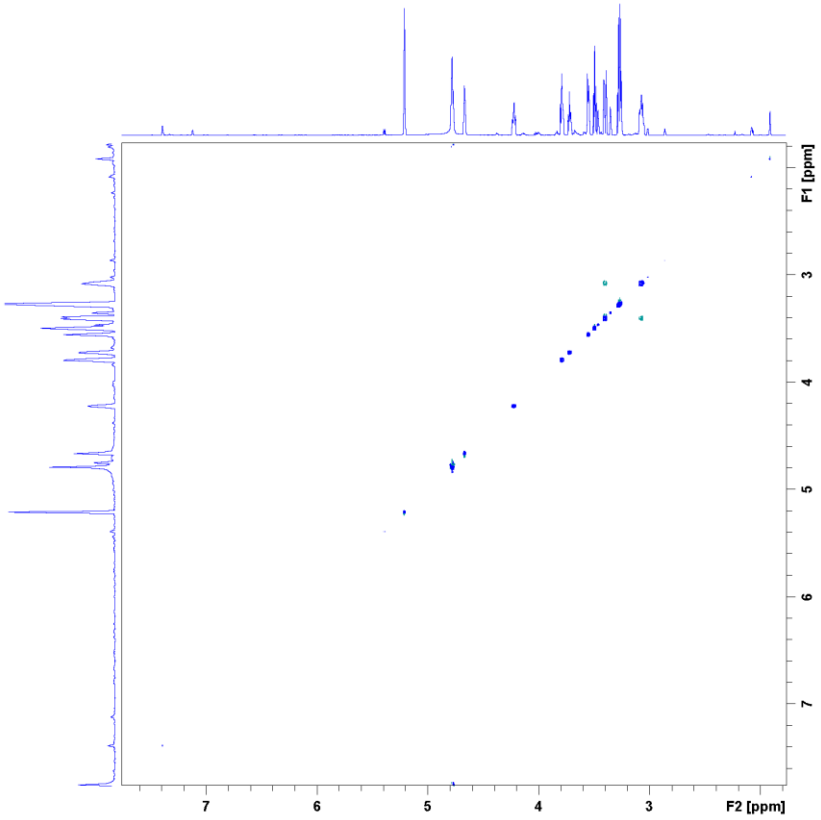


Glucose-6-phosphate (600 MHz, 15 mM, D_2O)

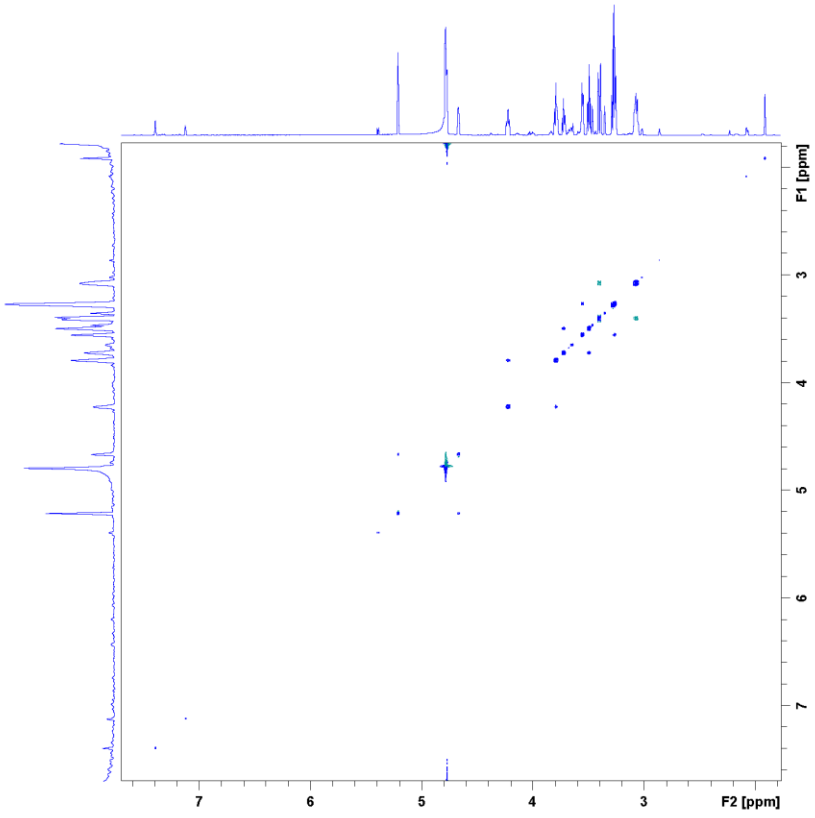


2D ^{1}H-^{1}H NOESY spectra with 1D spectrum projected onto F1 and F2 axes

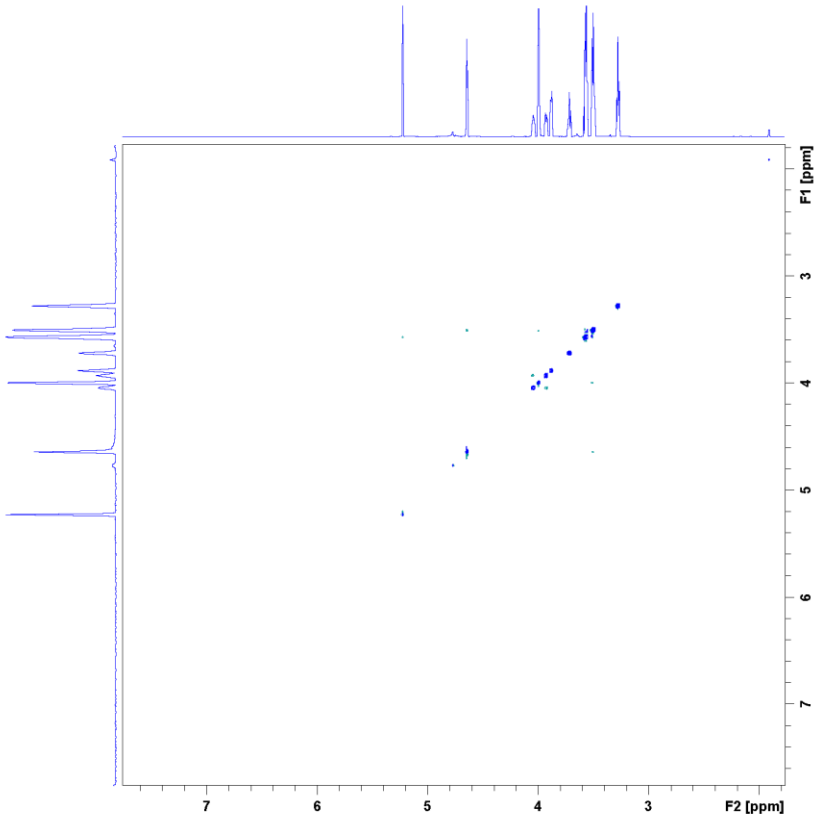
Sulfoquinovose (5 mM), no enzyme



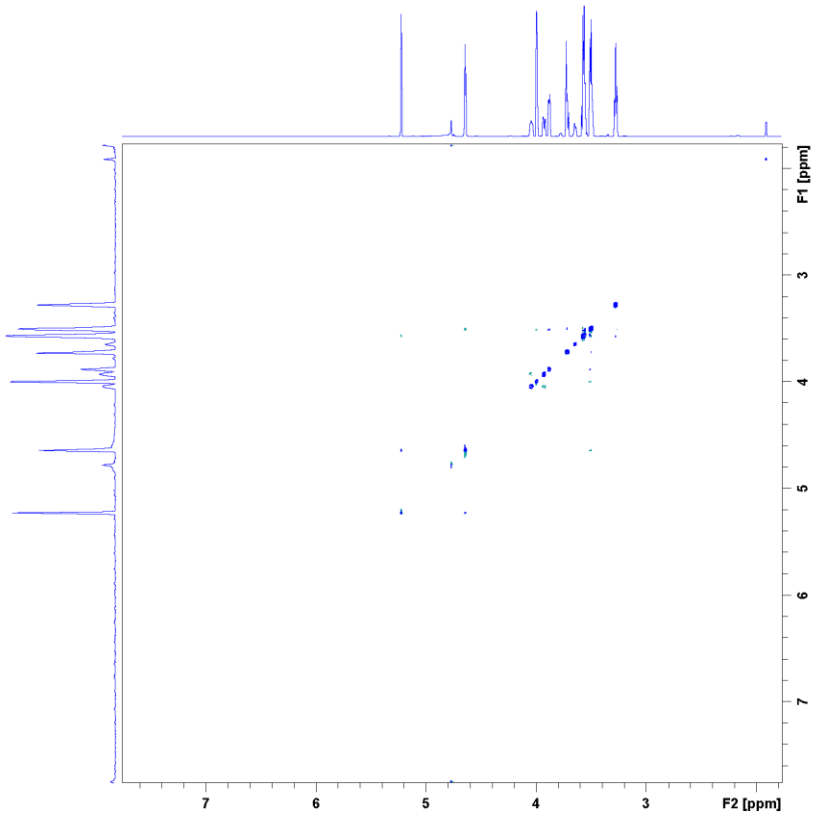
Sulfoquinovose (5 mM), with *Hs*SQM



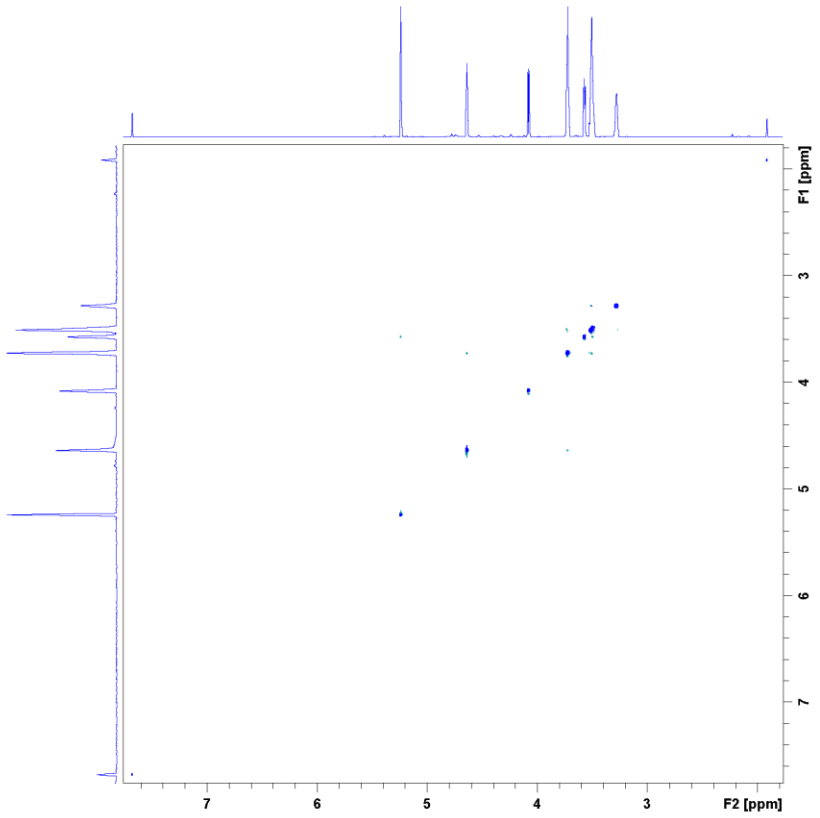
D-Glucose-6-phosphate (5 mM), no enzyme



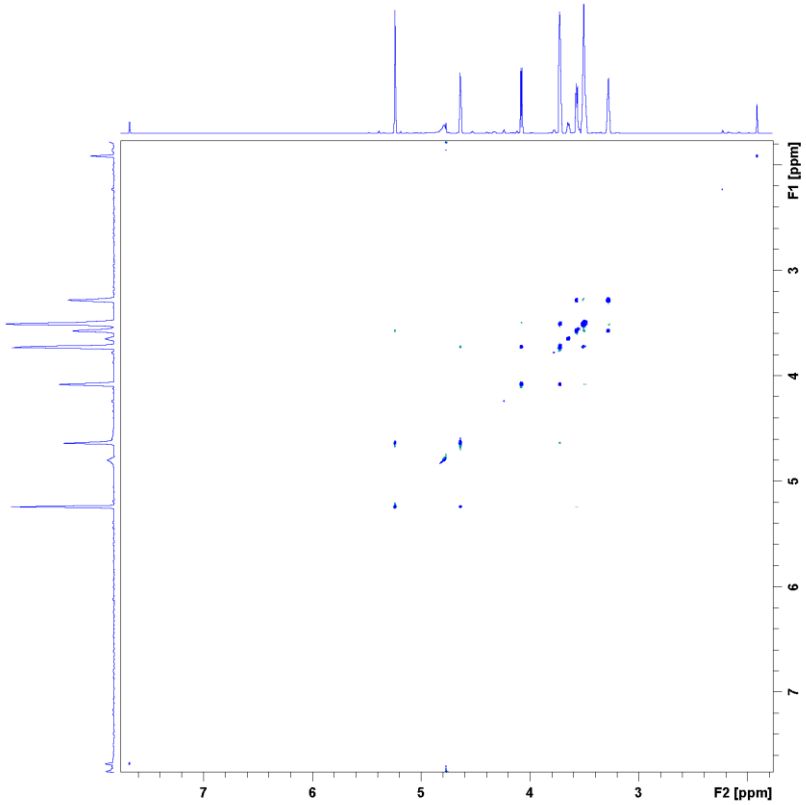
D-Glucose-6-phosphate (5 mM), with *Hs*SQM



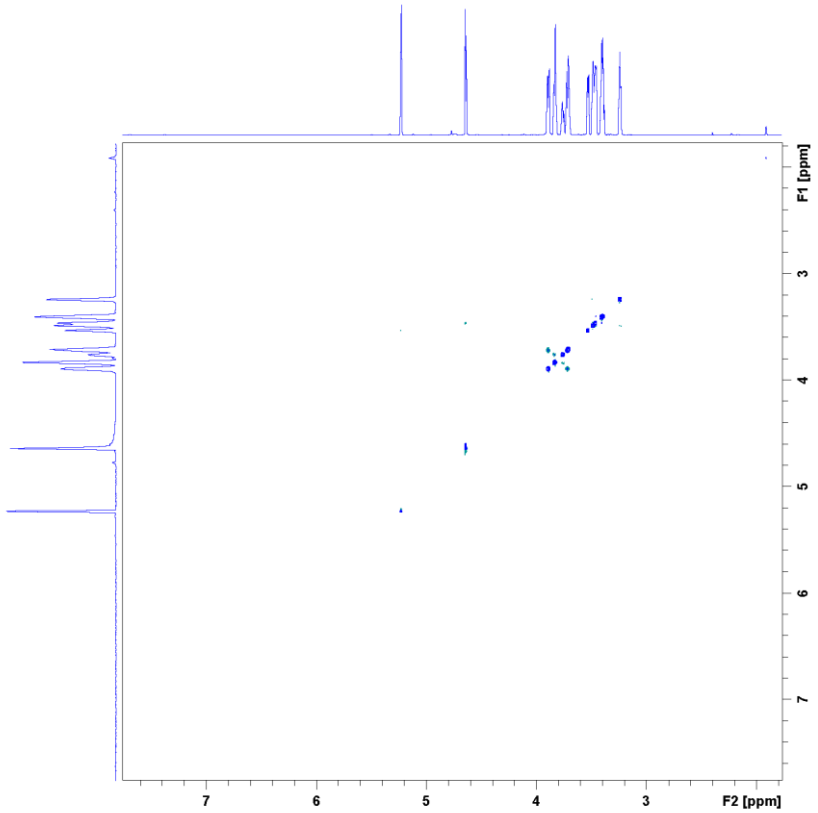
D-Glucuronic acid (5 mM), no enzyme



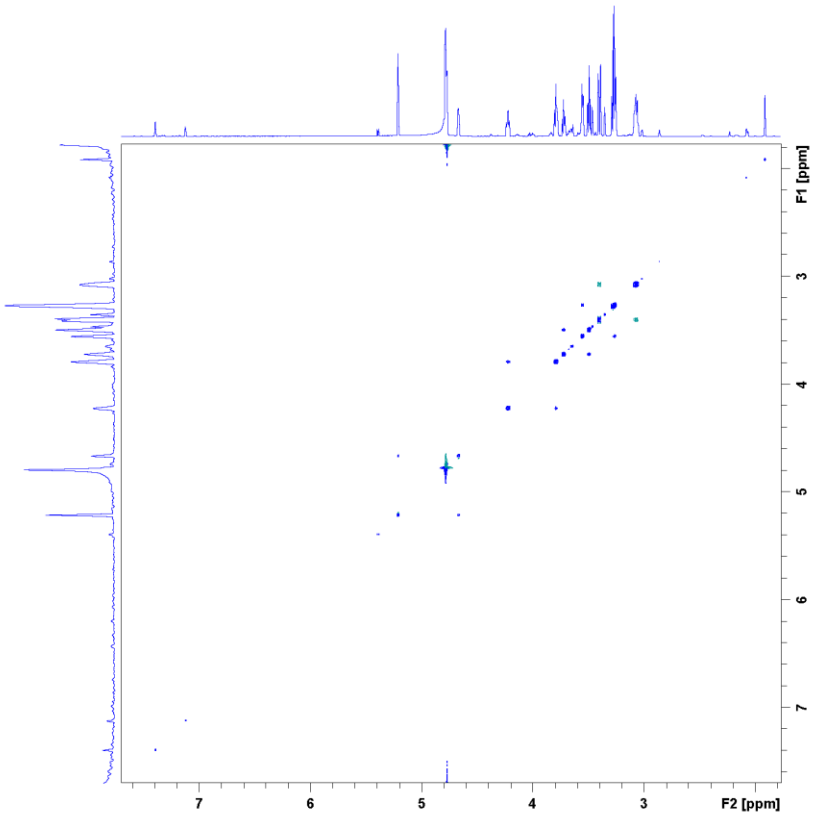
D-Glucuronic acid (5 mM), with *Hs*SQM



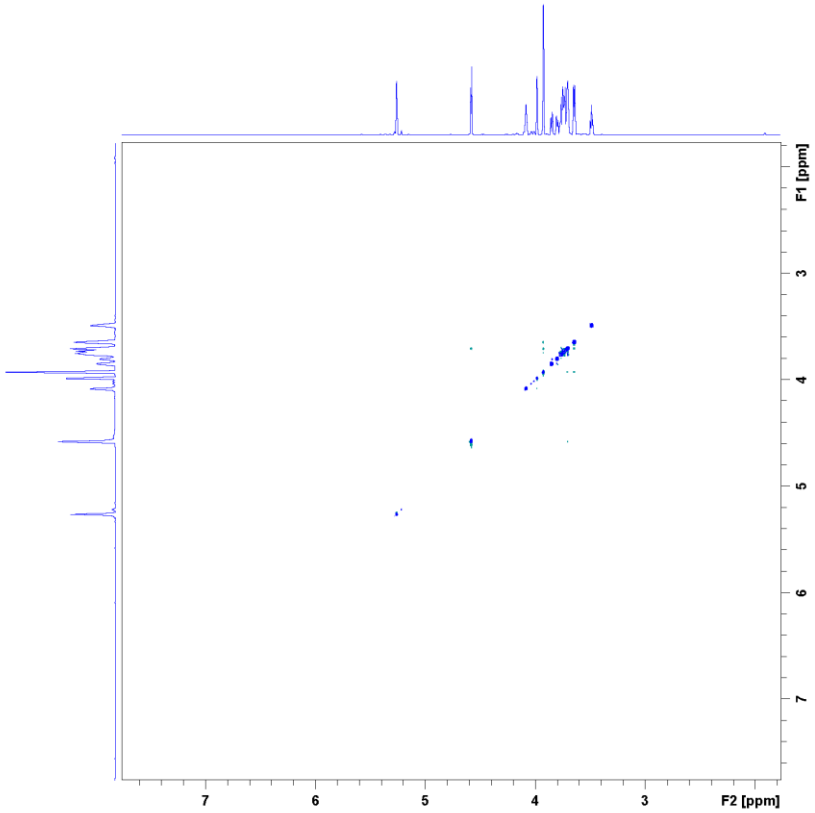
D-Glucose (5 mM), no enzyme



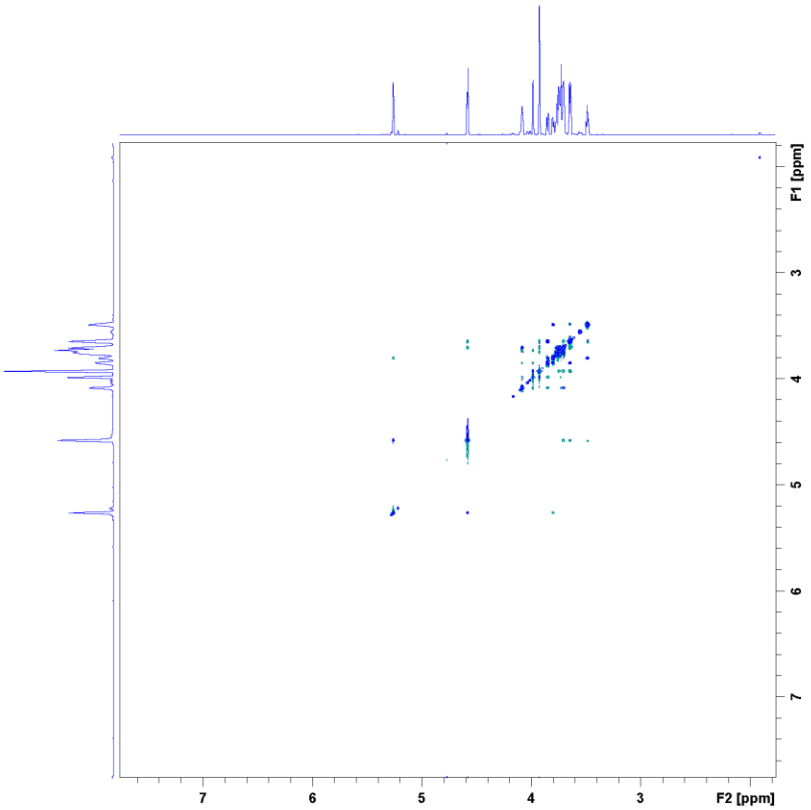
D-Glucose (5 mM), with *Hs*SQM



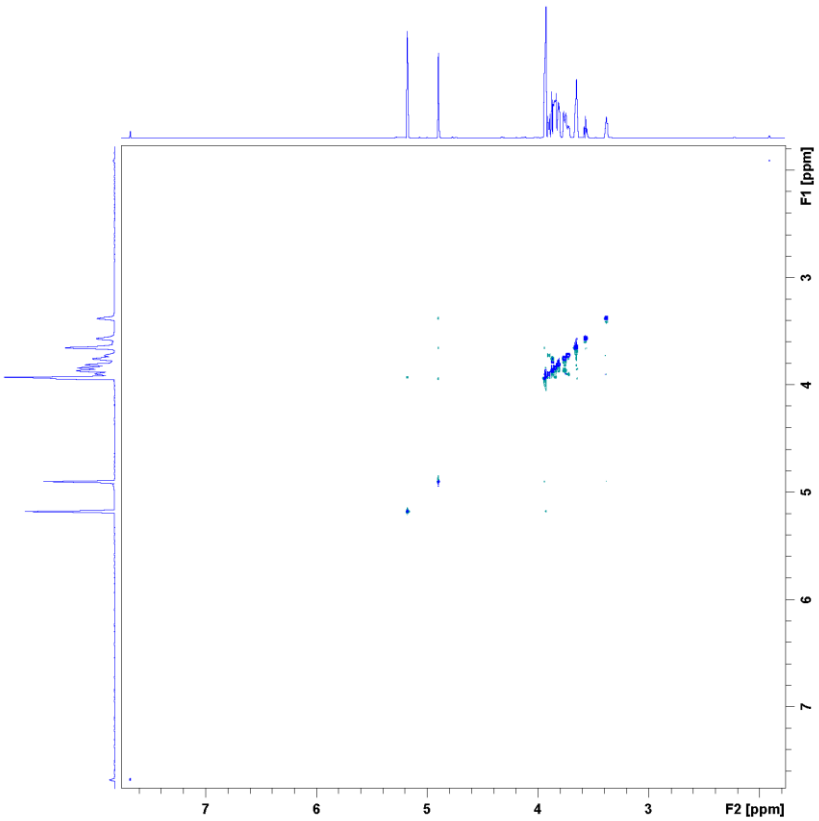
D-Galactose (5 mM), no enzyme



D-Galactose (5 mM), with *Hs*SQM



D-Mannose (5 mM), no enzyme



D-Mannose (5 mM), with *Hs*SQM