

# **NMR-Based Characterization of Citrus Tacle Juice and Low-Level NMR and UV – Vis Data Fusion for Monitoring Its Fractions from Membrane-Based Operations**

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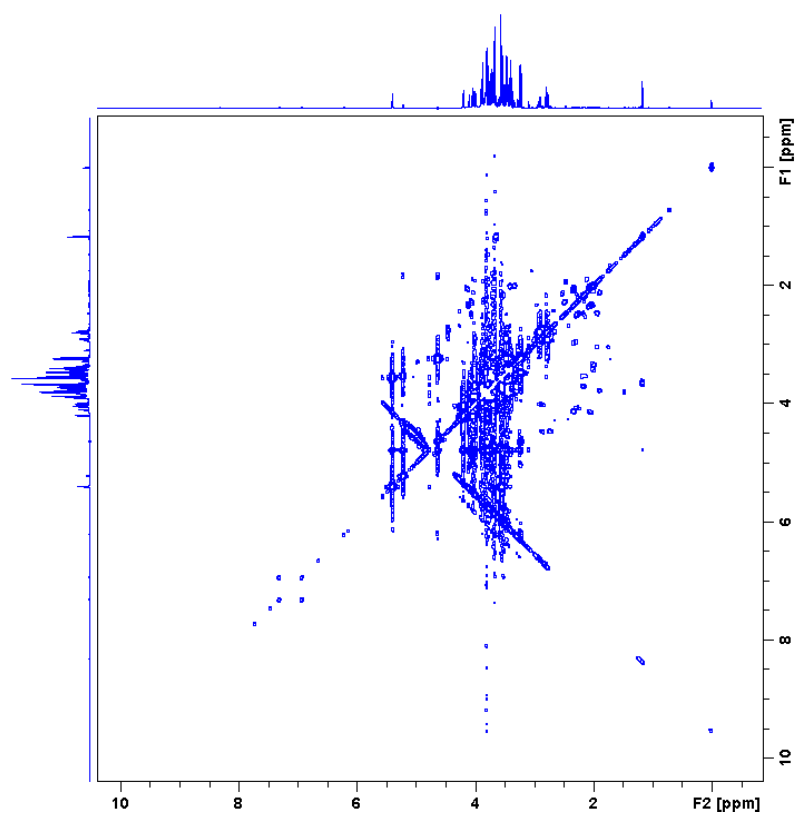
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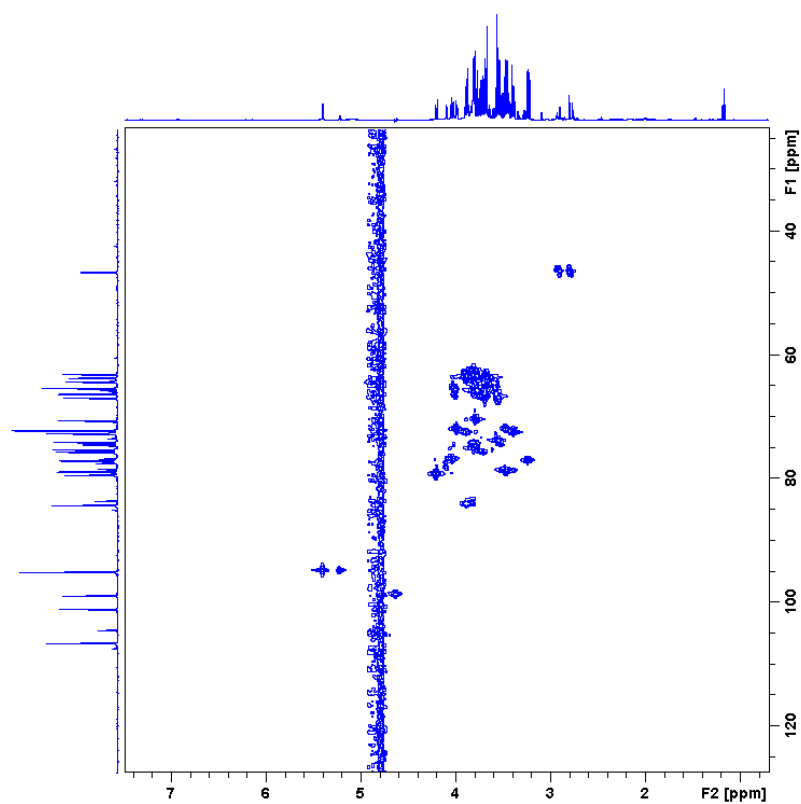
**Table S1:** Metabolites identified in the 500 MHz  $^1\text{H}$  Spectrum of the aqueous phase of Tacle juice at pH 3.41.

Compound	Assignment	<sup>1</sup> H (ppm)	Multiplicity	<sup>13</sup> C (ppm)	
Amino acids					
Valine	γ-CH <sub>3</sub>	0.98	d		
	γ'-CH <sub>3</sub>	1.04	d		
Isoleucine	γ-CH <sub>3</sub>	0.99			
	δ-CH <sub>3</sub>	0.95			
Leucine	γ-CH <sub>3</sub>	1.70			
	δ-CH <sub>3</sub>	0.95			
Alanine	α-CH	3.79	d		
	β-CH <sub>3</sub>	1.47			
Threonine	α-CH	3.96	d		
	γ-CH <sub>3</sub>	1.22			
Arginine	β-CH <sub>2</sub>	1.65;1.72	m		
	γ-CH <sub>2</sub>	1.90	m		
	δ-CH <sub>2</sub>	3.23			
GABA (γ-aminobutyric acid)	α-CH <sub>2</sub>	2.46	t		
	β-CH <sub>2</sub>	1.90	m		
	γ-CH <sub>2</sub>	3.03	t		
Glutamine	α-CH	3.79	m		
	β-CH <sub>2</sub>	2.13			
	γ-CH <sub>2</sub>	2.53			
Proline	α-CH	4.13	m		
	β-CH	2.33			
	β'-CH	2.06			
	γ-CH <sub>2</sub>	1.99			
	δ-CH	3.40			
	δ'-CH	3.33			
DMP (dimethylproline)	α-CH	4.07	m		
	β-CH	2.48			
	β'-CH	2.27			
	γ-CH <sub>2</sub>	2.16			
	δ-CH	3.53	s		
	δ'-CH	3.69			
	N-CH <sub>3</sub>	3.09			
	N-CH <sub>3</sub> '	3.28			
Tyrosine	C2,6H ring	7.31	d		
	C3,5H ring	6.91	d		
Carbohydrates					
α-glucose	CH-1	5.22	d	94.83 73.80	
	CH-2	3.53			
	CH-3	3.70			
	CH-4	3.46			
	CH-5	3.83			
	CH <sub>2</sub> -6,6	3.77;3.83			

β-glucose	CH-1	4.64	dd	98.65
	CH-2	3.23		76.93
	CH-3	3.48		78.54
	CH-4	3.38		72.38
	CH-5	3.46		78.62
	CH <sub>2</sub> -6,6	3.73; 3.81		63.52
Sucrose	CH-1 (Glc)	5.40	d	94.83
	CH-2	3.57		73.80
	CH-3	3.75		75.55
	CH-4	3.47		71.95
	CH-5	3.85		75.07
	CH <sub>2</sub> -6,6	3.80;3.82		62.88
	CH <sub>2</sub> -1' (Fru)	3.67		64.10
	CH-2'			104.2
	CH-3'	4.20		79.18
	CH-4'	4.04		76.93
	CH-5'	3.85		84.05
	CH <sub>2</sub> -6',6'	3.83		65.73
α-fructose	CH <sub>2</sub> -1,1	3.58		65.70
	CH-3	4.09		78.18
	CH-4	4.09		78.18
	CH-5	3.82		83.36
	CH <sub>2</sub> -6,6	3,68; 3.77		65.48
β-fructose	CH-3	3.78		70.34
	CH-4	3.88		72.45
	CH-5	3.99		77.20
	CH <sub>2</sub> -6,6	3.69; 4.01		66.67
Organic Acids				
Lactic acid	α-CH	3.71	d	
	β-CH <sub>3</sub>	1.22		
Succinic acid	α,β-CH <sub>2</sub>	2.64	s	
Malic acid	α-CH	4.46		
	β-CH <sub>2</sub>	2.72		
	β'-CH <sub>2</sub>	2.86		
Citric acid	αγ-CH	2.78	d	46.6
	α'γ'-CH	2.91	d	46.6
Aspartic acid	α-CH	4.00	dd	
	β-CH <sub>2</sub>	2.71		
	β'-CH <sub>2</sub>	2.84		
Formic acid	HCOOH	8.32	s	
Other compounds				
Ethanol	CH <sub>3</sub>	1.17	t	
	CH	3.67		
Methanol	CH <sub>3</sub>	3.32	s	
Phlorin	C4H ring	6.15	t	
	C2,6H ring	6.22	d	



**Figure S1:** 2D  $^1\text{H}$  COSY spectrum (Bruker pulse sequence: *cosygpprqf*) recorded on Tacle juice in  $\text{D}_2\text{O}$  (field strength of 11.74 T).



**Figure S2:** 2D  $^1\text{H}$ - $^{13}\text{C}$  HMQC spectrum (Bruker pulse sequence: *hmqcgpqf*) recorded on Tacle juice in  $\text{D}_2\text{O}$  (field strength of 11.74 T).