



Review

Supplementary Materials for “Processes, Challenges and Optimisation of Rum Production from Molasses—A Contemporary Review”

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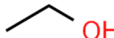
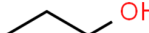
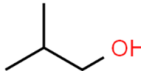
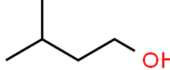
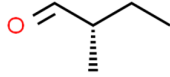
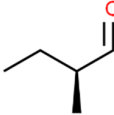
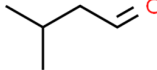
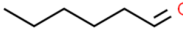
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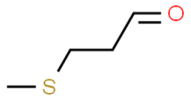
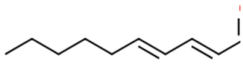
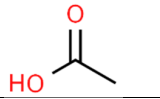
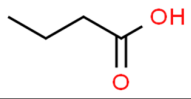
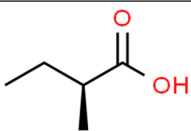
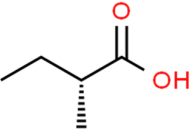
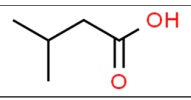
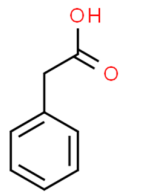
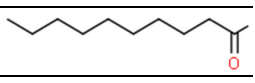
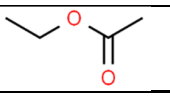
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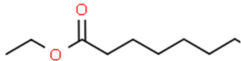
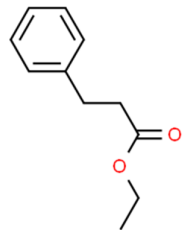
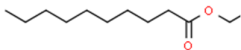
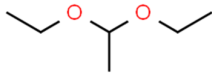
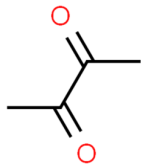
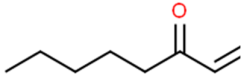
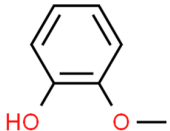
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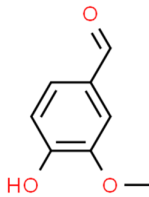
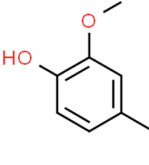
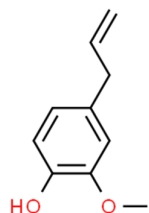
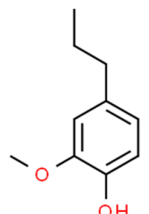
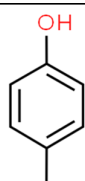
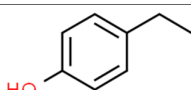
Table S1. Typical concentrations of the major volatile compounds found in rum produced from sugar cane molasses, alongside their odour threshold and odour activity value (OAV). Structures are from ChemSpider (<http://www.chemspider.com/>).

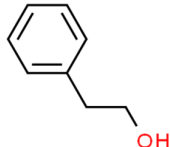
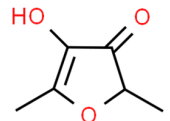
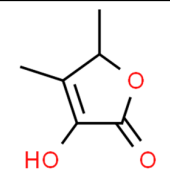
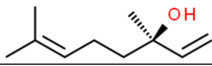
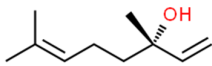
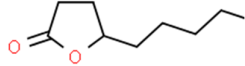
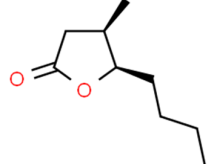
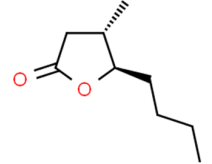
Compound	Typical concentration (mg/L)	Odour threshold		OAV ^	Odour quality	Boiling point (°C)	Structure
		Threshold (mg/L)	Matrix used for threshold testing				
Alcohols							
Methanol	20.6-49.1 [80]	10,000 [97]	Beer	<1	Alcohol, solvent [97]	65	
Ethanol	349,994 [78]	24.9 [78]	Water	14,056	Dissolvent, ethanol [78]	78	
	317,000 [55]	990 [55]	Water	320			
	309,000-322,000 [79]	24.9 [78]	Water	12,400-12,900			
1-propanol	136.1-186.5 [80]	800 [97]	Beer	<1	Alcohol-like [97]	97	
2-methyl-1-propanol (isobutyl alcohol)	98.5-109.4 [80]	160 [55] 10.069 [98]	40% ethanol	<1	Malty [55]	108	
	183 [55]		1				
	0.4-6.7 [79]		<1				
(S)-2-methyl-1-butanol	148 [55]	6.1 [55]	40% ethanol	24	Malty [55,79]	129	
	0.16-4.85 [79]	24 [79]	40% ethanol	<1			
3-methyl-1-butanol	909 [55]	56.1 [79]	40% ethanol	16	Malty [55,79]	131	
	0.7-19.3 [79]			<1			
	180-212.4 [80]			3-4			
Aldehydes							
Acetaldehyde	34.3-74.5 [80]	0.025 [99]	Water	1370-2980	Fresh, green [99]	20	
(S)-2-methylbutanal	0.885 [55]	0.020 [97]	40% ethanol	44	Malty [55,79]	90-92	
	0.008-0.061 [79]	0.033 [79] (for racemate)	40% ethanol	<1-2			
(R)-2-methylbutanal	0.456 [55]	0.110 [55]	40% ethanol	4	Malty [55,79]	~94	
	0.006-0.027 [79]	0.033 [79] (for racemate)	40% ethanol	<1			
3-methylbutanal (isovaleraldehyde)	2.080 [55] 0.034-0.315 [79]	0.0028 [100]	40% ethanol	743 12-110	Malty [55,79]	94	
Hexanal	0.004-0.044 [79]	0.0879 [79]	40% ethanol	<1	Green, grassy [79]	129	

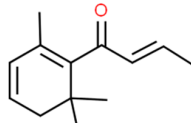
3-(methylthio)propanal (methional)	0.00336 [55]	0.0068 [55]	40% ethanol	<1	Cooked potato-like [55]	165	
(<i>E,E</i>)-2,4-decadienal	0.00232 [55] 0.0001 [79]	0.0011 [100]	40% ethanol	2 <1	Fatty, deep-fried [55,79]	115	
Carboxylic acids							
Acetic acid	121 [55] 0-55 [79]	230 [55] 75.521 [98]	40% ethanol 40% ethanol	<1 <1	Vinegar-like [55]	118	
Butanoic acid	0.462 [55] 0.172-0.629 [79]	6.9 [55] 1.2 [101]	40% ethanol 40% ethanol	<1 <1	Sweaty [101]	164	
(<i>S</i>)-2-methylbutanoic acid	0.216 [55] 0.022-0.028 [79]	3.5 [55]	40% ethanol	<1 <1	Sweaty [55] Fruity [79]	175	
(<i>R</i>)-2-methylbutanoic acid	0.0227 [55] 0.007-0.023 [79]	13 [55]	40% ethanol	<1 <1	Sweaty [55] Fruity [79]	176	
3-methylbutanoic acid	0.368 [55] 0.030-0.069 [79]	0.078 [55]	40% ethanol	5	Sweaty, fruity [79]	176	
Phenylacetic acid	0.0358 [55]	1.4 [55]	40% ethanol	<1	Beeswax-like, honey-like [55]	266	
Decanoic acid	1.240 [55] 0.195-0.635 [79]	2.8 [55]	40% ethanol	<1 <1	Soapy, musty [55]	269	
Esters							
Ethyl acetate	79.0-103.9 [80]	17 [102]	10% ethanol	5-8	Solvent, fruity, sweetish [102]	77	

Ethyl 2-methylpropanoate (ethyl isobutyrate)	0.14 [78]	0.0045 [100]	40% ethanol	31	Fruity, strawberry [78]	110	
Ethyl butanoate	0.441 [55] 4.19 [78] 0.075-0.532 [79]	0.0095 [100]	40% ethanol	46 442 8-110	Fruity [55,78]	121	
Ethyl pentanoate	0.0366 [55] 0.006-0.027 [79]	0.011 [55] 0.0030 [98]	40% ethanol 40% ethanol	3 2-9	Fruity [55]	145	
Ethyl (S)-2-methylbutanoate	0.0194 [55] 0.02 [78] 0.0069-0.0088 [79]	0.0002 [98] 0.0016 [78] 0.00022 [79]	40% ethanol Water 40% ethanol	97 12 40-56	Fruity [78]	133	
Ethyl 3-methylbutanoate (ethyl isovalerate)	32.0 [55] 0.0042-0.0064 [79]	0.0016 [79]	40% ethanol	20 3-4	Blueberry-like [55,79]	135	
3-methylbutyl acetate (isoamyl acetate)	1.860 [55] 0.49 [78] 0.027-0.076 [79]	0.245 [100]	40% ethanol	8 2 <1	Banana-like [78]	142	
Ethyl hexanoate	0.424 [55] 4.35 [78] 0.067-0.080 [79]	0.03 [55,100] 0.03 [100] 0.0297 [79]	40% ethanol 40% ethanol 40% ethanol	14 145 2-3	Fruity [55,79] Green apple [78]	168	
Ethyl cyclohexanoate	0.00107 [55] 0.0001-0.0012 [79]	0.0003 [55] 0.0016 [98]	40% ethanol 40% ethanol	4 <1	Fruity, sweet [55]	196	
2-phenylethyl acetate	0.12 [78]	0.108 [100]	40% ethanol	1	Rose, honey [78]	232	

Ethyl octanoate	3.610 [55] 4.12 [78]	0.147 [55,100]	40% ethanol	25 28	Fruity [78] Green [55]	208	
Ethyl 3-phenylpropanoate	0.0267 [55] 0.0005 [79]	0.014 [55]	40% ethanol	2 <1	Flowery [55,79]	248	
Ethyl decanoate (ethyl caprate)	9.24 [78]	0.42 [100]	40% ethanol	22	Brandy [78]	245-250	
Ethers							
1,1-diethoxyethane	20.8 [55] 9.36 [78] 4.05-5.31 [79]	0.719 [100]	40% ethanol	29 13 6-7	Fruity [78]	102	
Ketones							
2,3-butanedione	0.526 [55] 0.030-0.621 [79]	0.0028 [98]	40% ethanol	188 11-220	Butter-like [55,79]	88	
1-octen-3-one	0.00101 [55]	0.0026 [55]	40% ethanol	<1	Mushroom-like [55]	175	
Methoxyphenols							
2-methoxyphenol (guaicol)	0.399 [55] 0.65 [78] 0.001-0.016 [79]	0.0092 [100]	40% ethanol	43 71 <1-2	Gammon, smoky-like [78]	205	

Vanillin	1.200 [55] 2.84 [78] 0.002-0.912 [79]	0.022 [55,100]	40% ethanol	55 129 <1-42	Vanilla-like [78]	285	
4-ethylguaicol (4-ethyl-2-methoxyphenol)	0.110 [55] 0.128 [78] 0.0018-0.0025 [79]	0.0069 [100]	40% ethanol	16 17 <1	Phenolic, smoky, gammon-like [78]	237	
Eugenol (4-allyl-2-methoxyphenol)	0.001-0.018 [79] 0.09 [78]	0.0071 [100]	40% ethanol	<1-3 14	Spicy, clove-like [78]	254	
2-methoxy-4-propylphenol	0.0605 [55] 0.0004-0.0037 [79] 0.128 [78]	0.0044 [55] 0.00189 [101] 0.020 [78]	40% ethanol 40% ethanol Water	14 <1-2 17	Phenolic, smoked [78]	~250-264	
Other compounds							
4-methylphenol (p-cresol)	0.0323 [55] 0.0002-0.0015 [79]	0.089 [55] 0.0815 [79]	40% ethanol 40% ethanol	<1 <1	Fecal, horse stable-like [55,79]	202	
4-ethylphenol	1.450 [55] 0.0006-0.0017 [79]	0.173 [55,100]	40% ethanol	8 <1	Phenolic [55,79]	218	

2-phenylethanol	2.670 [55] 10.40 [78] 0.002-0.29 [79]	2.6 [100]	40% ethanol	1 4 <1	Floral, honey-like [78]	255	
Furaneol (4-hydroxy-2,5-dimethylfuran-3(2H)-one)	0.00354 [55]	0.350 [55]	40% ethanol	<1	Caramel-like[55]	216	
Sotolon (3-hydroxy-4,5-dimethylfuran-2(5H)-one)	0.0003-0.0015 [79] 0.00295 [55]	0.0242 [98] 0.00011 [55]	40% ethanol 40% ethanol	<1 27	Seasoning-like, spicy [79]	184	
(R)-linalool	0.0255 [55]	0.024 [55] (for racemate)	40% ethanol	~2	Citrus-like, flowery [55]	198	
(S)-linalool	0.0233 [55]	0.024 [55] (for racemate)	40% ethanol	~2	Citrus-like, flowery [55]	198	
γ-nonalactone	0.15 [78]	0.021 [100]	40% ethanol	7	Coconut-like [78]	122	
cis-whisky lactone (cis-oak lactone)	0.210 [55] 2.41 [78] 0.0004-0.318 [79]	0.067 [103]	30% ethanol	3 36 <1-5	Coconut-like [55,79] Woody, oaky [78]	Est. 247	
trans-whisky lactone (trans-oak lactone)	0.191 [55] 0.39 [78] 0.0004-0.020 [79]	0.790 [103]	30% ethanol	<1 <1 <1	Coconut-like Woody [78]	Est. 247	

<i>(E)</i> - β -Damascenone	0.328 [55]	0.0001 [100]	40% ethanol	3280	Baked apple-like, grape	116	
	0.11 [78]	0.0001 [100]	40% ethanol	1100	juice-like [55,79]		
	0.001-0.002 [79]	0.00014 [79]	40% ethanol	7-12	Peach jam, sweet [78]		

Abbreviations: ND = no data; MW = molecular weight; OAV = odour activity value

^ OAV is the ratio of the concentration present to the respective odour threshold for that compound. Compounds with OAV >1 are considered to be odour active.

