Fast and isothermal hydrothermal liquefaction of polysaccharide feedstocks

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5 Pages

1 Table

Table S1 Tentative identities of organic compounds in biocrudes produced by isothermal HTL at 350 $^{\circ}$ C set-point temperature, 31.6 min and fast HTL at 500 $^{\circ}$ C set-point temperature, 1 min for the polysaccharide feedstocks

Compound Group	Compound Identified	Starch		Cellulose		Amylopectin		Amylose		Pectin		Chitin	
		Iso.	Fast	Iso.	Fast	Iso.	Fast	Iso.	Fast	Iso.	Fast	Iso.	Fast
	2-Cyclopenten-1-one,3-methyl-	✓		√		✓		✓		√		с	
	2-Cyclopenten-1-one,2,3-dimethyl-	√		√		✓		√		√	√	√	
	2-Cyclopenten-1-one	√		√		√	√	√		√			
	Ethanone,1-(3-hydroxyphenyl)-	√	√	√		√			√		√		
	3,6-Heptanedione			√		√	√	√					
	2-Cyclohexen-1-one, 6-methyl-3-(1-methylethyl)-	√		√		1						√	
	2,5-Hexanedione	√		✓		✓	✓	✓					
	2-Cyclopenten-1-one,2-methyl-	✓		√		✓		✓		√		√	
	1,2-Cyclopentanedione,3-methyl-	√		√				√					
	2-Cyclopenten-1-one,3-ethyl-	√		√		√		√		√		√	
	Ethanone,1-(1-cyclohexen-1-yl)-	√		√				√		√		√	
Ketones	Cyclohexanone,3-ethenyl-	√		√		√		√		√		√	
	2-Cyclopenten-1-one,3,4-dimethyl-	√		√		√		√		√		√	
	4,4-Dimethyl-2-cyclopenten-1-one	√		√				√		√		√	
	2-Acetonylcyclopentanone	√		√									
	1,3-Cyclopentanedione, 2,4- dimethyl-	√											
	Cyclohept-4-enone	√											
	2-Cyclopenten-1-one, 3-ethyl-2- hydroxy-	√	✓			✓							
	3-Methylcyclopentane-1,2-dione					✓							
	3,4-dihydroxyphenyl-2-propanone					√							
	2-Cyclohexen-1-one, 3,4- dimethyl-							✓		✓			
	5-Hexen-2-one, 5-methyl-3- methylene-							✓					
	Cyclopentanone									✓		✓	
	3-Methyl-3-cyclohexen-1-one									✓			
	2-Cyclohexen-1-one,3-methyl-									✓			
	Cyclohexanone									√		√	-
	2-Cyclopenten-1-one, 2,3,4,5- tetramethyl-												
	3-Methylcyclopentane-1,2-dione		✓						✓		✓		
	Maltol		✓						√				
	Ethanone,1-(2,5-dihydroxyphenyl)-		✓								✓		
	1,2-Cyclopentanedione		✓				✓		✓				✓
	2-Cyclohexen-1-one,4-(1- methylethyl)- 5,9-Dodecadien-2-one,6,10-						✓		√ 				
	dimethyl-,(E,E))-								√				
	3-Buten-2-one, 4-(4-hydroxy-3-methoxyphenyl)-										✓		
	2-Hydroxy-3-propyl-2-cyclopenten- 1-one										✓		

Compound	Compound Identified	Starch		Cellulose		Amylopectin		Amylose		Pectin		Chitin	
Group		Iso.	Fast	Iso.	Fast	Iso.	Fast	Iso.	Fast	Iso.	Fast	Iso.	Fast
	Phenol	✓		√	√	√	√	√	√	√		√	√
	Phenol,2-methyl-	√		√		√		√		√		√	
	Phenol,3-methyl-	✓		√		√		√		√	√	√	
	Phenol,2,3-dimethyl-			√									
Phenols	Phenol,2,5-dimethyl-									√			
	Phenol,4-ethyl-2-methoxy-									√			
	Phenol,3,4-dimethyl-			√				√					
	Phenol,2,2'-methylenebis[6-(1,1-dimethylethyl)-4-methyl-		✓	✓	√	✓					✓		
	Phenol, 2-methoxy-											√	
	2-Methoxy-5-methylphenol				√								
	1H-Inden-1-one,2,3-dihydro-	✓		√		√		√		√		√	
Ludanan	7-Methylindan-1-one	✓		√		√		√		√			
Indanone derivatives	Indan-1,2-dione, 4,7-dimethyl-					√							
	1H-Inden-5-ol, 2,3-dihydro-			√		√		/		√			
	4-Hydroxy-1-indanone							√		√			
	1-Methylindan-2-one									√			
	2-Methyl-5-hydroxybenzofuran	1	√	√		√		√			√		
	2,4-Dimethylfuran	/	√	√		√		√					
	2(3H)-Benzofuranone					√							
	Benzofuran,4,7-dimethyl-							√					
	Benzofuran,2-methyl-							√		√			
Furan	2-Furancarboxaldehyde, 5-methyl-	✓			✓	✓	✓	✓	✓				✓
derivatives	5-Hydroxymethylfurfural		✓	✓	✓		✓		✓		✓		✓
	Benzofuran-2,3-dione,4,7-dimethyl- 2,3-dihydro-	✓											
	2-Furancarboxylic acid,2- methylpropyl ester		✓										
	2-Methyl-5-hydroxybenzofuran												
	2,5-Furandicarboxaldehyde		✓		✓		✓		✓				✓
	Furyl hydroxymethyl ketone				√		√		√				
	Furfural						✓						
	2-Acetyl-5-methylfuran						✓						
	2(5H)-Furanone						✓						
	2,2'-Bifuran				√								
	2(5H)-Furanone, 5,5-dimethyl-												√
	5-Acetoxymethyl-2-furaldehyde								✓				✓

Compound	Compound Identified	Starch		Cellulose		Amylopectin		Amylose		Pectin		Chitin	
Group		Iso.	Fast	Iso.	Fast	Iso.	Fast	Iso.	Fast	Iso.	Fast	Iso.	Fast
Benzene derivatives	Catechol		√			√				√	√		
	1,2-Benzenediol,4-methyl-	√	√	√		√				√	√		
	1,2-Benzenediol,3-methyl-	√	√	√		√					√		
uerry uerves	2-Coumaranone			√									
	1,3-Benzenediol,4-ethyl-		√	√						√			
	1,4-Benzenediol,2-methyl-								√				
	1,4-Benzenedicarboxaldehyde,2- methyl-	✓								✓			
	Benzene,ethoxy-											✓	
	Resorcinol,2-acetyl-		✓										
	Benzaldehyde, 3-hydroxy-		✓										
	Benzene,1,3-bis(1,1-dimethylethyl)-				√								
	Benzaldehyde, 3-hydroxy-3- Formylphenol										✓		
	Resorcinol,2-acetyl-										√		
	Hydrocoumarin										√		
	4-Hydroxy-2-methylbenzaldehyde										√		
	3-Hydroxy-2-methylbenzaldehyde										√		
	Vanillin										√		
	4-Ethoxystyrene										√		
Acids	2-Hexenoic acid,3,4,4-trimethyl-5-oxo-,(Z)-		✓										
	n-Hexadecanoic acid				✓		✓		√				
Alcohols	1-Dodecanol				√		✓		√				
	1-Decanol,2-hexyl-				√				√				
	1-Decanol, 2-octyl-				√								
	n-Nonadecanol-1				√								
	2-Isopropyl-5-methyl-1-heptanol								√				
Esters	2-Propenoic acid, pentadecyl ester				√		√		√				
	Hexadecanoic acid,2-hydroxy-1- (hydroxymethyl) ethyl ester				✓		√						
Hydrocarbons	Nonane,5-butyl-						✓						
	Eicosane				√				√				
	Heptadecane				√				√				√
	Tetracosane												√
	Tetratriacontane												√
	Hexatriacontane												√

Compound Group	Compound Identified		Starch		Cellulose		Amylopectin		Amylose		Pectin		Chitin	
		Iso.	Fast	Iso.	Fast	Iso.	Fast	Iso.	Fast	Iso.	Fast	Iso.	Fast	
Nitrogenous	2,5-Pyrrolidinedione, 1-methyl											✓		
compounds	2-acetyl pyrrole											✓	√	
	Pyridine											✓		
	1H-Indole, 2,3-dimethyl-											✓		
	Pyridine, 4-propyl-											✓		
	Pyrazine, methyl-											✓		
	2,6-Dimethylphenyl isocyanate											✓		
	Pyrazine, 2-ethyl-3-methyl-											✓		
	2-Acetyl-1-methylpyrrole											✓		
	2,5-Pyrrolidinedione, 1-ethyl											✓		
	Pyridine, 2-methyl-											✓		
	1,3-Benzoxazol-4-ol											✓		
	Acetamide											✓		
	1H-Pyrrole-2-carboxaldehyde												√	
	1H-Pyrrole-2-carboxaldehyde, 1- methyl-												√	
	2-Acetoxymethylpyridine												✓	
	4(1H)-Pyridinone, 2,3-dihydro-1- methyl-												√	
	3-(Furan-2-yl)-4-methyl-1,2,4- triazole												√	
	Acetamide, N-(2,4- dihydroxyphenyl)-												√	
	4-Hydroxy-6- (methylamino)pyrimidine												√	