Supporting Information for:

Aqueous stream characterization from biomass fast pyrolysis and catalytic fast pyrolysis

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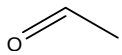
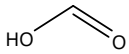
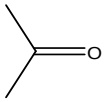
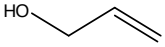
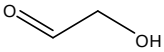
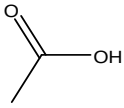
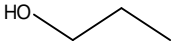
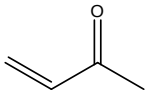
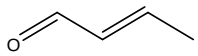
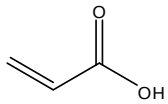
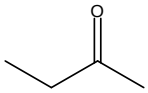
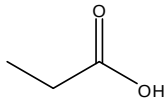
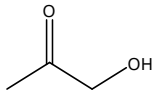
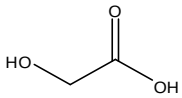
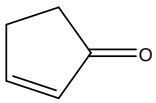
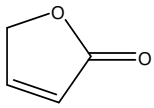
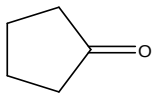
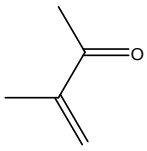
Table S1. Standard deviation of all compositional analysis from minimum triplicate independent analysis (n=≥3)

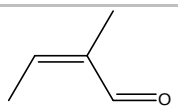
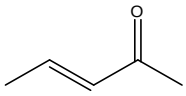
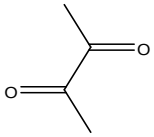
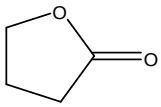
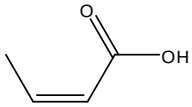
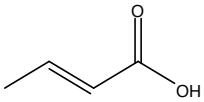
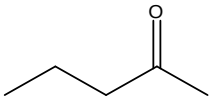
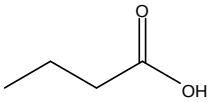
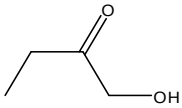
	Fast Pyrolysis		Catalytic Fast Pyrolysis		
	FP_{NREL}	**$SF5_{ISU}$**	**CFP_{NREL}** *ex-situ*	**$CFP_{RTI\text{-}pine}$** *in-situ*	**$CFP_{RTI\text{-}oak}$** *in-situ*
Water (wt%)	0.5	1.7	0.9	0.6	0.3
TOC (wt%)	1.0	0.6	0.5	0.3	0.3
TAN (mg NaOH g^{-1})	1.0	2.4	0.3	0.2	14.4
Carbonyl (mmole g^{-1})	0.5	0.0	3.6	0.2	0.1
COD (mg/g)	33	68	13	36	67
pH	0.1	0.1	0.1	0.0	0.1
Al (ppm)	1.5	0.4	27.9	3.8	1.8
Ca (ppm)	53.5	4.0	16.6	1.0	7.6
Cr (ppm)	ND	ND	21.1	ND	ND
Cu (ppm)	0.5	0.3	ND	0.9	4.6
Fe (ppm)	1.1	0.7	19.8	1.2	5.3
K (ppm)	ND	ND	ND	ND	ND
Mg (ppm)	12.9	0.9	3.2	0.4	1.8
Mn (ppm)	0.2	0.3	8.1	0.7	0.7
Na (ppm)	89.6	ND	10.5	5.9	41.1
Ni (ppm)	1.8	1.1	13.8	2.5	6.7
P (ppm)	ND	ND	77.7	ND	ND
S (ppm)	10.6	4.6	208.9	10.9	50.7
Zn (ppm)	0.5	0.5	1.6	0.7	4.8
C (wt%)	0.2	0.4	1.0	0.2	0.2
H (wt%)	0.3	0.0	6.9	0.6	1.0
N (wt%)	0.0	0.1	0.1	0.1	0.1

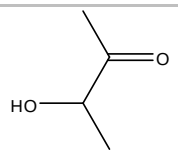
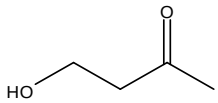
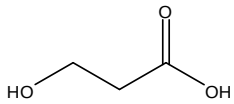
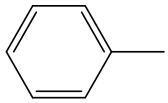
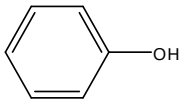
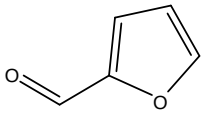
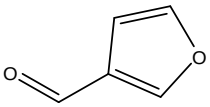
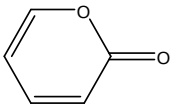
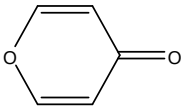
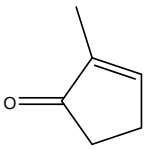
ND = not detected

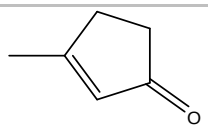
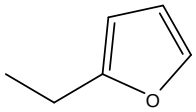
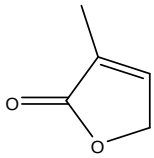
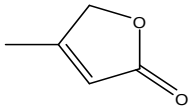
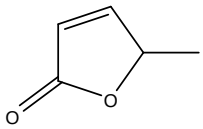
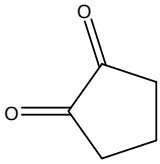
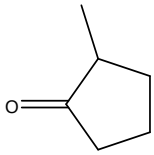
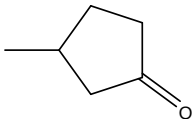
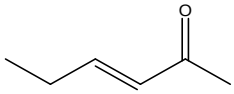
Table S2. Chemical compounds identified within aqueous streams and key marker ions for characterization, ordered by increasing molecular weight.

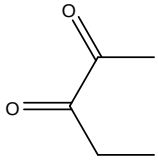
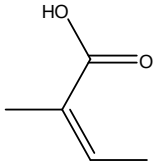
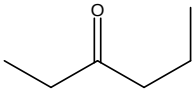
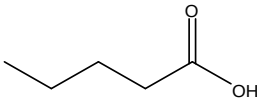
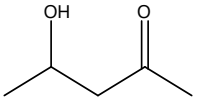
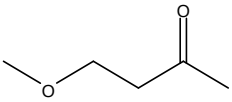
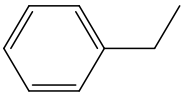
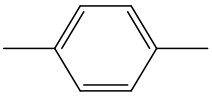
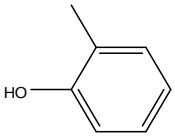
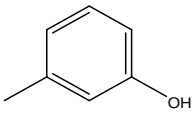
Identified compound (IUPAC)	Chemical structure	Chemical formula	Theoretical molecular weight (g mol^{-1})	Chemical present in select aqueous pyrolysis streams	Quantitation/ identification ions (Da)*
Methanol		CH_4O	32.03	FP_{NREL}, $SF5_{ISU}$, CFP_{NREL}, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 31 Da Fragment ions: 32, 29 Da LC-MS: $[M+H]^+$ 33 Da LC-RID
Acetaldehyde		C_2H_4O	44.03	$SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 44 Da Fragment ions: 29 Da LC-MS: $[M+H]^+$ 45 Da Product ions: 27 Da LC-RID
Formic acid		CH_2O_2	46.01	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$,	GC-MS: Q_{ion} 46 Da Fragment ions: 45, 29 Da LC-MS: $[M-H]^-$ 45 Da LC-UV_{210nm} LC-RID
Propan-2-one		C_3H_6O	58.04	FP_{NREL}, $SF5_{ISU}$, CFP_{NREL}, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 58 Da Fragment ions: 43 Da LC-MS: $[M+H]^+$ 59 Da Product ions: 43 Da LC-RID
Prop-2-en-1-ol		C_3H_6O	58.04	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$	GC-MS: Fragment ions: 57, 39, 31 Da
2-Hydroxyacetaldehyde		$C_2H_4O_2$	60.02	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 31 Da Fragment ions: 29 Da LC-RID
Acetic acid		$C_2H_4O_2$	60.02	FP_{NREL}, $SF5_{ISU}$, CFP_{NREL}, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 60 Da Fragment ions: 45, 43 Da LC-MS: $[M-H]^-$ 59 Da LC-UV_{210nm} LC-RID
Propan-1-ol		C_3H_8O	60.06	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 31 Da LC-MS: $[M+H]^+$ 61 Da Product ions: 43 Da
But-3-en-2-one		C_4H_6O	70.04	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 55 Da Fragment ions: 70, 43 Da LC-UV_{210nm}

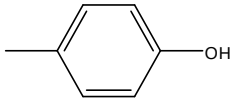
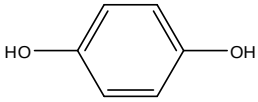
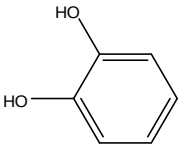
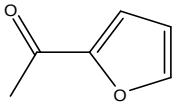
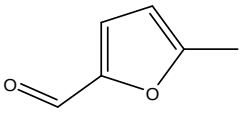
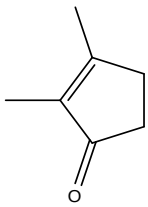
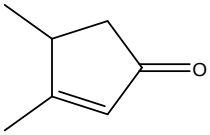
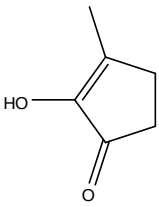
But-2-enal		C_4H_6O	70.04	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 70 Da Fragment ions: 41, 39 Da LC-RID
Prop-2-enoic acid		$C_3H_4O_2$	72.02	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$	GC-MS: Q_{ion} 72 Da Fragment ions: 55, 27 Da LC-UV_{210nm} LC-RID
Butan-2-one		C_4H_8O	72.06	$SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 72 Da Fragment ions: 43 Da LC-MS: $[M+H]^+$ 73 Da Product ions: 55, 43 Da
Propanoic acid		$C_3H_6O_2$	74.04	FP_{NREL}, $SF5_{ISU}$, CFP_{NREL}, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	LC-MS: $[M-H]^-$ 73 Da LC-UV_{210nm} LC-RID
1-Hydroxypropan-2-one		$C_3H_6O_2$	74.04	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 43 Da Fragment ions: 74, 31 Da LC-MS: $[M-H]^-$ 73 Da Product ions: 57, 55 Da
2-Hydroxyacetic acid		$C_2H_4O_3$	76.02	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	LC-MS: $[M-H]^-$ 75 Da Product ions: 73, 31 Da LC-UV_{210nm} LC-RID
Cyclopent-2-en-1-one		C_5H_6O	82.04	FP_{NREL}, $SF5_{ISU}$, CFP_{NREL}, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 82 Da Fragment ions: 54, 39 Da LC-MS: $[M+H]^+$ 83 Da
2*(5H)*-Furanone		$C_4H_4O_2$	84.02	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 55 Da Fragment ions: 84, 27 Da LC-MS: $[M+H]^+$ 85 Da Product ions: 67, 57 Da
Cyclopentanone		C_5H_8O	84.06	FP_{NREL}, $SF5_{ISU}$, CFP_{NREL}, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 55 Da Fragment ions: 84, 28 Da LC-MS: $[M+H]^+$ 85 Da
3-Methylbut-3-en-2-one		C_5H_8O	84.06	$SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Fragment ions: 84, 43, 41 Da
2-Methylbut-2-enal		C_5H_8O	84.06	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 55 Da Fragment ions: 84, 29 Da

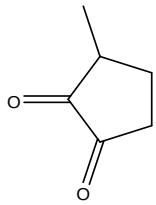
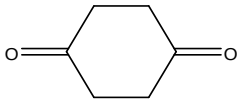
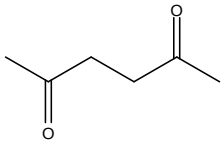
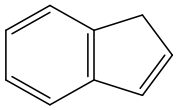
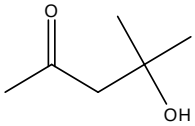
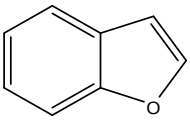
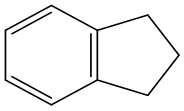
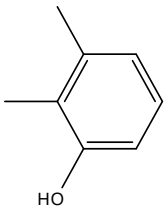
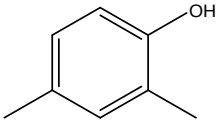
					
Pent-3-en-2-one		C_5H_8O	84.06	$CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Fragment ions: 69, 43, 41 Da LC-MS: $[M+H]^+$ 85 Da Product ions: 67, 43 Da
Butane-2,3-dione		$C_4H_6O_2$	86.04	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 43 Da Fragment ions: 86, 15 Da LC-MS: $[M+H]^+$ 87 Da Product ions: 69, 43 Da
Oxolan-2-one		$C_4H_6O_2$	86.04	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 86 Da Fragment ions: 42, 28 Da LC-MS: $[M+H]^+$ 87 Da Product ions: 69, 44 Da
(*Z*)-But-2-enoic acid		$C_4H_6O_2$	86.04	$SF5_{ISU}$	GC-MS: Fragment ions: 86, 41, 39 Da LC-MS:$[M-H]^-$ 85 Da Product ions: 41 Da $LC\text{-}UV_{210nm}$
(*E*)-But-2-enoic acid		$C_4H_6O_2$	86.04	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$	GC-MS: Q_{ion} 86 Da Fragment ions: 41, 39 Da LC-MS:$[M-H]^-$ 85 Da Product ions: 41 Da $LC\text{-}UV_{210nm}$
Pentan-2-one		$C_5H_{10}O$	86.07	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 86 Da Fragment ions: 43, 41 Da LC-MS: $[M+H]^+$ 87 Da Product ions: 69 Da
Butanoic acid		$C_4H_8O_2$	88.05	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 60 Da Fragment ions: 73, 41 Da LC-MS:$[M-H]^-$ 87 Da Product ions: 44 Da
1-Hydroxybutan-2-one		$C_4H_8O_2$	88.05	FP_{NREL}, $SF5_{ISU}$, CFP_{NREL}, $CFP_{RTI\text{-}pine}$	GC-MS: Q_{ion} 57 Da Fragment ions: 31, 29 Da LC-MS: $[M+H]^+$ 89 Da Product ions: 71 Da
3-Hydroxybutan-2-one		$C_4H_8O_2$	88.05	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 45 Da Fragment ions: 88, 43 Da

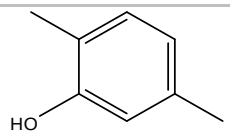
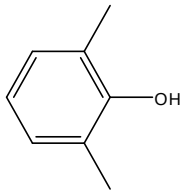
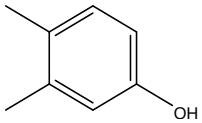
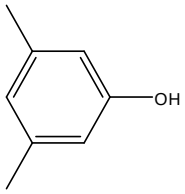
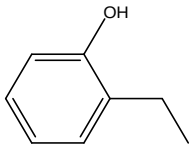
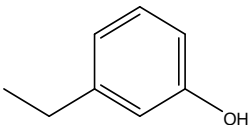
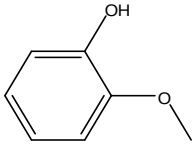
					LC-MS: $[M+H]^+$ 89 Da Product ions: 71, 43 Da
4-Hydroxybutan-2-one		$C_4H_8O_2$	88.05	$CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 43 Da Fragment ions: 70, 31 Da LC-MS: $[M+H]^+$ 89 Da Product ions: 71, 57 Da
3-Hydroxypropanoic acid		$C_3H_6O_3$	90.03	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 60 Da Fragment ions: 43, 42 Da LC-MS:$[M-H]^-$ 89 Da Product ions: 59, 43, 41 Da
Toluene		C_7H_8	92.06	$SF5_{ISU}$, CFP_{NREL}, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 91 Da Fragment ions: 92, 65 Da LC-UV_{264nm}
Phenol		C_6H_6O	94.04	FP_{NREL}, $SF5_{ISU}$, CFP_{NREL}, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 94 Da Fragment ions: 66, 65 Da LC-UV_{210nm}
Furan-2-carbaldehyde		$C_5H_4O_2$	96.02	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 96 Da Fragment ions: 95, 39 Da LC-UV_{210nm} LC-RID
Furan-3-carbaldehyde		$C_5H_4O_2$	96.02	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 95 Da Fragment ions: 96, 39 Da LC-UV_{210nm} LC-RID
Pyran-2-one		$C_5H_4O_2$	96.02	$SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Fragment ions: 96, 68, 39 Da
Pyran-4-one		$C_5H_4O_2$	96.02	FP_{NREL}	GC-MS: Fragment ions: 96, 69, 42 Da
2-Methylcyclopent-2-en-1-one		C_6H_8O	96.06	FP_{NREL}, $SF5_{ISU}$, CFP_{NREL}, $CFP_{RTI\text{-}pine}$, $CF_{PRTI\text{-}oak}$	GC-MS: Q_{ion} 96 Da Fragment ions: 67, 53 Da LC-MS:$[M+H]^+$ 97 Da Product ions: 82, 77 Da
3-Methylcyclopent-2-en-1-one		C_6H_8O	96.06	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 96 Da Fragment ions: 67, 53

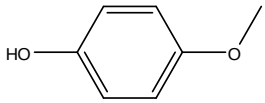
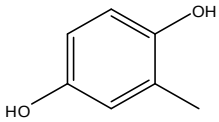
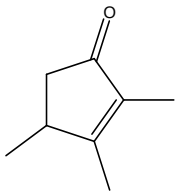
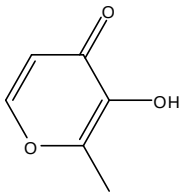
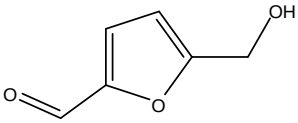
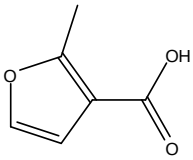
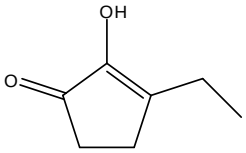
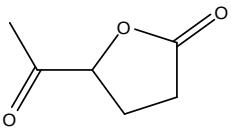
					LC-MS:$[M+H]^+$ 97 Da Product ions: 79, 77 Da
2-Ethylfuran		C_6H_8O	96.06	$CFP_{RTI\text{-}pine}$	GC-MS: Fragment ions: 96, 81, 53 Da LC-MS:$[M+H]^+$ 97 Da Product ions: 57 Da
3-Methyl-2(*5H)*-furanone		$C_5H_6O_2$	98.04	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 98 Da Fragment ions: 55, 43 Da LC-MS:$[M+H]^+$ 99 Da Product ions: 69 Da
4-Methyl-2(*5H)*-furanone		$C_5H_6O_2$	98.04	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 98 Da Fragment ions: 69, 41 Da LC-MS:$[M+H]^+$ 99 Da Product ions: 55 Da
5-Methyl-2(*5H)*-furanone		$C_5H_6O_2$	98.04	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 98 Da Fragment ions: 55, 43 Da LC-MS:$[M+H]^+$ 99 Da Product ions: 69 Da
Cyclopentane-1,2-dione		$C_5H_6O_2$	98.04	FP_{NREL}, $SF5_{ISU}$, CFP_{NREL}, $CFP_{RTI\text{-}pine}$	GC-MS: Q_{ion} 98 Da Fragment ions: 69, 55 Da LC-MS: $[M+H]^+$ 99 Da Product ions: 81, 71Da
2-Methylcyclopentan-1-one		$C_6H_{10}O$	98.07	$SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 98 Da Fragment ions: 55, 42 Da LC-MS: $[M+H]^+$ 99 Da Product ions: 83, 71Da LC-UV_{264nm}
3-Methylcyclopentan-1-one		$C_6H_{10}O$	98.07	$SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 98 Da Fragment ions: 69, 42 Da LC-MS: $[M+H]^+$ 99 Da Product ions: 83, 71Da LC-UV_{264nm}
Hex-3-en-2-one		$C_6H_{10}O$	98.07	$CFP_{RTI\text{-}oak}$	GC-MS: Fragment ions: 83, 55, 43 Da
Pentane-2,3-dione		$C_5H_8O_2$	100.05	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 57 Da Fragment ions: 43, 29

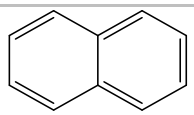
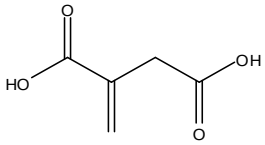
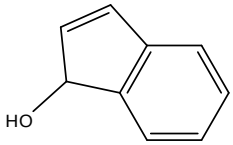
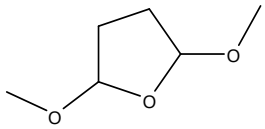
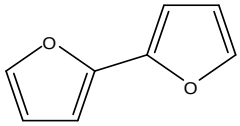
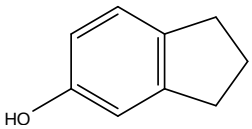
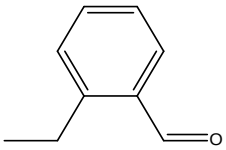
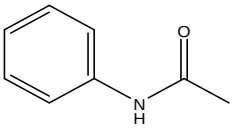
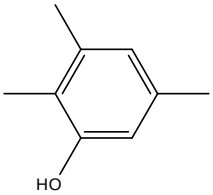
					Da LC-MS:$[M+H]^+$ 101 Da Product ions: 71, 59 Da
2-Methylbut-2-enoic acid		$C_5H_8O_2$	100.05	$SF5_{ISU}$, $CFP_{RTI\text{-}pine}$	GC-MS: Fragment ions: 100, 55, 39 Da LC-MS:$[M-H]^-$ 99 Da Product ions: 59 Da
Hexan-3-one		$C_6H_{12}O$	100.09	$CFP_{RTI\text{-}oak}$	GC-MS: Fragment ions: 71, 57, 43 Da LC-MS:$[M+H]^+$ 101 Da Product ions: 83, 59 Da
Pentanoic acid		$C_5H_{10}O_2$	102.07	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$	GC-MS: Fragment ions: 73, 60, 41 Da LC-MS:$[M-H]^-$ 101 Da Product ions: 54 Da
4-Hydroxypentan-2-one		$C_5H_{10}O_2$	102.07	$SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Fragment ions: 58, 45, 43 Da LC-RID
4-Methoxybutan-2-one		$C_5H_{10}O_2$	102.07	$CFP_{RTI\text{-}pine}$	GC-MS: Fragment ions: 87, 45, 43 Da
Ethylbenzene		C_8H_{10}	106.08	CFP_{NREL}	GC-MS: Q_{ion} 91 Da Fragment ions: 106, 51 Da LC-UV_{264nm}
1,4-Dimethylbenzene		C_8H_{10}	106.08	CFP_{NREL}	GC-MS: Q_{ion} 91 Da Fragment ions: 106, 105 Da LC-UV_{264nm}
2-Methylphenol		C_7H_8O	108.06	FP_{NREL}, $SF5_{ISU}$, CFP_{NREL}, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 108 Da Fragment ions: 107, 79 Da LC-MS: $[M+H]^+$ 109 Da Product ions: 79 Da LC-UV_{264nm}
3-Methylphenol		C_7H_8O	108.06	FP_{NREL}, $SF5_{ISU}$, CFP_{NREL}, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 108 Da Fragment ions: 107, 79 Da LC-MS: $[M+H]^+$ 109 Da Product ions: 91, 81 Da

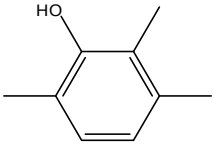
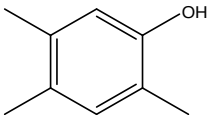
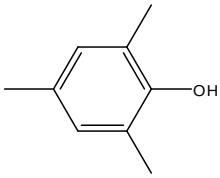
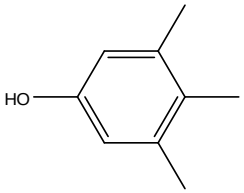
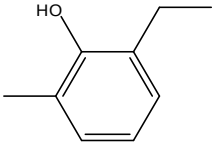
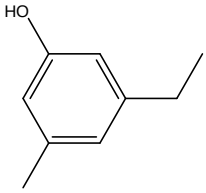
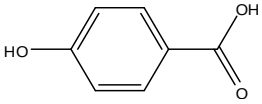
					LC-UV$_{264nm}$
4-Methylphenol		C_7H_8O	108.06	FP$_{NREL}$, SF5$_{ISU}$, CFP$_{NREL}$, CFP$_{RTI-pine}$, CFP$_{RTI-oak}$	GC-MS: Q$_{ion}$ 107 Da Fragment ions: 108, 77 Da LC-MS: [M+H]$^+$ 109 Da Product ions: 91, 81 Da LC-UV$_{264nm}$
Benzene-1,4-diol		$C_6H_6O_2$	110.04	FP$_{NREL}$, CFP$_{NREL}$	GC-MS: Q$_{ion}$ 110 Da Fragment ions: 81, 55 Da LC-UV$_{210nm}$
Benzene-1,2-diol		$C_6H_6O_2$	110.04	FP$_{NREL}$, SF5$_{ISU}$, CFP$_{NREL}$, CFP$_{RTI-pine}$, CFP$_{RTI-oak}$	GC-MS: Q$_{ion}$ 110 Da Fragment ions: 64, 63 Da LC-MS:[M-H]$^-$ 109 Da Product ions: 108, 91 Da LC-UV$_{210nm}$
1-(Furan-2-yl)ethanone		$C_6H_6O_2$	110.04	FP$_{NREL}$, SF5$_{ISU}$, CFP$_{RTI-pine}$, CFP$_{RTI-oak}$	GC-MS: Q$_{ion}$ 95 Da Fragment ions: 110, 39 Da LC-MS: [M+H]$^+$ 111 Da
5-Methylfuran-2-carbaldehyde		$C_6H_6O_2$	110.04	FP$_{NREL}$, SF5$_{ISU}$, CFP$_{RTI-pine}$, CFP$_{RTI-oak}$	GC-MS: Q$_{ion}$ 110 Da Fragment ions: 109, 53 Da LC-MS: [M+H]$^+$ 111 Da Product ions: 81, 51 Da
2,3-Dimethylcyclopent-2-en-1-one		$C_7H_{10}O$	110.07	FP$_{NREL}$, SF5$_{ISU}$, CFP$_{NREL}$, CFP$_{RTI-pine}$, CFP$_{RTI-oak}$	GC-MS: Q$_{ion}$ 110 Da Fragment ions: 67, 39 Da LC-MS: [M+H]$^+$ 111 Da Product ions: 93 Da
3,4-Dimethylcyclopent-2-en-1-one		$C_7H_{10}O$	110.07	CFP$_{RTI-pine}$, CFP$_{RTI-oak}$	GC-MS: Q$_{ion}$ 110 Da Fragment ions: 95, 67 Da LC-MS: [M+H]$^+$ 111 Da Product ions: 93 Da
2-Hydroxy-3-methylcyclopent-2-en-1-one		$C_6H_8O_2$	112.05	FP$_{NREL}$, SF5$_{ISU}$, CFP$_{NREL}$, CFP$_{RTI-pine}$, CFP$_{RTI-oak}$	GC-MS: Q$_{ion}$ 112 Da Fragment ions: 69, 55 Da LC-MS: [M+H]$^+$ 113 Da Product ions: 95 Da

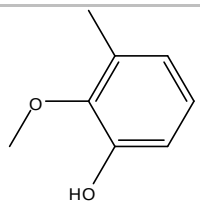
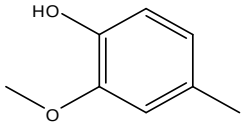
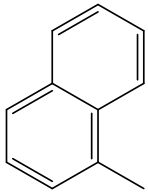
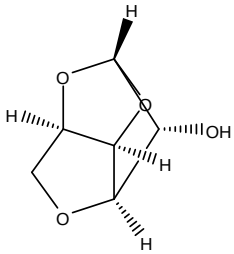
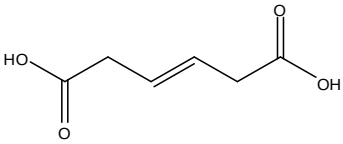
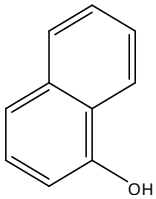
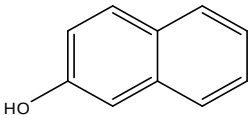
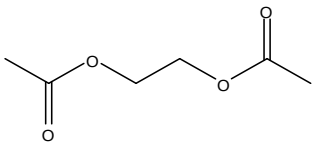
3-Methylcyclopentane-1,2-dione		$C_6H_8O_2$	112.05	FP_{NREL}, $SF5_{ISU}$, CFP_{NREL}, $CFP_{RTI\text{-}pine}$	GC-MS: Q_{ion} 112 Da Fragment ions: 55, 41 Da LC-MS: $[M+H]^+$ 113 Da Product ions: 95, 85, 67 Da
Cyclohexane-1,4-dione		$C_6H_8O_2$	112.05	FP_{NREL}, $SF5_{ISU}$	GC-MS: Q_{ion} 112 Da Fragment ions: 56, 28 Da
Hexane-2,5-dione		$C_6H_{10}O_2$	114.07	$SF5_{ISU}$	GC-MS: Fragment ions: 99, 71, 43 Da
1H-Indene		C_9H_8	116.06	CFP_{NREL}, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 116 Da Fragment ions: 115 Da
4-Hydroxy-4-methylpentan-2-one		$C_6H_{12}O_2$	116.08	FP_{NREL}, CFP_{NREL}, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 59 Da Fragment ions: 58, 43 Da LC-RID
1-Benzofuran		C_8H_6O	118.04	$SF5_{ISU}$, CFP_{NREL}, $CFP_{RTI\text{-}pine}$	GC-MS: Q_{ion} 118 Da Fragment ions: 90, 89 Da
2,3-Dihydro-*1H*-indene		C_9H_{10}	118.08	CFP_{NREL}	GC-MS: Q_{ion} 117 Da Fragment ions: 118, 115 Da
2,3-Dimethylphenol		$C_8H_{10}O$	122.07	$SF5_{ISU}$, CFP_{NREL}, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 107 Da Fragment ions: 122, 121 Da LC-MS: $[M+H]^+$ 123 Da Product ions: 107, 95 Da LC-UV_{210nm}
2,4-Dimethylphenol		$C_8H_{10}O$	122.07	FP_{NREL}, $SF5_{ISU}$, CFP_{NREL}, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 107 Da Fragment ions: 122, 121 Da LC-MS: $[M+H]^+$ 123 Da Product ions: 107, 95 Da LC-UV_{210nm}
2,5-Dimethylphenol		$C_8H_{10}O$	122.07	FP_{NREL}, $SF5_{ISU}$, CFP_{NREL}, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 107 Da Fragment ions: 122, 121 Da

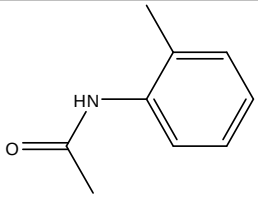
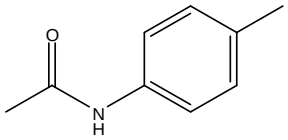
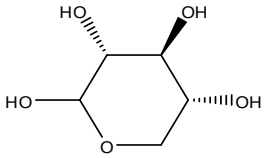
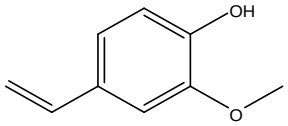
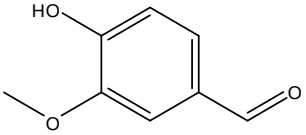
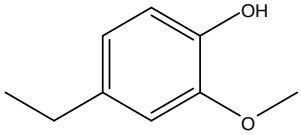
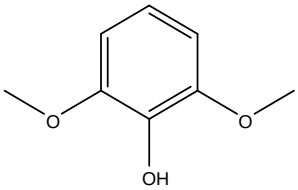
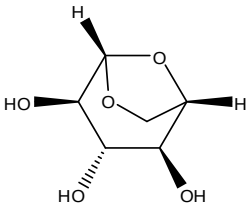
					LC-MS: $[M+H]^+$ 123 Da Product ions: 107 Da LC-UV_{210nm}
2,6-Dimethylphenol		$C_8H_{10}O$	122.07	FP_{NREL}, $SF5_{ISU}$, CFP_{NREL}, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 122 Da Fragment ions: 121, 107 Da LC-MS: $[M+H]^+$ 123 Da Product ions: 107, 93 Da LC-UV_{210nm}
3,4-Dimethylphenol		$C_8H_{10}O$	122.07	FP_{NREL}, $SF5_{ISU}$, CFP_{NREL}, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 122 Da Fragment ions: 121, 107 Da LC-MS: $[M+H]^+$ 123 Da Product ions: 105, 77 Da LC-UV_{210nm}
3,5-Dimethylphenol		$C_8H_{10}O$	122.07	FP_{NREL}, $SF5_{ISU}$, CFP_{NREL}, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 122 Da Fragment ions: 121, 107 Da LC-MS: $[M+H]^+$ 123 Da Product ions: 105, 51 Da LC-UV_{210nm}
2-Ethylphenol		$C_8H_{10}O$	122.07	FP_{NREL}, $SF5_{ISU}$, CFP_{NREL}, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 107 Da Fragment ions: 122, 77 Da LC-MS: $[M-H]^-$ 121 Da Product ions: 109 Da LC-UV_{264nm}
3-Ethylphenol		$C_8H_{10}O$	122.07	FP_{NREL}, $SF5_{ISU}$, CFP_{NREL}, $CFP_{RTI\text{-}pine}$,	GC-MS: Q_{ion} 107 Da Fragment ions: 122, 77 Da LC-MS: $[M-H]^-$ 121 Da Product ions: 109 Da LC-UV_{264nm}
2-Methoxyphenol		$C_7H_8O_2$	124.05	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 109 Da Fragment ions: 124, 81 Da LC-MS: $[M-H]^-$ 123 Da Product ions: 107 Da LC-UV_{210nm} LC-RID

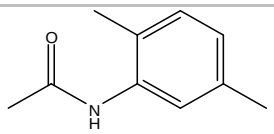
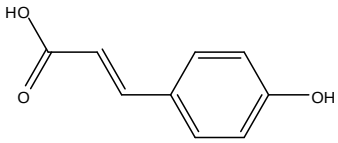
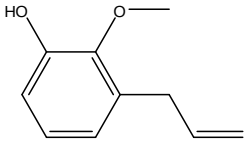
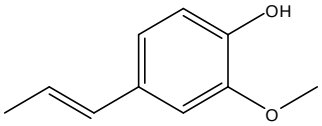
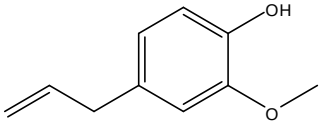
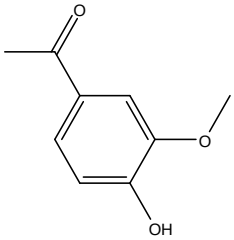
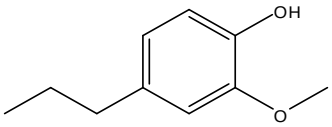
4-Methoxyphenol		$C_7H_8O_2$	124.05	$CFP_{RTI\text{-}oak}$	GC-MS: Fragment ions: 124, 109, 81 Da LC-MS: $[M\text{-}H]^-$ 123 Da Product ions: 107 Da $LC\text{-}UV_{210nm}$
2-Methylbenzene-1,4-diol		$C_7H_8O_2$	124.05	FP_{NREL} , CFP_{NREL}, $CFP_{RTI\text{-}pine}$	GC-MS: Q_{ion} 124 Da Fragment ions: 123, 95 Da LC-MS: $[M+H]^+$ 125 Da Product ions: 107, 97 Da
2,3,4-Trimethylcyclopent-2-en-1-one		$C_8H_{12}O$	124.09	$SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Fragment ions: 124, 109, 81 Da LC-MS: $[M+H]^+$ 125 Da Product ions: 107, 95 Da
3-Hydroxy-2-methylpyran-4-one		$C_6H_6O_3$	126.03	FP_{NREL}, $SF5_{ISU}$	GC-MS: Q_{ion} 126 Da Fragment ions: 71, 43 Da LC-MS: $[M+H]^+$ 127 Da Product ions: 109 Da
5-(Hydroxymethyl)furan-2-carbaldehyde		$C_6H_6O_3$	126.03	FP_{NREL}, $SF5_{ISU}$, CFP_{NREL}, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Fragment ions: 126, 97, 41 Da LC-MS: $[M+H]^+$ 127 Da Product ions: 109 Da
2-Methylfuran-3-carboxylic acid		$C_6H_6O_3$	126.03	FP_{NREL}, $SF5_{ISU}$, CFP_{NREL}	LC-MS: $[M\text{-}H]^-$ 125 Da Product ions: 109 Da $LC\text{-}UV_{210nm}$
3-Ethyl-2-hydroxycyclopent-2-en-1-one		$C_7H_{10}O_2$	126.07	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$	GC-MS: Q_{ion} 126 Da Fragment ions: 83, 55 Da LC-MS: $[M\text{-}H]^-$ 125 Da Product ions: 107 Da
5-Acetyldihydro-2(*3H*)-furanone		$C_6H_8O_3$	128.05	$SF5_{ISU}$	GC-MS: Fragment ions: 85, 43, 29 Da LC-MS: $[M+H]^+$ 129 Da Product ions: 113, 51 Da
Naphthalene		$C_{10}H_8$	128.06	CFP_{NREL}	GC-MS: Q_{ion} 128 Da

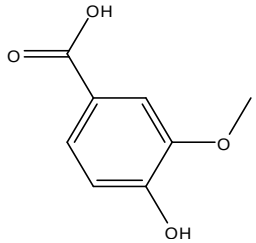
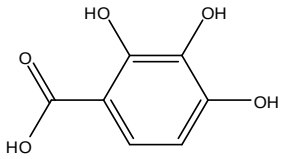
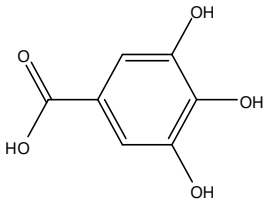
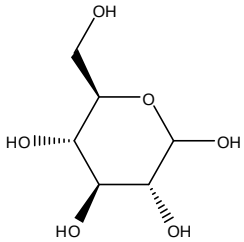
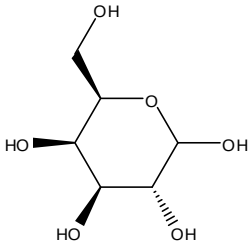
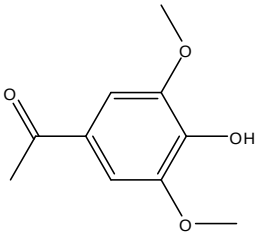
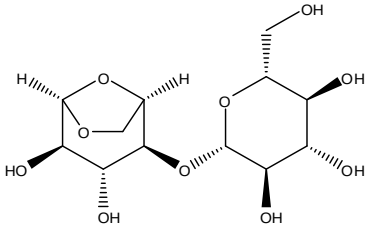
					Fragment ions: 129, 127 Da LC-UV$_{264nm}$
2-Methylidenebutanedioic acid		$C_5H_6O_4$	130.03	FP$_{NREL}$, SF5$_{ISU}$, CFP$_{RTI-pine}$	GC-MS: Fragment ions: 41, 39 Da LC-MS: $[M-H]^-$ 129 Da Product ions: 85, 41 Da LC-UV$_{210nm}$ LC-RID
1H-Inden-1-ol		C_9H_8O	132.06	CFP$_{NREL}$	GC-MS: Fragment ions: 132, 131, 103 Da
2,5-Dimethoxyoxolane		$C_6H_{12}O_3$	132.08	SF5$_{ISU}$, CFP$_{RTI-pine}$	GC-MS: Q_{ion} 101 Da Fragment ions: 72, 41 Da
2-(Furan-2-yl)furan		$C_8H_6O_2$	134.04	SF5$_{ISU}$, CFP$_{NREL}$,	GC-MS: Fragment ions: 134, 105, 78 Da
2,3-Dihydro-*1H*-inden-5-ol		$C_9H_{10}O$	134.07	SF5$_{ISU}$, CFP$_{NREL}$,	GC-MS: Fragment ions: 134, 133, 105 Da
2-Ethylbenzaldehyde		$C_9H_{10}O$	134.07	CFP$_{NREL}$	GC-MS: Fragment ions: 134, 133, 105 Da LC-UV$_{264nm}$
N-phenylacetamide		C_8H_9NO	135.07	CFP$_{RTI-pine}$, CFP$_{RTI-oak}$	GC-MS: Q_{ion} 93 Da Fragment ions: 135, 43 Da LC-MS: $[M+H]^+$ 136 Da Product ions: 94 Da
2,3,5-Trimethylphenol		$C_9H_{12}O$	136.09	SF5$_{ISU}$, CFP$_{NREL}$, CFP$_{RTI-oak}$	GC-MS: Q_{ion} 121 Da Fragment ions: 136, 135 Da LC-MS: $[M-H]^-$ 135 Da Product ions: 119, 79 Da LC-UV$_{264nm}$
2,3,6-Trimethylphenol		$C_9H_{12}O$	136.09	CFP$_{NREL}$, CFP$_{RTI-pine}$, CFP$_{RTI-oak}$	GC-MS: Fragment ions: 136, 121, 91 Da

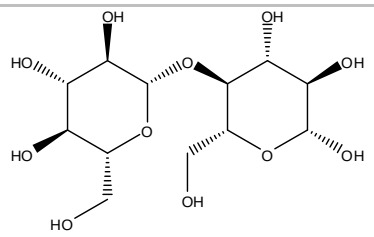
					LC-MS: $[M-H]^-$ 135 Da Product ions: 119, 79 Da LC-UV_{264nm}
2,4,5-Trimethylphenol		$C_9H_{12}O$	136.09	CFP_{NREL}	GC-MS: Fragment ions: 136, 135, 121 Da LC-MS: $[M-H]^-$ 135 Da Product ions: 119, 77 Da LC-UV_{264nm}
2,4,6-Trimethylphenol		$C_9H_{12}O$	136.09	CFP_{NREL}	GC-MS: Fragment ions: 136, 121, 91 Da LC-MS: $[M-H]^-$ 135 Da Product ions: 119, 79 Da LC-UV_{264nm}
3,4,5-Trimethylphenol		$C_9H_{12}O$	136.09	CFP_{NREL}, $CFP_{RTI-pine}$, $CFP_{RTI-oak}$	GC-MS: Fragment ions: 136, 121 91 Da LC-MS: $[M-H]^-$ 135 Da Product ions: 119, 77 Da LC-UV_{264nm}
2-Ethyl-6-methylphenol		$C_9H_{12}O$	136.09	CFP_{NREL}	GC-MS: Fragment ions: 136, 121, 77 Da LC-MS: $[M+H]^+$ 137 Da Product ions: 109 Da LC-UV_{210nm}
3-Ethyl-5-methylphenol		$C_9H_{12}O$	136.09	CFP_{NREL}	GC-MS: Fragment ions: 136, 121, 77 Da LC-MS: $[M+H]^+$ 137 Da Product ions: 109 Da LC-UV_{210nm}
4-Hydroxybenzoic acid		$C_7H_6O_3$	138.03	FP_{NREL}, $CFP_{RTI-oak}$	GC-MS: Fragment ions: 138, 121, 93 Da LC-MS: $[M-H]^-$ 137 Da Product ions: 93, 59 Da LC-UV_{210nm}
2-Methoxy-3-methylphenol		$C_8H_{10}O_2$	138.07	$SF5_{ISU}$	GC-MS: Fragment ions: 138, 123, 77 Da

					LC-MS: $[M-H]^-$ 137 Da Product ions: 122 , 107 Da LC-UV_{264nm}
2-Methoxy-4-methylphenol		$C_8H_{10}O_2$	138.07	FP_{NREL}, $SF5_{ISU}$, $CF_{PRTI\text{-}pine}$	GC-MS: Q_{ion} 138 Da Fragment ions: 123, 77 Da LC-MS: $[M-H]^-$ 137 Da Product ions: 122 Da LC-UV_{264nm}
1-Methylnaphthalene		$C_{11}H_{10}$	142.08	$SF5_{ISU}$, CFP_{NREL}	GC-MS: Q_{ion} 142 Da Fragment ions: 141, 115 Da LC-MS: $[M+H]^+$ 143 Da Product ions: 117 Da LC-UV_{264nm}
1,4:3,6-Dianhydro-*α*-d-glucopyranose		$C_6H_8O_4$	144.04	FP_{NREL}, $SF5_{ISU}$	GC-MS: Fragment ions: 144, 69 Da LC-MS: $[M-H]^-$ 143 Da Product ions: 113, 74, Da LC-ELSD
Hex-3-enedioic acid		$C_6H_8O_4$	144.04	$SF5_{ISU}$	GC-MS: Fragment ions: 126, 108, 55 Da LC-MS: $[M-H]^-$ 143 Da Product ions: 125 Da
Naphthalen-1-ol		$C_{10}H_8O$	144.06	CFP_{NREL}	GC-MS: Q_{ion} 144 Da Fragment ions: 116, 115 Da LC-MS: $[M-H]^-$ 143 Da Product ions: 125, 117 Da
Naphthalen-2-ol		$C_{10}H_8O$	144.06	CFP_{NREL}	GC-MS: Q_{ion} 144 Da Fragment ions: 116, 115 Da LC-MS: $[M-H]^-$ 143 Da Product ions: 125, 115 Da
2-Acetyloxyethyl acetate		$C_6H_{10}O_4$	146.06	$SF5_{ISU}$	GC-MS: Fragment ions: 86, 43, 15 Da
N-(2-methylphenyl)acetamide		$C_9H_{11}NO$	149.08	$CFP_{RTI\text{-}oak}$	

					GC-MS: Fragment ions: 149, 107, 106 Da LC-MS: $[M+H]^+$ 150 Da Product ions:108, 55 Da
N-(4-methylphenyl)acetamide		$C_9H_{11}NO$	149.08	$CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Fragment ions: 149, 107, 106 Da LC-MS: $[M+H]^+$ 150 Da Product ions:108, 93 Da
D-Xylose		$C_5H_{10}O_5$	150.05	FP_{NREL}, $SF5_{ISU}$	LC-MS: $[M-H]^-$ 149 Da Product ions: 131, 89 Da LC-ELSD
4-Ethenyl-2-methoxyphenol		$C_9H_{10}O_2$	150.07	FP_{NREL}, $SF5_{ISU}$	GC-MS: Q_{ion} 150 Da Fragment ions: 135, 107 Da LC-MS: $[M+H]^+$ 151 Da Product ions: 123, 109 Da
4-Hydroxy-3-methoxybenzaldehyde		$C_8H_8O_3$	152.05	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 151 Da Fragment ions: 152, 81 Da LC-MS: $[M-H]^-$ 151 Da Product ions: 136 Da
4-Ethyl-2-methoxyphenol		$C_9H_{12}O_2$	152.08	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 137 Da Fragment ions: 152 Da LC-MS: $[M+H]^+$ 153 Da Product ions:125, 93 Da
2,6-Dimethoxyphenol		$C_8H_{10}O_3$	154.06	FP_{NREL}, $SF5_{ISU}$, CFP_{NREL}, $CFP_{RTI\text{-}oak}$	GC-MS: Fragment ions: 154, 139, 111 Da LC-MS: $[M+H]^+$ 155 Da Product ions:123 Da
1,6-Anhydro-*β*-D-glucopyranose		$C_6H_{10}O_5$	162.05	FP_{NREL}, $SF5_{ISU}$	LC-MS: $[M-H]^-$ 161 Da Product ions: 143 Da LC-ELSD
N-(2,5-dimethylphenyl)acetamide		$C_{10}H_{13}NO$	163.10	$CFP_{RTI\text{-}oak}$	GC-MS: Fragment ions: 163, 121, 106 Da

					LC-MS: $[M+H]^+$ 164 Da Product ions:122 Da
3-(4-Hydroxyphenyl)prop-2-enoic acid		$C_9H_8O_3$	164.05	FP_{NREL}, $CFP_{RTI\text{-}oak}$	LC-MS: $[M-H]^-$ 163 Da Product ions: 119, 93 Da LC-UV_{210nm}
2-Methoxy-3-prop-2-enylphenol		$C_{10}H_{12}O_2$	164.08	$SF5_{ISU}$, $CFP_{RTI\text{-}pine}$	GC-MS: Fragment ions: 164, 149, 77 Da LC-MS: $[M+H]^+$ 165 Da Product ions:147, 123 Da LC-UV_{264nm}
2-Methoxy-4-prop-1-enylphenol		$C_{10}H_{12}O_2$	164.08	$SF5_{ISU}$, $CFP_{RTI\text{-}pine}$	GC-MS: Q_{ion} 164 Da Fragment ions: 149, 77 Da LC-MS: $[M+H]^+$ 165 Da Product ions:137, 124 Da LC-UV_{264nm}
2-Methoxy-4-prop-2-enylphenol		$C_{10}H_{12}O_2$	164.08	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Q_{ion} 164 Da Fragment ions: 149, 77 Da LC-MS: $[M+H]^+$ 165 Da Product ions:137, 124 Da
1-(4-Hydroxy-3-methoxyphenyl)-ethanone		$C_9H_{10}O_3$	166.06	FP_{NREL}, $SF5_{ISU}$, CFP_{NREL}, $CFP_{RTI\text{-}pine}$, $CFP_{RTI\text{-}oak}$	GC-MS: Fragment ions: 166, 151, 123 Da LC-MS: $[M-H]^-$ 165 Da Product ions:150, 121 Da
2-Methoxy-4-propylphenol		$C_{10}H_{14}O_2$	166.10	FP_{NREL}, $SF5_{ISU}$, $CFP_{RTI\text{-}pine}$	GC-MS: Q_{ion} 137 Da Fragment ions: 166, 122 Da LC-MS: $[M+H]^+$ 167 Da Product ions:125, 107 Da
4-Hydroxy-3-methoxybenzoic acid		$C_8H_8O_4$	168.04	FP_{NREL}	LC-MS: $[M-H]^-$ 167 Da Product ions:123, 108 Da LC-UV_{210nm}

					
2,3,4-Trihydroxybenzoic acid		$C_7H_6O_5$	170.02	$SF5_{ISU}$, $CFP_{RTI\text{-}pine}$	LC-MS: $[M\text{-}H]^-$ 169 Da Product ions:125, 97 Da LC-UV_{210nm}
3,4,5-Trihydroxybenzoic acid		$C_7H_6O_5$	170.02	FP_{NREL}, $SF5_{ISU}$	LC-MS: $[M\text{-}H]^-$ 169 Da Product ions:125, 79 Da LC-UV_{210nm}
D-Glucose		$C_6H_{12}O_6$	180.06	FP_{NREL}	LC-MS: $[M\text{-}H]^-$ 179 Da Product ions: 161, 143, 119 Da LC-ELSD
D-Galactose		$C_6H_{12}O_6$	180.06	FP_{NREL}	LC-MS: $[M\text{-}H]^-$ 179 Da Product ions: 161, 143, 80 Da LC-ELSD
1-(4-Hydroxy-3,5-dimethoxyphenyl)-ethanone		$C_{10}H_{12}O_4$	196.07	FP_{NREL}	GC-MS: Q_{ion} 181 Da Fragment ions: 196, 43 Da LC-MS: $[M+H]^+$ 197 Da Product ions:179, 155 Da LC-UV_{210nm}
1,6-Anhydro-*β*-D-cellobiose		$C_{12}H_{20}O_{10}$	324.11	FP_{NREL}	LC-MS: $[M\text{-}H]^-$ 323 Da Product ions: 179, 161, 143 Da LC-ELSD
D-Cellobiose		$C_{12}H_{22}O_{11}$	342.12	FP_{NREL}	

					LC-MS: $[M-H]^-$ 341 Da Product ions: 281, 179, 161 Da LC-ELSD

*Q_{ion} (GC-MS) indicates the ion from which the chemical was quantitated; Parent ion (LC-MS) indicates the most abundant ionization adduct formation, multiples adducts were found in this study for most chemicals between experiments

Table S3. Associated standards used to quantify analytes identified within aqueous fractions of fast pyrolysis and catalytic fast pyrolysis, including analysis deviation. Ordered alphabetically by IUPAC name.

IUPAC Name	Common Name	CAS	Supplier	Purity	Relative Standard Deviation*
1-(4-Hydroxy-3,5-dimethoxyphenyl)-ethanone	Acetosyringone	2478-38-8	Sigma Aldrich	≥97%	1.83%
1-(4-Hydroxy-3-methoxyphenyl)-ethanone	Acetovanillone	498-02-2	Sigma Aldrich	98%	2.36 – 14.09%
1-(Furan-2-yl)-ethanone	2-Acetylfuran	1192-62-7	Sigma Aldrich	99%	1.33 – 10.01%
1,4:3,6-Dianhydro-α-D-glucopyranose	Same	4451-30-3	LC Scientific	≥98%	0.59 – 1.61%
1,4-Dimethylbenzene	1,4-Xylene	106-42-3	AccuStandard[2]	≥98%	0.00%
1,6-Anhydro-β-D-cellobiose	Cellobiosan	35405-71-1	Santa Cruz Biotech	≥98%	3.32 – 6.85%
1,6-Anhydro-β-D-glucopyranose	Levoglucosan	498-07-7	Sigma Aldrich	≥99%	0.59 – 1.93%
1-Benzofuran	Benzofuran	271-89-6	AccuStandard[1]	≥98%	1.01 – 6.49%
1H-Indene	Indene	95-13-6	AccuStandard[2]	≥98%	0.00 – 5.59%
1-Hydroxybutan-2-one	Same	5077-67-8	AccuStandard[3]	≥98%	1.09 – 5.93 %
1-Hydroxypropan-2-one	Hydroxyacetone	116-09-6	AccuStandard[3]	≥98%	0.53 – 7.62%
1-Methylnaphthalene	Same	90-12-0	AccuStandard[2]	≥98%	0.00 – 3.15%
2(5H)-Furanone	2-Butenolide	497-23-4	Sigma Aldrich	98%	1.00 – 7.18%
2,3,4-Trihydroxybenzoic acid	Pyrogallolcarboxylic acid	610-02-6	Sigma Aldrich	≥97%	5.25%
2,3-Dihydro-1H-indene	Indane	496-11-7	AccuStandard[2]	≥98%	0.00 – 7.53%
2,3-Dimethylcyclopent-2-en-1-one	Same	1121-05-7	AccuStandard[3]	≥98%	1.00 – 5.54%
2,3-Dimethylphenol	2,3-Xylenol	526-75-0	AccuStandard[1]	≥98%	0.00 – 6.93%
2,4-Dimethylphenol	2,4-Xylenol	105-67-9	AccuStandard[1]	≥98%	0.55 – 7.00%
2,5-Dimethoxyoxolane	2-5-Dimethoxytetrahydrofuran	696-59-3	Sigma Aldrich	98%	3.89%
2,5-Dimethylphenol	2,5-Xylenol	95-87-4	Sigma Aldrich	≥99%	0.44 – 8.87%
2,6-Dimethoxyphenol	Syringol	91-10-1	Sigma Aldrich	99%	1.16 – 4.91%
2,6-Dimethylphenol	2,6-Xylenol	576-26-1	Sigma Aldrich	≥99.8%	0.27 – 12.63%
2-Ethylphenol	Same	90-00-6	Sigma Aldrich	99%	2.25 – 2.78%
2-Hydroxy-3-methylcyclopent-2-en-1-one	Cyclotene	80-71-7	AccuStandard[1]	≥98%	0.44 – 6.01%
2-Hydroxyacetaldehyde	Glycoaldehyde	141-46-8	Sigma Aldrich	97%	0.06 – 8.21%
2-Hydroxyacetic acid	Glycolic acid	79-14-1	TCI Chemicals	≥98%	0.94 –1.20%
2-Methoxy-4-methylphenol	Creosol	93-51-6	AccuStandard[1]	≥98%	0.35 – 6.64%
2-Methoxy-4-prop-1-enylphenol	Isoeugenol	97-54-1	AccuStandard[1]	≥98%	2.86 – 7.46%
2-Methoxy-4-prop-2-enylphenol	Eugenol	97-53-0	Sigma Aldrich	99%	0.72%
2-Methoxy-4-propylphenol	4-Propylquaiacol	2785-87-7	Sigma Aldrich	≥99%	2.44%
2-Methoxyphenol	Guaiacol	8001-58-9	Sigma Aldrich	≥99%	2.12 – 6.82%
2-Methylbenzene-1,4-diol	2-Methylhydroquinone	95-71-6	Sigma Aldrich	≥98%	1.83 – 7.01%
2-Methylbut-2-enal	Tiglic aldehyde	497-03-0	Sigma Aldrich	≥96%	0.82 – 7.49%
2-Methylcyclopent-2-en-1-one	2-Methyl-2-cyclopenten-1-one	1120-73-6	AccuStandard[1]	≥98%	0.79 – 13.47%
2-Methylcyclopentan-1-one	2-Methylcyclopentanone	1120-72-5	Sigma Aldrich	98%	13.80 - 15.17%
2-Methylfuran-3-carboxylic acid	2-Methyl-3-furoic acid	6947-94-0	Sigma Aldrich	97%	3.10 – 7.07%
2-Methylidenebutanedioic acid	Itaconic acid	97-65-4	Fluka Analytical	≥99%	3.70 – 9.34%
2-Methylphenol	*o*-Cresol	95-48-7	AccuStandard[1]	≥98%	1.05 – 5.27%
2,3,5-Trimethylphenol	Same	697-82-5	Sigma Aldrich	99%	4.68%
3-(4-Hydroxyphenyl)prop-2-enoic acid	*p*-Coumaric acid	501-98-4	Sigma Aldrich	≥98%	0.14 – 14.64%
3,4,5-Trihydroxybenzoic acid	Gallic acid	149-91-7	Sigma Aldrich	99.5%	0.94 – 3.69%
3,4-Dimethylcyclopent-2-en-1-one	Same	30434-64-1	2,3-Dimethylcyclopent-2-en-1-one used for quantitation		
3,4-Dimethylphenol	3,4-Xylenol	95-65-8	Sigma Aldrich	99%	7.18%
3,5-Dimethylphenol	3,5-Xylenol	108-68-9	Sigma Aldrich	≥99%	5.84%
3-Ethyl-2-hydroxycylcopent-2-en-1-one	Same	21835-01-8	AccuStandard[3]	≥98%	1.39 – 5.62%
3-Ethylphenol	Same	620-17-7	Sigma Aldrich	99%	23.77%
3-Hydroxy-2-methylpyran-4-one	Maltol	118-71-8	Sigma Aldrich	≥97%	1.29 – 9.26%
3-Hydroxybutan-2-one	Acetoin	513-86-0	AccuStandard[3]	≥98%	3.43 – 7.30%
3-Methyl-2(5H)-furanone	2-Methyl-2-Butenolide	22122-36-7	Sigma Aldrich	90%	0.68 – 8.33%
3-Methylcyclopent-2-en-1-one	3-Methyl-2-cyclopentenone	2758-18-1	Sigma Aldrich	97%	0.62 – 6.38%
3-Methylcyclopentan-1-one	3-Methylcyclopentanone	1757-42-2	Sigma Aldrich	99%	1.50 – 7.25%
3-Methylcyclopentane-1,2-dione	3-Methyl-1,2-cyclopentanedione	765-70-8	Sigma Aldrich	99%	1.45 – 11.16%
3-Methylphenol	*m*-Cresol	108-39-4	AccuStandard[2]	≥98%	0.39 – 6.74%
4-Ethenyl-2-methoxyphenol	4-Vinylguaiacol	7786-61-0	AccuStandard[1]	≥98%	1.14 – 5.89%
4-Ethyl-2-methoxyphenol	4-Ethylguaiacol	2785-89-9	AccuStandard[1]	≥98%	0.54 – 5.03%
4-Hydroxy-3-methoxybenzaldehyde	Vanillin	121-33-5	Sigma Aldrich	≥99%	0.86 – 7.37%
4-Hydroxy-3-methoxybenzoic acid	Vanillic acid	121-34-6	Sigma Aldrich	≥97%	0.70 – 2.87%
4-Hydroxy-4-methylpentan-2-one	Diacetone alcohol	123-42-2	Sigma Aldrich	99%	1.90 – 7.88%
4-Hydroxybenzoic acid	4-Carboxyphenol	99-96-7	Sigma Aldrich	≥99%	6.35 – 6.58%
4-Hydroxybutan-2-one	Methylalacetone	590-90-9	AccuStandard[3]	≥98%	1.32 – 14.40%

4-Methyl-2(5H)-furanone	Same	6124-79-4	TCI Chemicals	≥97%	0.52 – 8.00%
4-Methylphenol	*p*-Cresol	106-44-5	AccuStandard[1]	≥98%	0.55 – 5.95%
5-(Hydroxymethyl)-2-furancarbaldehyde	5-Hydroxymethylfurfural	67-47-0	Sigma Aldrich	≥98%	0.43 – 5.90%
5-Methyl-2(5H)-furanone	*β*-Angelica lactone	591-11-7	4-Methyl-2(5H)-furanone used for quantitation		
5-Methylfuran-2-carbaldehyde	5-Methylfurfural	620-02-0	Sigma Aldrich	99%	0.98 – 6.68%
Acetaldehyde	Same	75-07-0	Sigma Aldrich	≥99.5%	3.89 – 23.65%
Acetic acid	Same	64-19-7	Sigma Aldrich	≥99.8%	0.12 – 1.19%
Benzene-1,2-diol	Catechol	120-80-9	Sigma Aldrich	≥99.9%	2.49 - 6.21%
Benzene-1,4-diol	Hydroquinone	123-31-9	Sigma Aldrich	≥99%	2.81 – 5.89%
But-2-enal	Crotonaldehyde	123-73-9	Sigma Aldrich	≥99%	1.06 – 10.26%
But-2-enoic acid	Crotonic acid	107-93-7	Sigma Aldrich	98%	0.14 – 9.00%
But-3-en-2-one	Methyl vinyl ketone	78-94-4	AccuStandard[1]	≥98%	9.52 – 14.85%
Butane-2,3-dione	Diacetyl	431-03-8	Sigma Aldrich	≥99%	1.41 – 11.91%
Butanoic acid	Butyric acid	107-92-6	AccuStandard[3]	≥98%	1.09 – 7.10%
Cyclohexane-1,4-dione	Tetrahydroquinone	637-88-7	AccuStandard[3]	≥98%	2.92 – 10.82%
Cyclopent-2-en-1-one	2-Cyclopenten-1-one	930-30-3	AccuStandard[1]	≥98%	0.33 – 5.37%
Cyclopentane-1,2-dione	1,2-Cyclopentandione	3008-40-0	Sigma Aldrich	97%	0.29 – 8.95%
Cyclopentanone	Adipic ketone	120-92-3	AccuStandard[3]	≥98%	1.74 – 8.45%
D-Galactose	Galactose	59-23-4	Sigma Aldrich	≥99%	3.06%
D-Glucose	Glucose	50-99-7	Sigma Aldrich	≥99.5%	0.59 – 4.36%
D-Xylose	Xylose	58-86-6	Sigma Aldrich	≥99%	0.74 – 1.44%
Ethylbenzene	Same	100-41-4	AccuStandard[2]	≥98%	0.00 - 1.88%
Formic acid	Same	64-18-6	Sigma Aldrich	≥98%	2.23 – 16.78%
Furan-2-carbaldehyde	Furfural	98-01-1	Sigma Aldrich	99%	0.46 – 25.83%
Furan-3-carbaldehyde	3-Furaldehyde	498-60-2	Sigma Aldrich	≥97%	0.55 – 13.64%
Methanol	Same	67-56-1	Sigma Aldrich	≥98.5%	1.02 – 1.51%
N-(2,5-dimethylphenyl)acetamide	Same	2050-44-4	N-(2-methylphenyl)acetamide used for quantitation		
N-(2-methylphenyl)acetamide	o-Acetotoluidide	120-66-1	Sigma Aldrich	N/A	7.88%
N-(4-methylphenyl)acetamide	p-Acetotoluidide	103-89-9	N-(2-methylphenyl)acetamide used for quantitation		
Naphthalen-1-ol	1-Naphthol	90-15-3	Sigma Aldrich	≥99%	2.10%
Naphthalen-2-ol	2-Naphthol	135-19-3	Sigma Aldrich	99%	1.62%
Naphthalene	Naphthalin	91-20-3	AccuStandard[2]	≥98%	0.00%
N-phenylacetamide	Acetanilide	103-84-4	Elemental Microanalysis	99%	6.59%
Oxolan-2-one	ɣ-Butyrolactone	96-48-0	Sigma Aldrich	≥99%	0.49 – 5.87%
Pentan-2-one	Methyl propyl ketone	107-87-9	TCI Chemicals	≥97%	1.75 – 7.03%
Pentane-2,3-dione	Acetylpropionyl	600-14-6	Sigma Aldrich	97%	1.06 – 8.48%
Pentanoic acid	Valeric acid	109-52-4	Sigma Aldrich	≥99%	1.92 – 12.23%
Phenol	Hydroxybenzene	108-95-2	Sigma Aldrich	≥99.5%	0.67 – 6.09%
Prop-2-enoic acid	Acrylic acid	79-10-7	Sigma Aldrich	99%	0.15 – 6.85%
Propan-1-ol	Propanol	71-23-8	AccuStandard[3]	≥98%	1.02 – 4.13%
Propan-2-one	Acetone	67-64-1	Sigma Aldrich	≥99.9%	5.18 – 13.83%
Propanoic acid	Propionic acid	79-09-4	Sigma Aldrich	≥99.5%	0.39 – 16.08%
Toluene	Same	108-88-3	AccuStandard[1]	≥98%	0.00 – 6.66%

*Relative standard deviation range of analysis and shot-to-shot variability within each sample of triplicate independent experiments (n = 3). [1]Accustandard custom mix, purity adjusted for by concentration and certified – lot # 214041098; [2]lot # 214041230; [3]lot # 215031394.