Aqueous extractive upgrading of bio-oils created by tail-gas reactive pyrolysis to produce pure hydrocarbons and phenols

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Supplemental Materials

paraffins	naphtha	BTEX/aromatics	Phenols
2-methylbutane	decalin	Benzene	Phenol
2-methylpentane	cyclopentane	Toluene	o-cresol
2,4-dimethylpentane	cyclopentane, methyl	Ethyl Benzene	m-cresol
n-pentane	cyclohexane	p-xylene	p-cresol
n-hexane	cyclohexane, methyl-	o-xylene	2,4-dimethylphenol
n-heptane	cyclohexane, 1,3-dimethyl	benzene, n-propyl	4-ethylphenol
n-octane	cyclohexane, 1,2-dimethyl-(trans)	benzene, n-butyl	
n-nonane[1]	cyclohexane,1,2-dimethyl-(cis)		
n-decane	cyclohexane,ethyl-	PAHs	Methyl tetralins[3]
n-dodecane	cyclohexane,isopropyl-	Biphenyl	2-methyltetralin
n-tridecane	cyclohexane,n-propyl-	Fluorene	1-methyltetralin
n-tetradecane	cyclohexane,isobutyl-	Anthracene	6-methyltetralin
n-pentadecane	cyclohexane,t-butyl-		
n-hexadecane	cyclohexane,n-butyl-		
n-heptadecane			
n-octadecane	acids	naphthalenes	
n-nonadecane	Acetic Acid	naphthalene	
n-eicosane	Acetol	2-methyl naphthalene	
n-heneicosane		1-methyl naphthalene[2]	

Table S1 – lumped categories of compounds quantified by GC-MS. This list excludes compounds which were calibrated but did not appear beyond trace amounts. [1]Assumed to scale according to n-octane. [2]assumed to scale according to 2-methyl napththalene [3]assumed to scale according to tetralin.

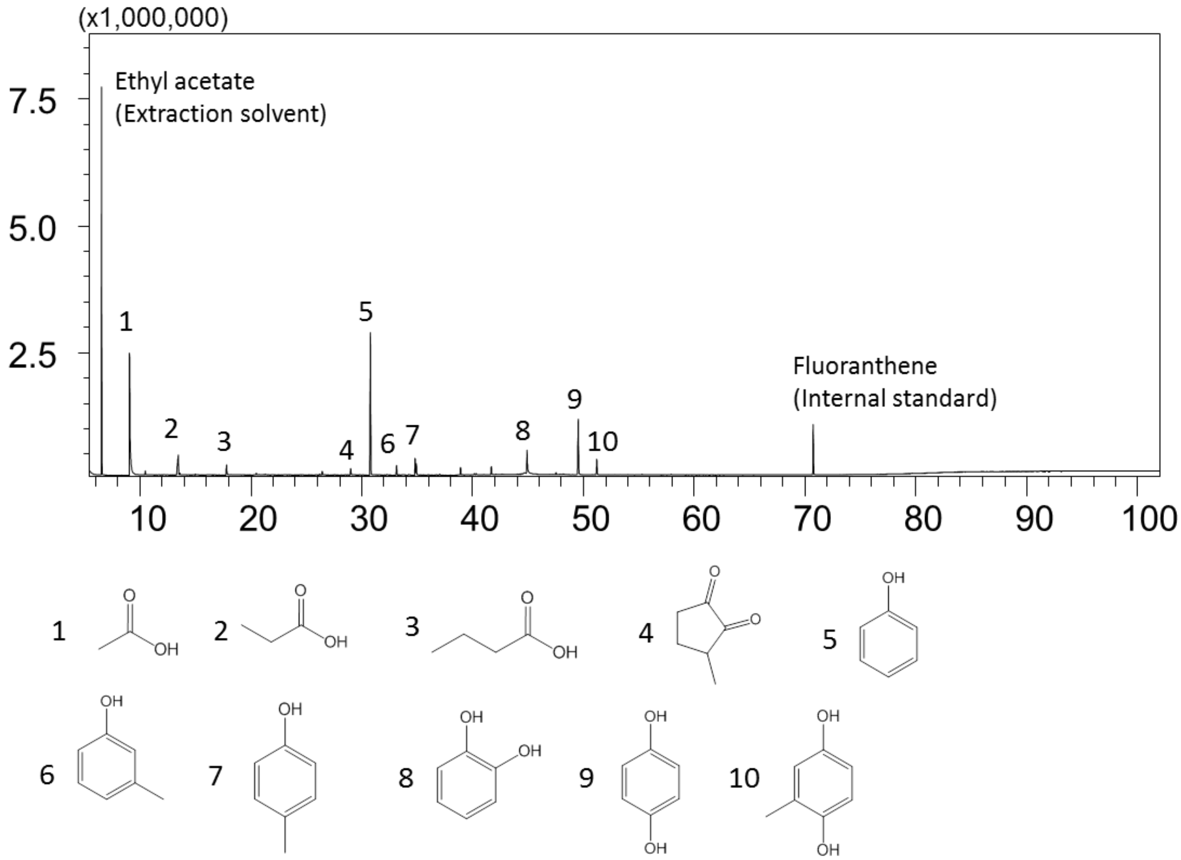

Figure S1 – chromatogram of organic compounds extracted from the 3a aqueous layer, post-acidification of phenolic salts.

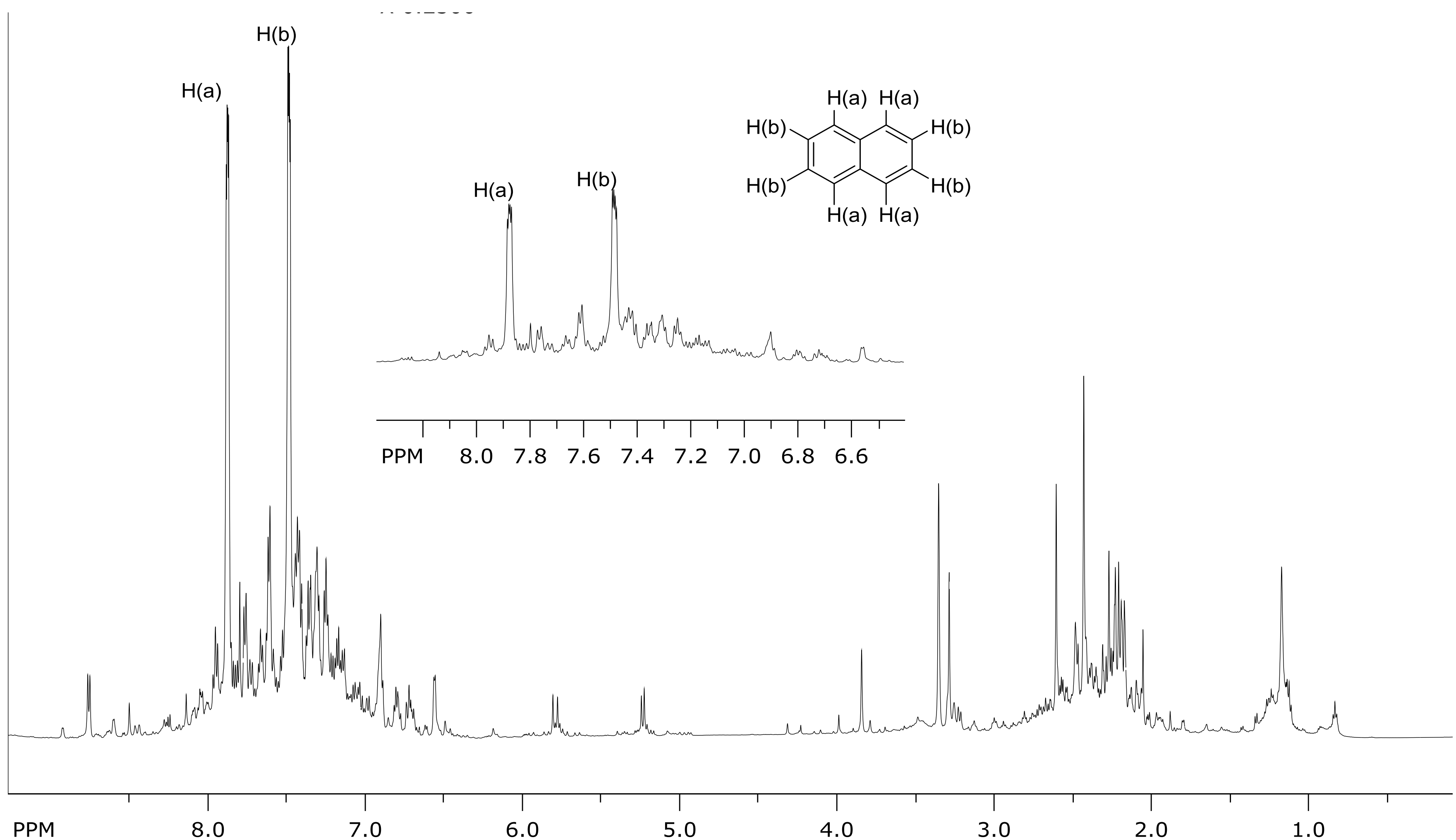

Figure S2. ^{1}H NMR (600 MHz, DMSO-d6) spectrum of fraction 2a hydrocarbons extracted from horse manure bio-oil. Peaks assigned to naphthalene are labeled.

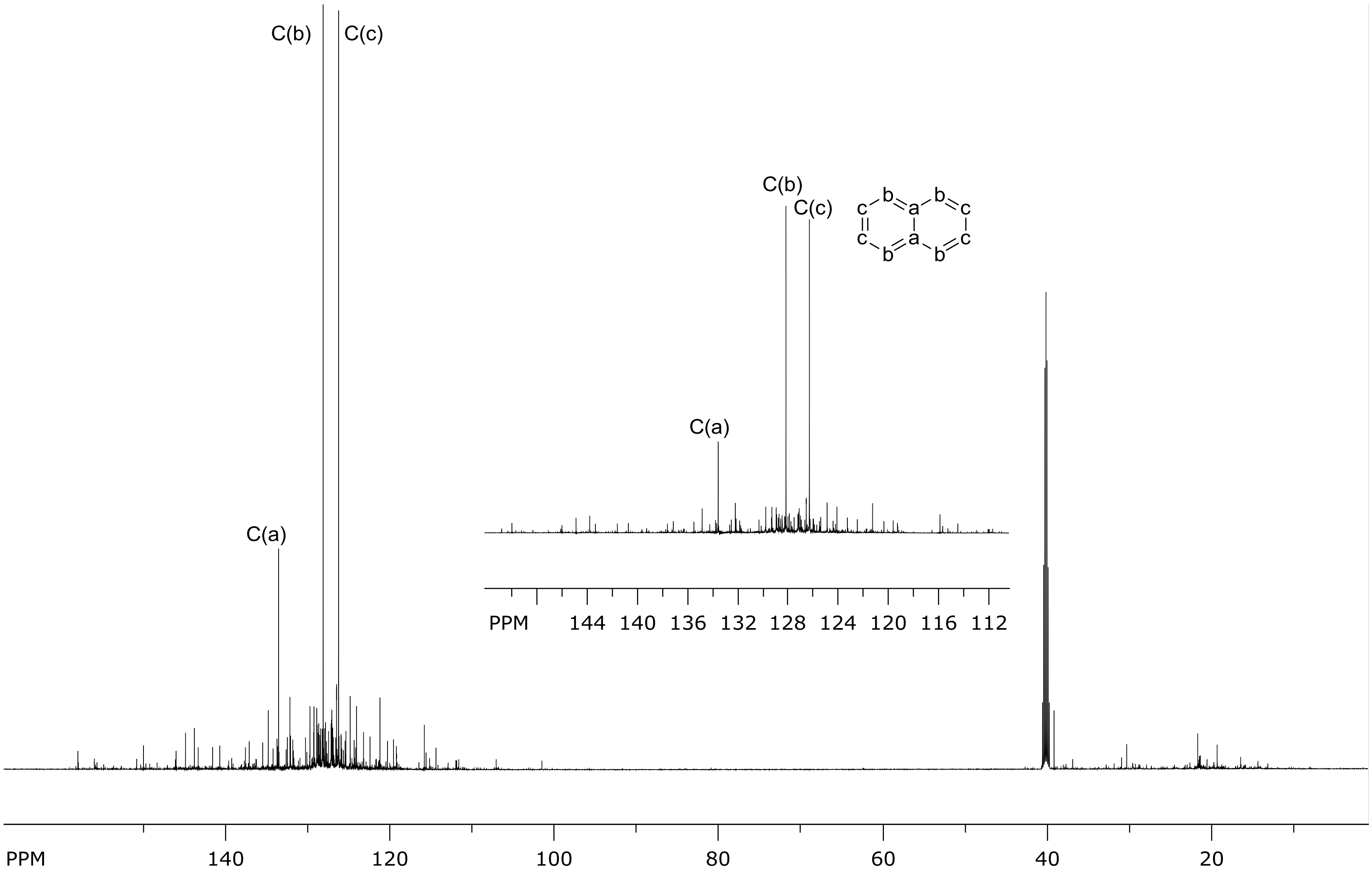

Figure S3 – $^{13}C\{^{1}H\}$ NMR spectrum (150 MHZ, DMSO-d_6) of fractions 2a hydrocarbons extracted from horse manure bio-oil. Peaks assigned to naphthalene are labeled.

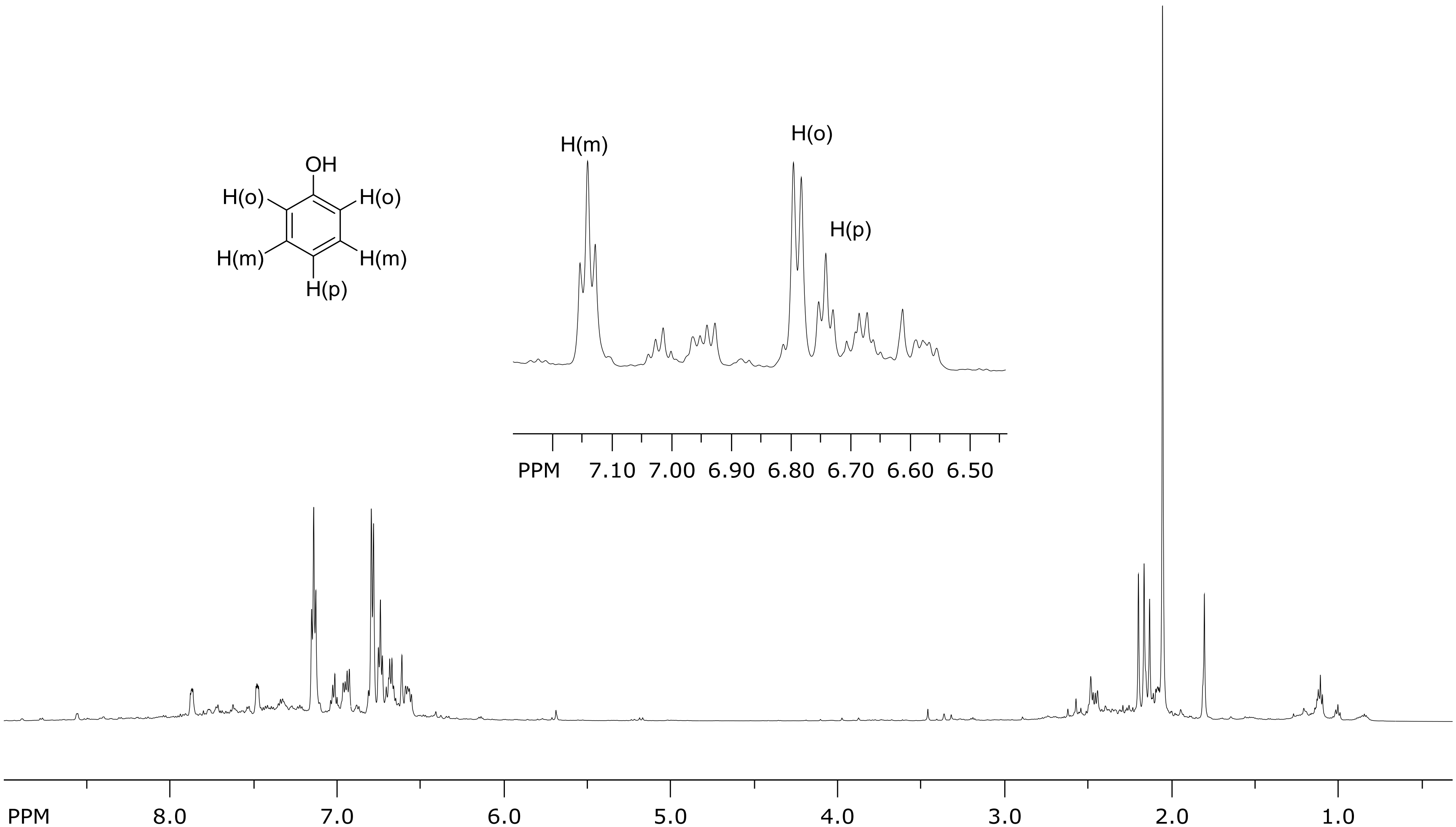

Figure S4 – 1H NMR spectrum (600 MHZ, DMSO-d_6) fractions 3a phenolics extracted from horse manure bio-oil. Peaks assigned to phenol are labeled.

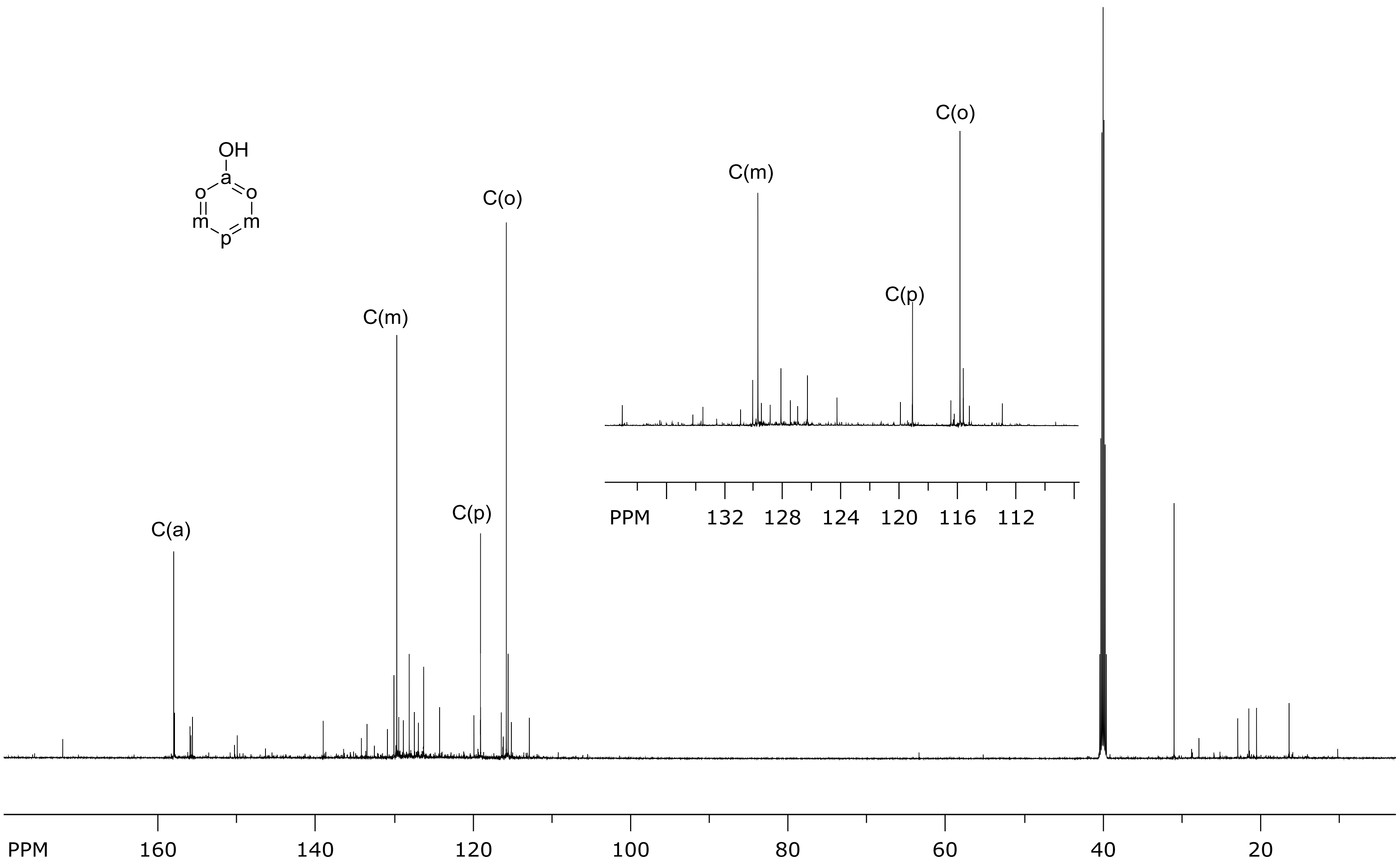

Figure S5 – $^{13}C\{^{1}H\}$ NMR spectrum (150 MHZ, DMSO-d_6) fractions 3a phenolics extracted from horse manure bio-oil. Peaks assigned to phenol are labeled.

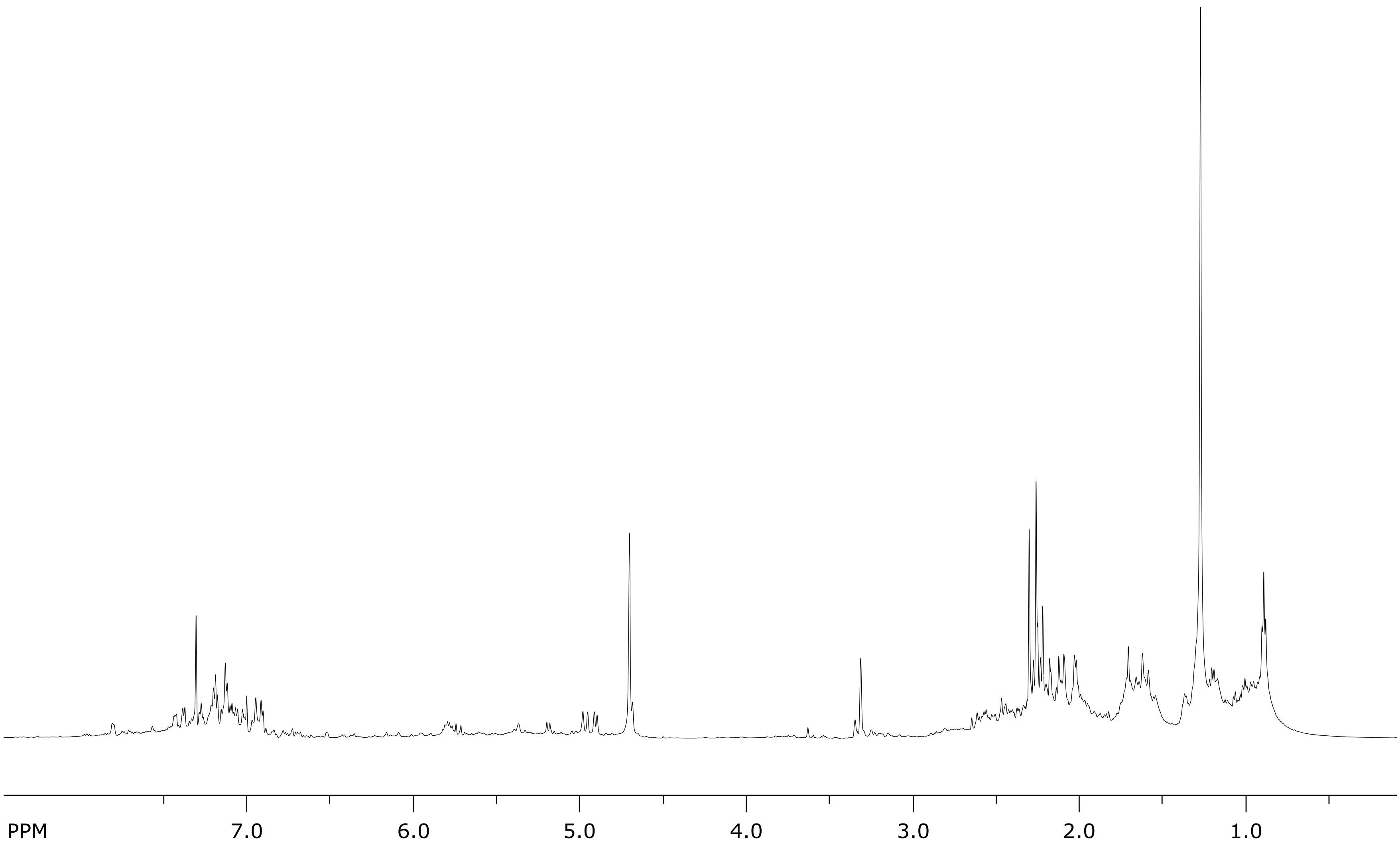

Figure S6. [1]H NMR (600 MHz, DMSO-d6) spectrum of fraction 2a hydrocarbons extracted from guayule bagasse bio-oil.

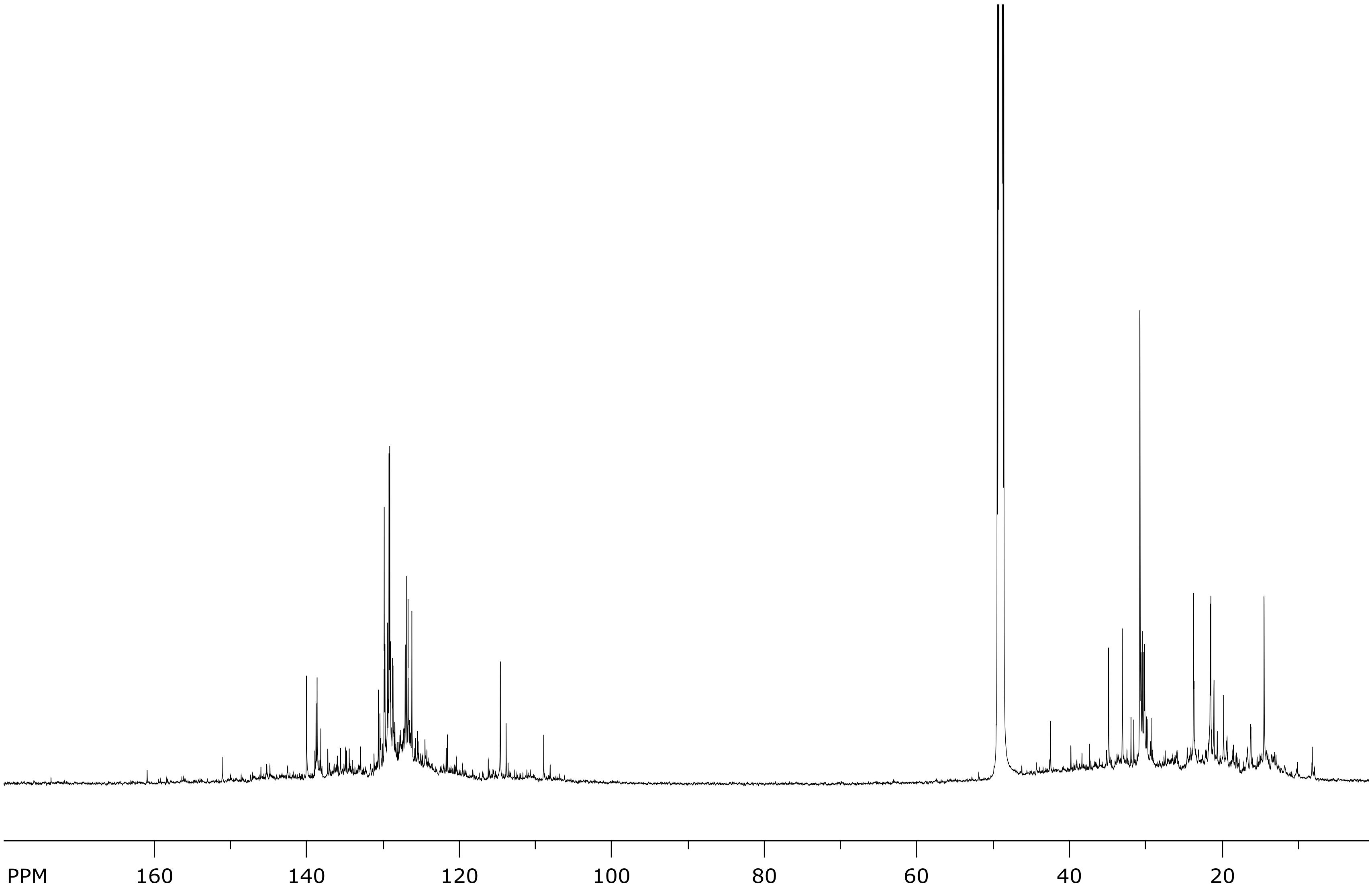

Figure S7– $^{13}C\{^{1}H\}$ NMR spectrum (150 MHZ, DMSO-d_6) of fractions 2a hydrocarbons extracted from guayule bagasse bio-oil.

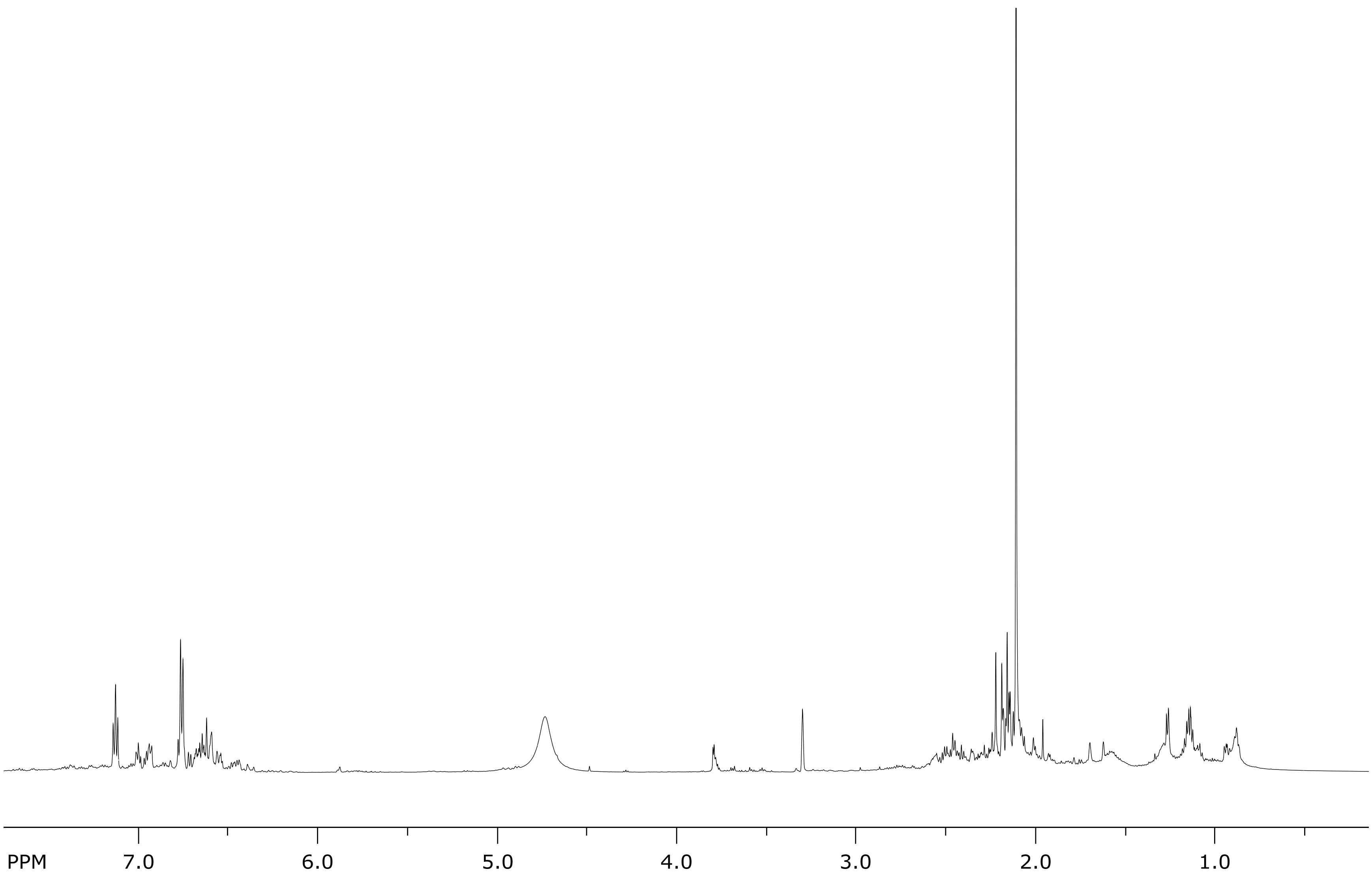

Figure S8 – 1H NMR spectrum (600 MHZ, DMSO-d_6) fractions 3a phenolics extracted from guayule bagasse bio-oil.

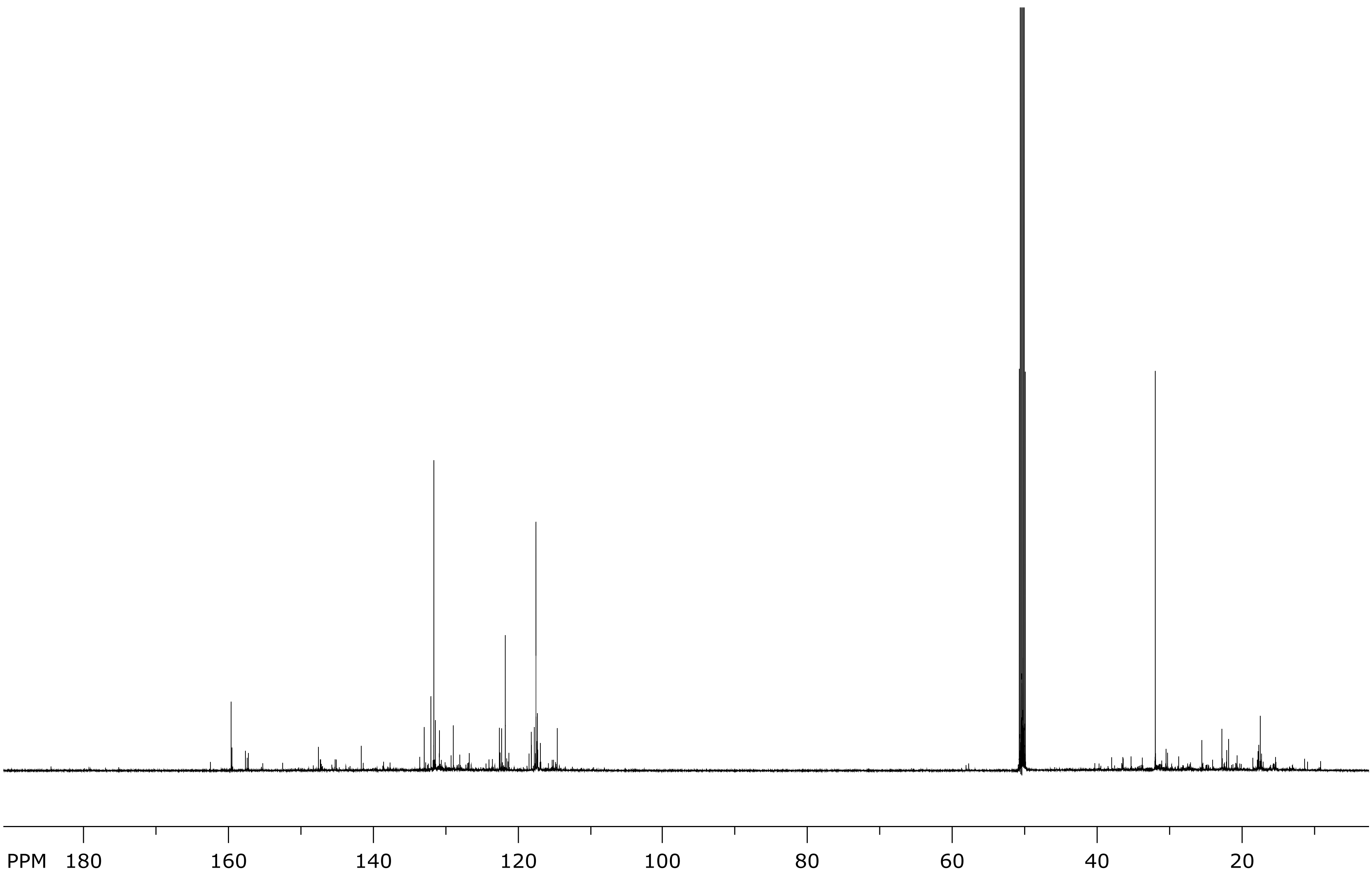

Figure S9– $^{13}C\{^{1}H\}$ NMR spectrum (150 MHZ, DMSO-d_6) of fractions 3a phenolics extracted from guayule bagasse bio-oil.

		horse litter	horse manure
wt% of biomass	biomass	100	100
	bio-oil	35	36.9
	total distillates	23.1	22.9
	HCs	9.9	12.6
	Phenols	11.4	8.0
	Acids	1.2	1.8
	total bottoms	10.9	9.2
	calcined coke	5.7	4.7
g/100g biomass	NaOH, in	2.6	1.8
	HCl, in	2.4	1.7
	NaCl, out*	3.8	2.7
	NaCl, recov	2.5	1.3

Table S2 – Calculated yields of product streams for horse litter and horse manure biomasses, normalized with respect to the amount of biomass fed. (*Calculated based on theoretical maximum from NaOH added)