Electronic Supplementary Information

An assessment of spent coffee grounds as a replacement for peat in the production of Scotch Whisky: chemical extraction and pyrolysis studies.

Details of Extraction Procedures

Extraction in methanol for 72 hours was determined to give best results. Though not an alcohol matrix (ethanol/water) that replicates whisky, methanol extraction produced more informative spectra. Longer extraction time lead to minimal increase in NMR signal intensity, while severely prolonging the analysis time for each sample. Heating the mixture resulted in loss of some signals. Methanol produces only two ^{1}H NMR signals (CH_3 singlet at 3.34 ppm and OH broad singlet around 4.9 ppm), which is (also) easier to suppress than multiple signals of the ethanol/water mixture, leading to fewer baseline distortions and a cleaner spectrum. However, ethanol/water mixture showed better results, in terms of number of signals and their intensity, for malt samples.

Peat	
P1 (kk67hp1) P2 (kk67hp1_2) P3 (kk67hp1_3)	0.5 g of peat stirred in 10 mL of methanol for 72 hours at room temperature
P4 (kk67hp2_1) P5 (kk67hp2_2) P6 (kk67hp2_3)	0.5 g of peat stirred in 10 mL of ethanol/water mixture (10 % ethanol v/v) for 72 hours at room temperature

Table S1. *Peat extraction details.*

Coffee Waste	
CW1 (kk67hcw2_2) CW2 (kkhcw2_3) CW3 (kkhcw2_4)	0.5 g of SCG from decaffeinated coffee stirred in 10 mL of methanol for 72 hours
CW4 (kk67hcw3_2) CW5 (kkhcw3_3) CW6 (kkhcw3_4)	0.5 g of SCG from decaffeinated coffee stirred in 10 mL of methanol/water mixture (60 % methanol v/v) for 90 minutes at 60 °C
CW7 (kk67hcw4_3) CW8 CW9	0.5 g of SCG from decaffeinated coffee stirred in 10 mL of water for 7 days at room temperature
CW10 (kk67hcw5_2) CW11 (kkhcw5_3) CW12 (kkhcw5_4)	0.5 g of SCG from decaffeinated coffee stirred in 10 mL of ethanol/water (10% of ethanol v/v) mixture for 72 hours at room temperature
CW13 (kk67hcw6_1) CW14 (kk67hcw6_2) CW15 (kk67hcw6_3)	0.5 g of SCG stirred in 10 mL of methanol for 72 hours at room temperature
CW16 (kk67hcw7_2) CW17 (kk67hcw7_3) CW18 (kk67hcw7_4)	0.5 g of SCG stirred in 10 mL of ethanol/water (10 % of ethanol v/v) mixture for 72 hours at room temperature
CW19 (kk67hcw8_1) CW20 (kk67hcw8_2)	0.5 g of SCG stirred in 10 mL of methanol/water (60 % of methanol v/v) mixture for 90 minutes at 60 °C

CW21 (kk67hcw8_3)	

Table S2. *Coffee waste extraction details.*

Peat Smoke	
PS1 (kk67hps2_1) PS2 (kk67hps3_1) PS3 (kk67hps6_1)	Smoke from burning 0.5 g of peat bubbled through 5 mL of methanol
PS4 (kk67hps5_1) PS5 (kk67hps5_2) PS6 (kk67hps5_3)	Smoke from burning 1 g of peat bubbled through 5 mL of methanol

Table S3. *Peat smoke collection details.*

Coffee Waste Smoke	
CWS1 (kk67hcws2_1) CWS2 (kk67hcws2_2) CWS3 (kk67hcws2_3)	Smoke from burning 0.5 g of SCG from decaffeinated coffee bubbled through 5 mL of ethanol/water (10 % of ethanol v/v) mixture
CWS4 (kk67hcws3_1) CWS5 (kk67hcws3_2) CWS6 (kk67hcws3_3)	Smoke from burning 0.5 g of SCG from decaffeinated coffee bubbled through 5 mL of methanol
CWS7 (kk67hcws5_1) CWS8 (kk67hcws7_1) CWS9 (kk67hcws8_1)	Smoke from burning 0.5 g of SCG bubbled through 5 mL of methanol
CWS10 (kk67hcws6_1) CWS11 (kk67hcws6_2) CWS12 (kk67hcws6_3)	Smoke from burning 1 g of SCG bubbled through 5 mL if methanol

Table S4. *Coffee waste smoke collection details.*

Industrially Peated Malt	
IPM1 (kk67hpm4_1) IPM2 (kk67hpm4_2) IPM3 (kk67hpm4_3)	0.5 g of industrially peated malt stirred in 10 mL of methanol for 72 hours at room temperature
IPM4 (kk67hpm5_1) IPM5 (kk67hpm5_2) IPM6 (kk67hpm5_3)	0.5 g of industrially peated malt stirred in 10 mL of ethanol/water (10 % of ethanol v/v) mixture.

Table S5. *Industrially peated malt extraction details.*

"Coffee Peated" Malt	
CPM1 (kk67hcpm9_1) CPM2 (kk67hcpm9_2) CPM3 (kk67hcpm9_3)	0.5 g of coffee peated malt stirred in 10 mL of water for 3 days at room temperature
CPM4 (kk67hcpm2_2) CPM5 (kkhcpm2_3) CPM6 (kkhcpm2_4)	0.5 g of coffee peated malt stirred in 10 mL of ethanol/water (10 % of ethanol v/v) mixture for 7 days at room temperature
CPM7 (kk67hcpm4_3) CPM8 CPM9	0.5 g of coffee peated malt stirred in 10 mL of water for 7 days at 70 °C
CPM10 (kk67hcpm5_3) CPM11	0.5 g of coffee peated malt stirred in 10 mL of methanol for 7 days at room temperature

CPM12	
CPM13 (kk67hcpm6_1) CPM14 (kk67hcpm6_2) CPM15 (kk67hcpm6_3)	0.5 g of light coloured coffee peated malt stirred in 10 mL of ethanol/water (10 % of ethanol) mixture for 72 hours at room temperature
CPM16 (kk67hcpm7_1) CPM17 (kk67hcpm7_2) CPM18 (kk67hcpm7_3)	0.5 g of dark coloured coffee peated malt stirred in 10 mL of ethanol/water (10 % of ethanol) mixture for 72 hours at room temperature

Table S6. *„Coffee peated" malt extraction details.*

NMR spectra – pure compounds

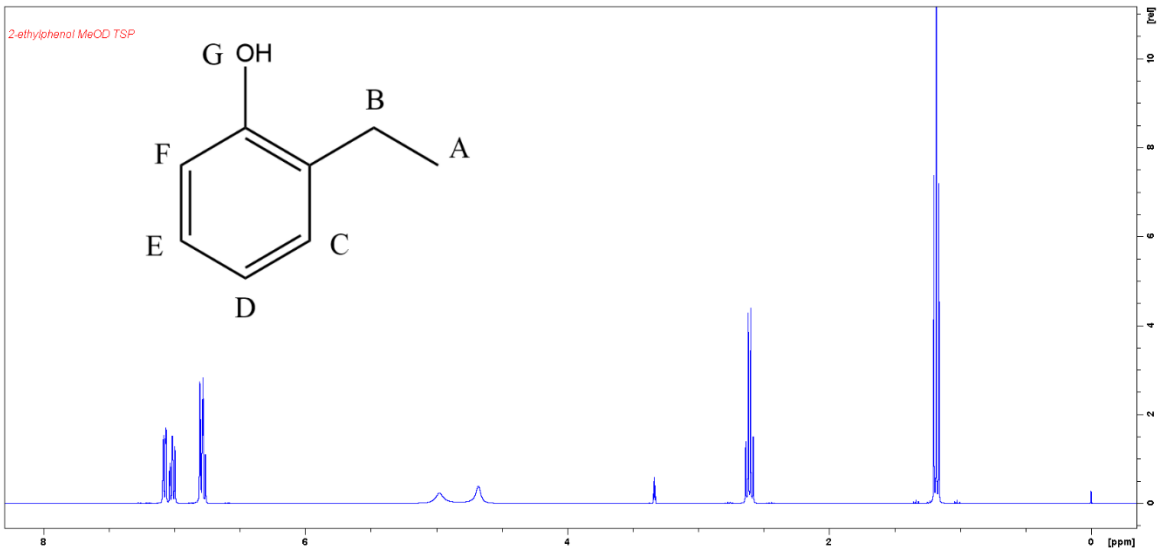

Figure S1. *^{1}H NMR spectrum of 2-ethylphenol in methanol-d_4 recorded at 400 MHz.*

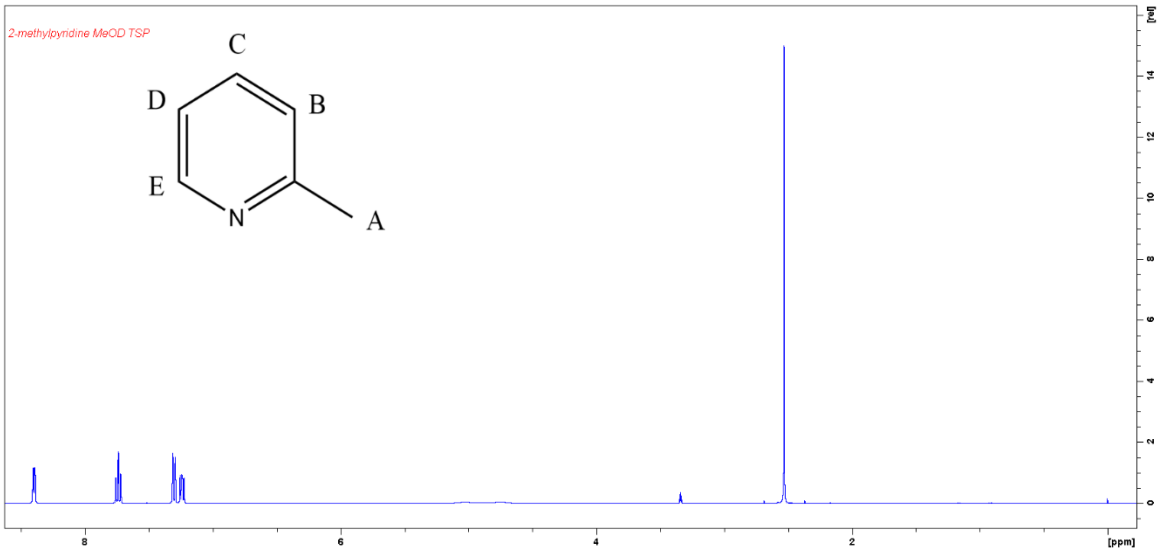

Figure S2. *^{1}H NMR spectrum of 2-methylpyridine in methanol-d_4 recorded at 400 MHz.*

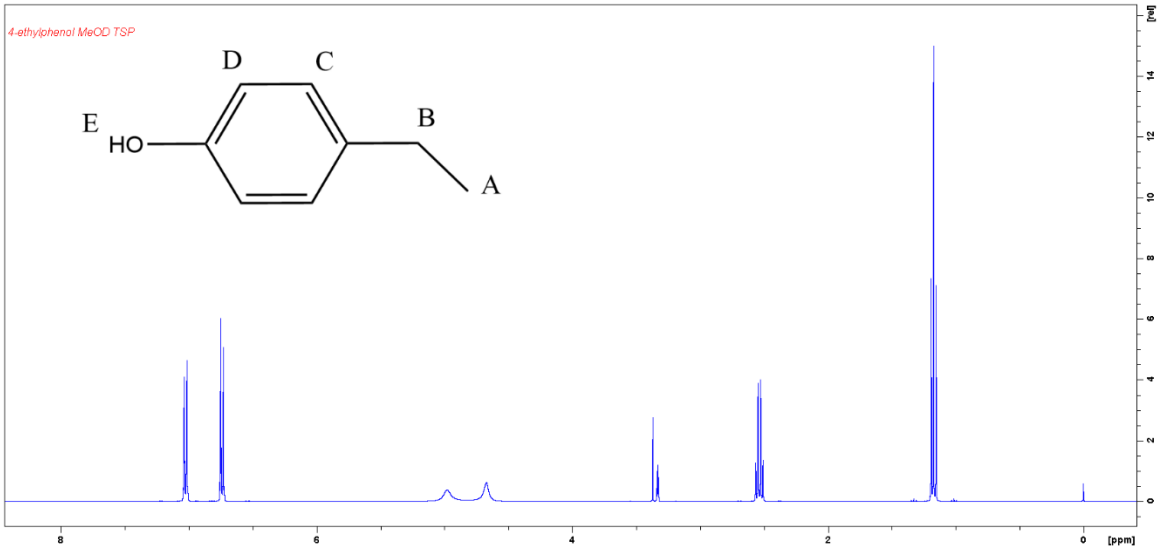

Figure S3. *^{1}H NMR spectrum of 4-ethylphenol in methanol-d_4 recorded at 400 MHz.*

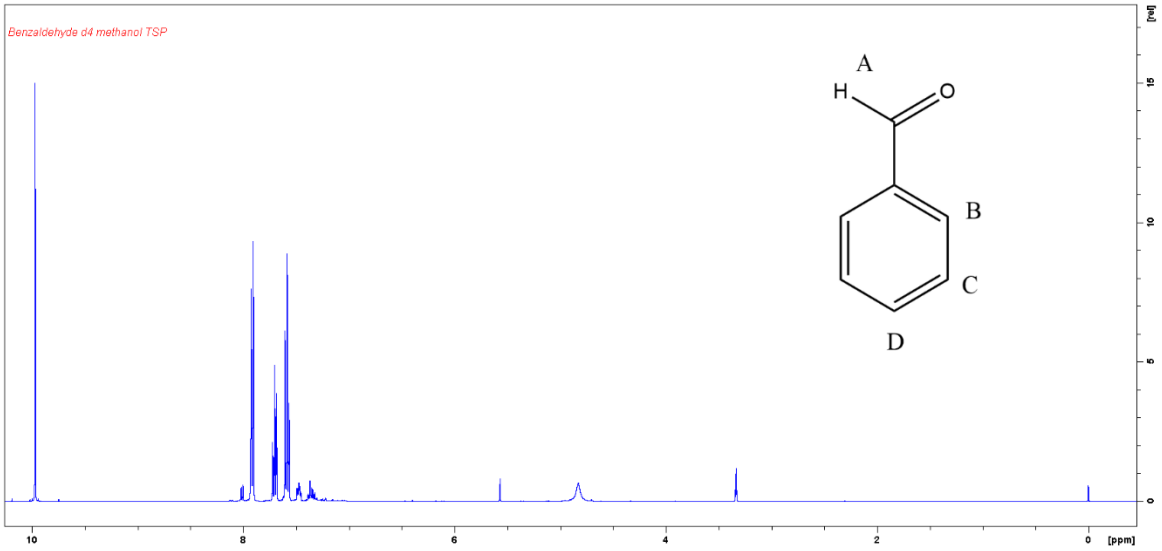

Figure S4. *^{1}H NMR spectrum of benzaldehyde in methanol-d_4 recorded at 400 MHz.*

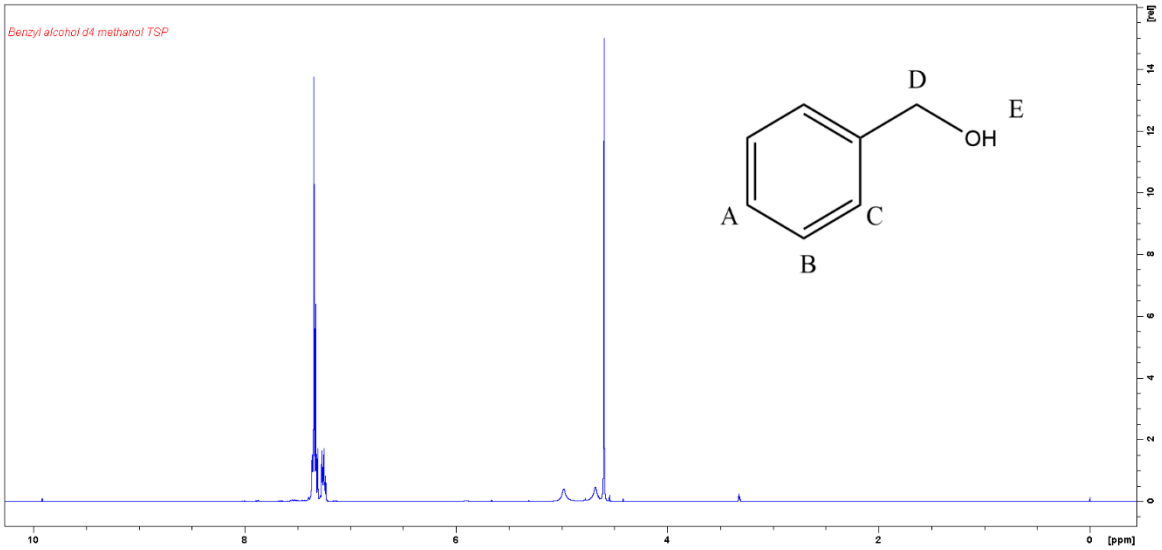

Figure S5. *^{1}H NMR spectrum of benzyl alcohol in methanol-d_4 recorded at 400 MHz.*

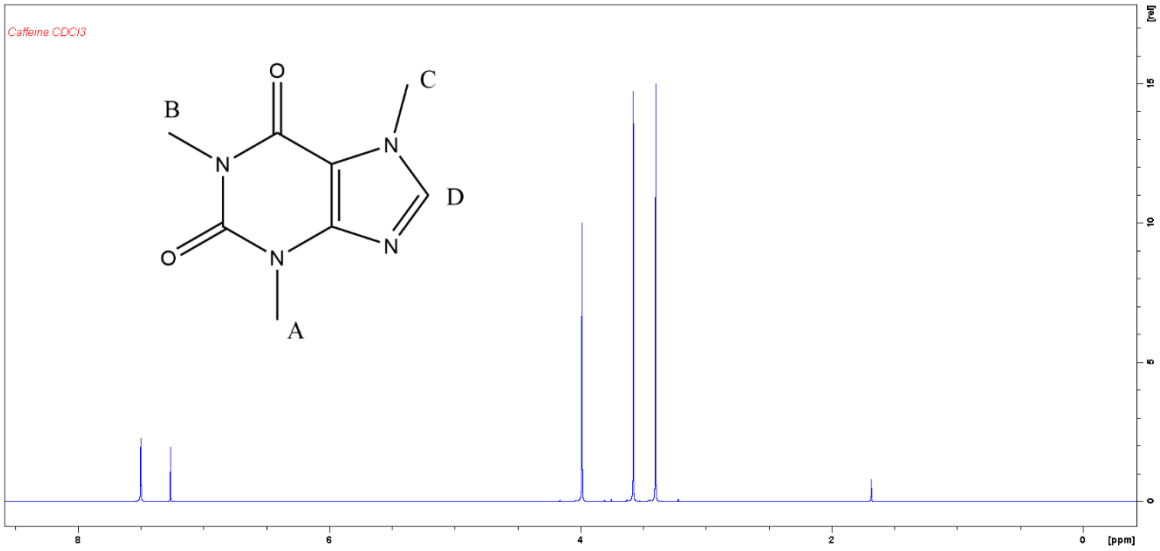

Figure S6. *^{1}H NMR spectrum of caffeine in $CDCl_3$ recorded at 400 MHz.*

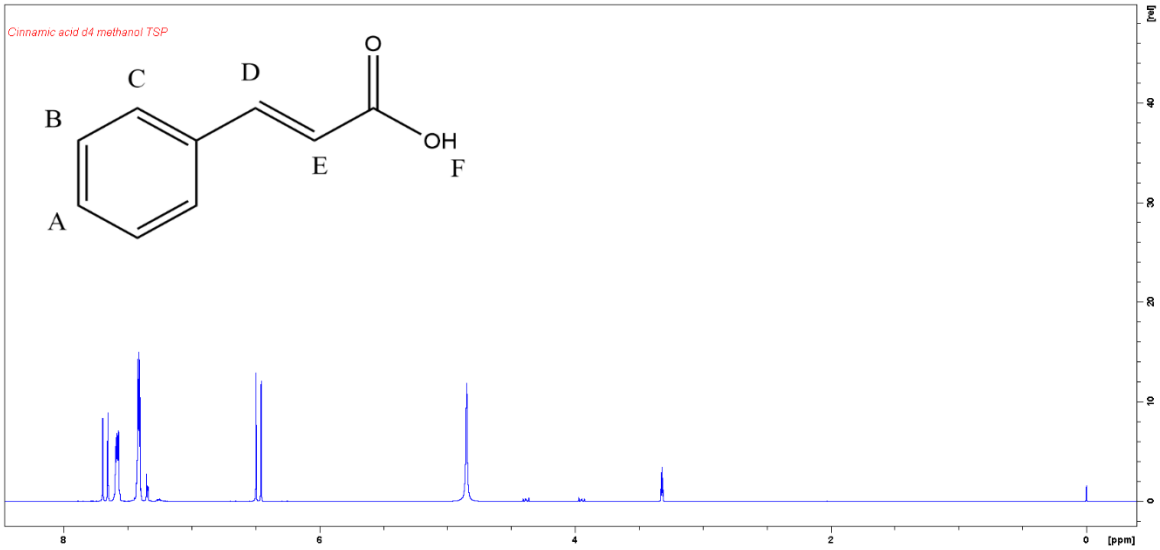

Figure S7. *^{1}H NMR spectrum of cinnamic acid in methanol-d_4 recorded at 400 MHz.*

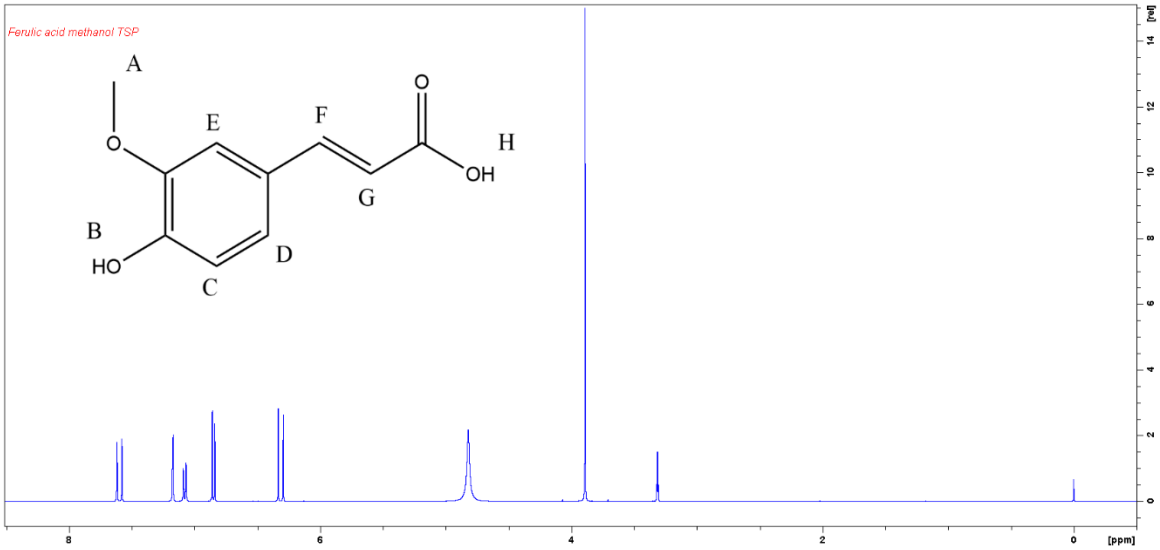

Figure S8. *^{1}H NMR spectrum of ferulic acid in methanol-d_4 recorded at 400 MHz.*

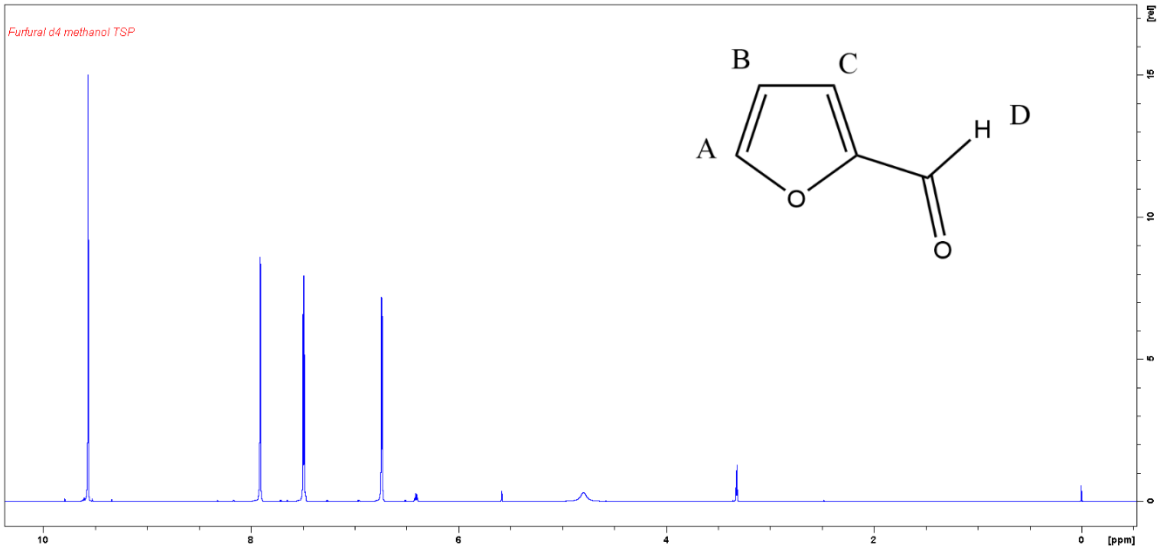

Figure S9. *^{1}H NMR spectrum of furfural in methanol-d_4 recorded at 400 MHz.*

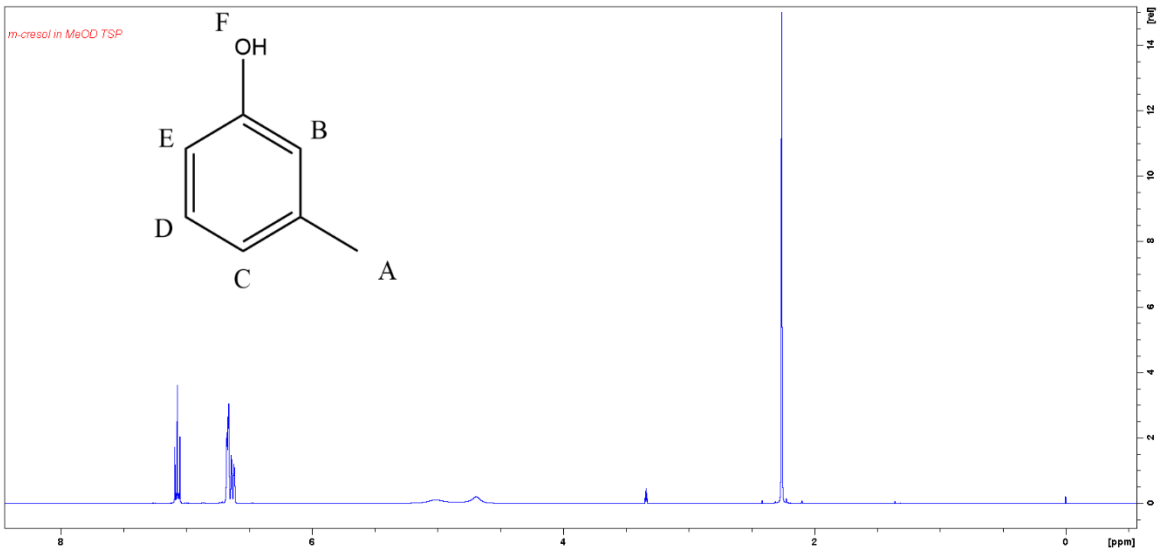

Figure S10. *^{1}H NMR spectrum of m-cresol in methanol-d_4 recorded at 400 MHz.*

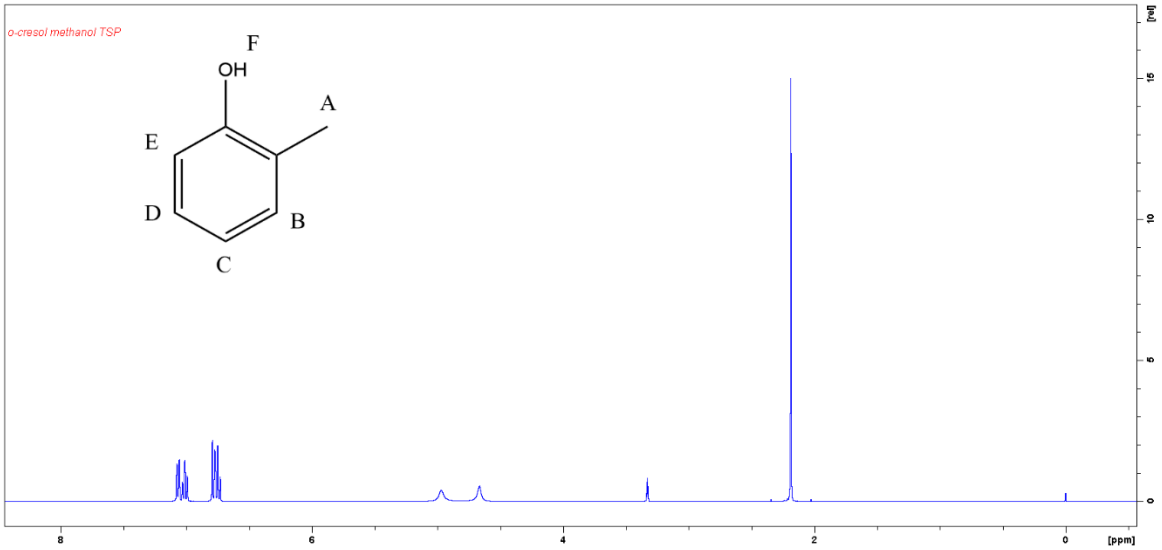

Figure S11. *^{1}H NMR spectrum of o-cresol in methanol-d_4 recorded at 400 MHz.*

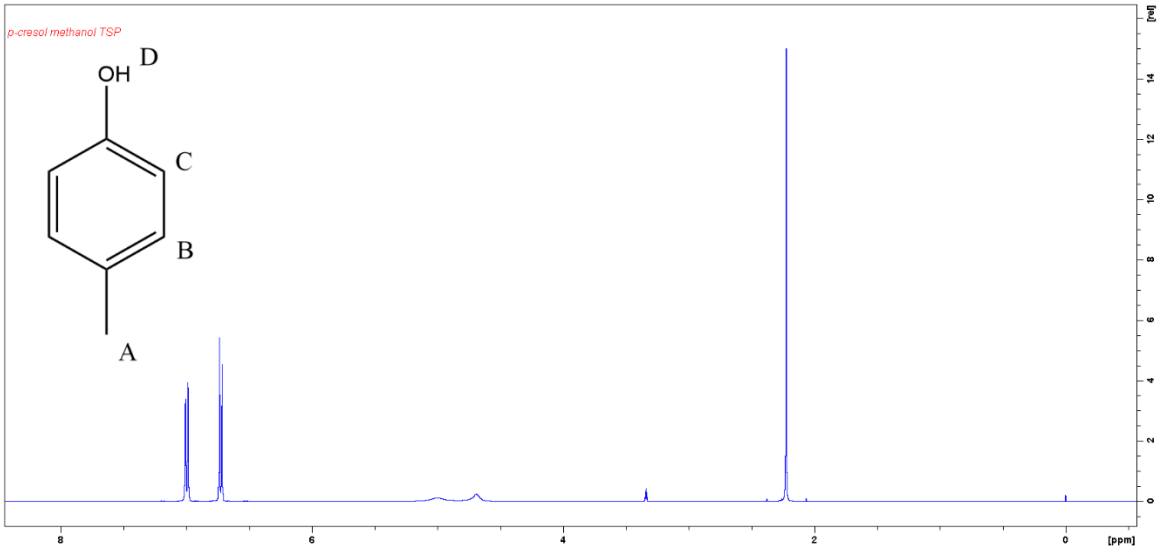

Figure S12. *^{1}H NMR spectrum of p-cresol in methanol-d_4 recorded at 400 MHz.*

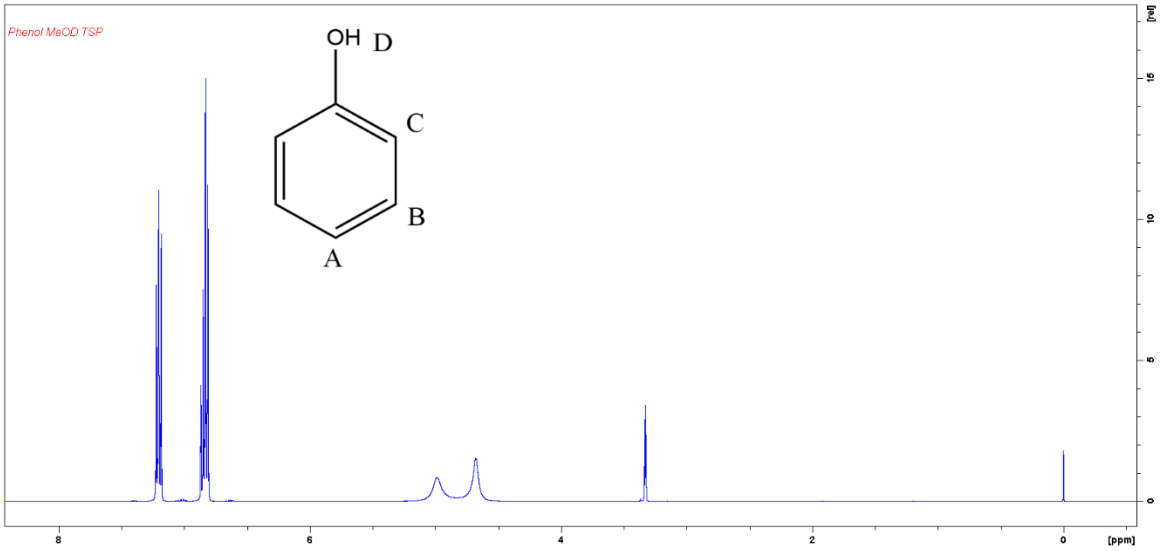

Figure S13. *^{1}H NMR spectrum of phenol in methanol-d_4 recorded at 400 MHz.*

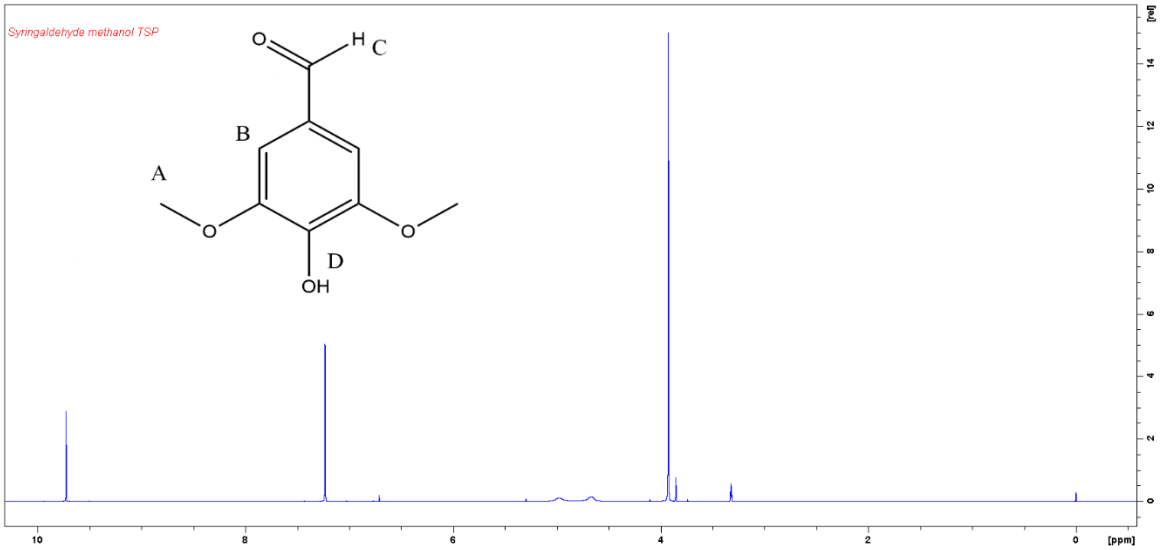

Figure S14. *^{1}H NMR spectrum of syringaldehyde in methanol-d_4 recorded at 400 MHz.*

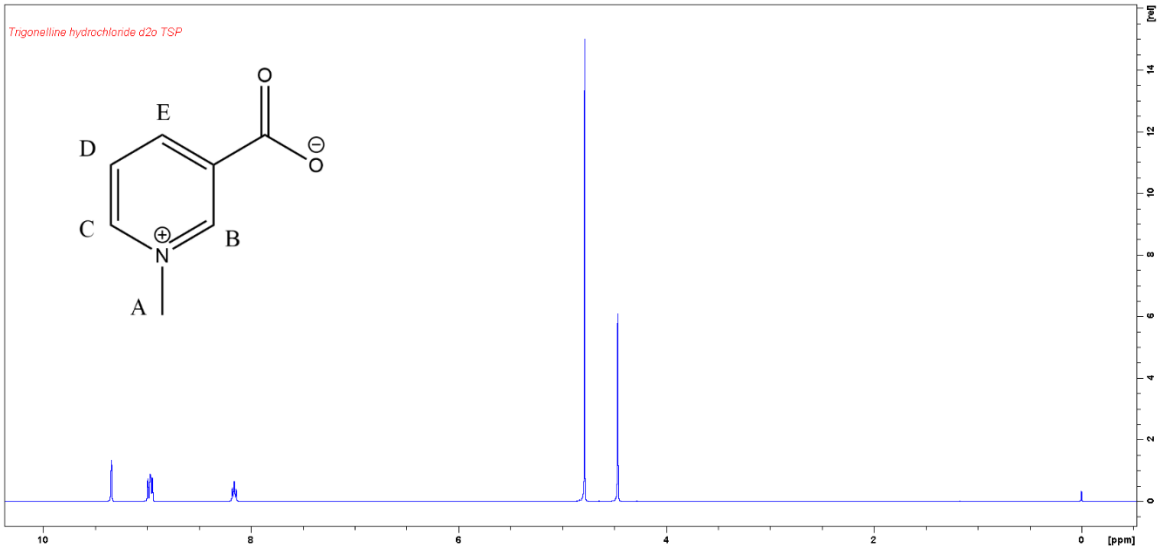

Figure S15. *^{1}H NMR spectrum of trigonelline hydrochloride in D_2O recorded at 400 MHz.*

Signal assignments – pure compounds

2-ethylphenol, $C_8H_{10}O$			
δ_H / ppm	Multiplicity	Integration	Inferences
1.18	Triplet, ^3J = 7.5 Hz	3H	CH_3 next to CH_2 (A)
2.61	Quartet, ^3J = 7.5 Hz	2H	CH_2 next to CH_3 and aromatic ring (B)
4.68	Broad singlet	~ 1H	OH (G)
6.78	Triplet of doublets, ^3J = 7.4 Hz, ^4J = 1.2 Hz	1H	Aromatic CH coupling to 2xCH, with long range coupling to CH (D)
6.80	Doublet of doublets, ^3J = 8.1 Hz, ^4J = 0.9 Hz	1H	Aromatic CH coupling to CH, with long range coupling to CH (F)
7.01	Triplet of doublets, ^3J = 7.7 Hz, ^4J = 1.7 Hz	1H	Aromatic CH coupling to 2xCH, with long range coupling to CH (E)
7.08	Doublet of doublets, ^3J = 7.4 Hz, ^4J = 1.3 Hz	1H	Aromatic CH coupling to CH, with long range coupling to CH (C)

Table S7. *Signal assignment for 2-ethylphenol.*

2-methylpyridine, C_7H_7N			
δ_H / ppm	Multiplicity	Integration	Inferences
2.53	Singlet	3H	CH_3 isolated, next to aromatic ring (A)
7.24	Doublet of doublet of doublets, ^3J = 7.5 Hz, ^3J = 5.1 Hz, ^4J = 1.1 Hz	1H	Aromatic CH, coupling to 2xCH (different coupling constants), with long range coupling to CH (D)
7.30	Doublet ^3J = 2.6 Hz	1H	Aromatic CH coupling to CH (B)
7.74	Triplet of doublets, ^3J = 7.7 Hz, ^4J = 1.8 Hz	1H	Aromatic CH coupling to 2xCH, with long range coupling to CH (C)
8.40	Doublet of doublets, ^3J = 5.0 Hz, ^4J = 1.6 Hz	1H	Aromatic CH coupling to 2xCH (different coupling constants) (E)

Table S8. *Signal assignment for 2-methylpyridine.*

4-ethylphenol, $C_8H_{10}O$			
δ_H / ppm	Multiplicity	Integration	Inferences
1.17	Triplet, ^3J = 7.6 Hz	3H	CH_3 next to CH_2 (A)

2.53	Quartet, ^3J = 7.6 Hz	2H	CH_2 next to CH_3 (B)
4.67	Broad singlet	~ 1H	OH (E)
6.74	AA'XX'	2H	2 x aromatic CH near OH (D)
7.02	AA'XX'	2H	2 x aromatic CH near CH_2CH_3

Table S9. *Signal assignment for 4-ethylphenol.*

Benzaldehyde, C_7H_6O			
δ_H / ppm	Multiplicity	Integration	Inferences
7.58	Triplet, ^3J = 7.6 Hz	2H	2 x aromatic CH, each next to 2xCH (C)
7.70	Triplet of triplets, ^3J = 7.4 Hz, ^4J = 1.8 Hz	1H	Aromatic CH next to 2xCH, long range coupling to 2xCH (D)
7.91	Doublet of doublets	2H	2 x aromatic CH, next to CH (B)
9.97	Singlet	1H	CHO, isolated (A)

Table S10. *Signal assignment for benzaldehyde.*

Benzyl alcohol, C_7H_8O			
δ_H / ppm	Multiplicity	Integration	Inferences
4.60	Singlet	2H	CH_2 isolated, next to OH (D)
4.68	Broad singlet	~0.5 H	OH
~7.3	Multiplet	5H	5x aromatic CH coupling to each other (A,B,C)

Table S11. *Signal assignment for benzyl alcohol.*

Caffeine, $C_8H_{10}O_2N_4$			
δ_H / ppm	Multiplicity	Integration	Inferences
3.40	Singlet	3H	CH_3 isolated, next to N (A)
3.58	Singlet	3H	CH_3 isolated, next to N (B)
3.98	Singlet	3H	CH_3 isolated, next to N (C)
7.47	Singlet	1H	Aromatic CH, isolated (D)

Table S12. *Signal assignment for caffeine.*

Cinnamic acid, $C_9H_8O_2$			
δ_H / ppm	Multiplicity	Integration	Inferences
6.48	Doublet, ^3J = 16 Hz	1H	Trans alkene CH, next to aromatic ring (D)
7.41	Multiplet	3H	3x aromatic CH, meta and para to substituent (A,B)
7.58	Multiplet	2H	2x aromatic CH, ortho to substituent (C)
7.67	Doublet, ^3J = 16 Hz	1H	Trans alkene CH, next to COOH (E)

Table S13. *Signal assignment for cinnamic acid.*

Ferulic acid, $C_{10}H_{10}O_3$			
δ_H / ppm	Multiplicity	Integration	Inferences
3.89	Singlet	3H	CH_3 isolated, next to O (A)
6.31	Doublet, ^3J = 16 Hz	1H	Trans alkene CH, next to aromatic ring (F)
6.85	Doublet, ^3J = 8.2 Hz	1H	Aromatic CH coupling to CH (C)
7.08	Doublet of doublets, ^3J = 8.3 Hz, ^4J = 1.9 Hz	1H	Aromatic CH coupling to CH, with long range coupling to CH (D)
7.17	Doublet, ^4J = 1.9 Hz	1H	Aromatic CH with long range coupling to CH (E)
7.60	Doublet, ^3J = 16 Hz	1H	Trans alkene CH, next to COOH (G)

Table S14. *Signal assignment for ferulic acid.*

Furfural, $C_5H_4O_2$			
δ_H / ppm	Multiplicity	Integration	Inferences
6.74	Doublet of doublets, ^3J = 3.6 Hz, ^3J = 1.7 Hz	1H	Aromatic CH coupling to 2xCH (with different coupling constants) (B)
7.49	Doublet of doublets, ^3J = 3.6 Hz, ^4J = 0.6 Hz	1H	Aromatic CH coupling to CH, with long range coupling to CH(C)
7.91	Doublet of doublets, ^3J = 1.6 Hz, ^4J = 0.8 Hz	1H	Aromatic CH coupling to CH, with long range coupling to CH(A)
9.57	Doublet, ^4J = 0.8 Hz	1H	CHO with long range coupling to CH(D)

Table S15. *Signal assignment for furfural.*

m-cresol C_7H_9O			
δ_H / ppm	Multiplicity	Integration	Inferences
2.26	Singlet	3H	CH_3 isolated, next to aromatic ring (A)
4.69	Broad singlet	~1H	OH (F)
6.63	Multiplet	1H	Aromatic CH ortho to OH (B)
6.67	Multiplet	2H	Aromatic CH ortho to OH and aromatic CH para to OH (C,E)
7.07	Triplet, ^3J = 8.0 Hz	1H	Aromatic CH meta to OH, coupling to 2xCH (D)

Table S16. *Signal assignment for m-cresol.*

o-cresol C_7H_9O			
δ_H / ppm	Multiplicity	Integration	Inferences
2.19	Singlet	3H	CH_3 isolated, next to aromatic ring (A)
4.67	Broad singlet	~1H	OH (F)
6.75	Triplet, ^3J = 7.4 Hz	1H	Aromatic CH coupling to 2xCH, para to OH (C)
6.78	Doublet, ^3J = 8.0 Hz	1H	Aromatic CH coupling to CH, ortho to OH (E)
7.01	Triplet, ^3J = 7.7 Hz	1H	Aromatic CH coupling to 2xCH, meta to OH (D)
7.06	Doublet, ^3J = 7.4 Hz	1H	Aromatic CH coupling to CH, meta to OH (B)

Table S17. *Signal assignment for o-cresol.*

p-cresol C_7H_9O			
δ_H / ppm	Multiplicity	Integration	Inferences
2.26	Singlet	3H	CH_3 isolated, next to aromatic ring (A)
4.69	Broad singlet	~1H	OH (D)
6.72	Doublet, ^3J = 8.5 Hz	2H	2x aromatic CH next to CH (C)
6.99	Doublet, ^3J = 8.0 Hz	2H	2x aromatic CH next to CH (B)

Table S18. *Signal assignment for p-cresol.*

Syringaldehyde $C_9H_{10}O_4$			
δ_H / ppm	Multiplicity	Integration	Inferences
3.92	Singlet	6H	2x CH_3 isolated, next to O (A)
7.23	Singlet	2H	2x Aromatic CH (B)
9.72	Singlet	1	CHO

Table S19. *Signal assignment for syringaldehyde.*

Trigonelline hydrochloride $C_7H_8O_2NCl$			
δ_H / ppm	Multiplicity	Integration	Inferences
4.46	Singlet	3H	CH_3 isolated, next to N (A)

8.16	Triplet ^{3}J = 7.0 Hz	1H	Aromatic CH next to 2 x CH (D)
8.96	Doublet, ^{3}J = 7.0 Hz	1H	Aromatic CH next to CH (E)
8.98	Doublet, ^{3}J = 8.3 Hz	1H	Aromatic CH next to CH (C)
9.34	Singlet	1	Aromatic CH isolated (B)

Table S20. *Signal assignment for trigonelline hydrochloride.*

NMR spectra

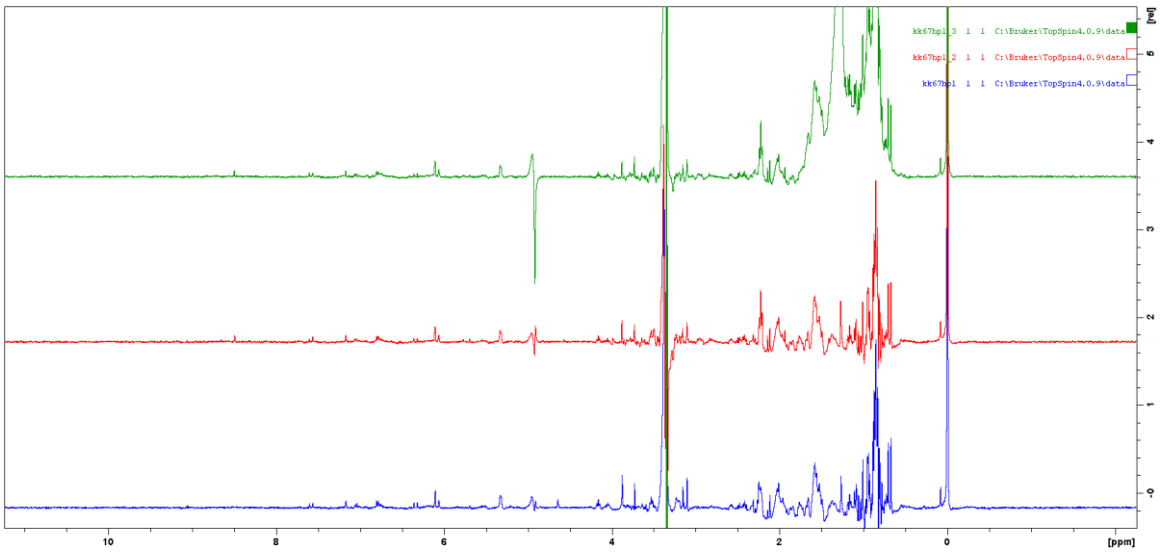

Figure S16. *^{1}H NMR spectra of P1 (bottom), P2 (middle), P3 (top) recorded at 400 MHz.*

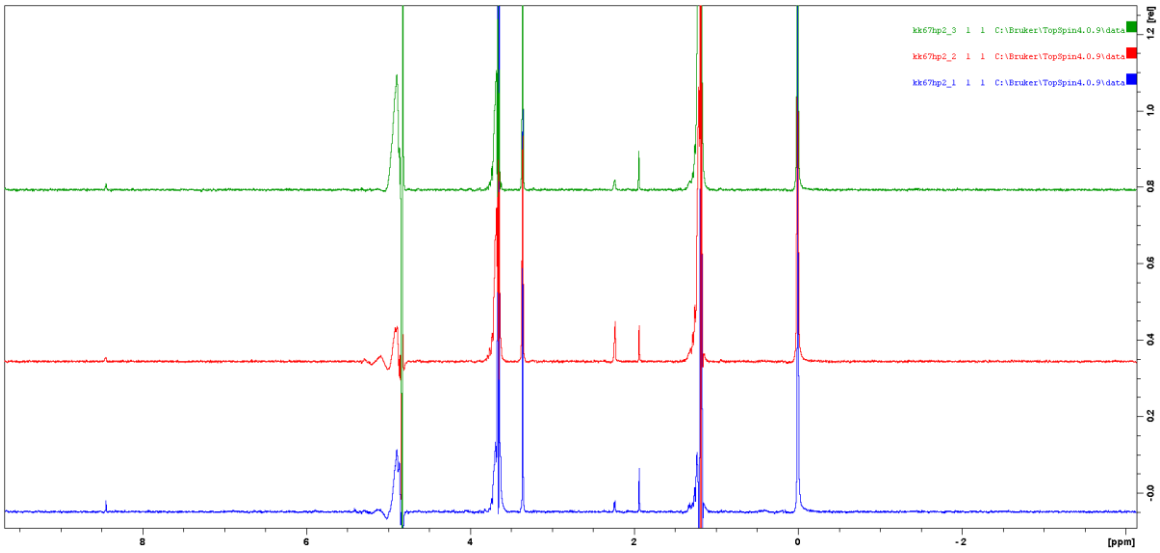

Figure S17. *^{1}H NMR spectra of P4 (bottom), P5 (middle), P6 (top) recorded at 400 MHz.*

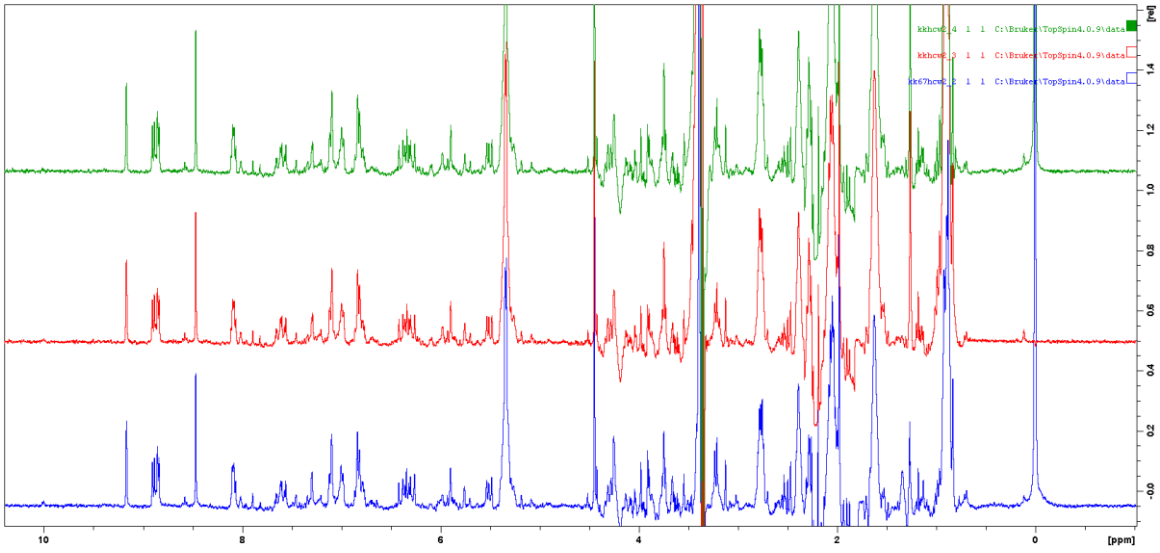

Figure S18. *^{1}H NMR spectra of CW1 (bottom), CW2 (middle), CW3 (top) recorded at 400 MHz.*

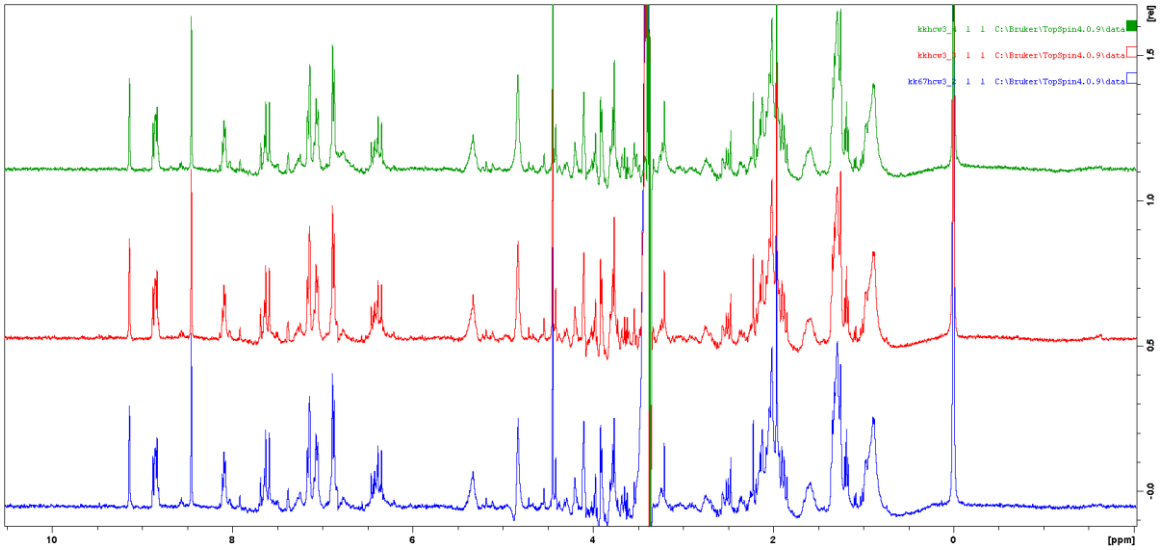

Figure S19. *^{1}H NMR spectra of CW4 (bottom), CW5 (middle), CW6 (top) recorded at 400 MHz.*

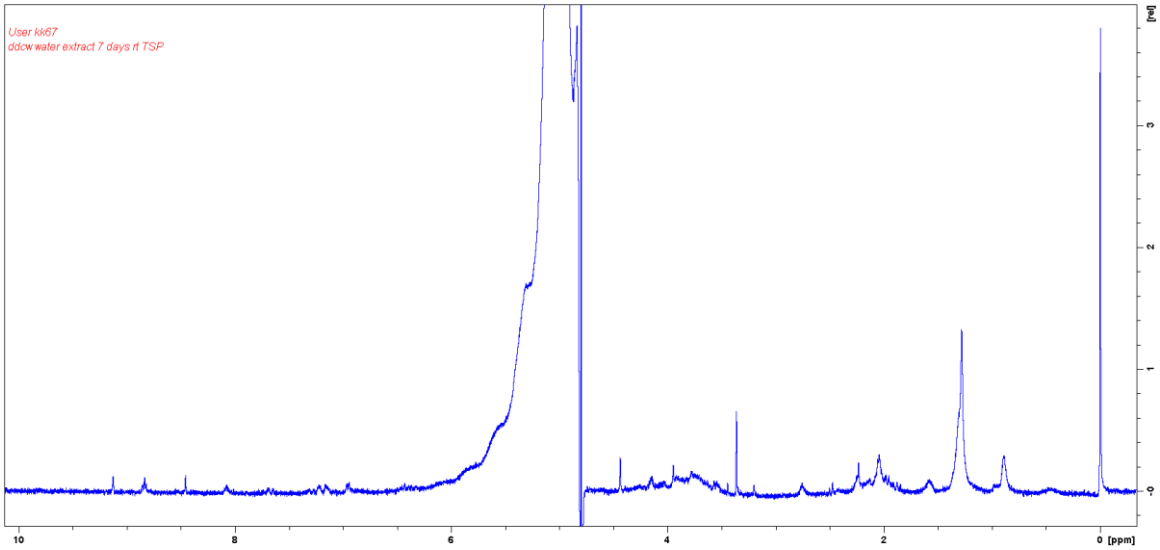

Figure S20. *^{1}H NMR spectra of CW7 recorded at 400 MHz.*

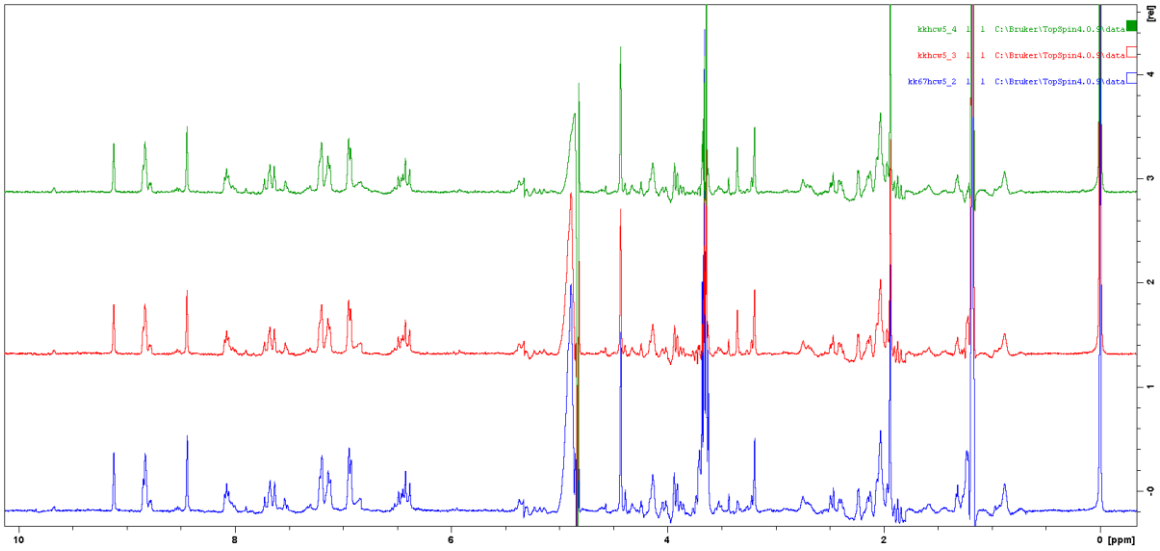

Figure S21. *^{1}H NMR spectra of CW10 (bottom), CW11 (middle), CW12 (top) recorded at 400 MHz.*

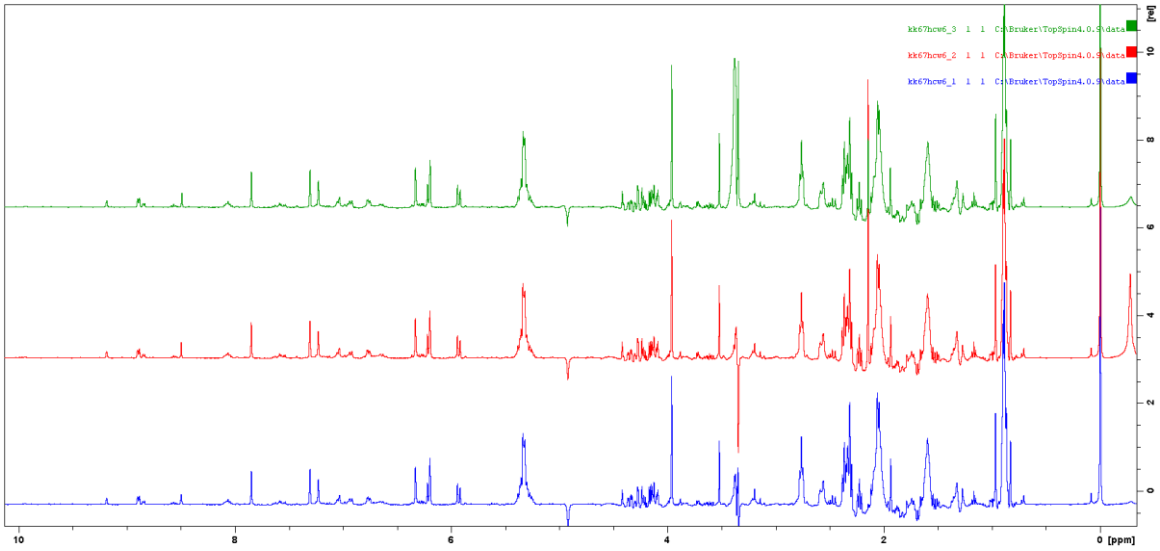

Figure S22. *^{1}H NMR spectra of CW13 (bottom), CW14 (middle), CW15 (top) recorded at 400 MHz.*

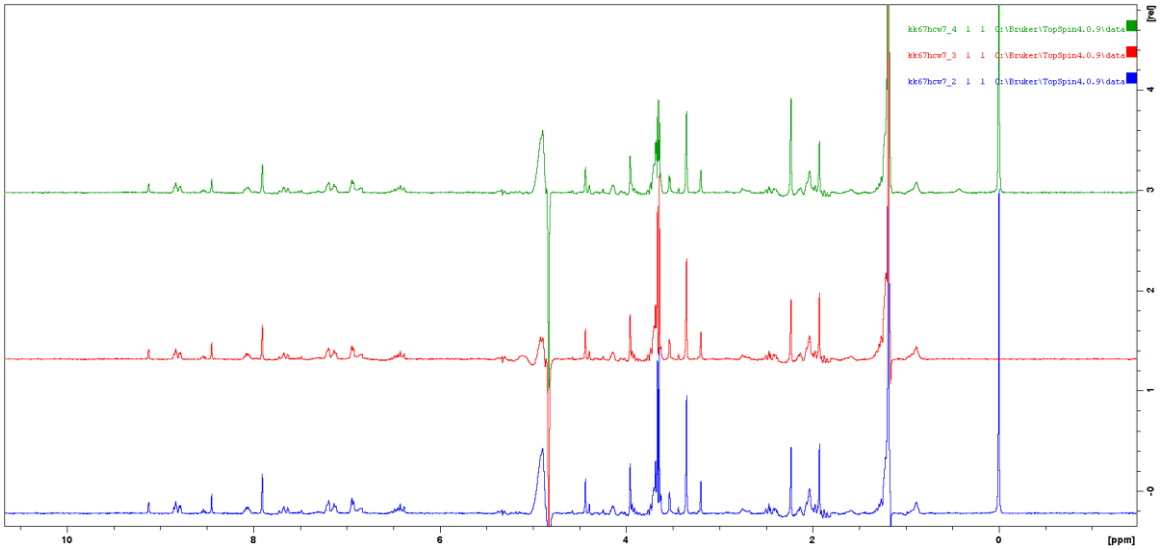

Figure S23. *^{1}H NMR spectra of CW16 (bottom) ,CW17 (middle), CW18 (top) recorded at 400 MHz.*

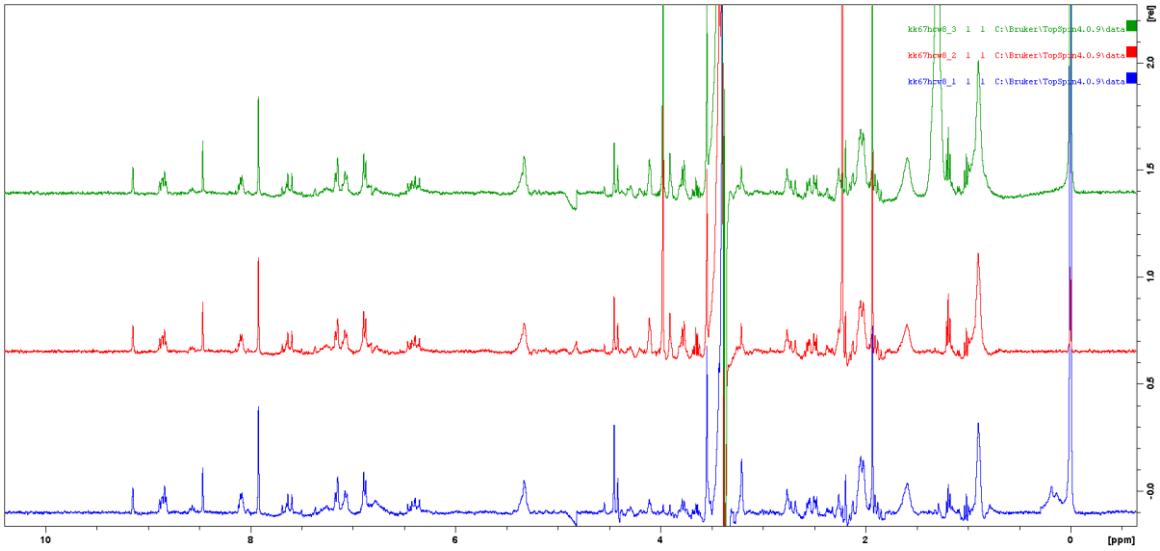

Figure S24. *^{1}H NMR spectra of CW19 (bottom), CW20 (middle), CW21 (top) recorded at 400 MHz.*

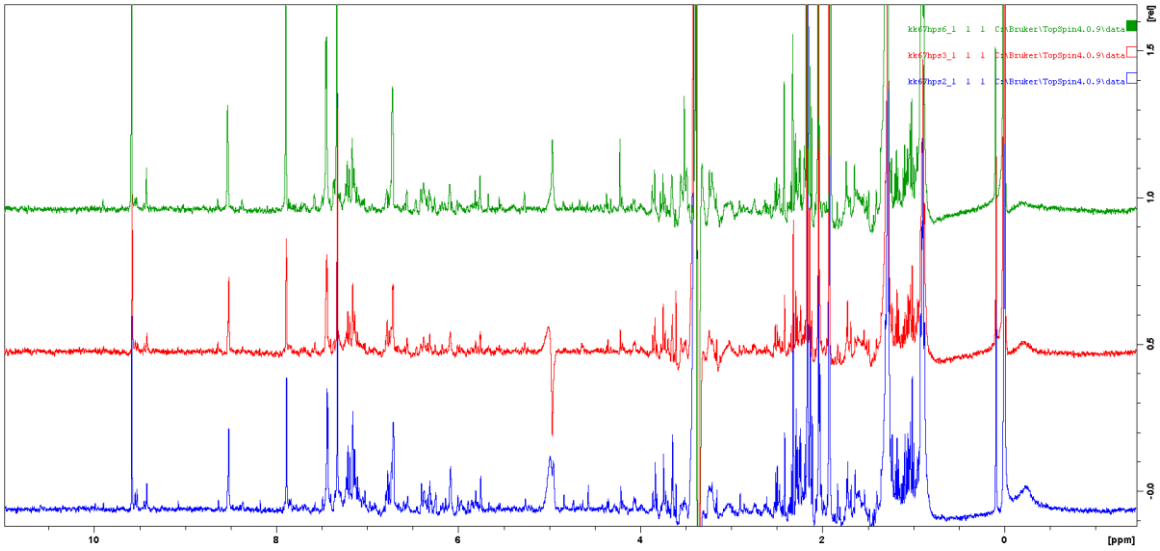

Figure S25. *^{1}H NMR spectra of PS1 (bottom), PS2 (middle), PS3 (top) recorded at 400 MHz.*

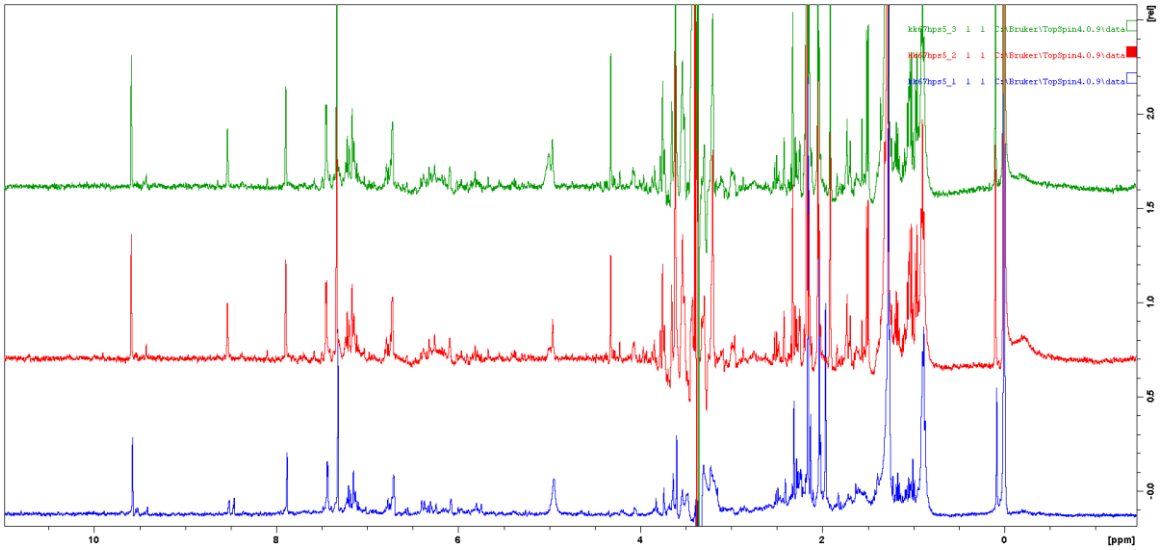

Figure S26. *^{1}H NMR spectra of PS4 (bottom), PS5 (middle), PS6 (top) recorded at 400 MHz.*

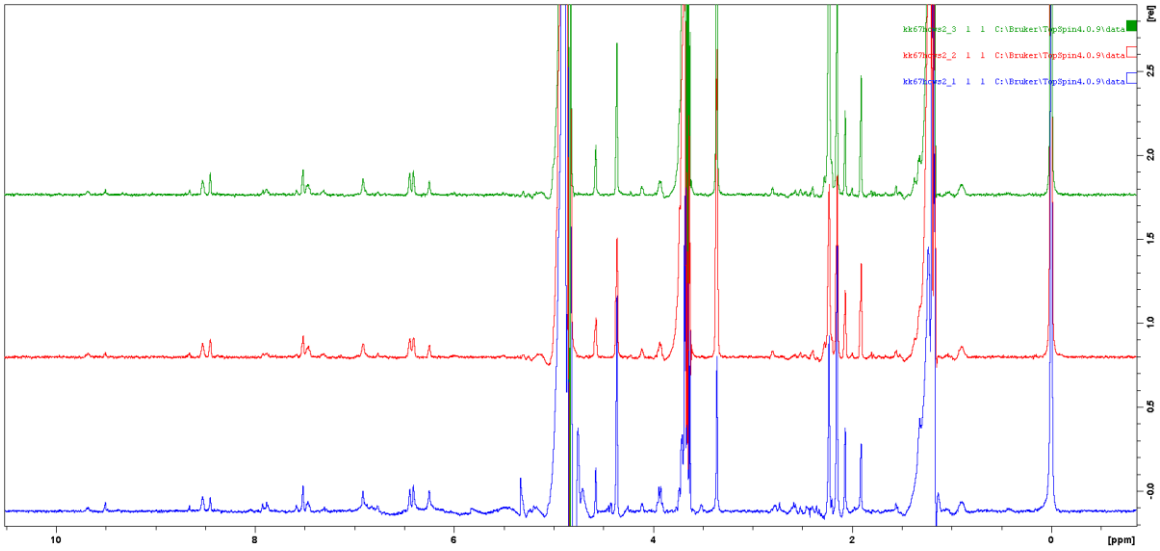

Figure S27. *^{1}H NMR spectra of CWS1 (bottom), CWS2 (middle), CWS3 (top) recorded at 400 MHz.*

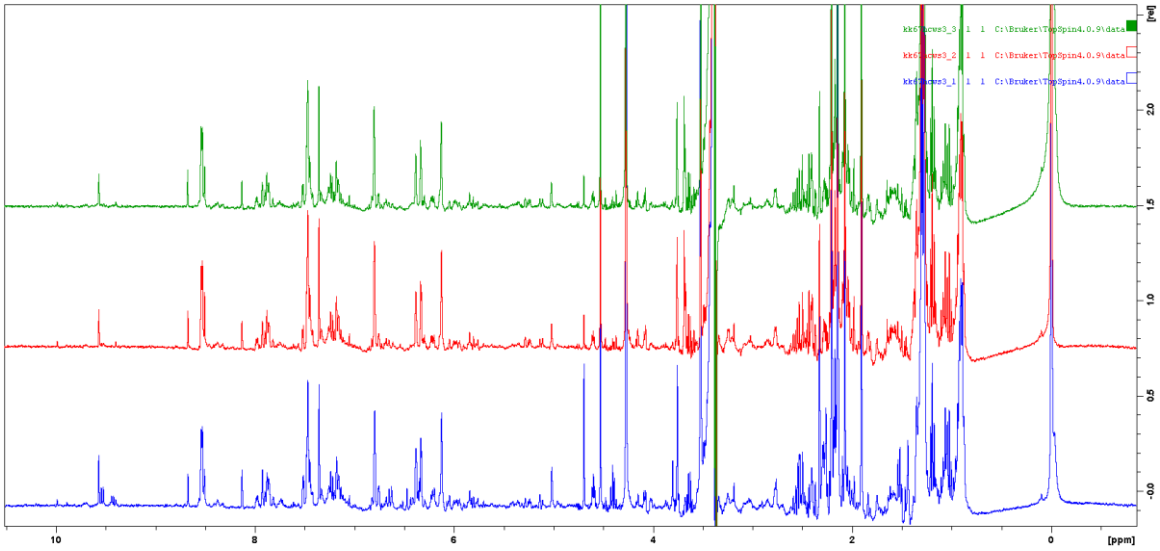

Figure S28. *^{1}H NMR spectra of CWS4 (bottom), CWS5 (middle), CWS6 (top) recorded at 400 MHz.*

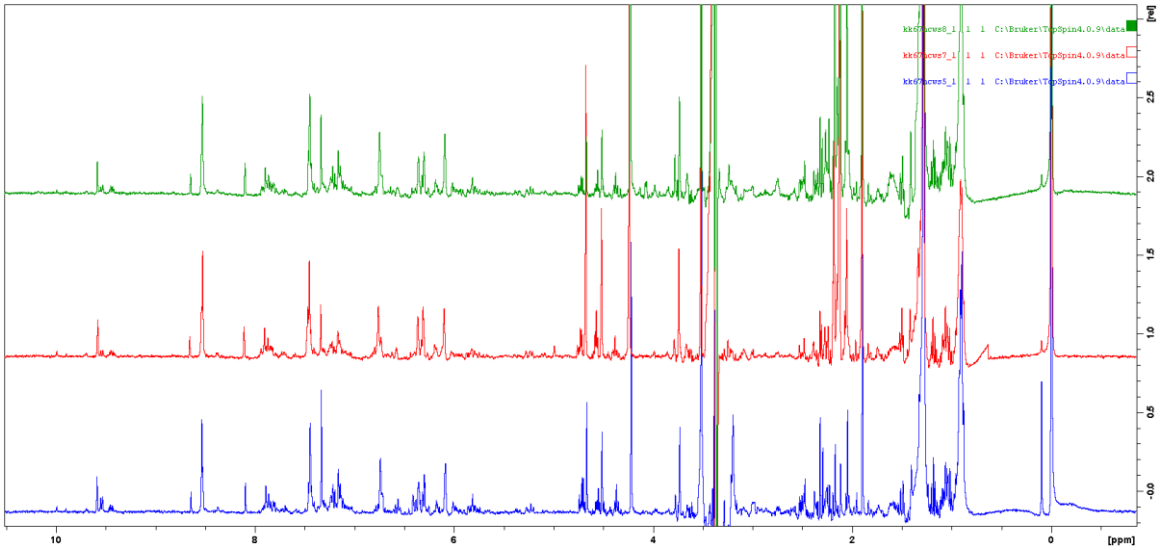

Figure S29. *^{1}H NMR spectra of CWS7 (bottom), CWS8 (middle), CWS9 (top) recorded at 400 MHz.*

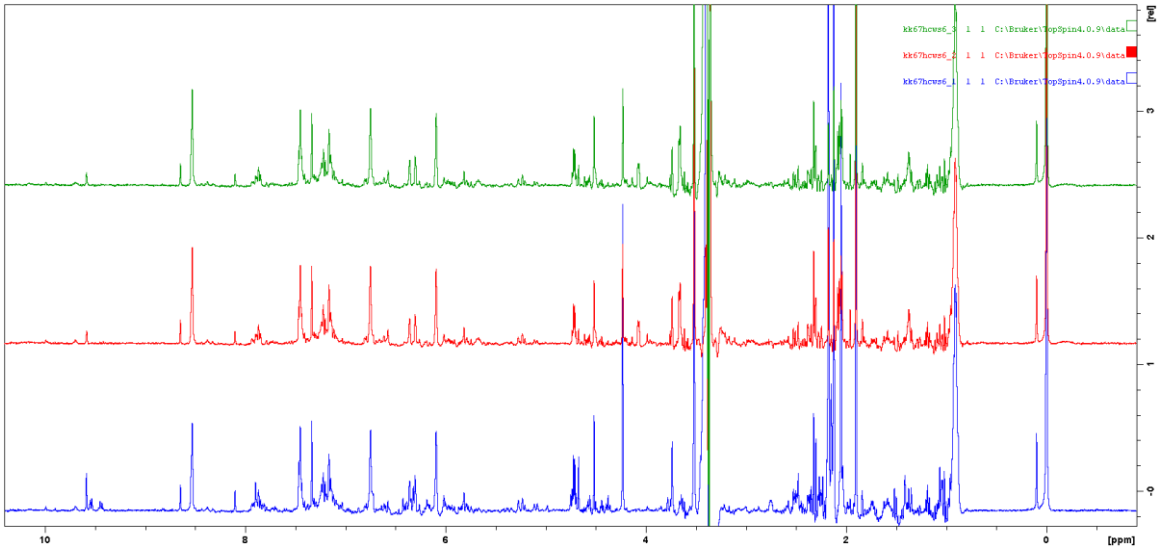

Figure S30. *^{1}H NMR spectra of CWS10 (bottom), CWS11 (middle), CWS 12 (top) recorded at 400 MHz.*

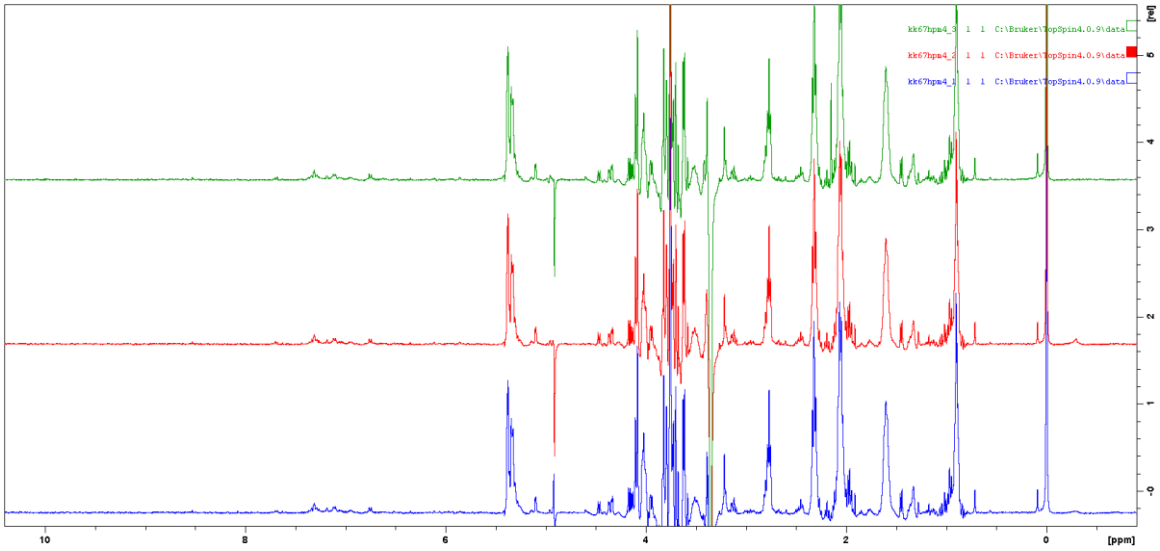

Figure S31. *^{1}H NMR spectra of IPM1 (bottom), IMP2 (middle), IPM3 (top) recorded at 400 MHz.*

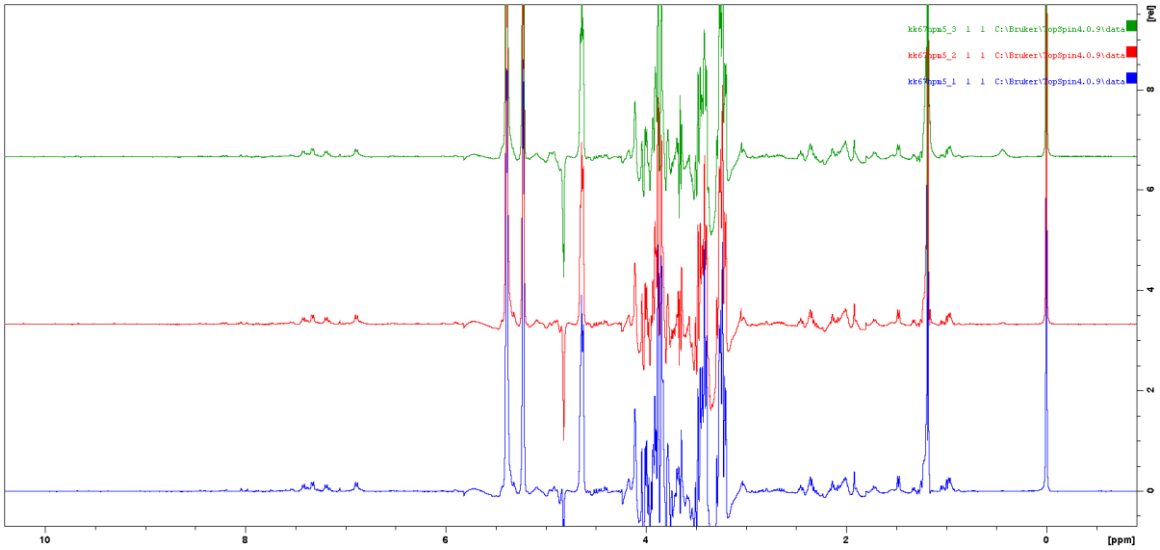

Figure S32. *^{1}H NMR spectra of IPM4 (bottom), IPM5 (middle), IPM6 (top) recorded at 400 MHz.*

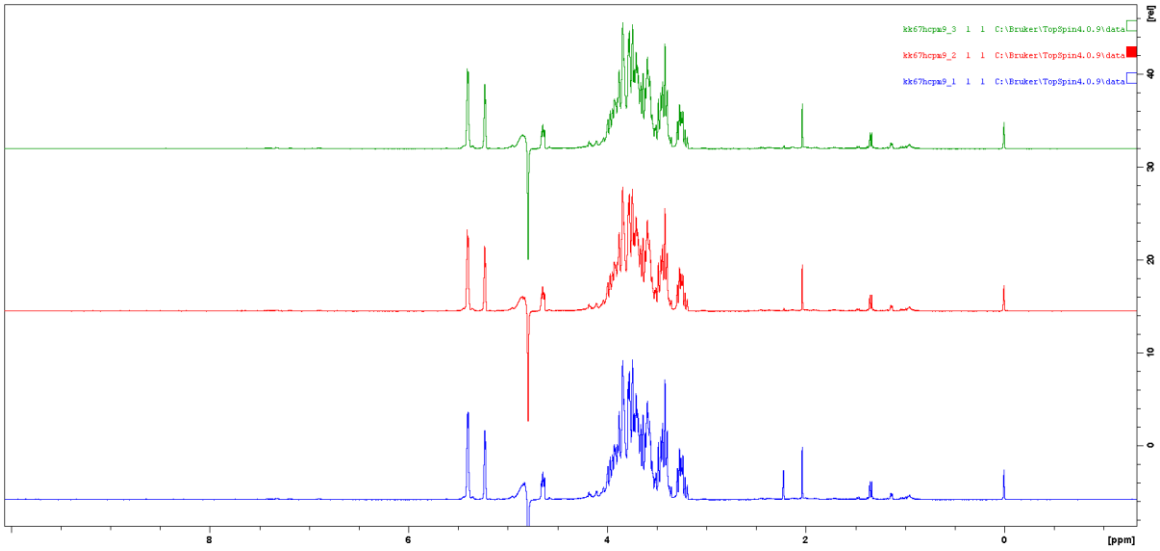

Figure S33. *^{1}H NMR spectra of CPM1 (bottom), CPM2 (middle), CPM3 (top) recorded at 400 MHz.*

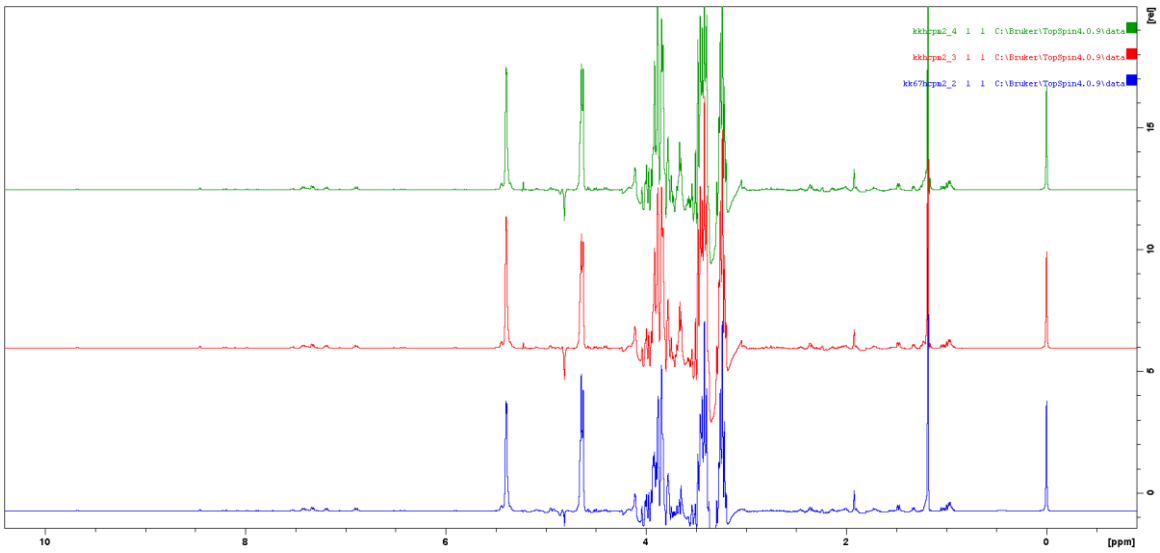

Figure S34. *^{1}H NMR of CPM4 (bottom), CPM5 (middle), CPM6 (top) recorded at 400 MHz.*

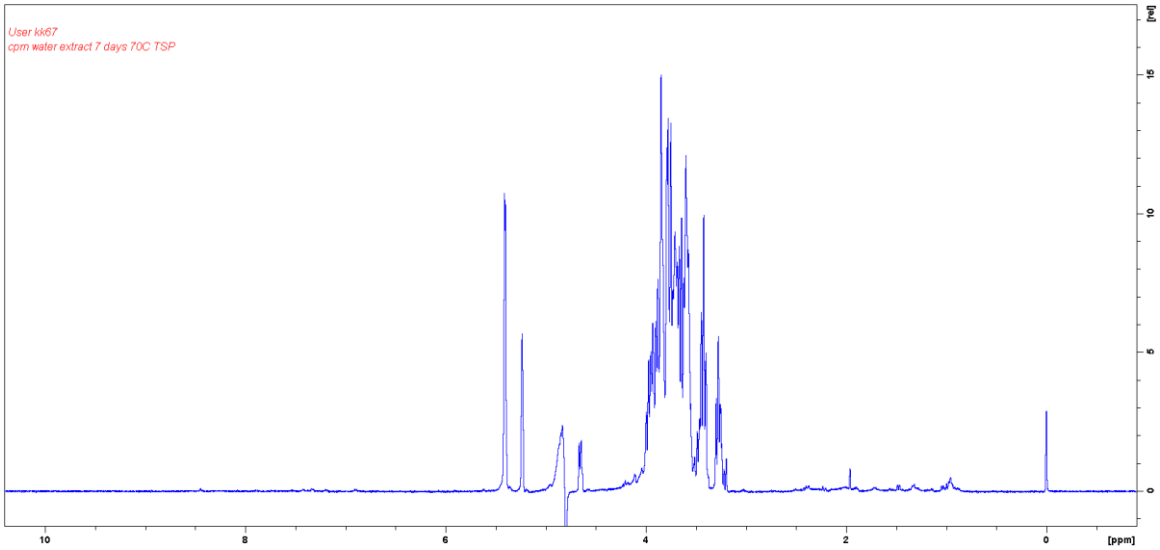

Figure S35. *^{1}H NMR of CPM7 recorded at 400 MHz.*

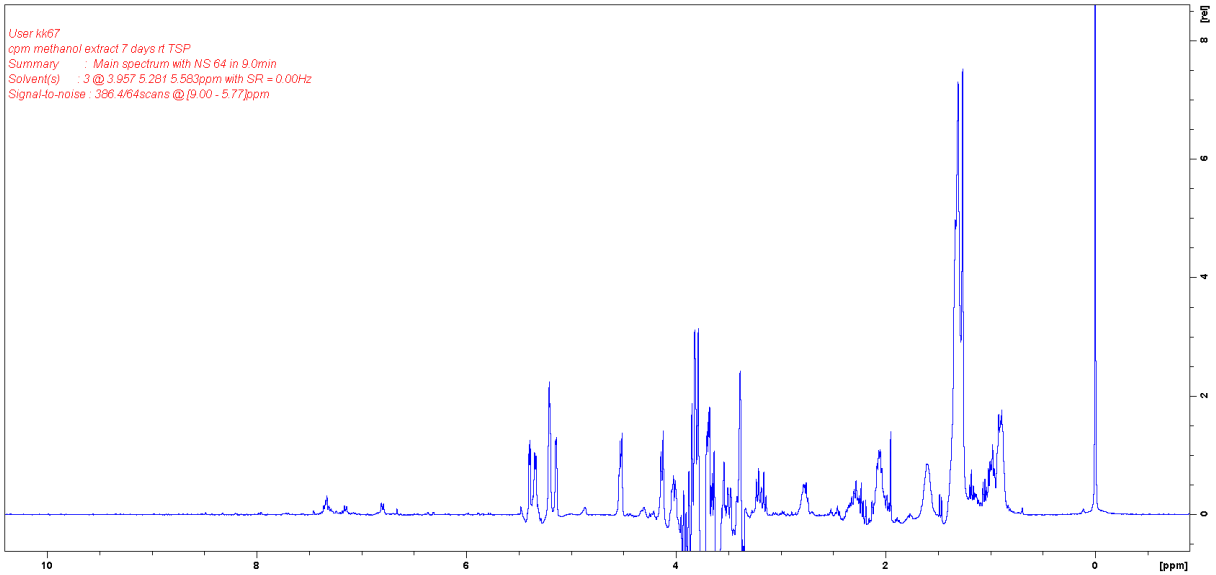

Figure S36. *^{1}H NMR spectrum of CPM10 recorded at 400 MHz.*

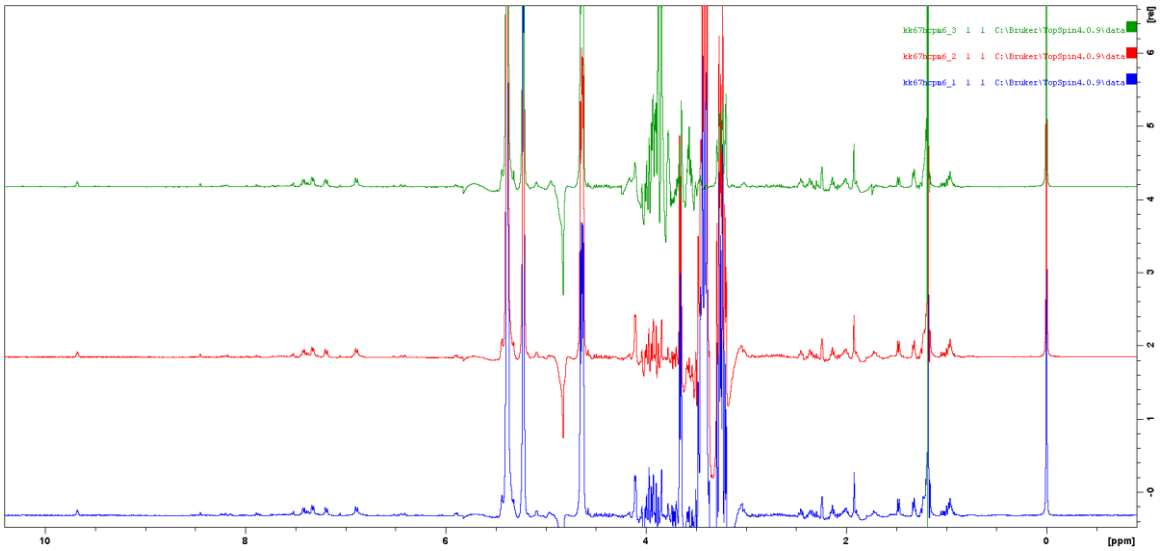

Figure S37. *^{1}H NMR spectrum of CPM13 (bottom), CPM14 (middle), CPM 15 (top) recorded at 400 MHz.*

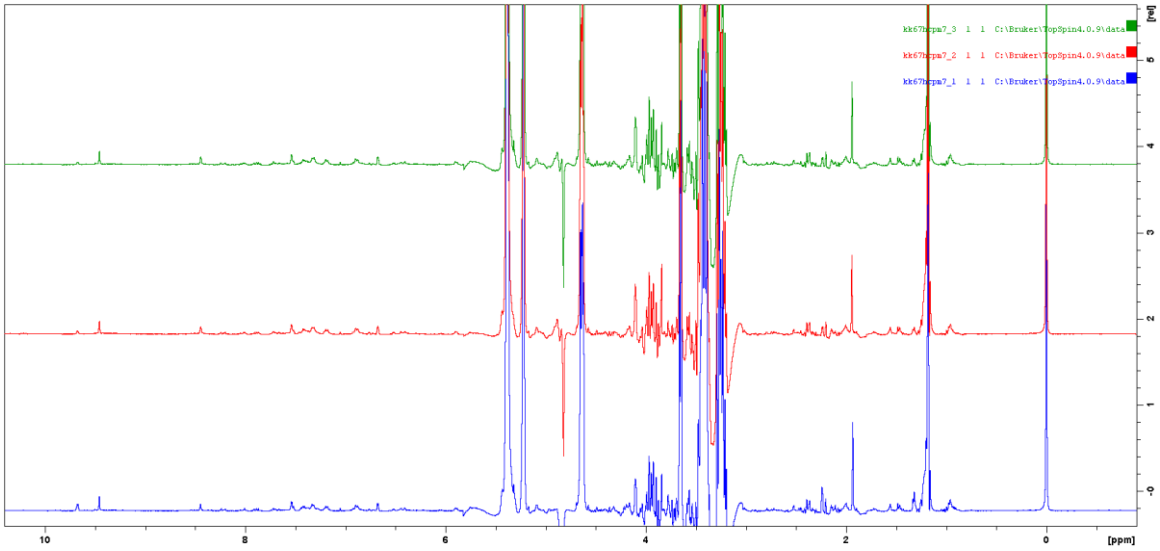

Figure S38. *^{1}H NMR spectrum of CPM16 (bottom), CPM17 (middle), CPM18 (top) recorded at 400 MHz.*

NMR signal assignment

δ_H / ppm	Multiplicity	Inferences
0	Singlet	TSP 3xCH_3
0.81	Doublet, J = 4.9 Hz	Long chain alkanes/ alkenes/alcohols/esters
0.85	Triplet, J = 8.0 Hz	Long chain alkanes CH_3 groups
0.88	Singlet	Long chain alkanes/ alkenes/alcohols/esters
0.94	Multiplet	Long chain alkanes/ alkenes/alcohols/esters
1.00	Singlet	Long chain alkanes/ alkenes/alcohols/esters
1.05	Doublet, J = 11 Hz	Long chain alkanes/ alkenes/alcohols/esters
1.10	Doublet, J = 7.8 Hz	Long chain alkanes/ alkenes/alcohols/esters
1.17	Triplet, J = 6.9 Hz	Ethylphenol CH_3
1.58		Long chain alkanes CH_2 groups
2.01	Singlet	Acetic acid/acetate CH_3
2.14	Singlet	Acetone 2xCH_3
2.25	Multiplet	o-cresol CH_3, p-cresol CH_3
2.48	Quartet J = 7.3 Hz	Ethylphenol CH_3
3.38	Distorted	Water, methanol CH_3, suppressed
3.73	Singlet	Glycine
3.88	Singlet	Ferulic acid OCH_3
4.64	Singlet	o-cresol, p-cresol OH
4.96	Distorted	Methanol OH, suppressed
6.06	Singlet	Long chain alkene CHs
6.11	Singlet	Long chain alkene CHs
6.34	Doublet, J = 16 Hz	Ferulic acid trans alkene CH
6.75	Multiplet	o-cresol aromatic CH
6.80	Doublet, J = 8.2 Hz	Ferulic acid aromatic CH, overlap with o-cresol, p-cresol aromatic CHs
7.05	Doublet J = 7.9 Hz	Ferulic acid aromatic CH, overlap with o-cresol, p-cresol aromatic CHs
7.17	Singlet	Ferulic acid aromatic CH
7.58	Doublet J = 16 Hz	Ferulic acid trans alkene CH
8.50	Singlet	Formic acid CH, present only in P2 and P3

Table S21. *Signal assignments for P1, P2, P3.*

δ_H / ppm	Multiplicity	Inferences
0	Singlet	TSP 3xCH_3
0.83	Singlet	Long chain alkanes/ alkenes/alcohols/esters
0.88	Multiplet	Long chain alkanes CH_3 groups
1.18	Triplet, J = 7.1 Hz	2-ethylphenol CH_3
1.26	Singlet	Lactic acid CH_3
1.34	Multiplet	Long chain alkanes/ alkenes/alcohols/esters
1.62	Broad Singlet	Long chain alkanes CH_2 groups
1.98	Singlet	Acetic acid/acetate CH_3
2.05	Multiplet	Quinic acid
2.19	Singlet	o-cresol CH_3
2.26	Singlet	p-cresol CH_3
2.48	Doublet, J = 11 Hz	Quinic acid/quinides
2.53	Triplet, J = 7.4 Hz	Quinic acid/quinides
3.21	Singlet	Choline 3xCH_3
3.39	Distorted	Methanol CH_3, suppressed
3.89	Singlet	Ferulic acid OCH_3
4.44	Singlet	Trigonelline CH_3
5.34	Doublet, J = 5.7 Hz	Carbohydrate CH
5.48	Singlet	4,5 – caffeoylquinic acid
5.52	Doublet, J = 8.7 Hz	Carbohydrate glycosidic linkage CH
6.34	Doublet, J = 16 Hz	Ferulic acid trans alkene CH
6.40	Doublet, J = 16 Hz	Cinnamic acid trans alkene CH
6.82	Multiplet	p-cresol, overlap with phenol and 2-ethylphenol
6.99	Multiplet	2-ethylphenol
7.09	Multiplet	p-cresol, overlap with phenol an 2-ethylphenol
7.29	Singlet	Phenol aromatic CHs
7.58	Doublet, J = 16 Hz	Ferulic acid trans alkene CH
7.59	Doublet, J = 16 Hz	Cinnamic acid trans alkene CH
7.89	Singlet	Pyridine aromatic CH
8.08	Multiplet	Trigonelline aromatic CH
8.46	Singlet	Formic acid CH
8.84	Doublet, J = 5.9 Hz	N-methylpyridinium aromatic CH
8.89	Doublet, J = 8.2 Hz	Trigonelline aromatic CH
9.16	Singlet	Trigonelline aromatic CH

Table S22. *Signal assignment for CW1, CW2, CW3.*

δ_H / ppm	Multiplicity	Inferences
0	Singlet	TSP 3xCH_3
0.83	Singlet	Long chain alkanes/ alkenes/alcohols/esters
0.89	Multiplet	Long chain alkanes CH_3 groups
0.97	Singlet	Long chain alkanes/ alkenes/alcohols/esters
1.17	Triplet, J = 7.1 Hz	Ethylphenol CH_3
1.27	Singlet	Lactic acid CH_3
1.36	Singlet	Long chain alkanes/ alkenes/alcohols/esters
1.50	Doublet, J = 7.0 Hz	Long chain alkanes/ alkenes/alcohols/esters
1.60	Broad Singlet	Long chain alkanes CH_2 groups
1.94	Singlet	Acetic acid/acetate CH_3
2.05	Multiplet	Quinic acid

2.12	Singlet	Acetone 2xCH_3
2.32	Triplet, J = 7.4 Hz	Glutamic acid CH_2, overlap with cresols
2.37	Triplet, J = 7.3 Hz	Glutamic acid CH_2
2.46	Doublet, J = 11 Hz	Quinic acid/qunides
2.56	Multiplet	Quinic acid/quinides
3.20	Singlet	Choline 3xCH_3
3.35	Distorted	Methanol CH_3, suppressed
3.52	Singlet	Caffeine CH_3
3.71	Multiplet	Glutamic acid CH
3.88	Singlet	Ferulic acid CH_3
3.96	Singlet	Caffeine CH_3
4.42	Singlet	Trigonelline CH_3
5.33	Doublet, J = 7.6 Hz	Carbohydrate CH
6.28	Doublet, J = 16 Hz	Ferulic acid trans alkene CH
6.29	Doublet, J = 16 Hz	Cinnamic acid trans alkene CH
6.33	Singlet	Caffeic acid
6.76	Multiplet	Overlapping p-cresol, o-cresol, ethylphenol
6.93	Multiplet	Overlapping o-cresol, p-cresol
7.04	Multiplet	Overlapping p-cresol, o-cresol, ethylphenol
7.05	Singlet	Ferulic acid aromatic CH
7.31	Singlet	Caffeic acid
7.55	Doublet, J = 16 Hz	Ferulic acid trans alkene CH
7.57	Doublet, J = 16 Hz	Cinnamic acid trans alkene CH
7.85	Singlet	Caffeine CH
8.06	Multiplet	Trigonelline aromatic CH
8.50	Singlet	Formic acid CH
8.84	Doublet, J = 6.2 Hz	N-methylpyridinium aromatic CH
8.89	Doublet, J = 6.7 Hz	Trigonelline aromatic CH
9.19	Singlet	Trigonelline aromatic CH

Table S23. *Signal assignment for CW13, CW14, CW15.*

δ_H / ppm	Multiplicity	Inferences
0	Singlet	TSP 3xCH_3
0.89	Multiplet	Long chain alkanes CH_3 groups
1.01	Triplet, J = 7.4 Hz	Long chain alkanes/ alkenes/alcohols/esters
1.09	Triplet, J = 7.3 Hz	Long chain alkanes/ alkenes/alcohols/esters
1.18	Triplet, J = 7.0 Hz	4-ethylphenol CH_3
1.28	Multiplet	Long chain alkanes CH_2 groups
1.64	Singlet	Squalene
1.68	Singlet	Squalene
2.04	Singlet	Acetic acid/acetate CH_3
2.16	Singlet	Acetone 2xCH_3
2.19	Singlet	Hydroxyacetone CH_3
2.24	Multiplet	*o*-Cresol CH_3, overlap with other signals
2.27	Singlet	*p*-Cresol CH_3
2.32	Singlet	Toluene CH_3
2.41	Singlet	5-methylfurfural CH_3
2.50	Quartet, J = 7.4 Hz	4-ethylphenol CH_2
3.38	Distorted	Methanol CH_3 suppressed
3.60	Singlet	Levoglucosan CH

3.64	Multiplet	Levoglucosan CH
3.74	Singlet	Guaiacol OCH_3, overlap with levoglucosan CH
4.06	Doublet, J = 6.6 Hz	Levoglucosan CH
4.21	Singlet	Hydroxyacetone CH_2
4.57	Singlet	Benzyl alcohol CH_2
4.99	Broad singlet	Methanol OH, suppressed
5.80	Singlet	Long chain alkenes CH
6.24	Singlet	5-methylfurfural aromatic CH
6.55	Multiplet	5-HMF aromatic CH
6.71	Doublet of doublets, J = 3.5 Hz, J = 1.5 Hz	Furfural aromatic CH
6.73	Multiplet	Phenol aromatic CH
6.76	Multiplet	Overlapping phenol, 4-ethylphenol, guaiacols, cresols
7.04	Multiplet	4-ethylphenol aromatic CH
7.08	Singlet	Guaiacol derivative
7.11	Doublet, J = 7.7	Phenol aromatic CH, overlap with *o*-Cresol, *p*-Cresol
7.15	Singlet	5-methylfurfural, overlap with toluene
7.20	Doublet, J = 7.1 Hz	5-methylfurfural
7.32	Singlet	Benzyl alcohol, overlap with 3-methylpyridazine
7.44	Doublet, J = 3.6 Hz	Furfural aromatic CH
7.49	Singlet	Naphthalene aromatic CH
7.88	Singlet	Furfural, overlap with naphthalene
8.52	Singlet	Pyridine aromatic CH
9.07	Singlet	3-methylpyridazine CH
9.42	Singlet	Hydroxyacetaldehyde CHO
9.54	Doublet, J =7.0 Hz	5-HMF CHO, overlap with 5-methylfurfural CHO
9.58	Singlet	Furfural CHO

Table S24. *Signal assignment for PS1, PS2, PS3.*

δ_H / ppm	Multiplicity	Inferences
0	Singlet	TSP 3xCH_3
0.91	Multiplet	Long chain alkanes CH_3 groups
1.03	Triplet, J = 7.5 Hz	Long chain alkanes/ alkenes/alcohols/esters
1.06	Triplet, J = 7.0 Hz	Long chain alkanes/ alkenes/alcohols/esters
1.20	Triplet, J = 7.0 Hz	4-ethylphenol CH_3
1.28	Singlet	Long chain alkanes CH_2 groups
1.30	Doublet, J = 5.2 Hz	Long chain alkanes CH_2 groups
1.35	Singlet	Methylglyoxal CH_3
1.44	Singlet	Squalene
1.52	Singlet	Squalene
2.08	Singlet	Acetic acid/acetate CH_3
2.10	Singlet	Ethyl acetate isolated CH_3
2.15	Singlet	Acetone 2xCH_3
2.21	Singlet	Hydroxyacetone CH_3
2.27	Singlet	*p*-Cresol CH_3
2.33	Singlet	Toluene CH_3
2.41	Multiplet	5-methylfurfural CH_3, overlap with other signals
2.43	Singlet	Methylpyridine/methylpyrazine CH_3
2.51	Multiplet	Methylpyridine/methylpyrazine CH_3, overlapping
2.56	Multiplet	4-ethylphenol, overlapping with other signals

3.39	Distorted	Methanol CH_3 suppressed
3.68	Multiplet	Levoglucosan CH
3.76	Singlet	Guaiacol OCH_3, overlap with levoglucosan
3.81	Singlet	Guaiacol derivative OCH_3
4.08	Multiplet	Levoglucosan CH
4.15	Singlet	Hydroxyacetone CH_2
4.53	Singlet	Benzyl alcohol CH_2
5.12	Doublet, J = 11 Hz	Vinylguaiacol alkene CH
5.80	Singlet	Long chain alkenes CH
5.84	Singlet	Long chain alkenes CH
6.13	Singlet	Long chain alkenes CH
6.21	Multplet	5-methylfurfural CH
6.33	Doublet, J = 2.9 Hz	2-methylfuran CH
6.38	Multiplet	2-methylfuran
6.64	Doublet, J = 9.3 Hz	5-HMF CH
6.76	Doublet, J = 3.5 Hz	Furfural CH
6.80	Singlet	Overlapping *p*-cresol, *o*-cresol, guaiacol derivatives, phenol
7.05	Multiplet	4-ethylphenol aromatic CH
7.12	Multiplet	Phenol CH
7.18	Multiplet	5-methylfurfural, overlap with toluene
7.36	Singlet	Benzyl alcohol aromatic CHs, overlap with
7.47	Multiplet	2-methylfuran, overlap with 2-methylpyridine
7.52	Doublet, J = 3.5 Hz	Furfural aromatic CH
7.62	Triplet, J = 7.1 Hz	Benzaldehyde aromatic CH
7.74	Triplet, J = 5.4 Hz	Benzaldehyde aromatic CH
7.88	Multiplet	Overlapping 5-HMF, 2-methylpyridine, naphthalene
7.93	Singlet	Furfural aromatic CH, overlap with benzaldehyde
8.13	Singlet	Dimethylpyrazine
8.51	Singlet	2-methylpyrazine aromatic CH
8.54	Doublet, J = 4.6 Hz	2-methylpyridine, 2-methylpyrazine aromatic CH
9.42	Triplet, J = 8.3 Hz	Hydroxyacetaldehyde CHO
9.54	Doublet, J = 7.6 Hz	5-HMF CHO overlap with 5-methylfurfural CHO
9.57	Singlet	Furfural CHO
9.89	Singlet	Vanilin CHO
9.99	Singlet	Benzaldehyde CHO

Table S25. *Signal assignment for CWS4, CWS5, CWS6.*

δ_H / ppm	Multiplicity	Inferences
0	Singlet	TSP 3xCH_3
0.90	Multiplet	Long chain alkanes CH_3 groups
1.02	Triplet, J = 7.5 Hz	Long chain alkanes/ alkenes/alcohols/esters
1.05	Multiplet	Long chain alkanes/ alkenes/alcohols/esters
1.19	Triplet, J = 7.0 Hz	4-ethylphenol CH_3
1.28	Multiplet	Long chain alkanes CH_2 groups
1.41	Singlet	Squalene
1.49	Singlet	Squalene
2.05	Singlet	Acetic acid/acetate CH_3
2.06	Singlet	Ethyl acetate isolated CH_3
2.12	Singlet	Hydroxyacetone CH_3

2.17	Singlet	Acetone 2xCH_3
2.23	Singlet	*o*-cresol CH_3
2.30	Singlet	*p*-cresol CH_3
2.32	Singlet	Toluene CH_3
2.47	Singlet	Methylpyridines/methylpyrazines CH_3
2.51	Multiplet	Methylpyridines/methylpyrazines CH_3
2.53	Singlet	2-methylpyridine CH_3
3.38	Distorted	Methanol CH_3 suppressed
3.62	Doublet, J = 6.9 Hz	Levoglucosan CH
3.73	Singlet	Guaiacol OCH_3 overlap with levoglucosan CH
3.78	Singlet	Levoglucosan CH
3.96	Multiplet	Levoglucosan CH
4.52	Singlet	Benzyl alcohol CH_2
5.80	Doublet, J = 3.9 Hz	Long chain alkene CHs
5.81	Singlet	Long chain alkene CHs
6.09	Multiplet	Long chain alkene CHs
6.30	Doublet, J = 3.0 Hz	2-methylfuran CH
6.36	Doublet, J = 2.2 Hz	2-methylfuran CH
6.58	Doublet, J = 9.4 Hz	5-HMF aromatic CH
6.72	Doublet of doublets, J = 3.6 Hz, J = 1.8 Hz	Furfural aromatic CH
6.74	Multiplet	Phenol aromatic CH
6.78	Multiplet	Overlapping *p*-cresol, *o*-cresol, phenol, 4-ethylphenol
7.04	Multiplet	Overlapping *p*-cresol, guaiacol derivatives, 4-ethylphenol
7.11	Multiplet	Overlapping *o*-cresol, guaiacol derivatives, phenol
7.16	Singlet	5-methylfurfural, overlap with toluene
7.22	Singlet	2-methylpyridine CH
7.34	Singlet	Benzyl alcohol aromatic CHs
7.45	Multiplet	Overlapping 2-methylfuran, furfural
7.84	Singlet	Pyridine aromatic CH
7.86	Singlet	Naphthalene aromatic CH
7.89	Singlet	Furfural aromatic CH
7.93	Multiplet	Benzaldehyde
8.53	Singlet	Pyridine aromatic CH, 2 methylpyridine overlap
8.64	Singlet	Methylpyridine/methylpyrazine
9.54	Singlet	5-methylfurfural CHO
9.55	Singlet	5-HMF CHO
9.59	Singlet	Furfural CHO
9.70	Multiplet	Syringaldehyde CHO
9.90	Singlet	Vanilin CHO
9.99	Singlet	Benzaldeyde CHO

Table S26. *Signal assignment for CWS7, CWS8, CWS9.*

δ_H / ppm	Multiplicity	Inferences
0	Singlet	TSP 3xCH_3
0.98	Multiplet	Long chain alkanes CH_3 groups
1.18	Distorted	Ethanol CH_3 suppressed
1.33	Doublet, J = 6.5 Hz	Lactic acid CH_3
1.92	Singlet	Acetic acid/acetate CH_3
2.08	Multiplet	Cresol CH_3

2.34	Multiplet	Cresol CH_3
2.46	Triplet, J = 8.6 Hz	Ethylphenol CH_2
3.23	Triplet, J = 8.4 Hz	Beta glucose CH
3.27	Multiplet	Glucose/mannose CH
3.42	Triplet, J = 8.7 Hz	Sucrose CH
3.86	Distorted	Ethanol CH_2 suppressed
3.90	Singlet	Carbohydrate CH
3.91	Singlet	Carbohydrate CH
3.96	Doublet, J = 9.4 Hz	Carbohydrate CH
4.00	Doublet, J = 5.5 Hz	Carbohydrate CH
4.04	Singlet	Carbohydrate CH
4.11	Singlet	Carbohydrate CH
4.63	Doublet, J = 7.5 Hz	Beta glucose/mannose anomeric CH
4.64	Doublet, J = 8.0 Hz	Beta glucose/mannose anomeric CH
5.22	Doublet, J = 2.8 Hz	Alpha glucose anomeric CH
5.39	Doublet, J = 2.7 Hz	Sucrose glycosidic linkage CH
6.89	Doublet, J = 8.0 Hz	Phenol, overlap with *p*-cresol
7.19	Doublet, J = 8.0 Hz	Phenol, overlap with *p*-cresol
7.38	Doublet, J = 6.9 Hz	Flavonoids
7.42	Doublet, J = 7.1 Hz	Flavonoids
7.54	Doublet, J = 9.0 Hz	Flavonoids
7.74	Doublet, J = 7.7 Hz	Flavonoids
7.98	Singlet	Flavonoids
8.04	Singlet	Pyridine/pyrazine derivative
8.19	Singlet	Pyridine/pyrazine derivative
8.45	Singlet	Pyridine/pyrazine derivative

Table S27. *Signal assignment for IPM4, IMP5, IPM6.*

δ_H / ppm	Multiplicity	Inferences
0	Singlet	TSP 3xCH_3
0.96	Multiplet	Long chain alkanes CH_3 groups
1.18	Distorted	Ethanol CH_3 suppressed
1.32	Doublet, J = 4.7 Hz	Lactic acid CH_3
1.93	Singlet	Acetic acid/ acetate CH_3
2.08	Singlet	Cresol CH_3
2.20	Singlet	Acetone 2xCH_3
2.24	Singlet	Acetaldehyde CH_3
2.46	Doublet, J = 2.8 Hz	Ethylphenol CH_2
3.23	Triplet, J = 8.3 Hz	Beta glucose CH
3.27	Triplet, J = 8.5 Hz	Glucose/mannose CH
3.41	Triplet, J = 9.1 Hz	Sucrose CH
3.66	Doublet, J = 6.8 Hz	Carbohydrate CH
3.86	Distorted	Ethanol CH_2 suppressed
3.90	Singlet	Carbohydrate CH
3.93	Singlet	Carbohydrate CH
3.97	Triplet, J = 8.9 Hz	Carbohydrate CH
4.10	Doublet, J = 5.5 Hz	Carbohydrate CH
4.63	Doublet, J = 7.4 Hz	Beta glucose/mannose anomeric CH
4.64	Doublet, J = 8.0 Hz	Beta glucose/mannose anomeric CH
5.22	Doublet, J = 3.2 Hz	Alpha glucose anomeric CH

5.39	Doublet, J = 3.4 Hz	Sucrose glycosidic linkage CH
6.41	Singlet	2-methylfuran
6.44	Singlet	2-methylfuran
6.68	Doublet, J = 3.3 Hz	Furfural CH
6.89	Doublet, J = 8.4 Hz	Phenol, overlap with *p*-cresol
7.19	Doublet, J = 8.0 Hz	Phenol, overlap with *p*-cresol
7.42	Doublet, J = 7.2 Hz	Flavonoids
7.52	Singlet	Flavonoids
7.54	Doublet, J = 3.2 Hz	Furfural CH
7.73	Doublet, J = 7.7 Hz	Flavonoids
7.88	Doublet, J = 7.9 Hz	Flavonoids
7.91	Singlet	Furfural CH
8.01	Singlet	Pyridine/pyrazine derivatives
8.20	Multiplet	Pyridine/pyrazine derivatives
8.24	Singlet	Pyridine/pyrazine derivatives
8.45	Singlet	Pyridine/pyrazine derivatives
9.46	Singlet	Furfural CHO
9.68	Doublet, J = 2.8 Hz	Acetaldehyde CHO

Table S28. *Signal assignment for CPM16, CPM17, CPM18*

Thermogravimetric analysis

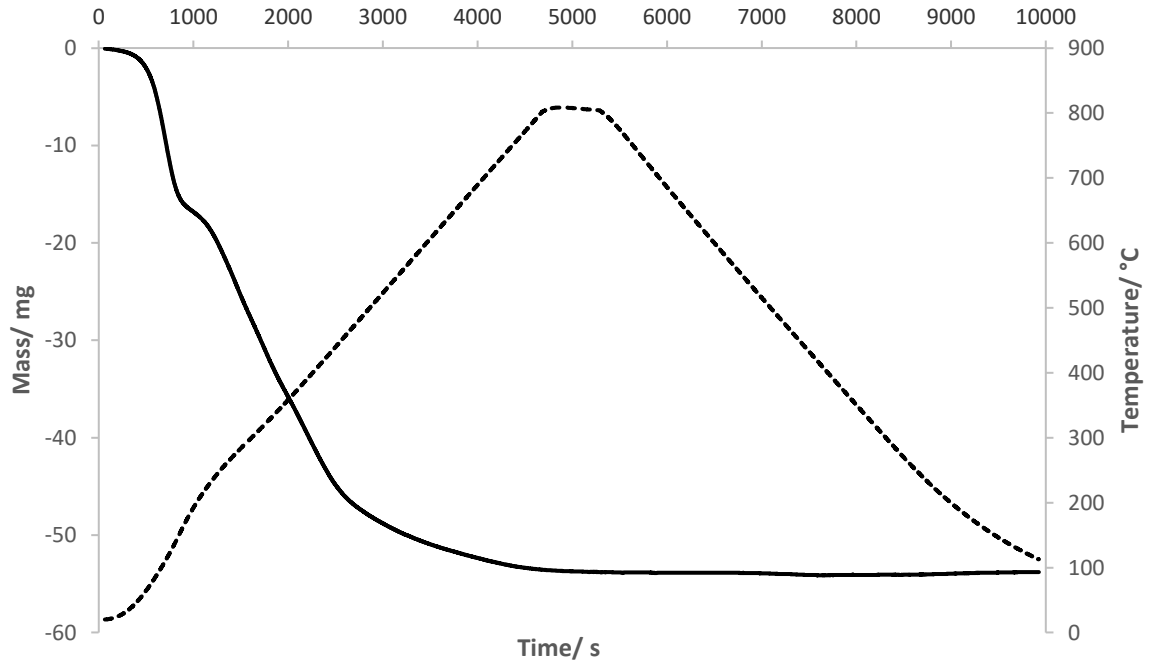

Figure S39. *TGA data for peat sample. Solid line is mass (mg) against time (s), dotted line is temperature (°C) against time (s).*

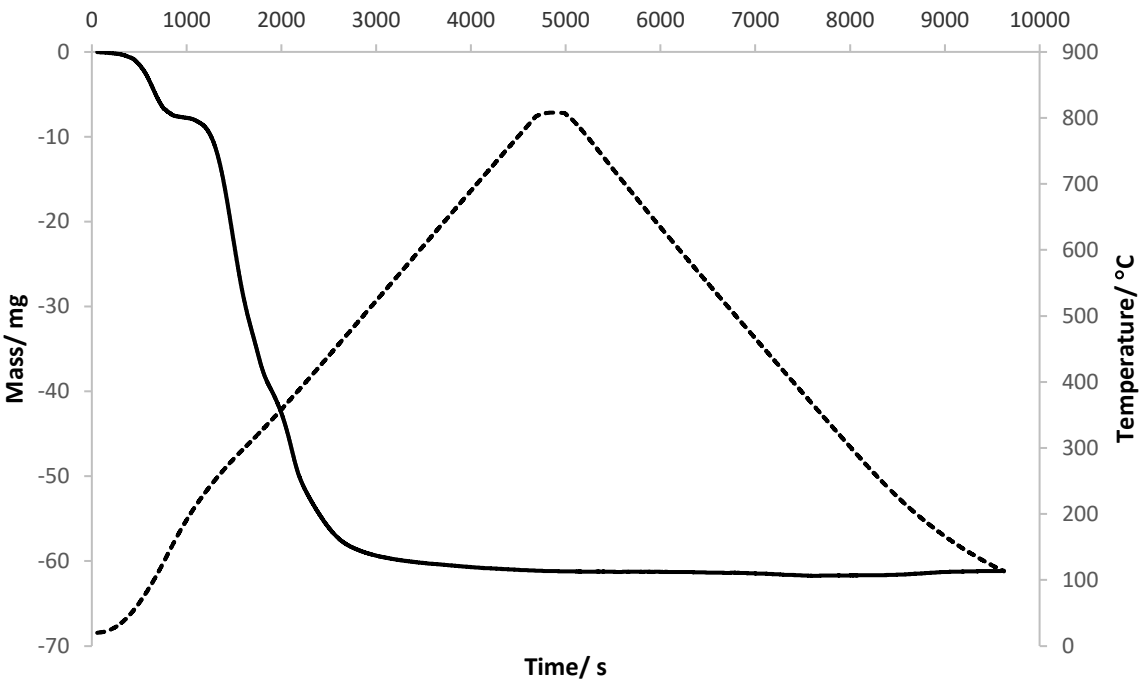

Figure S40. *TGA data for spent coffee grounds. Solid line is mass (mg) against time (s), dotted line is temperature (°C) against time (s).*

Pyrolysis - Gas Chromatography/Mass Spectrometry

Component RT (mins)	Compound Name	Match Factor (%)	Molecular Formula	Component Area	Library File	Total area	Compound %	Stdva	CV%
66.20166687	Stigmastan-3,5-diene	90.9829884	C29H48	4654316.148	NIST14.L	381456681.4	1.220142778	273796.563	5.882638
62.85195835	Squalene	97.64731317	C30H50	4448940.419	NIST14.L	381456681.4	1.166302921	29660.1408	0.708255
2.908294933	Toluene	98.22116701	C7H8	2635175.525	NIST14.L	238342058.8	1.105627575	88708.3405	2.383897
9.226297765	3-Methylpyridazine	94.77178725	C5H6N2	4187776.123	NIST14.L	381456681.4	1.097837927	180856.206	6.863156
32.63351764	.beta.-D-Glucopyranose, 1,6-anhydro-	89.45095624	C6H10O5	3721148.237	NIST14.L	381456681.4	0.975510043	66791.8635	2.248798
69.02551425	.gamma.-Sitosterol	88.41623864	C29H50O	2795371.419	NIST14.L	381456681.4	0.732814905	126681.328	4.531825
4.177502827	Furfural	96.60810416	C5H4O2	2647670.14	NIST14.L	381456681.4	0.694094577	104531.422	3.948053
13.12959273	p-Cresol	94.35235121	C7H8O	2575825.992	NIST14.L	381456681.4	0.675260421	114299.781	4.437403
71.20598595	1-Decanol, 2-hexyl-	82.89560501	C16H34O	2495826.874	NIST14.L	381456681.4	0.654288415	114105.872	4.571866
9.283459567	Phenol	88.0963478	C6H6O	2207481.799	NIST14.L	381456681.4	0.578697899	78734.3208	3.918489
72.31851004	1-Heneicosanol	91.00486606	C21H44O	2009302.908	NIST14.L	381456681.4	0.526744715	53350.9674	2.792799
23.24884163	Ethanone, 1-(2-hydroxy-5-methylphenyl)-	93.41281053	C9H10O2	1910304.571	NIST14.L	381456681.4	0.500792007	82783.3729	5.079118
57.80470481	Behenic alcohol	96.12863074	C22H46O	1876088.824	NIST14.L	381456681.4	0.491822248	37909.0909	2.411978
57.80577812	1-Docosene	94.88682061	C22H44	1781551.767	NIST14.L	381456681.4	0.467039078	66781.5018	4.292509
54.54281269	Tricosane	94.32590536	C23H48	1629876.998	NIST14.L	381456681.4	0.427277087	51697.2293	3.357916

31.86481133	Guanidine, methyl-	83.07343929	C2H7N3	1629109.525	NIST14.L	381456681.4	0.427075892	2879.92854	0.188592
57.94406137	Hexacosane	94.40478508	C26H54	1571701.111	NIST14.L	381456681.4	0.412026106	28226.8681	1.851119
47.50839024	n-Hexadecanoic acid	95.52141659	C16H32O2	1555768.418	NIST14.L	381456681.4	0.407849304	5450.70519	0.367035
56.20522762	1-Nonadecene	94.59355285	C19H38	1527070.659	NIST14.L	381456681.4	0.400326101	30376.4575	2.072245
56.20539002	1-Octadecanol	94.31216782	C18H38O	1524854.226	NIST14.L	381456681.4	0.399745056	12057.5193	0.874088
52.53950402	1-Eicosanol	97.09106393	C20H42O	1485064.32	NIST14.L	381456681.4	0.389314015	35646.7603	2.705312
19.74393448	Benzofuran, 2,3-dihydro-	86.9909605	C8H8O	1465871.93	LIGNOCELLULOSIC 2019.L	381456681.4	0.384282673	1376.55394	0.110378
17.91495783	2-Methoxy-5-methylphenol	90.71244499	C8H10O2	1379440.667	NIST14.L	381456681.4	0.361624461	9556.40512	0.795479
60.93931994	n-Heptadecanol-1	94.54644529	C17H36O	1317658.133	NIST14.L	381456681.4	0.345427986	41370.3262	3.943463
5.659571231	Styrene	92.1750442	C8H8	1247131.079	NIST14.L	381456681.4	0.326939111	29512.7997	2.905837
13.30740445	Mequinol	96.41746512	C7H8O2	1201339.601	NIST14.L	381456681.4	0.314934738	30161.0912	3.04008
17.93083067	Phenol, 2-methoxy-4-methyl-	90.02378522	C8H10O2	1185634.324	LIGNOCELLULOSIC 2019.L	381456681.4	0.310817553	28814.4038	3.195158
67.69076117	Tetracosane	88.09018839	C24H50	1049086.173	NIST14.L	381456681.4	0.275021051	8900.50015	0.992322
21.72194075	Phenol, 4-ethyl-2-methoxy-	96.35620884	C9H12O2	1015638.526	NIST14.L	381456681.4	0.266252651	12397.4532	1.394845
66.44331598	Heneicosane	90.51871805	C21H44	992114.9234	NIST14.L	381456681.4	0.260085869	14518.8599	1.665506
54.54261097	Octacosane	93.80645197	C28H58	988178.2871	NIST14.L	381456681.4	0.259053868	3816.32587	0.441431
8.153865195	2-Furancarboxaldehyde, 5-methyl-	86.50254483	C6H6O2	901814.7335	NIST14.L	381456681.4	0.236413406	2439.20384	0.282489
61.23527603	2-Pentacosanone	85.78416705	C25H50O	896936.6841	NIST14.L	381456681.4	0.235134611	14452.6361	1.720154
62.43510922	Dodecyl nonyl ether	86.60211561	C21H44O	888805.1281	NIST14.L	381456681.4	0.2330029	11468.4871	1.438697
45.40954533	Nonadecane	96.14747665	C19H40	871738.5453	NIST14.L	381456681.4	0.228528844	4150.66619	0.524107
68.29981188	Stigmasterol	84.2841983	C29H48O	864535.8467	NIST14.L	381456681.4	0.226640635	2562.64668	0.341136
3.46768513	2-Amino-oxazole	83.91079534	C3H4N2O	863469.5202	NIST14.L	381456681.4	0.226361095	8883.80738	1.207701
52.53332423	1-Hexadecanol	97.09143412	C16H34O	841970.2891	NIST14.L	381456681.4	0.220725008	8743.0246	1.328954
52.65413074	Docosane	95.67017335	C22H46	840194.493	NIST14.L	381456681.4	0.220259477	8893.40076	1.381798
13.33171996	Phenol, 2-methoxy-	95.43963259	C7H8O2	832149.1732	NIST14.L	381456681.4	0.218150373	12600.3301	2.005901
12.18993561	Phenol, 2-methyl-	94.16390007	C7H8O	797144.1106	NIST14.L	381456681.4	0.208973692	11317.7252	1.815906
68.7513789	16-Hentriacontanone	85.3953551	C31H62O	791949.6127	NIST14.L	381456681.4	0.207611939	14461.9331	2.410565
41.97090627	Octadecane	96.87403059	C18H38	751210.2929	NIST14.L	381456681.4	0.196932006	14852.8582	2.551014
14.33180001	Levoglucosenone	92.46547978	C6H6O3	735596.8134	NIST14.L	381456681.4	0.192838886	11367.2646	2.138878
63.82718133	Hexadecane	86.68932177	C16H34	716480.2192	NIST14.L	381456681.4	0.187827414	10881.4771	2.455293

5.006249488	Benzene, 1,3-dimethyl-	94.54502839	C8H10	657887.7483	NIST14.L	381456681.4	0.172467224	10156.0288	2.311172
62.10173392	Tetracosanoic acid	85.17727678	C24H48O2	643610.9714	NIST14.L	381456681.4	0.168724524	12545.8033	2.919245
48.0569705	9-Eicosene, (E)-	96.26026006	C20H40	628163.0059	NIST14.L	381456681.4	0.164674794	13302.0352	3.114663
17.20776256	Phenol, 4-ethyl-	88.70188903	C8H10O	623255.1134	NIST14.L	381456681.4	0.163388176	16016.138	3.782598
31.96972364	Acetic acid	85.61584253	C2H4O2	614855.2682	LIGNOCELLULOSIC 2019.L	381456681.4	0.161186132	16127.2934	3.875219
48.2262575	Eicosane	96.26557542	C20H42	599939.5004	NIST14.L	381456681.4	0.157275919	13587.1341	3.392079
62.38955402	Formic acid, undecyl ester	81.25086033	C12H24O2	590875.1498	NIST14.L	381456681.4	0.154899672	12694.539	3.34227
38.4862303	Heptadecane	95.30062564	C17H36	582233.4662	NIST14.L	381456681.4	0.152634229	12581.2526	3.371412
9.535591447	Oxazolidine, 2,2-diethyl-3-methyl-	84.05647615	C8H17NO	553627.4443	NIST14.L	381456681.4	0.145135076	12253.6165	3.367082
62.43338726	Oxalic acid, allyl octadecyl ester	82.27561722	C23H42O4	547908.6226	NIST14.L	381456681.4	0.143635887	11008.6481	3.129783
52.05644574	Octadecanoic acid	91.05805207	C18H36O2	531459.139	NIST14.L	381456681.4	0.139323589	9994.2091 6	2.941376
16.20758901	Phenol, 3,4-dimethyl-	80.4826499	C8H10O	474369.6068	NIST14.L	381456681.4	0.124357399	8552.3854 8	2.571805
9.186458586	Cyclopropane, 1-hexyl-2-methyl-	86.95002234	C10H20	443184.4818	NIST14.L	381456681.4	0.116182126	4362.2662 8	1.345792
57.86305373	5-Eicosene, (E)-	87.73207894	C20H40	431356.4434	NIST14.L	381456681.4	0.113081371	4852.9678 8	1.541764
24.98377928	Phenol, 2,6-dimethoxy-	90.21852464	C8H10O3	427077.8067	NIST14.L	381456681.4	0.111959713	2731.1470 5	0.874371
30.6745369	n-Tridecan-1-ol	93.96486168	C13H28O	423416.3565	NIST14.L	381456681.4	0.110999853	3703.5063 4	1.195819
61.00427914	1-Iodoundecane	83.1688353	C11H23I	423251.9382	NIST14.L	381456681.4	0.110956675	1147.6750 7	0.381656
2.192383122	Furan, 2,5-dimethyl-	87.09375156	C6H8O	419725.2657	NIST14.L	381456681.4	0.110032223	7377.8534 6	2.584156
30.67444523	1-Tridecene	93.27682209	C13H26	416164.7158	NIST14.L	381456681.4	0.109098814	6179.1095 1	2.16607
4.801248387	Ethylbenzene	92.2160456	C8H10	400554.8099	NIST14.L	381456681.4	0.105006631	174.854451	0.062293
18.28440375	Decane	89.03466668	C10H22	363923.9248	NIST14.L	381456681.4	0.095403736	21908.3488	7.860781
55.7818388	Eicosanoic acid	88.91224896	C20H40O2	351738.374	NIST14.L	381456681.4	0.092209258	20217.8848	7.322933
56.28729901	Sulfurous acid, 2-ethylhexyl isohexyl ester	89.71224605	C14H30O3S	351679.0066	NIST14.L	381456681.4	0.092193694	19720.2375	7.261787
30.98337363	Undecane, 4,7-dimethyl-	93.83413385	C13H28	339780.042	NIST14.L	381456681.4	0.089074345	20538.4104	7.592754
18.79628622	1,4:3,6-Dianhydro-.alpha.-d-glucopyranose	84.66017119	C6H8O4	332544.0808	NIST14.L	381456681.4	0.087177417	2924.2715 6	1.08571
26.94394589	Tetradecane	89.98601759	C14H30	324141.0889	NIST14.L	381456681.4	0.084974547	4409.2732 4	1.644215
62.44545329	Borane, diethyl(decyloxy)-	81.1443389	C14H31BO	320180.1607	NIST14.L	381456681.4	0.083936178	18168.6661	7.152681
41.96744223	Tridecane, 2-methyl-	90.51410409	C14H30	315955.3357	NIST14.L	381456681.4	0.082828628	5932.8921 4	2.397628
67.65337543	1-[1,2,4]Triazol-1-ylethanone	82.51581111	C4H5N3O	314767.1985	NIST14.L	381456681.4	0.082517154	2567.8197	1.057533
22.69842704	Tridecane	91.33438069	C13H28	312355.7725	NIST14.L	381456681.4	0.081884992	3877.0358 5	1.599844

57.80679885	Pentane, 2-isocyano-2,4,4-trimethyl-	81.08329533	C9H17N	311199.4716	NIST14.L	381456681.4	0.081581864	1806.00237	0.780586
51.51778625	11-Hexadecen-1-ol, (Z)-	80.54579031	C16H32O	309704.6291	NIST14.L	381456681.4	0.081189987	21720.7007	9.833324
5.59883192	1,3,5,7-Cyclooctatetraene	83.28945709	C8H8	300709.5317	NIST14.L	381456681.4	0.078831895	13089.813	6.414766
26.6124489	1-Tetradecene	93.88118985	C14H28	286166.7715	NIST14.L	381456681.4	0.075019468	18104.1781	9.064943
3.302902541	Heptane, 4-methylene-	87.58217915	C8H16	285503.4345	NIST14.L	381456681.4	0.074845572	11657.2592	6.317314
39.55886592	1-Undecene, 5-methyl-	87.8230804	C12H24	285268.212	NIST14.L	381456681.4	0.074783908	8765.01074	4.941679
59.50456824	2-Bromotetradecane	87.6507392	C14H29Br	282024.8784	NIST14.L	381456681.4	0.073933658	8535.61166	4.937308
9.529096078	Octane	89.38532963	C8H18	281727.4087	NIST14.L	381456681.4	0.073855675	16298.5166	9.972036
2.635174669	Pyridine	82.95883138	C5H5N	280698.2407	NIST14.L	381456681.4	0.073585876	7641.68344	5.045301
30.67586851	1-Pentadecene	94.9005809	C15H30	280682.0695	NIST14.L	381456681.4	0.073581637	5930.14394	3.94366
4.148076521	Furan, 2-methyl-	87.55766565	C5H6O	278704.4763	NIST14.L	381456681.4	0.073063205	1995.64293	1.40959
63.81725529	Tridecane, 6-methyl-	86.55211389	C14H30	276256.2269	NIST14.L	381456681.4	0.072421389	515.442294	0.365246
7.95997177	Benzene, 1-ethyl-2-methyl-	88.76765573	C9H12	276089.9804	NIST14.L	381456681.4	0.072377807	1241.75114	0.908213
13.42262785	Cyclopropane, octyl-	95.38379893	C11H22	271561.7684	NIST14.L	381456681.4	0.071190723	1082.49887	0.830655
61.66167991	1,4-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	89.68533297	C24H38O4	270713.704	NIST14.L	381456681.4	0.0709684	11515.2411	9.562252
51.50522812	1,15-Pentadecanediol	81.88480629	C15H32O2	270679.3603	NIST14.L	381456681.4	0.070959397	1535.34095	1.361178
4.147277961	1,2,4,5-Tetrazine	85.21311085	C2H2N4	270500.1442	NIST14.L	381456681.4	0.070912415	2799.50391	2.539714
30.99095947	Tetradecane, 4-methyl-	85.40941082	C15H32	270236.1463	NIST14.L	381456681.4	0.070843207	9049.52118	8.229606
13.42224024	1-Undecene	95.36405886	C11H22	269341.7905	NIST14.L	381456681.4	0.070608749	9551.65524	9.051769
30.54933708	Ethanone, 1-(3-hydroxy-4-methoxyphenyl)-	88.27126882	C9H10O3	268168.9777	LIGNOCELLULOSIC2019.L	381456681.4	0.070301293	10325.3481	9.796628
9.187300582	1-Decanol	90.0018239	C10H22O	255570.3412	NIST14.L	381456681.4	0.066998523	9566.55377	9.124004
22.42121556	m-Aminophenylacetylene	84.18036448	C8H7N	254011.9559	NIST14.L	381456681.4	0.066589987	9815.19613	9.620384
21.19315633	1,4-Benzenediol, 2-methoxy-	81.07118925	C7H8O3	247448.4428	NIST14.L	381456681.4	0.064869343	7290.57658	7.424443
30.67902128	1-Dodecene	93.81577608	C12H24	246332.1188	NIST14.L	381456681.4	0.064576695	6649.27557	6.886551
76.23815471	2-Hepten-4-one, 6-methyl-	81.88243432	C8H14O	242812.164	NIST14.L	381456681.4	0.063653929	6707.54813	6.998957
15.68324334	1H-Indene, 1-methyl-	82.91436202	C10H10	242338.3946	NIST14.L	381456681.4	0.063529729	5057.45729	5.489196
59.50754705	Undecane, 3,8-dimethyl-	80.6219317	C13H28	240498.2553	NIST14.L	381456681.4	0.063047331	5818.71702	6.378609
2.914923625	Ethane, 1,1-difluoro-	86.7621437	C2H4F2	231364.8239	NIST14.L	381456681.4	0.060652975	5391.35575	6.154528
48.22086822	Decane, 2,9-dimethyl-	92.64169854	C12H26	231061.7825	NIST14.L	381456681.4	0.060573531	4092.86057	4.674397
2.584272522	Bi-2-cyclohexen-1-yl	87.51590132	C12H18	227673.8677	NIST14.L	381456681.4	0.059685379	4070.63757	0.684992

31.00069476	Undecane, 5,7-dimethyl-	89.34963801	C13H28	221175.564	NIST14.L	381456681.4	0.05798183	4048.41457	0.668645
5.924823106	Nonane	90.46321289	C9H20	220888.6818	NIST14.L	381456681.4	0.05790662 3	4026.19157	0.668947
23.2597775	N-Acetyl-4-hydroxyphenylacetamide	81.13225676	C10H11NO3	219630.8783	NIST14.L	381456681.4	0.05757688 6	4003.96857	0.685526
34.54211238	1-Undecanol	94.13530953	C11H24O	206297.7755	NIST14.L	381456681.4	0.05408157 3	3981.74557	0.66958
13.79928485	Undecane	86.60796986	C11H24	204057.5296	NIST14.L	381456681.4	0.05349428 6	3959.52257	0.660264
15.68493281	5-Hepten-2-one, 7-phenyl-	80.8447115	C13H16O	202306.0475	NIST14.L	381456681.4	0.05303513	3937.29957	0.677855
3.309031756	Cyclopropane, pentyl-	93.44687828	C8H16	195823.1394	NIST14.L	381456681.4	0.05133561 7	3915.07657	0.679884
18.29471897	Dodecane	90.20309659	C12H26	191890.1135	NIST14.L	381456681.4	0.05030456 2	3892.85357	0.711358
22.70078047	Decane, 2,4-dimethyl-	91.3879886	C12H26	186192.0395	NIST14.L	381456681.4	0.04881079 5	3870.63057	0.733221
22.66021588	Naphthalene, 2-methyl-	88.80129021	C11H10	184528.7417	NIST14.L	381456681.4	0.04837475 7	3848.40757	0.766631
9.186254944	1-Decen-3-one	85.18926761	C10H18O	182764.1688	NIST14.L	381456681.4	0.04791216 9	3826.18457	0.763645
66.8563506	Vitamin E	82.24842555	C29H50O2	177369.0931	NIST14.L	381456681.4	0.04649783 4	3803.96157	0.741132
39.56055089	1-Nonanol, 4,8-dimethyl-	88.09526752	C11H24O	175642.6089	NIST14.L	381456681.4	0.04604523 1	3781.73857	0.743326
39.57036045	1-Undecene, 7-methyl-	88.32403363	C12H24	175211.6548	NIST14.L	381456681.4	0.04593225 5	3759.51557	0.764751
72.31000519	Oxalic acid, allyl hexadecyl ester	82.06309601	C21H38O4	174599.253	NIST14.L	381456681.4	0.04577171 2	3737.29257	0.802144
10.26521477	N-Benzoyltyramine	82.14335141	C15H15NO2	172879.8838	NIST14.L	381456681.4	0.04532097 4	3715.06957	1.060542
77.00498792	1H-Tetrazol-5-amine	90.78000545	CH3N5	171687.8555	NIST14.L	381456681.4	0.04500848	3692.84657	1.246061
7.973094444	Benzene, 1-ethyl-4-methyl-	89.50776902	C9H12	169200.7778	NIST14.L	381456681.4	0.04435648 6	3670.62357	1.317645
10.2791761	Benzene, 1,3,5-trimethyl-	81.7045823	C9H12	165433.8537	LIGNOCELLULOSIC 2019a.L	381456681.4	0.04336897 5	3648.40057	1.673158
8.788977826	4-Chloro-1-azabicyclo[2.2.2]octane	81.08437634	C7H12ClN	163442.2129	NIST14.L	381456681.4	0.04284686 1	3626.17757	2.111821
3.462760998	Pentane, 2,2-dimethyl-	86.41152789	C7H16	151461.3878	NIST14.L	381456681.4	0.03970605 2	3603.95457	2.124605
31.36210293	1,1,4,5,6-Pentamethyl-2,3-dihydro-1H-indene	85.47428441	C14H20	145893.674	NIST14.L	381456681.4	0.03824645 9	3581.73157	2.131065
14.34610408	Methane, chlorofluoro-	84.04894092	CH2ClF	144916.1403	NIST14.L	381456681.4	0.03799019 6	3559.50857	2.741585
17.11362863	Naphthalene	88.11614313	C10H8	141576.1521	NIST14.L	381456681.4	0.03711460 8	3537.28557	2.498504
82.62210548	Hexane, 2,2,5-trimethyl-	82.29352052	C9H20	141121.8892	NIST14.L	381456681.4	0.03699552 2	3515.06257	2.490799
65.61655856	.beta.-Tocopherol	85.94490014	C28H48O2	138872.9682	NIST14.L	381456681.4	0.03640596	3492.83957	2.515133
18.70436848	Benzofuran, 4,7-dimethyl-	85.11237295	C10H10O	136724.631	NIST14.L	381456681.4	0.03584276 7	3470.61657	2.538399
13.93936874	Benzofuran, 2-methyl-	90.54410998	C9H8O	130318.7439	NIST14.L	381456681.4	0.03416344 5	3448.39357	2.646122
15.94663083	Naphthalene, 1,2-dihydro-	83.76047638	C10H10	127118.1111	NIST14.L	381456681.4	0.03332439	3426.17057	2.695265
2.907430158	Ethene, 1,2-difluoro-	80.26251249	C2H2F2	124649.0193	NIST14.L	381456681.4	0.03267711	3403.94757	2.730826

8.264872433	2,3-Pentanedione	82.46384805	C5H8O2	120423.9477	LIGNOCELLULOSIC 2019a.L	381456681.4	0.031569495	3381.72457	2.808183
9.137465789	Mesitylene	89.43287684	C9H12	112795.016	NIST14.L	381456681.4	0.029569548	3359.50157	2.978413
67.85718235	Acetic acid, 7,7,10a,12a-tetramethyl-2,5-dioxo-1,2,3,4,4a,4b,5,7,8,9,10,10a,10b,11,12,12a-hexadecahydro-1-azachrysen-8-yl ester	81.85807701	C23H33NO4	110229.0984	NIST14.L	381456681.4	0.028896885	3337.27857	3.027584
39.85368929	Ethanone, 1-(4-hydroxy-3,5-dimethoxyphenyl)-	85.96337002	C10H12O4	109962.9887	NIST14.L	381456681.4	0.028827124	3315.05557	3.014701
8.620513271	Benzene, 1,2,3-trimethyl-	87.47977431	C9H12	105884.4933	NIST14.L	381456681.4	0.027757934	3292.83257	3.109835
3.822364697	Aniline	85.05011101	C6H7N	105522.5195	NIST14.L	381456681.4	0.027663041	3270.60957	3.099442
38.35568285	Valylvaline, N,N'-dimethyl-n-butoxycarbonyl-, isohexyl ester	80.02193488	C23H44N2O5	105396.9627	NIST14.L	381456681.4	0.027630126	3248.38657	3.08205
7.654398945	Benzene, propyl-	93.59566042	C9H12	104850.3879	NIST14.L	381456681.4	0.027486884	3226.16357	3.076921
18.58284475	Decanal	84.12835535	C10H20O	104470.8848	NIST14.L	381456681.4	0.027387352	3203.94057	3.066826
56.11399331	Cyclopentane, 1,1,3-trimethyl-	85.08641294	C8H16	102024.9894	NIST14.L	381456681.4	0.026746153	3181.71757	3.118567
10.86193296	N-Cyanomethyl-N-methylacetamide	84.312863	C5H8N2O	99213.98788	NIST14.L	381456681.4	0.026009241	3159.49457	3.184525
10.86193306	1,2,4-Cyclopentanetrione	86.13871116	C5H4O3	98930.2431	NIST14.L	381456681.4	0.025934857	3137.27157	3.171196
39.85368899	4-Methoxyphenol, TMS derivative	83.87584124	C10H16O2Si	98196.95209	NIST14.L	381456681.4	0.025742622	3115.04857	3.172246
3.767450244	2-Isopropylimidazole	80.96383991	C6H10N2	96554.50408	NIST14.L	381456681.4	0.025312005	3092.82557	3.203191
32.33199656	2-Propanone, 1-(4-hydroxy-3-methoxyphenyl)-	84.59106306	C10H12O3	95836.40059	NIST14.L	381456681.4	0.025123797	3070.60257	3.204004
19.85414448	Phenol, 2-(1-methylethyl)-	83.97303687	C9H12O	92134.76242	NIST14.L	381456681.4	0.024153401	3048.37957	3.30861
13.71527829	1H-Indazole, 4-methyl-	82.85018525	C8H8N2	91222.34319	NIST14.L	381456681.4	0.023914208	3026.15657	3.317341
33.76308966	Naphthalene, 1,4,6-trimethyl-	89.17944826	C13H14	90369.17879	NIST14.L	381456681.4	0.023690548	3003.93357	3.324069
50.69483354	Carbonic acid, prop-1-en-2-yl tetradecyl ester	83.92094917	C18H34O3	87963.9145	NIST14.L	381456681.4	0.023060001	2981.71057	3.389697
35.49813497	9H-Xanthene	80.2644387	C13H10O	87559.11019	NIST14.L	381456681.4	0.022953888	2959.48757	3.379988
6.356499824	Ethanone, 1-(2-furanyl)-	81.69565636	C6H6O2	85261.37741	NIST14.L	381456681.4	0.022351523	2937.26457	3.445012
59.49900248	Cyclobutanone, 2,3,3-trimethyl-	87.11360822	C7H12O	85252.07772	NIST14.L	381456681.4	0.022349085	2915.04157	3.41932
54.30349063	2-Heptadecenal	85.9869471	C17H32O	82720.74121	NIST14.L	381456681.4	0.021685488	2892.81857	3.49709
25.67090464	Biphenyl	85.77047024	C12H10	78860.43037	demo.mslibrary.xml	381456681.4	0.020673496	2870.59557	3.640096
36.31816821	1,3-Dioxolane	86.60285626	C3H6O2	77852.75918	NIST14.L	381456681.4	0.020409332	2848.37257	3.658666
26.9415944	4-Pentenylamine, N,N-dimethyl-	80.31716538	C7H15N	76842.0405	NIST14.L	381456681.4	0.020144369	2826.14957	3.677869

33.63071158	O-(2,6-Dimethylpyrid-3-yl)-N-phenylbenzimidate	81.82857652	C20H18N2O	76201.42508	NIST14.L	381456681.4	0.01997643	2803.92657	3.679625
72.29803414	3-Hexene, 2,2-dimethyl-, (Z)-	82.53385097	C8H16	73855.8887	NIST14.L	381456681.4	0.01936154	2781.70357	3.766394
13.71486963	1H-Pyrrolo[2,3-b]pyridine, 2-methyl-	83.69479819	C8H8N2	71487.68573	NIST14.L	381456681.4	0.01874070 9	2759.48057	3.860078
55.16157217	(E)-4-Oxohex-2-enal	88.68180804	C6H8O2	67845.22224	NIST14.L	381456681.4	0.01778582 6	2737.25757	4.034562
44.78105325	Oxalic acid, allyl pentadecyl ester	87.1752568	C20H36O4	67422.9204	NIST14.L	381456681.4	0.01767511 8	2715.03457	4.026872
30.99966329	Naphtho[2,1-b]furan	81.4983558	C12H8O	67257.10156	NIST14.L	381456681.4	0.01763164 9	2692.81157	4.003758
4.832073964	Acetic anhydride	80.24333415	C4H6O3	66795.08084	NIST14.L	381456681.4	0.01751052 8	2670.58857	3.998182
11.73532691	Benzene, (2-methylpropyl)-	89.58540051	C10H14	66356.69069	NIST14.L	381456681.4	0.01739560 3	2648.36557	3.991106
14.06945692	Nonanal	80.27353486	C9H18O	65864.10468	NIST14.L	381456681.4	0.01726647	2626.14257	3.987214
3.850529967	Pyridine, 2-methyl-	89.35903274	C6H7N	63986.09146	NIST14.L	381456681.4	0.01677414 4	2603.91957	4.069509
14.06945706	Acetic acid, trichloro-, heptyl ester	80.15938271	C9H15Cl3O2	63464.98965	NIST14.L	381456681.4	0.01663753 5	2581.69657	4.067907
13.74404085	Thiodiglycolic anhydride	88.66095478	C4H4O3S	62688.59061	NIST14.L	381456681.4	0.016434	2559.47357	4.082838
18.91198422	Butane, 2,2-dimethyl-	80.21441207	C6H14	62468.6843	NIST14.L	381456681.4	0.01637635 1	2537.25057	4.061636
18.55004101	3-Undecene, 9-methyl-, (E)-	80.33454572	C12H24	61418.76977	NIST14.L	381456681.4	0.01610111 3	2515.02757	4.094884
37.69505822	1-Nonanol	84.89458663	C9H20O	60648.83128	NIST14.L	381456681.4	0.01589927 1	2492.80457	4.110227
37.69625218	Cyclooctane, methyl-	86.45086681	C9H18	58675.21841	NIST14.L	381456681.4	0.01538188 2	2470.58157	4.210605
59.58937755	Acenaphtho[1,2-b]quinoxaline, 9-methoxy-	81.31708379	C19H12N2O	57920.07264	NIST14.L	381456681.4	0.01518391 9	2448.35857	4.227133
10.28539008	.beta.-Methoxy-.alpha.-phenylphenethyl alcohol	82.86052827	C15H16O2	57407.62245	NIST14.L	381456681.4	0.01504957 8	2426.13557	4.226156
18.5504474	4-Undecene, 5-methyl-	81.22461173	C12H24	56370.77354	NIST14.L	381456681.4	0.01477776 5	2403.91257	4.264466
10.46920883	Benzeneethanol, .beta.-ethenyl-	88.75720824	C10H12O	56313.2792	NIST14.L	381456681.4	0.01476269 3	2381.68957	4.229357
2.240839195	Propanediamide, 2-amino-	90.06766422	C3H7N3O2	56146.43188	NIST14.L	381456681.4	0.01471895 4	2359.46657	4.202345
52.75235047	Cyclooctane, 1,4-dimethyl-, trans-	85.22652127	C10H20	56134.86559	NIST14.L	381456681.4	0.01471592 1	2337.24357	4.163622
26.34872829	Benzene, 1,3,5-trimethyl-2-(1,2-propadienyl)-	84.17447037	C12H14	54779.20947	NIST14.L	381456681.4	0.01436053 2	2315.02057	4.226093
7.023803154	Pyridine, 2,3-dimethyl-	81.07220036	C7H9N	54085.72255	NIST14.L	381456681.4	0.01417873 3	2292.79757	4.239192
11.33599295	2,4,6-Cycloheptatrien-1-one, 4-methyl-	81.89533247	C8H8O	53283.42415	NIST14.L	381456681.4	0.01396840 8	2270.57457	4.261315
7.237581413	Octane, 3-methyl-	82.55613547	C9H20	51122.26612	NIST14.L	381456681.4	0.01340185 4	2248.35157	4.397989
9.149750624	1,3-Dioxane, 5-fluoro-2-methyl-, cis-	80.22110064	C5H9FO2	50935.64433	NIST14.L	381456681.4	0.01335293	2226.12857	4.370473
20.79632912	2-Ethyl-1-H-indene	80.96021032	C11H12	50739.8279	NIST14.L	381456681.4	0.01330159 6	2203.90557	4.343542
50.69064103	Carbonic acid, decyl prop-1-en-2-yl ester	81.36431378	C14H26O3	49995.99831	NIST14.L	381456681.4	0.01310659 9	2181.68257	4.363714
51.3735361	Cyclohexane, ethenyl-	84.53251205	C8H14	48866.46989	NIST14.L	381456681.4	0.01281049	2159.45957	4.419103

48.36084059	1,7-Dimethyl-4-(1-methylethyl)cyclodecane	82.08732774	C15H30	46850.09824	NIST14.L	381456681.4	0.012281892	2137.23657	4.561861
10.76115011	Diglycolic acid, di(3-phenylpropyl) ester	86.11201807	C22H26O5	45128.39806	NIST14.L	381456681.4	0.011830543	2115.01357	4.686658
10.48746321	3-Phenyl-1-propanol, acetate	81.155676	C11H14O2	42420.20646	NIST14.L	381456681.4	0.011120583	2092.79057	4.933476
29.45954763	1-Phenyl-5-methylheptane	80.01532439	C14H22	41816.70038	NIST14.L	381456681.4	0.010962372	2070.56757	4.951533
39.96009104	5-Hexen-3-one	86.78875675	C6H10O	37790.75918	NIST14.L	381456681.4	0.009906896	2048.34457	5.420226
18.91431588	Hexane, 2,2,5,5-tetramethyl-	82.07767578	C10H22	36144.63845	NIST14.L	381456681.4	0.009475424	2026.12157	5.605594
8.2096499	1-Hexanone, 5-methyl-1-phenyl-	80.70318075	C13H18O	33948.07839	NIST14.L	381456681.4	0.008899589	2003.89857	5.902834
3.466095971	3-Pentanone, 2,4-dimethyl-	89.98359703	C7H14O	33473.61516	NIST14.L	381456681.4	0.008775207	1981.67557	5.920112
58.70200227	Phthalic acid, bis(2-pentyl) ester	80.39932478	C18H26O4	32389.79693	NIST14.L	381456681.4	0.008491081	1959.45257	6.049598
14.55503096	1,3-Benzodioxol-2-one	88.42660937	C7H4O3	27770.18298	NIST14.L	381456681.4	0.007280036	1937.22957	6.975934
5.919899886	Sydnone, 3-(1-methylethyl)-	81.19545001	C5H8N2O2	26238.82084	NIST14.L	381456681.4	0.006878585	1915.00657	7.298371
54.69877718	Butanimidamide	80.43827969	C4H10N2	26092.75778	NIST14.L	381456681.4	0.006840294	1892.78357	7.254057
41.25991051	Thiophene-2-carboxylic acid, 2,2,2-trifluoroethyl ester	87.9113504	C7H5F3O2S	25199.0004	NIST14.L	381456681.4	0.006605993	1870.56057	7.423154
7.504051347	Oxazole, 4,5-dihydro-2-methyl-	88.27832266	C4H7NO	24128.40564	NIST14.L	381456681.4	0.006325333	1848.33757	7.660422
15.23246214	2-Azetidinone, 1-isopropyl-3,3-dimethyl-4-phenyl-	83.58849886	C14H19NO	16911.15393	NIST14.L	381456681.4	0.004433309	1171.11457	6.925101
25.95020608	1,2,3-Trimethyldiaziridine	86.84306402	C4H10N2	15194.94952	NIST14.L	381456681.4	0.003983401	448.891573	2.954216
20.71874044	Ethaneperoxoic acid, 1-cyano-1-phenylbutyl ester	87.03542359	C13H15NO3	14887.73579	NIST14.L	381456681.4	0.003902864	426.668573	2.865906
7.849912604	N-Ethylformamide	84.58038903	C3H7NO	14396.74691	NIST14.L	381456681.4	0.003774145	404.445573	2.809284
38.64441702	3-Nitro-1-phenyl-1-butanone	81.71644059	C10H11NO3	13184.5727	NIST14.L	381456681.4	0.003456375	382.222573	2.899014
50.97458946	3H-Pyrazol-3-one, 2,4-dihydro-4,5-dimethyl-	82.26276203	C5H8N2O	9703.637176	NIST14.L	381456681.4	0.002543837	359.999573	3.709945

Table S29. *Py-GC/MS data for peat.*

Component RT (mins)	Compound Name	Match Factor (%)	Molecular Formula	Component Area	Library File	Total area	Compound %	Stdva	CV %
48.20887761	n-Hexadecanoic acid	85.83462455	C16H32O2	46211177.1	NIST14.L	1056874332	4.372438208	130976.5539	0.283430465
51.8706594	9,12-Octadecadienoic acid (Z,Z)-	80.86781863	C18H32O2	26326250.27	NIST14.L	1056874332	2.4909537	90556.40512	0.343977605
58.38063518	5-Pregnen-3.beta.-ol-20-one, formate	85.53772227	C22H32O3	25762022.12	NIST14.L	1056874332	2.437567206	41370.32618	0.160586487
51.87029704	2-Methylbicyclo[3.2.1]octane	84.04203204	C9H16	22920473.78	NIST14.L	1056874332	2.168703798	29512.79974	0.128761735
43.69972103	Caffeine	94.39784317	C8H10N4O2	11205760.9	demo.mslibrary.xml	1056874332	1.060273733	30161.09112	0.269157012
62.86076828	Squalene	98.32259329	C30H50	10445193.33	NIST14.L	1056874332	0.988309887	28814.40382	0.275862781

52.38854722	Octadecanoic acid	94.42345466	C18H36O2	9499706.327	NIST14.L	1056874332	0.898849186	8900.500154	0.093692372
55.97728678	Eicosanoic acid	93.39846252	C20H40O2	6058863.584	NIST14.L	1056874332	0.573281364	12397.45318	0.204616807
74.17690141	Octacosanol	82.18058604	C28H58O	4599021.023	NIST14.L	1056874332	0.435153063	14518.85993	0.315694576
4.853969719	2-Furanmethanol	96.69541408	C5H6O2	4565141.686	LIGNOCELLULOSIC 2019.L	1056874332	0.431947446	3816.325865	0.083597096
75.12936559	1-Dodecanol, 2-hexyl-	87.54524498	C18H38O	4472421.633	NIST14.L	1056874332	0.423174402	2439.203844	0.054538772
31.02102171	Pentadecane	98.90223543	C15H32	4047553.392	NIST14.L	1056874332	0.382973952	14452.63614	0.35707092
2.910889397	Toluene	96.40378815	C7H8	3267641.352	NIST14.L	1056874332	0.309179744	11468.48706	0.350971414
9.3170024	Phenol	97.30140941	C6H6O	2851231.135	NIST14.L	1056874332	0.269779558	4150.666191	0.145574525
13.89106906	Formic acid, 2-propenyl ester	86.38053855	C4H6O2	2693078.956	NIST14.L	1056874332	0.254815438	2562.646682	0.09515676
7.049657527	1,2-Cyclopentanedione	95.75580352	C5H6O2	2660110.068	NIST14.L	1056874332	0.251695967	8883.807376	0.333963902
75.11679393	Carbonic acid, eicosyl vinyl ester	81.56197365	C23H44O3	2549814.548	NIST14.L	1056874332	0.241259956	8743.024596	0.342888647
19.55635947	Catechol	87.07766287	C6H6O2	2297871.061	NIST14.L	1056874332	0.217421409	8893.400759	0.387027841
13.81521873	Diazene, bis(1,1-dimethylethyl)-	86.23701187	C8H18N2	2295739.891	NIST14.L	1056874332	0.21721976	10881.47706	0.473985625
10.94490416	1,2-Cyclopentanedione, 3-methyl-	96.86539523	C6H8O2	2246421.755	NIST14.L	1056874332	0.212553346	10156.02876	0.452098042
9.314195394	3-Methylpyridazine	94.57823875	C5H6N2	2000339.76	NIST14.L	1056874332	0.189269405	12545.80326	0.627183617
7.019315026	2-Cyclopenten-1-one, 2-hydroxy-	90.2073132	C5H6O2	1964610.205	NIST14.L	1056874332	0.185888724	13302.0352	0.677082668
66.18992458	Stigmasta-3,5-diene	93.88691329	C29H48	1963715.713	NIST14.L	1056874332	0.185804088	16016.13801	0.8156037
4.186436333	3,5-Dimethylpyrazole	80.37549085	C5H8N2	1879001.492	NIST14.L	1056874332	0.177788545	16127.29341	0.858290612
30.38751447	n-Butyl nitrite	82.1775379	C4H9NO2	1802714.151	NIST14.L	1056874332	0.170570341	13587.13412	0.753704303
13.82356898	Trimethylaluminum	87.40514428	C3H9Al	1772266.029	NIST14.L	1056874332	0.167689381	12694.53903	0.716288572
30.86777357	N-Carbethoxy-N-methoxyamine	93.46281302	C4H9NO3	1749254.437	NIST14.L	1056874332	0.165512056	12581.25255	0.719235137
2.6519934	Pyridine	95.2258505	C5H5N	1713996.52	NIST14.L	1056874332	0.162176	12253.61651	0.7149149
30.41577582	Butanoic acid	89.0314709	C4H8O2	1641456.369	NIST14.L	1056874332	0.155312351	11008.64814	0.670663464
37.85972791	E-2-Octadecadecen-1-ol	84.70194777	C18H36O	1425815.576	NIST14.L	1056874332	0.134908715	9994.209165	0.700946836
52.65072479	Hexadecanamide	86.88218236	C16H33NO	1374755.99	NIST14.L	1056874332	0.130077527	8552.385481	0.622102071
10.9017843	2-Cyclopenten-1-one, 2-hydroxy-3-methyl-	94.99434632	C6H8O2	1307097.399	NIST14.L	1056874332	0.123675763	4362.266279	0.333736895
73.4368536	1-Decanol, 2-hexyl-	84.0231861	C16H34O	1304915.225	NIST14.L	1056874332	0.123469289	4852.967876	0.371899092
6.546421364	2(5H)-Furanone	95.04268367	C4H4O2	1279458.486	NIST14.L	1056874332	0.121060607	2731.147054	0.21346117
4.860903975	3-Butyn-1-ol	91.42763389	C4H6O	1274790.113	NIST14.L	1056874332	0.120618892	3703.506338	0.29051891
53.54378496	Isopropyl linoleate	87.63622469	C21H38O2	1221070.709	NIST14.L	1056874332	0.115536036	1147.675067	0.093989239

45.41152181	Hexadecanenitrile	85.74345066	C16H31N	1208504.249	NIST14.L	1056874332	0.114347015	7377.85346	0.610494623
45.41138737	Tetradecanenitrile	85.90083774	C14H27N	1197287.111	NIST14.L	1056874332	0.113285665	6179.109514	0.516092544
38.49856753	Heptadecane	97.6515712	C17H36	1150536.054	NIST14.L	1056874332	0.108862144	174.8544506	0.015197651
53.40033944	Linoelaidic acid	87.60503554	C18H32O2	1136861.118	NIST14.L	1056874332	0.10756824	21908.34876	1.927091042
6.935707032	1H-Tetrazole	93.48824074	CH2N4	1089008.348	NIST14.L	1056874332	0.103040477	20217.88478	1.856540846
37.34268022	6,9-Heptadecadiene	92.21846063	C17H32	1061532.508	NIST14.L	1056874332	0.10044075	19720.23748	1.857713949
59.12549399	Docosanoic acid	88.70139197	C22H44O2	1056076.888	NIST14.L	1056874332	0.099924547	20538.41038	1.944783623
79.49068381	Nitric acid, nonyl ester	81.00295728	C9H19NO3	1032763.579	NIST14.L	1056874332	0.097718674	2924.271562	0.283150144
6.929187052	Methoxyacetonitrile	92.35170155	C3H5NO	1031088.75	NIST14.L	1056874332	0.097560204	4409.273241	0.427632756
51.78494111	Ethanone, 1-(1H-pyrrol-2-yl)-	85.391026	C6H7NO	1024408.025	NIST14.L	1056874332	0.096928083	18168.66614	1.7735771
23.27788166	4-Hydroxy-2-methylacetophenone	88.95560161	C9H10O2	1007692.909	NIST14.L	1056874332	0.095346521	5932.892138	0.588759937
3.32499077	l-Alanine, N-methoxycarbonyl-, butyl ester	80.32973347	C9H17NO4	1004076.568	NIST14.L	1056874332	0.095004348	2567.819698	0.255739431
68.99066251	.gamma.-Sitosterol	83.67384016	C29H50O	976825.7471	NIST14.L	1056874332	0.092425913	3877.03585	0.39690148
2.801237355	Methanamine, N,N-difluoro-	91.90306041	CH3F2N	942187.0757	NIST14.L	1056874332	0.089148449	1806.002371	0.19168193
53.54078491	1,8,11-Heptadecatriene, (Z,Z)-	81.92319939	C17H30	936669.4348	NIST14.L	1056874332	0.088626377	21720.70071	2.318929166
32.06606398	.beta.-D-Glucopyranose, 1,6-anhydro-	81.37983915	C6H10O5	928718.9206	NIST14.L	1056874332	0.087874111	13089.81301	1.409448297
30.86775128	Pentanoic acid	85.19485408	C5H10O2	888668.5946	NIST14.L	1056874332	0.084084604	18104.17809	2.037224923
26.62138888	1-Tetradecene	95.30087098	C14H28	868168.1155	NIST14.L	1056874332	0.082144877	11657.25923	1.342742151
2.191294289	Furan, 2,5-dimethyl-	87.09220116	C6H8O	864842.2509	LIGNOCELLULOSIC 2019.L	1056874332	0.081830188	8765.010744	1.013480867
13.34711283	Ethanone, 1-(2-methyl-1-cyclopenten-1-yl)-	81.9902009	C8H12O	844795.8979	NIST14.L	1056874332	0.079933429	8535.611663	1.010375605
22.45718336	Indole	92.18547347	C8H7N	805862.6859	NIST14.L	1056874332	0.076249622	16298.51656	2.022493018
22.45718413	m-Aminophenylacetylene	92.00609878	C8H7N	801240.3012	NIST14.L	1056874332	0.075812259	7641.683439	0.953731786
13.34415195	Phenol, 2-methoxy-	89.42063234	C7H8O2	774632.5884	NIST14.L	1056874332	0.073294673	5930.143943	0.765542792
37.33019512	cis-7-Dodecen-1-ol	89.54522418	C12H24O	764953.602	NIST14.L	1056874332	0.072378861	1995.642933	0.26088418
26.95503708	Tetradecane	96.88544017	C14H30	761456.1457	NIST14.L	1056874332	0.072047936	515.4422938	0.067691659
37.61612235	8-Heptadecene	91.33408997	C17H34	722149.2299	NIST14.L	1056874332	0.06832877	1241.751143	0.171952152
4.207675464	Furfural	97.20605088	C5H4O2	711265.2635	NIST14.L	1056874332	0.067298944	1082.498874	0.152193412
68.28555407	Stigmasterol	85.5342604	C29H48O	703708.0703	NIST14.L	1056874332	0.066583893	11515.24107	1.636366209
26.61760836	1-Tetradecanol	94.5246448	C14H30O	676306.0731	NIST14.L	1056874332	0.063991153	1535.340953	0.227018655
54.19673247	Octadecanoic acid, 2-propenyl ester	82.07766687	C21H40O2	642913.1587	NIST14.L	1056874332	0.060831561	2799.503906	0.435440443

18.05195267	1,4:3,6-Dianhydro-.alpha.-d-glucopyranose	86.38647891	C6H8O4	637574.518	NIST14.L	1056874332	0.060326427	9049.52118	1.419366823
14.85633257	2-Cyclopenten-1-one, 3-ethyl-2-hydroxy-	88.12326992	C7H10O2	629685.1997	NIST14.L	1056874332	0.05957995	9551.655235	1.516893718
5.605464566	Styrene	95.9457212	C8H8	618607.9902	NIST14.L	1056874332	0.05853184	10325.34814	1.669126216
22.71036771	Tridecane	92.80953382	C13H28	616599.395	NIST14.L	1056874332	0.058341789	9566.553772	1.551502296
65.43712364	Stigmasta-5,22-dien-3-ol, acetate, (3.beta.,22Z)-	86.20441	C31H50O2	612231.6505	NIST14.L	1056874332	0.057928519	9815.196132	1.603183391
4.394494633	1H-Pyrrole, 1-methyl-	89.48024134	C5H7N	607790.5425	NIST14.L	1056874332	0.057508308	7290.576578	1.199521228
16.20788953	Benzene, pentyl-	91.72434947	C11H16	596918.426	NIST14.L	1056874332	0.056479603	6649.27557	1.11393371
13.43870733	Cyclopropane, octyl-	90.66770831	C11H22	580972.193	NIST14.L	1056874332	0.054970792	6707.548127	1.154538583
13.438268	1-Nonanol	90.86450292	C9H20O	576881.7762	NIST14.L	1056874332	0.054583763	5057.457293	0.876688691
3.482586032	Carbonocyanidic acid, ethyl ester	80.64885588	C4H5NO2	573408.0564	NIST14.L	1056874332	0.054255084	5818.717023	1.014760249
4.169309337	2-Cyclopenten-1-one	98.36304158	C5H6O	572632.1637	NIST14.L	1056874332	0.05418167	3848.407573	0.672055783
23.27817765	Ethanone, 1-(2-hydroxy-5-methylphenyl)-	91.10191044	C9H10O2	567199.3975	NIST14.L	1056874332	0.053667629	3826.184573	0.674574866
65.62332789	.beta.-Tocopherol	91.82940846	C28H48O2	565390.0911	NIST14.L	1056874332	0.053496435	3803.961573	0.672803014
30.68613129	1-Pentadecene	94.69928643	C15H30	562332.5139	NIST14.L	1056874332	0.053207131	3781.738573	0.672509321
55.41673664	Pyrrolo[1,2-a]pyrazine-1,4-dione, hexahydro-3-(phenylmethyl)-	80.98579177	C14H16N2O2	550256.853	NIST14.L	1056874332	0.052064549	3759.515573	0.683229214
3.303265436	Cyclopropane, pentyl-	85.95084012	C8H16	511609.9227	NIST14.L	1056874332	0.048407829	3737.292573	0.730496499
12.26514786	Phenol, 2-methyl-	89.42458935	C7H8O	505218.7496	NIST14.L	1056874332	0.047803105	3715.069573	0.735338816
4.806574006	Ethylbenzene	93.35870788	C8H10	503395.3783	NIST14.L	1056874332	0.047630558	4070.637573	0.808636263
26.95403684	Undecane, 4,7-dimethyl-	95.94912402	C13H28	495154.7961	NIST14.L	1056874332	0.046850868	4048.414573	0.817605849
17.92083868	1-Dodecene	96.11250097	C12H24	485996.4465	NIST14.L	1056874332	0.045984317	4026.191573	0.828440537
9.533861841	Decane	90.35336057	C10H22	480901.3484	NIST14.L	1056874332	0.045502226	4003.968573	0.832596662
3.299489833	Cyclobutane, 1,2-diethyl-, trans-	93.69525892	C8H16	471983.4001	NIST14.L	1056874332	0.044658422	3981.745573	0.843619833
40.4931726	5-Heptadecene, 1-bromo-	82.87890031	C17H33Br	467249.343	NIST14.L	1056874332	0.044210492	3048.379573	0.652409601
26.2735501	1H-Indole, 4-methyl-	93.88217595	C9H9N	457871.6369	NIST14.L	1056874332	0.043323186	3026.156573	0.660918111
5.608048932	1,3,5,7-Cyclooctatetraene	92.40194938	C8H8	454634.6157	NIST14.L	1056874332	0.043016904	3003.933573	0.66073578
4.41421271	1H-Pyrrole, 2-methyl-	88.46962259	C5H7N	453879.5974	NIST14.L	1056874332	0.042945465	2981.710573	0.656938666
30.67880144	1-Tridecene	94.64455408	C13H26	441993.4491	NIST14.L	1056874332	0.041820814	2959.487573	0.669577248
5.017152959	Benzene, 1,3-dimethyl-	86.00985368	C8H10	440657.2999	NIST14.L	1056874332	0.041694389	2937.264573	0.666564374
6.336238547	Ethanone, 1-(2-furanyl)-	97.60071101	C6H6O2	439601.5201	NIST14.L	1056874332	0.041594493	2915.041573	0.663109985
52.73913056	2-Cyclopenten-1-one, 3-methyl-	87.74016444	C6H8O	437410.3232	NIST14.L	1056874332	0.041387165	2892.818573	0.661351235

3.30631386	Cyclobutane, 1,2-diethyl-, cis-	90.29001018	C8H16	431708.7294	NIST14.L	1056874332	0.040847688	2870.595573	0.664938042
4.920747845	Pyridine, 3-methyl-	82.85721361	C6H7N	417645.6274	NIST14.L	1056874332	0.039517057	2848.372573	0.682007038
67.87403116	Campesterol	80.62159161	C28H48O	405832.8771	NIST14.L	1056874332	0.03839935	2826.149573	0.696382608
34.54976448	1-Dodecanol	94.91292437	C12H26O	400148.4291	NIST14.L	1056874332	0.037861496	2803.926573	0.700721625
46.25798612	Hexadecanoic acid, methyl ester	87.14109511	C17H34O2	393850.8293	NIST14.L	1056874332	0.037265625	2781.703573	0.706283538
11.74501439	Benzene, n-butyl-	89.78036016	C10H14	392714.4709	NIST14.L	1056874332	0.037158105	2759.480573	0.702668421
12.2641817	p-Cresol	90.77254863	C7H8O	392468.5648	NIST14.L	1056874332	0.037134837	2737.257573	0.697446323
34.54433041	3-Hexadecene, (Z)-	95.12316518	C16H32	392460.1151	NIST14.L	1056874332	0.037134038	2715.034573	0.691798853
18.29890737	Dodecane	93.3348761	C12H26	390163.9735	NIST14.L	1056874332	0.03691678	2270.574573	0.581953929
22.3506024	Cyclopropane, nonyl-	95.82222596	C12H24	381630.713	NIST14.L	1056874332	0.036109375	2248.351573	0.589143247
8.172025802	2,4-Dimethylfuran	86.26793818	C6H8O	373279.55	NIST14.L	1056874332	0.035319199	2226.128573	0.596370354
4.169313803	Furan, 3-methyl-	85.64136943	C5H6O	370082.6449	LIGNOCELLULOSIC 2019.L	1056874332	0.035016712	2203.905573	0.595517137
32.23211028	Isoxazolidine	88.82853482	C3H7NO	347046.6472	NIST14.L	1056874332	0.032837078	2181.682573	0.628642458
26.26590808	1H-Indole, 6-methyl-	93.41944426	C9H9N	334431.8697	NIST14.L	1056874332	0.031643485	2159.459573	0.645709865
51.90747135	4-Cyclopentene-1,3-dione	80.05097484	C5H4O2	334249.1106	NIST14.L	1056874332	0.031626192	2137.236573	0.639414289
2.324047782	Propanediamide, 2-amino-	87.6748617	C3H7N3O2	332181.4112	NIST14.L	1056874332	0.03143055	2115.013573	0.636704374
5.019056039	2,4-Pentanedione, ion(1-), lithium	80.63976014	C5H7LiO2	330375.1526	NIST14.L	1056874332	0.031259644	2092.790573	0.633458829
16.37776327	Phenol, 3,4-dimethyl-	85.72698932	C8H10O	326122.8067	NIST14.L	1056874332	0.030857293	2070.567573	0.634904254
34.83400383	Hexadecane	91.27440584	C16H34	323620.7864	NIST14.L	1056874332	0.030620555	2048.344573	0.632945923
26.27455173	1H-Indole, 7-methyl-	92.99170941	C9H9N	320874.2802	NIST14.L	1056874332	0.030360684	2026.121573	0.631437824
6.129080569	2-Cyclopenten-1-one, 2-methyl-	88.18035328	C6H8O	317596.1881	NIST14.L	1056874332	0.030050516	2003.898573	0.630958005
54.55012649	2-Bromotetradecane	86.19282513	C14H29Br	312664.9591	NIST14.L	1056874332	0.02958393	1981.675573	0.633801619
17.30208338	Phenol, 4-ethyl-	81.69760202	C8H10O	301138.7687	NIST14.L	1056874332	0.028493337	1959.452573	0.650680941
63.81650126	Sulfurous acid, 2-ethylhexyl nonyl ester	81.80422547	C17H36O3S	297608.1592	NIST14.L	1056874332	0.028159276	1892.783573	0.635998549
20.75556463	Benzene, hexyl-	84.61567653	C12H18	296601.8068	NIST14.L	1056874332	0.028064056	1870.560573	0.630663917
13.34689645	Mequinol	90.02999868	C7H8O2	279381.3955	NIST14.L	1056874332	0.026434685	1848.337573	0.661582197
22.35168421	1-Decanol	95.7264715	C10H22O	270498.5121	NIST14.L	1056874332	0.025594198	1171.114573	0.432946771
6.420893675	Butyrolactone	92.29426041	C4H6O2	267327.9678	NIST14.L	1056874332	0.025294206	448.8915733	0.167917924
63.81726993	Nonadecane	87.12489114	C19H40	263675.2774	NIST14.L	1056874332	0.024948593	426.6685733	0.161815919
4.415193761	Pyrazine	84.64871886	C4H4N2	261933.0445	NIST14.L	1056874332	0.024783745	3981.745573	1.520138699

15.6919788	Naphthalene, 1,2-dihydro-	83.04867473	C10H10	259389.6214	NIST14.L	1056874332	0.02454309	3959.522573	1.52647687
18.03183073	Acetic acid, 2-fluoroethyl ester	87.02567937	C4H7FO2	258287.295	NIST14.L	1056874332	0.02443879	3937.299573	1.524387629
9.188128957	1-Decene	94.30161764	C10H20	257379.0497	NIST14.L	1056874332	0.02435285	3915.076573	1.521132578
63.81618053	Dodecane, 2,6,11-trimethyl-	85.76509535	C15H32	252092.9802	NIST14.L	1056874332	0.02385269	3892.853573	1.544213397
6.916402034	Vinyl crotonate	84.89079042	C6H8O2	250164.917	NIST14.L	1056874332	0.02367026	3870.630573	1.54723157
3.465445066	Octane	90.09464558	C8H18	248226.7651	NIST14.L	1056874332	0.02348687	3848.407573	1.550359636
30.39193127	1H-Tetrazole, 1,5-dimethyl-	82.05404931	C3H6N4	247582.9533	NIST14.L	1056874332	0.02342596	3826.184573	1.545415192
18.86014116	2-Acetyl-2-methyltetrahydrofuran	85.56518542	C7H12O2	245932.5444	NIST14.L	1056874332	0.0232698	3803.961573	1.546749977
20.05228707	2,3-Anhydro-d-mannosan	82.1196919	C6H8O4	242557.3585	NIST14.L	1056874332	0.02295044	3781.738573	1.559111048
21.06535666	Benzene, (1,3-dimethylbutyl)-	84.87593269	C12H18	242122.2149	NIST14.L	1056874332	0.02290972	3270.609573	1.350809373
10.58007761	Limonene	88.21872813	C10H16	241131.5374	NIST14.L	1056874332	0.02281553	3248.386573	1.347142978
6.423887097	Acetaldehyde, dimethylhydrazone	82.43757866	C4H10N2	237845.0543	NIST14.L	1056874332	0.02250457	3226.163573	1.356413983
18.85987847	3H-1,2,4-Triazol-3-one, 1,2-dihydro-	87.12562079	C2H3N3O	235971.2444	NIST14.L	1056874332	0.02232727	3203.940573	1.357767376
3.584078325	4-Octene, (E)-	80.64392242	C8H16	235503.0242	NIST14.L	1056874332	0.02228297	3181.717573	1.351030452
3.842784512	Pyridine, 2-methyl-	85.29518594	C6H7N	234414.2486	NIST14.L	1056874332	0.02217995	3159.494573	1.34782531
9.188910978	Cyclopropane, 1-hexyl-2-methyl-	92.15951646	C10H20	230293.1235	NIST14.L	1056874332	0.02179002	3137.271573	1.362294942
56.72077935	Linoleic acid ethyl ester	82.42811832	C20H36O2	230080.2525	NIST14.L	1056874332	0.02176978	3115.048573	1.353896538
6.940678482	1H-Pyrrole, 2,5-dimethyl-	85.80214948	C6H9N	225987.5033	NIST14.L	1056874332	0.02138262	3092.825573	1.368582567
5.934253551	Nonane	82.96746159	C9H20	223689.8442	NIST14.L	1056874332	0.02116522	3070.602573	1.372705401
7.96974019	1-Hexanone, 5-methyl-1-phenyl-	80.57864065	C13H18O	221827.7508	NIST14.L	1056874332	0.02098903	2559.473573	1.153811263
4.160574736	1-Propene, 3-azido-	86.34663921	C3H5N3	217961.3324	NIST14.L	1056874332	0.02062322	2537.250573	1.164082888
62.43873621	Oxalic acid, allyl decyl ester	85.20124815	C15H26O4	213503.4501	NIST14.L	1056874332	0.02020104	2515.027573	1.177979828
15.64101379	Benzene, 1-methyl-4-(1-propynyl)-	81.90457634	C10H10	212880.3339	NIST14.L	1056874332	0.02014245	2492.804573	1.170988662
5.188443703	2-Propanone, 1-(acetyloxy)-	91.07276413	C5H8O3	212837.6097	NIST14.L	1056874332	0.02013840	2470.581573	1.160782428
25.20993515	Benzene, heptyl-	84.61473202	C13H20	207036.2523	NIST14.L	1056874332	0.01958948	2448.358573	1.182574813
10.5774588	D-Limonene	86.45163667	C10H16	205627.2453	NIST14.L	1056874332	0.01945616	2426.135573	1.179870678
11.12892338	Benzene, 1-propynyl-	82.10796151	C9H8	203983.1133	NIST14.L	1056874332	0.01930060	2403.912573	1.178486069
66.43531637	3-Ethyl-3-methylheptane	84.19512976	C10H22	194753.4581	NIST14.L	1056874332	0.01842730	2381.689573	1.222925434
16.61940171	Benzene, (1-methylbutyl)-	92.17862508	C11H16	194363.311	NIST14.L	1056874332	0.01839039	2359.466573	1.213946481
21.59611199	1H-Inden-1-one, 2,3-dihydro-	91.21936557	C9H8O	189206.5234	NIST14.L	1056874332	0.01790246	2337.243573	1.235286993
18.31791691	Heptanediamide, N,N'-di-benzoyloxy-	80.88133881	C21H22N2O6	187167.0796	NIST14.L	1056874332	0.01770949	2315.020573	1.236873802

3.465727609	Pentane, 2,2-dimethyl-	83.93289317	C7H16	186602.3587	NIST14.L	1056874332	0.017656059	2292.797573	1.228707713
54.54214032	Sulfurous acid, 2-ethylhexyl hexyl ester	81.94322193	C14H30O3S	184143.246	NIST14.L	1056874332	0.017423381	2270.574573	1.233047979
3.583747667	1,2-Cyclohexanedione	89.30687093	C6H8O2	183588.7005	NIST14.L	1056874332	0.017370911	2248.351573	1.224667732
14.07563816	Cyclopentane, hexyl-	81.68188024	C11H22	182248.3066	NIST14.L	1056874332	0.017244085	2226.128573	1.221481075
8.287324307	2,3-Pentanedione	86.65120537	C5H8O2	181051.0479	NIST14.L	1056874332	0.017130802	2203.905573	1.217284074
61.00345987	Decane, 3,8-dimethyl-	84.24353237	C12H26	180301.0025	NIST14.L	1056874332	0.017059834	2181.682573	1.210022431
62.4388907	Octane, 2,4,6-trimethyl-	85.80879581	C11H24	180145.9328	NIST14.L	1056874332	0.017045161	2159.459573	1.198727909
66.84376747	Vitamin E	92.6769218	C29H50O2	179811.6463	NIST14.L	1056874332	0.017013531	2137.236573	1.188597411
3.342573047	Propanoic acid, 2-oxo-, methyl ester	91.20344765	C4H6O3	179653.9351	NIST14.L	1056874332	0.016998609	2115.013573	1.177270942
21.75324153	Phenol, 4-ethyl-2-methoxy-	83.52947605	C9H12O2	179271.0738	NIST14.L	1056874332	0.016962383	2092.790573	1.167388876
14.07579121	3-Undecene, (E)-	80.85194993	C11H22	178997.689	NIST14.L	1056874332	0.016936516	2070.567573	1.156756596
2.966360821	1-Hydroxy-2-butanone	80.25681507	C4H8O2	178508.5122	NIST14.L	1056874332	0.016890231	2048.344573	1.147477254
3.581542211	2-Heptene, 3-methyl-	87.36664616	C8H16	176842.5196	NIST14.L	1056874332	0.016732597	2026.121573	1.145720824
7.080711739	Pyridine, 2,5-dimethyl-	89.87270661	C7H9N	175478.2298	NIST14.L	1056874332	0.016603509	2003.898573	1.141964206
21.99241223	Naphthalene, 2-methyl-	85.11563014	C11H10	175456.1729	NIST14.L	1056874332	0.016601422	1981.675573	1.129441923
77.90960641	1-[1,2,4]Triazol-1-ylethanone	83.69794999	C4H5N3O	173760.3909	NIST14.L	1056874332	0.01644097	1959.452573	1.127675049
63.81908343	Octane, 2,7-dimethyl-	92.57056966	C10H22	170429.6011	NIST14.L	1056874332	0.016125815	1937.229573	1.136674358
15.94268498	2-Methylindene	84.43401075	C10H10	169719.9703	NIST14.L	1056874332	0.016058671	1915.006573	1.128333083
19.67422414	1H-Benzimidazole, 5,6-dimethyl-	81.72163131	C9H10N2	168851.6963	NIST14.L	1056874332	0.015976516	1892.783573	1.120973976
7.657137671	4,5-Dihydro-2(1H)-pentalenone	94.15932273	C8H8O	168593.9587	NIST14.L	1056874332	0.015952129	1870.560573	1.109506288
7.661008884	Benzene, propyl-	92.04893245	C9H12	168264.9605	NIST14.L	1056874332	0.015921	1848.337573	1.098468492
18.04381207	CH3NHCH2CN	83.12185943	C3H6N2	167085.5089	NIST14.L	1056874332	0.015809402	1171.114573	0.700907326
41.73194492	2-Methyl-1-undecanol	81.50484002	C12H26O	165802.0979	NIST14.L	1056874332	0.015687967	448.8915733	0.270739381
16.37391737	4-(2-Ethylhexoxy)ethylbenzene	80.66531653	C16H26O	165708.7933	NIST14.L	1056874332	0.015679139	16127.29341	9.732309965
9.531337709	Undecane, 3,5-dimethyl-	87.02557121	C13H28	164683.134	NIST14.L	1056874332	0.015582092	13587.13412	8.250470943
54.78647827	Pentadecanal-	81.87982239	C15H30O	163275.7133	NIST14.L	1056874332	0.015448924	12694.53903	7.77490955
61.67201657	1,4-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester	86.79904931	C24H38O4	161597.1645	NIST14.L	1056874332	0.015290102	12581.25255	7.78556517
17.135808	Naphthalene	87.60138952	C10H8	160231.3906	NIST14.L	1056874332	0.015160874	12253.61651	7.647450643
18.03130564	2-Carbomethoxyaziridine	86.74445568	C4H7NO2	159170.7984	NIST14.L	1056874332	0.015060523	11008.64814	6.916248618
18.93239998	Crotonyl isothiocyanate	83.62659657	C5H5NOS	157673.7263	NIST14.L	1056874332	0.014918872	9994.209165	6.338538066

7.345153862	4-Hexen-2-one	94.44404408	C6H10O	149846.8796	NIST14.L	1056874332	0.014178306	8552.385481	5.707416466
54.5437748	Undecane, 3,8-dimethyl-	85.46403704	C13H28	147477.1178	NIST14.L	1056874332	0.013954083	4362.266279	2.957927538
62.54013852	Pentanamide	81.43338445	C5H11NO	142306.6837	NIST14.L	1056874332	0.013464863	4852.967876	3.410217811
27.17112912	7-Tetradecene, (Z)-	84.45240409	C14H28	141464.4014	NIST14.L	1056874332	0.013385168	2731.147054	1.930624968
79.58940605	5H-Tetrazol-5-amine	90.28699395	CH3N5	134718.5049	NIST14.L	1056874332	0.012746808	3703.506338	2.749070249
25.21243076	Benzeneacetic acid, 2-propenyl ester	81.03607333	C11H12O2	134412.8084	NIST14.L	1056874332	0.012717956	1147.675067	0.853843529
3.448592519	1H-Tetrazol-5-amine	91.73372191	CH3N5	133357.4713	NIST14.L	1056874332	0.012618101	7377.85346	5.532388541
17.48717455	Cyclohexene, 3,4-diethenyl-, cis-	81.90203985	C10H14	132484.8749	NIST14.L	1056874332	0.012535537	6179.109514	4.664011284
8.622201345	Benzene, 1,2,3-trimethyl-	81.93669183	C9H12	131686.6773	NIST14.L	1056874332	0.012460013	174.8544506	0.132780669
50.58403699	Decane, 6-ethyl-2-methyl-	88.8331261	C13H28	131533.5066	NIST14.L	1056874332	0.01244552	2198.348757	1.671322247
38.37090705	2-Methylbenzylamine, N,N-diheptyl-	80.19749935	C22H39N	131324.3329	NIST14.L	1056874332	0.012425728	2017.884785	1.536565799
8.622851853	Benzene, 1-ethyl-4-methyl-	83.70971905	C9H12	127802.0874	NIST14.L	1056874332	0.012092458	1920.237478	1.502508698
3.458674535	2,4-Dimethyl-oxetane	80.03986126	C5H10O	119634.8127	NIST14.L	1056874332	0.011319682	20538.41038	17.16758685
8.429623688	Propanoic acid, 1-methylpropyl ester	83.33979023	C7H14O2	119604.5277	NIST14.L	1056874332	0.011316816	1720.700714	1.438658509
57.83100529	Oxalic acid, allyl hexadecyl ester	83.35774693	C21H38O4	119057.9559	NIST14.L	1056874332	0.011265101	3089.813013	2.59521759
25.42952877	Benzene, (1-methylhexyl)-	80.15855228	C13H20	114238.8889	NIST14.L	1056874332	0.010809127	1804.178094	1.579302907
3.028947865	2-Methoxy-1,3-dioxolane	85.33236201	C4H8O3	113732.8725	NIST14.L	1056874332	0.010761248	1157.259227	1.017523959
18.90279856	4-Hexen-3-one	89.23357487	C6H10O	113245.2928	NIST14.L	1056874332	0.010715114	8765.010744	7.739845541
11.30851651	Benzeneacetaldehyde	86.24949333	C8H8O	109934.6796	NIST14.L	1056874332	0.010401869	8535.611663	7.764257553
21.98357316	1H-Indene-1-methanol, .alpha.-methyl-, acetate	90.17092238	C13H14O2	108330.965	NIST14.L	1056874332	0.010250127	16298.51656	15.04511343
7.358700645	2(5H)-Furanone, 5-methyl-	87.34120209	C5H6O2	107640.6572	NIST14.L	1056874332	0.010184811	7641.683439	7.099253794
38.23157432	Decane, 3-chloro-	81.70753938	C10H21Cl	107582.2028	NIST14.L	1056874332	0.010179281	5930.143943	5.512197919
41.96737308	Heptane, 2,6-dimethyl-	86.52515297	C9H20	102699.1356	NIST14.L	1056874332	0.009717251	1995.642933	1.943193505
38.23152144	1-Octene, 6-methyl-	83.50570537	C9H18	102093.9708	NIST14.L	1056874332	0.009659992	515.4422938	0.504870454
53.12944859	Norbornane, 2-isobutyl-	83.94063799	C11H20	100110.4017	NIST14.L	1056874332	0.009472309	1241.751143	1.240381741
41.96711604	Decane, 2,4-dimethyl-	85.69520721	C12H26	99072.94445	NIST14.L	1056874332	0.009374146	1082.498874	1.092628144
15.83510353	5-Pentylcyclohexa-1,3-diene	85.30643073	C11H18	95927.54037	NIST14.L	1056874332	0.009076532	11515.24107	12.00410334
18.87805895	2-(E)-Hexen-1-ol, (4S)-4-amino-5-methyl-	80.97110983	C7H15NO	95084.46621	NIST14.L	1056874332	0.008996762	1535.340953	1.614712701
12.18404394	Benzene, 1-methyl-4-propyl-	83.83516866	C10H14	94704.83653	NIST14.L	1056874332	0.008960842	2799.503906	2.956030556
9.398983506	1,3-Cyclohexanedione	84.67017631	C6H8O2	94451.01786	NIST14.L	1056874332	0.008936826	9049.52118	9.581179097
8.421583843	Allyl thiopropionate	84.63186745	C6H10OS	94108.65464	NIST14.L	1056874332	0.008904432	9551.655235	8.149603426

30.48854007	1H-Indole, 2,5-dimethyl-	81.2118312	C10H11N	92967.73052	NIST14.L	1056874332	0.008796479	10325.34814	7.10637861
65.15281254	Decane, 1-iodo-	83.93449048	C10H21I	92646.79475	NIST14.L	1056874332	0.008766113	9566.553772	8.325833503
64.09440918	Cyclopentaneethanol, .beta.,2,3-trimethyl-	84.63794238	C10H20O	91747.86948	NIST14.L	1056874332	0.008681058	9815.196132	6.69800987
11.30863533	Spiro[2,4]hepta-4,6-diene	87.83676925	C7H8	87882.00621	NIST14.L	1056874332	0.008315275	7290.576578	8.295869533
63.80694386	2H-Pyran, 3,4-dihydro-6-methyl-	83.04196742	C6H10O	85125.76458	NIST14.L	1056874332	0.008054483	6649.27557	7.811119938
50.45761747	1-Tetradecyne	85.8524861	C14H26	85117.83186	NIST14.L	1056874332	0.008053733	6707.548127	7.880308956
4.820757641	2-Butanone	84.08560222	C4H8O	84607.85383	NIST14.L	1056874332	0.008005479	5057.457293	5.977526984
16.50168256	2,3-Furandione, dihydro-4,4-dimethyl-	82.99141845	C6H8O3	83774.86161	NIST14.L	1056874332	0.007926663	5818.717023	6.945659964
20.08074635	Sulfoxide, methyl phenethyl	80.08568556	C9H12OS	83747.76438	NIST14.L	1056874332	0.007924099	5391.355753	6.43761155
8.421916156	Oxalic acid, isobutyl propyl ester	83.53634075	C9H16O4	82181.93097	NIST14.L	1056874332	0.007775942	4092.860573	4.980243863
50.45136735	Cyclohexanepropanol-	81.31867854	C9H18O	81218.07881	NIST14.L	1056874332	0.007684743	4070.637573	5.011984564
50.45571772	Cyclohexaneethanol	84.85948085	C8H16O	79580.26304	NIST14.L	1056874332	0.007529775	4048.414573	5.087209339
27.17190741	6-Tridecene, 7-methyl-	86.51381299	C14H28	79486.53452	NIST14.L	1056874332	0.007520907	4026.191573	5.065249854
27.1722131	Cyclopentane, 1,1-dimethyl-	83.42160803	C7H14	78814.74188	NIST14.L	1056874332	0.007457343	4003.968573	5.080227985
10.44305124	Benzenamine, 4-methoxy-	81.98158855	C7H9NO	78588.85038	NIST14.L	1056874332	0.007435969	3981.745573	5.066552767
10.48316078	Benzeneethanol, .beta.-ethenyl-	90.69545301	C10H12O	78548.29772	NIST14.L	1056874332	0.007432132	3959.522573	5.040876363
56.30296541	3,5-Dimethyl-4-octanone	80.20211874	C10H20O	78450.39825	NIST14.L	1056874332	0.007422869	3937.299573	5.018839497
17.70166432	Furan, 2,3-dihydro-	84.1005643	C4H6O	78220.48258	NIST14.L	1056874332	0.007401115	3915.076573	5.005180797
53.13811223	2,2'-Bi-1,3-dioxolane	85.57290023	C6H10O4	78213.55599	NIST14.L	1056874332	0.007400459	3892.853573	4.977210822
25.43352701	1-Methyl-2-n-hexylbenzene	83.5729159	C13H20	78165.86509	NIST14.L	1056874332	0.007395947	3870.630573	4.951816972
7.358557283	2,4-Azetidinedione, 3,3-diethyl-1-methyl-	89.01097112	C8H13NO2	77857.07222	NIST14.L	1056874332	0.007366729	3848.407573	4.942913294
29.66638041	Benzene, (1-methylheptyl)-	84.59226876	C14H22	76798.7627	NIST14.L	1056874332	0.007266594	3826.184573	4.982091428
18.53734066	5-Undecene, 8-methyl-, (E)-	84.19996469	C12H24	76267.62451	NIST14.L	1056874332	0.007216338	3803.961573	4.987649212
57.95952112	Nonane, 2,2,4,4,6,8,8-heptamethyl-	80.37799038	C16H34	76154.18901	NIST14.L	1056874332	0.007205605	3781.738573	4.965896982
8.423249352	2-Butanone, 1-(acetyloxy)-	87.93532776	C6H10O3	74017.0659	NIST14.L	1056874332	0.007003393	3759.515573	5.079255071
8.423150409	Ethane-1,1-diol dipropanoate	83.00336194	C8H14O4	71660.86235	NIST14.L	1056874332	0.006780453	3737.292573	5.215249232
22.66999126	Succinic acid, 2,4,6-trichlorophenyl 2-naphthylmethyl ester	84.0550809	C21H15Cl3O4	71524.39298	NIST14.L	1056874332	0.006767574	3715.069573	5.194129469
10.8628572	1,4-Cyclohex-2-enedione	81.89728629	C6H6O2	71322.09406	NIST14.L	1056874332	0.006748399	3692.846573	5.177703518
24.49062416	2,5,6-Trimethylbenzimidazole	80.86318256	C10H12N2	69308.80204	NIST14.L	1056874332	0.006557904	3670.623573	5.296042444
9.709461536	2-Furanone, 2,5-dihydro-3,5-dimethyl	83.63684449	C6H8O2	69029.21203	NIST14.L	1056874332	0.006531449	3648.400573	5.285299464

57.95531541	Hexane, 3,3-dimethyl-	82.76061502	C8H18	68913.22616	NIST14.L	1056874332	0.006520475	3626.177573	5.261947198
10.47597823	Indane	88.61345439	C9H10	67825.31623	NIST14.L	1056874332	0.006417538	3603.954573	5.313583148
53.15158379	N-Ethylformamide	91.2847327	C3H7NO	65485.8414	NIST14.L	1056874332	0.006196181	3581.731573	5.46947477
50.45120516	Cyclohexane, cyclopropyl-	84.26306549	C9H16	64994.34894	NIST14.L	1056874332	0.006149676	3559.508573	5.476643172
37.69585025	2-Pentyn-4-one	81.74732147	C5H6O	61843.53665	NIST14.L	1056874332	0.005851551	3537.285573	5.719733645
6.111132163	Pyridine, 2-ethyl-	86.21899033	C7H9N	60014.13943	NIST14.L	1056874332	0.005678456	3515.062573	5.857057364
31.57692261	Cyclohexane, 1,2-dimethyl-, cis-	82.50792915	C8H16	59109.59077	NIST14.L	1056874332	0.005592868	3492.839573	5.90909111
21.32831366	Pyrazine, 2-methyl-5-(1-methylethyl)-	82.13654851	C8H12N2	58472.78732	NIST14.L	1056874332	0.005532615	3470.616573	5.935438915
13.05533785	2,4,5-Trihydroxypyrimidine	84.59579464	C4H4N2O3	58095.56679	NIST14.L	1056874332	0.005496923	3448.393573	5.935725846
14.24928111	1H-Isoindole, 2,3-dihydro-	83.45151148	C8H9N	57922.37326	NIST14.L	1056874332	0.005480536	3426.170573	5.915107376
35.02327928	Cyclooctane, 1,4-dimethyl-, trans-	85.30966424	C10H20	57898.61371	NIST14.L	1056874332	0.005478287	3403.947573	5.879152117
41.18829543	2-Oxobicyclo(3.2.2)nona-3,6-dien-1-yl benzoate	81.17026918	C16H14O3	57498.54649	NIST14.L	1056874332	0.005440434	3381.724573	5.881408801
3.748092015	Cyclopropane, [(1-propenyloxy)methyl]-	83.39955826	C7H12O	56121.15019	NIST14.L	1056874332	0.005310106	3359.501573	5.986159518
45.38000978	1H-Indene, 2-phenyl-	83.79472459	C15H12	55723.81176	NIST14.L	1056874332	0.005272511	3337.278573	5.988963188
14.41922331	1-Pentanol, 2-methyl-	94.26327667	C6H14O	54384.87987	NIST14.L	1056874332	0.005145823	3315.055573	6.095546374
21.32843863	Phenol, 3-ethyl-5-methyl-	80.42496536	C9H12O	51480.43232	NIST14.L	1056874332	0.004871008	3292.832573	6.396279955
7.399606301	Benzeneethanol, .beta.-ethenyl-.alpha.-methyl-	91.94503301	C11H14O	44291.69345	NIST14.L	1056874332	0.004190819	3270.609573	7.384250452
15.59802863	Benzene, 1-isocyano-3-methyl-	85.36816622	C8H7N	42967.36292	NIST14.L	1056874332	0.004065513	3248.386573	7.560125529
30.35971254	2-Heptyne-4-one	81.45817246	C7H10O	42669.96485	NIST14.L	1056874332	0.004037374	3226.163573	7.560736422
56.2247937	Cyclohexane, (2-methylpropyl)-	80.16439102	C10H20	42642.64739	NIST14.L	1056874332	0.004034789	3203.940573	7.513465438
12.96105616	Indan, 1-methyl-	80.53644055	C10H12	41304.9599	NIST14.L	1056874332	0.003908219	3181.717573	7.702991557
10.94501255	Bicyclo[2.2.2]oct-2-ene	85.73039219	C8H12	39996.68792	NIST14.L	1056874332	0.003784432	3159.494573	7.899390519
32.79941621	Glutaric acid, ethyl 3-heptyl ester	82.11989377	C14H26O4	39491.83514	NIST14.L	1056874332	0.003736663	3137.271573	7.944101767
13.02395411	1,2,4-Triazin-3-amine, 5,6-dimethyl-	90.71499989	C5H8N4	39034.55904	NIST14.L	1056874332	0.003693396	3115.048573	7.980232516
40.04306092	3-Methylbenzoic acid, 2,5-dichlorophenyl ester	83.34237252	C14H10Cl2O2	38876.67297	NIST14.L	1056874332	0.003678457	3092.825573	7.95547905
7.408677935	Propanoic acid, 2-methyl-, 3-phenylpropyl ester	83.9649377	C13H18O2	37910.33836	NIST14.L	1056874332	0.003587024	3070.602573	8.099644334
5.258782875	1,2,4-Triazine	81.78233106	C3H3N3	37879.86582	NIST14.L	1056874332	0.003584141	3048.379573	8.04749306
10.3715088	2-Cyclopenten-1-one, 3,4-dimethyl-	81.3004937	C7H10O	35484.6154	NIST14.L	1056874332	0.003357506	3026.156573	8.52808052
20.57428612	1H-Indene, 1,1-dimethyl-	84.1692413	C11H12	34904.68512	NIST14.L	1056874332	0.003302633	3003.933573	8.606104204
21.23819128	Phenol, 4-butyl-	81.76209852	C10H14O	34118.87157	NIST14.L	1056874332	0.003228281	2981.710573	8.73918285

40.06154958	Piperazine-2,5-dione, 4-(4-methylbenzoyl)-	80.89643288	C12H12N2O3	33542.74013	NIST14.L	1056874332	0.003173768	2959.487573	8.823034617
32.51575291	1-Methyl-3-phenyl-2,4,5-trioxoimidazolidine	82.74020507	C10H8N2O3	31759.03791	NIST14.L	1056874332	0.003004997	2937.264573	9.248594312
15.24752738	Benzene, 4-ethenyl-1,2-dimethyl-	83.30042979	C10H12	31489.29602	NIST14.L	1056874332	0.002979474	2915.041573	9.257245927
11.41202565	Cyclopentene, 3-methyl-	80.35305347	C6H10	30049.50542	NIST14.L	1056874332	0.002843243	2892.818573	9.626842549
18.53586673	1,6-Diazabicyclo[4.1.0]heptane	86.5187159	C5H10N2	28501.04206	NIST14.L	1056874332	0.002696673	1870.595573	6.563253263
7.201592311	Furan, 2,3,5-trimethyl-	82.92275893	C7H10O	27273.81005	NIST14.L	1056874332	0.002580611	1848.372573	6.777097039
64.20723736	Phthalic acid, cyclobutyl propyl ester	80.39184825	C15H18O4	26990.14952	NIST14.L	1056874332	0.002553771	1826.149573	6.765985389
3.227108663	3-Hexanone, 2-methyl-	85.58306738	C7H14O	25385.6266	NIST14.L	1056874332	0.002401953	803.9265733	3.166857316
15.72066746	Dimethylaminoethyltrifluorophosphorane	83.84838702	C4H11F3NP	25059.76434	NIST14.L	1056874332	0.002371121	781.7035733	3.11935724
56.48761365	Tetramethyl orthocarbonate	80.13199951	C5H12O4	24905.24957	NIST14.L	1056874332	0.002356501	759.4805733	3.049479874
8.886463541	Semioxamazide	88.220641	C2H5N3O2	23031.33946	NIST14.L	1056874332	0.002179194	1737.257573	7.543015795
61.23528366	Oxirane, tetramethyl-	80.04634622	C6H12O	20711.31962	NIST14.L	1056874332	0.001959677	815.0345733	3.93521315
7.193556266	1-(3H-Imidazol-4-yl)-ethanone	81.97769797	C5H6N2O	19158.64179	NIST14.L	1056874332	0.001812764	692.8115733	3.616183135
6.800938824	1H-Pyrrole-2-carboxaldehyde, 1-methyl-	83.79539911	C6H7NO	17805.75421	NIST14.L	1056874332	0.001684756	770.5885733	4.327750255
39.55789715	1-Butanol, 2-methyl-	84.19103979	C5H12O	17730.59871	NIST14.L	1056874332	0.001677645	648.3655733	3.656760745
3.329520781	Acetamide, 2,2'-thiobis-	85.19248542	C4H8N2O2S	17625.86447	NIST14.L	1056874332	0.001667735	626.1425733	3.552407737
19.20936351	Methanamine, 1-methoxy-N-methyl-N-nitroso-	82.54000977	C3H8N2O2	16970.15051	NIST14.L	1056874332	0.001605692	503.9195733	2.969446694
15.98655477	Dimethylphosphinic fluoride	83.77588696	C2H6FOP	16958.97362	NIST14.L	1056874332	0.001604635	781.6965733	4.609338932
61.2334108	2-Pentanone, 4-hydroxy-4-methyl-	85.48660619	C6H12O2	16390.13665	NIST14.L	1056874332	0.001550812	559.4735733	3.413477173
62.96663713	Butanal, O-methyloxime	82.77532777	C5H11NO	15664.22303	NIST14.L	1056874332	0.001482127	537.2505733	3.429793946
12.85059748	1H-Pyrazole, 5-methoxy-1,3-dimethyl-	86.71094567	C6H10N2O	14904.2738	NIST14.L	1056874332	0.001410222	515.0275733	3.455569727
36.37353957	Pyrazine, isopropenyl-	85.11752374	C7H8N2	13461.8955	NIST14.L	1056874332	0.001273746	792.8045733	5.889249203
60.59222936	Propane, 1-(1-methylethoxy)-	84.72055873	C6H14O	9692.905714	NIST14.L	1056874332	0.000917129	770.5815733	7.949954286

Table S30. *Py-GC/MS data for spent coffee grounds.*

```
;lc1pncwgpps
;avance-version (17/02/22)
;1D version of noesyprph using presaturation during relaxation delay
;and mixing time
;using shaped pulse for off-resonance presaturation
;with cp-decoupling on f2 - channel during acquisition and end of presat time and mixing time
;
;$CLASS=HighRes
;$DIM=1D
;$TYPE=
;$SUBTYPE=
;$COMMENT=

prosol relations=<lcnmr>

#include <Avance.incl>
#include <Delay.incl>
#include <Grad.incl>

"d11=30m"
"d12=20u"

"p0=p1*cnst12"

"if (d1/p18 < 1) {l6=1;} else {l6=d1/p18;}"
"if (d2/p18 < 1) {l8=0;} else {l8=d2/p18;}"
"l7=trunc(d8/p18)"

"DELTA=d8-(p18*l7)"

"acqt0=-p0*2/3.1416"

1 ze
  d12 pl14:f2
2 30m do:f2

#   ifdef FLAG_BLK
  4u BLKGRAD
#   else
  4u
#   endif /*FLAG_BLK*/

3 p18:sp6:f1 ph29
  4u
  lo to 3 times l6
  4u cpd2:f2
   4 p18:sp6:f1 ph29
  4u
  lo to 4 times l8
  4u do:f2
  50u UNBLKGRAD
  p16:gp1
  d16 pl1:f1
  p1 ph1
  4u
  p1 ph2
  d12 cpd2:f2
  DELTA
5 p18:sp6:f1 ph29
```

```
  4u
  lo to 5 times l7
  p16:gp2
  d16 pl1:f1

#   ifdef FLAG_BLK
  4u
#   else
  4u BLKGRAD
#   endif /*FLAG_BLK*/

  p0 ph3
  go=2 ph31
  30m do:f2 mc #0 to 2 F0(zd)

#   ifdef FLAG_BLK
  4u BLKGRAD
#   else
  4u
#   endif /*FLAG_BLK*/

exit

ph1=0 2
ph2=0 0 0 0 0 0 0 0 2 2 2 2 2 2 2 2
ph3=0 0 2 2 1 1 3 3
ph29=0
ph31=0 2 2 0 1 3 3 1 2 0 0 2 3 1 1 3

;pl1 : f1 channel - power level for pulse (default)
;pl14: f2 channel - power level for low power cpd decoupling
;sp6: f1 channel - shaped pulse for presaturation
;p0 : for any flip angle
;p1 : f1 channel -  90 degree high power pulse
;p16: homospoil/gradient pulse
;p18: f1 channel - presaturation using shaped pulse
;p31: f2 channel - 90 degree pulse for low power decoupling sequence
;d1 : relaxation delay; 1-5 * T1                [ca. 1-2sec]
;d2: relaxation delay with decoupling [e.g. 1s]
;d8 : mixing time                          [ca. 80 msec]
;d11: delay for disk I/O                        [30 msec]
;d12: delay for power switching                    [20 usec]
;d16: delay for homospoil/gradient recovery
;cnst12: as multiplier for flip angle (1 = 90o)          [1]
;l6: p18 * l6 = total duration of presaturation
;               during relaxation delay         [16]
;l7: p18 * l7 = total duration of presaturation
;               during mixing time              [1]
;l8: p18*l8 = total duration of presaturation with decoupling
;ns: 8 * n, total number of scans: NS * TD0
;ds: 4
;cpdprg2 : garp.p31 (decoupling sequence for low power cpd decoupling)

;use 100msec pulse of square shape defined by 1000 points

;for z-only gradients:
;gpz1: 50%
;gpz2: -10%
```

```
;use gradient files:
;gpnam1: SMSQ10.100
;gpnam2: SMSQ10.100

                                ;preprocessor-flags-start
;FLAG_BLK: for BLKGRAD before d1 rather than go
;           option -DFLAG_BLK: (eda: ZGOPTNS)
                                ;preprocessor-flags-end

;$Id: lc1pncwgpps,v 1.4 2017/02/22 15:52:05 ber Exp $
```

Figure S41. Pulse programme for Bruker sequence lc1pndcgpps