Electronic Supplementary Material (ESI) for Analytical Methods.

Electronic Supplementary Information

Rapid detection of toxic compounds in tobacco smoke condensates using high-resolution ^{1}H-nuclear magnetic resonance spectroscopy

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This supplementary information includes details of the chemical standards used for NMR analysis; details of the NMR chemical shifts for the Hoffmann analytes; data mining for validation of the protocol; expanded views of the NRM spectra, and a comprehensive list of the relative recorded chemical shifts of HPHCs detected in different types of cigarette.

Supplementary Table S1. List of chemical standards used for NMR

Name	CAS	Purity (%)	Supplier
Acetaldehyde	75-07-0	99.0%	
Isoprene	78-79-5	99.0%	
Nicotine	54-11-5	99.5%	
Acetone	67-64-1	99.9%	
Acrolein	107-02-8	95.0%	
Toluene	108-88-3	99.5%	
Catechol	120-80-9	99.5%	
Hydroquinone	123-31-9	99.0%	
Formaldehyde	50-00-0	unknown	
Acrylonitrile	107-13-1	99.0%	
Propionaldehyde	123-38-6	98.5%	
Crotonaldehyde	123-73-9	98.5%	
Butyraldehyde	123-72-8	99.5%	
Butanone (methyl ethyl ketone)	78-93-3	99.5%	
Benzene	71-43-2	99.5%	
Pyridine	110-86-1	99.5%	
Phenol	108-95-2	99.93%,	
Styrene	100-42-5	99.5%	
o-Cresol (2-methylphenol)	95-48-7	99.0%	
m-Cresol (3-methylphenol)	108-39-4	99.0%),	
p-Cresol (4-methylphenol)	106-44-5	99.0%	LGC Standards (UK)
Resorcinol	108-46-3	99.5%	
Quinoline	91-22-5	98.1%	
N-nitrosonornicotine	80508-23-2	98.5%	
1-Aminonaphthalene	134-32-7	99.5%	
2-Aminonaphthalene	91-59-8	99.5%	
3-Aminobiphenyl	2243-47-2	99.5%	
N-Nitrosoanatabine	887407-16-1	98.0%	
N-Nitrosoanabasine	37620-20-5	98.0%	
N-Nitrosonornicotine ketone	64091-91-4	98.0%	
Benzo(a)pyrene	50-32-8	99.6%	
4-aminobiphenyl	92-67-1	99.5%	
Acetamide	60-35-5	99%	
Anabasine	13078-04-1	97%	
o-Anisidine	90-04-0	99%	
Pyrrolidine	123-75-1	99.5%	
N-Nitrosopyrrolidine	930-55-2	99.6%	
Vynilacetate	108-05-4	99%	
Nitrobenzene	98-95-3	99.9%	
o-Toluidine	95-53-4	99%	
2-Nitropropane	79-46-9	98.5%	
N-Nitrosodiethanolamine	1116-54-7	99.9%	
N-Nitrosopiperidine	100-75-4	99.9%	

Name	CAS	Purity (%)	Supplier
Chrysene	218-01-9	98.7%	LGC Standards (UK)
5-Methyl-chrysene	3697-24-3	98.7%	
Benzo(b)fluoranthene	205-99-2	99.8%	
Dibenzo(a,h)pyrene	189-64-0	98%	
N-Nitrosomethylethylamine	10595-95-6	99.5%	
Acrylamide	110-26-9	99.9%	
Benzo(a)anthracene	56-55-3	99.9%	
Indeno[1,2,3–c,d]pyrene	193-39-5	99%	
Naphthalene	91-20-3	99%	
Propylene oxide	75-56-9	99%	
N-Nitrosodiethylamine	55-18-5	99%	
Dibenzo(a,e)pyrene	192-65-4	99%	
Deuterated methanol	811-98-3	99.8% atom D	Cambridge Isotope Laboratories (via LGC Standards)
1,3-Butadiene dissolved in toluene (20% w/w)	106-99-0	unknown	
Ethylbenzene	100-41-4	99.8%	Sigma Aldrich (UK)
2,5-Dimethylaniline	95-78-3	99.0%	
Acetamide	60-35-5	99.0%	
o-Anisidine	90-04-0	99.0%	
Benzo(k)fluoranthene	207-08-9	99.0%	
2,3-Benzofuran	271-89-6	99.0%	
Coumarine	91-64-5	99.0%	
Urethane	51-79-6	99.0%	
Caffeic acid	331-39-5	98.0%	
TSP (3-(trimethylsilyl)propionic-2,2,3,3-d_4 acid sodium salt)	24493-21-8	98 % atom D	

Supplementary Table S2. NMR chemical shifts of the Hoffman analytes detected in 3R4F cigarette TSC.

Compound	NMR detectable in TSC	Chemical shifts in CD3OD	Chemical shifts observed in 3R4F TSC	LOD (µg/cig.) 1
Acetaldehyde	yes	4.6885, 4.6782, 4.6679, 4.6576, 1.2585, 1.2481	4.6826, 4.6723, 4.6620, 4.6517, 1.2528, 1.2424	4.08
Isoprene	yes	6.482, 6.4606, 6.4471, 6.4257, 5.2021, 5.2009, 5.1997, 5.1671, 5.166, 5.1648, 5.0625, 5.0412, 4.9913, 4.9886, 4.9679, 4.9664, 4.9631	6.4669, 6.4455, 6.4319, 6.4107, 5.1858, 5.1509, 5.0473, 5.026, 4.9759, 4.9527, 4.9515, 4.948, 4.9463	6.30
Nicotine	yes	8.5025, 8.4991, 8.4483, 8.4453, 8.4386, 8.4355, 7.8705, 7.867, 7.8635, 7.8547, 7.8512, 7.8477, 7.4412, 7.4314, 7.4256, 7.4158, 2.4076, 2.389, 2.3712, 2.3526, 2.3087, 2.2982, 2.2931, 2.2898, 2.2831, 2.2793, 2.2736, 2.2676, 2.264, 2.2574, 2.254, 2.2488, 2.2383, 2.0113, 2.008, 2.0043, 1.9981, 1.9923, 1.9863, 1.9822, 1.9762, 1.9703, 1.9671, 1.9631, 1.9599, 1.9573, 1.9514, 1.941, 1.9347, 1.9304, 1.9232, 1.9181, 1.913, 1.911, 1.9044, 1.9, 1.8935, 1.8871, 1.8823, 1.876, 1.8744, 1.8239, 1.8125, 1.8052, 1.8017, 1.7988, 1.7939, 1.7903, 1.7871, 1.7831, 1.78, 1.7768, 1.7716, 1.7684, 1.7654, 1.758, 1.7463.	8.5427, 8.5394, 8.499, 8.496, 8.4892, 8.4863, 7.9026, 7.8993, 7.8959, 7.8868, 7.8834, 7.88, 7.4711, 7.4611, 7.4553, 7.4455, 2.1378	15.01
Acetone	yes	2.154	2.1374	5.37
1,3-Butadiene	no, due to volatility at room temp.	7.222, 7.207, 7.1922, 7.1564, 7.1399, 7.1386, 7.1188, 7.1045, 7.0905, 6.3934, 6.3913, 6.3773, 6.3631, 6.3587, 6.3449, 6.3401, 6.3263, 6.3124, 6.3102, 5.22, 5.2176, 5.2153, 5.2014, 5.1875, 5.185, 5.1829, 5.0923, 5.0755, 5.0725, 2.318, 2.1902, 2.1522	7.2, 7.1927, 7.1783, 7.1393, 7.1181, 7.1045, 7.0908, 6.3789–6.3219 cluster, 5.217, 5.1851 triplet, 5.0915 doublet, 5.0716 doublet, 2.3182	NA
Acrolein	yes	9.5535, 9.5392, 6.5638, 6.5613, 6.5425, 6.4271, 6.393, 6.386, 6.3725, 6.369, 6.3538, 6.3344, 6.3193	9.5358, 9.5218, 6.546, 6.5432, 6.5418, 6.5279, 6.5244, 6.379, 6.3773, 6.3748, 6.368, 6.3545, 6.3503, 6.336	5.19
Toluene	yes	7.2246, 7.2096, 7.1948, 7.1563, 7.1414, 7.1217, 7.1071, 2.3211	7.2081, 7.193, 7.1781, 7.1395, 7.1246, 7.1058, 7.0906, 7.0764, 2.3042	8.52
Catechol	yes	6.752, 6.7449, 6.7403, 6.7332, 6.6542, 6.6471, 6.6424, 6.6353	6.7368, 6.7297, 6.7251, 6.7179, 6.6387, 6.6316, 6.6269, 6.6198	10.19
Hydroquinone	yes	6.6081	6.5934	10.19
Formaldehyde	yes	4.6422	4.6277	2.78
Acrylonitrile	yes	6.2798, 6.2781, 6.2442, 6.2424, 6.1527, 6.151, 6.1291, 6.1274, 5.8843, 5.8607, 5.8486, 5.8251	6.264, 6.2622, 6.2283, 6.2265, 6.1369, 6.1352, 6.1134, 6.1117, 5.8682, 5.8446, 5.8324	4.91
Propionaldehyde	yes	4.4162, 4.4052, 4.3942, 1.5861, 1.571,	4.4018, 4.391, 4.3796,	5.37

		1.5532, 1.5419, 1.5268, 0.9232, 0.9082, 0.8932	0.9086, 0.8939, 0.8791	
Crotonaldehyde	yes	9.4549, 9.4389, 7.0446, 7.0307, 7.0132, 6.9994, 2.0353, 2.032, 2.0216, 2.0184	9.4396, 9.4237	6.48
Butyraldehyde	no, obscured by other peaks	0.9515, 0.9373, 0.9231, 0.9085.	Peak overlap, no isolated peaks found	NA
Butanone (methyl ethyl ketone)	yes	2.5166, 2.502, 2.4873, 2.4726, 2.1241, 1.0245, 1.0098, 0.9952	2.5019, 2.4872, 2.4726, 2.4582, 2.1094, 1.0099, 0.9952, 0.9804	6.69
Benzene	yes	7.3267	7.3117	7.22
Pyridine	close to detection limit	8.5359, 7.8517, 7.4497, 7.4379, 7.4344, 7.4227, 7.3273	7.836, 7.4339, 7.4228, 7.4195, 7.4079,	7.32
Phenol	close to detection limit	7.3266, 7.1651, 7.1501, 7.1331, 6.800, 6.7851, 6.7641, 6.7621, 6.7468	8.0682, 7.1498, 7.1183, 6.7699, 6.7481, 6.7318	8.70
Styrene	close to detection limit	7.4181, 7.4031, 7.3263, 7.3159, 7.3013, 7.2952, 7.2857, 7.2397, 7.2248, 7.2104, 6.7539, 6.7317, 6.7176, 6.696, 5.7792, 5.7773, 5.744, 5.7418, 5.2189, 5.197, 4.5879	8.0683, 7.4041, 7.389, 7.2876, 5.7649, 5.729, 4.5732	9.63
o-Cresol (2-methylphenol)	at absolute LOD	7.032, 7.0177, 6.9779, 6.9591, 6.9463, 6.7148, 6.7006, 6.6908, 6.6773, 2.1623	6.6915, 6.6764	10.00
m-Cresol (3-methylphenol)	at absolute LOD	7.0362, 7.0199, 7.0049, 6.6245, 6.6098, 6.5905, 6.5559, 6.5392	7.022, 6.9937	10.00
p-Cresol (4-methylphenol)	close to detection limit	6.9657, 6.9495, 6.656, 6.6391, 2.2138	6.9507, 6.9341, 6.6414, 6.6248	10.00
Resorcinol	no			NA
Quinoline	no			NA
N-Nitrosonornicotine	no	Below detection limits. NMR overspike data acquired but no peaks observed at this concentration		NA
1-Aminonaphthalene	no			NA
2-Aminonaphthalene	no			NA
3-Aminobiphenyl	no			NA
N-Nitrosoanatabine	no	8.5243, 8.5196, 8.4931, 8.4904, 8.4834, 8.4807, 8.4569, 8.4498, 8.3993, 7.8253, 7.8093, 7.7171, 7.701, 7.4539, 7.4451, 7.4379, 7.429, 7.4183, 7.4084, 7.4022, 7.3924, 6.4908, 6.478, 6.2093, 6.2013, 6.1919, 6.0296, 6.025, 6.0131, 6.0086, 6.0034, 5.9236, 5.753, 5.7432, 5.7321, 4.7379, 4.7321, 4.7215, 4.6969, 4.6738, 4.2638, 4.2268, 3.564, 3.5589, 3.554, 3.523, 3.5178, 3.5131, 2.9955, 2.9888, 2.9843, 2.9809	8.48163 doublet, 8.47187 doublet, 8.44795 doublet, 8.43777 doublet, 8.3869 doublet, 7.80676 2 quintets, 7.69872 2 quintets, 7.4302 quartet, 7.3946 quartet, 6.4804, 6.1907 triplet, 6.0069 cluster, 5.7346 cluster, 4.7261 quintet, 4.2535 cluster, 4.217 cluster, 2.9727 quintet	NA

N-Nitrosoanabasine	no	8.5032, 8.4943, 8.4522, 8.4435, 8.2819, 7.8179, 7.8018, 7.5876, 7.5716, 7.4897, 7.4801, 7.4739, 7.464, 7.4397, 7.4299, 7.4238, 7.4141, 6.2916, 5.7977, 5.7873, 5.7769, 4.2616, 4.2509, 4.2404, 4.2338, 4.2229, 4.2126, 3.7822, 3.7744, 3.7572, 3.748, 3.7303, 3.7222, 2.5423, 2.5344, 2.5149, 2.5049, 2.4947, 2.4508, 2.4232, 2.1856, 2.1762, 2.1667, 2.1579, 2.1485, 2.1388, 2.1299, 2.1204, 1.9797, 1.9565, 1.8173, 1.812, 1.8079, 1.8035, 1.7952, 1.7847, 1.6883, 1.6775, 1.666, 1.6119, 1.6033, 1.5941, 1.5855	8.4907, 8.4813 doublet, 8.4352 doublet, 8.2672 doublet, 7.7976 doublet of quintets, 7.5671 doublet of quintets, 7.4517, 7.4276, 7.4177, 7.411, 7.4016, 5.7755, 4.2382 triplet, 4.2105 triplet, 3.7659 doublet, 3.7397 doublet, 3.7136 doublet, 3.3993	NA
N-Nitrosonornicotine ketone	no	9.0958, 9.0926, 9.082, 9.0789, 8.7322, 8.7289, 8.7224, 8.7191, 8.3747, 8.3708, 8.3669, 8.3588, 8.355, 8.3509, 7.5835, 7.5737, 7.5676, 7.5577, 4.2742, 4.2602, 4.2462, 3.7935, 3.7637, 3.7494, 3.1065, 3.04, 3.0264, 3.0127, 2.2295, 2.2157, 2.2019, 2.1881, 2.1743, 2.151, 1.9729, 1.9587, 1.9446	9.0816 doublet, 9.0682 doublet, 8.7176 doublet, 8.7077 doublet, 8.3579 triplet, 8.3415 triplet, 7.5571 quartet, 4.2474 triplet, 3.7805, 3.7364 triplet, 3.1389, 3.1259, 3.0936, 3.0135 triplet, 2.1887 triplet, 1.9316	NA
Benzo(a)pyrene	no	9.153, 9.1347, 9.1177, 8.5763, 8.3849, 8.3667, 8.3352, 8.3191, 8.2792, 8.2636, 8.1289, 8.1143, 8.0554, 8.0372, 8.0117, 7.9965, 7.9813, 7.9672, 7.9489, 7.8645, 7.8618, 7.851, 7.8481, 7.8449, 7.8342, 7.8314, 7.8048, 7.8026, 7.7888, 7.7865, 7.7752, 7.773, 2.152	9.12 triplet, 8.36 doublet, 8.3195, 8.2549 doublet, 8.0986, 8.0397, 8.0219, 7.9963, 7.9814, 7.9665, 7.9512, 7.9335, 7.833 triplet, 7.7733 triplet	NA
4-Aminobiphenyl	no	7.5142, 7.5118, 7.4974, 7.4953, 7.3818,7.3765, 7.3724, 7.3634, 7.3594, 7.3541, 7.3453, 7.3291, 7.2209, 7.2186, 7.2061, 7.1914, 6.7979, 6.7925, 6.7884, 6.7795, 6.7754	7.5005 triplet, 7.3656 triplet, 7.3485, 7.3336, 7.3179, 6.7815 triplet, 6.7644 triplet	NA

[1] Calculated from the nicotine standard and projected to S/N 3:1.

Supplementary Table S3. Summary of NMR validation data[a].

Compound	3R4F 1st replicate	3R4F 2nd replicate	3R4F 3rd replicate	3R4F 4th replicate	3R4F 5th replicate	CM6
Acetaldehyde	Yes	Yes	yes	yes	yes	yes
Isoprene	yes	Yes	yes	yes	yes	yes
Nicotine	yes	Yes	yes	yes	yes	yes
Acetone	yes	Yes	yes	yes	yes	yes
1,3-Butadiene	no (volatile at RT)	no (volatile at RT)	no (volatile at RT)	no (volatile at RT)	no (volatile at RT)	no (volatile at RT)
Acrolein	yes	Yes	yes	yes	yes	yes
Toluene	yes	Yes	yes	yes	yes	yes
Catechol	yes	yes	yes	yes	yes	yes
Hydroquinone	yes	yes	yes	yes	yes	yes
Formaldehyde	yes (partially overlapped by a multiplet)	yes (partially overlapped by a multiplet)	yes (partially overlapped by a multiplet)	yes (partially overlapped by a multiplet)	yes (partially overlapped by a multiplet)	yes
Acrylonitrile	yes	yes	yes	yes	yes	yes
Propionaldehyde	yes	yes	yes	yes	yes	yes
Crotonaldehyde	yes	yes	yes	yes	yes	yes
Butyraldehyde	yes	yes	yes	yes	yes	yes
Butanone	yes	yes	yes	yes	yes	yes
Benzene	yes	yes	yes	yes	yes	yes
Pyridine	Close to LOD	Close to LOD	Close to LOD	Close to LOD	Close to LOD	Close to LOD
Phenol	yes	Yes	yes	yes	yes	yes
Styrene	close to LOD (some peaks not detected)	close to LOD (some peaks not detected)	close to LOD (some peaks not detected)	close to LOD (some peaks not detected)	close to LOD (some peaks not detected)	yes (weak)
o-Cresol	close to LOD	close to LOD	close to LOD	close to LOD	close to LOD	yes (weak)
m-Cresol	no	no	no	no	no	no
p-Cresol	close to LOD	close to LOD	close to LOD	close to LOD	close to LOD	close to LOD
Resorcinol	no	no	no	no	no	no
Quinoline	no	no	no	no	no	no
N-Nitrosonornicotine	no	no	no	no	no	no
1-Aminonaphtalene	no	no	no	no	no	no
2-Aminonaphtalene	no	no	no	no	no	no
3-Aminobiphenyl	no	no	no	no	no	no
N-Nitrosoanatabine	no	no	no	no	no	no
N-Nitrosoanabasine	no	no	no	no	no	no
N-Nitrosonornicotine-	no	no	no	no	no	no

Compound	3R4F 1st replicate	3R4F 2nd replicate	3R4F 3rd replicate	3R4F 4th replicate	3R4F 5th replicate	CM6
ketone						
Benzopyrene	no	no	no	no	no	no
4-Aminobiphenil	no	no	no	no	no	no

[a]"Yes" - detected; "no" - not detected. The first replicate of 3R4F was lost during NMR sample preparation.

Supplementary Table S4. NMR peaks for compounds detected in the TSC of the sample ISO 3R4F.

Compound	NMR detectable in TSC	Peaks observable in TSC, ppm[a]					
		Ref	1st replicate	2nd replicate	3rd replicate	4th replicate	5th replicate
Acetaldehyde	yes	(4.6826)	4.6830	4.6831	4.6828	4.6830	4.6833
		(4.6723)	4.6728	4.6728	4.6726	4.6726	4.6730
		(4.6620)	4.6623	4.6625	4.6623	4.6625	4.6627
		(4.6517)	4.6519	4.6521	4.65195	4.65195	4.6525
		(1.2528)	1.2530	1.2530	1.2528	1.2530	1.2532
		(1.2424)	1.2426	1.24265	1.2425	1.24265	1.2428
Isoprene	yes	(6.4669)	6.4668	6.4668	6.4668	6.4668	6.4670
		(6.4455)	6.4454	6.4454	6.4454	6.4455	6.4456
		(6.4319)	6.4318	6.4318	6.4318	6.4318	6.4320
		(6.4107)	6.4104	6.4106	6.4106	6.4104	6.4108
		(5.1858)	5.1857	5.1857	5.1857	5.1857	5.1860
		(5.1509)	5.1508	5.1508	5.1508	5.1508	5.1511
		(5.0473)	5.0475	5.0475	5.0475	5.0475	5.0475
		(5.0260)	5.0260	5.0260	5.0260	5.0260	5.0260
		(4.9759)	4.9759	4.9759	4.9759	4.9759	4.9759
		(4.9527)	4.9529	4.9529	4.9529	4.9529	4.9529
		(4.9515)	4.9520	4.9520	4.9520	4.9520	4.9520
		(4.9480)	4.9480	4.9480	4.9480	4.9480	4.9481
		(4.9463)	4.9463	4.9463	4.9463	4.9463	4.9463
Nicotine	yes	(8.5430)	8.5723	8.5691	8.5815	8.5815	8.5657
		(8.5394)	8.5679	8.5653	8.5724	8.5724	8.5620
		(8.4990)	8.5341	8.5300	8.54505	8.54505	8.5261
		(8.496)	8.5311	8.5270	8.5421	8.5421	8.5233
		(8.4892)	8.5243	8.5203	8.53515	8.5356	8.5164
		(8.4863)	8.5214	8.5174	8.5325	8.5326	8.5134
		(7.9026)	7.9263	7.9246	7.9340	7.9346	7.9226
		(7.8993)	7.9264	7.92455	7.9304	7.9311	7.9194
		(7.8959)	7.9189	7.9174	7.9267	7.9273	7.91575
		(7.8868	7.9105	7.910895	7.9182	7.9186	7.9071

Compound	NMR detectable in TSC	Peaks observable in TSC, ppm[a]					
		Ref	1st replicate	2nd replicate	3rd replicate	4th replicate	5th replicate
		)					
		(7.8834)	7.90685	7.9051	7.9146	7.9151	7.9035
		(7.8800)	7.9030	7.9015	7.9108	7.9115	7.8997
		(7.4711)	7.4947	7.4922	7.5025	7.5025	7.4898
		(7.4611)	7.4849	7.4822	7.49265	7.4930	7.4792
		(7.4553)	7.479	7.4777	7.4868	7.4868	7.4773
		(7.4455)	7.4692	7.4665	7.4743	7.4748	7.4641
		(2.1967)	2.1967	2.1968	2.1967	2.1967	2.1967
Acetone	yes	(2.1374)	2.1376	2.1376	2.1376	2.1376	2.138076
1,3 Butadiene	no	(7.2081)	7.2081	7.2081	7.2081	7.2081	7.2081
		(7.1927)	7.1931	7.1931	7.1931	7.1931	7.1933
		(7.1783)	7.1782	7.1782	7.1782	7.1782	7.1785
		(7.1393)	7.1393	7.1393	7.1393	7.1393	7.1397
		(7.1181)	7.1245	7.1245	7.1245	7.1245	7.1245
		(7.1045)	7.1068	7.1068	7.1068	7.1068	7.1068
		(7.0906)	7.0906	7.0906	7.0906	7.0906	7.0906
		(6.338)	6.338	6.338	6.338	6.338	6.338
		(5.2036)	5.2036	5.2036	5.2036	5.2036	5.2036
		(5.217)	5.217	5.217	5.217	5.217	5.217
		(5.1851)	5.1858	5.1858	5.1858	5.1858	5.1860
		(5.0915)	5.0915	5.0915	5.0915	5.0915	5.0915
		(5.0716)	5.078	5.078	5.078	5.078	5.078
		(2.3182)	2.3042	2.3042	2.3042	2.3042	2.3042
Acrolein	yes	(9.5358)	9.5354	9.5354	9.5358	9.5358	9.5354
		(9.5218)	9.5215	9.5215	9.5215	9.5215	9.5215
		(6.5460)	6.5463	6.5466	6.5463	6.5466	6.5470
		(6.5432)	6.5437	6.5437	6.5435	6.5437	6.5441
		(6.5418)	6.5422	6.5422	6.5422	6.5425	6.5430
		(6.5279)	6.5285	6.5285	6.5283	6.5285	6.5289
		(6.5244)	6.5247	6.5247	6.5247	6.5250	6.5254
		(6.3790)	6.3796	6.3796	6.3794	6.3795	6.3797
		(6.3773)	6.3776	6.3778	6.3776	6.3779	6.3782
		(6.3748)	6.37495	6.3751	6.37495	6.3751	6.37545
		(6.3680)	6.3683	6.3683	6.3683	6.3683	6.3686
		(6.3545)	6.3549	6.3549	6.3549	6.3549	6.3552
		(6.3503)	6.3506	6.3506	6.3506	6.3506	6.3509

Compound	NMR detectable in TSC	Peaks observable in TSC, ppm[a]					
		Ref	1st replicate	2nd replicate	3rd replicate	4th replicate	5th replicate
		(6.3360)	6.3360	6.3360	6.3360	6.3360	6.33655
Toluene	yes	(7.2081)	7.2081	7.2081	7.2081	7.2081	7.2084
		(7.1930)	7.1930	7.1930	7.1930	7.1930	7.1934
		(7.1781)	7.1781	7.1781	7.1781	7.1781	7.1784
		(7.1395)	7.1395	7.1395	7.1395	7.1395	7.1395
		(7.1246)	7.1247	7.1247	7.1247	7.1247	7.1247
		(7.1058)	7.1063	7.1063	7.1063	7.1063	7.1063
		(7.0906)	7.0906	7.0908	7.0906	7.0906	7.0908
		(7.0764)	7.0764	7.0764	7.0764	7.0764	7.0764
		(2.3042)	2.3042	2.3042	2.3042	2.3042	2.3042
Catechol	yes	(6.7368)	6.7372	6.7372	6.7372	6.7372	6.7376
		(6.7297)	6.7301	6.7301	6.7301	6.7301	6.7306
		(6.7251)	6.7255	6.7255	6.7255	6.7255	6.7258
		(6.7179)	6.7182	6.7182	6.7182	6.7182	6.7187
		(6.6387)	6.6389	6.6389	6.6389	6.6392	6.6394
		(6.6316)	6.6319	6.6319	6.6317	6.6319	6.6321
		(6.6269)	6.6272	6.6273	6.6272	6.6272	6.6275
		(6.6198);	6.6198	6.6201	6.6198	6.6198	6.6204
Hydroquinone	yes	(6.5934);	6.5939	6.5939	6.5939	6.5939	6.5942
Formaldehyde	yes	(4.6277)	4.6277 (partially overlapped by a multiplet)	4.6277 (partially overlapped by a multiplet)	4.6277 (partially overlapped by a multiplet)	4.6277 (partially overlapped by a multiplet)	4.6277 (partially overlapped by a multiplet)
Acrylonitrile	yes	(6.2640)	6.2641	6.2641	6.2641	6.2641	6.2647
		(6.2622)	6.2622	6.2624	6.2622	6.2625	6.2629
		(6.2283)	6.2285	6.2285	6.2285	6.2285	6.2289
		(6.2265)	6.2266	6.2266	6.2266	6.2266	6.2270
		(6.1369)	6.1373	6.1371	6.1371	6.1371	6.1373
		(6.1352)	6.1355	6.1355	6.1355	6.1355	6.1361
		(6.1134)	6.1136	6.1136	6.1136	6.1136	6.1142
		(6.1117)	6.1118	6.1118	6.1118	6.1118	6.1125
		(5.8682)	5.8682	5.8682	5.8682	5.8682	5.8684
		(5.8446)	5.8445	5.8445	5.8445	5.8445	5.8448

Compound	NMR detectable in TSC	Peaks observable in TSC, ppm[a]					
		Ref	1st replicate	2nd replicate	3rd replicate	4th replicate	5th replicate
		(5.8324)	5.83245	5.83245	5.83245	5.83245	5.83245
Propionaldehyde	yes	(4.4018)	4.40215	4.40215	4.40215	4.40215	4.4024
		(4.3910)	4.39135	4.39135	4.39135	4.39135	4.39171
		(4.3796)	4.3797	4.3800	4.37965	4.3800	4.3804
		(0.9086)	0.9085	0.9085	0.9085	0.9085	0.9085
		(0.8939)	0.8938	0.8938	0.8938	0.8938	0.8940
		(0.8791)	0.8790	0.8790	0.8790	0.8790	0.8792
Crotonaldehyde	yes	(9.4396)	9.4395	9.4395	9.4395	9.4395	9.4397
		(9.4237)	9.4235	9.4235	9.4235	9.4235	9.4237
Butyraldehyde	no	not detected	not detected	not detected	not detected	not detected	not detected
Butanone	yes	(2.5019)	2.5022	2.5022	2.5018	2.5022	2.5023
		(2.4872)	2.4874	2.4874	2.4872	2.4874	2.4876
		(2.4726)	2.4728	2.4728	2.4728	2.4728	2.4730
		(2.4582)	2.4585	2.4587	2.4582	2.4582	2.4588
		(2.1094)	2.1094	2.1096	2.1094	2.1096	2.1099
		(1.0099)	1.0098	1.0098	1.0098	1.0098	1.0101
		(0.9952)	0.9950	0.9950	0.9950	0.9950	0.9954
		(0.9804)	0.9802	0.9802	0.9802	0.9802	0.9802
Benzene	yes	(7.3117)	7.31175	7.31175	7.3116	7.31175	7.31120
Pyridine	close to LOD	(7.8360)	7.8370	7.8370	7.8370	7.8370	7.8370
		(7.4339)	7.4380	7.4380	7.4410	7.4410	7.4380
		(7.4228)	7.4227	7.4227	7.4227	7.4227	7.4227
		(7.4195)	7.4193	7.4193	7.4193	7.4193	7.4193
		(7.4079)	7.4074	7.4074	7.4074	7.4074	7.4074
Phenol	yes	(8.0682)	8.0686	8.0690	8.0688	8.0690	8.0692
		(7.1498)	7.1504	7.1504	7.1504	7.1504	7.1504
		(7.1183)	7.1184	7.1184	7.1184	7.1184	7.1189
		(6.7699)	6.7701	6.7701	6.7701	6.7701	6.7701
		(6.7481)	6.74805	6.74805	6.74805	6.74805	6.7479
		(6.7318)	6.7318	6.7318	6.7318	6.7318	6.7318
Styrene	close to LOD	(8.0683)	8.06855	8.0689	8.0689	8.0689	8.0689
		(7.4041)	7.4038	7.4038	7.4026	7.4026	7.4038
		(7.3890	7.3880	7.3880	7.3880	7.3880	7.3890

Compound	NMR detectable in TSC	Peaks observable in TSC, ppm[a]					
		Ref	1st replicate	2nd replicate	3rd replicate	4th replicate	5th replicate
		)					
		(7.2876)	7.2868	7.2868	7.2868	7.2868	7.2871
		(5.7649)	–	–	–	–	–
		(5.7294)	–	–	–	–	–
		(4.5732)	4.5732	4.5732	4.5732	4.5732	4.5732
o-Cresol	close to LOD	(6.6915)	–	–	–	–	–
		(6.6859)	6.6858	6.6858	6.6858	6.6858	6.6859
m-Cresol	no	–	–	–	–	–	–
p-Cresol	close to LOD	(6.9507)	6.9507	6.9508	6.9508	6.9510	6.9511
		(6.9341)	6.9340	6.9340	6.9340	6.9340	6.9340
		(6.6414)	6.6415	6.6415	6.6415	6.6415	6.6415
		(6.6248)	6.6240	6.6240	6.6240	6.6240	6.6248
Resorcinol	no	–	–	–	–	–	–
Quinoline	no	–	–	–	–	–	–
N-Nitrosonornicotine	no	–	–	–	–	–	–
1-Aminonaphtalene	no	–	–	–	–	–	–
2-Aminonaphtalene	no	–	–	–	–	–	–
3-Aminobiphenyl	no	–	–	–	–	–	–
N-Nitrosoanatabine	no	–	–	–	–	–	–
N-Nitrosoanabasine	no	–	–	–	–	–	–
N-Nitrosonornicotine-ketone	no	–	–	–	–	–	–
Benzo(a)pyrene	no	–	–	–	–	–	–

[a] Each column shows the resonances peaks detected for each compound. The first replicate was lost during NMR sample preparation.

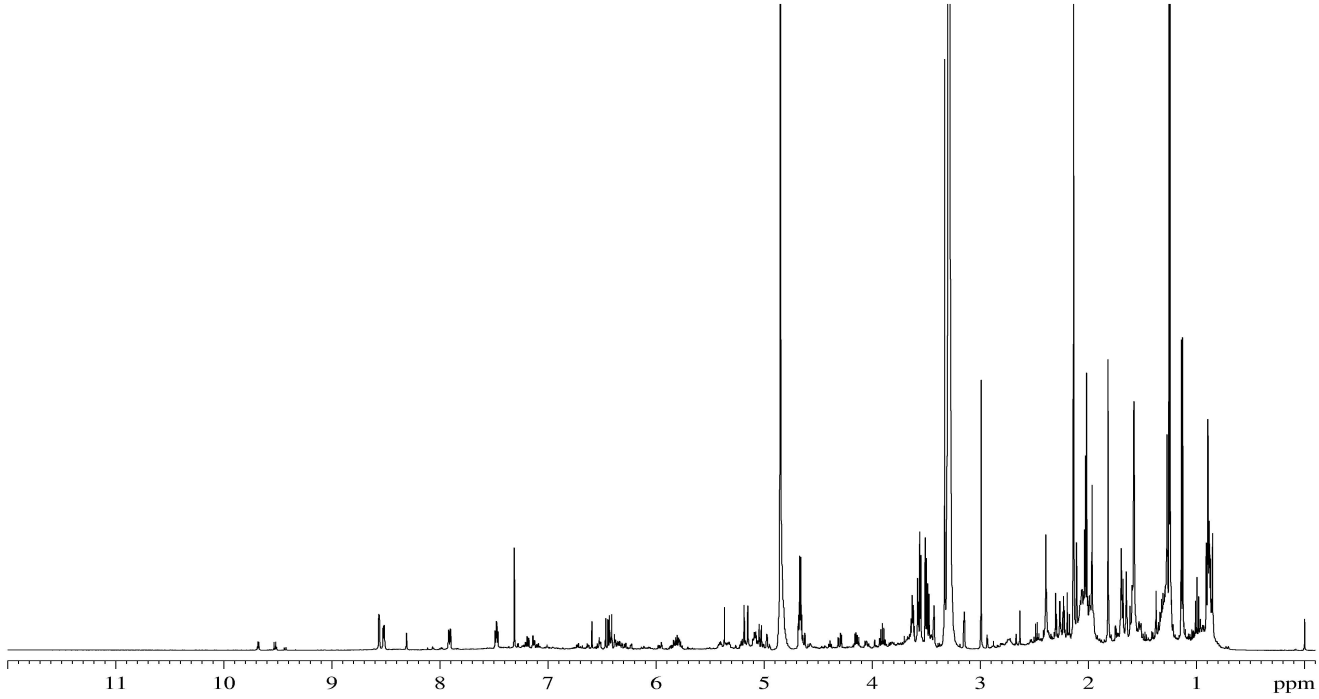
Supplementary Table S5. NMR peaks for compounds detected in the CM6 tobacco smoke condensate.

Compound name	NMR detectable in TSC	Peaks observed in TSC, ppm [1]
Acetaldehyde	yes	4.6836 (4.6826); 4.6733 (4.6723); 4.6630 (4.6620); 4.6526 (4.6517); 1.2535 (1.2528) 1.2432 (1.2424)
Isoprene	yes	6.4673 (6.4669); 6.4460 (6.4455) 6.4323 (6.4319); 6.4110 (6.4107); 5.1863 (5.1858); 5.1514 (5.1509); 5.0481 (5.0473); 5.0268 (5.026); 4.9764 (4.9759); 4.9534 (4.9527); (4.9515) not detected; (4.948) not detected; (4.9463) not detected
Nicotine	yes	8.5402 (8.543); 8.5363 (8.5394); 8.4954 (8.4990); 8.4922 (8.496); 8.4856 (8.4892); 8.4825 (8.4863); 7.9015 (7.9026); 7.8978 (7.8993); 7.8941 (7.8959); 7.8857 (7.8868); 7.8821 (7.8834); 7.8780 (7.8800); 7.4691 (7.4711); 7.4594 (7.4611); 7.4533 (7.4553); 7.4434 (7.4455); 2.1975 (previously unassigned)
Acetone	yes	2.1383 (previously unassigned)
1,3 Butadiene	Close to LOD	7.2 (7.2); 7.1938 (7.1927); 7.1789 (7.1783); 7.1401 (7.1393); 7.1194 (7.1181); 7.1082 (7.1045); 7.0912 (7.0908); (6.3504) not detected 5.218 (5.217); 5.1857 (5.1851, center of triplet); (5.0716) not detected; (5.0915) not detected; (2.3182) not detected
Acrolein	yes	9.5363 (9.5358); 9.5224 (9.5218); 6.5470 (6.5460); 6.5444 (6.5432); 6.3802 (6.3790); 6.3782 (6.3773); 6.37615 (6.3748); 6.3689 (6.3680); 6.3554 (6.3545); 6.3511 (6.3503); 6.3368 (6.3360);
Toluene	yes	7.2086 (7.2081); 7.1937 (7.1930); 7.1788 (7.1781); 7.1395 (7.1395); 7.1252 (7.1246); 7.1071 (7.1058); 7.0910 (7.0906); 7.0772 (7.0764); 2.30495 (2.3042)
Catechol	yes	6.7377 (6.7368); 6.7306 (6.7297); 6.7258 (6.7251); 6.7189 (6.7179); 6.6396 (6.6387); 6.6325 (6.6316); 6.6278 (6.6269); 6.6207 (6.6198)
Hydroquinone	yes	6.59465 (6.5934)
Formaldehyde	yes	4.6282 (4.6277)

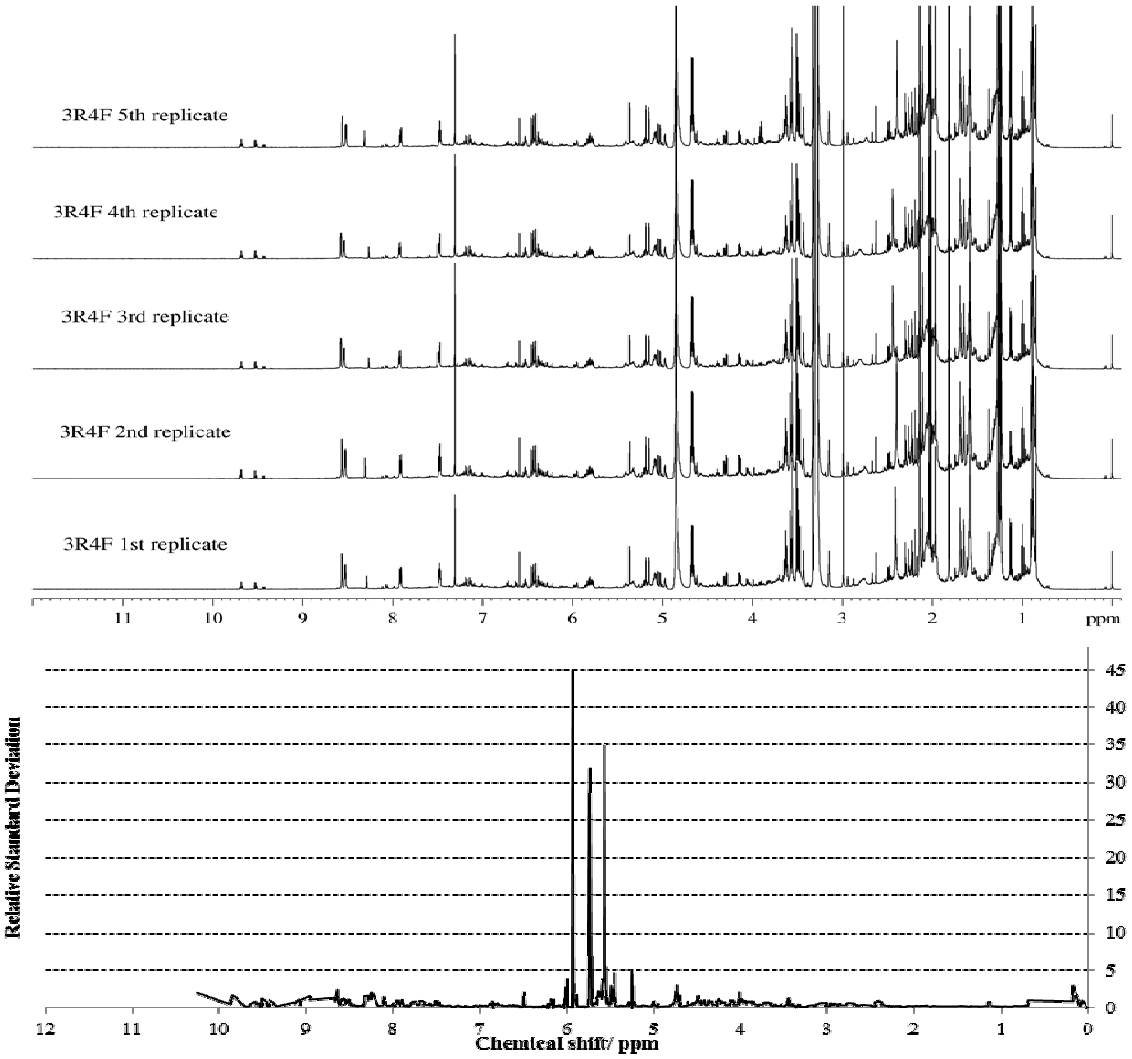
Compound name	NMR detectable in TSC	Peaks observed in TSC, ppm [1]
Acrylonitrile	yes	6.2649 (6.2640); 6.2623 (6.2622); 6.2293 (6.2283); 6.2272 (6.2265); 6.1381 (6.1369); 6.1364 (6.1352), 6.1146 (6.1134); 6.1126 (6.1117); 5.8690 (5.8682); 5.8453 (5.8446); 5.8331 (5.8324)
Propionaldehyde	yes	4.4027 (4.4018); 4.3918 (4.3910); 0.9090 (0.9086); 0.8945 (0.8939); 0.8797 (0.8791)
Crotonaldehyde	yes	9.4399 (9.4396); 9.4241 (9.4237)
Butyraldehyde	no	–
Butanone	yes	2.5027 (2.5019); 2.4878 (2.4872); 2.4730 (2.4726); 2.4590 (2.4582); 2.1102 (2.1094); 1.010 (1.0099); 0.9957 (0.9952); 0.9809 (0.9804)
Benzene	yes	7.3123 (7.3117)
Pyridine	yes	7.8370 (7.8360); All other peaks not detected
Phenol	yes	8.0690 (8.0682); 7.1503 (7.1498); 7.1192 (7.1183); 6.7714 (6.7699); 6.7487 (6.7481); 6.73345 (6.7318)
Styrene	yes	8.0683 (8.0683); 7.4076 (7.4041); 7.3687 (7.3890); 7.2872 (7.2876); 5.7668 (5.7649); 5.7303 (5.7290); 4.5733 (4.5732)
o-Cresol	yes	6.6920 (6.6915); 6.6870 (6.6859)
m-Cresol	no	–
p-Cresol	yes	6.95165 (6.9507); 6.9343 (6.9341); 6.6422 (6.6414); 6.62485 (6.6248)
Resorcinol	no	–
Quinoline	no	–
N-Nitrosonornicotine	no	–
1-Aminonaphtalene	no	–
2-Aminonaphtalene	no	–
3-Aminobiphenyl	no	–
N-Nitrosoanatabine	no	–
N-Nitrosoanabasine	no	–
N-Nitrosonornicotine-ketone	no	–
Benzopyrene	no	–
4-Aminobiphenil	no	–

[1] For each detected peak, the corresponding resonance frequency of the database is reported in parentheses.

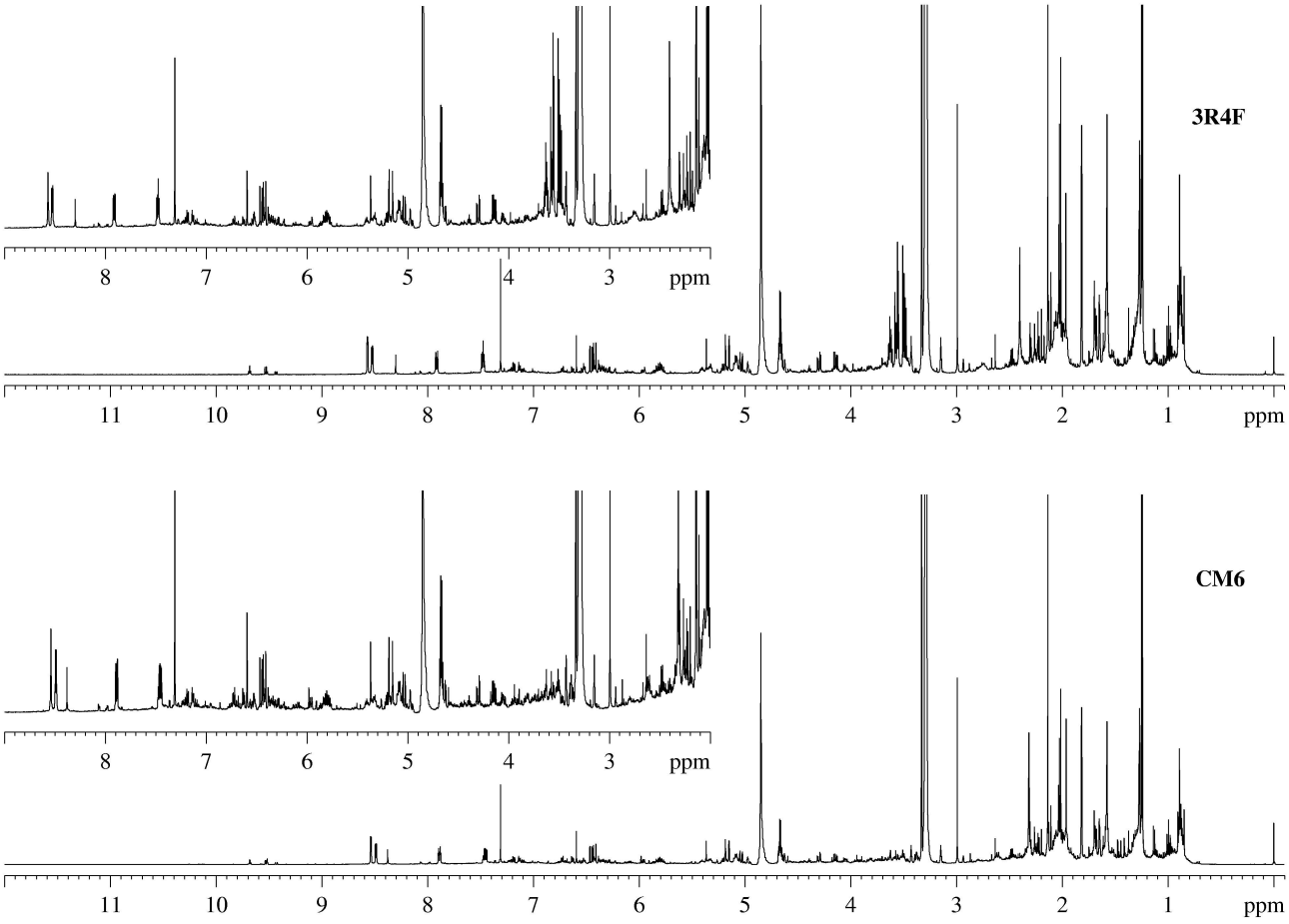
Supplementary Figure S1. Expanded ^{1}H NMR spectrum of 3R4F smoke condensate (see also Figure 2).



Supplementary Table Figure S2. Expanded stacked plot of the NMR spectra of five replicates of 3R4F smoke condensate, along with a plot of the relative standard deviation (see also Figure 3).



Supplementary Figure S3. Expanded stacked plot of the NMR spectra of 3R4F and CM6 smoke condensates. The NMR spectral profiles of these two samples showed a difference of 10% when peak areas where compared (see also Figure 4).



Supplementary Table S6. The relative recorded chemical shifts of HPHCs detected in different types of cigarette.

Compound	NMR detectability in TSC	Chemical shift in CD3OD	Type of cigarette smoke condensate		
			CM6	3R4F (from 10 cig)	3R4F (from 5 cig)
Caffeic acid	Detected	6.7526	?	?	?
		6.76903	6.7485	6.7485	6.7482
		6.9074 (doublet)	6.9053 (doublet not resolved	6.9053 (doublet not resolved)	6.9053 (doublet not resolved)
		6.9113 (doublet)	6.9053 (doublet not resolved)	6.9053 (doublet not resolved)	6.9053 (doublet not resolved)
		6.9236 (doublet)	6.9209 (doublet not resolved)	6.9209 (doublet not resolved)	6.9209 (doublet not resolved)
		6.9277 (doublet)	6.9209 (doublet not resolved)	6.9209 (doublet not resolved)	6.9209 (doublet not resolved)
		7.017	7.0125	7.0125	7.018
		7.0212	7.0163	7.0163	7.0157
		7.4963	?	?	?
		7.5281	?	?	?
4-(Nitroso-methylamino)-1-(3-pyridyl)-1-butanone	Detected	1.9786	1.992	1.9908	1.9913
		1.9925	2.004	2.004	2.004
		2.1806	2.1637	2.1637	2.1637
		2.1939	2.1761	?	?
		2.2079	2.1887	?	2.1881
		2.2217	2.23064	2.23064	2.23064
		2.2351	2.2447	2.2447	2.2447
		3.0175	3.0154	3.0143	3.0151
		3.0307	-?	3.0295	3.0307
		3.0448	-?	?	3.0448
		3.1122	3.1281	3.1281	3.1281
		3.1551	?	?	?
		3.1687	?	?	?
		3.1823	?	?	?
		3.7407	?	?	?
		3.7598	?	?	?
		3.7694	-?	?	?
		3.7997	3.7778	3.7793	3.7794
		4.2525	4.2304	shoulder at 4.2305	shoulder at 4.2301
		4.2662	shoulder at 4.2446	shoulder at 4.2446	shoulder at 4.2446

Compound	NMR detectability in TSC	Chemical shift in CD3OD	Type of cigarette smoke condensate		
			CM6	3R4F (from 10 cig)	3R4F (from 5 cig)
		4.2806	4.259	4.259	4.259
		7.5629	?	?	?
		7.5642	?	?	?
		7.5726	?	7.5552	7.5552
		7.574	?	7.5568	7.5563
		7.5787	?	7.5586	7.5589
		7.5801	?	7.5598	7.5589
		7.5886	?	?-	7.5679
		7.59	?	?	7.5692
		8.3462	?	obscured	obscured
		8.3502	?	obscured	obscured
		8.3564	?-	obscured	obscured
		8.3604	?-	obscured	obscured
		8.364	?	obscured	obscured
		8.376	?	8.342	?
		8.3803	?	8.346	?
		8.7252	?	?	8.6906
		8.7289	?	?	8.693
		8.7351	?-	?	8.7
		8.7385	?	?	8.7029
		9.0846	?	?	?
		9.0895	?	9.0638	9.0632
		9.09844	9.06736	9.0674	9.0705
		9.1028	9.06527	9.0744	9.0715
Acetamide	Detected	1.9305	1.9182	1.9181	1.9177
5-Methyl chrysene	Detected	7.5987	?	7.5992	?
		7.6132	?	?	?
		7.6448	?	?	?
		7.661	?	7.6318	?
		7.6746	?	7.6539	?
		7.9048	?	7.8901	?
		7.9184	?	7.9039	?
		7.9355	?	7.9201	?
		8.019	?	8.0042	?
		8.0369	?	8.0241	?
		8.0463	?	?	?
Chrysene	Detected	7.6299	?	?	?
		7.6324	?	?	?
		7.646	?	?	?
		7.6598	?	7.65975	?
		7.66	?	?	?

Compound	NMR detectability in TSC	Chemical shift in CD3OD	Type of cigarette smoke condensate		
			CM6	3R4F (from 10 cig)	3R4F (from 5 cig)
		7.6624	?	7.6621	?
		7.7064	?	7.7064	?
		7.7091	?	7.7094	?
		7.72026	?	7.7202	?
		7.72303	?	7.7234	?
		7.7258	?	7.7261	?
		7.73705	?	7.7372	?
		7.73966	?	7.7396	?
		8.016	?	?	?
		8.0319	?	?	?
		8.0439	?	8.044	?
		8.0621	?	8.0622	?
		8.798	-?	?	?
		8.816	-?	?	?
		8.854	-?	?	?
		8.8706	-?	?	?
o-Anisidine	Detected	3.8351	3.8192	3.8192	3.8192
		6.6721	?	?	?
		6.6761	6.672	6.672	6.672
		6.6867	?	?	?
		6.6906	?	?	?
		6.7016	6.6916	6.6916	shoulder
		6.7059	6.6956	6.6956	
		6.7095	obscured	obscured	obscured
		6.7128	obscured	obscured	obscured
		6.7247	?	?	?
		6.72766	?	?	?
		6.73906	obscured	obscured	obscured
		6.74202	obscured	obscured	obscured
		6.7457	6.733	6.733	6.728 (shoulder)
		6.7498	obscured	obscured	obscured
		6.76072	?	?	?
		6.76481	obscured	obscured	obscured
		6.81596	?	?	6.8058
		6.8191	?	?	6.8086
		6.8316	?	?	6.8203
		6.8344	?	?	6.8231
Pyrrolidine	Detected	1.6918	obscured	obscured	obscured
		1.7055	obscured	obscured	obscured
		1.7129	1.9853	1.9853	1.9853
		1.7192	1.9894	1.9894	1.9894
		1.7252	1.9978	obscured	obscured

Compound	NMR detectability in TSC	Chemical shift in CD_3OD	Type of cigarette smoke condensate		
			CM6	3R4F (from 10 cig)	3R4F (from 5 cig)
		1.7327	obscured	obscured	obscured
		1.7465	?	?	?
		2.7957	3.2079	3.2076	3.2076
		2.8085	3.2221	3.2203	3.2214
Ethyl benzene	Detected	1.2029	1.186	1.186	1.186
		1.2083	1.2011	1.2011	1.2011
		1.2352	obscured	obscured	obscured
		2.6043	2.5866	2.58676	2.5865
		2.6206	2.6015	2.6015	2.6015
		2.635	shoulder of peak at 2.6201	2.6171	2.6171
		2.6509	obscured	obscured	obscured
		3.3106	obscured	obscured	obscured
		7.1165	7.1514	7.1509	7.1509
		7.1306	7.165	7.165	7.165
		7.1439	7.168	7.168	7.168
		7.1709	obscured	obscured	obscured
		7.1514	obscured	obscured	obscured
		7.2428	obscured	obscured	obscured
		7.2577	7.226	7.2234	7.226
o-Toluidine	Detected	2.141	?	?	?
		6.60398 (doublet)	obscured	obscured	obscured
		6.6062 (doublet)	obscured	obscured	obscured
		6.619 (doublet)	6.612 (doublet not resolved)	6.612 (doublet not resolved)	6.612 (doublet not resolved)
		6.62094 (doublet)	6.612 (doublet not resolved)	6.612 (doublet not resolved)	6.612 (doublet not resolved)
		6.63355 (doublet)	6.6247	6.6247	6.6247
		6.6357 (doublet)	obscured	obscured	obscured
		6.6971 (doublet)	6.692 (doublet)	6.692 (doublet)	6.692 (doublet)
		6.713 (doublet)	6.7066 (doublet)	6.7066 (doublet)	6.7066 (doublet)
		6.9289	-?	-?	-?
		6.9444	6.9336	6.9336	6.9336
		6.9626	6.9559	6.9559	6.9559
		6.9786	6.9713	6.9713	6.9713
N-Nitroso-methyl ethyl amine	Detected	1.0598	?	?	?
		1.0742	?	?	?
		1.0888	?	?	?
		1.3432	?	?	?
		1.3576	?	?	?
		1.3721	?	?	?

Compound	NMR detectability in TSC	Chemical shift in CD3OD	Type of cigarette smoke condensate		
			CM6	3R4F (from 10 cig)	3R4F (from 5 cig)
		3.05847	?	?	?
		3.6263	obscured	obscured	obscured
		3.6408	obscured	obscured	obscured
		3.6553	obscured	obscured	obscured
		3.67	obscured	obscured	obscured
		3.734	?	?	3.662
		4.1583	obscured	obscured	obscured
		4.168	4.168	4.168	4.168
		4.1823	?	?	?
		4.20194	?	?	4.1776
N-Nitroso-morpholine	Detected	3.6279	3.6216	3.6214	3.6205
		3.6382	3.6322	3.6319	3.6314
		3.6489	3.6422	3.6422	3.6422
		4.2478	shoulder	shoulder	shoulder
		4.2596	4.2596	4.2596	4.2572
		4.2698	shoulder	shoulder	shoulder
		4.2798	?	?	?
Anabasine	Detected	1.555	?	?	?
		1.562	?	?	?
		1.58	?	?	?
		1.582	?	?	?
		1.5969	?	?	?
		1.601	?	?	?
		1.6216	?	?	?
		1.6272	?	?	?
		1.6842	?	?	?
		1.6894	?	shoulder at 1.9361	shoulder at 1.9554
		1.6946	?	?	?
		1.6995	?	?	?
		1.705	?	?	?
		1.7082	?	?	?
		1.71243	?	?	?
		1.8177	2.0505	2.0505	2.0505
		1.8218	?	?	?
		1.8281	?	?	?
		1.8383	2.0717	2.0732	2.0714
		1.8468	?	?	?
		1.9275	?	?	?
		2.7722	?	?	?
		2.7776	2.7755	2.7755	2.7752

Compound	NMR detectability in TSC	Chemical shift in CD3OD	Type of cigarette smoke condensate		
			CM6	3R4F (from 10 cig)	3R4F (from 5 cig)
		2.7961	?	?	?
		2.8017	?	?	?
		2.8198	?	?	?
		2.8254	?	?	?
		3.1469	?	3.1717	3.1719
		3.14695	?	?	?
		3.1677	obscured by peak at 3.1877	obscured by peak at 3.1877	obscured by peak at 3.1877
		3.1712	?	?	?
		3.1757	?	?	?
		3.6894	?	?	?
		3.6949	obscured by peak at 3.4684	obscured by peak at 3.4686	obscured by peak at 3.4687
		3.7114	obscured by peak at 3.4879	obscured by peak at 3.4879	obscured by peak at 3.4879
		3.7158	obscured by peak at 3.4879	obscured by peak at 3.4879	obscured by peak at 3.4879
		7.4023 (center of doublet)	?	7.5264	7.5264
		7.4126 (center of a doublet)	?	7.53715	7.5359
		7.4188 (center of a doublet)	?	7.54475	7.5436
		7.4286 (center of a doublet)	?	shoulder	shoulder
		7.85401 (double triplet)	?	?	?
		7.85742 (double triplet)	?	?	?
		7.86112 (double triplet)	?	?	?
		7.86974 (double triplet)	?	?	?
		7.87333 (double triplet)	?	?	?
		7.87685 (double triplet)	?	?	?
		8.4235	?	8.691	8.691
		8.4266	?	8.693	8.693
		8.4332	?	8.7	8.699
		8.4364	?	8.7035	8.7033
		8.5458	?	8.7372	8.7345
		8.5499	?	8.7419	8.7394
2,3 Benzofuran	Detected	6.82382	?	6.80552	obscured
		6.8256	?	6.80552	obscured
		6.82805	?	6.8088	obscured
		6.8299	?	6.8088	obscured
		7.1995	obscured	obscured	obscured
		7.2012	obscured	obscured	obscured
		7.2144	obscured	obscured	obscured
		7.2157	obscured	obscured	obscured

Compound	NMR detectability in TSC	Chemical shift in CD3OD	Type of cigarette smoke condensate		
			CM6	3R4F (from 10 cig)	3R4F (from 5 cig)
		7.2291	obscured	obscured	obscured
		7.2311	obscured	obscured	obscured
		7.2622	7.2423	7.2423	7.2423
		7.2647	7.2441	7.2441	7.2441
		7.2788	?	?	?
		7.2809	?	?	?
		7.29304	obscured	obscured	obscured
		7.29546	obscured	obscured	obscured
		7.47199	obscured	obscured	obscured
		7.4733	obscured	obscured	obscured
		7.48839	obscured	obscured	obscured
		7.48977	obscured	obscured	obscured
		7.59619	7.5762	7.5762	7.576
		7.61153	Obscured	obscured	obscured
		7.7265	?	?	?
		7.73089	?	?	?