

Supplement of

**Molecular Composition of Oxygenated Nitrogen-Containing Organic Compounds
Emitted from Combustion of the Three Biomass Macro-Components**

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Supplementary text

HR-MS analysis and instrument settings.

To minimize the well-known “matrix effects” during the HR-MS analysis processes, a widely used method is adoption the same carbon concentrations for analysis.(Jiang et al., 2021; Kellerman et al., 2014) Here, filters with same OC contents ($\sim 50 \mu\text{g C}$) were punched and extracted with the mixture of methanol and dichloromethane (v:v=1:1) to obtain the polar and less-polar OC fractions in the OAs. The combined extracts were then filtered and concentrated, stored in -20°C before further analysis.

A high-resolution Q-Exactive Orbitrap mass spectrometer equipped with a heated ESI source (Thermo Electron, Inc.) were used for the molecular composition analysis . As indicated in many previous studies, the ESI technique is focused on the analysis of polar compounds, such as acid, alcohol. Furthermore, the difference in the operation modes of negative and positive modes for these ionization techniques also influence the detected compound composition, because previous studies have shown that the compounds detected in negative modes always have higher oxidation degree than that of positive (Hoffmann et al., 2011; Jiang et al., 2018; Laskin et al., 2018). That means the compounds detected in negative are more oxidized, while a large number of reduced compounds could be identified in the positive modes.

Samples were directly injected through a syringe at a flow rate of $5 \mu\text{L}/\text{min}$, and an average mass spectrum of 5 min detection was obtained. The sources were operated in both negative and positive modes using spray voltages of 3.2 kV and 3.5 kV for ESI- and ESI+ at vaporizer temperature of 350°C , and spray currents of $10 \mu\text{A}$ and $5 \mu\text{A}$ for APCI- and APCI+ at vaporizer temperature of 400°C , respectively. Mass spectra data acquired in all modes was set in the range of m/z 90–800 with a mass resolving power of 120000 at m/z 200.

All the mass peaks with a signal-to-noise ratio (s/n) higher than 4 were exported using the Xcalibur software (V2.3, Thermo Scientific), and subsequently processed via an open-source R package of MFAssignR to obtain the elemental compositions (Schum et al., 2020). Before the formular assignment, all mass peaks were recalibrated with a series of O_xH_y compounds auto-selected by the function “recalibrate” in DOMAssignR. The final mass peaks obtained in the negative modes were assigned to the form of $\text{C}_x\text{H}_y\text{O}_{1-30}\text{N}_{0-5}\text{S}_{0-2}$ with several restrictions, H/C: 0.3-3; O/C: 0-2.5; DBE–O (double bond equivalents minus oxygen count): -20 -25. For the mass peaks obtained in the positive modes, O number allowed to be absent, and $[\text{H}]^+$ or $[\text{Na}]^+$ adducts were allowed to be present. Then, all the assigned formula can be classified into 4 groups (CHO, CHON, CHOS and CHNOS) based on the elemental composition for the negative modes, and additional groups of CH, CHN, CHS and CHNS can be determined in the positive modes. Molecules presented in the blank sample were all subtracted from the samples.

HR-MS data analysis and aromatic compounds classification

A series of elemental ratios (e.g., H/C and O/C), double bonds equivalent (DBE), modified aromatic index (AI_{mod}), (Koch and Dittmar, 2016) aromaticity equivalent (X_c) (Yassine et al., 2014) were calculated according to the equations reported in previous studies. The DBE and AI_{mod} can be calculated as:

$$DBE = (2c + 2 - h + n) / 2$$

$$AI_{mod} = (1 + c - 0.5o - s - 0.5h) / (c - 0.5o - s - n)$$

Where c, h, o, n and s represent the carbon, hydrogen, oxygen, nitrogen and sulfur atom numbers in the assigned formulae. Noted that the AI_{mod} could be set to 0 if $(c - 0.5o - s - n) \leq 0$ or $AI_{mod} < 0$. It is usually believed that a compounds with AI_{mod} higher than 0.5 may therefore contain a benzene ring, and AI_{mod} higher than 0.67 suggest the compounds may have condensed aromatic compounds. As mentioned earlier, the AI_{mod} cutoff could not identify the aromatic compounds effectively if it contained long-chain alkyl groups. In this study, due to the abundant cyclic structures containing in cellulose and hemicellulose, both DBE and AI_{mod} are insufficient to determine whether benzene-ring structures are present in the combustion products. And thus, the modified index of aromaticity equivalent (X_c) was also applied here and combined with the usages of AI_{mod} thresholds to identified the benzene-ring containing aromatic compounds. The X_c can be calculated using the following equation:

$$X_c = (3[DBE - (m \times o + n \times s)] - 2) / (DBE - (m \times o + n \times s))$$

Where m and n correspond to the fraction of oxygen and sulfur involved in the π -bond structure of the compound, respectively. If $DBE \leq (m \times o + n \times s)$, then $X_c = 0$ is assumed. For chemical classes including alcohol, ether, sulfide, disulfide, sulfinic and sulfonic acids, $m = n = 0$ should be used. And for chemical classes including carboxylic acid, ester and nitro, $m = 0.5$ was adopted. Here, as mentioned in previous study, a $m = n = 0.5$ was used here to minimize the complexity of the calculation, which is consistent with the calculations for biomass burning adopted by the authors who have proposed this index. A value of $X_c \geq 2.5000$ was supposed as the unambiguous minimum criterion for the presence of an aromatic structure. $X_c \geq 2.7143$, 2.8000, 2.8333, 2.9231 were considered as the thresholds for molecules containing cores of naphthalene, anthracene, pyrene and ovalene, respectively. Notably, the only use of X_c criteria may also lead to the loss in identification of benzene-ring containing aromatic compounds, such as methoxyphenol ($X_c = 2.33$). Therefore, those compounds with $AI_{mod} \geq 0.5$ but $X_c < 2.5$ were also included in the main text analysis parts. It should be also mentioned that the compounds with $AI_{mod} \geq 0.5$ but $X_c < 2.5$ are all composed by the compounds having carbon number lower than 14, therefore the compounds with AI_{mod} in the range of [0.5, 0.67] can therefore have 1 benzene-ring. And the compounds with $AI_{mod} \geq 0.67$, but C number in the range of [6, 10] could also be classified in the 1 benzene-ring compound group. The other compounds with $AI_{mod} \geq 0.67$ could be all classified in the 2 benzene-ring compound group.

Nevertheless, the aromatic compounds screen out using these criteria may not all contain aromatic rings, which means that the proportion of aromatic compounds may be overestimated. An important possible reason for this overestimation is that AI_{mod} or X_c index cannot distinguish between benzene rings and compounds

with multiple rings. Especially in the OAs from the combustion of cellulose and hemicellulose, polymeric structures with multiple pyran rings are likely to be identified as having a benzene ring structure during analysis. Given that the complexity in the molecular composition of aromatic compounds, the workflow describe above still was a simple and effective method for aromatic compound classification.

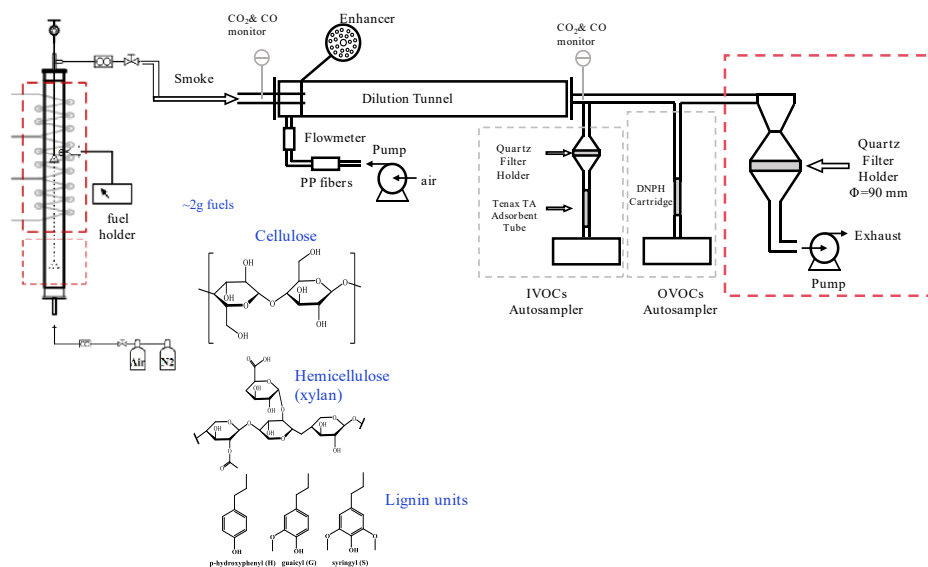


Figure S1. Fuel structures, combustion, dilution and sampling system used in this work.

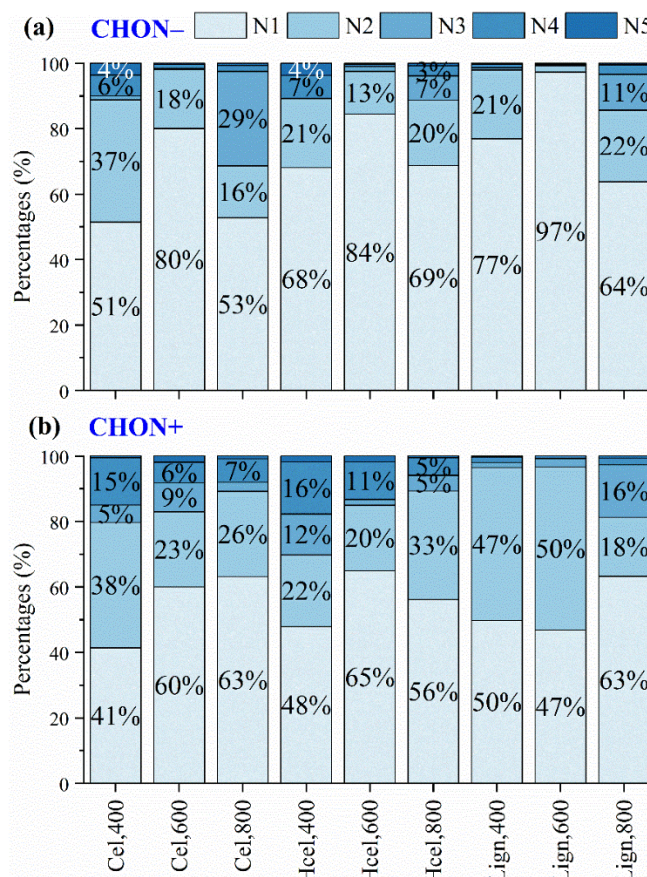


Figure S2. The molecular distribution of CHON- and CHON+ compounds with the number of nitrogen atoms.

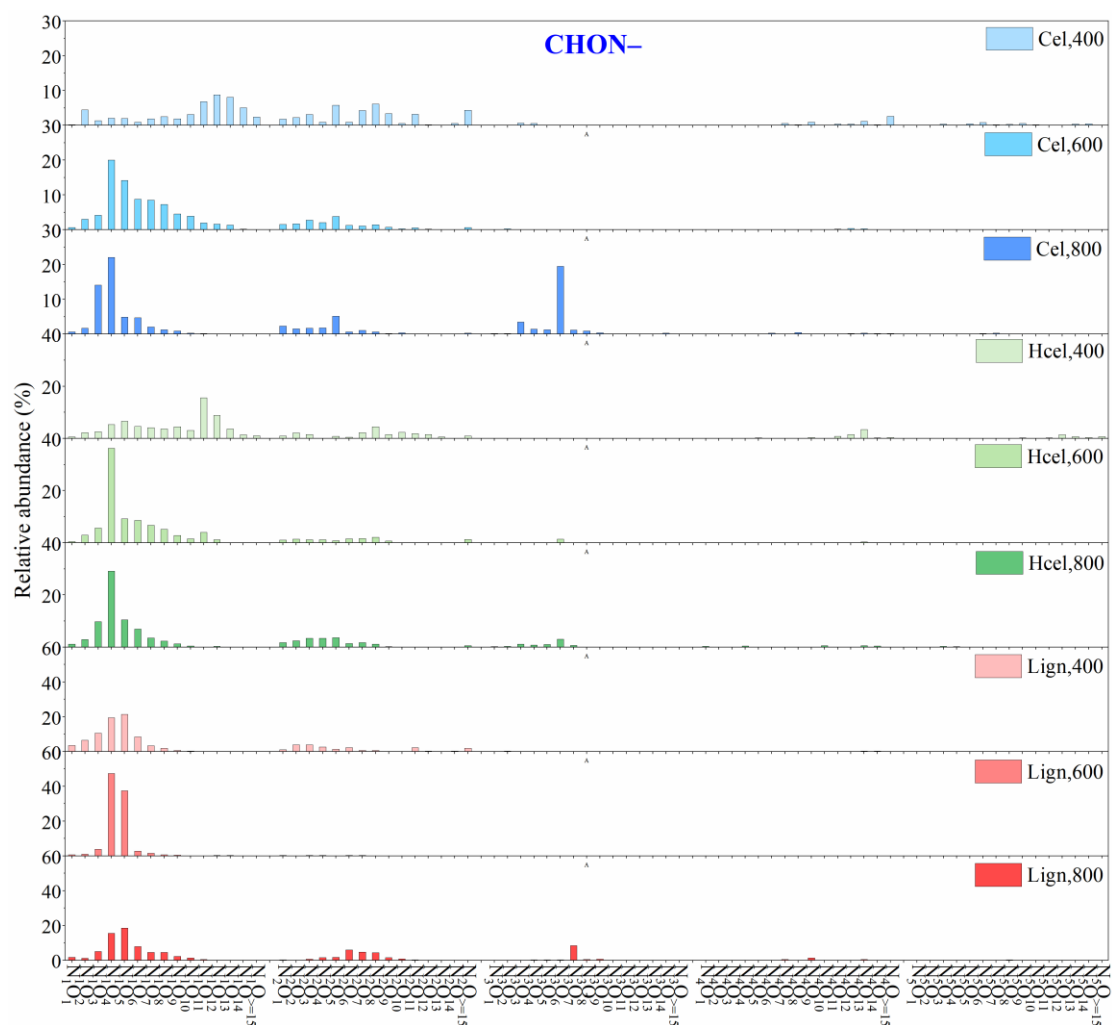


Figure S3. Classification of CHON- compounds into different subgroups according to the number of N and O atoms in their molecules.

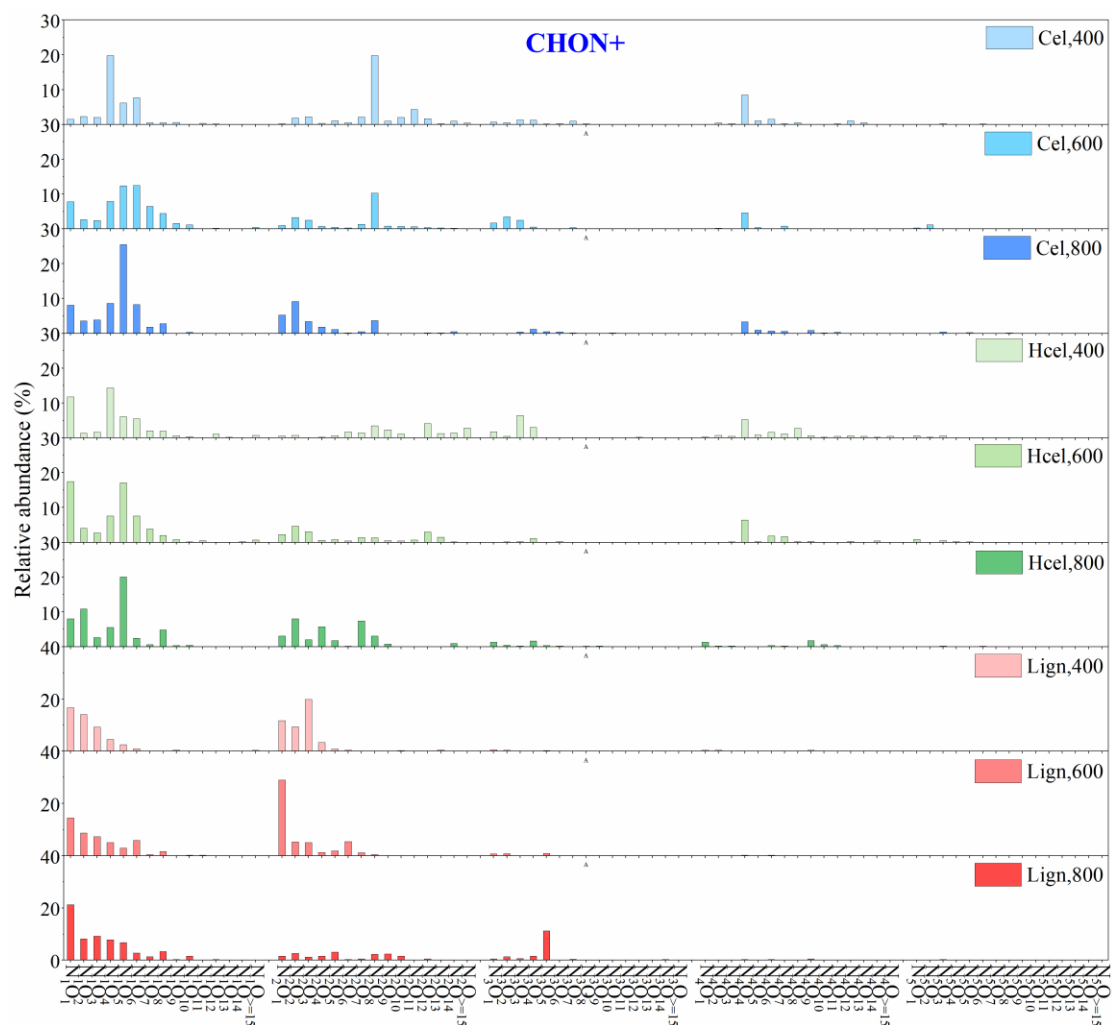


Figure S4. Classification of CHON⁺ compounds into different subgroups according to the number of N and O atoms in their molecules.

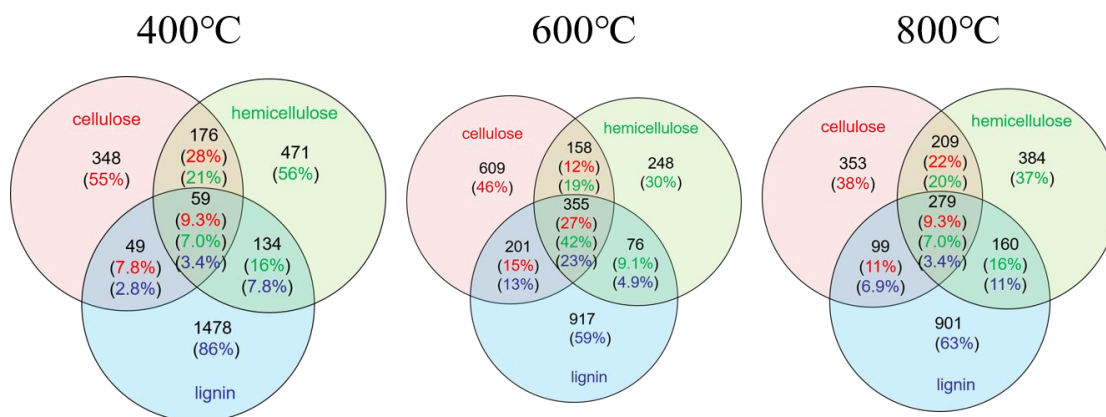


Figure S5. Venn diagrams showing the relative distributions of all CHON formulae present in OAs from the TMBCs at the IGT of 400 °C, 600 °C and 800 °C, respectively. Percentages in areas of overlap are formula number percentages of CHON compounds that appear in the corresponding samples. Percentages in areas with no overlap are unique to that individual sample.

Table S1. The intensity-weighted average values of atoms number, elemental ratios, molecular weight (MW), double-bond equivalents (DBEs) and aromaticity index (AI_{mod} and X_C) for the CHON compounds.

		Cellulose			Hemicellulose			Lignin		
		400°C	600°C	800°C	400°C	600°C	800°C	400°C	600°C	800°C
Modified combustion efficiency (MCE)		0.89	0.97	0.98	0.96	0.84	0.92	0.92	0.95	0.99
CHON−	Formula number	327	996	689	396	565	808	894	774	1042
	Formula (%)	14	39	27	15	25	34	40	41	53
	Intensity (%)	1.3	12	11	1.5	5.2	18	14	60	52
CHON+	Formula number	309	505	333	451	332	300	1098	946	455
	Formula (%)	24	38	34	29	28	34	48	45	30
	Intensity (%)	4.3	8.1	6.9	3.4	5.5	8.4	29	32	11

Table S2. The intensity-weighted average values of atoms number, elemental ratios, molecular weight (MW), double-bond equivalents (DBEs) and aromaticity index (AI_{mod} and X_C) for the CHON– compounds.

	Cellulose			Hemicellulose			Lignin		
	400°C	600°C	800°C	400°C	600°C	800°C	400°C	600°C	800°C
MW*	347	267	261	324	261	241	253	192	255
C*	13.34	11.76	12.38	12.17	11.83	11.10	11.99	7.98	10.80
H*	13.83	12.20	9.42	13.33	12.02	10.42	12.66	7.95	8.50
O*	9.31	5.99	4.87	8.90	5.61	4.78	4.89	4.58	5.92
N*	1.73	1.24	1.82	1.58	1.19	1.47	1.27	1.04	1.54
MW*	347	267	261	324	261	241	253	192	255
O/C*	0.76	0.54	0.45	0.81	0.52	0.47	0.45	0.59	0.60
H/C*	1.07	1.04	0.83	1.16	1.02	0.95	1.05	0.99	0.81
N/C*	0.16	0.12	0.17	0.15	0.12	0.15	0.12	0.14	0.16
O/N*	6.91	5.35	3.25	7.01	5.03	3.81	4.08	4.47	4.43
DBE*	8.29	7.29	9.57	7.30	7.42	7.63	7.30	5.53	8.32
DBE/C*	0.63	0.64	0.77	0.59	0.65	0.71	0.64	0.70	0.78
nO_{eff}^*	5.84	3.50	1.24	5.74	3.23	1.83	2.34	2.49	2.84
AI_{mod}^*	0.35	0.43	0.61	0.31	0.47	0.55	0.47	0.48	0.60
X_C^*	1.67	2.37	2.56	1.63	2.36	2.49	2.42	2.36	2.49

Table S3. The intensity-weighted average values of atoms number, elemental ratios, molecular weight (MW), double-bond equivalents (DBEs) and aromaticity index (AI_{mod} and X_C) for the CHON+ compounds.

	Cellulose			Hemicellulose			Lignin		
	400°C	600°C	800°C	400°C	600°C	800°C	400°C	600°C	800°C
MW*	373	337	288	345	348	316	306	385	291
C*	18.66	17.31	14.54	16.70	18.59	16.74	18.16	23.88	15.08
H*	25.56	23.84	22.05	23.36	27.44	22.15	23.89	32.08	22.83
O*	6.01	5.13	4.31	5.78	4.62	4.38	2.64	2.72	4.05
N*	1.94	1.67	1.57	2.02	1.66	1.61	1.56	1.57	1.59
MW*	373	337	288	345	348	316	306	385	291
O/C*	0.44	0.41	0.41	0.43	0.37	0.41	0.18	0.20	0.34
H/C*	1.32	1.33	1.47	1.34	1.41	1.43	1.31	1.33	1.51
N/C*	0.19	0.15	0.17	0.18	0.16	0.15	0.11	0.11	0.14
O/N*	3.70	3.97	3.41	3.58	3.45	3.21	1.92	2.07	2.90
DBE*	7.85	7.22	5.30	7.03	6.70	7.47	8.00	9.63	5.46
DBE/C*	0.51	0.50	0.46	0.51	0.46	0.45	0.48	0.46	0.40
nO_{eff}^*	2.12	1.79	1.18	1.73	1.30	1.16	-0.49	-0.42	0.87
AI_{mod}^*	0.31	0.27	0.23	0.31	0.23	0.27	0.36	0.34	0.23
X_C^*	1.58	1.99	1.92	1.71	1.95	1.90	2.54	2.52	1.72

Table S4. The intensity-weighted average values of atoms number, elemental ratios, molecular weight (MW), double-bond equivalents (DBEs) and aromaticity index (AI_{mod} and X_C) for the CHON compounds.

			Cellulose			Hemicellulose			Lignin		
			400°C	600°C	800°C	400°C	600°C	800°C	400°C	600°C	800°C
CHON-	O/N $\geq$ 3	Formula number	272	806	407	345	475	484	590	614	833
		Formula (%)	83	81	59	87	84	60	66	79	80
		Intensity (%)	75	83	56	87	89	71	76	96	80
CHON+	O/N $\geq$ 3	Formula number	200	334	166	283	185	137	368	401	213
		Formula (%)	65	66	50	63	56	46	34	42	47
		Formula (%)	72	65	57	56	52	50	20	31	42
Common CHON compounds with O/N $\geq$ 3		Formula number	12	153	52	13	51	36	123	117	39
		% of total CHON+	6.0	46	31	4.6	28	26	33	29	18
		% of CHON+ with O/N $\geq$ 3	3.9	30.3	15.6	2.9	15.4	12.0	11.2	12.4	8.6
		% of total CHON+ intensity	1.8	27	19	4.4	9.5	7.7	10	7.9	5.4

Table S5. The most 50 intense aromatic CHON– compounds detected in the organic aerosols from the cellulose combustion at 400 °C, 600 °C and 800 °C.

400 °C			600 °C			800 °C		
Formula	Ring number	RI%	Formula	Ring number	RI%	Formula	Ring number	RI%
C ₆ H ₅ NO ₄	1	17	C ₇ H ₅ NO	1	6.1	C ₅ H ₆ N ₂ O	0	4.4
C ₉ H ₈ N ₂ O	2	14	C ₈ H ₈ N ₂ O	1	11	C ₄ H ₅ N ₃ O ₃	0	2.2
C ₉ H ₁₀ N ₂ O	1	14	C ₆ H ₅ NO ₄	1	100	C ₆ H ₅ NO ₄	1	59
C ₉ H ₉ NO ₂	1	87	C ₉ H ₁₀ N ₂ O	1	5.8	C ₇ H ₇ NO ₄	1	31
C ₁₀ H ₈ N ₂ O ₂	2	43	C ₉ H ₉ NO ₂	1	12	C ₈ H ₅ NO ₄	1	5.2
C ₁₀ H ₁₀ N ₂ O ₃	1	41	C ₈ H ₉ NO ₃	1	6.8	C ₉ H ₉ NO ₃	1	1.7
C ₉ H ₄ N ₂ O ₅	2	100	C ₇ H ₇ NO ₄	1	77	C ₉ H ₁₁ NO ₃	1	1.8
C ₁₁ H ₁₁ NO ₄	1	17	C ₆ H ₅ NO ₅	1	43	C ₈ H ₉ NO ₄	0	9.3
C ₆ H ₁₁ NO ₈	0	26	C ₁₀ H ₁₀ N ₂ O	2	5.8	C ₇ H ₉ N ₃ O ₃	1	16
C ₁₂ H ₉ NO ₅	2	11	C ₈ H ₉ NO ₄	0	70	C ₈ H ₁₁ NO ₄	0	1.7
C ₆ H ₄ N ₂ O ₉	0	17	C ₇ H ₇ NO ₅	0	51	C ₁₀ H ₇ NO ₃	2	1.7
C ₈ H ₁₂ N ₂ O ₉	0	18	C ₉ H ₇ NO ₄	1	6.2	C ₁₀ H ₉ NO ₃	1	1.8
C ₇ H ₁₀ N ₂ O ₁₁	0	33	C ₁₀ H ₁₁ NO ₃	1	7.4	C ₉ H ₇ NO ₄	1	9.1
C ₁₈ H ₆ N ₂ O ₄	5	10	C ₉ H ₉ NO ₄	1	8.5	C ₉ H ₉ NO ₄	1	3.0
C ₁₂ H ₆ N ₄ O ₇	2	11	C ₉ H ₁₁ NO ₄	0	22	C ₆ H ₃ N ₃ O ₅	1	3.1
C ₉ H ₁₂ N ₂ O ₁₁	0	14	C ₄ H ₉ NO ₈	0	13	C ₉ H ₁₁ NO ₄	0	1.8
C ₁₀ H ₁₅ NO ₁₁	0	11	C ₈ H ₉ NO ₅	0	18	C ₁₀ H ₉ NO ₄	1	6.2
C ₁₉ H ₁₃ N ₃ O ₃	4	13	C ₈ H ₁₃ NO ₅	0	6.3	C ₁₀ H ₁₁ NO ₄	1	2.8
C ₁₃ H ₁₁ N ₅ O ₆	2	11	C ₁₀ H ₁₀ N ₂ O ₃	1	14	C ₉ H ₁₀ N ₂ O ₄	1	1.8
C ₁₆ H ₆ N ₂ O ₇	4	12	C ₁₀ H ₉ NO ₄	1	7.3	C ₁₀ H ₁₃ NO ₄	0	1.6
C ₁₁ H ₁₇ NO ₁₁	0	17	C ₁₀ H ₁₁ NO ₄	1	8.9	C ₉ H ₄ N ₂ O ₅	2	3.1
C ₁₄ H ₁₅ NO ₉	1	10	C ₉ H ₉ NO ₅	1	6.8	C ₁₁ H ₁₁ NO ₄	1	2.6
C ₁₅ H ₆ N ₂ O ₈	3	27	C ₁₀ H ₁₃ NO ₄	0	6.4	C ₁₀ H ₉ NO ₅	1	1.7
C ₁₂ H ₁₅ NO ₁₁	0	12	C ₉ H ₁₁ NO ₅	0	15	C ₁₂ H ₇ NO ₄	2	1.8
C ₇ H ₁₆ N ₂ O ₁₄	0	11	C ₉ H ₄ N ₂ O ₅	2	37	C ₁₀ H ₆ N ₂ O ₅	2	6.3
C ₁₆ H ₆ N ₂ O ₈	3	11	C ₁₁ H ₁₁ NO ₄	1	8.8	C ₁₂ H ₁₃ NO ₄	1	1.6
C ₁₆ H ₈ N ₂ O ₈	3	19	C ₁₀ H ₉ NO ₅	1	6.2	C ₁₀ H ₉ NO ₆	1	1.8
C ₁₃ H ₄ N ₄ O ₉	3	18	C ₁₀ H ₁₁ NO ₅	1	8.4	C ₁₀ H ₁₂ N ₂ O ₅	1	1.8
C ₁₆ H ₂₀ N ₂ O ₈	1	22	C ₁₀ H ₁₃ NO ₅	0	6.6	C ₈ H ₇ N ₃ O ₆	1	23
C ₁₂ H ₁₉ NO ₁₂	0	85	C ₁₁ H ₁₁ NO ₅	1	10	C ₁₀ H ₁₁ NO ₆	0	2.4
C ₁₆ H ₁₅ NO ₁₀	1	11	C ₁₀ H ₉ NO ₆	1	7.2	C ₇ H ₅ N ₃ O ₇	1	2.7
C ₁₂ H ₁₇ NO ₁₃	0	26	C ₁₁ H ₁₃ NO ₅	1	6.7	C ₁₁ H ₇ N ₃ O ₄	2	2.0
C ₁₂ H ₁₉ NO ₁₃	0	43	C ₁₀ H ₁₁ NO ₆	0	7.2	C ₁₂ H ₁₃ NO ₅	1	2.4
C ₂₀ H ₈ N ₂ O ₇	5	12	C ₁₂ H ₁₃ NO ₅	1	6.8	C ₁₆ H ₉ NO ₃	4	59
C ₁₅ H ₂₁ NO ₁₁	0	11	C ₁₁ H ₁₁ NO ₆	1	8.4	C ₁₃ H ₉ N ₃ O ₄	2	2.3
C ₁₄ H ₁₉ NO ₁₂	0	11	C ₁₁ H ₁₃ NO ₆	0	8.9	C ₁₇ H ₁₁ NO ₃	4	3.1
C ₂₇ H ₁₁ NO ₃	7-9	13	C ₁₂ H ₁₃ NO ₆	1	9.7	C ₁₈ H ₉ NO ₃	4	1.9
C ₁₇ H ₁₉ NO ₁₀	1	13	C ₁₂ H ₁₅ NO ₆	0	6.1	C ₁₃ H ₁₁ N ₃ O ₅	2	2.0
C ₁₆ H ₁₉ NO ₁₁	0	15	C ₁₃ H ₁₃ NO ₆	1	5.8	C ₂₁ H ₁₀ N ₂ O	6	5.9
C ₁₄ H ₁₉ NO ₁₃	0	18	C ₁₂ H ₁₃ NO ₇	1	6.7	C ₁₆ H ₈ N ₂ O ₅	4	3.0
C ₁₆ H ₁₉ NO ₁₂	0	18	C ₁₂ H ₁₅ NO ₇	0	5.9	C ₂₀ H ₁₁ NO ₃	5	1.8
C ₂₂ H ₁₄ N ₂ O ₇	4	19	C ₁₃ H ₁₅ NO ₇	1	6.1	C ₁₅ H ₇ N ₃ O ₆	3	3.4
C ₁₆ H ₂₁ NO ₁₂	0	11	C ₁₅ H ₁₅ NO ₆	1	5.8	C ₁₅ H ₆ N ₂ O ₇	3	2.5
C ₁₅ H ₂₁ NO ₁₃	0	13	C ₁₄ H ₁₅ NO ₇	1	5.8	C ₁₄ H ₇ N ₃ O ₇	3	2.3
C ₁₄ H ₂₁ NO ₁₄	0	33	C ₁₅ H ₁₅ NO ₇	1	6.2	C ₂₂ H ₁₁ NO ₃	6	1.8
C ₈ H ₁₀ N ₄ O ₁₇	0	27	C ₁₅ H ₁₇ NO ₇	1	5.8	C ₁₅ H ₅ N ₃ O ₈	3	2.5
C ₁₂ H ₆ N ₂ O ₁₇	0	10	C ₁₆ H ₁₇ NO ₈	1	5.8	C ₂₀ H ₁₀ N ₂ O ₅	5	13

C ₁₈ H ₂₃ NO ₁₃	0	15	C ₁₀ H ₁₇ NO ₁₃	0	5.8	C ₁₅ H ₅ N ₃ O ₉	3	1.8
C ₁₇ H ₂₃ NO ₁₄	0	10	C ₁₇ H ₁₇ NO ₈	1	6.0	C ₁₉ H ₉ N ₃ O ₆	4	100
C ₁₈ H ₂₅ NO ₁₅	0	11	C ₂₇ H ₄₁ NO ₇	1	11	C ₈ H ₁₅ N ₃ O ₁₄	0	2.1

Table S6. The most 50 intense aromatic CHON⁺ compounds detected in the organic aerosols from the cellulose combustion at 400 °C, 600 °C and 800 °C.

400 °C			600 °C			800 °C		
Formula	Ring number	RI%	Formula	Ring number	RI%	Formula	Ring number	RI%
C ₅ H ₅ NO	0	3.3	C ₅ H ₅ NO	0	21	C ₅ H ₅ NO	0	11
C ₆ H ₇ NO	1	2.1	C ₆ H ₇ NO	1	17	C ₄ H ₆ N ₂ O	0	4.7
C ₇ H ₁₅ NO ₂	0	7.0	C ₅ H ₆ N ₂ O ₂	0	4.5	C ₅ H ₆ N ₂ O	0	11
C ₅ H ₆ N ₄ O ₄	0	41	C ₇ H ₉ NO	1	4.7	C ₄ H ₇ NO ₂	0	6.9
C ₇ H ₁₅ NO ₄	0	16	C ₆ H ₈ N ₂ O ₂	0	6.9	C ₆ H ₇ NO	1	45
C ₁₀ H ₁₀ N ₂ O ₃	1	10	C ₇ H ₉ NO ₂	0	4.1	C ₆ H ₈ N ₂ O	1	20
C ₁₂ H ₆ N ₂ O ₂	3	7.1	C ₈ H ₈ N ₂ O ₂	1	5.8	C ₇ H ₉ NO	1	8.6
C ₁₀ H ₅ N ₃ O ₄	2	6.0	C ₁₁ H ₁₁ NO	2	4.4	C ₇ H ₁₀ N ₂ O	1	9.9
C ₁₅ H ₅ NO ₂	4	2.5	C ₆ H ₁₁ NO ₄	0	5.4	C ₆ H ₈ N ₂ O ₂	0	19
C ₉ H ₁₉ NO ₅	0	3.8	C ₈ H ₁₀ N ₂ O ₃	1	6.6	C ₆ H ₁₀ N ₂ O ₂	0	13
C ₅ H ₁₀ N ₄ O ₆	0	5.1	C ₅ H ₆ N ₄ O ₄	0	47	C ₅ H ₈ N ₂ O ₃	0	8.4
C ₁₅ H ₇ N ₃ O	4	3.0	C ₄ H ₉ NO ₈	0	8.6	C ₉ H ₁₁ NO ₂	1	6.6
C ₇ H ₉ N ₃ O ₇	0	3.0	C ₈ H ₁₃ NO ₅	0	19	C ₈ H ₁₀ N ₂ O ₂	1	4.7
C ₁₆ H ₉ N ₃ O ₂	4	2.5	C ₉ H ₁₅ NO ₅	0	20	C ₈ H ₁₂ N ₂ O ₂	0	4.7
C ₁₁ H ₁₉ NO ₈	0	2.2	C ₉ H ₁₅ NO ₆	0	4.1	C ₆ H ₉ NO ₄	0	4.7
C ₁₅ H ₂₂ N ₄ O ₄	1	2.1	C ₉ H ₇ NO ₆	1	20	C ₉ H ₈ N ₂ O ₂	1	11
C ₁₁ H ₁₄ N ₄ O ₈	0	2.2	C ₉ H ₉ NO ₇	0	5.3	C ₆ H ₁₁ NO ₄	0	8.1
C ₁₈ H ₃₇ NO ₄	0	3.7	C ₅ H ₁₂ N ₄ O ₇	0	8.2	C ₉ H ₁₀ N ₂ O ₂	1	4.7
C ₁₈ H ₁₁ N ₃ O ₃	4	6.4	C ₁₁ H ₁₇ NO ₆	0	5.1	C ₉ H ₁₂ N ₂ O ₂	1	5.3
C ₅ H ₁₂ N ₄ O ₁₂	0	5.0	C ₁₁ H ₁₅ NO ₆	0	4.3	C ₈ H ₁₀ N ₂ O ₃	1	5.2
C ₁₉ H ₃₉ NO ₄	0	11	C ₁₅ H ₁₅ NO ₄	2	4.0	C ₅ H ₆ N ₄ O ₄	0	26
C ₂₀ H ₄₁ NO ₄	0	2.7	C ₁₂ H ₁₅ NO ₆	0	6.7	C ₇ H ₁₅ NO ₄	0	18
C ₁₄ H ₁₅ NO ₉	1	2.7	C ₁₁ H ₁₇ NO ₇	0	4.5	C ₄ H ₉ NO ₈	0	24
C ₆ H ₁₄ N ₄ O ₁₃	0	2.5	C ₁₂ H ₁₇ NO ₇	0	7.0	C ₁₀ H ₁₃ NO ₃	1	5.5
C ₂₀ H ₈ N ₂ O ₅	6	3.3	C ₁₂ H ₁₅ NO ₇	0	14	C ₈ H ₁₃ NO ₅	0	41
C ₂₀ H ₃₉ NO ₅	0	2.7	C ₁₅ H ₁₅ NO ₅	2	4.5	C ₉ H ₁₅ NO ₅	0	25
C ₂₀ H ₄₁ NO ₅	0	4.1	C ₂₀ H ₂₁ N ₃ O	4	7.5	C ₉ H ₇ NO ₆	1	18
C ₁₈ H ₁₂ N ₂ O ₇	3	2.8	C ₁₃ H ₁₉ NO ₇	0	5.2	C ₁₁ H ₁₅ NO ₅	0	6.5
C ₂₃ H ₄₇ NO ₃	0	2.2	C ₂₂ H ₂₅ N ₃ O	4	8.3	C ₁₁ H ₁₇ NO ₅	0	6.4
C ₂₁ H ₄₁ NO ₅	0	3.7	C ₂₂ H ₂₅ N ₃ O ₂	3	4.2	C ₁₀ H ₁₅ NO ₆	0	7.8
C ₂₁ H ₄₁ NO ₄	0	7.0	C ₂₃ H ₂₇ N ₃ O ₂	3	13	C ₁₂ H ₁₇ NO ₅	0	6.5
C ₂₀ H ₁₂ N ₂ O ₇	4	2.2	C ₂₄ H ₂₉ N ₃ O ₂	3	12	C ₁₂ H ₁₉ NO ₅	0	6.1
C ₂₁ H ₄₃ NO ₅	0	4.5	C ₂₅ H ₃₁ N ₃ O ₂	3	4.8	C ₁₃ H ₁₉ NO ₅	0	5.0
C ₂₀ H ₁₂ N ₂ O ₈	4	100	C ₁₈ H ₁₄ N ₂ O ₈	2	100	C ₁₆ H ₂₉ NO ₃	0	6.2
C ₂₃ H ₄₅ NO ₅	0	4.5	C ₂₅ H ₃₁ N ₃ O ₃	3	9.9	C ₉ H ₁₈ N ₂ O ₈	0	4.9
C ₂₂ H ₄₃ NO ₆	0	7.9	C ₂₂ H ₄₃ NO ₆	0	6.6	C ₁₃ H ₁₉ NO ₆	0	9.3
C ₂₆ H ₅₃ NO ₄	0	5.9	C ₂₆ H ₃₃ N ₃ O ₃	3	13	C ₁₈ H ₃₇ NO ₄	0	5.4
C ₂₄ H ₄₅ NO ₆	0	23	C ₂₆ H ₅₃ NO ₄	0	4.9	C ₁₀ H ₂₀ N ₄ O ₉	0	9.2
C ₃₀ H ₆₁ NO ₄	0	2.9	C ₂₄ H ₄₅ NO ₆	0	28	C ₂₁ H ₃₂ N ₂ O ₂	1	16
C ₁₉ H ₂₂ N ₂ O ₁₄	0	3.6	C ₂₃ H ₂₂ N ₂ O ₁₁	2	4.1	C ₂₀ H ₂₉ N ₃ O ₄	1	12
C ₂₃ H ₂₂ N ₂ O ₁₁	2	9.4	C ₃₂ H ₆₅ NO ₄	0	4.7	C ₁₇ H ₃₇ N ₅ O ₃	0	4.7
C ₂₅ H ₂₀ N ₂ O ₁₁	4	9.4	C ₃₂ H ₁₈ N ₂ O ₇	7-9	7.6	C ₂₀ H ₁₂ N ₂ O ₈	4	30
C ₂₄ H ₁₈ N ₂ O ₁₂	3	5.9	C ₃₄ H ₆₉ NO ₄	0	19	C ₂₄ H ₄₅ NO ₆	0	24

C ₃₃ H ₅₉ NO ₄	0	5.2	C ₃₄ H ₅₅ NO ₅	1	4.8	C ₃₀ H ₃₆ N ₂ O ₄	4	9.1
C ₃₄ H ₆₉ NO ₄	0	23	C ₃₄ H ₅₇ NO ₅	1	32	C ₃₂ H ₆₅ NO ₄	0	6.9
C ₃₆ H ₇₃ NO ₄	0	14	C ₃₆ H ₇₃ NO ₄	0	11	C ₃₂ H ₅₅ NO ₅	1	5.1
C ₃₈ H ₇₇ NO ₄	0	3.8	C ₄₀ H ₅₉ N ₅ O ₂	4	12	C ₂₉ H ₅₄ N ₄ O ₅	0	5.7
C ₄₀ H ₇₉ NO ₃	0	3.1	C ₄₁ H ₆₁ NO ₆	2	12	C ₃₄ H ₆₉ NO ₄	0	13
C ₄₀ H ₈₁ NO ₃	0	2.7	C ₅₀ H ₆₉ NO	6	6.0	C ₃₄ H ₅₅ NO ₅	1	22
C ₄₀ H ₈₁ NO ₄	0	2.0	C ₅₁ H ₇₁ NO	6	12	C ₃₄ H ₅₇ NO ₅	1	100

Table S7. The most 50 intense aromatic CHON– compounds detected in the organic aerosols from the hemicellulose combustion at 400 °C, 600 °C and 800 °C.

400 °C			600 °C			800 °C		
Formula	Ring number	RI%	Formula	Ring number	RI%	Formula	Ring number	RI%
C ₃ H ₃ NO ₃	0	17	C ₈ H ₈ N ₂ O	1	3.8	C ₄ H ₅ NO ₃	0	7.2
C ₄ H ₄ N ₂ O ₂	0	8.7	C ₈ H ₉ NO ₂	1	2.9	C ₇ H ₅ NO	1	3.1
C ₈ H ₈ N ₂ O	1	14	C ₆ H ₅ NO ₄	1	100	C ₇ H ₇ NO ₂	1	2.3
C ₈ H ₇ NO ₂	1	27	C ₇ H ₇ NO ₄	1	93	C ₈ H ₈ N ₂ O	1	3.9
C ₆ H ₅ NO ₄	1	43	C ₇ H ₁₀ N ₂ O ₃	0	3.2	C ₆ H ₅ NO ₄	1	100
C ₆ H ₇ NO ₅	0	21	C ₆ H ₅ NO ₅	1	3.4	C ₈ H ₈ N ₂ O ₂	1	2.3
C ₉ H ₈ N ₂ O ₂	1	14	C ₉ H ₉ NO ₃	1	3.6	C ₈ H ₇ NO ₃	1	2.8
C ₉ H ₈ N ₂ O ₃	1	20	C ₈ H ₇ NO ₄	1	3.4	C ₇ H ₇ NO ₄	1	42
C ₈ H ₅ NO ₅	1	36	C ₉ H ₁₁ NO ₃	1	3.3	C ₈ H ₅ NO ₄	1	5.4
C ₇ H ₅ NO ₆	1	12	C ₈ H ₉ NO ₄	0	35	C ₉ H ₁₁ NO ₃	1	2.5
C ₁₀ H ₉ NO ₄	1	20	C ₈ H ₁₁ NO ₄	0	2.9	C ₇ H ₅ NO ₅	1	9.7
C ₉ H ₇ NO ₅	1	9.3	C ₁₀ H ₇ NO ₃	2	3.2	C ₈ H ₉ NO ₄	0	13
C ₁₀ H ₉ NO ₅	1	15	C ₁₀ H ₉ NO ₃	1	3.9	C ₁₀ H ₇ NO ₃	2	3.9
C ₉ H ₉ NO ₆	0	10	C ₉ H ₇ NO ₄	1	3.7	C ₉ H ₇ NO ₄	1	8.8
C ₁₁ H ₁₃ NO ₆	0	15	C ₉ H ₉ NO ₄	1	6.9	C ₉ H ₉ NO ₄	1	5.8
C ₈ H ₁₁ NO ₉	0	8.8	C ₉ H ₁₁ NO ₄	0	8.1	C ₉ H ₁₁ NO ₄	0	3.1
C ₆ H ₁₂ N ₂ O ₁₀	0	11	C ₁₀ H ₉ NO ₄	1	7.1	C ₁₁ H ₉ NO ₃	2	3.5
C ₉ H ₁₃ NO ₉	0	12	C ₁₀ H ₁₁ NO ₄	1	7.5	C ₁₀ H ₉ NO ₄	1	7.5
C ₈ H ₁₃ NO ₁₀	0	20	C ₉ H ₁₁ NO ₅	0	3.1	C ₁₀ H ₁₁ NO ₄	1	4.2
C ₈ H ₁₃ NO ₁₁	0	67	C ₆ H ₂ N ₂ O ₇	1	4.3	C ₉ H ₉ NO ₅	1	7.2
C ₈ H ₁₅ NO ₁₁	0	100	C ₁₁ H ₁₁ NO ₄	1	5.8	C ₁₀ H ₁₃ NO ₄	0	2.6
C ₉ H ₁₅ NO ₁₁	0	22	C ₁₀ H ₉ NO ₅	1	3.6	C ₆ H ₂ N ₂ O ₇	1	5.5
C ₁₃ H ₁₅ NO ₈	0	8.2	C ₉ H ₉ NO ₆	0	4.5	C ₁₂ H ₉ NO ₃	2	3.1
C ₈ H ₁₃ NO ₁₂	0	18	C ₁₂ H ₁₃ NO ₄	1	3.2	C ₁₂ H ₁₁ NO ₃	2	2.6
C ₁₀ H ₁₄ N ₂ O ₁₀	0	12	C ₁₁ H ₁₁ NO ₅	1	4.3	C ₁₁ H ₁₁ NO ₄	1	3.1
C ₁₀ H ₁₇ NO ₁₁	0	41	C ₁₁ H ₁₃ NO ₅	1	4.6	C ₁₀ H ₉ NO ₅	1	5.1
C ₉ H ₁₇ NO ₁₂	0	64	C ₁₂ H ₄ N ₂ O ₄	3	3.4	C ₁₂ H ₁₁ NO ₄	1	3.0
C ₁₀ H ₁₅ NO ₁₂	0	19	C ₁₀ H ₁₁ NO ₆	0	3.9	C ₁₂ H ₁₃ NO ₄	1	2.7
C ₁₅ H ₆ N ₂ O ₈	3	23	C ₁₃ H ₁₁ NO ₄	2	3.1	C ₁₁ H ₁₂ N ₂ O ₄	1	2.2
C ₁₆ H ₈ N ₂ O ₈	3	19	C ₁₂ H ₁₁ NO ₅	1	3.4	C ₁₁ H ₁₁ NO ₅	1	4.6
C ₁₃ H ₁₇ NO ₁₁	0	8.9	C ₁₂ H ₁₃ NO ₅	1	3.0	C ₁₄ H ₉ NO ₃	3	2.5
C ₁₆ H ₁₉ NO ₉	1	11	C ₁₁ H ₁₃ NO ₆	0	3.6	C ₁₁ H ₁₃ NO ₅	1	3.3
C ₁₁ H ₁₉ NO ₁₃	0	18	C ₁₃ H ₁₁ NO ₅	2	3.3	C ₁₀ H ₁₂ N ₂ O ₅	1	6.0
C ₁₀ H ₆ N ₄ O ₁₂	1	11	C ₁₃ H ₁₃ NO ₅	1	4.4	C ₁₂ H ₁₃ NO ₅	1	3.0
C ₈ H ₁₇ N ₅ O ₁₂	0	16	C ₁₃ H ₁₅ NO ₅	1	3.3	C ₁₁ H ₁₁ NO ₆	1	2.5
C ₁₀ H ₈ N ₄ O ₁₂	0	8.9	C ₁₂ H ₁₃ NO ₆	1	3.4	C ₁₂ H ₁₅ NO ₅	1	2.6
C ₁₃ H ₁₉ NO ₁₂	0	14	C ₁₄ H ₁₅ NO ₅	1	3.0	C ₈ H ₅ N ₃ O ₇	1	2.3
C ₂₀ H ₈ N ₂ O ₇	5	11	C ₁₃ H ₁₃ NO ₆	1	4.0	C ₁₁ H ₁₃ NO ₆	0	3.7

C ₁₄ H ₁₉ NO ₁₂	0	10	C ₁₃ H ₁₅ NO ₆	1	3.0	C ₁₃ H ₉ NO ₅	2	4.1
C ₁₁ H ₈ N ₄ O ₁₃	1	10	C ₁₆ H ₂₉ NO ₃	0	3.6	C ₁₆ H ₉ NO ₃	4	10
C ₁₁ H ₁₀ N ₄ O ₁₃	0	15	C ₁₄ H ₁₇ NO ₆	1	3.5	C ₁₃ H ₁₅ NO ₅	1	2.3
C ₉ H ₂₁ N ₅ O ₁₃	0	10	C ₈ H ₁₅ NO ₁₁	0	20	C ₁₂ H ₁₃ NO ₆	1	3.4
C ₁₂ H ₈ N ₄ O ₁₃	1	12	C ₁₅ H ₁₇ NO ₇	1	3.3	C ₁₃ H ₁₃ NO ₆	1	2.5
C ₁₆ H ₂₁ NO ₁₂	0	10	C ₁₀ H ₁₇ NO ₁₁	0	4.1	C ₁₆ H ₂₉ NO ₃	0	6.6
C ₁₅ H ₂₁ NO ₁₃	0	9.0	C ₉ H ₁₇ NO ₁₂	0	6.2	C ₁₆ H ₂₇ N ₃ O ₃	1	2.6
C ₁₅ H ₂₃ NO ₁₃	0	9.1	C ₁₅ H ₆ N ₂ O ₈	3	3.9	C ₁₅ H ₆ N ₂ O ₇	3	2.3
C ₁₄ H ₂₃ NO ₁₄	0	13	C ₁₆ H ₈ N ₂ O ₈	3	3.8	C ₂₀ H ₁₀ N ₂ O ₅	5	3.4
C ₁₆ H ₂₃ NO ₁₃	0	10	C ₁₉ H ₉ N ₃ O ₆	4	12	C ₁₉ H ₉ N ₃ O ₆	4	21
C ₂₀ H ₁₈ N ₂ O ₁₀	2	13	C ₂₇ H ₄₁ NO ₇	1	9.8	C ₂₄ H ₂₀ N ₄ O	6	2.5
C ₂₂ H ₂₄ N ₂ O ₁₃	1	8.7	C ₃₉ H ₄₆ N ₂ O ₆	5	8.8	C ₁₉ H ₄₂ N ₄ O ₁₀	0	4.2

Table S8. The most 50 intense aromatic CHON⁺ compounds detected in the organic aerosols from the hemicellulose combustion at 400 °C, 600 °C and 800 °C.

400 °C			600 °C			800 °C		
Formula	Ring number	RI%	Formula	Ring number	RI%	Formula	Ring number	RI%
C ₅ H ₅ NO	0	100	C ₅ H ₅ NO	0	40	C ₅ H ₅ NO	0	21
C ₆ H ₇ NO	1	8.4	C ₅ H ₆ N ₂ O	0	6.4	C ₄ H ₇ NO ₂	0	10
C ₉ H ₁₁ NO ₂	1	4.0	C ₆ H ₇ NO	1	17	C ₆ H ₇ NO	1	11
C ₅ H ₆ N ₄ O ₄	0	25	C ₆ H ₈ N ₂ O	1	7.6	C ₆ H ₈ N ₂ O	1	17
C ₅ H ₈ N ₄ O ₄	0	9.4	C ₇ H ₉ NO	1	7.0	C ₇ H ₉ NO	1	5.8
C ₇ H ₁₅ NO ₄	0	11	C ₆ H ₈ N ₂ O ₂	0	9.5	C ₆ H ₉ NO ₂	0	3.7
C ₆ H ₈ N ₄ O ₅	0	4.4	C ₈ H ₉ NO ₂	1	7.3	C ₇ H ₁₀ N ₂ O	1	5.3
C ₄ H ₁₀ N ₄ O ₆	0	3.8	C ₇ H ₁₀ N ₂ O ₂	0	7.5	C ₆ H ₈ N ₂ O ₂	0	8.8
C ₁₁ H ₈ N ₄ O ₃	2	3.6	C ₁₀ H ₉ NO	2	10	C ₁₀ H ₉ NO	2	4.4
C ₉ H ₇ NO ₆	1	16	C ₉ H ₁₁ NO ₂	1	7.0	C ₇ H ₁₄ N ₂ O ₂	0	3.9
C ₁₆ H ₁₀ N ₂ O	4	4.4	C ₈ H ₁₀ N ₂ O ₂	1	11	C ₈ H ₁₀ N ₂ O ₂	1	5.6
C ₁₆ H ₉ N ₃ O ₂	4	4.4	C ₁₁ H ₁₁ NO	2	24	C ₆ H ₁₁ NO ₄	0	4.9
C ₁₉ H ₉ N ₃ O	6	16	C ₇ H ₁₀ N ₂ O ₃	0	26	C ₈ H ₁₄ N ₂ O ₃	0	4.4
C ₉ H ₁₂ N ₄ O ₇	0	6.8	C ₁₂ H ₉ NO	2	5.8	C ₄ H ₉ NO ₈	0	37
C ₁₀ H ₁₄ N ₄ O ₈	0	6.0	C ₈ H ₁₀ N ₂ O ₃	1	6.5	C ₁₃ H ₁₃ NO	2	11
C ₁₉ H ₁₁ N ₃ O ₃	5	59	C ₇ H ₁₁ NO ₄	0	7.4	C ₉ H ₁₃ NO ₄	0	6.6
C ₁₁ H ₁₄ N ₄ O ₈	0	5.5	C ₉ H ₁₁ NO ₃	1	6.2	C ₈ H ₁₃ NO ₅	0	11
C ₉ H ₁₉ NO ₁₂	0	6.2	C ₅ H ₆ N ₄ O ₄	0	57	C ₁₀ H ₁₅ NO ₄	0	9.4
C ₁₃ H ₂₁ NO ₈	0	7.4	C ₇ H ₁₅ NO ₄	0	19	C ₉ H ₁₃ NO ₅	0	4.3
C ₁₉ H ₃₉ NO ₄	0	37	C ₁₂ H ₁₃ NO	2	6.6	C ₉ H ₁₅ NO ₅	0	5.9
C ₂₀ H ₁₃ N ₃ O ₄	4	18	C ₈ H ₁₃ NO ₅	0	13	C ₁₃ H ₂₇ NO ₂	0	6.1
C ₂₀ H ₄₁ NO ₄	0	6.3	C ₄ H ₁₀ N ₄ O ₆	0	10	C ₁₀ H ₁₅ NO ₅	0	10
C ₁₈ H ₃₀ N ₄ O ₄	1	4.7	C ₉ H ₁₉ NO ₅	0	5.3	C ₁₁ H ₁₅ NO ₅	0	4.1
C ₂₀ H ₂₉ N ₃ O ₄	1	5.8	C ₉ H ₉ NO ₇	0	5.4	C ₈ H ₁₈ N ₂ O ₇	0	30
C ₂₀ H ₃₉ NO ₅	0	8.8	C ₁₀ H ₁₉ NO ₈	0	5.6	C ₁₂ H ₁₇ NO ₆	0	3.7
C ₂₀ H ₄₁ NO ₅	0	8.5	C ₉ H ₁₂ N ₄ O ₇	0	18	C ₉ H ₂₀ N ₂ O ₇	0	3.7
C ₂₁ H ₄₃ NO ₄	0	6.7	C ₁₂ H ₁₇ NO ₇	0	5.2	C ₁₀ H ₁₈ N ₂ O ₇	0	13
C ₂₂ H ₄₅ NO ₄	0	3.6	C ₁₃ H ₁₀ N ₂ O ₈	1	13	C ₁₀ H ₂₀ N ₂ O ₇	0	3.8
C ₂₁ H ₄₁ NO ₄	0	5.9	C ₁₀ H ₁₄ N ₂ O ₁₂	0	33	C ₉ H ₁₈ N ₂ O ₈	0	15
C ₂₁ H ₄₃ NO ₅	0	11	C ₂₁ H ₃₂ N ₂ O ₂	1	13	C ₁₁ H ₁₈ N ₂ O ₈	0	11
C ₁₈ H ₁₄ N ₂ O ₈	2	22	C ₂₀ H ₂₉ N ₃ O ₄	1	8.1	C ₁₃ H ₁₉ NO ₈	0	5.0
C ₂₃ H ₄₁ NO ₄	0	3.7	C ₁₁ H ₁₆ N ₂ O ₁₃	0	6.5	C ₂₂ H ₂₅ N ₃ O	4	3.9
C ₂₂ H ₄₃ NO ₆	0	7.2	C ₁₅ H ₁₇ NO ₁₁	0	6.2	C ₂₂ H ₁₆ N ₂ O ₂	5	15

C ₂₃ H ₄₅ NO ₇	0	4.6	C ₁₄ H ₁₆ N ₂ O ₁₃	0	7.0	C ₁₀ H ₂₀ N ₄ O ₉	0	15
C ₂₄ H ₄₅ NO ₆	0	11	C ₂₂ H ₄₃ NO ₆	0	8.8	C ₂₁ H ₁₄ N ₂ O ₄	4	20
C ₂₄ H ₄₇ NO ₆	0	8.6	C ₂₄ H ₄₅ NO ₆	0	46	C ₂₂ H ₁₄ N ₂ O ₄	5	25
C ₂₁ H ₁₈ N ₂ O ₁₀	2	3.5	C ₂₉ H ₃₉ N ₅ O	4	7.0	C ₂₀ H ₂₉ N ₃ O ₄	1	8.9
C ₁₉ H ₂₀ N ₂ O ₁₃	1	5.5	C ₂₄ H ₁₈ N ₂ O ₁₁	4	5.8	C ₁₉ H ₂₉ N ₃ O ₄	1	5.3
C ₂₅ H ₂₄ N ₂ O ₉	3	6.3	C ₂₇ H ₅₀ N ₄ O ₄	0	12	C ₉ H ₁₈ N ₂ O ₁₄	0	8.3
C ₂₂ H ₂₀ N ₂ O ₁₂	2	31	C ₃₆ H ₁₇ NO ₅	10	6.1	C ₁₀ H ₂₂ N ₄ O ₁₀	0	4.9
C ₂₂ H ₂₈ N ₂ O ₁₄	0	4.0	C ₃₂ H ₅₅ NO ₅	1	6.2	C ₂₂ H ₄₀ N ₄ O	1	9.2
C ₃₄ H ₆₉ NO ₄	0	25	C ₃₄ H ₆₉ NO ₄	0	24	C ₂₂ H ₁₆ N ₂ O ₅	4	9.7
C ₃₆ H ₇₃ NO ₄	0	14	C ₃₄ H ₅₅ NO ₅	1	16	C ₂₇ H ₃₆ N ₂ O ₂	3	9.1
C ₃₅ H ₅₄ N ₂ O ₁₀	1	3.7	C ₃₄ H ₅₇ NO ₅	1	100	C ₂₂ H ₂₀ N ₂ O ₇	3	7.5
C ₃₄ H ₆₄ N ₄ O ₈	0	3.8	C ₃₁ H ₅₈ N ₄ O ₆	0	7.1	C ₃₄ H ₁₃ NO ₂	10	55
C ₃₉ H ₆₂ N ₂ O ₉	1	4.6	C ₄₉ H ₆₇ NO	6	14	C ₃₃ H ₃₈ N ₂ O ₂	5	8.0
C ₃₇ H ₆₈ N ₄ O ₈	0	4.1	C ₅₀ H ₆₉ NO	6	23	C ₃₂ H ₆₅ NO ₄	0	3.9
C ₃₇ H ₇₀ N ₄ O ₉	0	5.5	C ₅₁ H ₇₁ NO	6	28	C ₃₂ H ₅₅ NO ₅	1	3.9
C ₄₅ H ₇₂ N ₂ O ₆	2	5.0	C ₅₁ H ₇₁ NO ₂	6	13	C ₃₄ H ₅₅ NO ₅	1	23
C ₃₆ H ₇₁ NO ₁₅	0	5.9	C ₃₆ H ₇₁ NO ₁₅	0	5.2	C ₃₄ H ₅₇ NO ₅	1	100

Table S9. The most 50 intense aromatic CHON– compounds detected in the organic aerosols from the lignin combustion at 400 °C, 600 °C and 800 °C.

400 °C			600 °C			800 °C		
Formula	Ring number	RI%	Formula	Ring number	RI%	Formula	Ring number	RI%
C ₇ H ₅ NO	1	23	C ₄ H ₅ NO ₃	0	0.4	C ₇ H ₅ NO	1	13
C ₇ H ₆ N ₂ O	1	2.5	C ₇ H ₅ NO	1	2.2	C ₆ H ₅ NO ₄	1	81
C ₇ H ₅ NO ₂	1	12	C ₅ H ₇ NO ₃	0	0.6	C ₈ H ₇ NO ₃	1	21
C ₈ H ₄ N ₂ O	2	5.2	C ₇ H ₅ NO ₂	1	1.2	C ₇ H ₇ NO ₄	1	32
C ₉ H ₇ NO	2	4.0	C ₈ H ₄ N ₂ O	2	0.5	C ₈ H ₅ NO ₄	1	22
C ₈ H ₅ NO ₂	1	3.5	C ₈ H ₇ NO ₂	1	0.5	C ₇ H ₅ NO ₅	1	6.9
C ₈ H ₇ NO ₂	1	5.7	C ₆ H ₅ NO ₄	1	54	C ₈ H ₉ NO ₄	0	12
C ₆ H ₅ NO ₄	1	17	C ₈ H ₅ NO ₃	1	0.6	C ₇ H ₇ NO ₅	0	55
C ₉ H ₇ NO ₂	1	4.4	C ₈ H ₇ NO ₃	1	8.5	C ₉ H ₇ NO ₄	1	4.7
C ₈ H ₅ NO ₃	1	9.4	C ₆ H ₃ NO ₅	1	0.8	C ₁₃ H ₇ NO	3	4.0
C ₉ H ₉ NO ₂	1	2.9	C ₇ H ₇ NO ₄	1	69	C ₈ H ₆ N ₂ O ₄	1	8.9
C ₈ H ₇ NO ₃	1	10	C ₆ H ₅ NO ₅	1	0.7	C ₇ H ₄ N ₂ O ₅	1	4.5
C ₃ H ₈ N ₂ O ₆	0	9.7	C ₉ H ₇ NO ₃	1	0.4	C ₈ H ₇ NO ₅	1	48
C ₇ H ₇ NO ₄	1	38	C ₉ H ₉ NO ₃	1	1.5	C ₉ H ₁₁ NO ₄	0	5.3
C ₁₀ H ₉ NO ₂	1	2.9	C ₈ H ₇ NO ₄	1	1.7	C ₇ H ₅ NO ₆	1	8.9
C ₉ H ₇ NO ₃	1	11	C ₇ H ₅ NO ₅	1	0.4	C ₈ H ₉ NO ₅	0	10
C ₉ H ₉ NO ₃	1	5.3	C ₈ H ₉ NO ₄	0	48	C ₅ H ₂ N ₂ O ₇	0	13
C ₈ H ₉ NO ₄	0	33	C ₇ H ₇ NO ₅	0	100	C ₁₀ H ₁₁ NO ₄	1	6.4
C ₇ H ₇ NO ₅	0	100	C ₁₀ H ₉ NO ₃	1	0.5	C ₉ H ₉ NO ₅	1	62
C ₁₁ H ₉ NO ₂	2	3.8	C ₁₀ H ₁₁ NO ₃	1	0.5	C ₈ H ₇ NO ₆	1	16
C ₁₀ H ₉ NO ₃	1	7.4	C ₉ H ₉ NO ₄	1	2.4	C ₆ H ₂ N ₂ O ₇	1	20
C ₉ H ₇ NO ₄	1	3.4	C ₈ H ₇ NO ₅	1	2.2	C ₇ H ₆ N ₂ O ₆	1	25
C ₉ H ₉ NO ₄	1	4.8	C ₉ H ₁₁ NO ₄	0	6.9	C ₁₀ H ₁₁ NO ₅	1	12
C ₉ H ₁₁ NO ₄	0	5.9	C ₈ H ₉ NO ₅	0	36	C ₉ H ₉ NO ₆	0	9.3
C ₈ H ₉ NO ₅	0	9.2	C ₁₀ H ₉ NO ₄	1	0.5	C ₈ H ₈ N ₂ O ₆	0	4.5
C ₁₁ H ₁₁ NO ₃	1	2.7	C ₁₀ H ₁₁ NO ₄	1	1.1	C ₁₂ H ₇ NO ₄	2	10
C ₁₀ H ₉ NO ₄	1	2.8	C ₉ H ₉ NO ₅	1	0.7	C ₈ H ₉ NO ₇	0	4.6
C ₁₀ H ₁₁ NO ₄	1	3.6	C ₁₀ H ₁₃ NO ₄	0	1.1	C ₇ H ₇ NO ₈	0	12

C ₁₂ H ₁₁ NO ₃	2	3.1	C ₉ H ₁₁ NO ₅	0	2.1	C ₁₀ H ₉ NO ₆	1	6.3
C ₁₁ H ₉ NO ₄	1	3.1	C ₆ H ₂ N ₂ O ₇	1	0.9	C ₁₁ H ₁₃ NO ₅	1	5.8
C ₁₁ H ₁₁ NO ₄	1	2.8	C ₁₁ H ₁₃ NO ₄	1	0.4	C ₉ H ₈ N ₂ O ₆	1	13
C ₁₀ H ₉ NO ₅	1	2.7	C ₁₀ H ₁₁ NO ₅	1	0.6	C ₁₀ H ₁₁ NO ₆	0	8.4
C ₁₃ H ₁₃ NO ₃	2	2.6	C ₉ H ₉ NO ₆	0	0.9	C ₉ H ₁₀ N ₂ O ₆	0	8.8
C ₁₂ H ₁₁ NO ₄	1	4.9	C ₁₀ H ₁₃ NO ₅	0	0.4	C ₁₀ H ₁₃ NO ₆	0	11
C ₁₂ H ₁₃ NO ₄	1	3.7	C ₉ H ₅ N ₃ O ₅	2	0.8	C ₇ H ₄ N ₂ O ₈	1	9.1
C ₁₁ H ₁₁ NO ₅	1	3.3	C ₁₀ H ₉ NO ₆	1	0.4	C ₇ H ₆ N ₂ O ₈	0	15
C ₁₁ H ₁₃ NO ₅	1	2.4	C ₁₁ H ₁₃ NO ₅	1	0.6	C ₁₀ H ₁₀ N ₂ O ₆	1	6.3
C ₁₃ H ₁₃ NO ₄	1	2.4	C ₁₀ H ₁₁ NO ₆	0	0.9	C ₁₀ H ₉ NO ₇	1	6.9
C ₁₂ H ₁₃ NO ₅	1	2.8	C ₁₁ H ₁₁ NO ₆	1	0.4	C ₁₁ H ₁₃ NO ₆	0	4.1
C ₁₁ H ₁₁ NO ₆	1	20	C ₁₃ H ₁₁ NO ₅	2	0.4	C ₁₆ H ₉ NO ₃	4	10
C ₁₅ H ₂₄ N ₂ O ₂	1	2.6	C ₁₆ H ₉ NO ₃	4	0.4	C ₉ H ₈ N ₂ O ₈	0	4.4
C ₁₅ H ₁₅ NO ₆	1	2.7	C ₁₄ H ₁₃ NO ₅	2	0.4	C ₁₁ H ₁₂ N ₂ O ₇	1	4.4
C ₁₉ H ₃₇ NO ₃	0	3.0	C ₁₃ H ₁₁ NO ₆	1	1.0	C ₉ H ₈ N ₂ O ₉	0	4.3
C ₁₇ H ₃₆ N ₂ O ₆	0	5.7	C ₁₄ H ₁₃ NO ₆	1	0.7	C ₉ H ₁₀ N ₂ O ₉	0	5.1
C ₂₀ H ₃₉ NO ₅	0	5.2	C ₁₅ H ₁₅ NO ₆	1	0.7	C ₂₀ H ₁₁ NO ₃	5	5.2
C ₁₉ H ₁₆ N ₂ O ₁₁	2	17	C ₁₄ H ₁₃ NO ₇	1	0.6	C ₁₆ H ₇ N ₃ O ₇	4	100
C ₂₇ H ₁₆ N ₂ O ₁₁	6	2.8	C ₁₆ H ₁₇ NO ₆	1	0.4	C ₁₅ H ₅ N ₃ O ₉	3	4.0
C ₂₀ H ₂₄ N ₂ O ₁₆	0	2.4	C ₁₅ H ₁₅ NO ₇	1	1.1	C ₁₆ H ₆ N ₄ O ₉	4	12
C ₂₃ H ₂₂ N ₂ O ₁₄	2	2.9	C ₁₆ H ₁₇ NO ₇	1	0.8	C ₂₁ H ₁₀ N ₄ O ₉	5	4.2
C ₁₉ H ₂₄ N ₂ O ₂₂	0	4.8	C ₉ H ₉ NO ₁₃	0	1.1	C ₃₃ H ₄₇ N ₃ O ₇	2	6.4

Table S10. The most 50 intense aromatic CHON⁺ compounds detected in the organic aerosols from the lignin combustion at 400 °C, 600 °C and 800 °C.

400 °C			600 °C			800 °C		
Formula	Ring number	RI%	Formula	Ring number	RI%	Formula	Ring number	RI%
C ₅ H ₅ NO	0	34	C ₅ H ₅ NO	0	15	C ₅ H ₅ NO	0	6.9
C ₅ H ₉ NO	0	3.2	C ₄ H ₇ NO ₂	0	1.9	C ₆ H ₇ NO	1	17
C ₆ H ₇ NO	1	13	C ₆ H ₇ NO	1	11	C ₆ H ₁₃ NO	0	5.9
C ₆ H ₁₃ NO	0	2.5	C ₆ H ₁₃ NO	0	0.9	C ₄ H ₈ N ₂ O ₂	0	5.2
C ₇ H ₉ NO	1	8.8	C ₆ H ₈ N ₂ O	1	1.4	C ₆ H ₉ NO ₃	0	7.2
C ₈ H ₁₁ NO	1	5.0	C ₇ H ₉ NO	1	4.5	C ₈ H ₁₃ NO ₂	0	5.0
C ₆ H ₉ NO ₃	0	4.1	C ₅ H ₁₁ N ₃ O	0	1.5	C ₁₁ H ₇ NO	2	16
C ₉ H ₁₃ NO	1	3.2	C ₈ H ₁₁ NO	1	1.7	C ₁₀ H ₁₅ NO	1	5.4
C ₉ H ₁₄ N ₂ O	1	5.8	C ₆ H ₉ NO ₃	0	4.2	C ₆ H ₁₁ NO ₄	0	4.9
C ₁₀ H ₁₅ NO	1	3.4	C ₉ H ₁₁ NO	1	0.9	C ₁₂ H ₉ NO	2	6.4
C ₁₁ H ₁₁ NO	2	2.6	C ₉ H ₁₄ N ₂ O	1	1.2	C ₁₂ H ₇ NO	3	7.0
C ₁₀ H ₁₆ N ₂ O	1	5.6	C ₁₀ H ₁₅ NO	1	0.9	C ₁₂ H ₁₁ NO	2	9.9
C ₁₁ H ₁₇ NO	1	2.6	C ₁₁ H ₉ NO	2	1.5	C ₈ H ₁₅ NO ₃	0	12
C ₁₂ H ₁₁ NO	2	5.8	C ₁₁ H ₁₁ NO	2	1.3	C ₄ H ₉ NO ₈	0	23
C ₉ H ₁₆ N ₂ O ₂	0	2.7	C ₁₀ H ₁₆ N ₂ O	1	1.0	C ₁₀ H ₁₃ NO ₃	1	5.1
C ₁₁ H ₁₈ N ₂ O	1	5.9	C ₁₂ H ₁₁ NO	2	1.9	C ₁₃ H ₁₃ NO	2	20
C ₁₁ H ₁₁ NO ₂	1	3.7	C ₉ H ₁₁ NO ₃	1	1.0	C ₉ H ₉ NO ₅	1	17
C ₁₂ H ₁₁ NO ₂	2	12	C ₁₁ H ₁₁ NO ₂	1	0.9	C ₁₅ H ₉ NO	4	13
C ₁₃ H ₁₃ NO	2	6.8	C ₄ H ₉ NO ₈	0	5.4	C ₁₃ H ₁₇ NO ₂	1	5.9
C ₁₀ H ₁₈ N ₂ O ₂	0	2.9	C ₁₂ H ₁₁ NO ₂	2	2.8	C ₁₆ H ₉ NO	4	6.6
C ₁₂ H ₂₀ N ₂ O	1	5.4	C ₁₁ H ₉ NO ₃	2	1.1	C ₈ H ₁₅ N ₃ O ₅	0	100
C ₁₂ H ₁₃ NO ₂	1	6.0	C ₁₀ H ₁₃ NO ₃	1	1.0	C ₁₁ H ₁₁ N ₃ O ₄	1	5.8
C ₁₄ H ₁₅ NO	2	3.8	C ₁₃ H ₁₃ NO	2	2.0	C ₁₂ H ₂₃ NO ₃	0	28

C ₁₃ H ₁₃ NO ₂	2	16	C ₁₂ H ₁₃ NO ₂	1	1.1	C ₁₃ H ₂₁ NO ₃	0	6.0
C ₁₃ H ₂₂ N ₂ O	1	3.5	C ₁₄ H ₁₅ NO	2	1.2	C ₁₉ H ₁₁ NO	5	8.6
C ₁₃ H ₁₅ NO ₂	1	2.9	C ₁₃ H ₁₃ NO ₂	2	3.7	C ₁₈ H ₂₉ NO ₂	1	4.9
C ₁₂ H ₁₃ NO ₃	1	4.7	C ₁₂ H ₁₁ NO ₃	2	1.5	C ₁₆ H ₃₁ NO ₃	0	8.7
C ₁₄ H ₁₅ NO ₂	2	13	C ₁₄ H ₁₅ NO ₂	2	2.6	C ₉ H ₁₈ N ₂ O ₈	0	7.1
C ₁₃ H ₁₃ NO ₃	2	6.4	C ₁₁ H ₁₄ N ₂ O ₃	1	0.9	C ₁₉ H ₃₅ NO ₂	0	5.8
C ₁₃ H ₁₅ NO ₃	1	6.9	C ₁₃ H ₁₃ NO ₃	2	3.5	C ₁₂ H ₁₈ N ₂ O ₈	0	7.7
C ₁₅ H ₂₀ N ₂ O	2	2.5	C ₁₅ H ₁₇ NO ₂	2	1.3	C ₁₄ H ₃₁ N ₃ O ₅	0	14
C ₁₅ H ₁₇ NO ₂	2	7.2	C ₈ H ₁₅ N ₃ O ₅	0	3.5	C ₂₁ H ₂₇ NO	2	7.8
C ₁₄ H ₁₅ NO ₃	2	8.6	C ₁₄ H ₁₅ NO ₃	2	2.6	C ₁₈ H ₃₇ NO ₄	0	5.1
C ₁₄ H ₁₇ NO ₃	1	3.5	C ₁₅ H ₁₇ NO ₃	2	1.1	C ₂₁ H ₂₉ NO	2	18
C ₁₆ H ₁₉ NO ₂	2	3.5	C ₁₄ H ₁₈ N ₂ O ₃	1	1.1	C ₁₈ H ₂₉ NO ₄	0	16
C ₁₆ H ₂₂ N ₂ O	2	6.1	C ₁₅ H ₂₀ N ₂ O ₃	1	0.9	C ₂₄ H ₂₅ NO	4	6.8
C ₁₅ H ₁₇ NO ₃	2	5.6	C ₁₇ H ₂₄ N ₂ O ₃	1	0.9	C ₂₁ H ₂₇ NO ₂	2	12
C ₁₇ H ₂₄ N ₂ O	2	2.9	C ₁₈ H ₂₆ N ₂ O ₃	1	1.4	C ₁₀ H ₂₀ N ₄ O ₉	0	4.8
C ₁₆ H ₁₉ NO ₃	2	2.9	C ₂₀ H ₃₉ N ₃ O ₂	0	2.0	C ₂₀ H ₃₇ NO ₄	0	6.9
C ₁₆ H ₂₂ N ₂ O ₂	1	3.9	C ₁₂ H ₂₃ NO ₁₁	0	0.9	C ₂₀ H ₂₉ N ₃ O ₄	1	10
C ₉ H ₁₇ NO ₉	0	4.2	C ₂₁ H ₃₂ N ₂ O ₂	1	1.0	C ₂₁ H ₃₀ N ₂ O ₄	1	5.0
C ₁₇ H ₂₄ N ₂ O ₂	1	5.5	C ₂₁ H ₃₀ N ₂ O ₆	1	0.9	C ₁₈ H ₃₄ N ₂ O ₅	0	29
C ₁₈ H ₂₆ N ₂ O ₂	1	3.2	C ₂₃ H ₂₈ N ₂ O ₆	2	1.3	C ₂₁ H ₄₃ NO ₅	0	10
C ₁₇ H ₂₄ N ₂ O ₃	1	4.2	C ₂₆ H ₃₆ N ₂ O ₆	2	13	C ₁₉ H ₂₃ NO ₈	1	5.7
C ₁₉ H ₃₁ NO ₂	1	4.8	C ₂₈ H ₄₉ NO ₄	0	1.3	C ₂₇ H ₃₆ N ₂ O ₂	3	6.5
C ₁₈ H ₂₆ N ₂ O ₃	1	3.9	C ₃₄ H ₆₉ NO ₄	0	0.9	C ₂₁ H ₂₇ NO ₁₀	1	16
C ₁₉ H ₂₈ N ₂ O ₄	1	2.6	C ₃₄ H ₅₇ NO ₅	1	1.2	C ₂₆ H ₄₃ NO ₅	1	6.1
C ₁₅ H ₁₈ N ₂ O ₁₃	0	4.7	C ₄₁ H ₆₁ NO ₆	2	19	C ₃₄ H ₆₉ NO ₄	0	13
C ₂₈ H ₄₉ NO ₄	0	4.1	C ₄₉ H ₆₆ N ₂ O	6	100	C ₂₈ H ₅₈ N ₂ O ₁₀	0	13
C ₄₄ H ₅₈ N ₂ O ₃	6	100	C ₅₀ H ₆₈ N ₂ O	6	1.1	C ₃₈ H ₇₂ N ₂ O ₉	0	18

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