



Supplement of

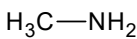
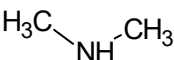
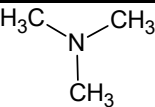
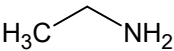
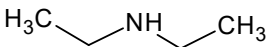
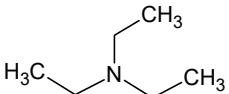
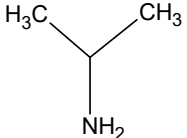
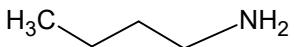
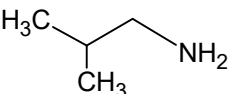
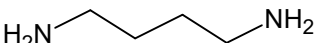
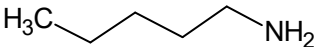
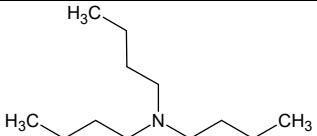
Enhancing characterization of organic nitrogen components in aerosols and droplets using high-resolution aerosol mass spectrometry

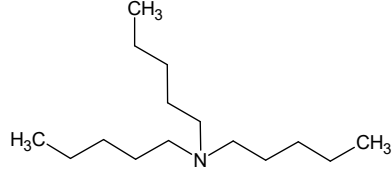
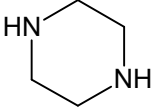
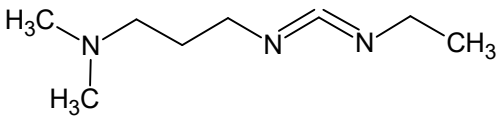
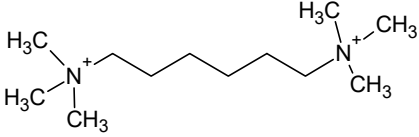
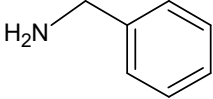
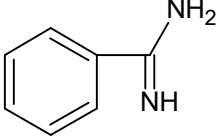
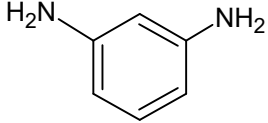
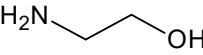
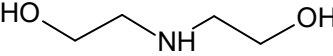
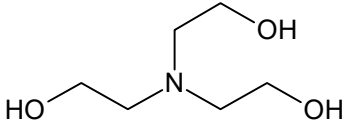
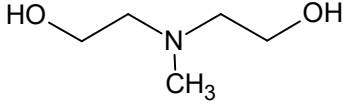
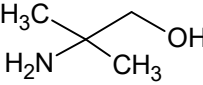
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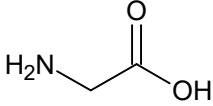
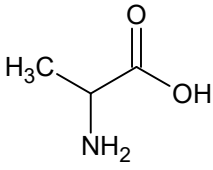
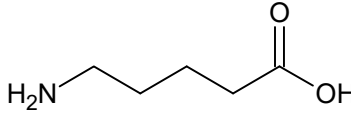
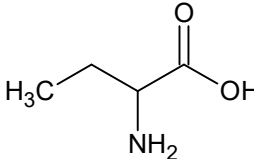
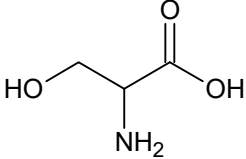
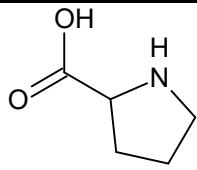
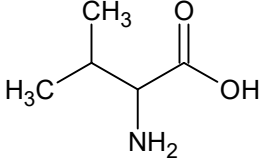
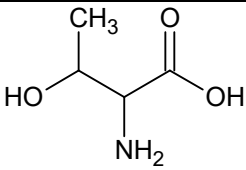
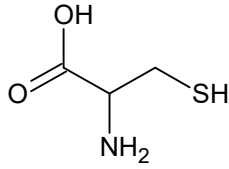
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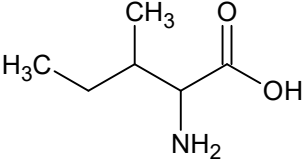
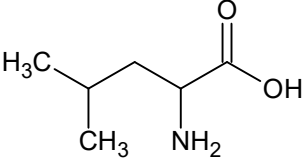
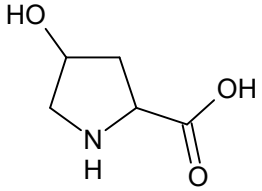
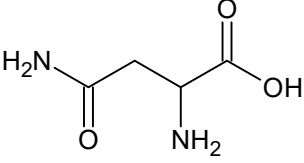
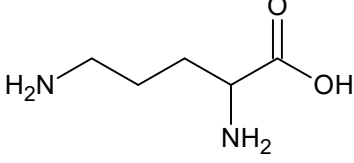
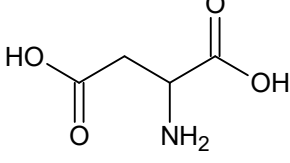
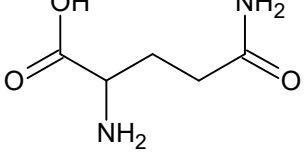
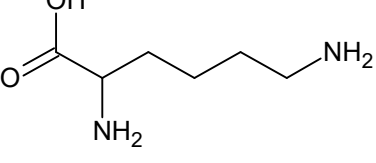
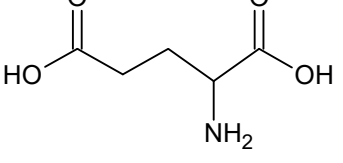
Table S1. List of N-containing organic (ON) standards analyzed in this study.

No.	Name	Abbr.	Functional Groups	Chemical Formula	Molecular weight	Structure
1	Methylamine (Hydrochloride)	MA	Amine	CH ₅ N (HCl)	31.0571 (36.4610)	
2	Dimethylamine (Hydrochloride)	DMA	Amine	C ₂ H ₇ N (HCl)	45.0837 (36.4610)	
3	Trimethylamine (Hydrochloride)	TMA	Amine	C ₃ H ₉ N (HCl)	59.1103 (36.4610)	
4	Ethylamine (Hydrochloride)	EA	Amine	C ₂ H ₇ N (HCl)	45.0837 (36.4610)	
5	Diethylamine (Hydrochloride)	DEA	Amine	C ₄ H ₁₁ N (HCl)	73.1368 (36.4610)	
6	Triethylamine (Hydrochloride)	TEA	Amine	C ₆ H ₁₅ N (HCl)	101.1900 (36.4610)	
7	Isopropylamine (Hydrochloride)	iPPA	Amine	C ₃ H ₉ N (HCl)	59.11 (36.4610)	
8	Butylamine (Hydrochloride)	BTA	Amine	C ₄ H ₁₁ N (HCl)	73.14 (36.4610)	
9	Isobutylamine (Hydrochloride)	iBTA	Amine	C ₄ H ₁₁ N (HCl)	73.14 (36.4610)	
10	1,4-Diaminobutane (Hydrochloride)	BDA	Amine	C ₄ H ₁₂ N ₂ (2HCl)	88.15 (72.9220)	
11	Pentylamine (Hydrochloride)	PTA	Amine	C ₅ H ₁₃ N (HCl)	87.16 (36.4610)	
12	Tributylamine (Hydrochloride)	TBA	Amine	C ₁₂ H ₂₇ N (HCl)	185.3495 (36.4610)	

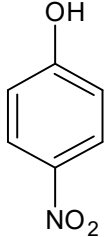
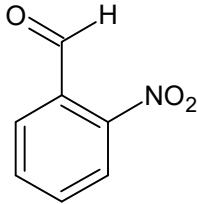
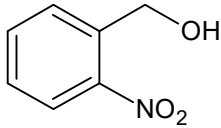
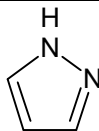
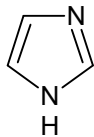
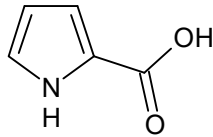
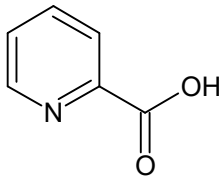
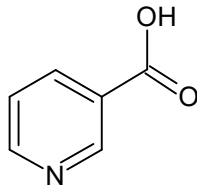
13	Tri-n-amyliamie (Hydrochloride)	TAA	Amine	$C_{15}H_{33}N$ (HCl)	227.4292 (36.4610)	
14	Piperazine (Dihydrochloride)	PIP	Amine	$C_4H_{10}N_2$ (2HCl)	86.1356 (72.9220)	
15	1-(3-Dimethylaminopropyl)-3-ethylcarbodiimide (Hydrochloride)	DMPED	Amine	$C_8H_{17}N_3$ (HCl)	155.2407 (36.4610)	
16	Hexamethonium chloride	HM	Amine	$C_{12}H_{30}N_2(Cl_2)$	202.3800 (70.9060)	
17	Benzylamine (Hydrochloride)	BZA	Amine	C_7H_9N (HCl)	107.1531 (36.4610)	
18	Benzamidine (Hydrochloride)	BZD	Amine	$C_7H_8N_2$ (HCl)	120.1518 (36.4610)	
19	1,3-phenylenediamine (Dihydrochloride)	PHLDA	Amine	$C_6H_8N_2$ (2HCl)	108.1411 (72.9220)	
20	Ethanolamine Also tried MEA.HCl	EAOH	Amine	C_2H_7NO	61.0831	
21	Diethanolamine (Hydrochloride)	DEAOH	Amine	$C_4H_{11}NO_2$ (HCl)	105.1356 (36.4610)	
22	Triethanolamine	TEAOH	Amine	$C_6H_{15}NO_3$	149.1882	
23	Methyldiethanolamine (Hydrochloride)	MDEA	Amine	$C_5H_{13}NO_2$ (HCl)	119.1622 (36.4610)	
24	2-Amino-2-methyl-1-propanol (Hydrochloride)	AMP	Amine	$C_4H_{11}NO$ (HCl)	89.1362 (36.4610)	

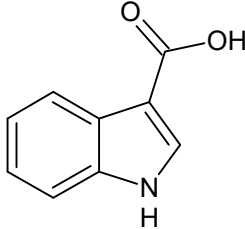
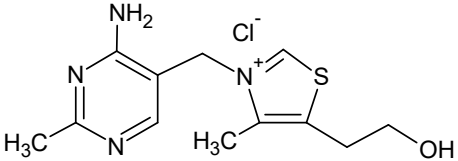
25	Bis(2-hydroxypropyl)amine	BOHA	Amine	$C_6H_{15}NO_2$	133.1888	
26	4-Aminophenol (Hydrochloride)	APA	Amine	C_6H_7NO (HCl)	109.1259 (36.4610)	
27	Ethylene diamine tetraacetic acid	EDTA	Amine	$C_{10}H_{16}N_2O_8$	292.2426	
28	Urea	UREA	Amide	CH_4N_2O	60.0553	
29	Benzamide	BZAM	Amide	C_7H_7NO	121.1366	
30	N,N'-Methylenebisacrylamide	NMAM	Amide	$C_7H_{10}N_2O_2$	154.1665	
31	Nicotinamide	NCAM	Amide	$C_6H_6N_2O$	122.1246	
32	Pyrazinecarboxamide	PRCAM	Amide	$C_5H_5N_3O$	123.1127	
33	Acetaminophenol	AAP	Amide	$C_8H_9NO_2$	151.1626	

34	Glycine	GLY	Amino Acid	$C_2H_5NO_2$	75.0666	
35	L-Alanine	ALA	Amino Acid	$C_3H_7NO_2$	89.0932	
36	γ -Aminobutyric acid	GABA	Amino Acid	$C_4H_9NO_2$	103.1198	
37	R-2-aminobutyric acid	RGABA	Amino Acid	$C_4H_9NO_2$	103.1198	
38	L-Serine	SER	Amino Acid	$C_3H_7NO_3$	105.0926	
39	L-Proline	PRO	Amino Acid	$C_5H_9NO_2$	115.1305	
40	L-Valine	VAL	Amino Acid	$C_5H_{11}NO_2$	117.1463	
41	L-Threonine	THR	Amino Acid	$C_4H_9NO_3$	119.1192	
42	L-Cysteine	CYS	Amino Acid	$C_3H_7NO_2S$	121.1580	

43	L-Isoleucine	ILE	Amino Acid	$C_6H_{13}NO_2$	131.1729	
44	L-Leucine	LEU	Amino Acid	$C_6H_{13}NO_2$	131.1729	
45	trans-4-hydroxyl-proline	PROOH	Amino Acid	$C_5H_9NO_3$	131.1299	
46	L-Asparagine	ASN	Amino Acid	$C_4H_8N_2O_3$	132.1179	
47	L-Ornithine (Hydrochloride)	ORN	Amino Acid	$C_5H_{12}N_2O_2$ (HCl)	132.1610 (34.4610)	
48	L-Aspartic Acid	ASP	Amino Acid	$C_4H_7NO_4$	133.1027	
49	L-Glutamine	GLN	Amino Acid	$C_5H_{10}N_2O_3$	146.1445	
50	L-Lysine	LYS	Amino Acid	$C_6H_{14}N_2O_2$	146.1876	
51	L-Glutamic Acid	GLU	Amino Acid	$C_5H_9NO_4$	147.1293	

52	L-Methionine	MET	Amino Acid	$C_5H_{11}NO_2S$	149.2110	
53	L-Histidine (Monochloride. Monohydrate)	HIS	Amino Acid	$C_6H_9N_3O_2$ (HCl·H ₂ O)	155.1546 (36.4610+18.013)	
54	L-Methionine Sulfoxide	METSO	Amino Acid	$C_5H_{11}NO_3S$	165.2110	
55	L-Phenylalanine	PHE	Amino Acid	$C_9H_{11}NO_2$	165.1891	
56	L-Arginine (Hydrochloride)	ARG	Amino Acid	$C_6H_{14}N_4O_2$ (HCl)	174.2010 (36.4610)	
57	L-Tyrosine	TYR	Amino Acid	$C_9H_{11}NO_3$	181.1885	
58	L-Tryptophan	TRP	Amino Acid	$C_{11}H_{12}N_2O_2$	204.2252	
59	4-Aminobenzoic acid	ABA	Amino acid	$C_7H_7NO_2$	137.1360	
60	4-Nitroimidazole	NID	Nitro- compounds	$C_3H_3N_3O_2$	113.0748	

61	4-Nitrophenol	NPH	Nitro-compounds	$C_6H_5NO_3$	139.1088	
62	2-Nitrobenzaldehyde	NBAD	Nitro-compounds	$C_7H_5NO_3$	151.1195	
63	2-nitrobenzyl alcohol	NBAC	Nitro-compounds	$C_7H_7NO_3$	153.1354	
64	Pyrazole	PRZ	N-heterocycle	$C_3H_4N_2$	68.0773	
65	Imidazole	ID	N-heterocycle	$C_3H_4N_2$	68.0773	
66	Pyrrole-2-carboxylic acid	PRCA	N-heterocycle	$C_5H_5NO_2$	111.0987	
67	2-Picolinic acid	PCA	N-heterocycle	$C_6H_5NO_2$	123.1094	
68	Nicotinic acid	NCA	N-heterocycle	$C_6H_5NO_2$	123.1094	

69	Indole-3-carboxylic acid	IDCA	N-heterocycle	C ₉ H ₇ NO ₂	161.1574	
70	Thiamine (hydrochloride)	THA	N-heterocycle	C ₁₂ H ₁₇ ClN ₄ OS (HCl)	300.8076 (36.4610)	
71	Amino acid standard	AS	Amino Acid	-	-	Physiological acidics and neutrals
72	Protein	PROTEIN	Protein	-	-	Cytochrome C from horse heart
73	Elliott Soil	HA	Humic substance	-	-	Standard HA from IHSS*, No. 1S102H
74	Waskish Peat	FA	Humic substance	-	-	Reference HA from IHSS, No. 1R107F
75	Suwannee River	NOM	Humic substance	-	-	Aquatic NOM (Natural Organic Matter) from IHSS, No. 1R101N

*International Humic Substances Society (<http://www.ihss.gatech.edu/>).

Table S2. List of the N-containing organic (ON) standards used to make the 1:1 (mass ratio) mixtures with sulfate (in ammonium sulfate).

No.	ID. in Table S1	Name	No.	ID. in Table S1	Name
1	1	Methylamine (Hydrochloride)	10	34	Glycine
2	2	Dimethylamine (Hydrochloride)	11	35	L-Alanine
3	3	Trimethylamine (Hydrochloride)	12	39	L-Proline
4	4	Ethylamine (Hydrochloride)	13	41	L-Threonine
5	5	Diethylamine (Hydrochloride)	14	42	L-Cysteine (Hydrochloride)
6	6	Triethylamine (Hydrochloride)	15	59	4-Aminobenzonic acid
7	20	Ethanolamine (Hydrochloride)	16	68	Nicotinic acid
8	19	1,3-phenylenediamine (Dihydrochloride)	17	23	Methyldiethanolamine (Hydrochloride)
9	33	Acetaminophenol	18	14	Piperazine (Dihydrochloride)

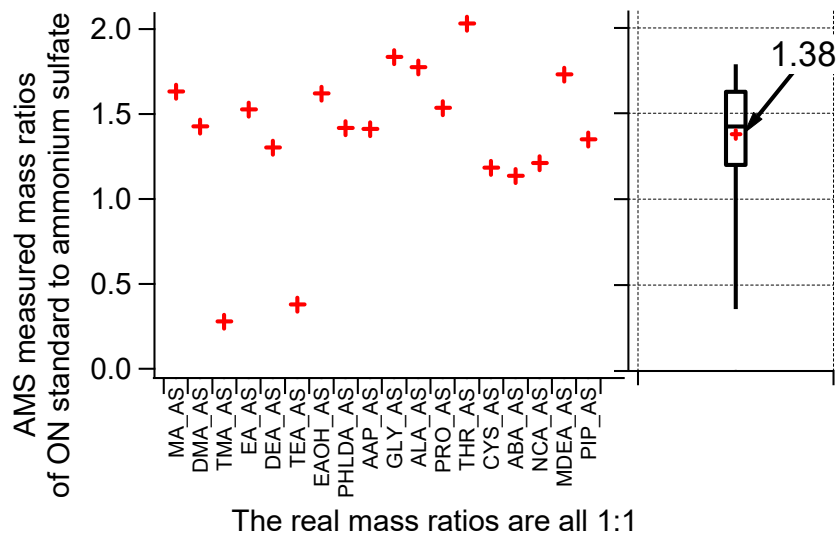


Figure S1. AMS measured mass ratios of the mixtures of different ON standards with ammonium sulfate. All mass ratios of the mixtures are prepared in 1:1 (the whiskers above and below the boxes indicate the 90th and 10th percentiles, the upper and lower boundaries of the boxes indicate the 75th and 25th percentiles, and the lines in the boxes indicate the median values and the cross symbols indicate the mean values).

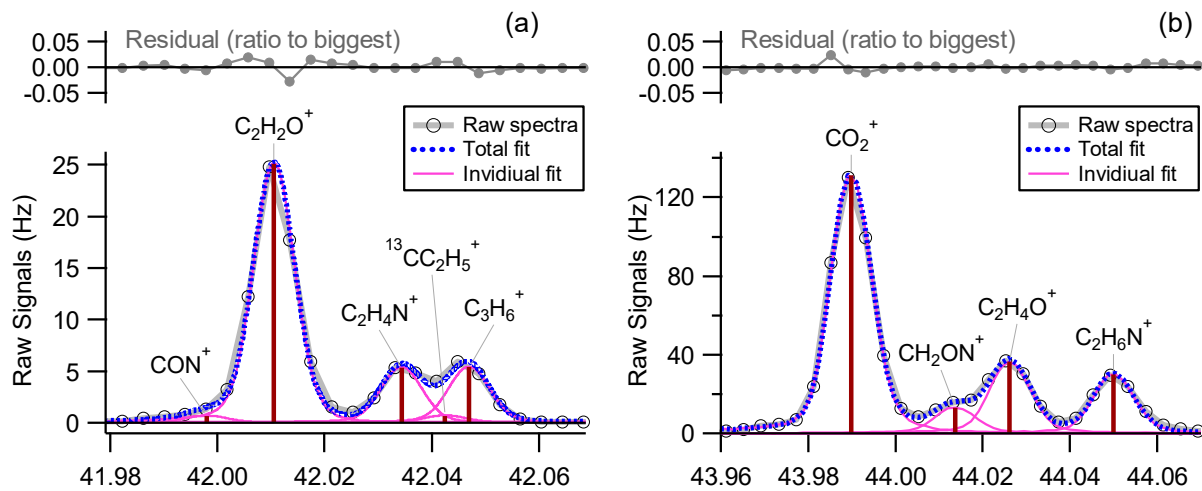
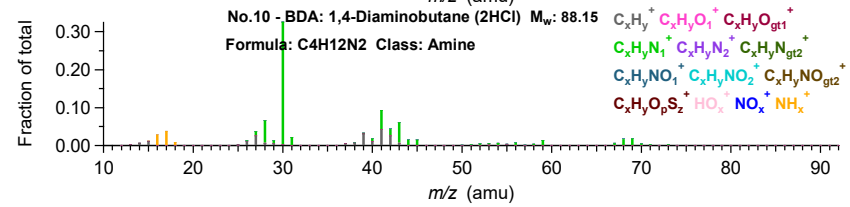
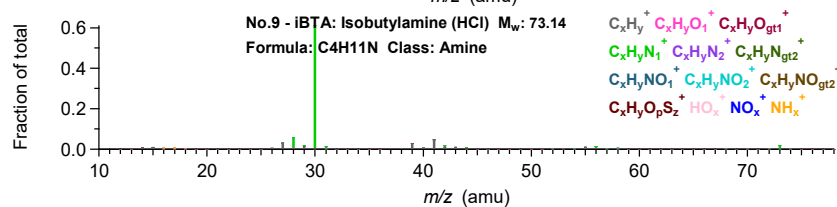
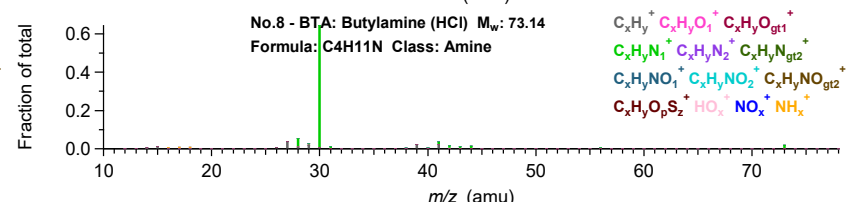
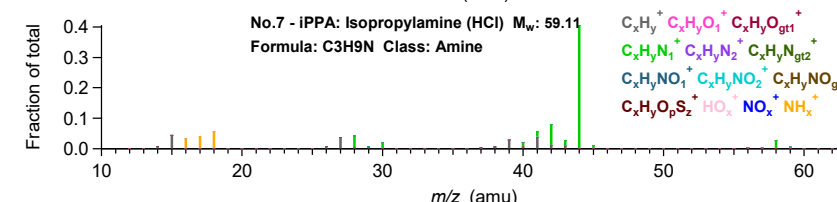
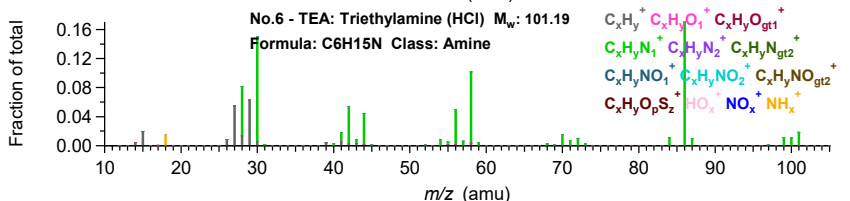
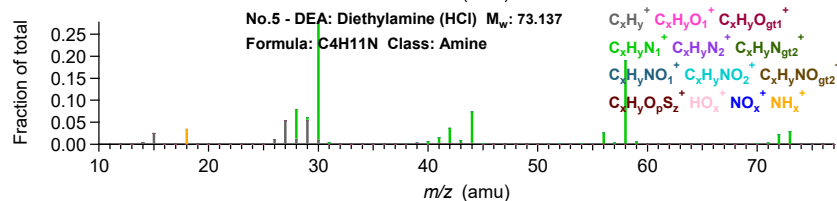
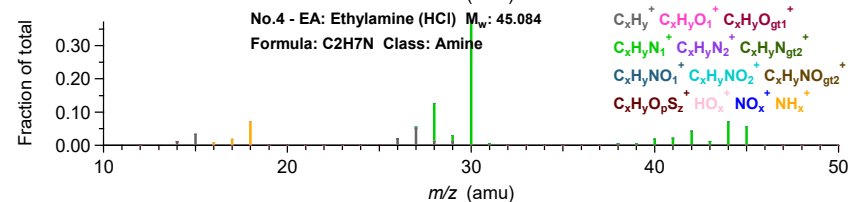
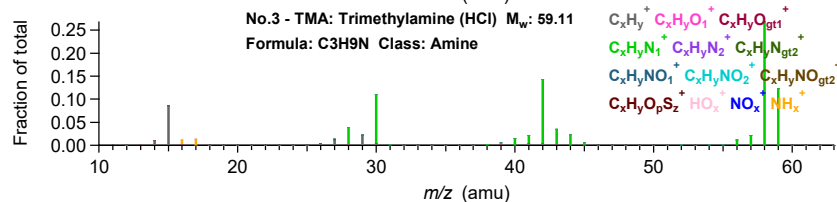
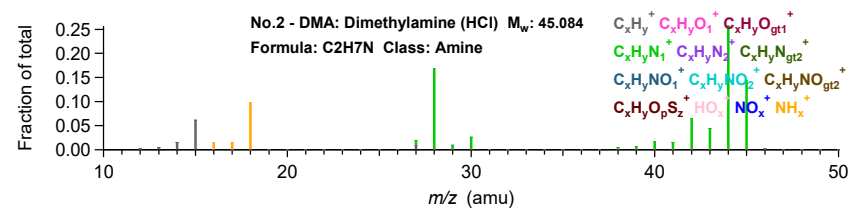
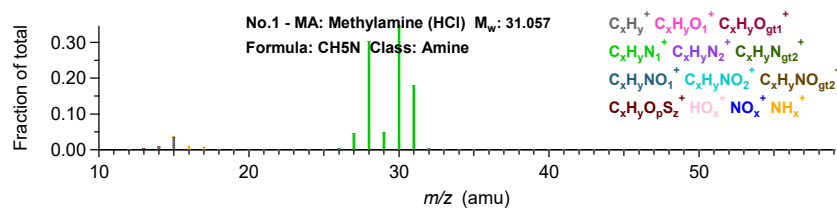
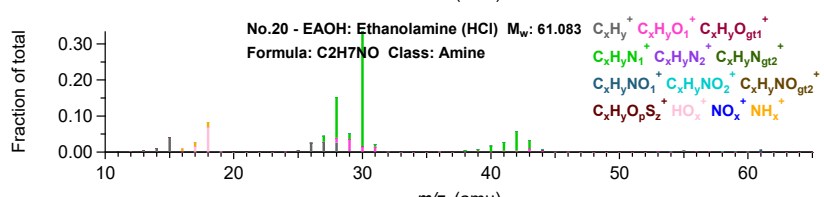
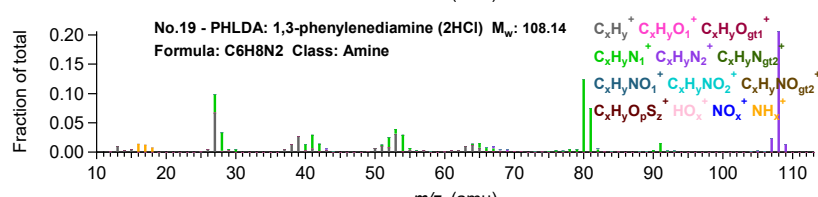
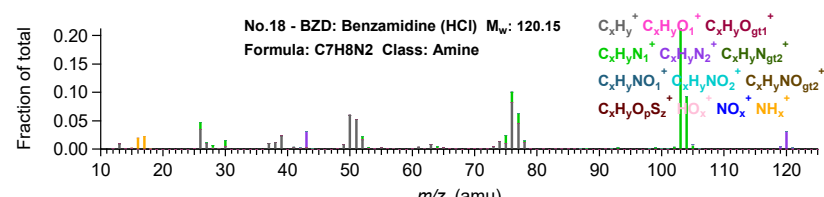
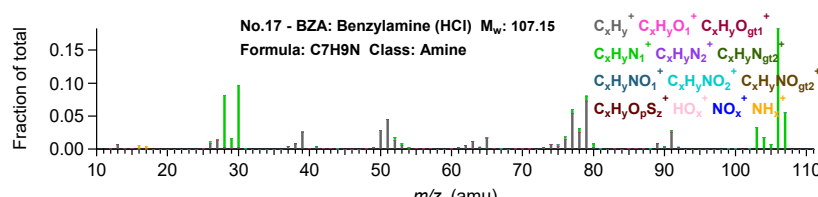
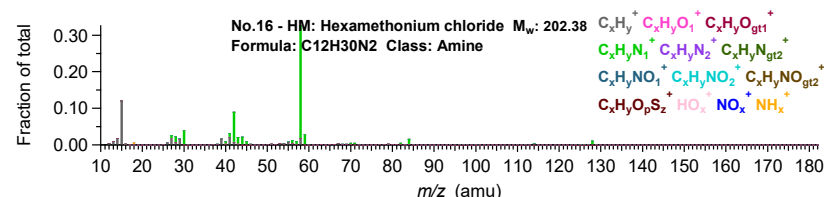
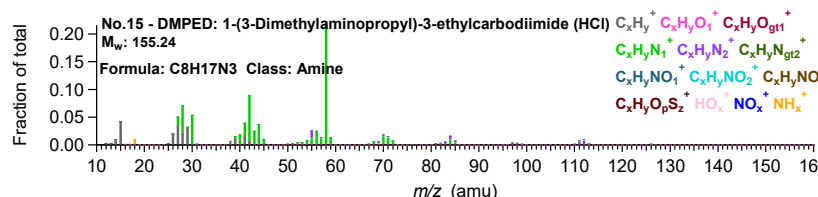
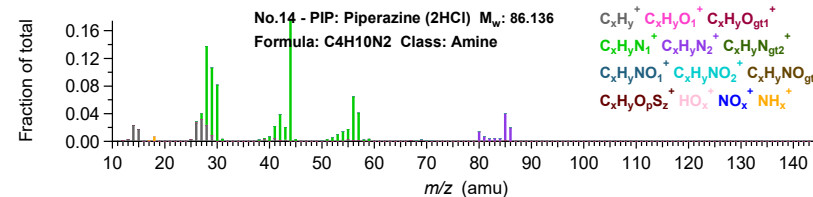
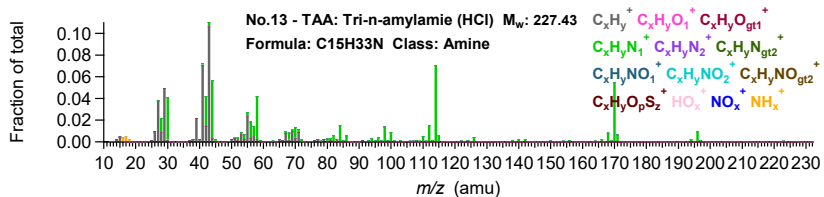
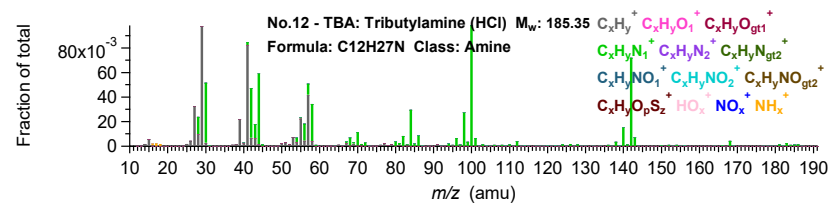
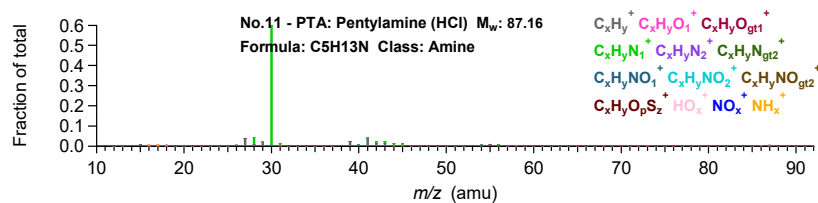
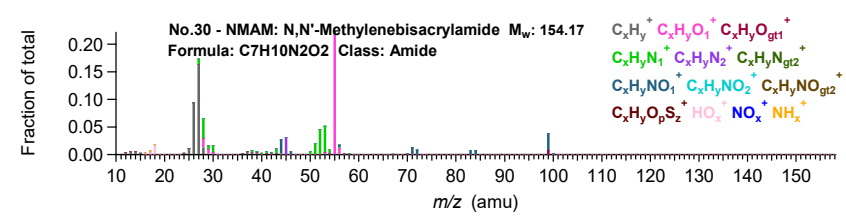
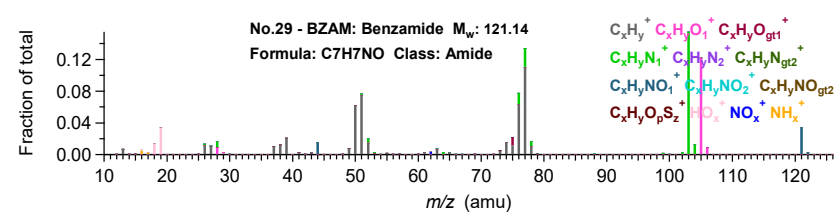
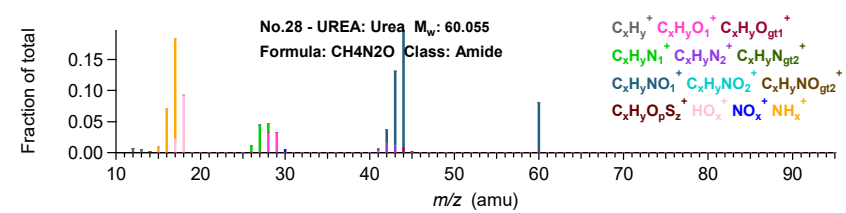
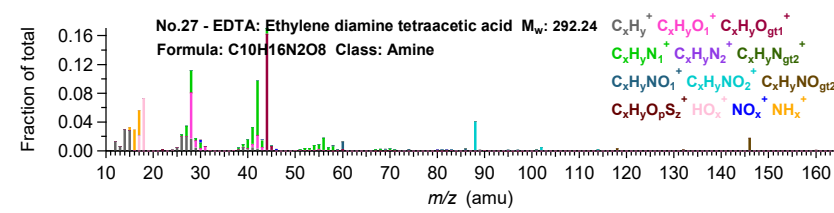
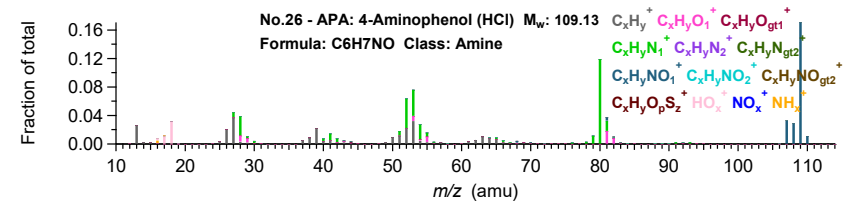
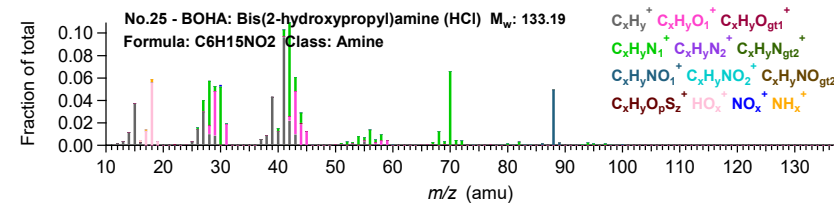
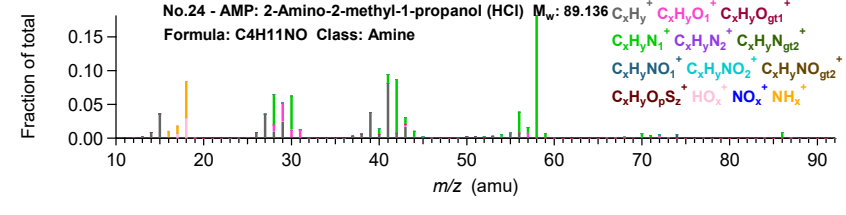
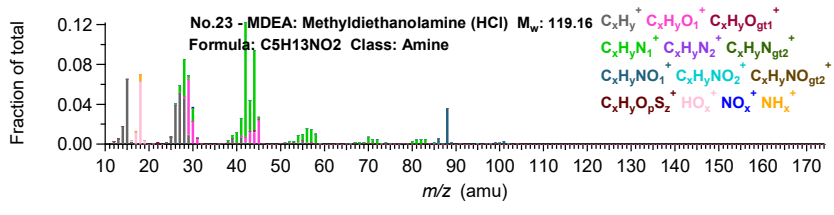
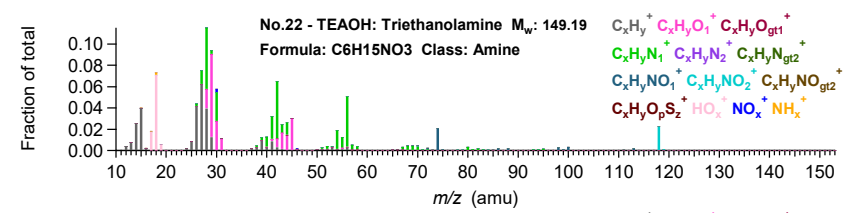
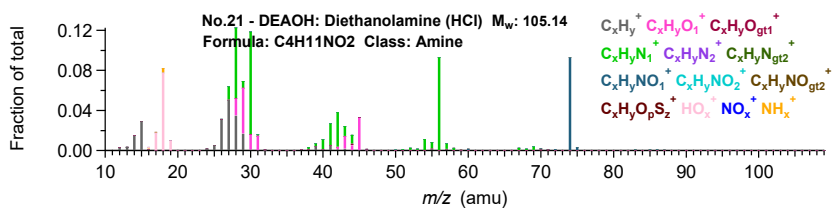
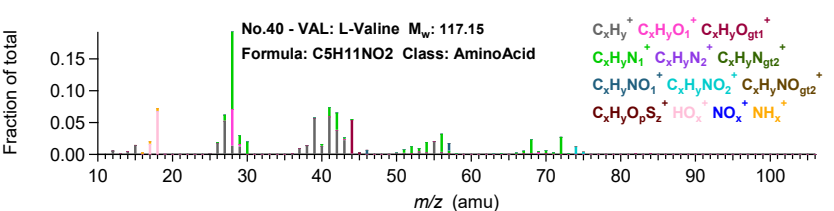
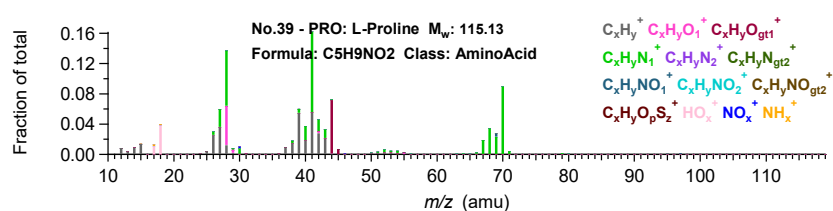
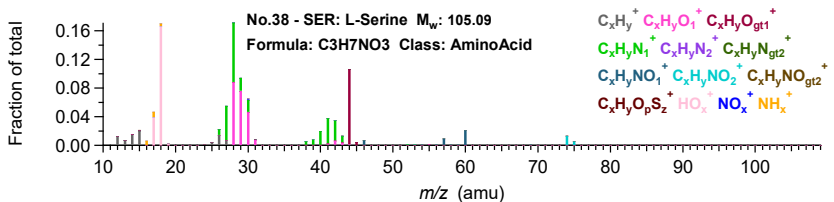
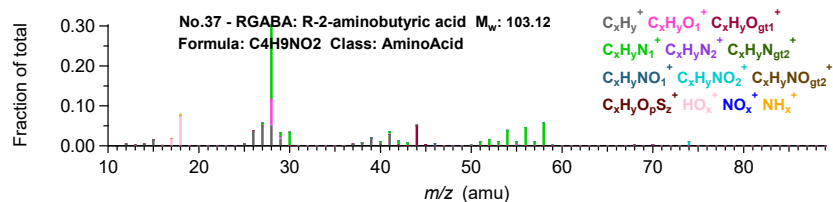
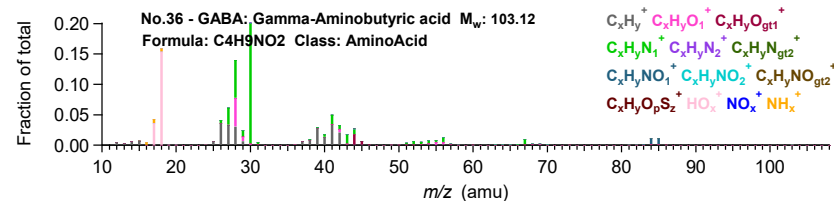
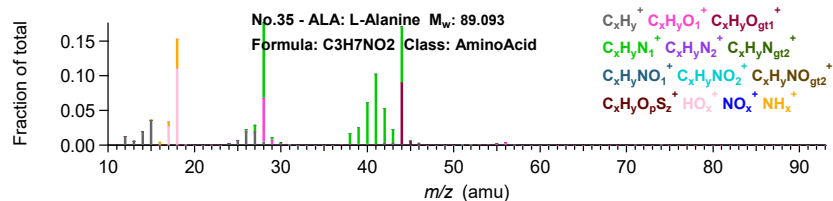
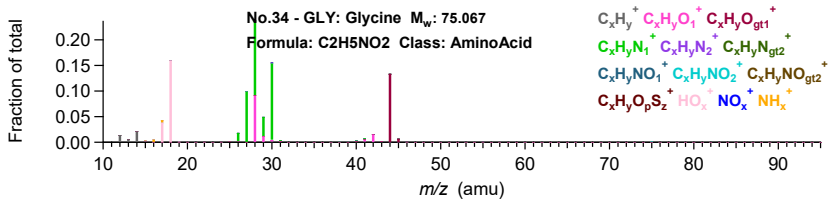
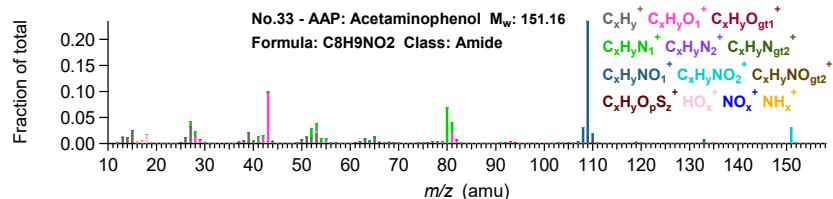
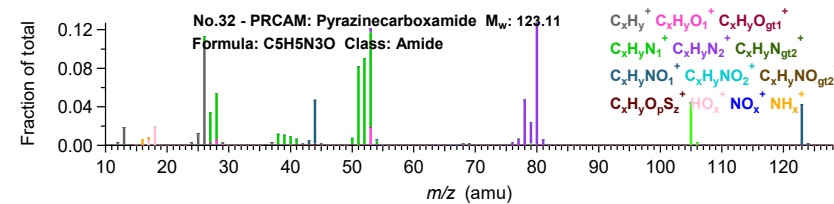
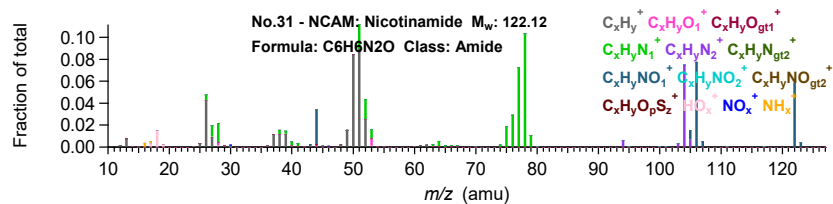


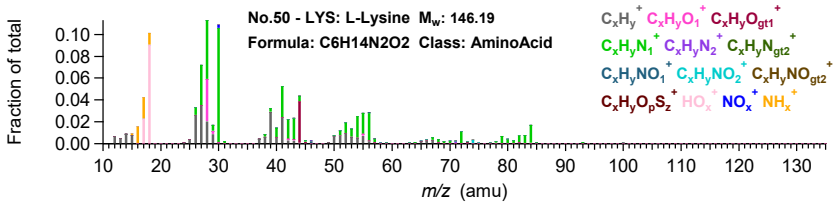
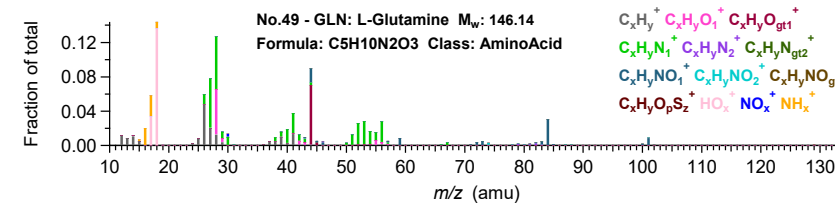
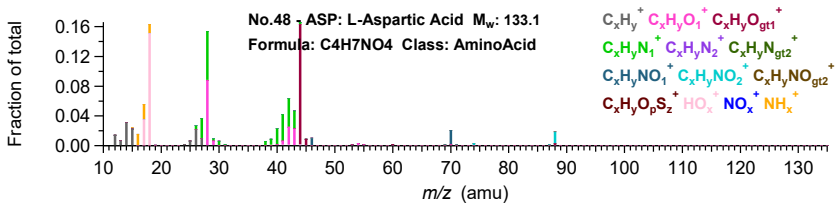
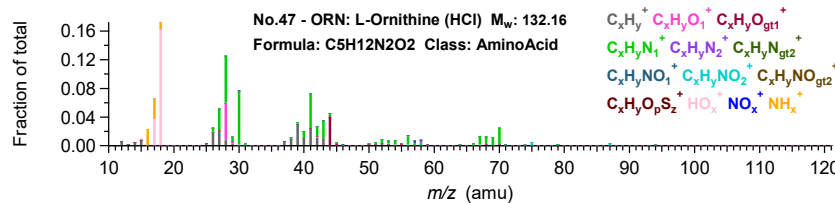
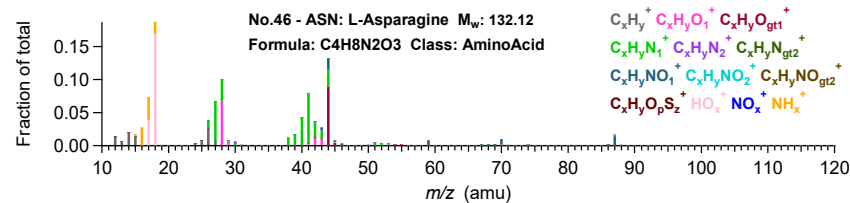
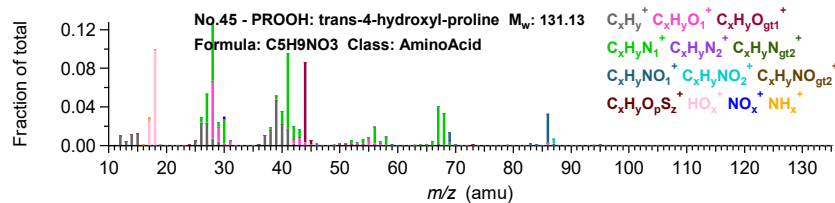
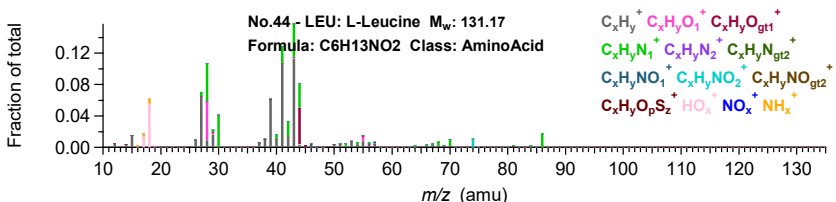
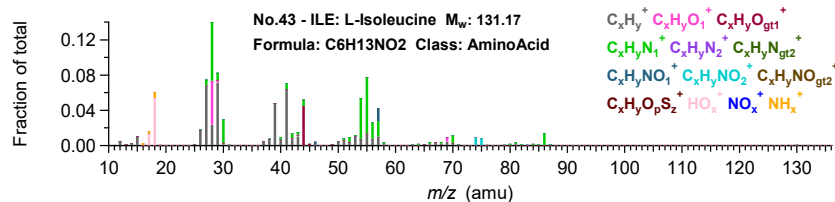
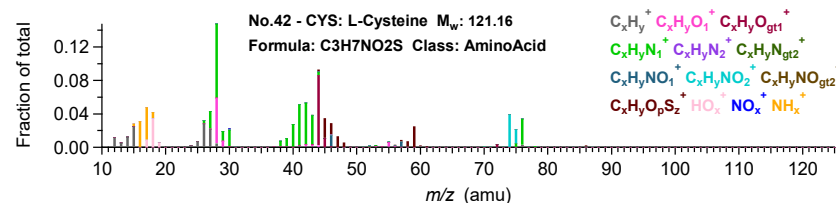
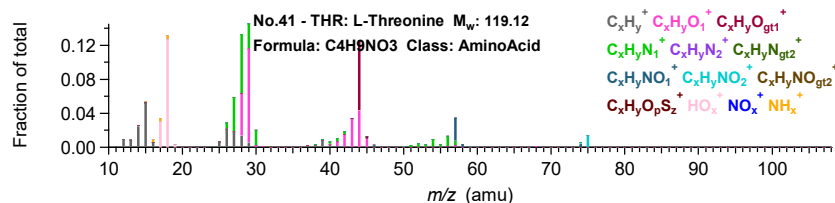
Figure S2. Examples of high resolution mass spectral analysis of (a) m/z 42 and (b) m/z 44.

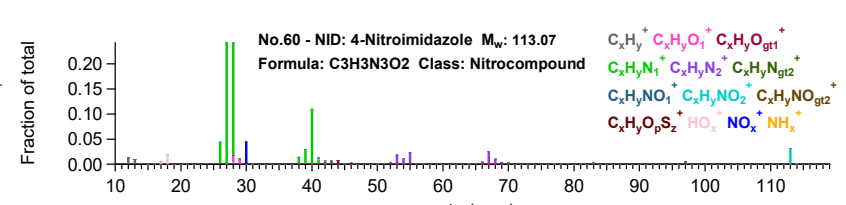
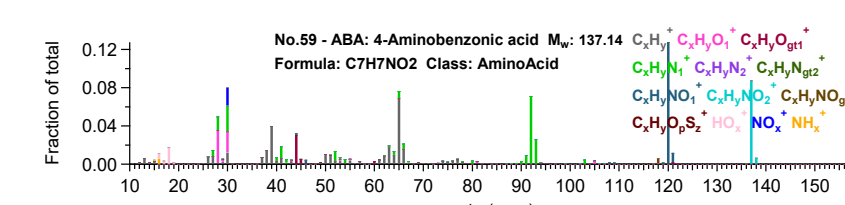
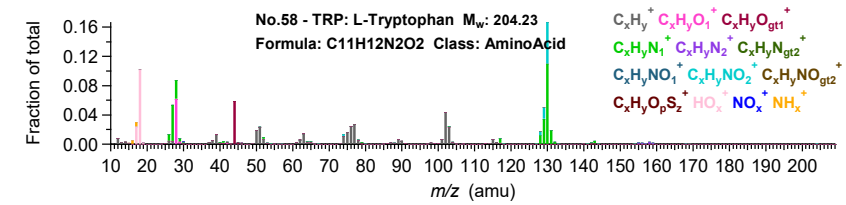
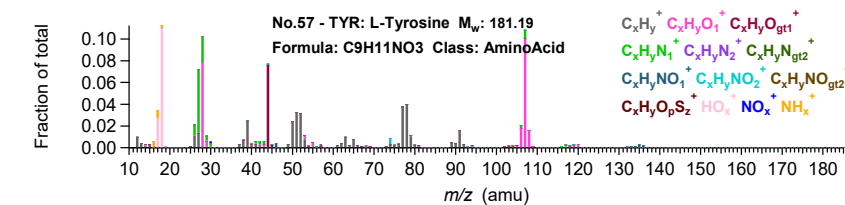
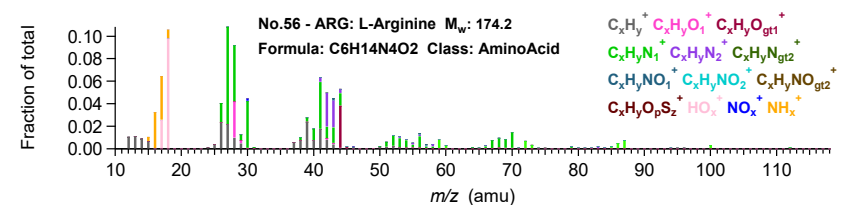
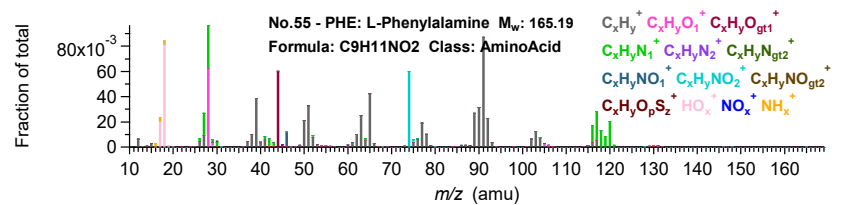
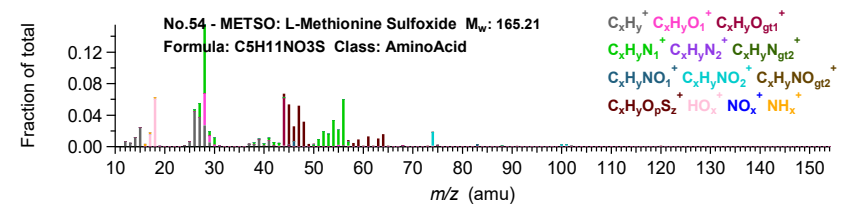
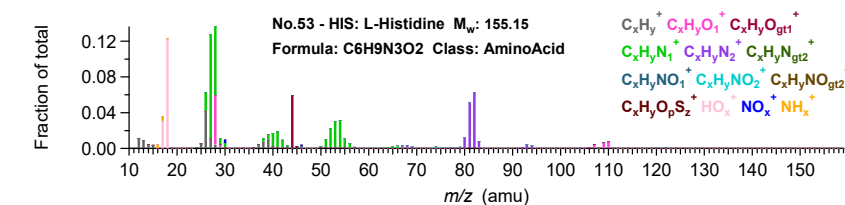
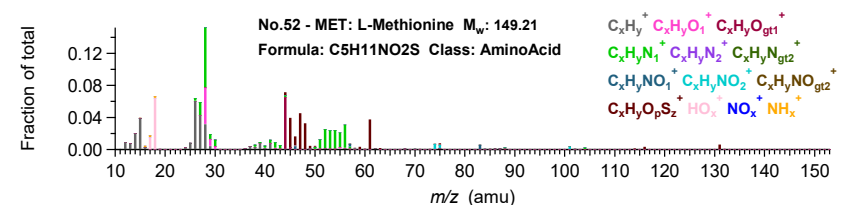
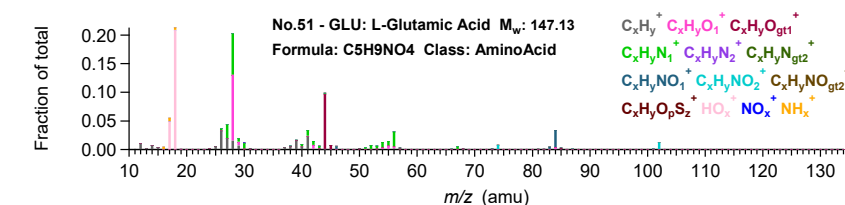


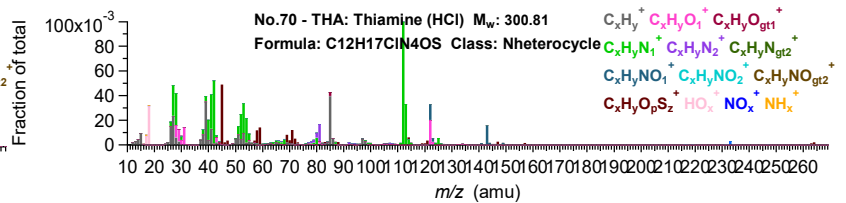
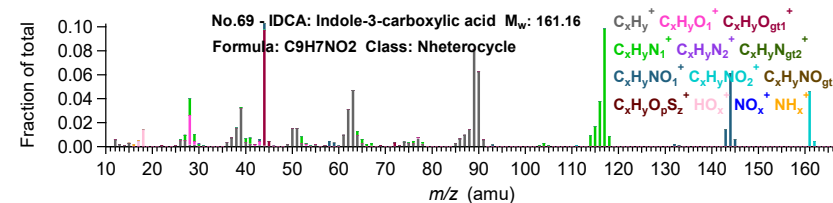
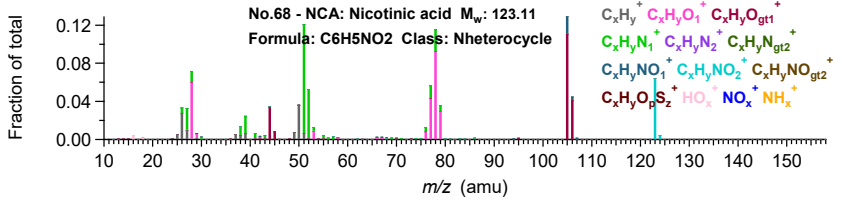
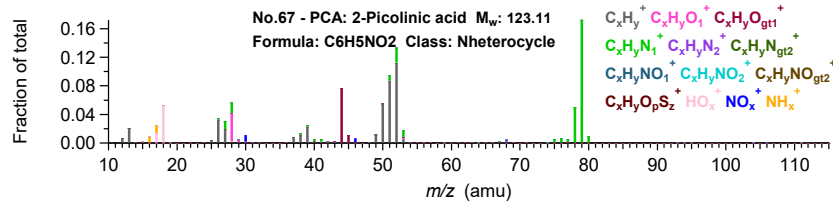
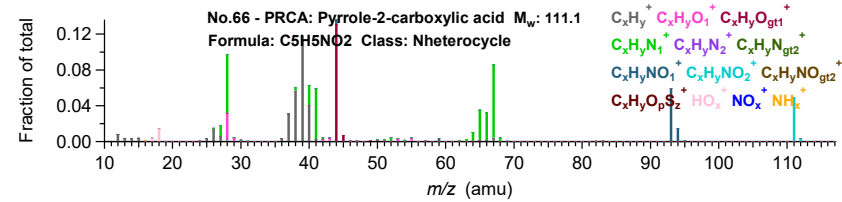
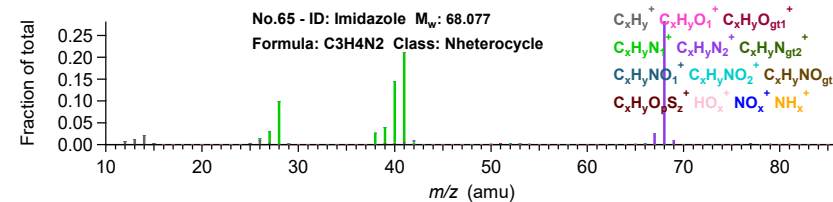
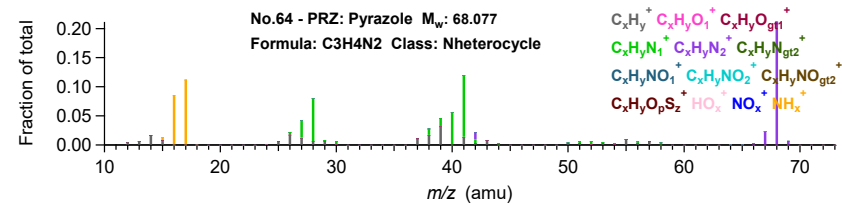
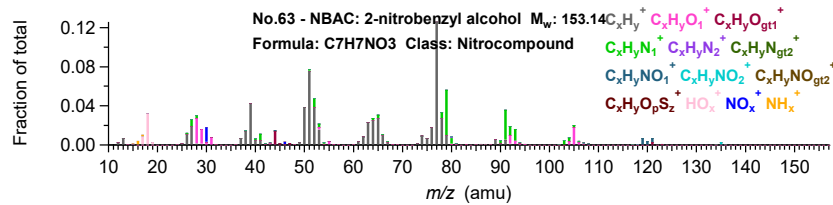
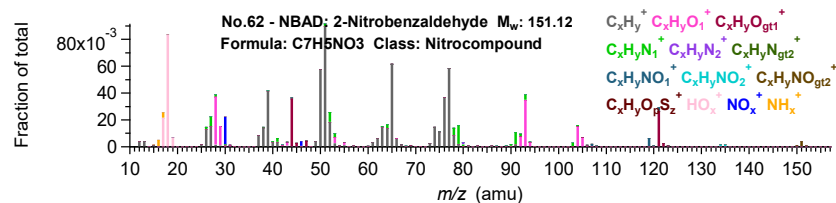
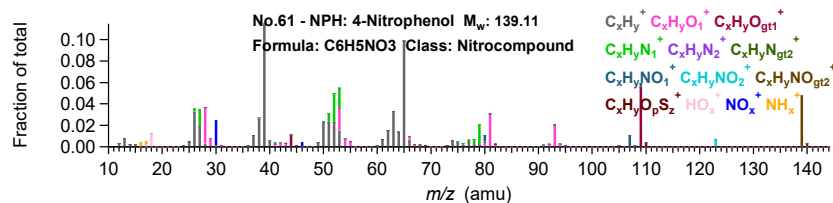












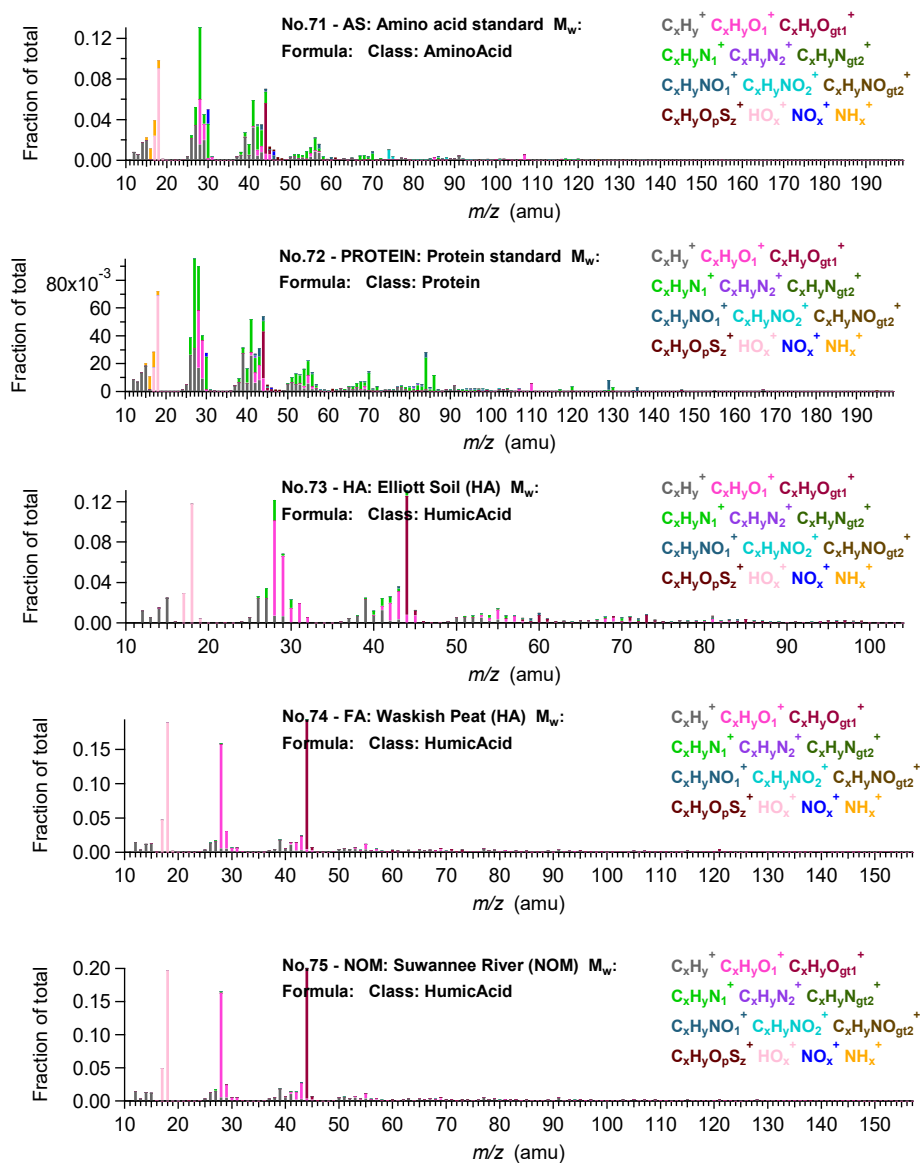


Figure S3. High resolution mass spectra of the 75 ON standards determined in this study.

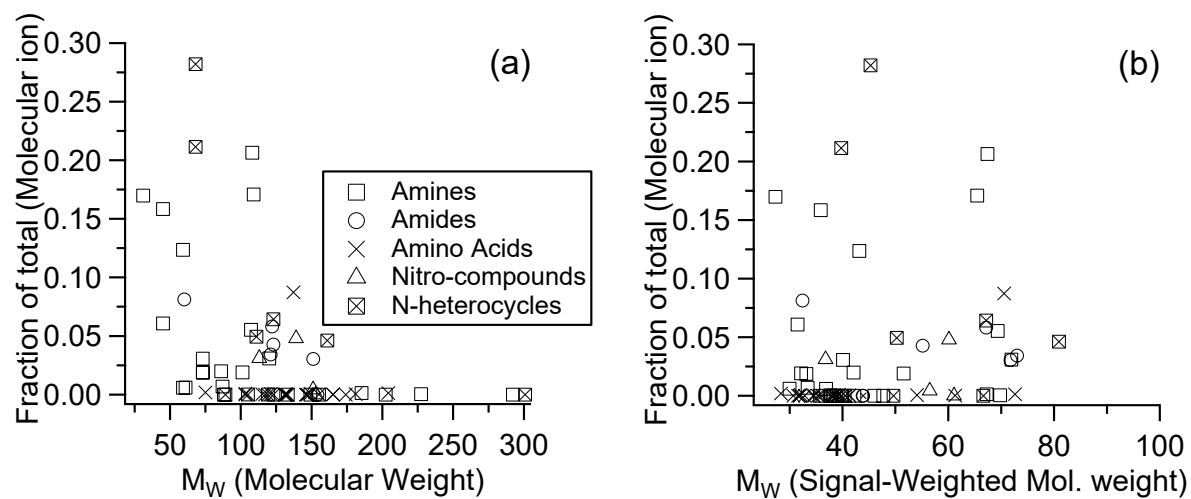


Figure S4. Mass fractions of the molecular ions in the HR-AMS spectra of the ON standards as a function of the molecular weights (M_w) (a), and the signal-weighted molecular weights (b) (calculated as $\sum f_i * i_{m/z}$, where $i_{m/z}$ is the exact mass of ion i and f_i is the mass fraction of that ion in the compound's spectrum).

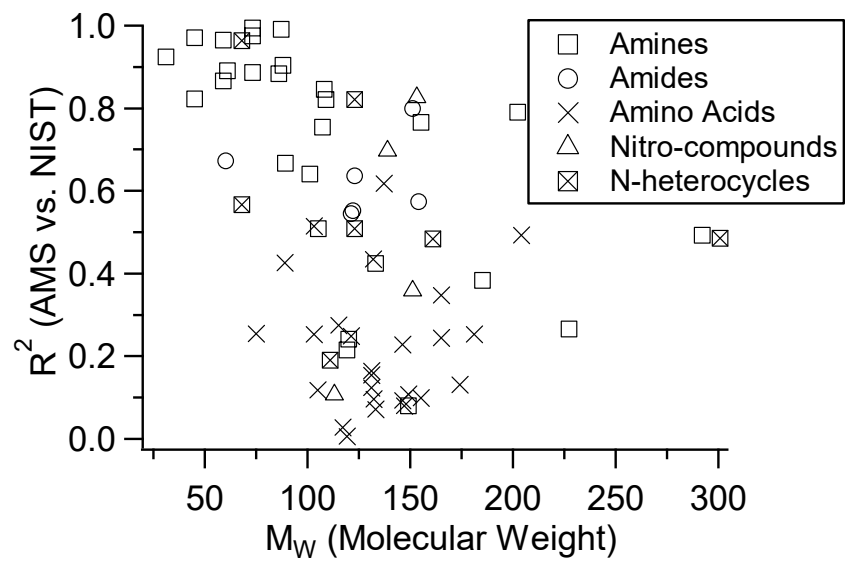


Figure S5. Correlation coefficients (Pearson's r^2) between the HR-AMS spectra and the NIST spectra as a function of the molecular weights of the ON standards.

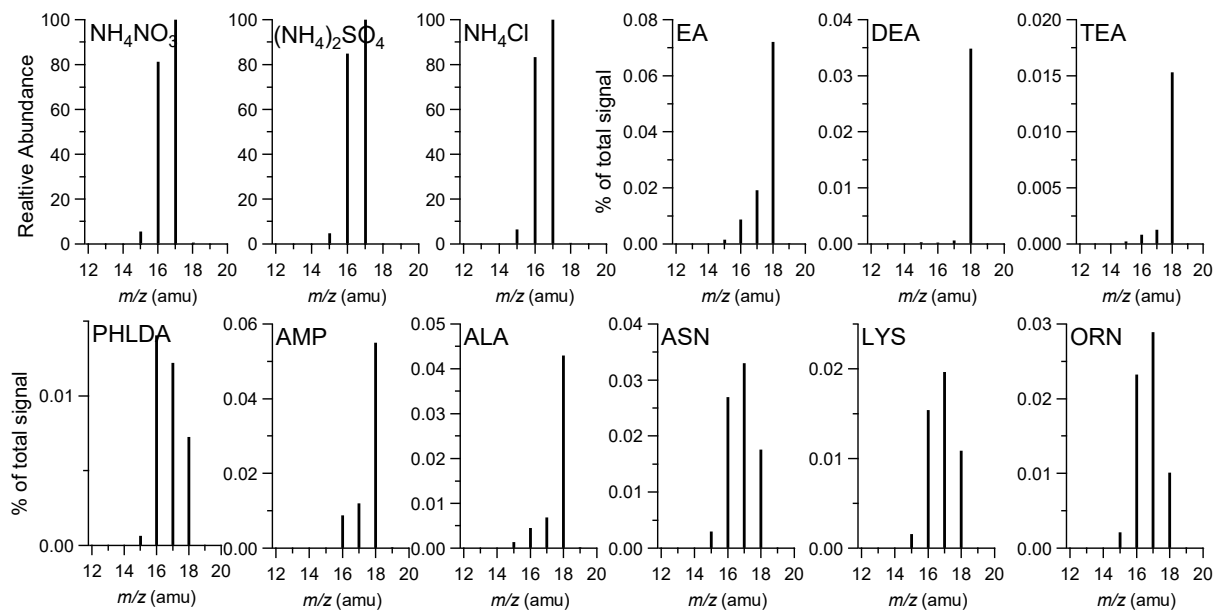


Figure S6. Mass fractional contributions of NH_x^+ ion fragments in the HR-AMS spectra of ammonium nitrate, ammonium sulfate and ammonium chloride, and a few selected amines and amino acids.

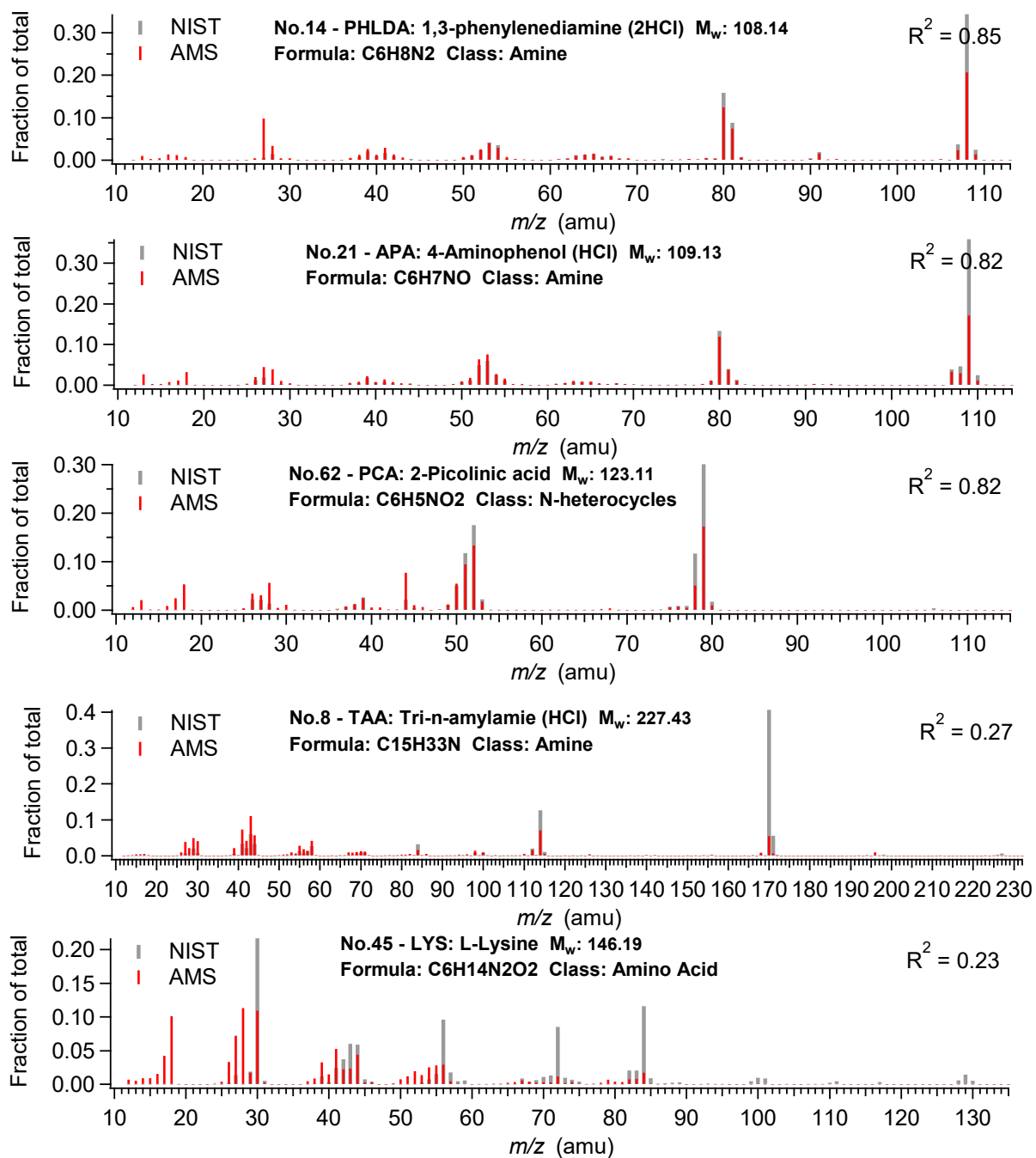


Figure S7. AMS spectra (summed in unit mass resolution from HR spectra) versus NIST spectra for a few selected ON standards.