

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN110323\
 Data File : VN079861.D
 Acq On : 03 Nov 2023 20:02
 Operator : JC\MD
 Sample : 05230-03 50X
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 60088

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110123W.M
 Title : SW846 8260

Signal : TIC: VN079861.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.289	50	57	64	rBV	33903	77861	3.23%	0.391%
2	2.665	115	121	129	rVB2	26082	50817	2.11%	0.255%
3	3.794	303	313	331	rBV	157704	436884	18.14%	2.195%
4	4.430	411	421	437	rBV	123945	385073	15.99%	1.934%
5	4.712	459	469	479	rBV	34401	110117	4.57%	0.553%
6	8.171	1046	1057	1061	rBV	220405	508007	21.10%	2.552%
7	8.229	1061	1067	1080	rVB	332650	757969	31.48%	3.808%
8	8.582	1118	1127	1141	rBV2	252315	740481	30.75%	3.720%
9	9.106	1206	1216	1230	rBV	548787	1115468	46.32%	5.604%
10	9.600	1287	1300	1312	rBV7	17954	48712	2.02%	0.245%
11	10.570	1457	1465	1470	rBV	820047	1486096	61.71%	7.465%
12	10.635	1470	1476	1490	rVV	1297144	2369602	98.40%	11.904%
13	11.870	1678	1686	1695	rBV	832220	1480568	61.48%	7.438%
14	11.965	1695	1702	1712	rVV	374036	657411	27.30%	3.303%
15	12.070	1712	1720	1732	rVV	1306806	2408156	100.00%	12.097%
16	12.400	1768	1776	1784	rBV	696886	1152176	47.84%	5.788%
17	12.700	1821	1827	1835	rBV	29668	50645	2.10%	0.254%
18	12.853	1846	1853	1862	rVB	613802	1028707	42.72%	5.168%
19	13.041	1877	1885	1889	rBV	64672	106703	4.43%	0.536%
20	13.100	1889	1895	1899	rVV	295322	514698	21.37%	2.586%
21	13.129	1899	1900	1904	rVV	121379	155297	6.45%	0.780%
22	13.176	1904	1908	1915	rVB	146997	231257	9.60%	1.162%
23	13.341	1927	1936	1943	rBV	132020	218537	9.07%	1.098%
24	13.488	1953	1961	1973	rVB	559385	916131	38.04%	4.602%
25	13.794	2006	2013	2031	rVB2	804846	1634597	67.88%	8.211%
26	13.994	2041	2047	2062	rVV3	128068	354449	14.72%	1.781%
27	14.182	2073	2079	2084	rBV2	17826	29539	1.23%	0.148%
28	14.247	2084	2090	2093	rVV2	33255	61854	2.57%	0.311%
29	14.276	2093	2095	2100	rVV2	29398	41461	1.72%	0.208%
30	14.329	2100	2104	2110	rVV	53920	85714	3.56%	0.431%
31	14.447	2119	2124	2131	rVB4	38234	68373	2.84%	0.343%
32	14.576	2141	2146	2151	rBV2	18294	28652	1.19%	0.144%
33	14.658	2151	2160	2162	rBV2	33690	56397	2.34%	0.283%
34	14.700	2162	2167	2170	rVV	49118	83821	3.48%	0.421%
35	14.935	2201	2207	2210	rBV2	37210	68434	2.84%	0.344%
36	15.053	2218	2227	2233	rBV2	69489	166836	6.93%	0.838%

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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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37	15.217	2249	2255	2262	rBV4	20292	36900	1.53%	0.185%
38	15.317	2267	2272	2278	rBV7	17612	35775	1.49%	0.180%
39	15.447	2286	2294	2300	rVB5	17850	46889	1.95%	0.236%
40	15.647	2321	2328	2334	rVB	49742	99351	4.13%	0.499%

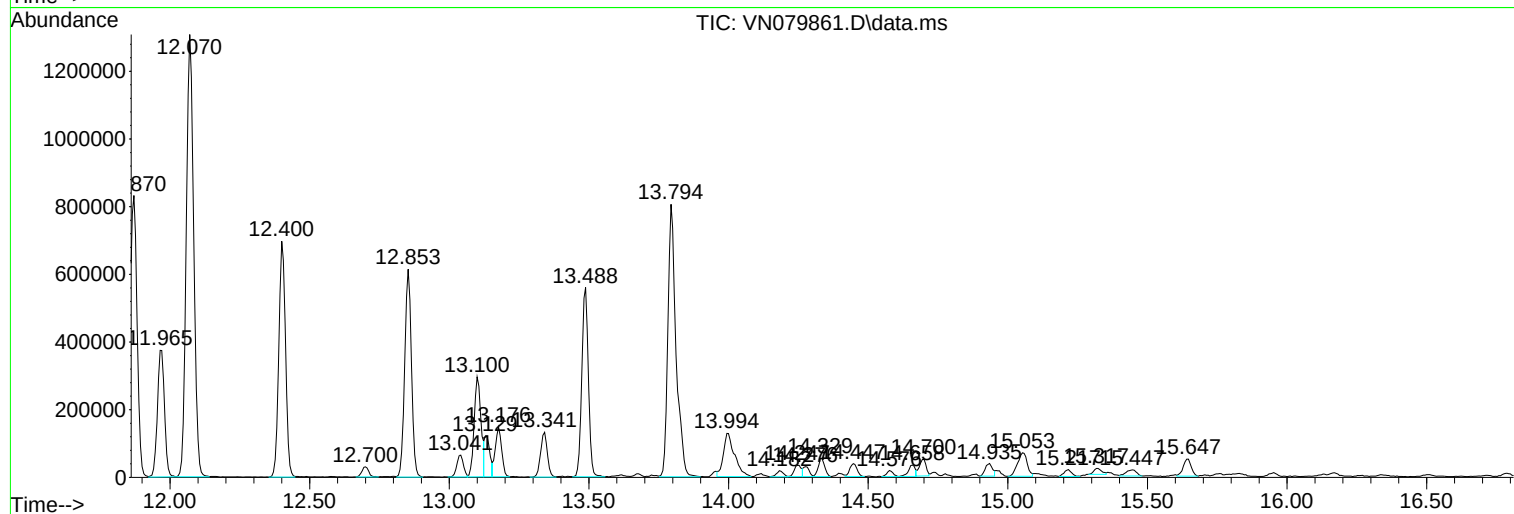
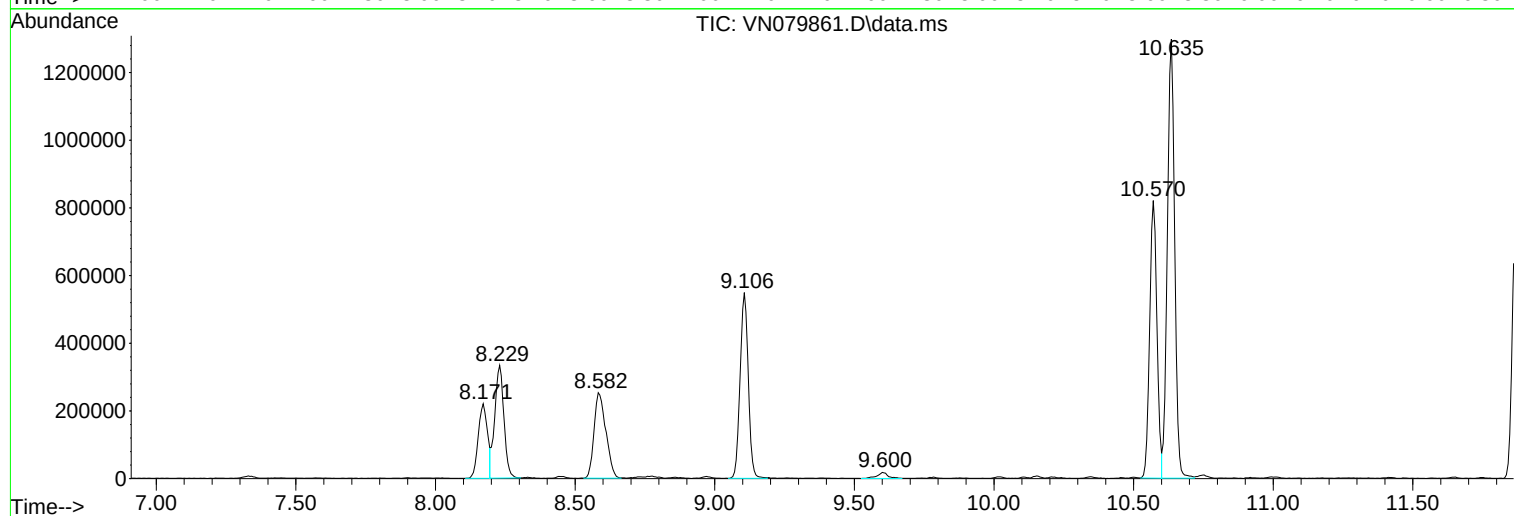
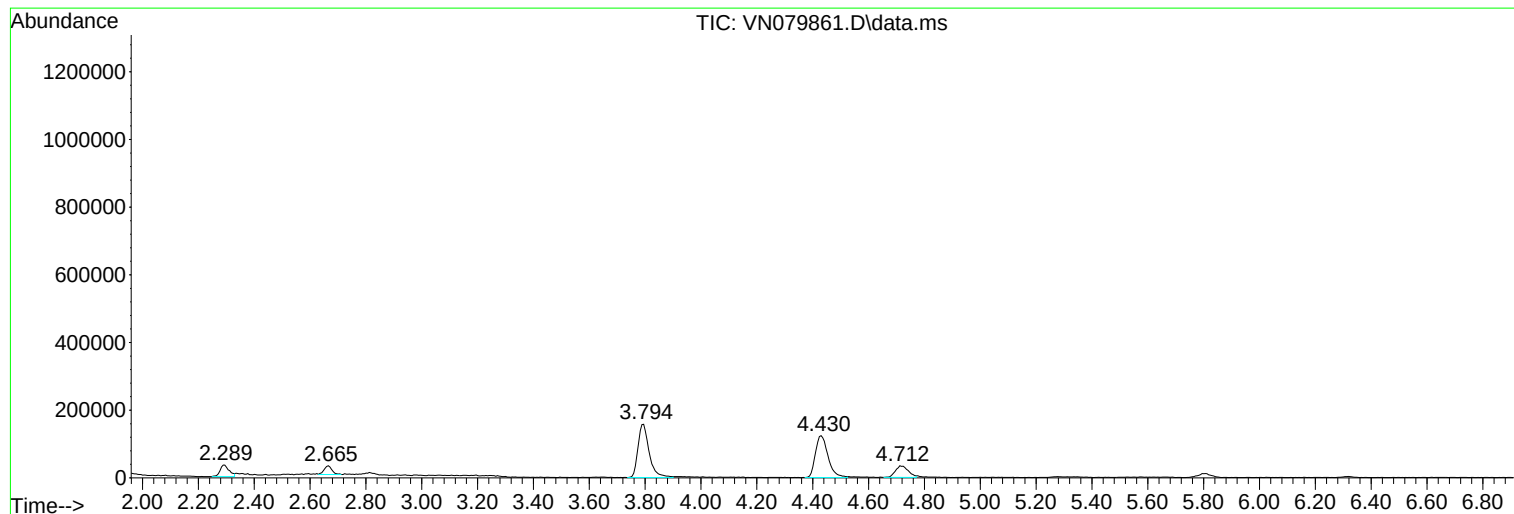
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110123W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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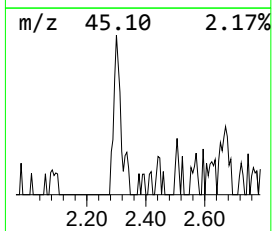
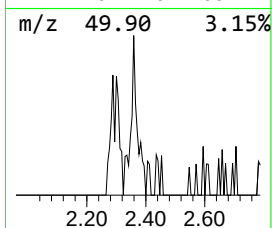
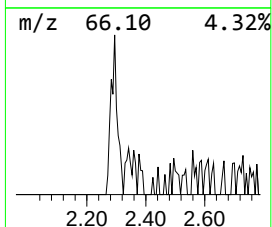
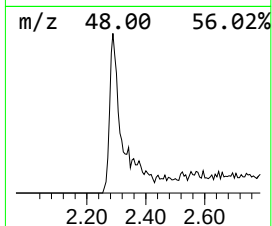
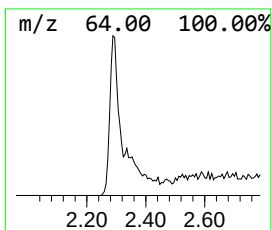
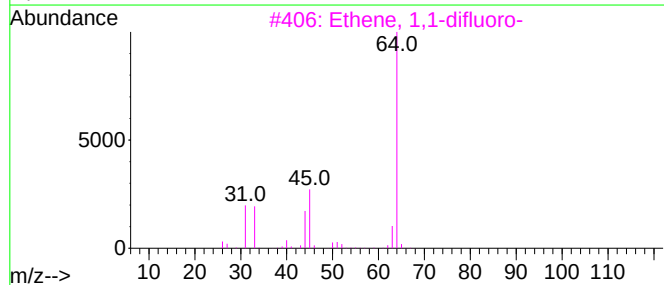
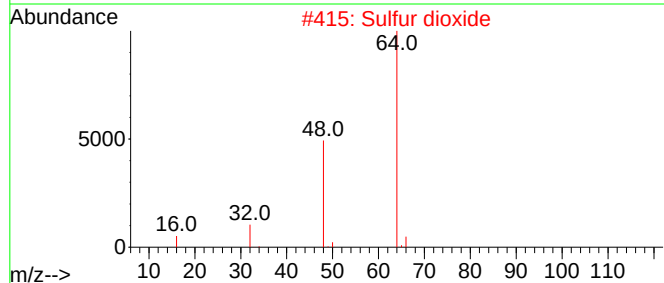
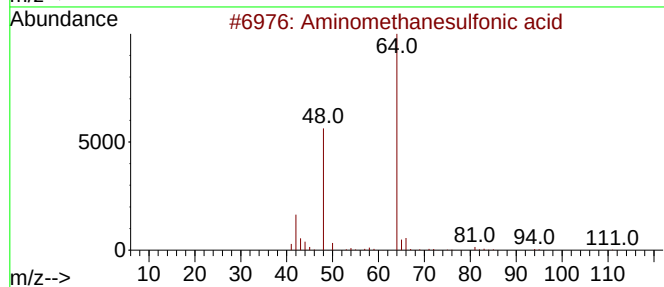
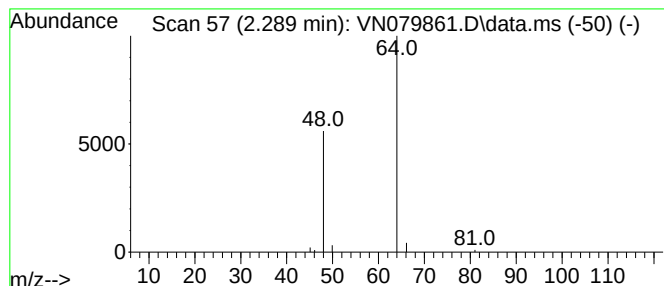
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110123W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Aminomethanesulfonic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.289	5.14 ug/l	77861	Pentafluorobenzene	8.229

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
2			Sulfur dioxide	64	O2S	007446-09-5	74
3			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	7
4			L-Cysteine sulfinic acid	153	C3H7NO4S	001115-65-7	4
5			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	4



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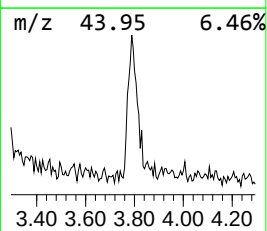
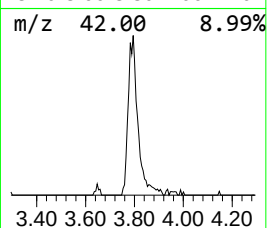
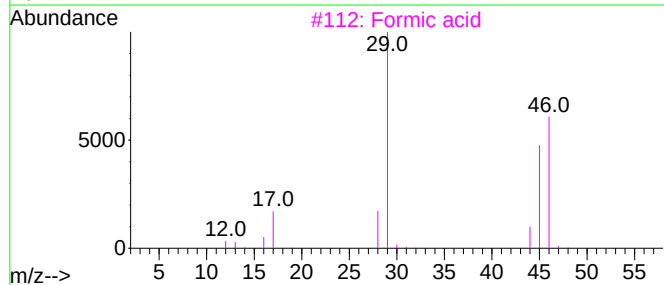
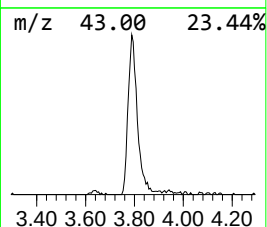
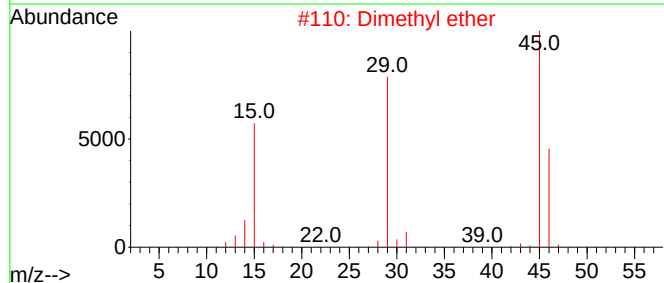
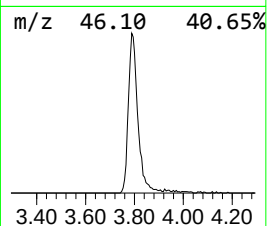
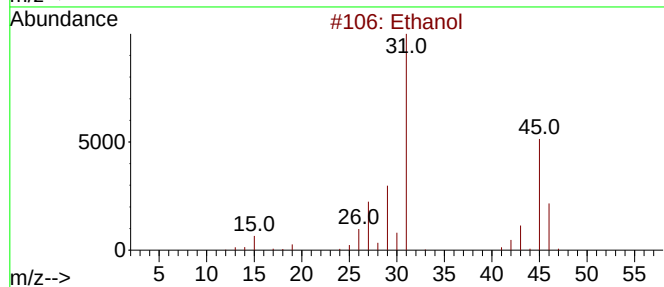
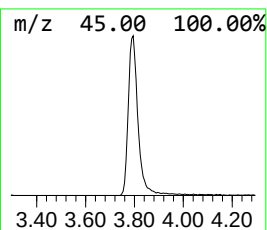
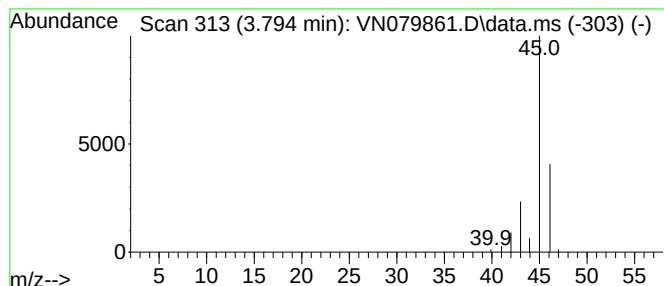
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Peak Number 2 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.794	28.82 ug/l	436884	Pentafluorobenzene	8.229

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	74
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Formic acid	46	CH2O2	000064-18-6	5
4			Methane, nitroso-	45	CH3NO	000865-40-7	4
5			Oxalic acid	90	C2H2O4	000144-62-7	4



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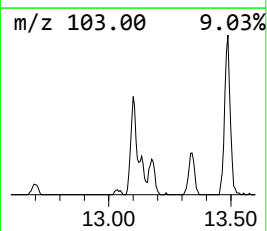
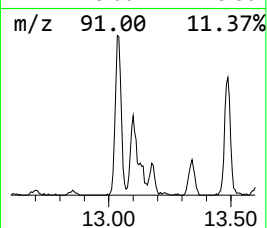
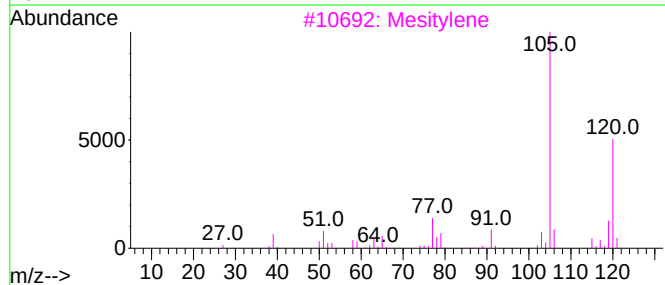
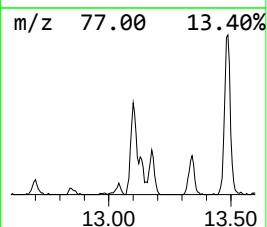
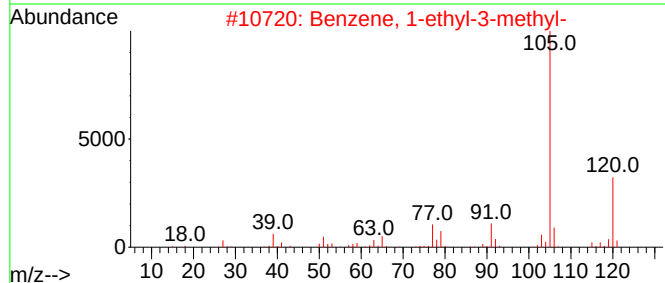
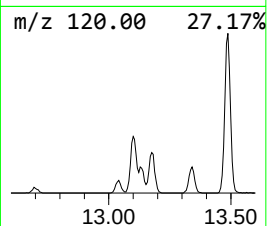
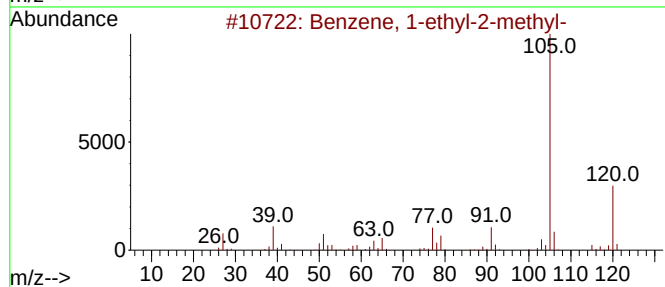
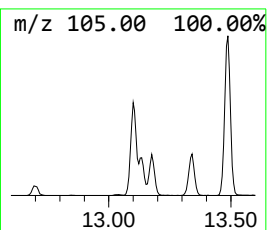
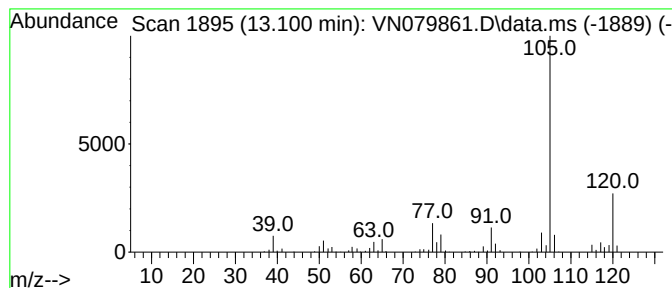
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110123W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.100	15.74 ug/l	514698	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
3			Mesitylene	120	C9H12	000108-67-8	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



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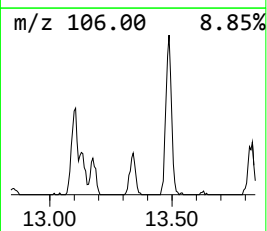
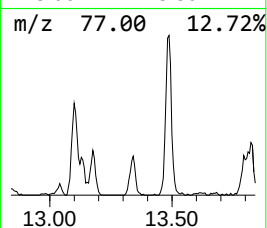
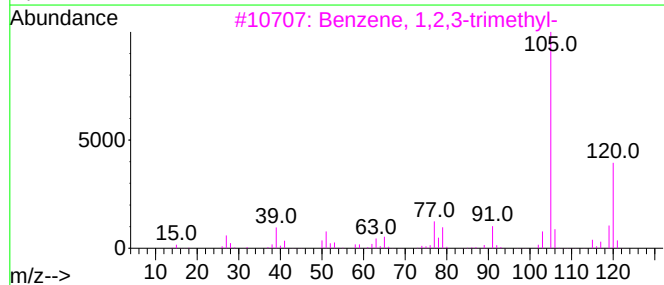
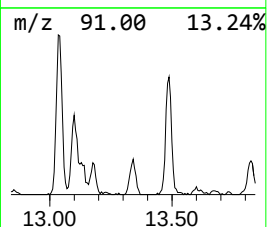
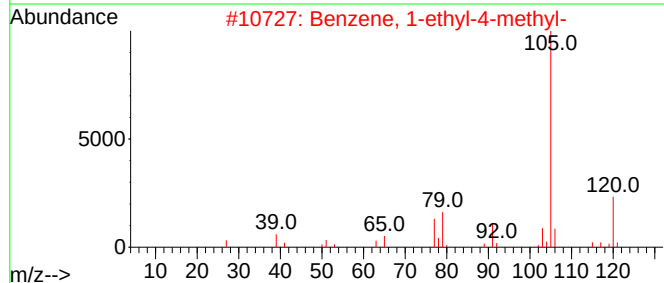
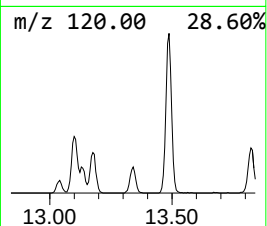
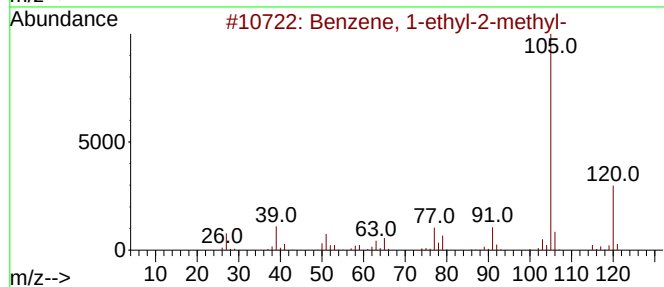
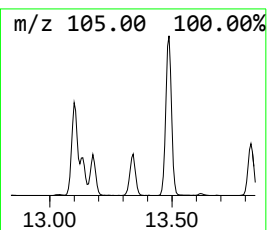
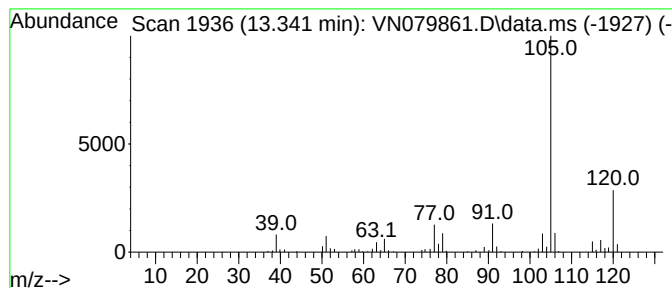
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Peak Number 5 Benzene, 1-ethyl-4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	6.68 ug/l	218537	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	90
5			Mesitylene	120	C9H12	000108-67-8	87



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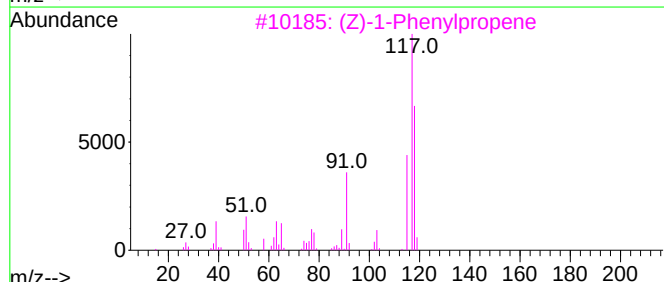
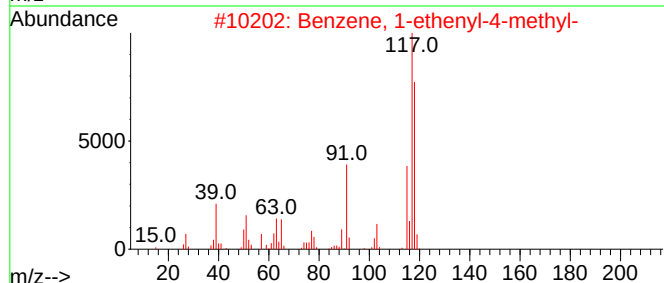
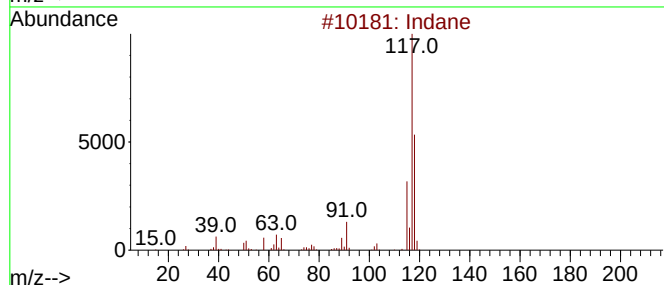
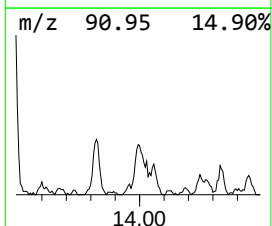
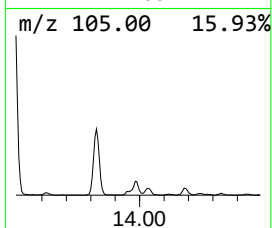
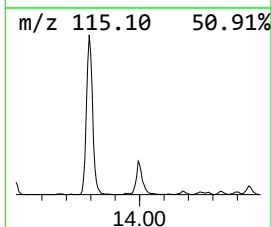
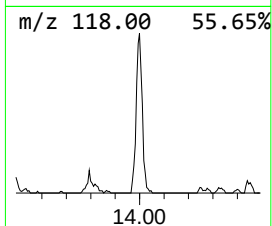
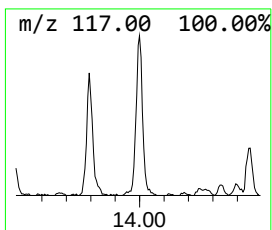
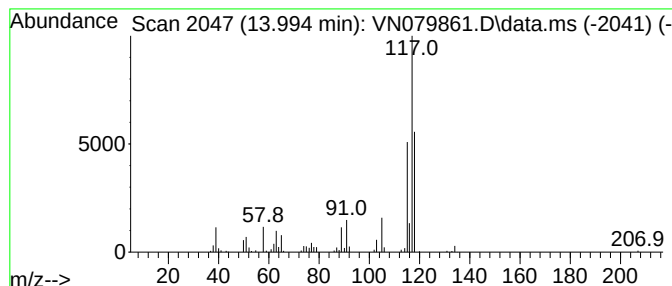
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.994	10.84 ug/l	354449	1,4-Dichlorobenzene-d4	13.794

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	76
2			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	70
3			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	64
4			Indane-5-carboxylic acid	162	C10H10O2	065898-38-6	59
5			Deltacyclene	118	C9H10	007785-10-6	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN110323\
Data File : VN079861.D
Acq On : 03 Nov 2023 20:02
Operator : JC\MD
Sample : 05230-03 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
60088

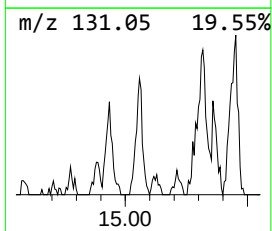
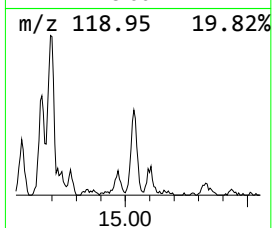
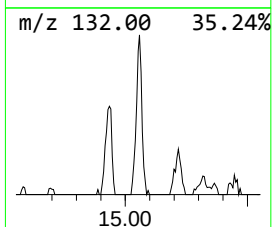
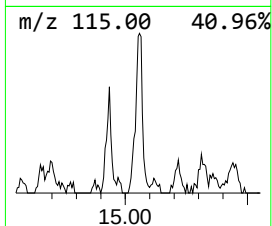
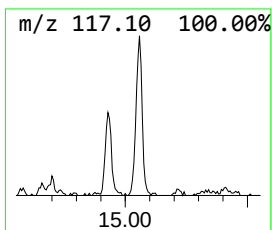
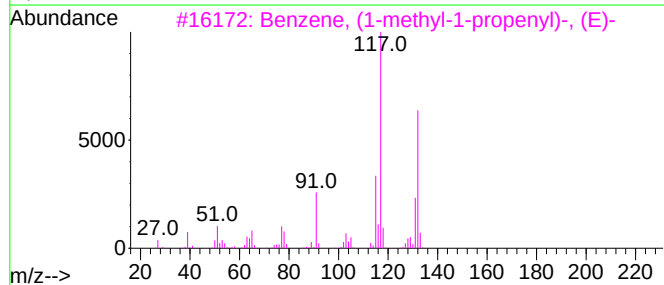
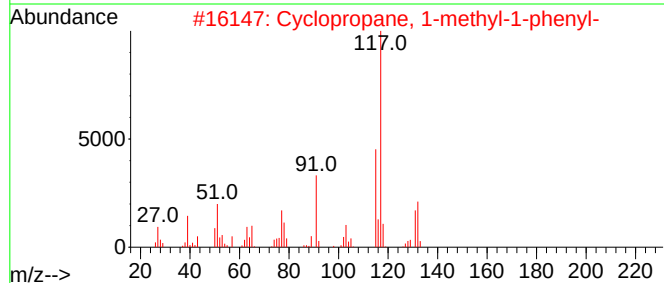
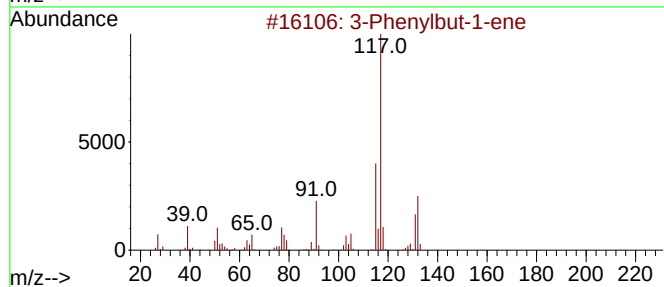
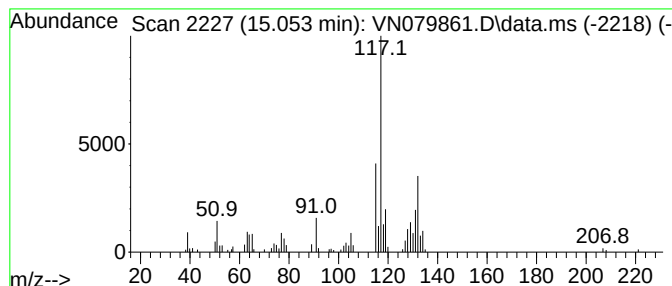
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 3-Phenylbut-1-ene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.053	5.10 ug/l	166836	1,4-Dichlorobenzene-d4	13.794

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Phenylbut-1-ene	132	C10H12	000934-10-1	81
2		Cyclopropane, 1-methyl-1-phenyl-	132	C10H12	002214-14-4	76
3		Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000768-00-3	74
4		Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	70
5		1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN110323\
Data File : VN079861.D
Acq On : 03 Nov 2023 20:02
Operator : JC\MD
Sample : 05230-03 50X
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
60088

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N110123W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Aminomethanesul...	2.289	5.1	ug/l	77861	1	8.229	757969	50.0
Ethanol	3.794	28.8	ug/l	436884	1	8.229	757969	50.0
Benzene, 1-ethy...	13.100	15.7	ug/l	514698	4	13.794	1634600	50.0
Benzene, 1-ethy...	13.341	6.7	ug/l	218537	4	13.794	1634600	50.0
Indane	13.994	10.8	ug/l	354449	4	13.794	1634600	50.0
3-Phenylbut-1-ene	15.053	5.1	ug/l	166836	4	13.794	1634600	50.0