

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN032622\
 Data File : VN071581.D
 Acq On : 26 Mar 2022 18:38
 Operator : JC\MD
 Sample : N2131-05
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-12

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\82N032522W.M
 Title : SW846 8260

Signal : TIC: VN071581.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.128	186	194	215	rVB	181297	455545	10.94%	1.401%
2	3.510	250	259	274	rVB	31485	75850	1.82%	0.233%
3	4.581	431	441	454	rBV3	11657	41758	1.00%	0.128%
4	5.075	512	525	531	rBV3	32531	115849	2.78%	0.356%
5	5.622	604	618	629	rBV	48656	164503	3.95%	0.506%
6	7.145	866	877	891	rVB3	94018	282668	6.79%	0.869%
7	8.016	1016	1025	1030	rBV	512405	1194986	28.69%	3.675%
8	8.081	1030	1036	1046	rVV	1016586	2385417	57.26%	7.336%
9	8.169	1047	1051	1064	rVB4	27558	71377	1.71%	0.220%
10	8.434	1087	1096	1110	rBV	536955	1236943	29.69%	3.804%
11	8.616	1122	1127	1137	rVV2	37823	105350	2.53%	0.324%
12	8.704	1137	1142	1151	rVB4	22604	64510	1.55%	0.198%
13	8.963	1177	1186	1200	rBV	1460445	2984723	71.65%	9.179%
14	9.881	1337	1342	1352	rVB2	22154	43124	1.04%	0.133%
15	10.010	1359	1364	1372	rVB2	25852	53291	1.28%	0.164%
16	10.439	1428	1437	1444	rBV	2299780	4165851	100.00%	12.812%
17	10.498	1444	1447	1461	rVB2	60381	135413	3.25%	0.416%
18	11.739	1649	1658	1669	rBV	2160126	3801571	91.26%	11.691%
19	11.839	1669	1675	1686	rVV	733614	1240355	29.77%	3.815%
20	11.951	1686	1694	1706	rVB	655322	1263056	30.32%	3.884%
21	12.275	1741	1749	1759	rVB	37166	65763	1.58%	0.202%
22	12.575	1792	1800	1807	rBV2	87875	147987	3.55%	0.455%
23	12.727	1818	1826	1837	rBV	1690144	2842742	68.24%	8.742%
24	12.916	1852	1858	1864	rBV	169021	285278	6.85%	0.877%
25	12.980	1864	1869	1871	rVV3	48760	87591	2.10%	0.269%
26	13.010	1871	1874	1878	rVV	125897	202912	4.87%	0.624%
27	13.057	1878	1882	1890	rVB	70250	118091	2.83%	0.363%
28	13.216	1902	1909	1917	rBV	220785	363490	8.73%	1.118%
29	13.363	1928	1934	1948	rVB	1336555	2183675	52.42%	6.716%
30	13.498	1948	1957	1963	rVB4	41807	93824	2.25%	0.289%
31	13.669	1979	1986	1999	rBV2	1790983	3462727	83.12%	10.649%
32	13.833	2008	2014	2016	rBV2	55459	87491	2.10%	0.269%
33	13.874	2016	2021	2025	rVV	270711	464246	11.14%	1.428%
34	13.916	2025	2028	2037	rVB4	52859	104201	2.50%	0.320%
35	14.127	2059	2064	2066	rBV	74640	119577	2.87%	0.368%
36	14.216	2073	2079	2084	rVB	126514	202832	4.87%	0.624%

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Max Peaks: 100

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37	14.274	2084	2089	2093	rVV5	23121	41767	1.00%	0.128%
38	14.327	2093	2098	2104	rVB2	107522	182458	4.38%	0.561%
39	14.539	2124	2134	2137	rBV	74153	134899	3.24%	0.415%
40	14.574	2137	2140	2146	rVB	79285	114806	2.76%	0.353%
41	14.804	2174	2179	2185	rBV2	64482	105972	2.54%	0.326%
42	14.927	2192	2200	2206	rBV2	126060	277757	6.67%	0.854%
43	15.192	2235	2245	2254	rVV6	24019	76745	1.84%	0.236%
44	15.310	2257	2265	2273	rVB3	30679	76650	1.84%	0.236%
45	15.504	2287	2298	2310	rBV	321878	639416	15.35%	1.966%
46	16.615	2480	2487	2496	rVB	64908	151456	3.64%	0.466%

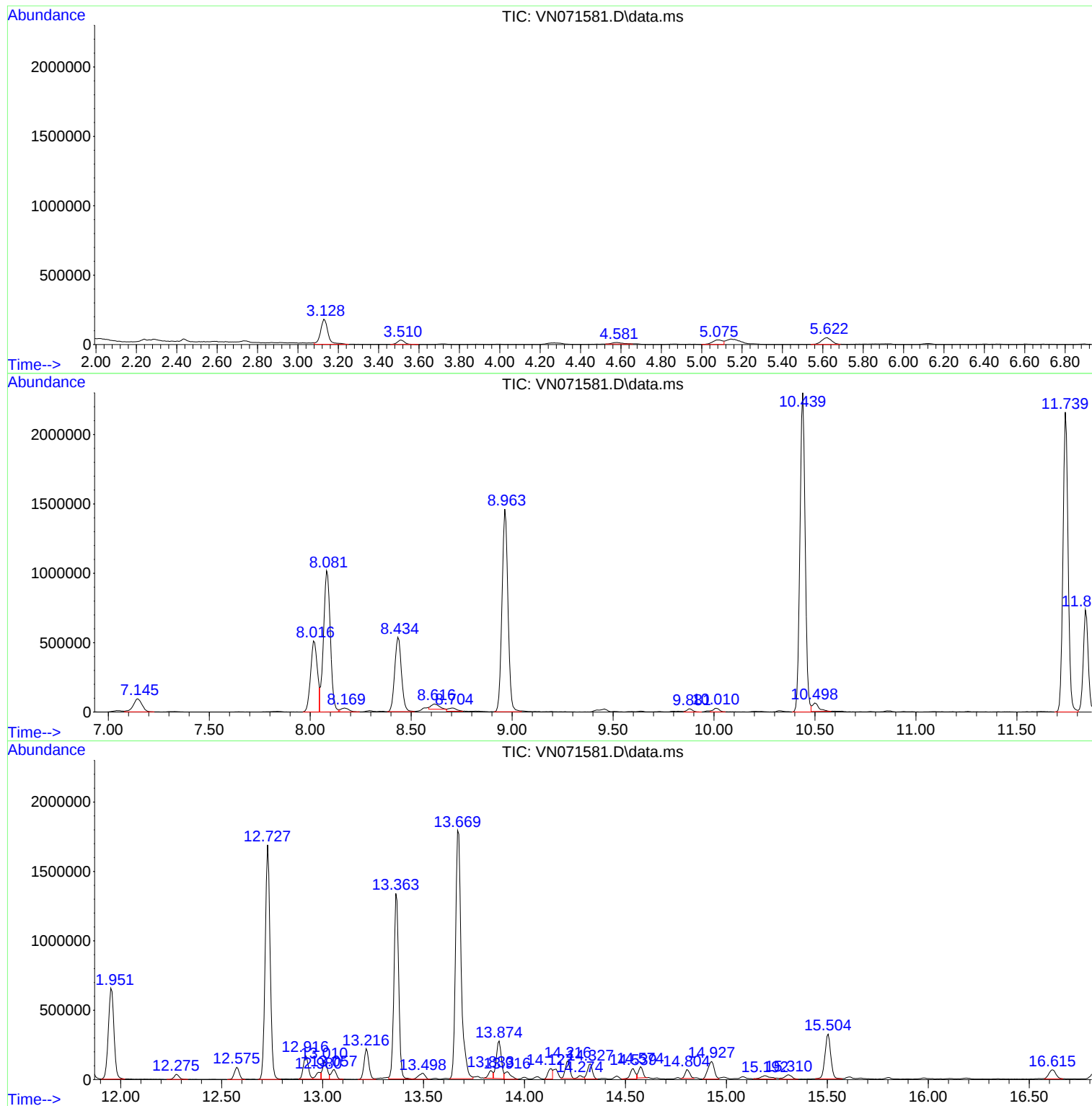
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032522W.M
Quant Title : SW846 8260

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



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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-12

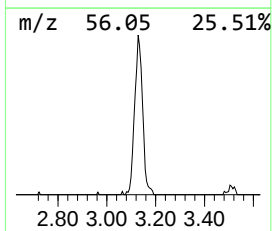
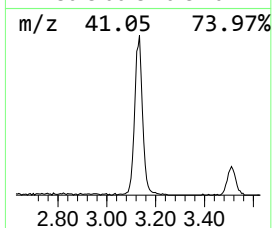
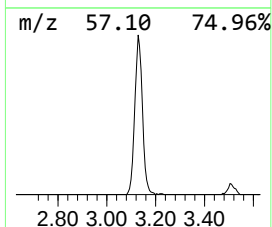
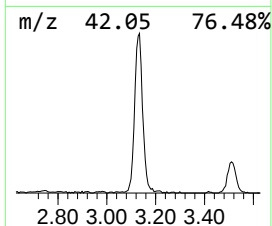
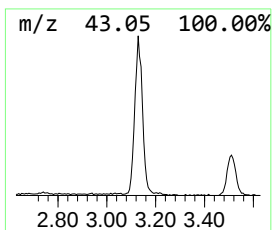
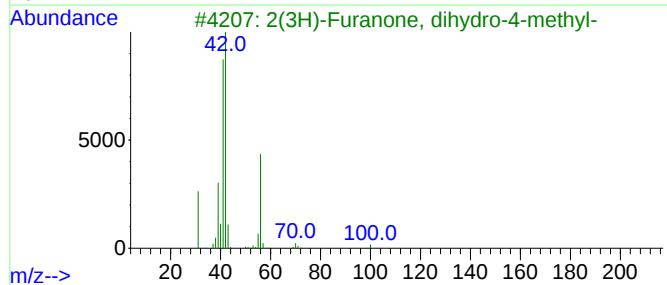
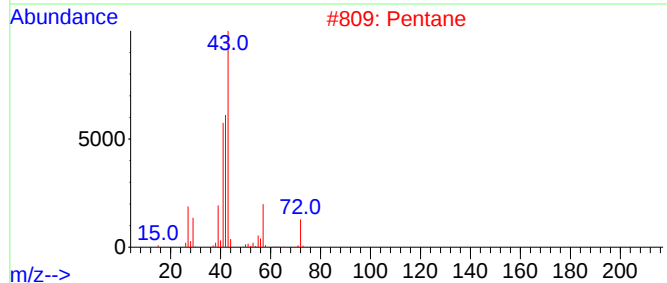
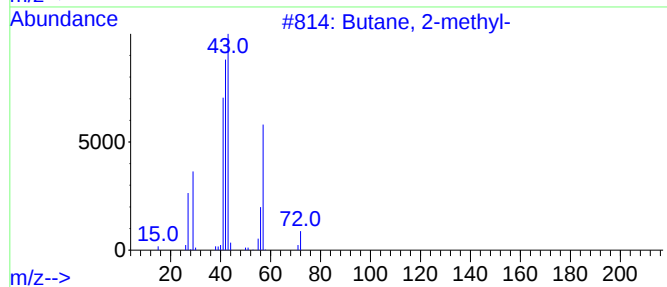
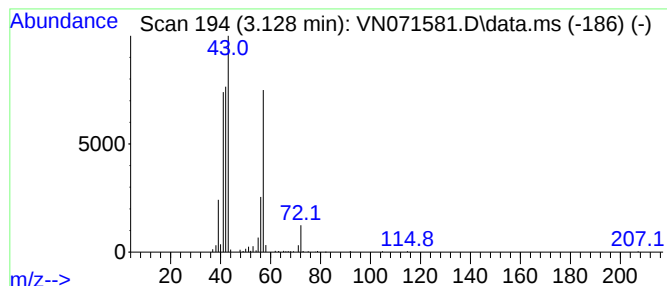
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032522W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.128	9.55 ug/l	455545	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	90
2			Pentane	72	C5H12	000109-66-0	72
3			2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	53
4			Oxirane, ethyl-	72	C4H8O	000106-88-7	50
5			Cyclobutane, methyl-	70	C5H10	000598-61-8	32



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Instrument :
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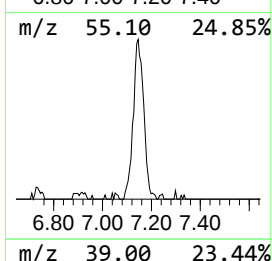
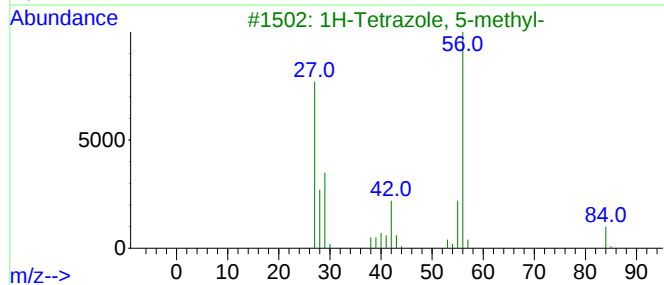
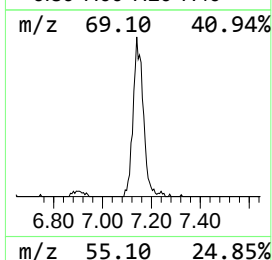
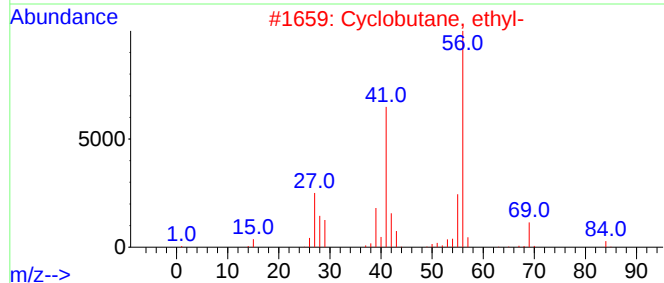
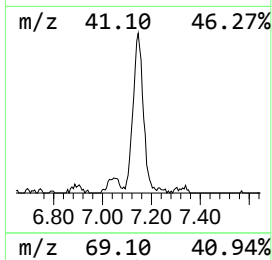
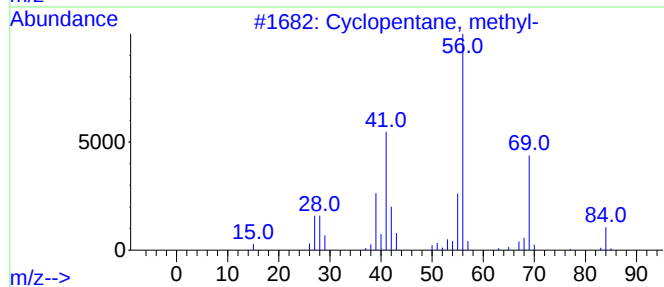
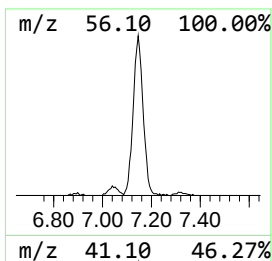
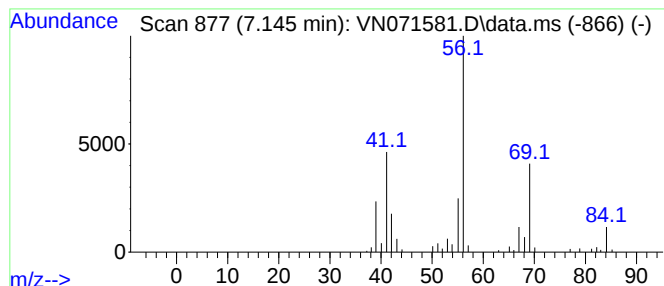
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032522W.M
Quant Title : SW846 8260

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

Peak Number 2 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.145	5.92 ug/l	282668	Pentafluorobenzene	8.081

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2			Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
3			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4			Cyclohexane	84	C6H12	000110-82-7	64
5			1-Pentanol, 3-methyl-	102	C6H14O	000589-35-5	45



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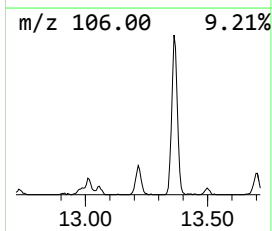
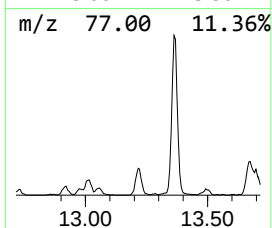
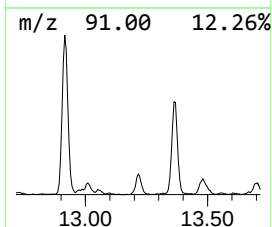
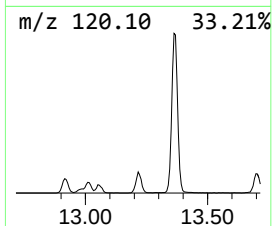
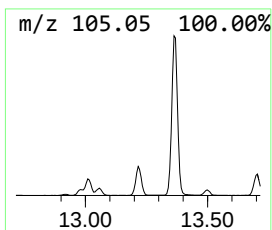
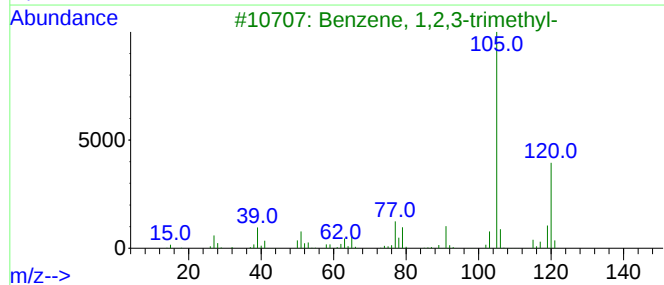
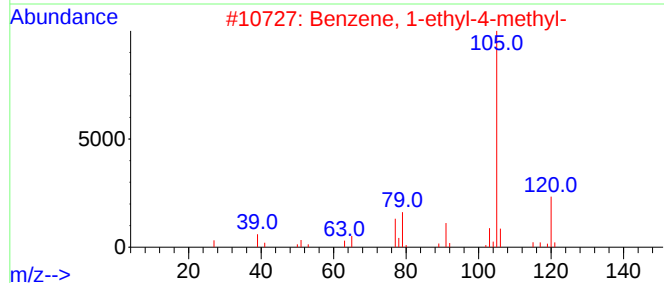
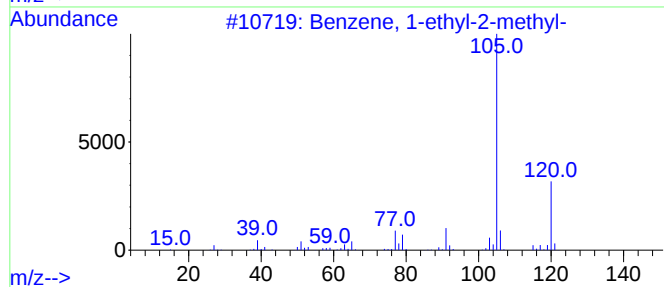
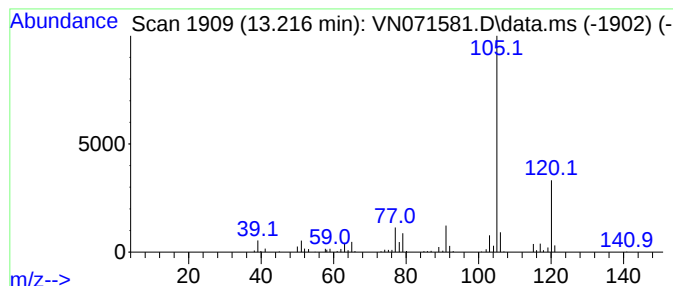
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N032522W.M
Quant Title : SW846 8260

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

Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.216	5.25 ug/l	363490	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
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	90



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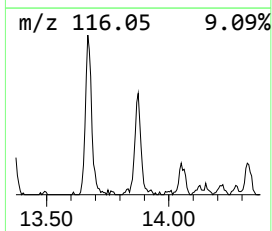
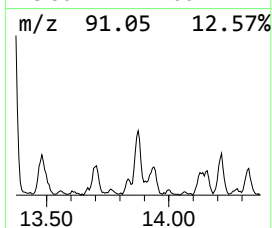
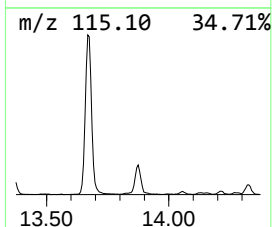
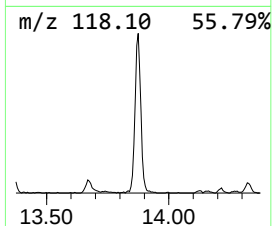
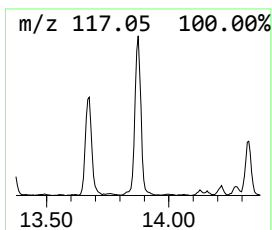
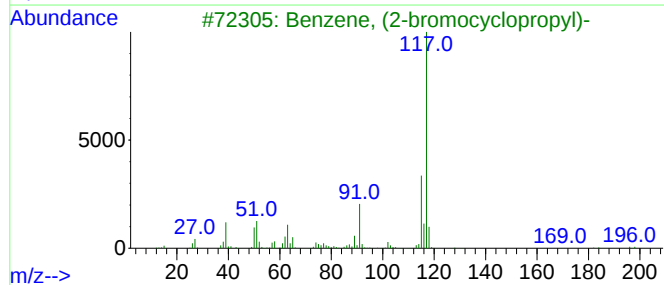
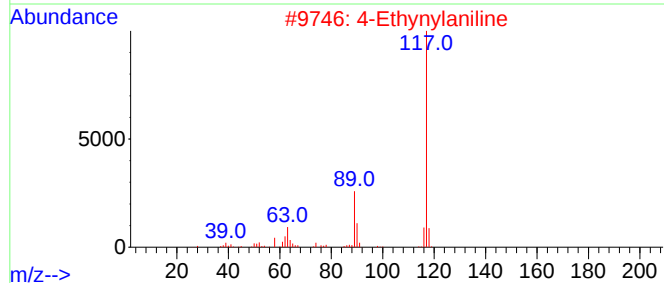
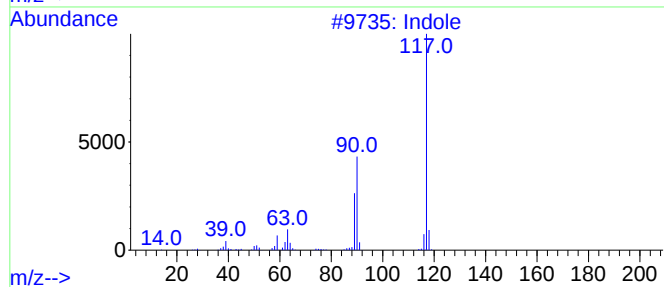
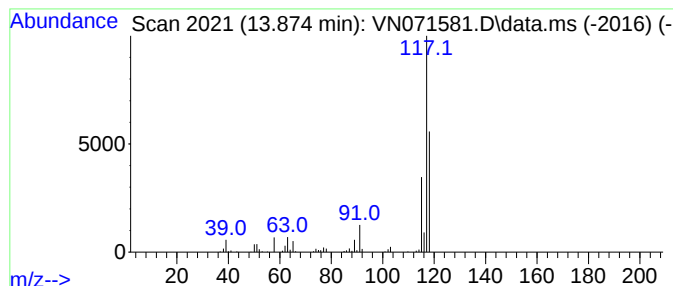
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown13.874 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	6.70 ug/l	464246	1,4-Dichlorobenzene-d4	13.669

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indole	117	C8H7N	000120-72-9	43
2			4-Ethynylaniline	117	C8H7N	014235-81-5	43
3			Benzene, (2-bromocyclopropyl)-	196	C9H9Br	036617-02-4	42
4			Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	40
5			trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	40



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methyl-	3.128	9.6	ug/l	455545	1	8.081	2385420	50.0
Cyclopentane, m...	7.145	5.9	ug/l	282668	1	8.081	2385420	50.0
Benzene, 1-ethy...	13.216	5.3	ug/l	363490	4	13.669	3462730	50.0
unknown13.874	13.874	6.7	ug/l	464246	4	13.669	3462730	50.0