

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021223\
 Data File : VX034133.D
 Acq On : 10 Feb 2023 22:27
 Operator : JC/MD
 Sample : VSTDCCC050
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 MSVOA_X
 LabSampleId :
 VSTDCCC050

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_X\Method\82X020423W.M
 Title : SW846 8260

Signal : TIC: VX034133.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.167	10	13	26	rVB	74260	82456	7.54%	0.258%
2	1.295	31	34	43	rVV	51072	61618	5.63%	0.193%
3	1.374	43	47	57	rVV	56980	66469	6.08%	0.208%
4	1.605	81	85	94	rVB	59508	70457	6.44%	0.221%
5	1.685	94	98	111	rVB	34739	47322	4.33%	0.148%
6	1.886	125	131	144	rBV	120502	173670	15.87%	0.544%
7	2.130	164	171	182	rBV	69962	100511	9.19%	0.315%
8	2.233	182	188	195	rVV	67311	102154	9.34%	0.320%
9	2.325	195	203	208	rVV2	227966	438195	40.05%	1.373%
10	2.374	208	211	219	rVV	98005	165048	15.09%	0.517%
11	2.453	219	224	229	rVV	64238	110927	10.14%	0.348%
12	2.514	229	234	249	rVV	89980	142301	13.01%	0.446%
13	2.666	249	259	262	rVV	111799	207611	18.98%	0.651%
14	2.697	262	264	273	rVV	67316	109882	10.04%	0.344%
15	2.788	273	279	297	rVV	92701	193525	17.69%	0.606%
16	2.953	299	306	318	rVV	28872	94778	8.66%	0.297%
17	3.063	318	324	326	rVV	152673	285348	26.08%	0.894%
18	3.099	326	330	347	rVB2	209183	554543	50.68%	1.738%
19	3.611	404	414	423	rBV	78654	184016	16.82%	0.577%
20	3.721	423	432	462	rVB2	295819	1027137	93.88%	3.219%
21	4.483	544	557	563	rBV3	149330	450122	41.14%	1.411%
22	4.550	563	568	576	rVB	82652	207834	19.00%	0.651%
23	4.635	576	582	589	rBV	53788	135894	12.42%	0.426%
24	4.715	589	595	596	rBV	22908	38724	3.54%	0.121%
25	4.904	615	626	634	rBV3	100797	320144	29.26%	1.003%
26	5.001	634	642	650	rVV	109269	341594	31.22%	1.071%
27	5.093	650	657	671	rVB2	76969	237118	21.67%	0.743%
28	5.385	692	705	712	rBV2	144821	438313	40.06%	1.374%
29	5.471	712	719	726	rVV	105710	330358	30.19%	1.035%
30	5.550	726	732	737	rVV	110611	309299	28.27%	0.969%
31	5.611	738	742	747	rVV	84461	210970	19.28%	0.661%
32	5.684	747	754	771	rVB3	166335	510399	46.65%	1.600%
33	5.952	789	798	805	rBV	59360	159711	14.60%	0.501%
34	6.038	805	812	818	rBV	149371	401462	36.69%	1.258%
35	6.336	850	861	880	rBV	77142	200746	18.35%	0.629%
36	6.757	922	930	943	rBV	152111	362988	33.18%	1.138%

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Integrator: RTE

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37	7.123	982	990	1001	rVB	144420	311999	28.52%	0.978%
38	7.379	1022	1032	1037	rBV	172475	392938	35.91%	1.231%
39	7.428	1037	1040	1055	rVB	125650	234094	21.40%	0.734%
40	7.580	1057	1065	1073	rBV	104244	203991	18.64%	0.639%
41	7.690	1073	1083	1094	rVB2	122671	266708	24.38%	0.836%
42	7.818	1094	1104	1117	rBV2	133803	374034	34.19%	1.172%
43	8.110	1145	1152	1162	rBV	26323	46496	4.25%	0.146%
44	8.238	1166	1173	1187	rVV	427729	684734	62.58%	2.146%
45	8.366	1187	1194	1204	rBV	154119	249315	22.79%	0.781%
46	8.574	1221	1228	1235	rBV	555454	885705	80.95%	2.776%
47	8.647	1235	1240	1246	rVV	297409	467501	42.73%	1.465%
48	8.714	1246	1251	1261	rVB	330720	519021	47.44%	1.627%
49	8.976	1288	1294	1306	rBV	163029	232034	21.21%	0.727%
50	9.116	1311	1317	1320	rVV	181040	264503	24.18%	0.829%
51	9.153	1320	1323	1336	rVV	193124	270740	24.75%	0.848%
52	9.275	1336	1343	1346	rVV	262763	416761	38.09%	1.306%
53	9.305	1346	1348	1363	rVV	174768	226016	20.66%	0.708%
54	9.427	1363	1368	1378	rVV	451578	624486	57.08%	1.957%
55	9.519	1378	1383	1388	rVV	136466	202211	18.48%	0.634%
56	9.580	1388	1393	1395	rVV	164048	213896	19.55%	0.670%
57	9.610	1395	1398	1410	rVB	107574	153193	14.00%	0.480%
58	10.055	1465	1471	1473	rBV	312590	474356	43.36%	1.487%
59	10.080	1473	1475	1483	rVV	318083	357798	32.70%	1.121%
60	10.165	1483	1489	1491	rVV	242030	363791	33.25%	1.140%
61	10.195	1491	1494	1505	rVV	420974	534306	48.83%	1.674%
62	10.299	1505	1511	1523	rVB	814127	1094112	100.00%	3.429%
63	10.647	1562	1568	1578	rBV2	600275	1040984	95.14%	3.262%
64	10.799	1587	1593	1597	rBV	132039	175275	16.02%	0.549%
65	10.842	1597	1600	1610	rVV	214873	262609	24.00%	0.823%
66	10.964	1614	1620	1625	rVV	460254	602956	55.11%	1.890%
67	11.018	1625	1629	1634	rVV	134852	162712	14.87%	0.510%
68	11.079	1634	1639	1651	rVB	263327	337510	30.85%	1.058%
69	11.201	1653	1659	1663	rBV2	325068	626944	57.30%	1.965%
70	11.238	1663	1665	1672	rVV2	199900	362171	33.10%	1.135%
71	11.305	1672	1676	1681	rVV	464413	566899	51.81%	1.777%
72	11.366	1681	1686	1692	rVV	373243	483081	44.15%	1.514%
73	11.451	1695	1700	1710	rVB	862717	1066487	97.48%	3.342%
74	11.713	1738	1743	1747	rBV2	648388	973163	88.95%	3.050%
75	11.750	1747	1749	1756	rVB	501472	538145	49.19%	1.686%
76	11.890	1764	1772	1780	rBV	489968	593180	54.22%	1.859%

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77	11.969	1780	1785	1788	rBV	374474	460150	42.06%	1.442%
78	12.012	1788	1792	1795	rBV3	602938	985691	90.09%	3.089%
79	12.335	1839	1845	1853	rBV	772954	960309	87.77%	3.009%
80	12.536	1873	1878	1885	rBV	267431	352467	32.21%	1.105%
81	12.945	1936	1945	1954	rBB2	93611	133356	12.19%	0.418%
82	13.103	1966	1971	1977	rBV	10626	14216	1.30%	0.045%
83	13.286	1995	2001	2011	rBV	511757	599278	54.77%	1.878%
84	13.585	2045	2050	2059	rBV	341547	425975	38.93%	1.335%
85	13.725	2067	2073	2077	rBV	263280	325783	29.78%	1.021%
86	13.774	2077	2081	2089	rVB	416873	493945	45.15%	1.548%
87	13.957	2106	2111	2123	rVB	332329	427915	39.11%	1.341%

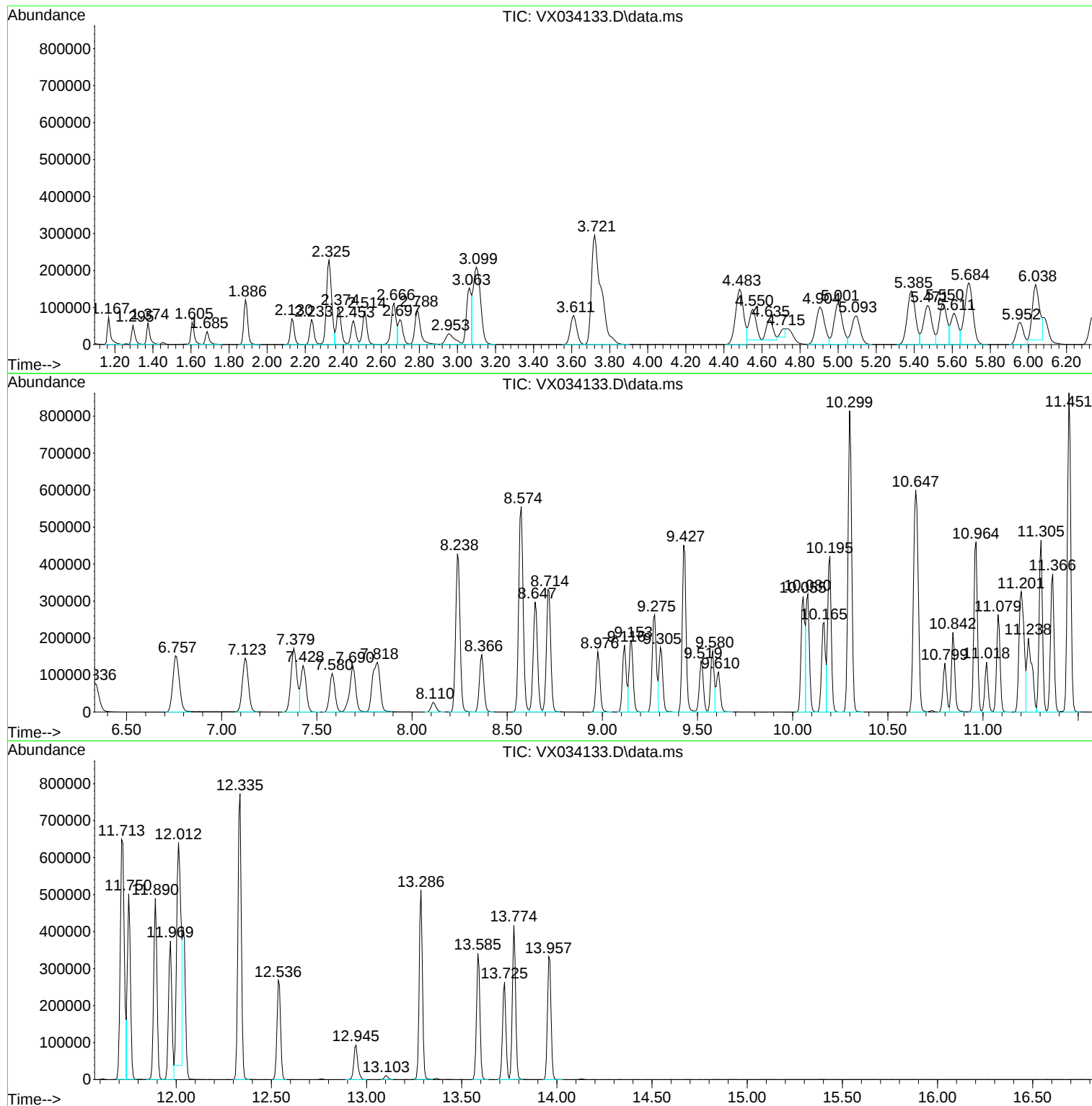
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LabSampleId :
VSTDCCC050

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020423W.M
Quant Title : SW846 8260

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



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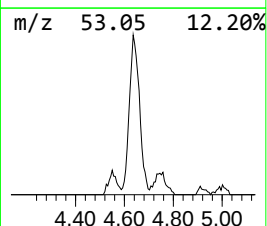
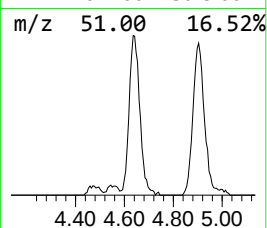
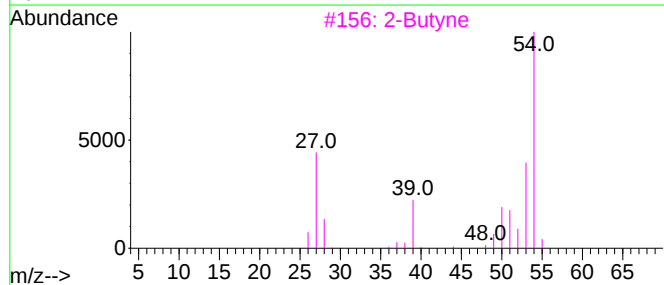
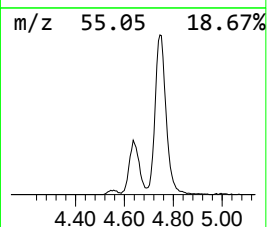
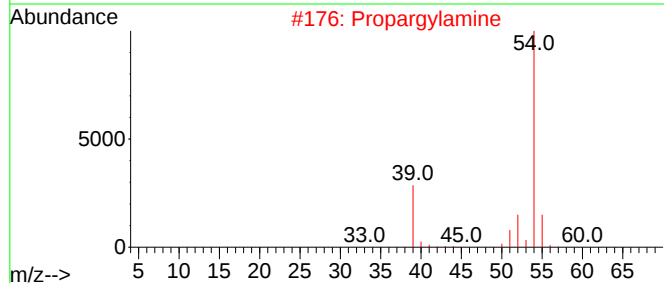
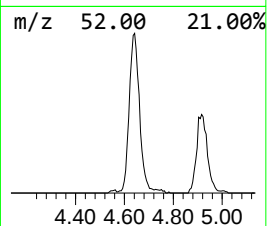
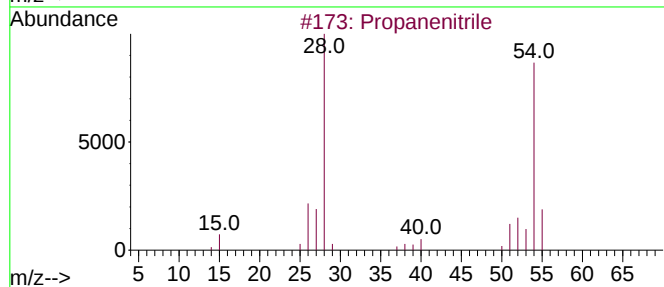
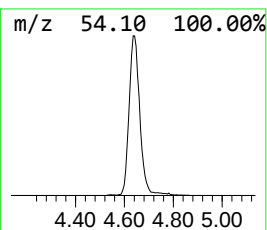
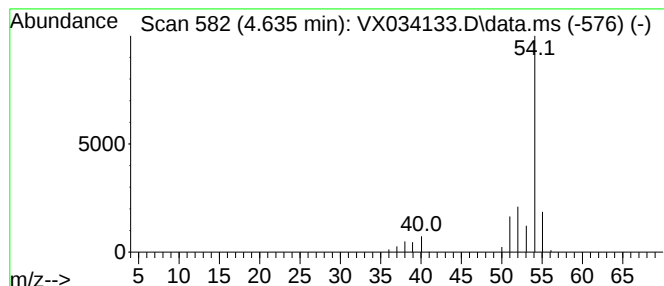
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020423W.M
Quant Title : SW846 8260

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

Peak Number 1 Propanenitrile Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.635	21.97 ug/l	135894	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanenitrile	55	C3H5N	000107-12-0	64
2			Propargylamine	55	C3H5N	002450-71-7	7
3			2-Butyne	54	C4H6	000503-17-3	7
4			1-Butyne	54	C4H6	000107-00-6	4
5			1,2-Butadiene	54	C4H6	000590-19-2	3



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_X
LabSampleId :
VSTDCCC050

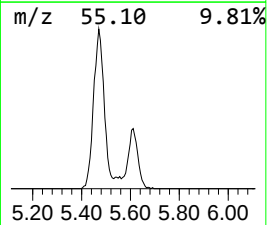
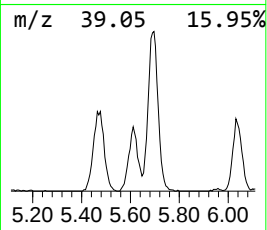
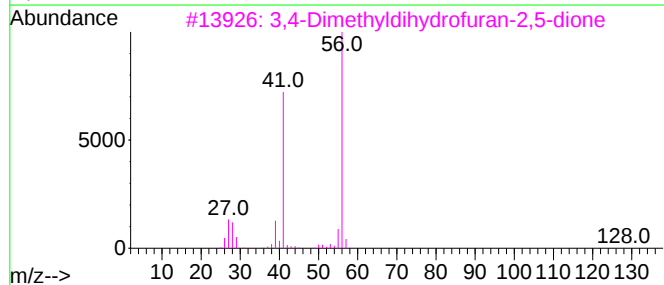
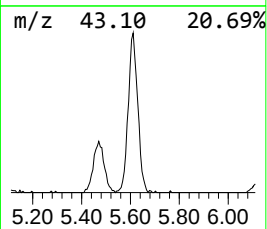
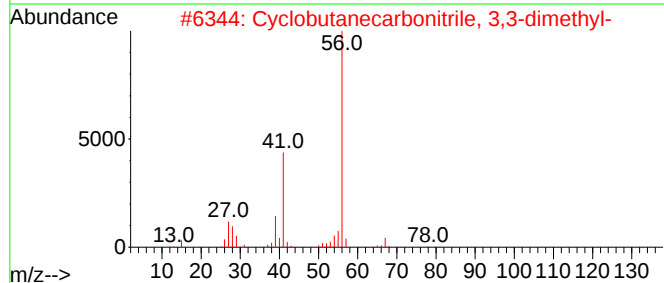
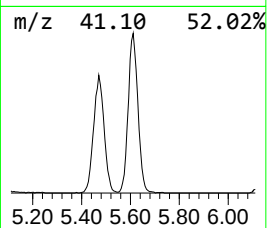
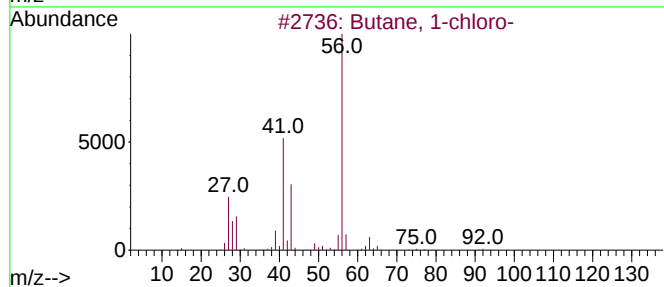
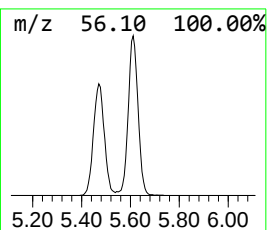
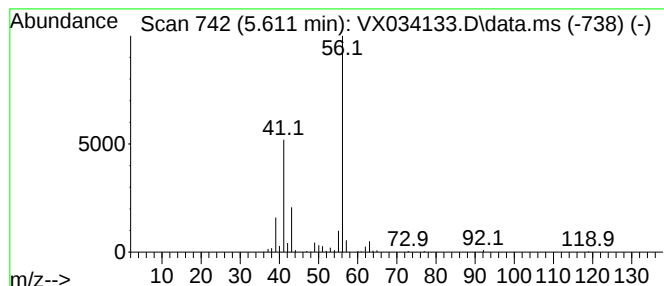
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020423W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.611	34.10 ug/l	210970	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 1-chloro-	92	C4H9Cl	000109-69-3	86
2			Cyclobutanecarbonitrile, 3,3-dim...	109	C7H11N	053783-86-1	72
3			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	50
4			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	39
5			Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	39



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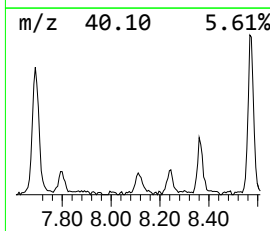
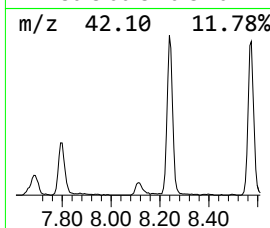
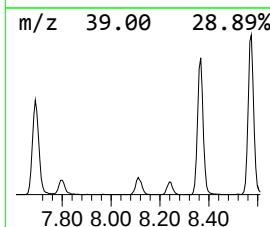
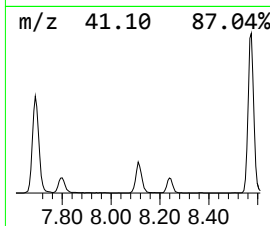
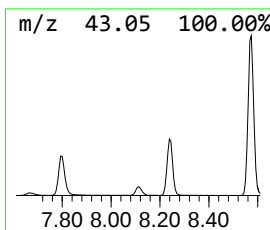
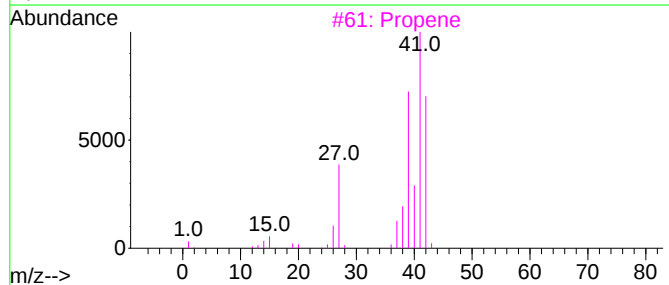
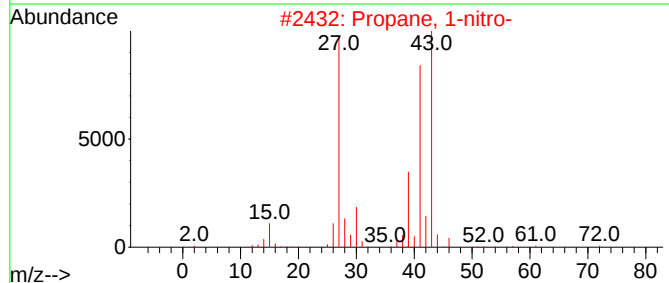
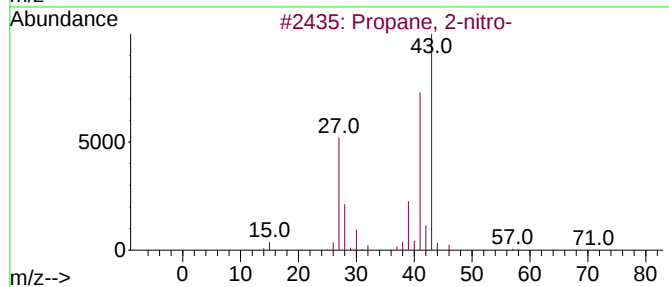
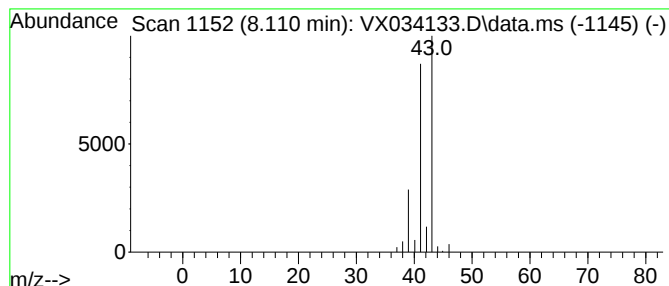
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020423W.M
Quant Title : SW846 8260

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

Peak Number 3 Propane, 2-nitro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.110	6.40 ug/l	46496	1,4-Difluorobenzene	6.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	74
2			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	74
3			Propene	42	C3H6	000115-07-1	9
4			Hydrogen azide	43	HN3	007782-79-8	4
5			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	4



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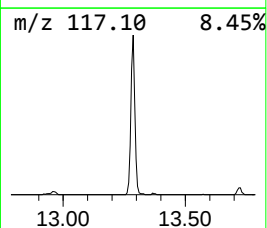
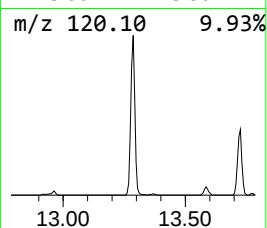
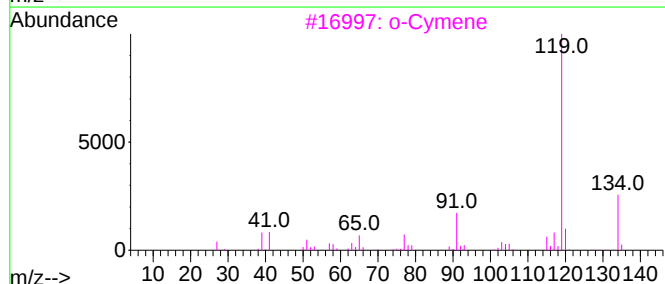
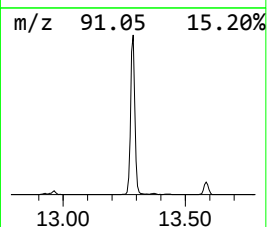
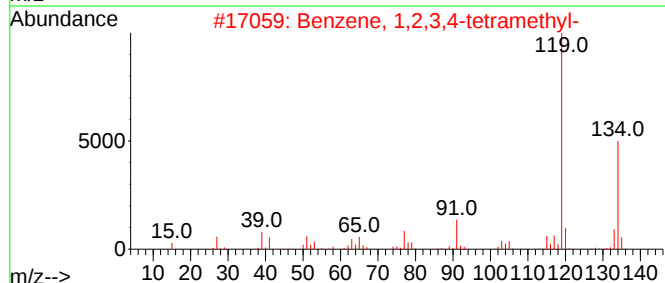
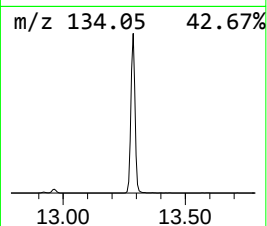
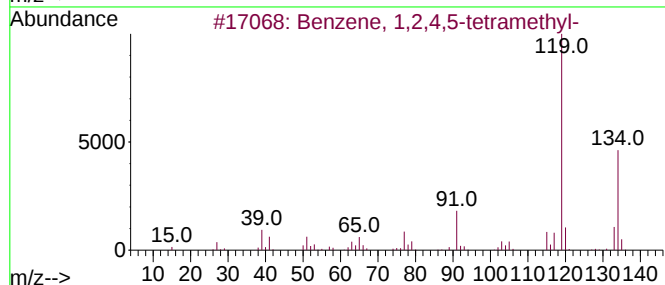
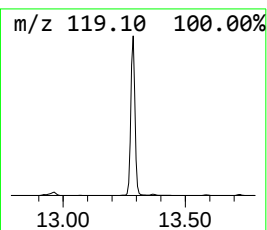
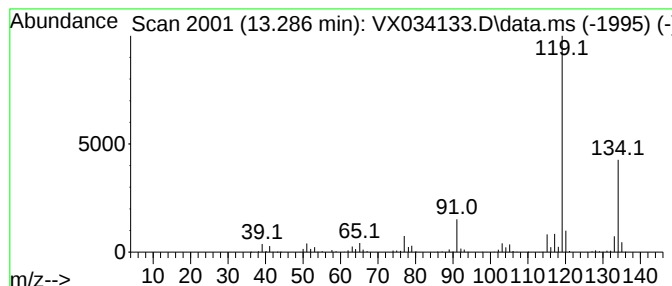
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020423W.M
Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.286	30.40 ug/l	599278	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
3			o-Cymene	134	C10H14	000527-84-4	96
4			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
5			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021223\
Data File : VX034133.D
Acq On : 10 Feb 2023 22:27
Operator : JC/MD
Sample : VSTDCCC050
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_X
LabSampleId :
VSTDCCC050

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020423W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanenitrile	4.635	22.0	ug/l	135894	1	5.550	309299	50.0
Butane, 1-chloro-	5.611	34.1	ug/l	210970	1	5.550	309299	50.0
Propane, 2-nitro-	8.110	6.4	ug/l	46496	2	6.757	362988	50.0
Benzene, 1,2,4,...	13.286	30.4	ug/l	599278	4	12.024	985691	50.0