

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
 Data File : VX027947.D
 Acq On : 04 Apr 2022 10:09
 Operator : JC/MD
 Sample : VSTDCCC050
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 2 Sample Multiplier: 1

Instrument :
 MSVOA_X
 LabSampleId :
 VSTDCCC050

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 1 % 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\82X032922W.M
 Title : SW846 8260

Signal : TIC: VX027947.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.166	10	13	21	rBV	61776	56130	6.83%	0.234%
2	1.294	31	34	43	rVB	38733	41393	5.04%	0.173%
3	1.374	43	47	50	rBV	43530	41530	5.05%	0.173%
4	1.599	80	84	92	rVB	32329	35466	4.32%	0.148%
5	1.685	93	98	105	rVB	26537	33144	4.03%	0.138%
6	1.886	125	131	139	rBV	80112	114096	13.89%	0.476%
7	2.130	166	171	180	rBV	52721	75615	9.20%	0.316%
8	2.233	183	188	196	rVB	45652	68508	8.34%	0.286%
9	2.325	196	203	208	rBV2	146216	286302	34.85%	1.195%
10	2.374	208	211	219	rVV	97385	154640	18.82%	0.645%
11	2.453	219	224	229	rVV	29180	48305	5.88%	0.202%
12	2.514	229	234	242	rVB	42245	69287	8.43%	0.289%
13	2.666	249	259	262	rBV	78561	151285	18.41%	0.631%
14	2.697	262	264	273	rVV	40475	63582	7.74%	0.265%
15	2.788	273	279	292	rVB	73827	135932	16.54%	0.567%
16	2.959	296	307	317	rBV2	28300	72419	8.81%	0.302%
17	3.062	317	324	326	rVV	125295	234903	28.59%	0.980%
18	3.099	327	330	348	rVB2	142689	354700	43.17%	1.480%
19	3.605	404	413	423	rBV	56250	132820	16.17%	0.554%
20	3.721	423	432	458	rVB2	247141	821640	100.00%	3.429%
21	4.483	543	557	563	rBV3	113523	358335	43.61%	1.495%
22	4.550	563	568	576	rVV	82665	230442	28.05%	0.962%
23	4.635	576	582	589	rVV2	56923	166909	20.31%	0.696%
24	4.715	589	595	615	rVV4	34934	162472	19.77%	0.678%
25	4.904	615	626	634	rVV3	73041	237680	28.93%	0.992%
26	4.995	634	641	650	rVV2	91942	288432	35.10%	1.204%
27	5.086	650	656	673	rVB2	56970	177666	21.62%	0.741%
28	5.385	692	705	712	rBV	100501	308707	37.57%	1.288%
29	5.471	712	719	725	rVV2	59707	185068	22.52%	0.772%
30	5.550	725	732	737	rVV	76533	216823	26.39%	0.905%
31	5.611	738	742	747	rVV	53670	133603	16.26%	0.558%
32	5.684	747	754	767	rVB3	111097	333020	40.53%	1.390%
33	5.958	787	799	805	rBV	41362	114531	13.94%	0.478%
34	6.038	805	812	818	rBV	96582	263627	32.09%	1.100%
35	6.336	852	861	877	rBV	59338	145339	17.69%	0.606%
36	6.757	920	930	941	rBV	105228	246115	29.95%	1.027%

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Integrator: RTE

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37	7.123	981	990	1003	rVB	97527	206202	25.10%	0.860%
38	7.379	1023	1032	1036	rBV	107941	235329	28.64%	0.982%
39	7.428	1036	1040	1054	rVB	88020	182664	22.23%	0.762%
40	7.580	1058	1065	1072	rBV	67032	130722	15.91%	0.545%
41	7.690	1072	1083	1093	rVV2	84818	193185	23.51%	0.806%
42	7.818	1093	1104	1121	rVB2	104714	302589	36.83%	1.263%
43	8.110	1145	1152	1160	rBV	24774	44769	5.45%	0.187%
44	8.238	1166	1173	1187	rVB	368871	593232	72.20%	2.475%
45	8.366	1187	1194	1203	rBV	119652	189185	23.03%	0.789%
46	8.574	1221	1228	1235	rBV	485063	762305	92.78%	3.181%
47	8.647	1235	1240	1246	rVV	211194	329440	40.10%	1.375%
48	8.720	1246	1252	1262	rVB	226677	353712	43.05%	1.476%
49	8.976	1287	1294	1303	rBV	130779	188849	22.98%	0.788%
50	9.116	1311	1317	1320	rBV	141722	199203	24.24%	0.831%
51	9.153	1320	1323	1334	rVB	147180	206151	25.09%	0.860%
52	9.275	1334	1343	1346	rBV	189123	290431	35.35%	1.212%
53	9.305	1346	1348	1354	rVB	132750	174993	21.30%	0.730%
54	9.433	1363	1369	1378	rBV	411498	570422	69.42%	2.380%
55	9.519	1378	1383	1388	rVV	105739	154203	18.77%	0.643%
56	9.580	1388	1393	1396	rVV	140056	191131	23.26%	0.798%
57	9.610	1396	1398	1404	rVB	75155	89939	10.95%	0.375%
58	10.055	1465	1471	1473	rBV	240570	348153	42.37%	1.453%
59	10.079	1473	1475	1483	rVV	234067	271315	33.02%	1.132%
60	10.165	1483	1489	1491	rVV	176154	251522	30.61%	1.050%
61	10.195	1491	1494	1501	rVV	315190	389140	47.36%	1.624%
62	10.299	1505	1511	1524	rVB	558438	781692	95.14%	3.262%
63	10.646	1562	1568	1580	rBV2	440473	771172	93.86%	3.218%
64	10.799	1588	1593	1597	rBV	103368	135638	16.51%	0.566%
65	10.842	1597	1600	1612	rVB	178767	212504	25.86%	0.887%
66	10.963	1614	1620	1625	rBV	357024	438357	53.35%	1.829%
67	11.018	1625	1629	1635	rVV	128376	154822	18.84%	0.646%
68	11.079	1635	1639	1645	rVB	193632	246899	30.05%	1.030%
69	11.201	1652	1659	1663	rBV2	244130	482376	58.71%	2.013%
70	11.238	1663	1665	1668	rVV	165344	248294	30.22%	1.036%
71	11.305	1672	1676	1681	rVV	371588	433612	52.77%	1.809%
72	11.366	1681	1686	1692	rVV	298573	375762	45.73%	1.568%
73	11.451	1695	1700	1710	rVB2	611683	806317	98.14%	3.365%
74	11.719	1738	1744	1747	rBV2	477485	677850	82.50%	2.829%
75	11.750	1747	1749	1756	rVB	345466	413574	50.34%	1.726%
76	11.890	1765	1772	1778	rBV	368817	455100	55.39%	1.899%

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77	11.969	1778	1785	1788	rBV	280883	340814	41.48%	1.422%
78	12.012	1788	1792	1796	rBV2	453326	810974	98.70%	3.384%
79	12.335	1840	1845	1857	rVB	630606	751623	91.48%	3.136%
80	12.542	1873	1879	1885	rVB2	202317	256413	31.21%	1.070%
81	12.945	1934	1945	1952	rBV2	78080	105834	12.88%	0.442%
82	13.103	1967	1971	1978	rVB	15098	18716	2.28%	0.078%
83	13.286	1996	2001	2011	rVB	376776	445795	54.26%	1.860%
84	13.591	2045	2051	2061	rVB	230644	294645	35.86%	1.230%
85	13.725	2068	2073	2077	rBV	182038	223269	27.17%	0.932%
86	13.774	2077	2081	2091	rVB	295954	369517	44.97%	1.542%
87	13.963	2106	2112	2121	rVB	239812	293795	35.76%	1.226%
88	14.134	2135	2140	2147	rBV	7434	9762	1.19%	0.041%

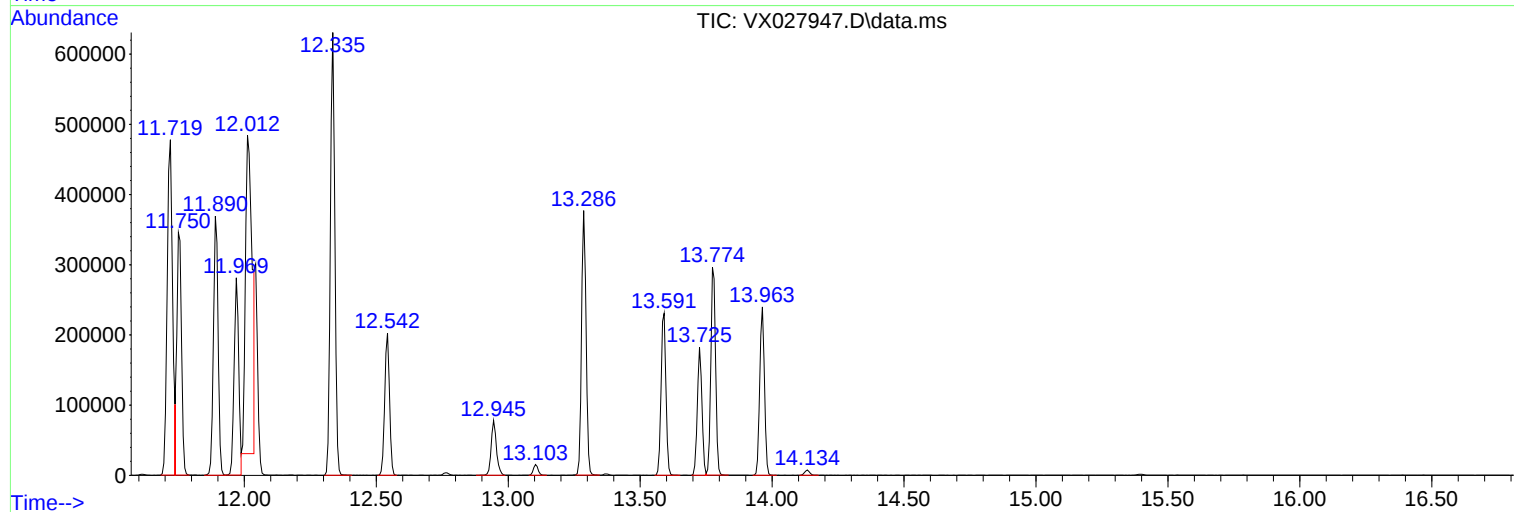
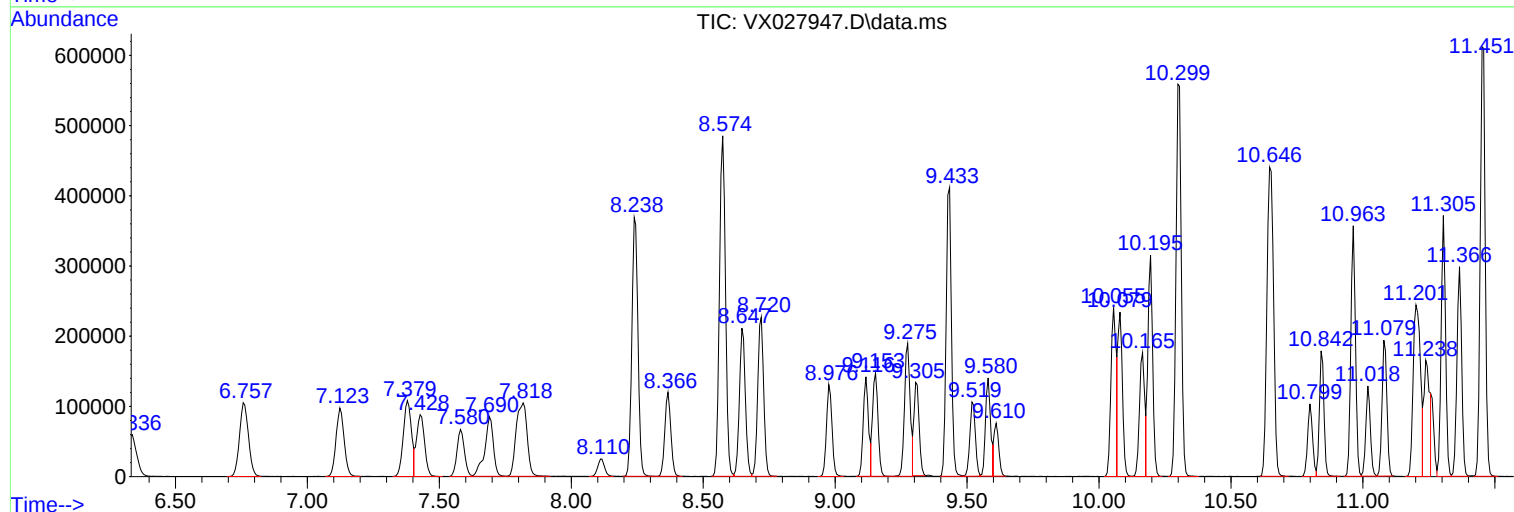
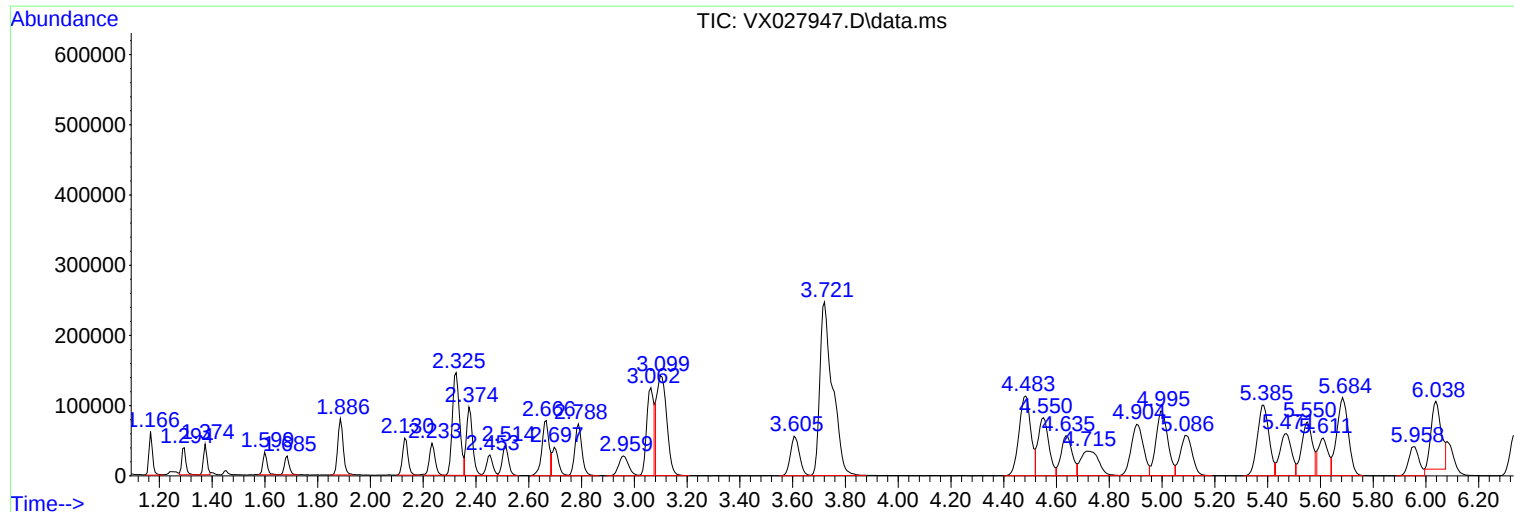
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ALS Vial : 2 Sample Multiplier: 1

Instrument :
MSVOA_X
LabSampleId :
VSTDCCC050

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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



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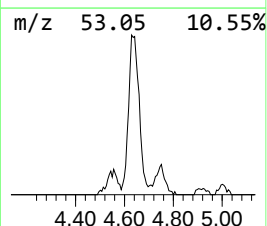
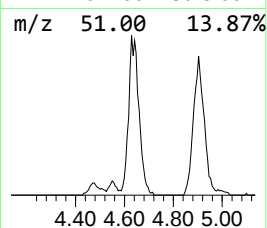
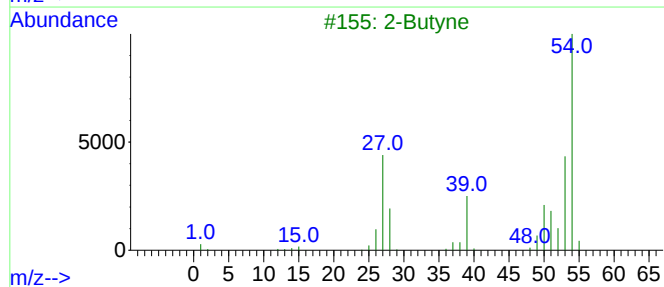
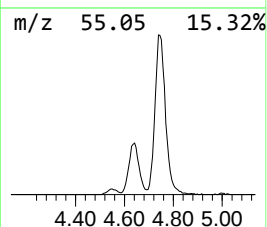
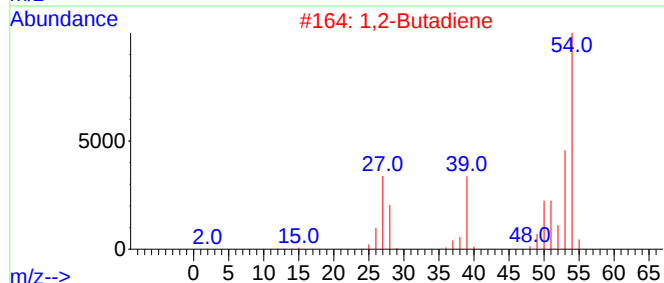
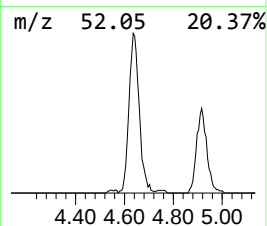
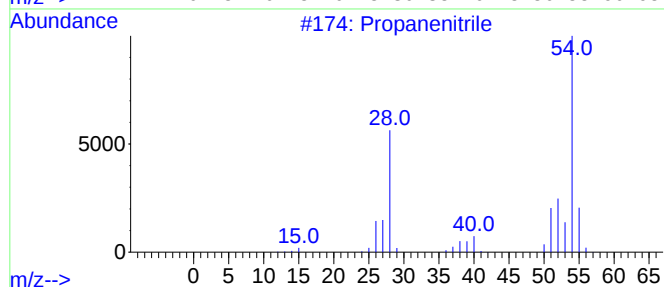
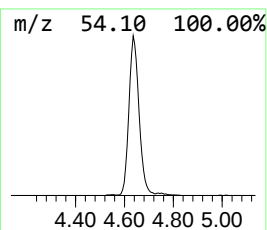
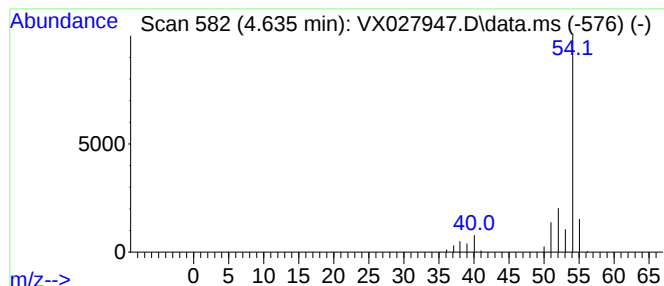
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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

Peak Number 1 Propanenitrile Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.635	38.49 ug/l	166909	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanenitrile	55	C3H5N	000107-12-0	64
2			1,2-Butadiene	54	C4H6	000590-19-2	9
3			2-Butyne	54	C4H6	000503-17-3	9
4			Propargylamine	55	C3H5N	002450-71-7	7
5			1-Butyne	54	C4H6	000107-00-6	4



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VSTDCCC050

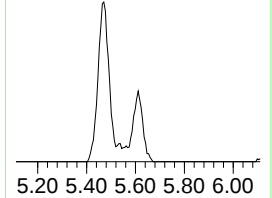
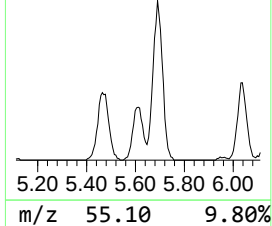
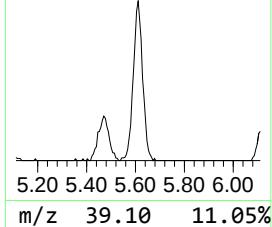
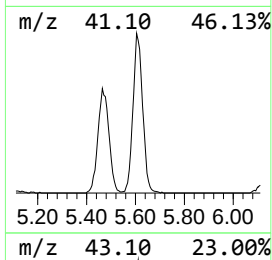
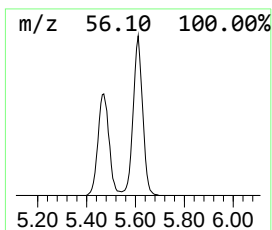
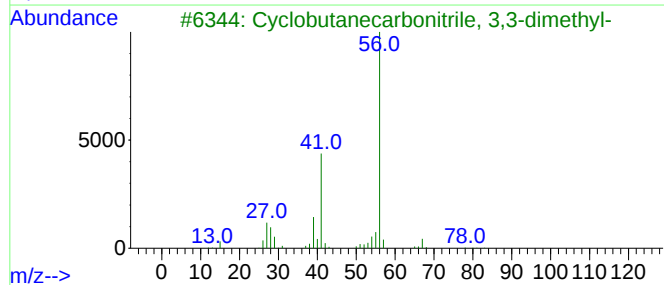
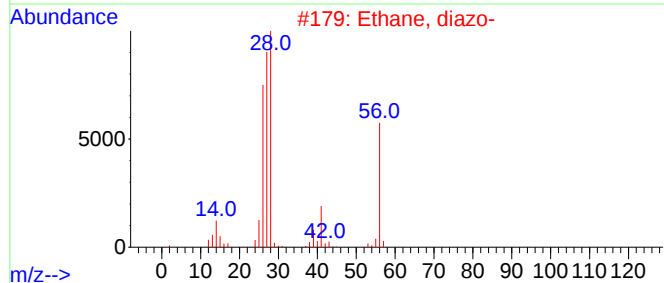
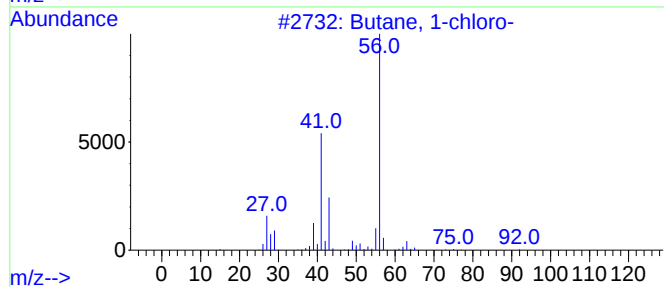
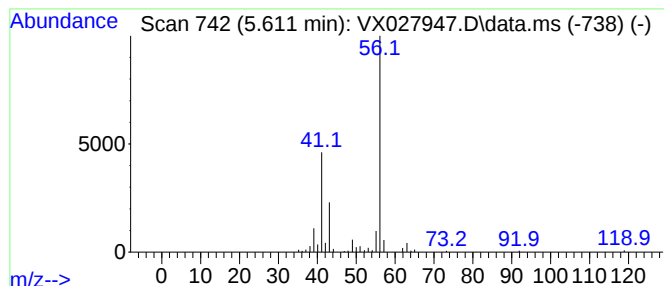
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.611	30.81 ug/l	133603	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 1-chloro-	92	C4H9Cl	000109-69-3	91
2			Ethane, diazo-	56	C2H4N2	001117-96-0	50
3			Cyclobutanecarbonitrile, 3,3-dimethyl-	109	C7H11N	053783-86-1	50
4			Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	39
5			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	39



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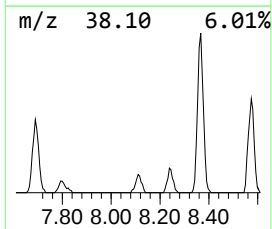
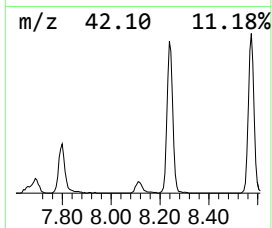
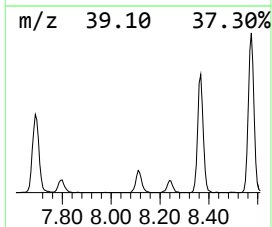
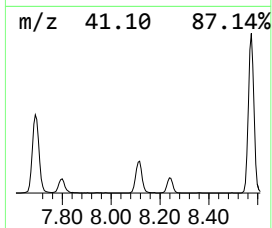
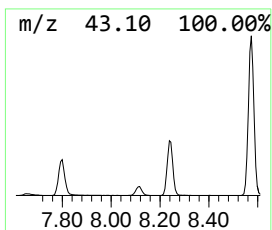
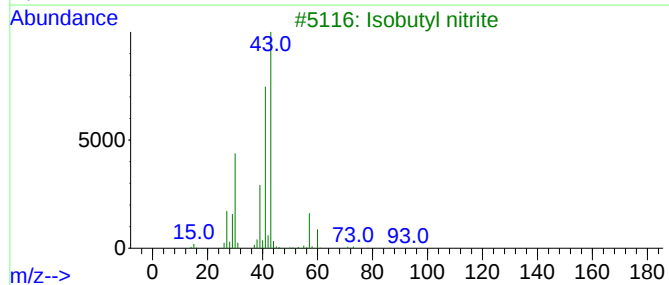
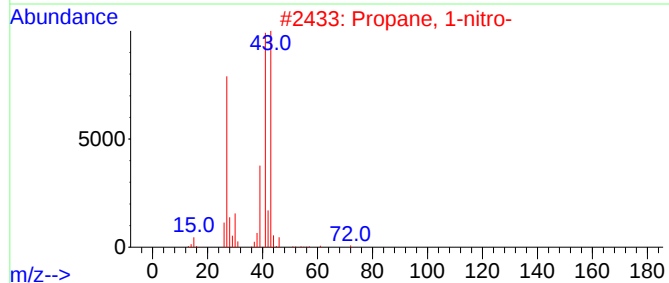
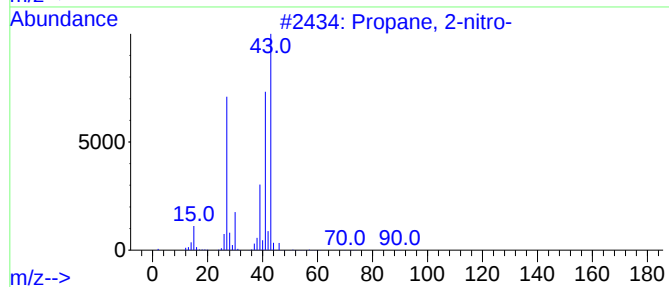
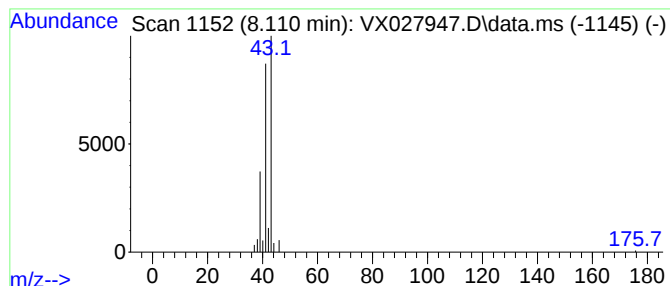
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.M
Quant Title : SW846 8260

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	9.10 ug/l	44769	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			Isobutyl nitrite	103	C4H9NO2	000542-56-3	43
4			Propene	42	C3H6	000115-07-1	9
5			Propanamide, 2,2-dimethyl-	101	C5H11NO	000754-10-9	9



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LabSampleId :
VSTDCCC050

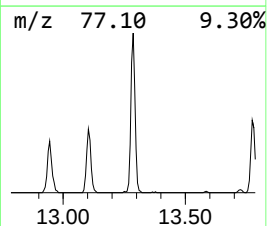
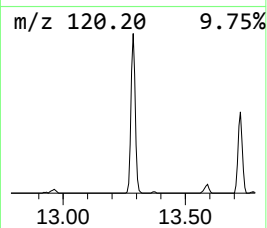
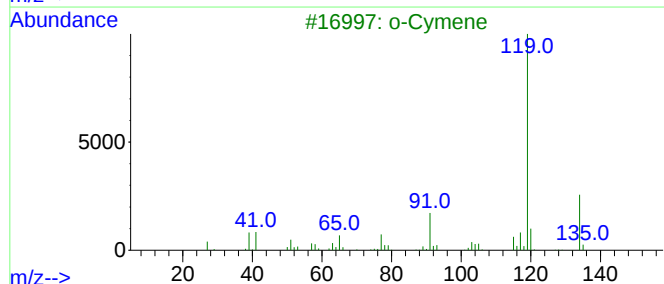
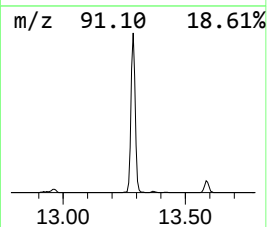
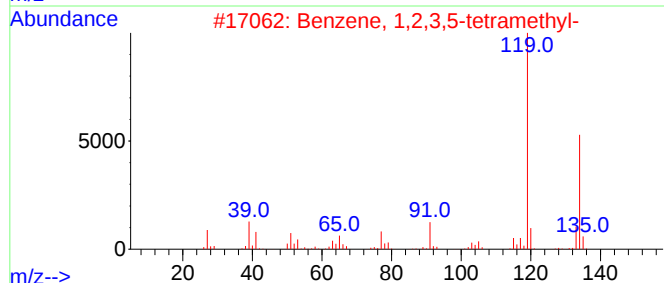
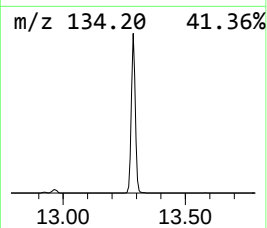
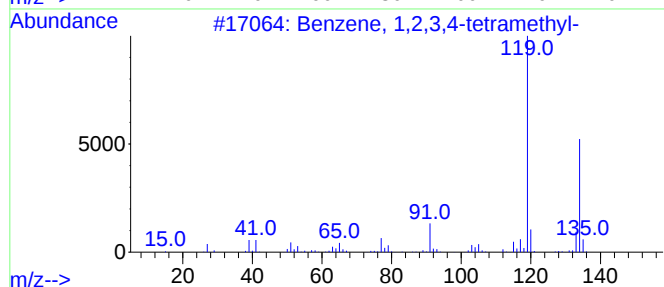
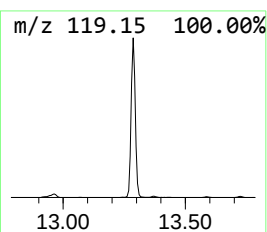
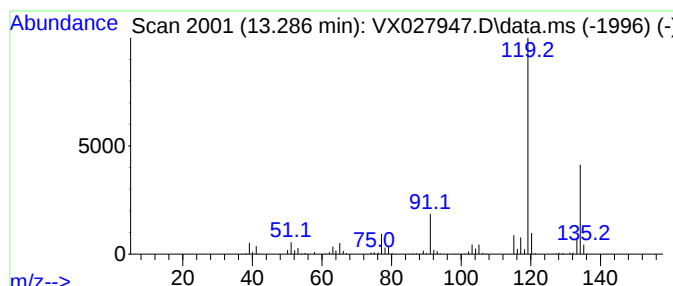
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Quant Title : SW846 8260

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

Peak Number 4 Benzene, 1,2,3,4-tetramethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.286	27.49 ug/l	445795	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	96
2			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
3			o-Cymene	134	C10H14	000527-84-4	95
4			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94
5			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX040422\
Data File : VX027947.D
Acq On : 04 Apr 2022 10:09
Operator : JC/MD
Sample : VSTDCCC050
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 2 Sample Multiplier: 1

Instrument :
MSVOA_X
LabSampleId :
VSTDCCC050

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032922W.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	38.5	ug/l	166909	1	5.550	216823	50.0
Butane, 1-chloro-	5.611	30.8	ug/l	133603	1	5.550	216823	50.0
Propane, 2-nitro-	8.110	9.1	ug/l	44769	2	6.757	246115	50.0
Benzene, 1,2,3,...	13.286	27.5	ug/l	445795	4	12.024	810974	50.0