

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012721\
 Data File : VX020771.D
 Acq On : 27 Jan 2021 15:34
 Operator : JC/SP
 Sample : VX0127WBS01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VX0127WBS01

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\82X012521W.M
 Title : SW846 8260

Signal : TIC: VX020771.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.185	12	16	24	rVB	172593	163481	5.69%	0.335%
2	1.313	34	37	44	rVB	142917	136497	4.75%	0.279%
3	1.392	47	50	59	rVB	144968	138911	4.84%	0.284%
4	1.624	84	88	93	rVB	119809	126432	4.40%	0.259%
5	1.709	97	102	110	rVB	74207	96687	3.37%	0.198%
6	1.910	130	135	144	rBV	171781	258235	8.99%	0.528%
7	2.166	171	177	185	rBV	119715	171406	5.97%	0.351%
8	2.270	189	194	202	rVV	62045	100444	3.50%	0.206%
9	2.355	202	208	214	rVV2	289460	556790	19.38%	1.139%
10	2.416	214	218	225	rVV	159706	265111	9.23%	0.542%
11	2.489	225	230	235	rVV	83459	141329	4.92%	0.289%
12	2.544	235	239	250	rVB	134170	225461	7.85%	0.461%
13	2.703	255	265	269	rBV	147129	272676	9.49%	0.558%
14	2.745	269	272	279	rVB	66822	113249	3.94%	0.232%
15	2.831	279	286	301	rVB	155145	298706	10.40%	0.611%
16	3.007	304	315	325	rBV	59697	145119	5.05%	0.297%
17	3.117	325	333	334	rBV	241937	407505	14.19%	0.834%
18	3.666	414	423	433	rBV	109777	260980	9.09%	0.534%
19	3.782	433	442	466	rVV2	444219	1494825	52.04%	3.059%
20	4.556	552	569	575	rBV4	205932	645084	22.46%	1.320%
21	4.629	575	581	589	rVB	117757	291806	10.16%	0.597%
22	4.714	589	595	602	rBV2	80297	198204	6.90%	0.406%
23	4.800	602	609	610	rBV	32806	62918	2.19%	0.129%
24	4.989	626	640	648	rBV5	114116	408212	14.21%	0.835%
25	5.086	648	656	663	rVV	160079	485264	16.89%	0.993%
26	5.172	663	670	685	rVB	106130	330018	11.49%	0.675%
27	5.458	703	717	725	rBV	308265	932345	32.46%	1.908%
28	5.544	725	731	737	rVV2	156163	462003	16.08%	0.945%
29	5.623	737	744	750	rVV	348253	1001425	34.86%	2.049%
30	5.678	751	753	759	rVV	127600	282231	9.83%	0.577%
31	5.757	759	766	779	rVB5	219270	664384	23.13%	1.359%
32	6.025	798	810	817	rBV	214916	564682	19.66%	1.155%
33	6.104	817	823	829	rBV	199788	500105	17.41%	1.023%
34	6.409	862	873	885	rBV	107820	271990	9.47%	0.557%
35	6.824	931	941	959	rBV	512126	1187755	41.35%	2.430%
36	7.184	991	1000	1011	rBV	193508	413320	14.39%	0.846%

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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	7.433	1032	1041	1046	rBV2	245422	559327	19.47%	1.144%
38	7.482	1046	1049	1060	rVB	174574	334455	11.64%	0.684%
39	7.635	1067	1074	1081	rBV2	129401	239787	8.35%	0.491%
40	7.744	1081	1092	1102	rVV2	157861	362609	12.62%	0.742%
41	7.866	1102	1112	1125	rVB2	177838	517023	18.00%	1.058%
42	8.159	1153	1160	1170	rBV	32155	59047	2.06%	0.121%
43	8.287	1173	1181	1195	rBV	638132	978351	34.06%	2.002%
44	8.409	1195	1201	1209	rVV	210515	344660	12.00%	0.705%
45	8.616	1227	1235	1242	rBV	825449	1276826	44.45%	2.613%
46	8.689	1242	1247	1254	rVV	1027452	1642417	57.18%	3.361%
47	8.762	1254	1259	1269	rVB	489106	733614	25.54%	1.501%
48	9.019	1294	1301	1313	rBV	223442	322349	11.22%	0.660%
49	9.159	1318	1324	1326	rBV	215800	305123	10.62%	0.624%
50	9.195	1326	1330	1340	rVB	267335	408348	14.22%	0.836%
51	9.317	1340	1350	1353	rBV	387647	609314	21.21%	1.247%
52	9.348	1353	1355	1361	rVB	245816	304890	10.61%	0.624%
53	9.470	1369	1375	1384	rBV	695106	933800	32.51%	1.911%
54	9.561	1384	1390	1395	rVV	187158	274002	9.54%	0.561%
55	9.616	1395	1399	1402	rVV	234690	315803	10.99%	0.646%
56	9.653	1402	1405	1413	rVB	140099	191614	6.67%	0.392%
57	10.092	1471	1477	1489	rBV2	1070249	2015091	70.15%	4.123%
58	10.201	1489	1495	1497	rVV	331042	446145	15.53%	0.913%
59	10.232	1497	1500	1511	rVV	606282	784555	27.31%	1.605%
60	10.341	1511	1518	1531	rVB	1143560	1508520	52.52%	3.087%
61	10.689	1568	1575	1584	rBV2	791582	1394044	48.53%	2.852%
62	10.835	1594	1599	1603	rBV	154888	218844	7.62%	0.448%
63	10.878	1603	1606	1616	rVV	307182	365947	12.74%	0.749%
64	11.000	1620	1626	1631	rVV	676281	823238	28.66%	1.684%
65	11.055	1631	1635	1640	rVV	207505	256992	8.95%	0.526%
66	11.122	1640	1646	1659	rVB	875652	1144047	39.83%	2.341%
67	11.238	1659	1665	1669	rBV2	472513	858439	29.89%	1.756%
68	11.280	1669	1672	1678	rVV2	296027	574598	20.00%	1.176%
69	11.341	1678	1682	1687	rVV	674906	791864	27.57%	1.620%
70	11.402	1687	1692	1698	rVV	536598	669662	23.31%	1.370%
71	11.494	1701	1707	1716	rVB2	1124832	1484134	51.67%	3.037%
72	11.756	1744	1750	1753	rBV2	817444	1169945	40.73%	2.394%
73	11.792	1753	1756	1762	rVB	657811	783913	27.29%	1.604%
74	11.927	1773	1778	1785	rVB	619127	756189	26.33%	1.547%
75	12.006	1785	1791	1794	rBV	464495	594192	20.69%	1.216%
76	12.055	1794	1799	1810	rVB4	1384359	2872434	100.00%	5.877%

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 ClientSampleId :
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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

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77	12.372	1845	1851	1858	rBV	1097458	1312192	45.68%	2.685%
78	12.579	1878	1885	1891	rVB	344480	438395	15.26%	0.897%
79	12.981	1943	1951	1960	rVB2	110957	158307	5.51%	0.324%
80	13.323	2002	2007	2017	rBV	587440	699107	24.34%	1.430%
81	13.627	2050	2057	2065	rBV	411616	495405	17.25%	1.014%
82	13.762	2074	2079	2084	rBV	306962	388135	13.51%	0.794%
83	13.816	2084	2088	2096	rVB	489674	581664	20.25%	1.190%
84	13.999	2113	2118	2124	rBV	395178	498088	17.34%	1.019%

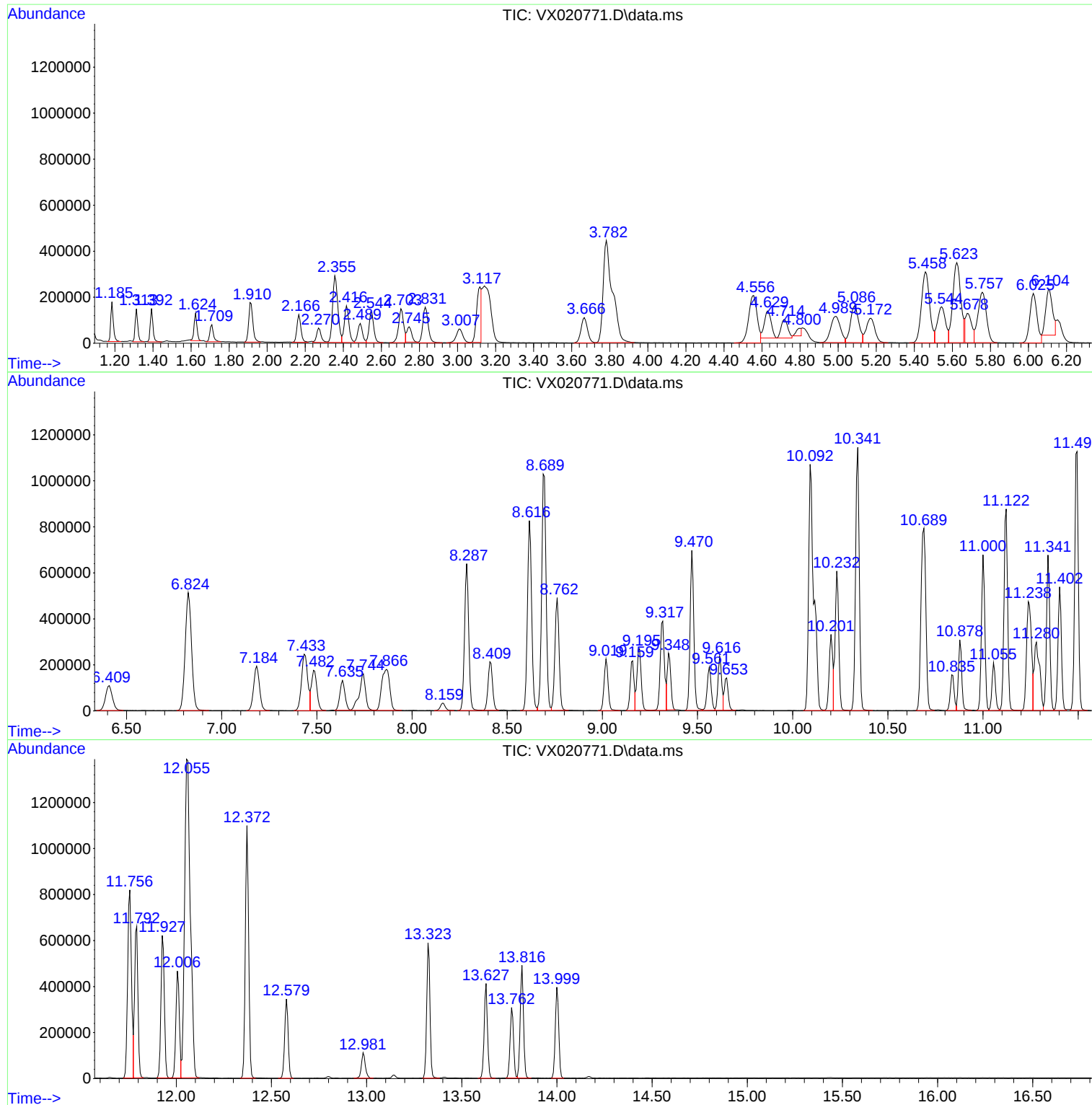
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Instrument :
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VX0127WBS01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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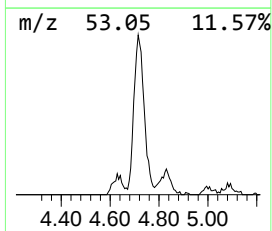
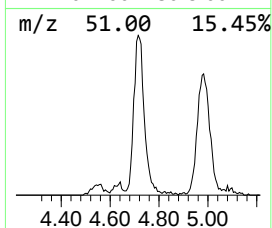
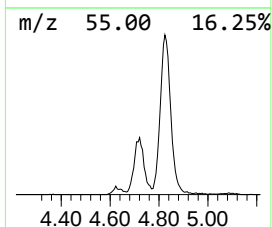
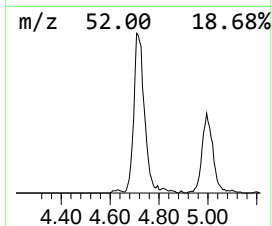
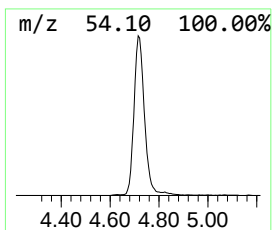
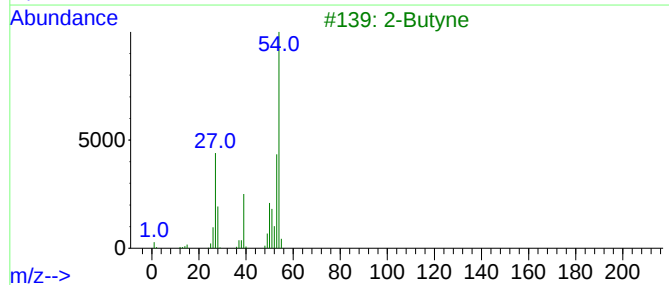
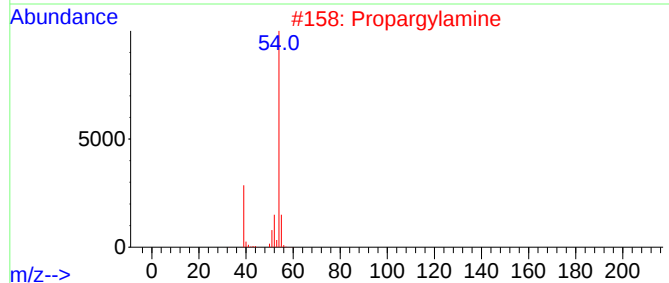
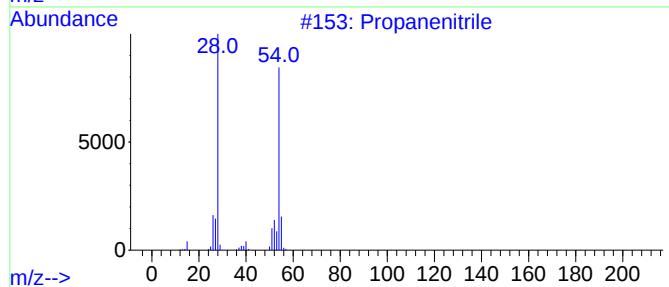
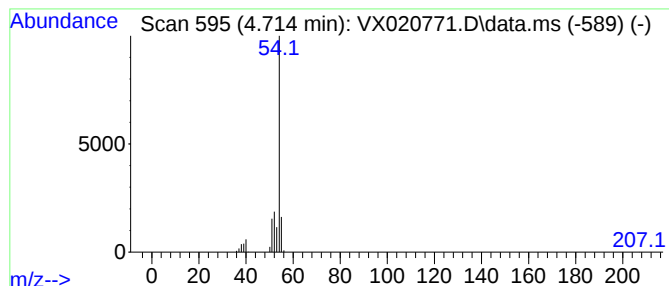
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propanenitrile Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.714	9.90 ug/l	198204	Pentafluorobenzene	5.623

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanenitrile	55	C3H5N	000107-12-0	43
2			Propargylamine	55	C3H5N	002450-71-7	7
3			2-Butyne	54	C4H6	000503-17-3	5
4			1,2-Butadiene	54	C4H6	000590-19-2	3
5			1-Butyne	54	C4H6	000107-00-6	3



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Misc : 5.0mL/MSVOA_X/WATER
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Instrument :
MSVOA_X
ClientSampleId :
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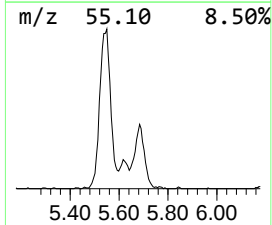
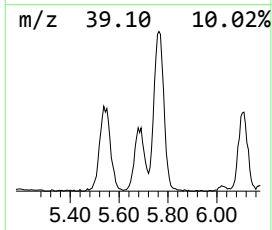
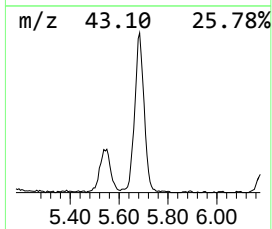
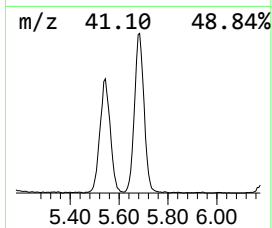
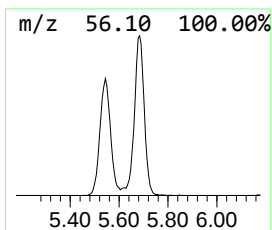
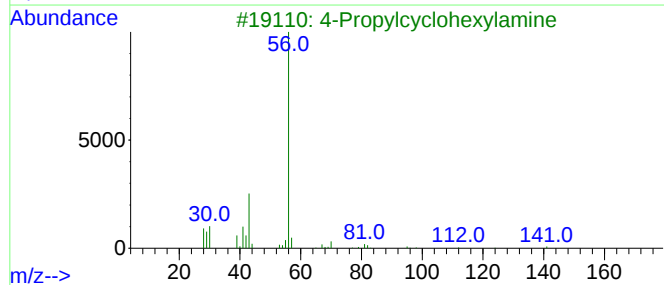
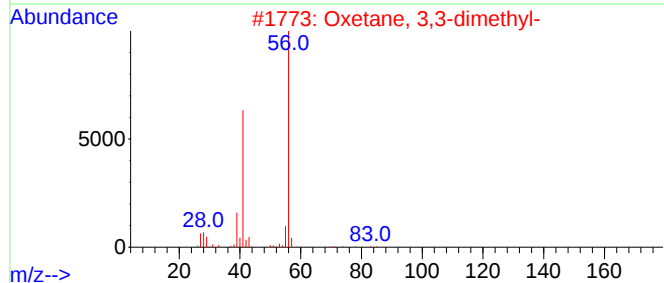
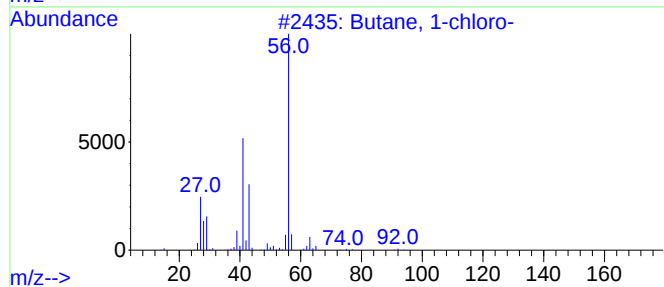
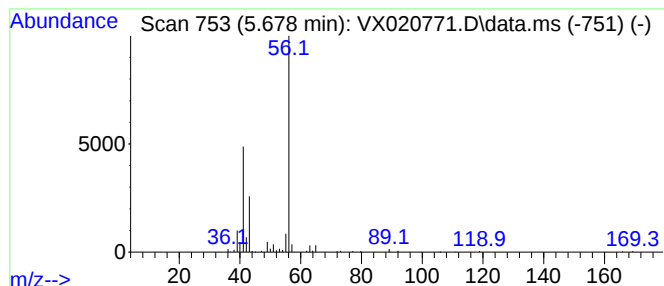
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.678	14.09 ug/l	282231	Pentafluorobenzene	5.623

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 1-chloro-	92	C4H9Cl	000109-69-3	86
2			Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	39
3			4-Propylcyclohexylamine	141	C9H19N	102653-37-2	9
4			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	9
5			Oxetane, 2,3,4-trimethyl-, (2.al...	100	C6H12O	032347-12-9	9



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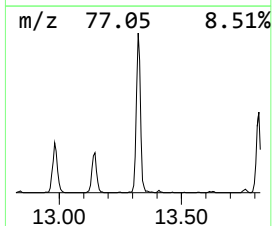
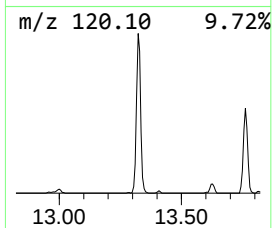
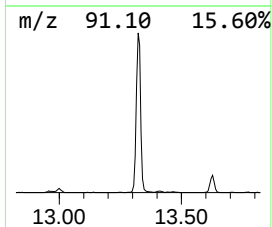
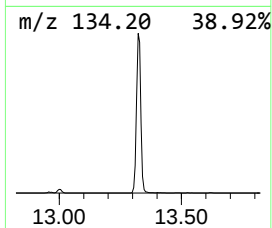
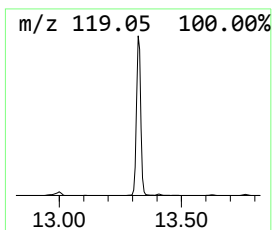
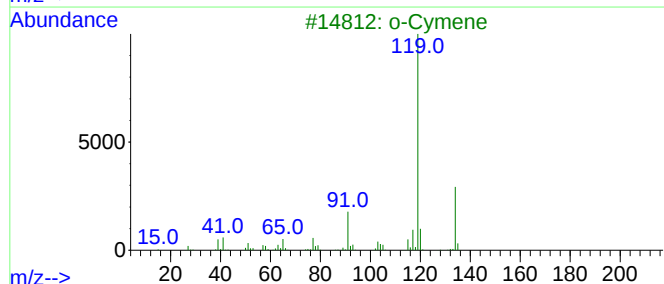
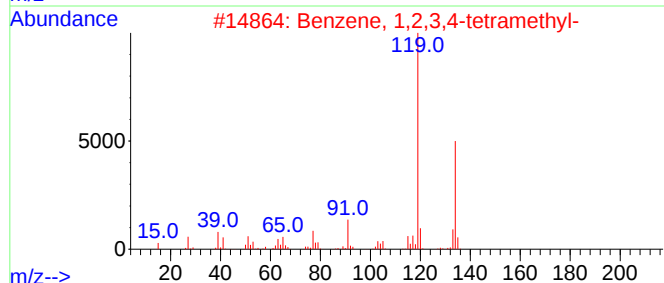
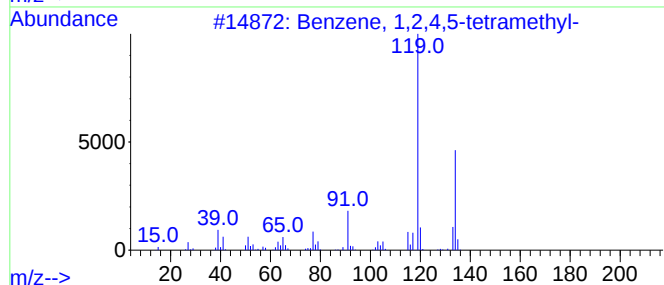
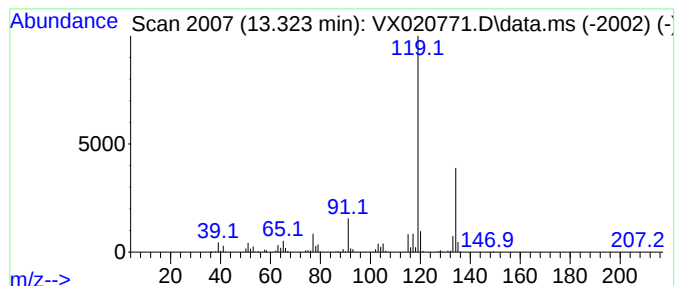
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.323	12.17 ug/l	699107	1,4-Dichlorobenzene-d4	12.061

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	95
4			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	95
5			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanenitrile	4.714	9.9	ug/l	198204	1	5.623	1001430	50.0
Butane, 1-chloro-	5.678	14.1	ug/l	282231	1	5.623	1001430	50.0
Benzene, 1,2,4,...	13.323	12.2	ug/l	699107	4	12.061	2872430	50.0