

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012621\
 Data File : VX020744.D
 Acq On : 26 Jan 2021 11:26
 Operator : JC/SP
 Sample : VX0126WBS01
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VX0126WBS01

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: VX020744.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	13	16	23	rVB	171320	160656	5.63%	0.327%
2	1.313	33	37	46	rVB	146666	140750	4.93%	0.286%
3	1.392	46	50	56	rBV	145887	141900	4.98%	0.289%
4	1.624	73	88	93	rBV	122979	162938	5.71%	0.331%
5	1.709	97	102	110	rVB	75699	100195	3.51%	0.204%
6	1.916	130	136	149	rVB	177632	268032	9.40%	0.545%
7	2.166	169	177	187	rBV	122344	177090	6.21%	0.360%
8	2.270	189	194	201	rBV	74635	110580	3.88%	0.225%
9	2.355	201	208	214	rBV2	289505	550645	19.31%	1.120%
10	2.416	214	218	225	rVB	146298	232226	8.14%	0.472%
11	2.489	225	230	235	rBV	76828	120458	4.22%	0.245%
12	2.544	235	239	255	rVB	135033	230992	8.10%	0.470%
13	2.703	255	265	269	rBV	148573	280636	9.84%	0.571%
14	2.745	269	272	279	rVB	68781	114976	4.03%	0.234%
15	2.831	279	286	303	rVB	159963	302669	10.61%	0.615%
16	3.008	303	315	325	rBV2	62937	154196	5.41%	0.314%
17	3.117	325	333	334	rBV	243111	419617	14.71%	0.853%
18	3.666	413	423	432	rBV	108022	264381	9.27%	0.538%
19	3.782	433	442	467	rVB2	459131	1538867	53.96%	3.129%
20	4.550	551	568	575	rBV3	211196	657715	23.06%	1.337%
21	4.629	575	581	589	rVV	139334	402536	14.11%	0.818%
22	4.715	589	595	602	rVV2	104915	304428	10.67%	0.619%
23	4.806	602	610	626	rVV4	66180	307318	10.78%	0.625%
24	4.983	628	639	648	rVV3	116688	418130	14.66%	0.850%
25	5.086	648	656	664	rVV	163410	516696	18.12%	1.051%
26	5.172	664	670	686	rVB	107742	318502	11.17%	0.648%
27	5.458	704	717	725	rBV3	303700	929594	32.59%	1.890%
28	5.544	725	731	737	rVV2	156256	464172	16.27%	0.944%
29	5.623	737	744	751	rVV	351274	1031331	36.16%	2.097%
30	5.678	751	753	759	rVV	124800	276894	9.71%	0.563%
31	5.757	759	766	780	rVB2	224016	677449	23.75%	1.377%
32	6.025	799	810	817	rBV	214724	569407	19.96%	1.158%
33	6.105	817	823	829	rBV	200783	509419	17.86%	1.036%
34	6.409	862	873	886	rBV	110343	281464	9.87%	0.572%
35	6.824	929	941	955	rBV	504901	1189517	41.71%	2.419%
36	7.184	991	1000	1009	rBV	197107	414363	14.53%	0.842%

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Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

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37	7.434	1029	1041	1046	rBV	252642	570912	20.02%	1.161%
38	7.482	1046	1049	1059	rVB	175804	340247	11.93%	0.692%
39	7.635	1066	1074	1081	rBV	124387	241243	8.46%	0.490%
40	7.738	1081	1091	1102	rVB2	158594	370800	13.00%	0.754%
41	7.866	1102	1112	1122	rBV2	181744	529589	18.57%	1.077%
42	8.159	1152	1160	1168	rBV	34440	62901	2.21%	0.128%
43	8.287	1174	1181	1195	rBV	663274	997854	34.99%	2.029%
44	8.409	1195	1201	1212	rVB	216288	351277	12.32%	0.714%
45	8.616	1228	1235	1241	rBV	830229	1299734	45.57%	2.643%
46	8.689	1241	1247	1254	rVV	1027577	1634073	57.29%	3.322%
47	8.763	1254	1259	1268	rVB	481933	736482	25.82%	1.497%
48	9.019	1294	1301	1311	rBV	223129	323565	11.34%	0.658%
49	9.153	1317	1323	1326	rBV	218349	312765	10.97%	0.636%
50	9.195	1326	1330	1338	rVB	278524	411453	14.43%	0.837%
51	9.317	1341	1350	1353	rBV	365582	595626	20.88%	1.211%
52	9.348	1353	1355	1361	rVB	251285	303236	10.63%	0.617%
53	9.470	1369	1375	1384	rBV	706562	945934	33.17%	1.923%
54	9.561	1384	1390	1395	rVV	193892	275304	9.65%	0.560%
55	9.616	1395	1399	1402	rVV	250436	324323	11.37%	0.659%
56	9.647	1402	1404	1413	rVB	139290	192461	6.75%	0.391%
57	10.092	1471	1477	1480	rBV	1088412	1566680	54.93%	3.185%
58	10.201	1489	1495	1497	rBV	330021	448235	15.72%	0.911%
59	10.232	1497	1500	1510	rVB	618681	773371	27.12%	1.572%
60	10.342	1510	1518	1525	rBV	1103777	1513782	53.08%	3.078%
61	10.689	1567	1575	1584	rBV2	791191	1401255	49.13%	2.849%
62	10.835	1593	1599	1603	rBV	150927	217132	7.61%	0.441%
63	10.878	1603	1606	1618	rVV	326867	378666	13.28%	0.770%
64	11.000	1620	1626	1631	rVV	680727	829303	29.08%	1.686%
65	11.055	1631	1635	1640	rVV	216814	261957	9.18%	0.533%
66	11.122	1640	1646	1658	rVB	851984	1122689	39.36%	2.283%
67	11.238	1658	1665	1669	rBV2	469978	865841	30.36%	1.760%
68	11.280	1669	1672	1678	rVV2	287336	574455	20.14%	1.168%
69	11.341	1678	1682	1687	rVV	666003	789108	27.67%	1.604%
70	11.402	1687	1692	1697	rVV	527878	660006	23.14%	1.342%
71	11.488	1701	1706	1715	rVB2	1126434	1474886	51.71%	2.999%
72	11.756	1739	1750	1753	rBV2	831949	1200814	42.10%	2.442%
73	11.786	1753	1755	1762	rVB	653543	767382	26.91%	1.560%
74	11.927	1773	1778	1784	rBV	607942	748926	26.26%	1.523%
75	12.006	1786	1791	1794	rVV	487335	593107	20.80%	1.206%
76	12.055	1794	1799	1810	rVB4	1378067	2852124	100.00%	5.799%

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77	12.372	1845	1851	1863	rBV	1085579	1307871	45.86%	2.659%
78	12.579	1879	1885	1891	rBV	339876	443282	15.54%	0.901%
79	12.981	1942	1951	1959	rBV2	116975	165426	5.80%	0.336%
80	13.323	2002	2007	2018	rBV	607126	704257	24.69%	1.432%
81	13.628	2051	2057	2062	rBV	394803	491065	17.22%	0.998%
82	13.762	2074	2079	2083	rBV2	316920	386993	13.57%	0.787%
83	13.817	2083	2088	2099	rVB	485935	590428	20.70%	1.200%
84	14.000	2112	2118	2124	rBV	405111	493838	17.31%	1.004%

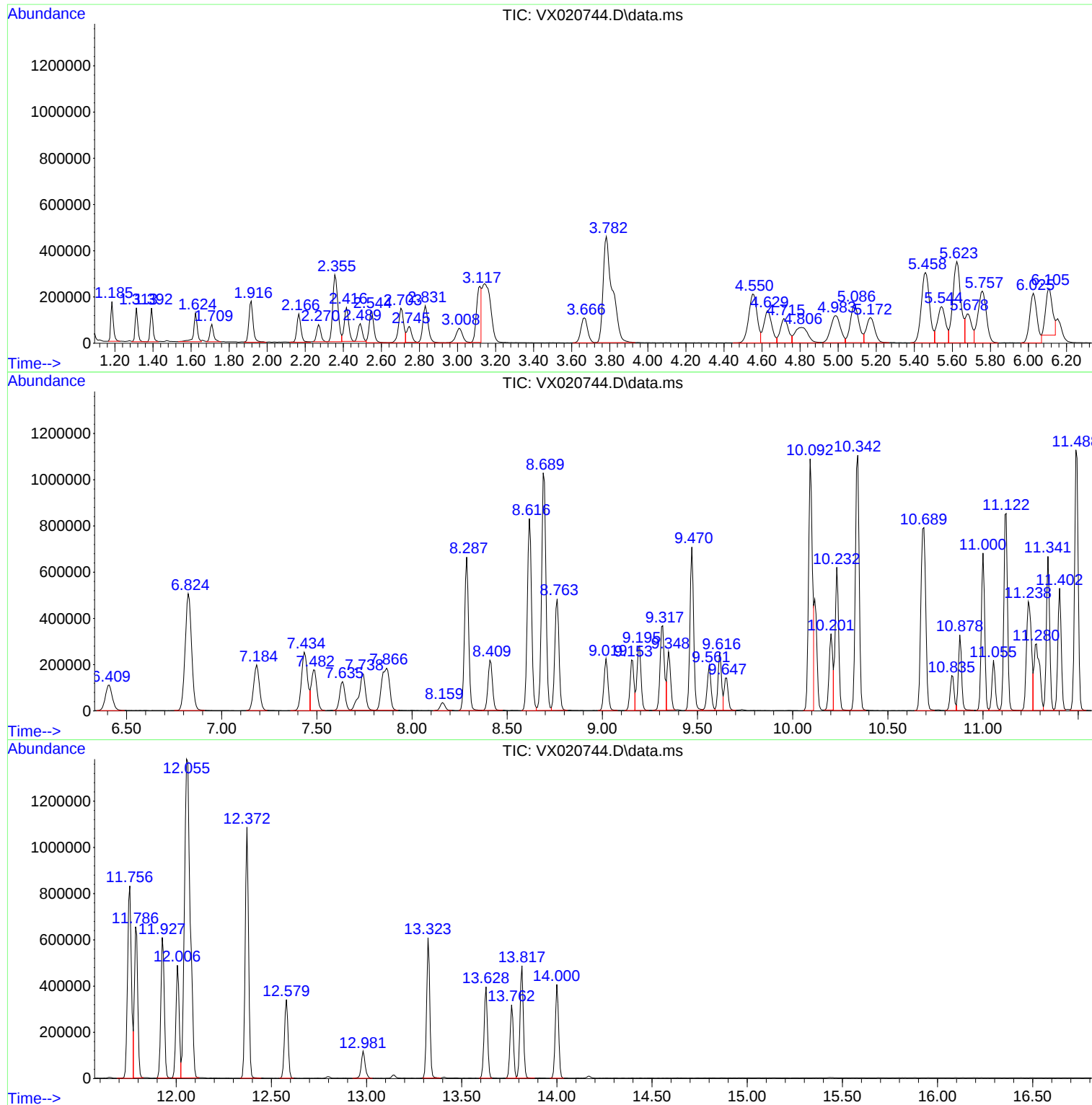
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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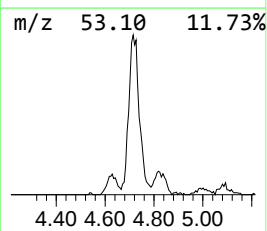
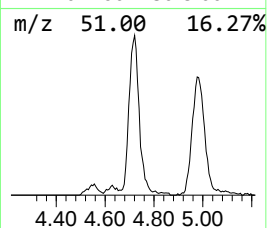
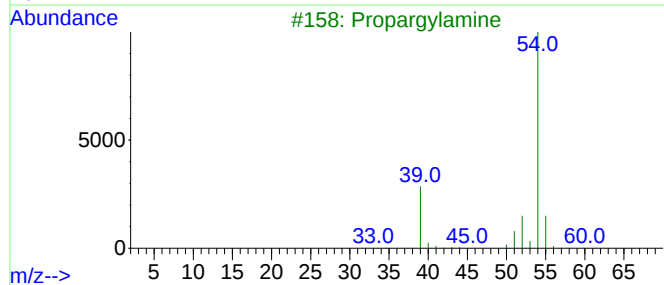
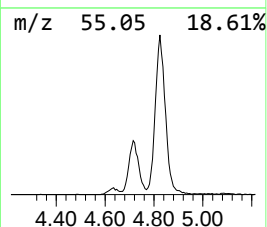
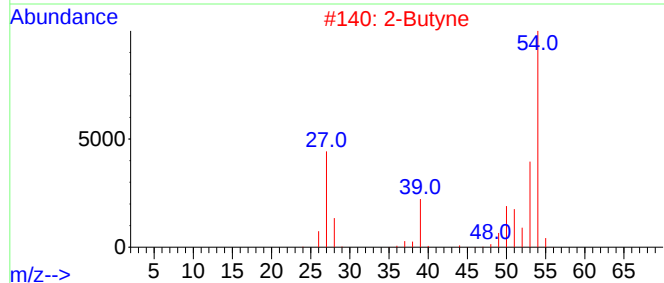
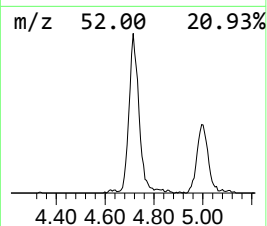
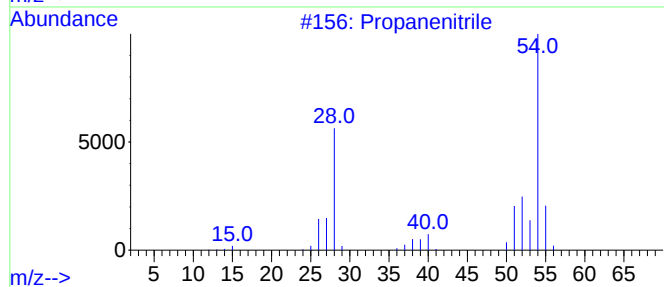
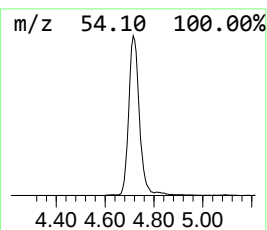
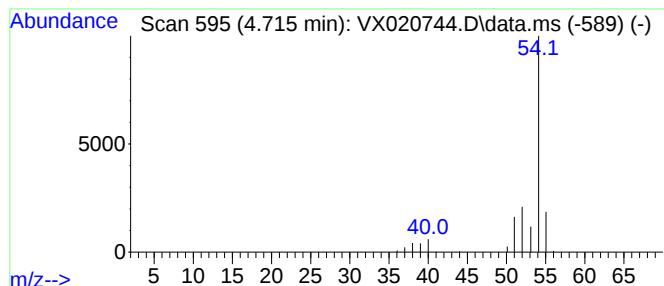
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

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

Peak Number 1 Propanenitrile Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.715	14.76 ug/l	304428	Pentafluorobenzene	5.623

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



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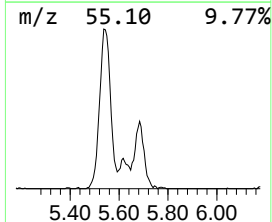
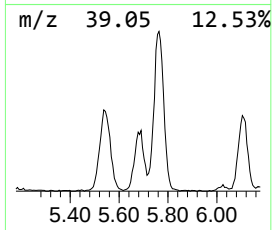
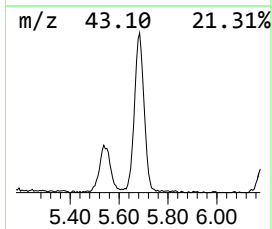
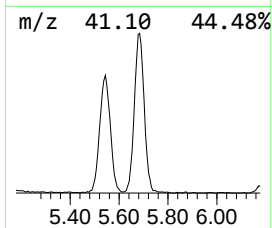
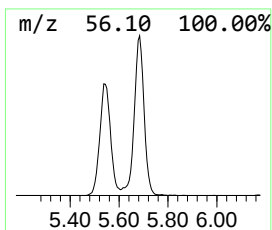
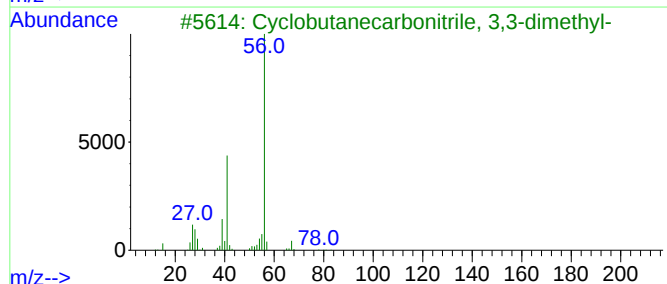
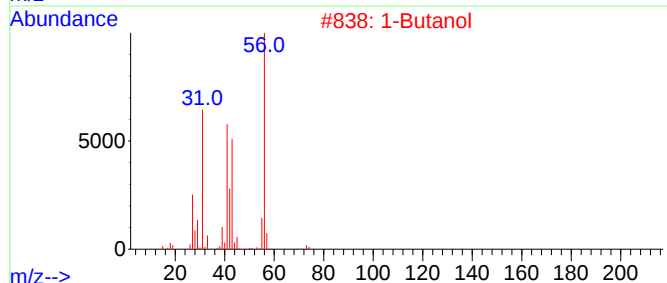
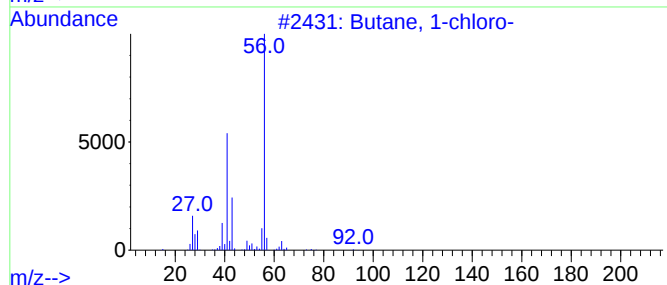
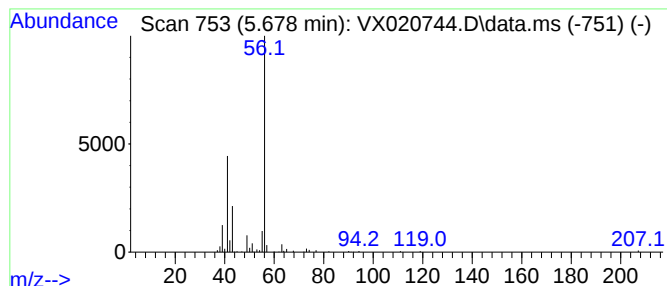
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Peak Number 2 Butane, 1-chloro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.678	13.42 ug/l	276894	Pentafluorobenzene	5.623

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 1-chloro-	92	C4H9Cl	000109-69-3	78
2			1-Butanol	74	C4H10O	000071-36-3	9
3			Cyclobutanecarbonitrile, 3,3-dim...	109	C7H11N	053783-86-1	9
4			Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	9
5			1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	9



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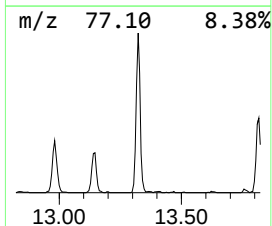
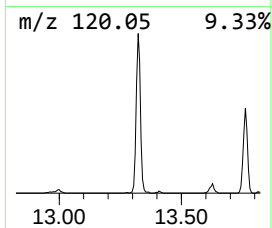
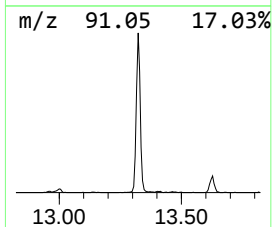
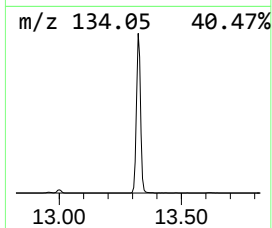
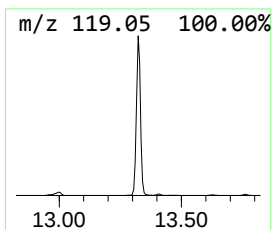
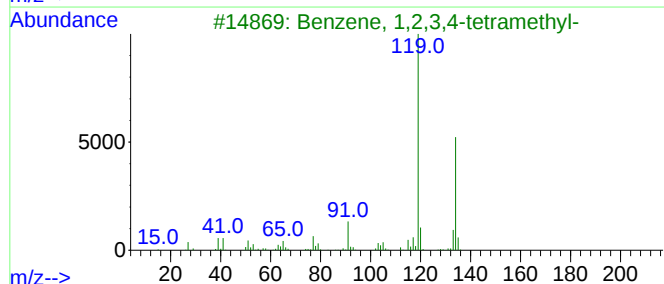
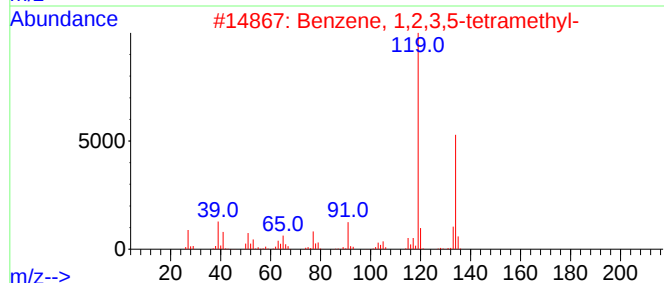
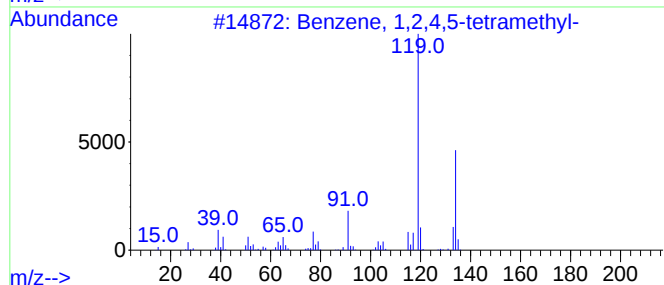
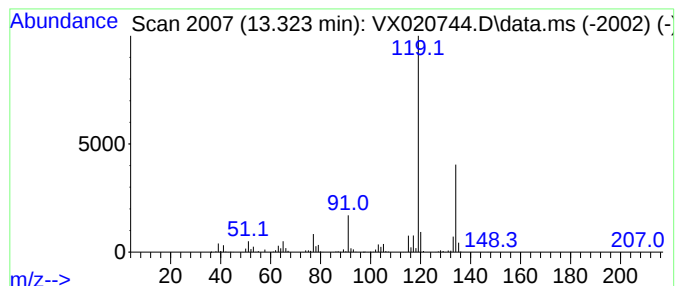
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.323	12.35 ug/l	704257	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, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	97
3			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	95
4			o-Cymene	134	C10H14	000527-84-4	95
5			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanenitrile	4.715	14.8	ug/l	304428	1	5.623	1031330	50.0
Butane, 1-chloro-	5.678	13.4	ug/l	276894	1	5.623	1031330	50.0
Benzene, 1,2,4,...	13.323	12.3	ug/l	704257	4	12.061	2852120	50.0