

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY012721\
 Data File : VY003948.D
 Acq On : 27 Jan 2021 13:01
 Operator : SY/MD
 Sample : VSTDIC100
 Misc : 5.00g/5mL/MSVOA_Y/SOIL
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 LabSampleId :
 VSTDIC100

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_Y\methods\82Y012721S.M

Title : SW846 8260

Signal : TIC: VY003948.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.906	9	14	29	rVB	176193	259799	6.00%	0.240%
2	2.119	44	49	62	rVB	234802	337490	7.79%	0.312%
3	2.259	62	72	89	rVB	256781	404209	9.33%	0.373%
4	2.558	112	121	128	rBV7	14616	49373	1.14%	0.046%
5	2.656	129	137	153	rVV	193882	426448	9.84%	0.394%
6	2.802	153	161	172	rVB	130269	260142	6.00%	0.240%
7	3.137	207	216	232	rBV	282454	685097	15.81%	0.633%
8	3.540	273	282	297	rBV	174540	419087	9.67%	0.387%
9	3.741	306	315	328	rBV	80159	207294	4.78%	0.191%
10	3.893	328	340	365	rVV3	420848	1972707	45.53%	1.822%
11	4.107	365	375	383	rVV	127460	366057	8.45%	0.338%
12	4.210	383	392	413	rVB	241583	686014	15.83%	0.634%
13	4.497	421	439	465	rVB	340643	1049349	24.22%	0.969%
14	4.735	465	478	495	rBV	261926	811805	18.74%	0.750%
15	4.978	501	518	536	rVB3	44480	195938	4.52%	0.181%
16	5.234	538	560	583	rBV3	561375	2478890	57.22%	2.290%
17	6.076	679	698	704	rBV2	833949	3096641	71.47%	2.860%
18	7.002	835	850	859	rBV2	860491	2461466	56.81%	2.274%
19	7.094	859	865	872	rBV3	177829	488869	11.28%	0.452%
20	7.350	892	907	924	rBV5	467237	1557250	35.94%	1.438%
21	7.521	924	935	948	rVB	357896	880076	20.31%	0.813%
22	7.716	954	967	974	rBV2	525861	1524730	35.19%	1.408%
23	7.795	974	980	988	rVV2	691506	1747017	40.32%	1.614%
24	7.923	988	1001	1015	rVB4	763334	2979734	68.78%	2.752%
25	8.167	1026	1041	1049	rBV3	890823	2253562	52.01%	2.082%
26	8.252	1049	1055	1057	rBV	244545	494602	11.42%	0.457%
27	8.697	1120	1128	1140	rVB	234378	466236	10.76%	0.431%
28	8.947	1155	1169	1182	rBV	616520	1171626	27.04%	1.082%
29	9.191	1199	1209	1212	rBV	855058	1769890	40.85%	1.635%
30	9.307	1221	1228	1234	rBV2	518817	1115621	25.75%	1.030%
31	9.362	1234	1237	1249	rVB	235968	406660	9.39%	0.376%
32	9.502	1252	1260	1274	rVB	420778	800673	18.48%	0.740%
33	9.728	1288	1297	1301	rBV	65460	126240	2.91%	0.117%
34	9.788	1301	1307	1316	rVB	1218880	2033473	46.93%	1.878%
35	9.935	1323	1331	1339	rBV	617692	1043648	24.09%	0.964%
36	10.075	1347	1354	1364	rVB	1279120	2133243	49.24%	1.970%

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Integrator: RTE

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37	10.185	1364	1372	1377	rVV	1021101	1773897	40.94%	1.638%
38	10.246	1377	1382	1393	rVB	1163395	2045517	47.21%	1.889%
39	10.471	1410	1419	1423	rBV	582268	998647	23.05%	0.922%
40	10.514	1423	1426	1432	rVV	474847	694910	16.04%	0.642%
41	10.581	1432	1437	1442	rVV	59608	109561	2.53%	0.101%
42	10.648	1442	1448	1454	rVV	520381	862687	19.91%	0.797%
43	10.721	1454	1460	1466	rVV	994714	1650572	38.10%	1.525%
44	10.794	1466	1472	1475	rVV	501014	840373	19.40%	0.776%
45	10.837	1475	1479	1488	rVV	961575	1471640	33.97%	1.359%
46	10.935	1488	1495	1499	rVV	422011	625168	14.43%	0.577%
47	10.989	1499	1504	1511	rVV	393556	656849	15.16%	0.607%
48	11.093	1511	1521	1529	rVB	232403	385898	8.91%	0.356%
49	11.520	1577	1591	1597	rBV2	1064071	2227373	51.41%	2.057%
50	11.593	1597	1603	1613	rVV	2167105	3451071	79.65%	3.188%
51	11.703	1613	1621	1631	rVB	2344711	4332535	100.00%	4.002%
52	12.038	1667	1676	1687	rBV2	2026151	4067918	93.89%	3.757%
53	12.148	1687	1694	1699	rBV	587799	851080	19.64%	0.786%
54	12.209	1699	1704	1711	rVB2	297061	487023	11.24%	0.450%
55	12.331	1715	1724	1729	rBV	1575810	2364214	54.57%	2.184%
56	12.379	1729	1732	1738	rVB	317951	464473	10.72%	0.429%
57	12.483	1743	1749	1758	rVB2	882872	1420045	32.78%	1.312%
58	12.611	1758	1770	1776	rBV3	1193909	2998563	69.21%	2.770%
59	12.672	1776	1780	1787	rVB	1530794	2283678	52.71%	2.109%
60	12.757	1787	1794	1799	rBV	1207815	1870889	43.18%	1.728%
61	12.812	1799	1803	1807	rVV	1584631	2388561	55.13%	2.206%
62	12.855	1807	1810	1818	rVB	1232982	1791095	41.34%	1.654%
63	13.074	1839	1846	1850	rBV	1458039	2350356	54.25%	2.171%
64	13.117	1850	1853	1860	rVB2	1953380	3014488	69.58%	2.784%
65	13.257	1869	1876	1882	rBV	1418127	2164974	49.97%	2.000%
66	13.367	1887	1894	1900	rBV	2717384	4104367	94.73%	3.791%
67	13.446	1900	1907	1916	rVB2	1198161	2252361	51.99%	2.080%
68	13.696	1941	1948	1952	rBV	1467789	2154858	49.74%	1.990%
69	13.739	1952	1955	1963	rVB	967821	1371361	31.65%	1.267%
70	13.965	1985	1992	1999	rVB	812719	1341947	30.97%	1.240%
71	14.355	2049	2056	2064	rVB2	134535	259492	5.99%	0.240%
72	14.513	2074	2082	2087	rBV	25432	45020	1.04%	0.042%
73	14.672	2101	2108	2115	rBV	1365622	1951587	45.04%	1.803%
74	15.007	2149	2163	2171	rBV	854877	1377373	31.79%	1.272%
75	15.111	2171	2180	2187	rVB	853240	1361047	31.41%	1.257%
76	15.239	2193	2201	2209	rBV	615239	1044854	24.12%	0.965%

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LabSampleId :
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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

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Title : SW846 8260

77	15.422	2221	2231	2240	rBV	683677	1195012	27.58%	1.104%
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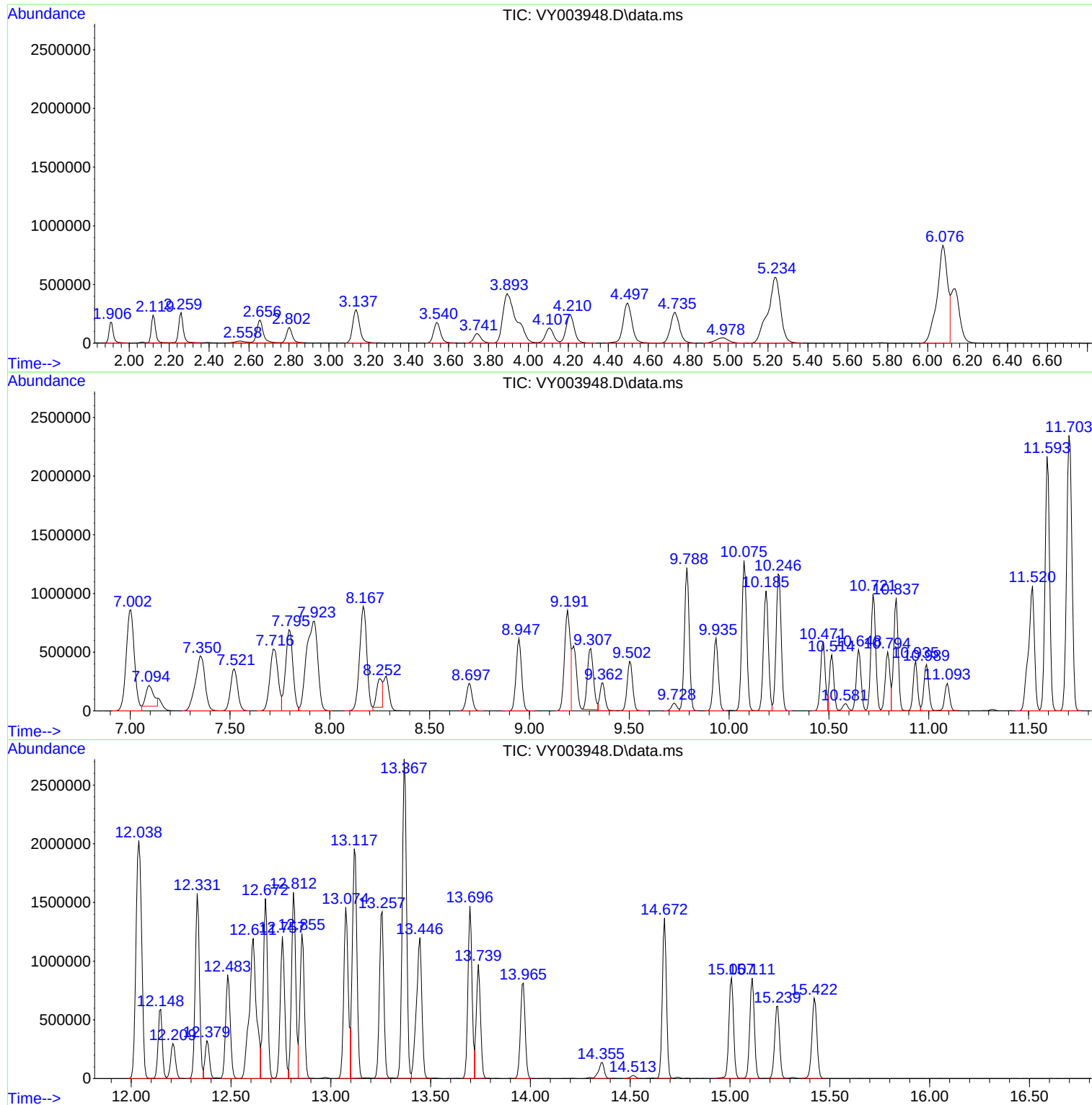
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_Y
LabSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y012721S.M
Quant Title : SW846 8260

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



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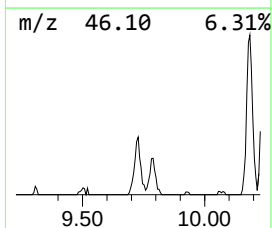
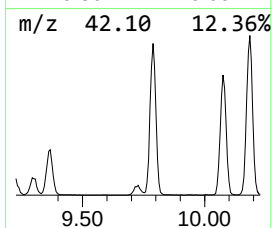
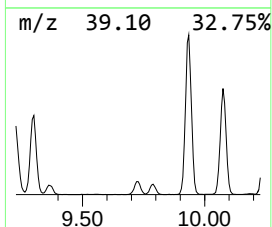
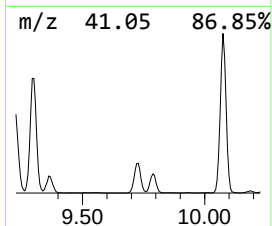
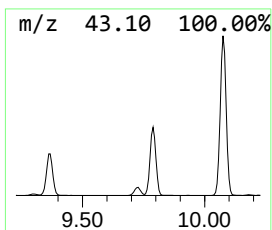
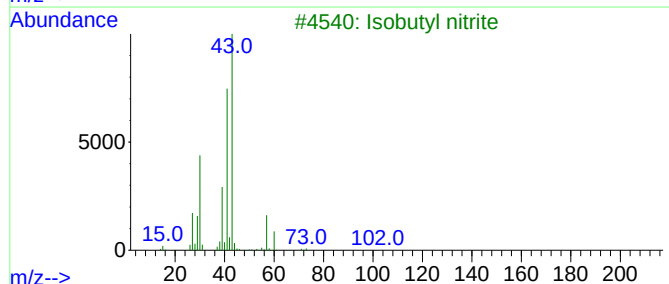
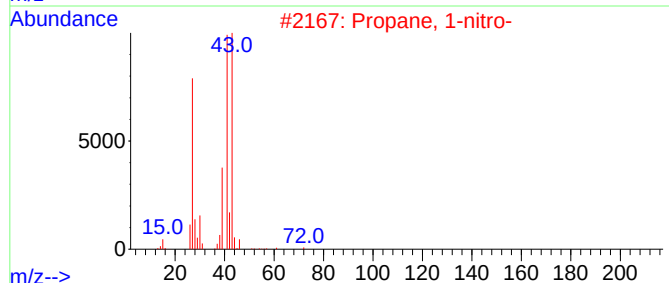
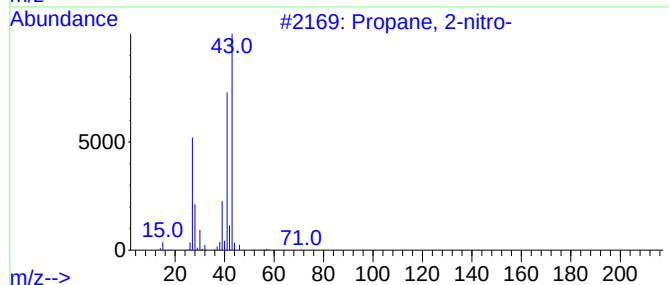
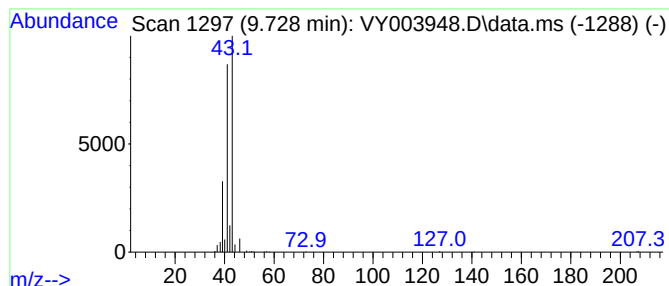
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y012721S.M
Quant Title : SW846 8260

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

Peak Number 1 Propane, 2-nitro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.728	13.54 ug/l	126240	1,4-Difluorobenzene	8.697

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	56
2			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	45
3			Isobutyl nitrite	103	C4H9NO2	000542-56-3	39
4			Propene	42	C3H6	000115-07-1	9
5			Propanamide, 2,2-dimethyl-	101	C5H11NO	000754-10-9	9



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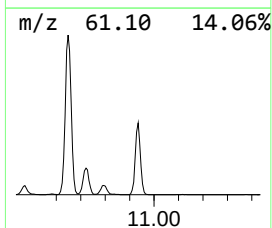
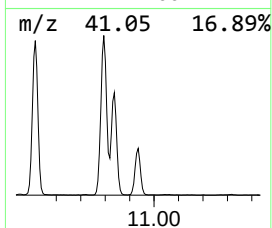
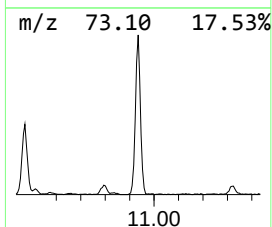
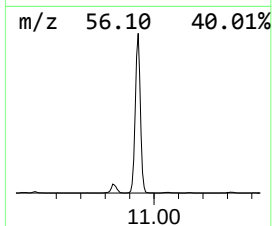
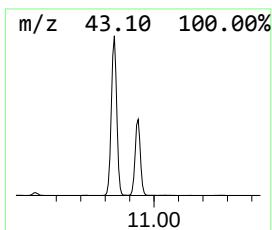
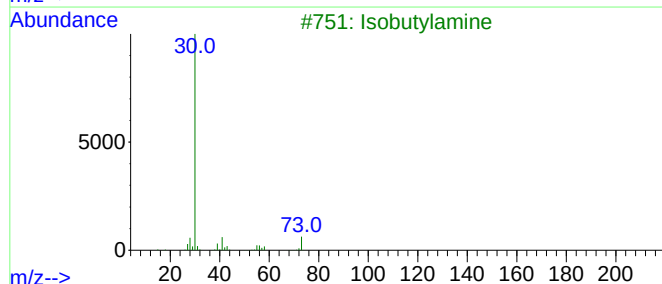
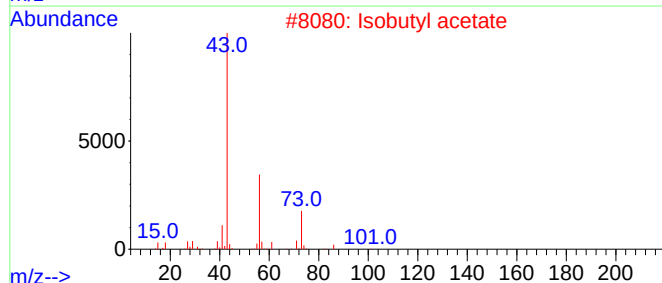
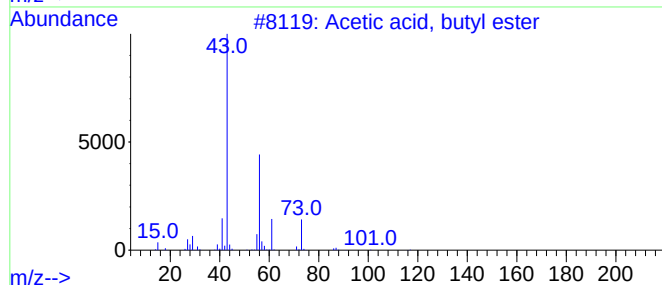
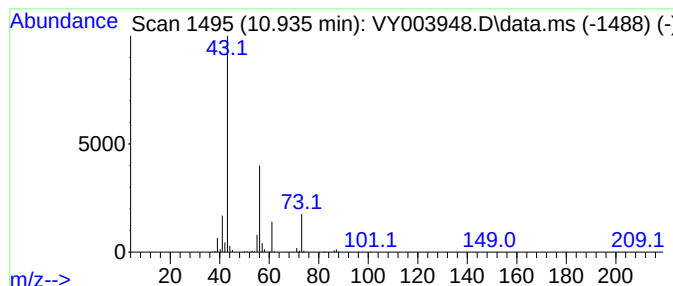
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Acetic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.935	14.03 ug/l	625168	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2			Isobutyl acetate	116	C6H12O2	000110-19-0	40
3			Isobutylamine	73	C4H11N	000078-81-9	9
4			1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	9
5			2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9



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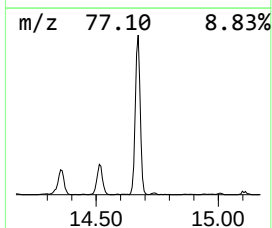
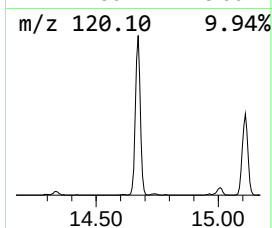
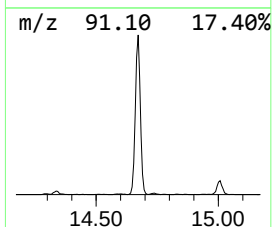
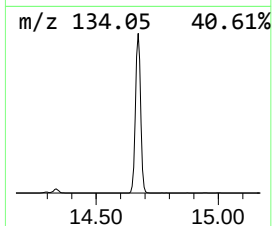
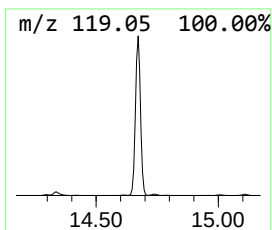
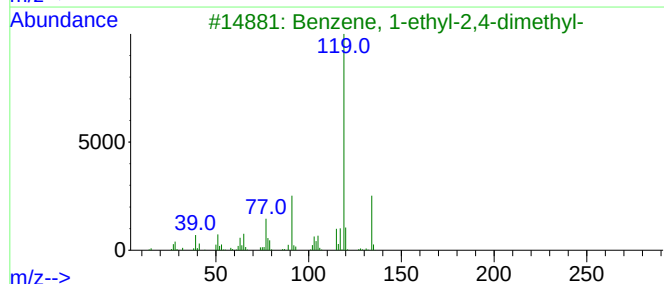
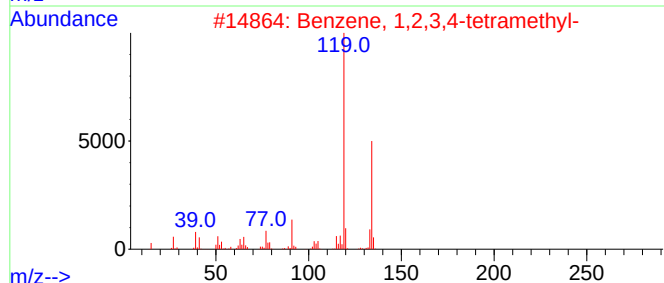
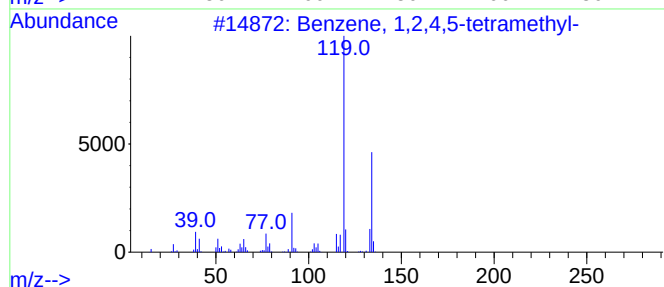
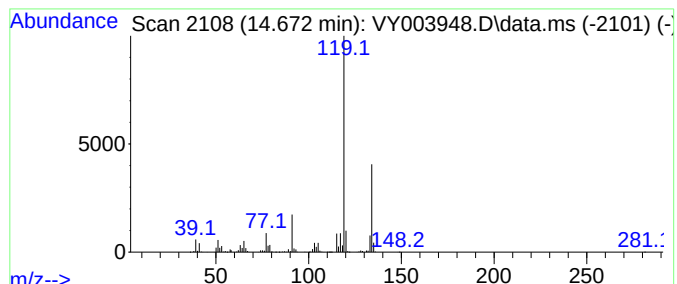
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.672	43.32 ug/l	1951590	1,4-Dichlorobenzene-d4	13.428

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	95
3			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	95
4			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94
5			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2-nitro-	9.728	13.5	ug/l	126240	2	8.697	466236	50.0
Acetic acid, bu...	10.935	14.0	ug/l	625168	3	11.496	2227370	50.0
Benzene, 1,2,4,...	14.672	43.3	ug/l	1951590	4	13.428	2252360	50.0