

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY012721\
 Data File : VY003949.D
 Acq On : 27 Jan 2021 13:24
 Operator : SY/MD
 Sample : VSTDIC150
 Misc : 5.00g/5mL/MSVOA_Y/SOIL
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 LabSampleId :
 VSTDIC150

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: VY003949.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	8	14	26	rBV	260228	380685	6.43%	0.261%
2	2.119	44	49	60	rBV	354346	502327	8.48%	0.344%
3	2.260	66	72	85	rBV	384582	600738	10.14%	0.411%
4	2.564	110	122	127	rBV7	21382	74308	1.25%	0.051%
5	2.644	128	135	151	rVV	270708	622257	10.51%	0.426%
6	2.796	153	160	175	rVB	166457	353099	5.96%	0.242%
7	3.131	205	215	232	rBV	354859	866424	14.63%	0.593%
8	3.540	273	282	297	rBV	227062	556186	9.39%	0.381%
9	3.741	306	315	328	rBV	116778	303709	5.13%	0.208%
10	3.893	328	340	349	rBV3	551642	2155903	36.41%	1.477%
11	4.107	365	375	383	rBV	162548	449185	7.59%	0.308%
12	4.204	383	391	411	rVB	321834	904022	15.27%	0.619%
13	4.497	420	439	455	rBV	458420	1436198	24.25%	0.984%
14	4.735	465	478	498	rVB	340899	1074261	18.14%	0.736%
15	4.979	502	518	535	rVB4	55808	242915	4.10%	0.166%
16	5.235	539	560	580	rBV2	773448	3434816	58.00%	2.352%
17	6.076	679	698	704	rBV2	1173222	4345590	73.38%	2.976%
18	6.996	833	849	859	rBV2	1187548	3414997	57.67%	2.339%
19	7.094	859	865	886	rVB3	300485	1172314	19.80%	0.803%
20	7.356	892	908	925	rBV4	665391	2239198	37.81%	1.534%
21	7.521	925	935	953	rVB	499221	1205047	20.35%	0.825%
22	7.722	955	968	974	rBV2	725794	2079240	35.11%	1.424%
23	7.795	974	980	988	rVV2	883346	2172765	36.69%	1.488%
24	7.917	988	1000	1016	rVB4	991326	3859140	65.17%	2.643%
25	8.167	1028	1041	1049	rBV3	1221534	3031014	51.18%	2.076%
26	8.252	1049	1055	1057	rVV	379936	810017	13.68%	0.555%
27	8.277	1057	1059	1069	rVB	410723	744121	12.57%	0.510%
28	8.697	1119	1128	1137	rVB	221069	429685	7.26%	0.294%
29	8.947	1158	1169	1183	rVB	801741	1583592	26.74%	1.085%
30	9.191	1195	1209	1212	rBV	1142066	2407672	40.66%	1.649%
31	9.307	1221	1228	1233	rBV2	716508	1537600	25.97%	1.053%
32	9.362	1233	1237	1249	rVB	349590	625749	10.57%	0.429%
33	9.502	1252	1260	1274	rVB	596000	1089369	18.40%	0.746%
34	9.722	1289	1296	1301	rBV	94300	183213	3.09%	0.125%
35	9.789	1301	1307	1317	rVV	1725804	2782429	46.99%	1.906%
36	9.935	1321	1331	1339	rBV	788334	1352301	22.84%	0.926%

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Integrator: RTE

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Filtering: 5

Sampling : 1

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Max Peaks: 100

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37	10.075	1347	1354	1364	rVB	1813609	3003013	50.71%	2.057%
38	10.185	1364	1372	1377	rVV	1390118	2383523	40.25%	1.632%
39	10.246	1377	1382	1392	rVB	1671137	2769833	46.77%	1.897%
40	10.471	1409	1419	1422	rBV	786393	1319956	22.29%	0.904%
41	10.514	1422	1426	1432	rVV	679151	1039845	17.56%	0.712%
42	10.581	1432	1437	1442	rVV	42877	81527	1.38%	0.056%
43	10.648	1442	1448	1454	rVV	705005	1179385	19.92%	0.808%
44	10.721	1454	1460	1466	rVV	1348047	2238705	37.81%	1.533%
45	10.795	1466	1472	1475	rVV	696669	1165188	19.68%	0.798%
46	10.837	1475	1479	1488	rVV	1338700	2059310	34.78%	1.410%
47	10.935	1488	1495	1499	rVV	566833	870328	14.70%	0.596%
48	10.990	1499	1504	1512	rVV	540683	895069	15.12%	0.613%
49	11.093	1513	1521	1528	rVB	317218	524887	8.86%	0.359%
50	11.520	1576	1591	1597	rBV2	1429223	2760572	46.62%	1.891%
51	11.593	1597	1603	1613	rVV	3038812	4700394	79.38%	3.219%
52	11.703	1613	1621	1634	rVB	3324619	5921691	100.00%	4.056%
53	12.038	1666	1676	1687	rBV2	2814174	5517181	93.17%	3.779%
54	12.142	1687	1693	1699	rVV	711472	1046085	17.67%	0.716%
55	12.209	1699	1704	1715	rVB	386913	634740	10.72%	0.435%
56	12.331	1716	1724	1729	rVV	2088805	3152209	53.23%	2.159%
57	12.380	1729	1732	1738	rVV	465681	671061	11.33%	0.460%
58	12.483	1742	1749	1757	rVV2	1162760	1844398	31.15%	1.263%
59	12.611	1758	1770	1776	rVV3	1634207	4062755	68.61%	2.782%
60	12.672	1776	1780	1787	rVV	2057129	3055841	51.60%	2.093%
61	12.758	1787	1794	1799	rVV	1616976	2502849	42.27%	1.714%
62	12.813	1799	1803	1807	rVV	2189173	3183019	53.75%	2.180%
63	12.855	1807	1810	1823	rVB	1662898	2381062	40.21%	1.631%
64	13.075	1839	1846	1849	rBV	1995619	2926482	49.42%	2.004%
65	13.117	1849	1853	1860	rVB2	2642949	4217751	71.23%	2.889%
66	13.251	1867	1875	1882	rBV	1843934	2822668	47.67%	1.933%
67	13.367	1887	1894	1900	rVV	3629647	5454991	92.12%	3.736%
68	13.447	1900	1907	1916	rVB2	1507643	2744126	46.34%	1.879%
69	13.697	1941	1948	1952	rBV	2104331	3039752	51.33%	2.082%
70	13.739	1952	1955	1965	rVB	1321611	1900908	32.10%	1.302%
71	13.959	1984	1991	2000	rVB	1059936	1734200	29.29%	1.188%
72	14.355	2049	2056	2063	rVB2	187635	352958	5.96%	0.242%
73	14.513	2075	2082	2090	rBV2	36383	61604	1.04%	0.042%
74	14.672	2101	2108	2115	rVB	1614145	2312171	39.05%	1.584%
75	15.007	2149	2163	2171	rBV	1104851	1740808	29.40%	1.192%
76	15.111	2172	2180	2187	rBV	1116288	1729801	29.21%	1.185%

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Instrument :
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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
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Stop Thrs : 0 Peak Location: TOP

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77	15.233	2193	2200	2208	rBV	842814	1421370	24.00%	0.973%
78	15.422	2221	2231	2241	rVB	929707	1566194	26.45%	1.073%

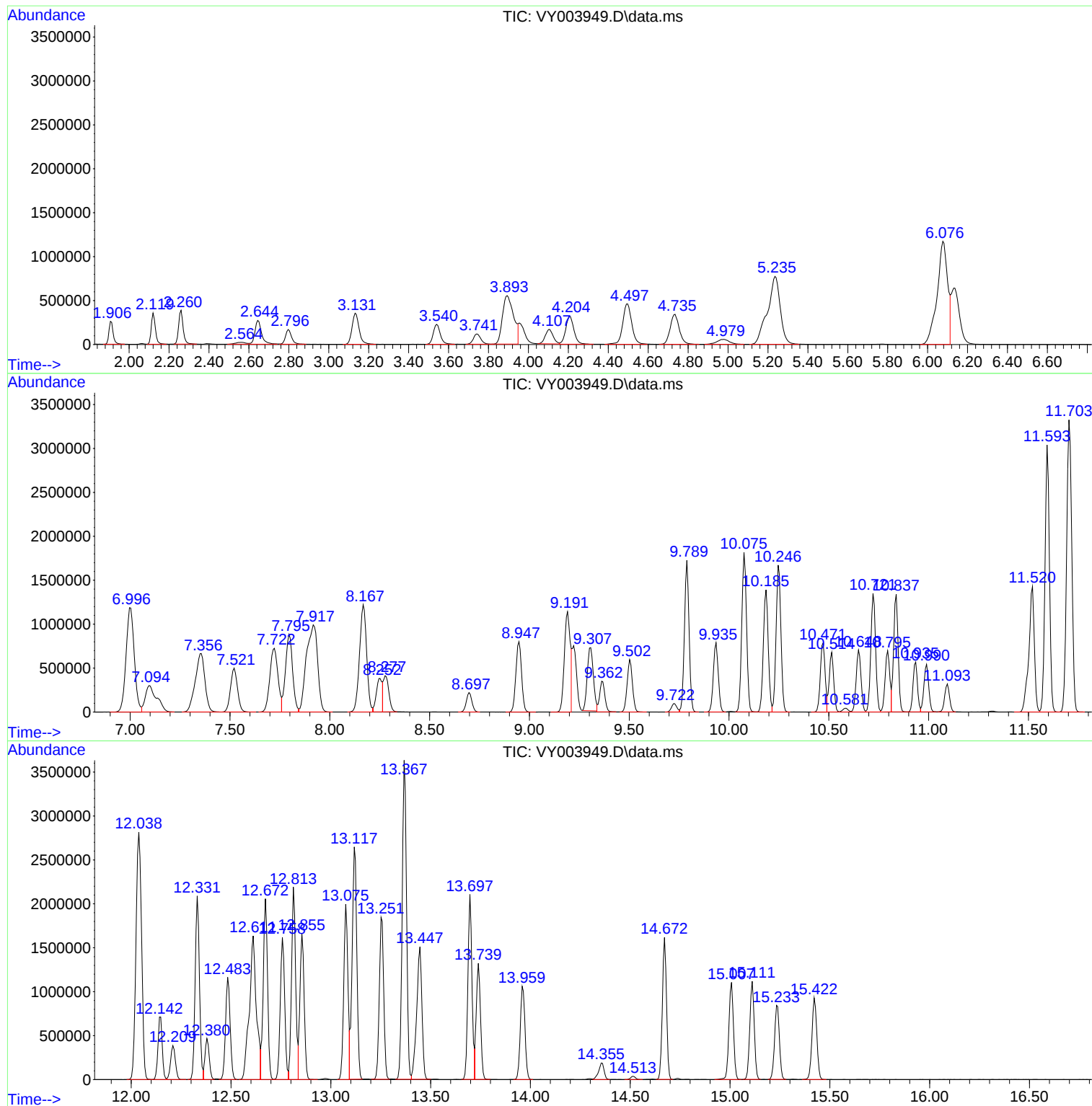
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Instrument :
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LabSampleId :
VSTDIC150

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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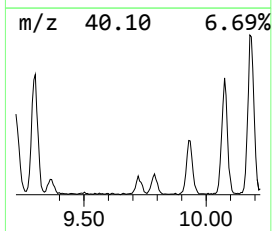
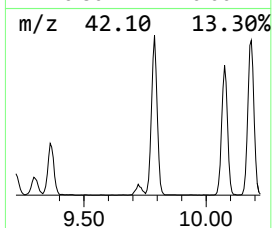
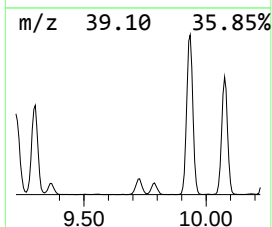
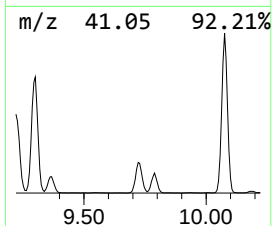
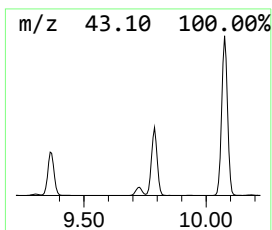
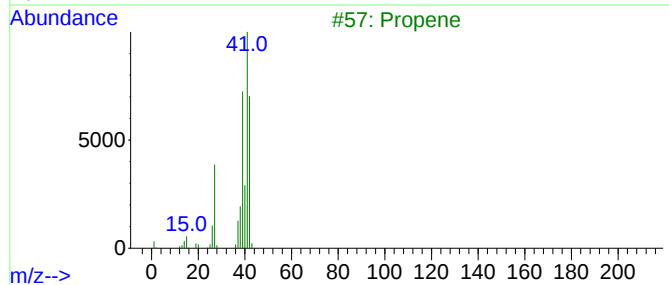
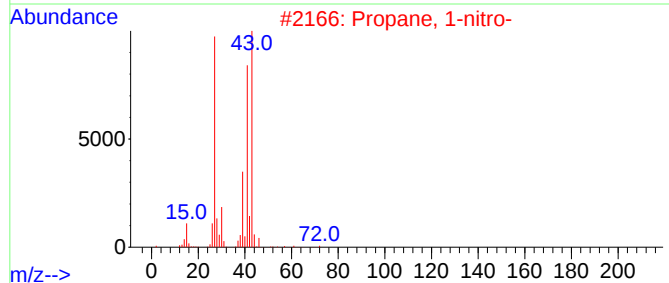
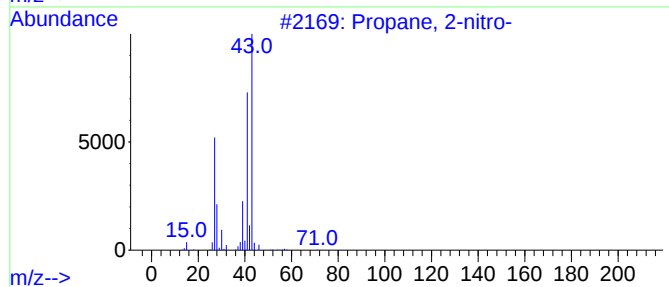
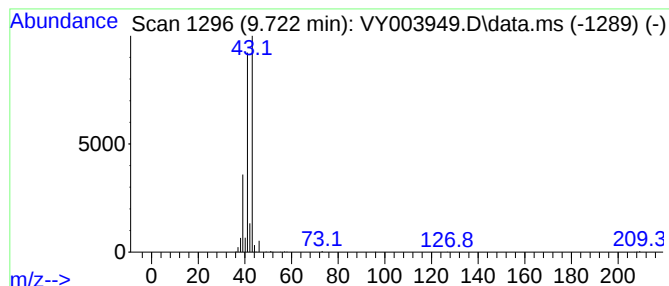
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y012721S.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.722	21.32 ug/l	183213	1,4-Difluorobenzene	8.697

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	64
2			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	64
3			Propene	42	C3H6	000115-07-1	9
4			Isobutyl nitrite	103	C4H9NO2	000542-56-3	9
5			Propanamide, 2,2-dimethyl-	101	C5H11NO	000754-10-9	9



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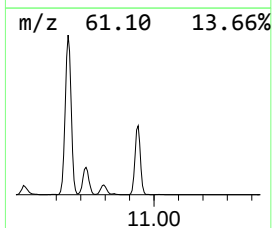
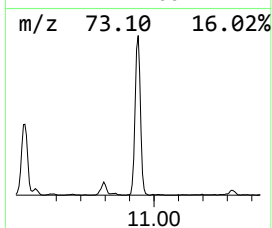
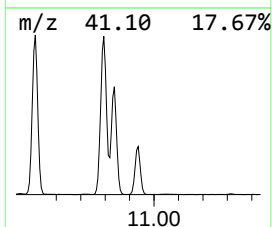
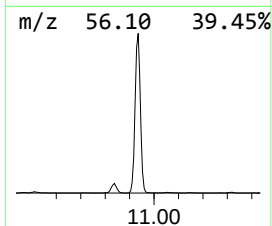
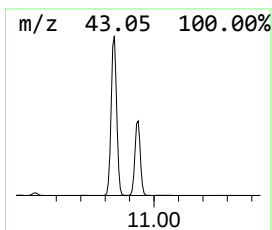
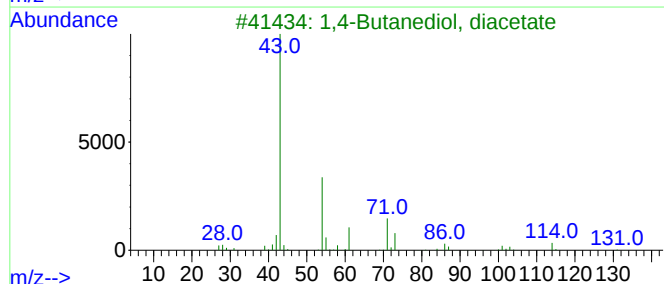
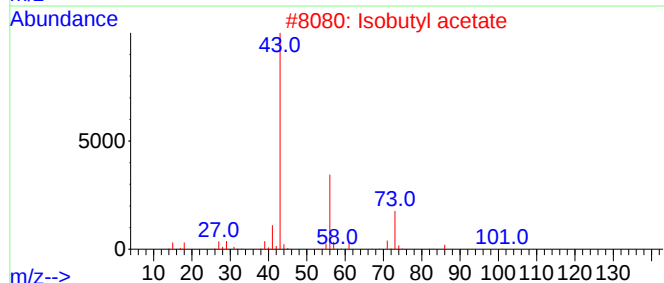
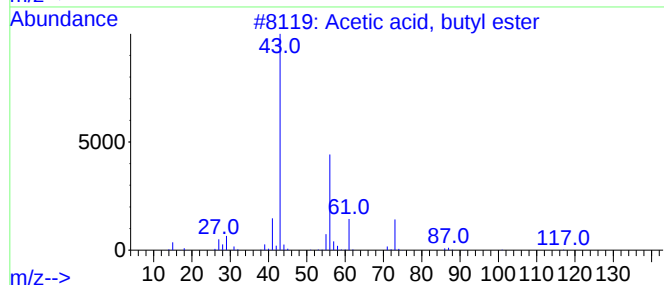
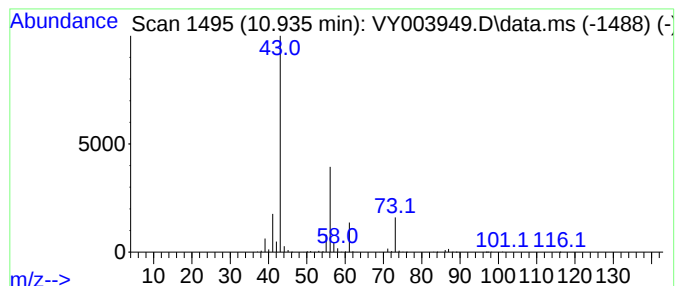
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Acetic acid, butyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.935	15.76 ug/l	870328	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			1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	17
4			1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	17
5			Isobutylamine	73	C4H11N	000078-81-9	9



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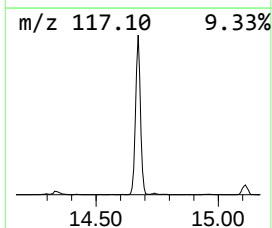
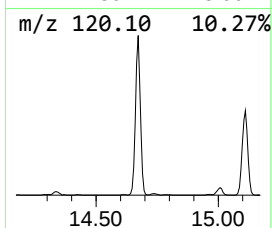
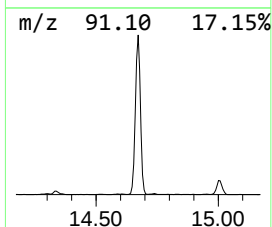
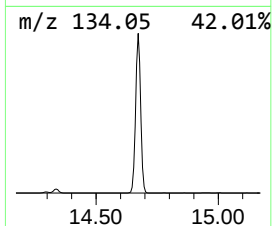
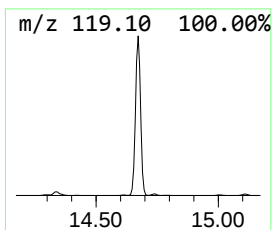
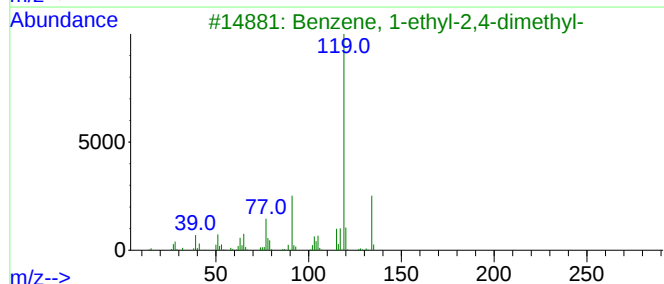
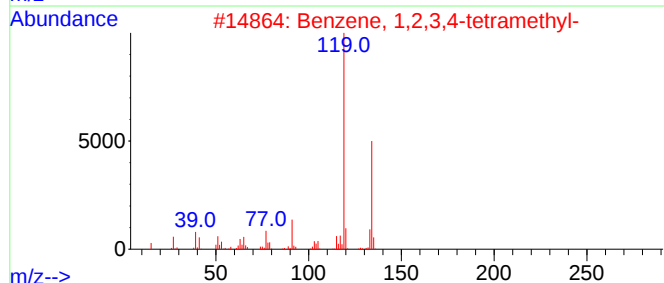
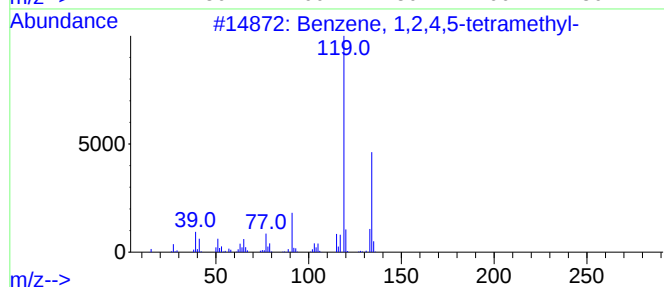
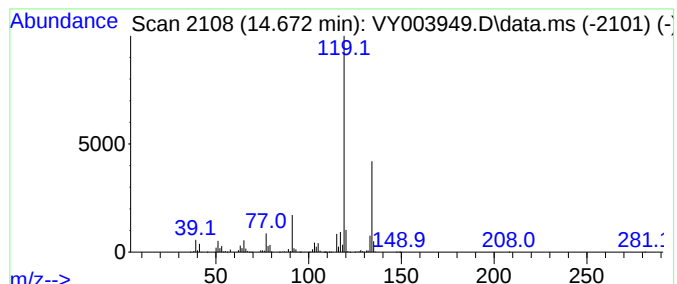
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.672	42.13 ug/l	2312170	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-	9.722	21.3	ug/l	183213	2	8.697	429685	50.0
Acetic acid, bu...	10.935	15.8	ug/l	870328	3	11.496	2760570	50.0
Benzene, 1,2,4,...	14.672	42.1	ug/l	2312170	4	13.428	2744130	50.0