

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY012721\
 Data File : VY003947.D
 Acq On : 27 Jan 2021 12:39
 Operator : SY/MD
 Sample : VSTDICCC050
 Misc : 5.00g/5mL/MSVOA_Y/SOIL
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 LabSampleId :
 VSTDICCC050

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: VY003947.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.912	10	15	25	rVB	74262	105750	5.97%	0.229%
2	2.119	44	49	61	rBV	109968	160059	9.04%	0.346%
3	2.259	65	72	83	rVB	104885	172352	9.73%	0.373%
4	2.662	131	138	150	rVB	94649	189204	10.68%	0.409%
5	2.808	153	162	170	rBV	51673	107255	6.06%	0.232%
6	3.137	208	216	233	rBV	118277	285621	16.13%	0.618%
7	3.546	274	283	295	rBV	76203	180192	10.17%	0.390%
8	3.747	305	316	329	rBV2	32865	88204	4.98%	0.191%
9	3.899	329	341	365	rVV3	171117	806372	45.53%	1.745%
10	4.107	367	375	384	rVV	48933	139815	7.89%	0.303%
11	4.210	384	392	405	rVB	102185	276944	15.64%	0.599%
12	4.497	421	439	454	rBV2	143622	441170	24.91%	0.955%
13	4.735	466	478	495	rBV2	113531	348355	19.67%	0.754%
14	4.972	499	517	532	rBV3	19434	92101	5.20%	0.199%
15	5.241	541	561	581	rVB4	238084	1034941	58.43%	2.240%
16	6.076	678	698	705	rBV2	351078	1349805	76.21%	2.921%
17	7.002	837	850	859	rBV2	360790	1026214	57.94%	2.221%
18	7.100	859	866	886	rVB4	87426	339646	19.18%	0.735%
19	7.356	893	908	924	rBV4	203831	668592	37.75%	1.447%
20	7.521	924	935	948	rVB	153548	373127	21.07%	0.808%
21	7.722	954	968	974	rBV2	227368	643220	36.32%	1.392%
22	7.801	974	981	989	rVV2	356354	876525	49.49%	1.897%
23	7.923	989	1001	1013	rVB3	316160	1241116	70.08%	2.686%
24	8.167	1025	1041	1049	rBV3	376466	984970	55.61%	2.132%
25	8.252	1049	1055	1057	rBV	105577	210896	11.91%	0.456%
26	8.697	1118	1128	1137	rBV	197829	387332	21.87%	0.838%
27	8.947	1159	1169	1180	rVB	251442	486536	27.47%	1.053%
28	9.191	1199	1209	1212	rBV	339228	721309	40.73%	1.561%
29	9.307	1221	1228	1234	rBV2	205984	464410	26.22%	1.005%
30	9.362	1234	1237	1246	rVB	99801	169079	9.55%	0.366%
31	9.502	1253	1260	1272	rVB	176661	335433	18.94%	0.726%
32	9.728	1287	1297	1301	rBV	27697	54219	3.06%	0.117%
33	9.789	1301	1307	1315	rVB	528489	877151	49.53%	1.898%
34	9.935	1323	1331	1339	rBV	256688	439005	24.79%	0.950%
35	10.075	1346	1354	1364	rBV	533101	875053	49.41%	1.894%
36	10.185	1364	1372	1377	rVV	458965	776860	43.86%	1.681%

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37	10.246	1377	1382	1392	rVB	500754	843548	47.63%	1.826%
38	10.471	1411	1419	1422	rBV	246175	394308	22.26%	0.853%
39	10.514	1422	1426	1432	rVV	199262	305610	17.26%	0.661%
40	10.581	1432	1437	1442	rVV	53592	95271	5.38%	0.206%
41	10.648	1442	1448	1454	rVV	213846	355889	20.09%	0.770%
42	10.721	1454	1460	1466	rVV	406407	685402	38.70%	1.483%
43	10.794	1466	1472	1475	rVV	208816	347422	19.62%	0.752%
44	10.837	1475	1479	1488	rVB	378057	564889	31.89%	1.223%
45	10.935	1488	1495	1499	rBV	164799	254965	14.40%	0.552%
46	10.990	1499	1504	1511	rVV	158480	269973	15.24%	0.584%
47	11.093	1515	1521	1527	rVB	98083	161455	9.12%	0.349%
48	11.319	1554	1558	1567	rVB	10834	19465	1.10%	0.042%
49	11.514	1577	1590	1597	rBV2	436129	1153843	65.15%	2.497%
50	11.593	1597	1603	1613	rVV	883587	1406151	79.39%	3.043%
51	11.703	1613	1621	1633	rVB	971023	1771118	100.00%	3.833%
52	12.038	1667	1676	1687	rBV2	804934	1644182	92.83%	3.558%
53	12.142	1687	1693	1699	rVV	236422	344522	19.45%	0.746%
54	12.209	1699	1704	1711	rVB	120775	197107	11.13%	0.427%
55	12.331	1716	1724	1729	rBV	643164	968652	54.69%	2.096%
56	12.380	1729	1732	1738	rVV	139122	198755	11.22%	0.430%
57	12.483	1742	1749	1759	rVB2	406190	681247	38.46%	1.474%
58	12.611	1759	1770	1776	rBV3	488895	1229817	69.44%	2.662%
59	12.672	1776	1780	1787	rVB	630146	937348	52.92%	2.029%
60	12.758	1787	1794	1798	rBV	506022	762898	43.07%	1.651%
61	12.812	1798	1803	1807	rVV	683454	1015535	57.34%	2.198%
62	12.855	1807	1810	1817	rVB	513566	736743	41.60%	1.594%
63	13.075	1839	1846	1849	rBV	601534	920566	51.98%	1.992%
64	13.117	1849	1853	1860	rVB2	812484	1306539	73.77%	2.828%
65	13.251	1868	1875	1887	rBV	589935	899951	50.81%	1.948%
66	13.367	1887	1894	1899	rVV	1134146	1701390	96.06%	3.682%
67	13.440	1899	1906	1917	rVB2	517991	1201762	67.85%	2.601%
68	13.696	1942	1948	1952	rBV	657649	974312	55.01%	2.109%
69	13.739	1952	1955	1962	rVB	409923	589956	33.31%	1.277%
70	13.959	1984	1991	1999	rVB2	351656	583964	32.97%	1.264%
71	14.361	2048	2057	2064	rVB2	54402	106593	6.02%	0.231%
72	14.672	2101	2108	2115	rBV	547618	792422	44.74%	1.715%
73	15.007	2150	2163	2171	rVB	341723	559027	31.56%	1.210%
74	15.111	2171	2180	2189	rBV2	347363	563363	31.81%	1.219%
75	15.233	2193	2200	2207	rBV	253725	427547	24.14%	0.925%
76	15.422	2220	2231	2242	rVB	287691	503300	28.42%	1.089%

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Instrument :
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LabSampleId :
VSTDICCC050

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

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Title : SW846 8260

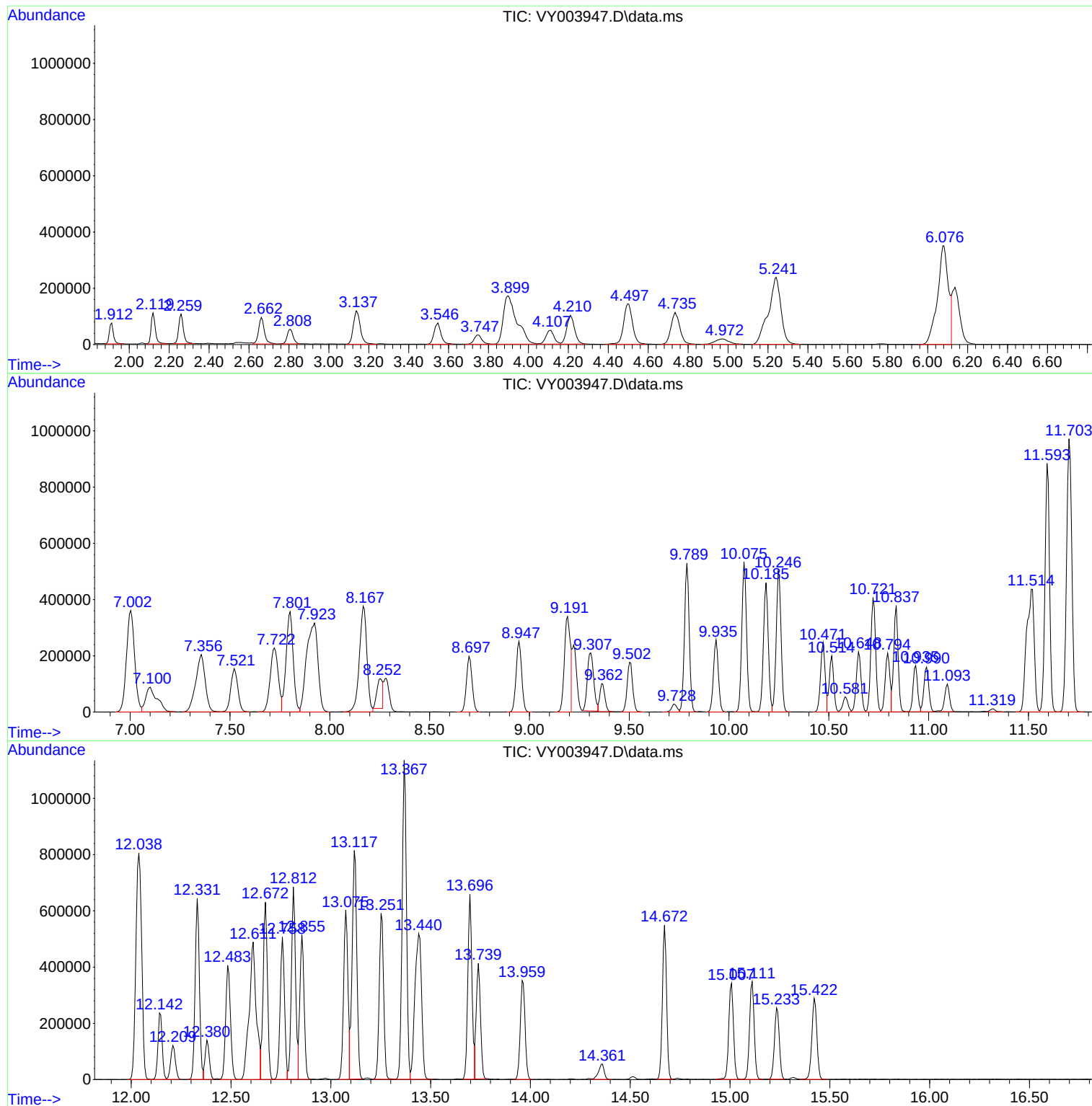
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LabSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y012721S.M
Quant Title : SW846 8260

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



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Instrument :
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LabSampleId :
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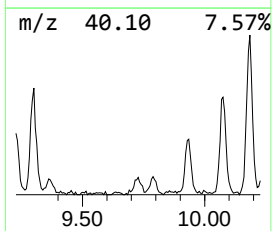
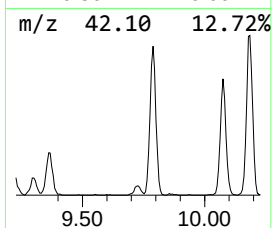
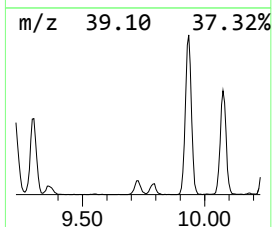
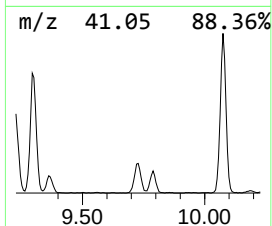
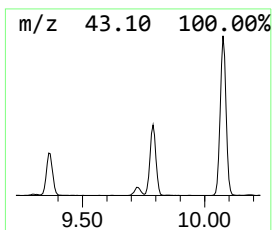
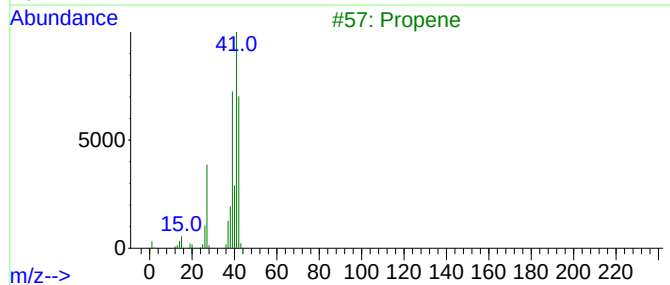
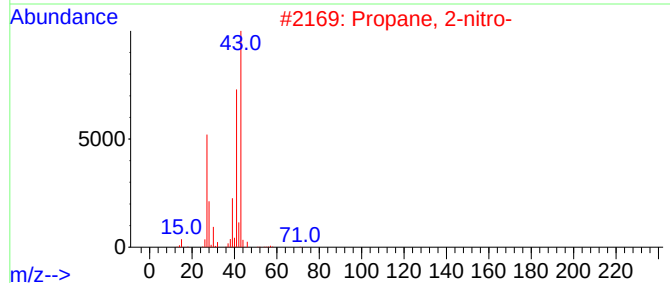
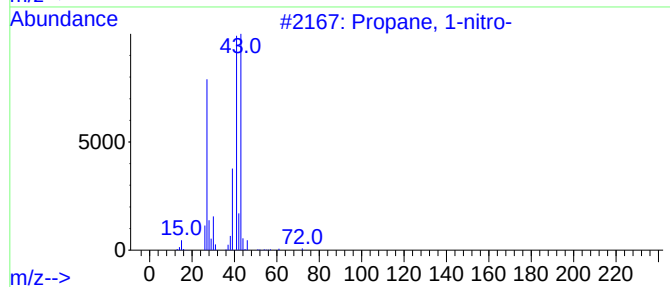
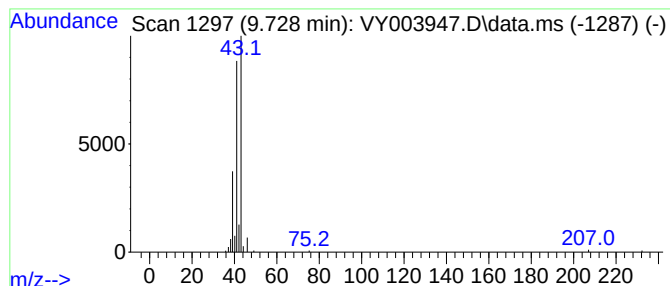
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.728	7.00 ug/l	54219	1,4-Difluorobenzene	8.697

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	64
2			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	40
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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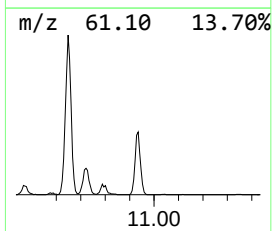
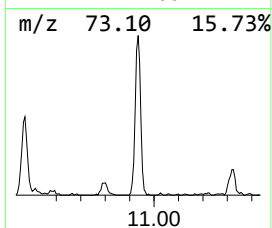
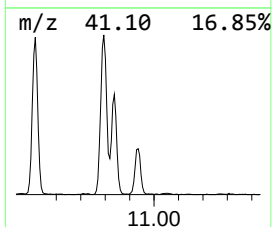
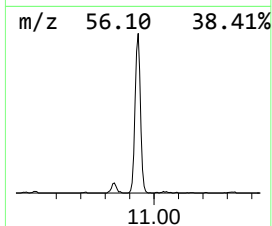
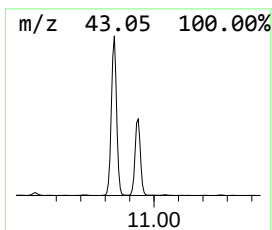
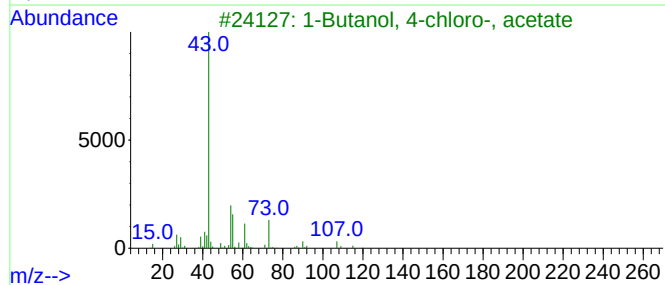
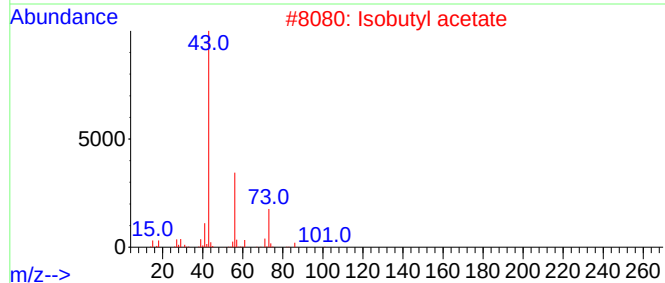
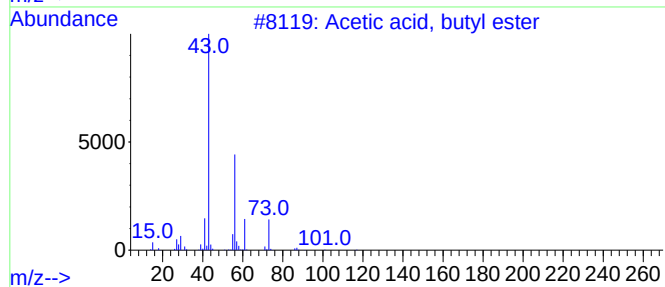
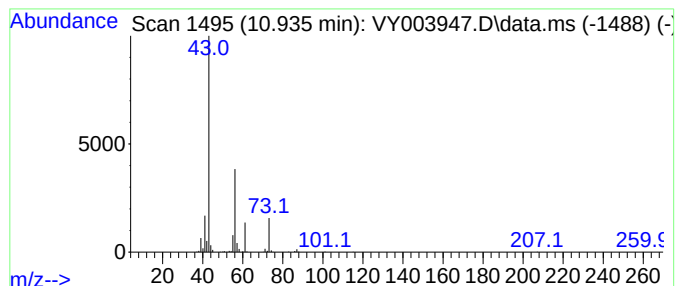
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Acetic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.935	11.05 ug/l	254965	Chlorobenzene-d5	11.496

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	74
2			Isobutyl acetate	116	C6H12O2	000110-19-0	40
3			1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	17
4			Isobutylamine	73	C4H11N	000078-81-9	9
5			Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	9



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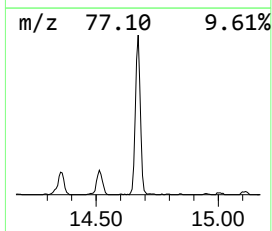
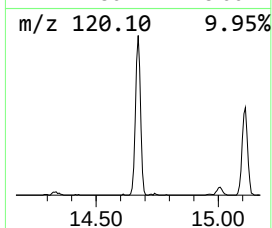
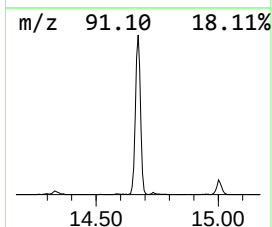
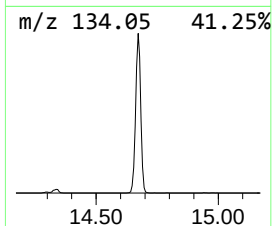
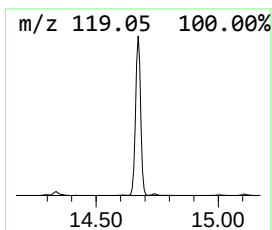
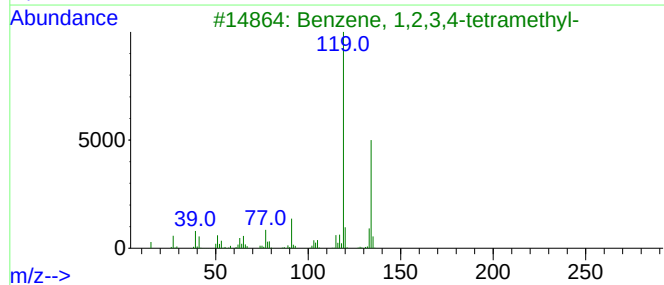
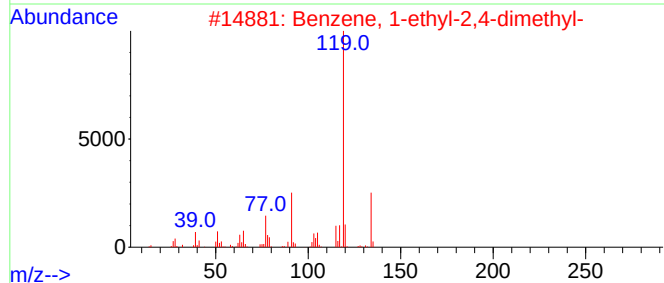
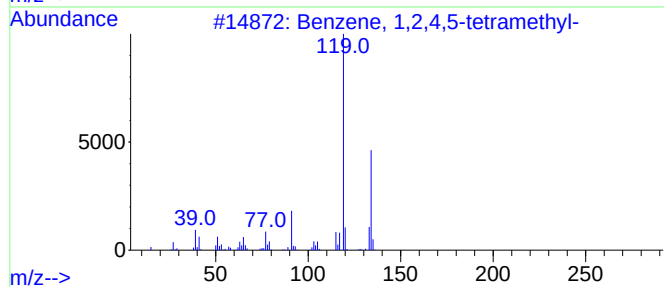
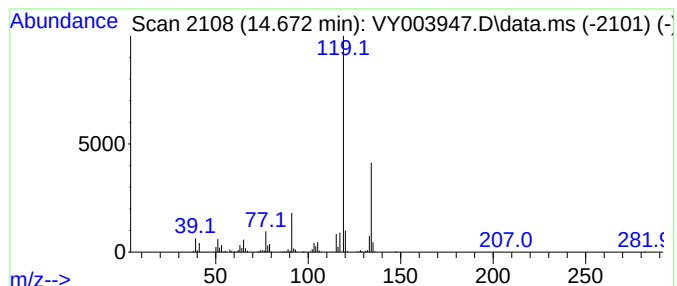
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.672	32.97 ug/l	792422	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-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	95
3			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94
4			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	94
5			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1-nitro-	9.728	7.0	ug/l	54219	2	8.697	387332	50.0
Acetic acid, bu...	10.935	11.0	ug/l	254965	3	11.496	1153840	50.0
Benzene, 1,2,4,...	14.672	33.0	ug/l	792422	4	13.428	1201760	50.0