

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY012721\
 Data File : VY003950.D
 Acq On : 27 Jan 2021 16:19
 Operator : SY/MD
 Sample : VSTDICV050
 Misc : 5.00g/5mL/MSVOA_Y/SOIL
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 ICVVY012721

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: VY003950.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	9	15	27	rVB	86207	121770	7.42%	0.285%
2	2.119	44	49	63	rVB	83581	121158	7.39%	0.283%
3	2.259	65	72	83	rBV	93652	147224	8.97%	0.344%
4	2.662	130	138	152	rVB	88273	177660	10.83%	0.416%
5	2.808	154	162	172	rVB	48013	100555	6.13%	0.235%
6	3.137	207	216	232	rVB	120020	283798	17.30%	0.664%
7	3.540	274	282	296	rVB	66485	157015	9.57%	0.367%
8	3.741	307	315	326	rBV	29299	74194	4.52%	0.174%
9	3.899	328	341	365	rVV3	167637	807961	49.25%	1.890%
10	4.107	365	375	383	rVV	52846	148976	9.08%	0.348%
11	4.204	383	391	405	rVB	89366	246032	15.00%	0.576%
12	4.497	420	439	457	rBV	124500	378268	23.06%	0.885%
13	4.728	465	477	496	rVB2	96989	304923	18.59%	0.713%
14	4.960	500	515	531	rBV3	17761	80253	4.89%	0.188%
15	5.234	538	560	579	rBV2	213078	936712	57.10%	2.191%
16	6.076	679	698	704	rBV2	296238	1155045	70.41%	2.702%
17	6.996	835	849	858	rBV2	329109	937801	57.17%	2.194%
18	7.088	858	864	871	rBV2	64038	176247	10.74%	0.412%
19	7.350	890	907	924	rBV5	176981	593471	36.18%	1.388%
20	7.521	924	935	946	rBV	134099	329223	20.07%	0.770%
21	7.716	955	967	974	rBV2	212641	613917	37.42%	1.436%
22	7.795	974	980	988	rVV2	327460	792128	48.29%	1.853%
23	7.917	988	1000	1013	rVB4	290197	1110579	67.70%	2.598%
24	8.167	1026	1041	1048	rBV3	327204	815541	49.72%	1.908%
25	8.246	1048	1054	1057	rBV	89825	190748	11.63%	0.446%
26	8.697	1113	1128	1136	rBV	176147	345514	21.06%	0.808%
27	8.947	1159	1169	1181	rVB	239733	459303	28.00%	1.074%
28	9.191	1198	1209	1212	rBV	305262	665996	40.60%	1.558%
29	9.301	1221	1227	1233	rBV2	198943	433682	26.44%	1.014%
30	9.362	1233	1237	1248	rVB	93088	158474	9.66%	0.371%
31	9.502	1252	1260	1268	rVB	162760	300744	18.33%	0.703%
32	9.721	1289	1296	1301	rBV	23361	44881	2.74%	0.105%
33	9.789	1301	1307	1315	rVB	435692	717065	43.71%	1.677%
34	9.935	1322	1331	1339	rVB	214665	386490	23.56%	0.904%
35	10.075	1346	1354	1363	rBV	462906	775014	47.24%	1.813%
36	10.185	1363	1372	1377	rVV	372875	652700	39.79%	1.527%

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Integrator: RTE

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Max Peaks: 100

Stop Thrs : 0

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37	10.246	1377	1382	1391	rVB	449038	760250	46.34%	1.778%
38	10.471	1410	1419	1422	rBV	211587	352439	21.48%	0.824%
39	10.514	1422	1426	1432	rVV	176199	268806	16.39%	0.629%
40	10.581	1432	1437	1442	rVV2	42818	77549	4.73%	0.181%
41	10.648	1442	1448	1454	rVV	196460	325829	19.86%	0.762%
42	10.721	1454	1460	1466	rVV	416007	686618	41.86%	1.606%
43	10.794	1466	1472	1475	rVV	181999	307791	18.76%	0.720%
44	10.837	1475	1479	1488	rVB	365559	557834	34.01%	1.305%
45	10.935	1488	1495	1499	rBV	147420	223806	13.64%	0.524%
46	10.990	1499	1504	1510	rVB	154257	261816	15.96%	0.612%
47	11.093	1515	1521	1528	rVB	94068	157756	9.62%	0.369%
48	11.520	1579	1591	1597	rBV2	397735	1037588	63.25%	2.427%
49	11.593	1597	1603	1613	rVV	830893	1305511	79.58%	3.054%
50	11.703	1613	1621	1630	rVV	909360	1634850	99.66%	3.824%
51	12.038	1668	1676	1687	rVB2	753546	1512192	92.18%	3.537%
52	12.148	1687	1694	1699	rBV	202545	300060	18.29%	0.702%
53	12.209	1699	1704	1713	rVB	126913	209202	12.75%	0.489%
54	12.331	1716	1724	1729	rBV	602869	917186	55.91%	2.145%
55	12.380	1729	1732	1738	rVB	123621	183503	11.19%	0.429%
56	12.483	1743	1749	1759	rVB2	364324	631941	38.52%	1.478%
57	12.611	1759	1770	1776	rBV3	463831	1151123	70.17%	2.693%
58	12.672	1776	1780	1787	rVB	587846	875186	53.35%	2.047%
59	12.758	1787	1794	1799	rBV	461595	714700	43.57%	1.672%
60	12.812	1799	1803	1807	rVV	622993	941722	57.41%	2.203%
61	12.855	1807	1810	1817	rVB	472808	688989	42.00%	1.612%
62	13.075	1839	1846	1850	rBV	571709	931417	56.78%	2.179%
63	13.117	1850	1853	1860	rVB2	766792	1196330	72.93%	2.798%
64	13.251	1868	1875	1882	rBV	565113	858197	52.32%	2.007%
65	13.367	1887	1894	1899	rBV	1087040	1640420	100.00%	3.837%
66	13.446	1899	1907	1918	rVB2	495546	1141038	69.56%	2.669%
67	13.696	1942	1948	1952	rBV	627282	918452	55.99%	2.148%
68	13.739	1952	1955	1962	rVB	397442	580437	35.38%	1.358%
69	13.965	1985	1992	2001	rVB	358210	584976	35.66%	1.368%
70	14.361	2049	2057	2063	rVB2	54618	104660	6.38%	0.245%
71	14.672	2101	2108	2115	rVB	547941	796385	48.55%	1.863%
72	15.007	2147	2163	2170	rBV	378908	594764	36.26%	1.391%
73	15.111	2173	2180	2188	rVV	399771	627994	38.28%	1.469%
74	15.239	2193	2201	2207	rBV	255847	432516	26.37%	1.012%
75	15.422	2220	2231	2240	rBV	291983	517083	31.52%	1.210%

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Integrator: RTE
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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

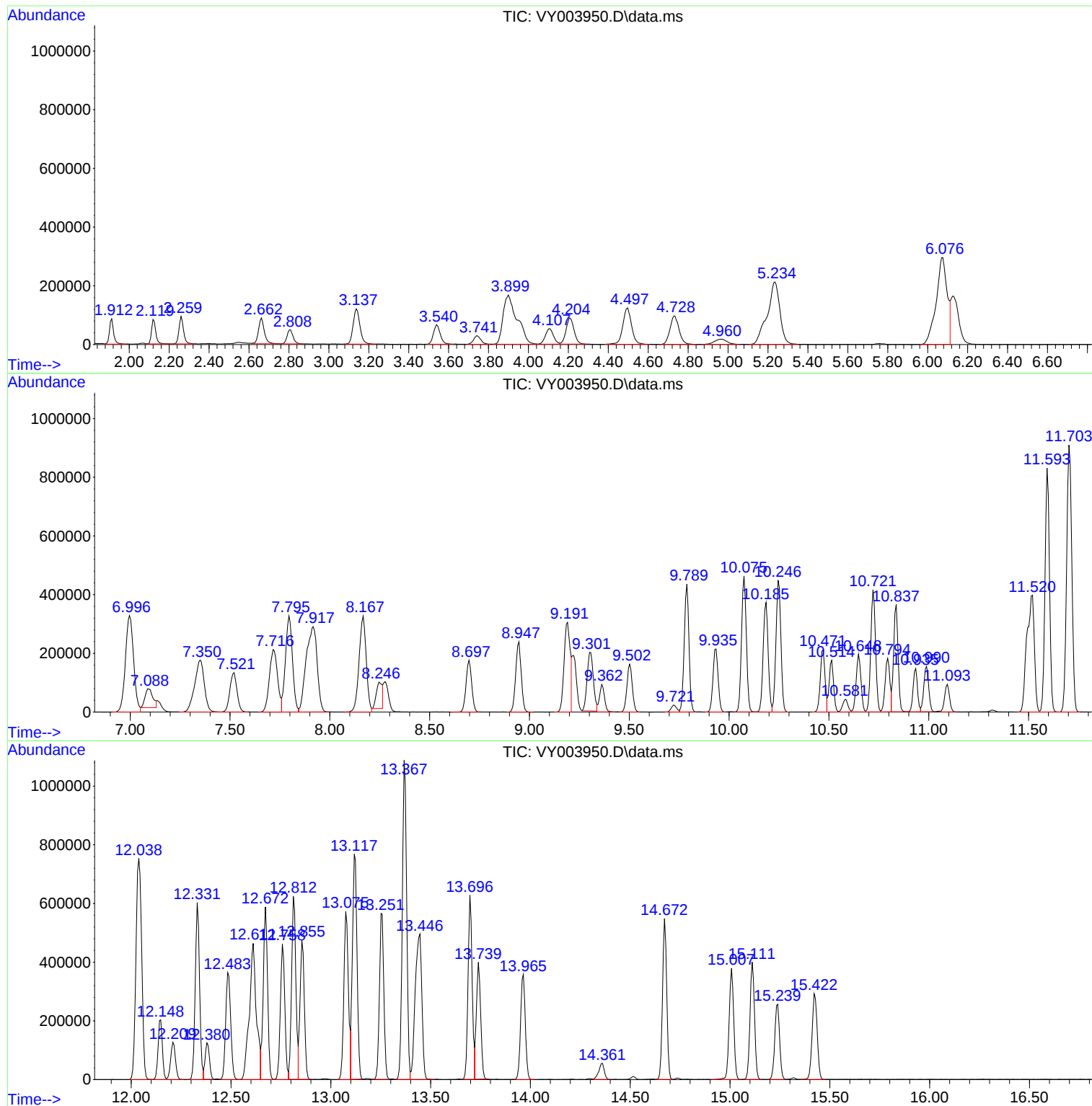
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y012721S.M
Quant Title : SW846 8260

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



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ClientSampleId :
ICVVY012721

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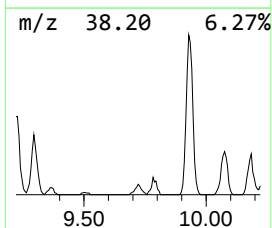
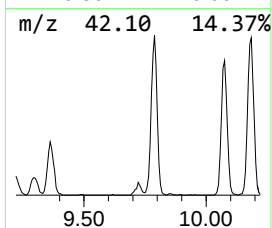
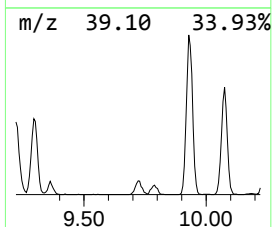
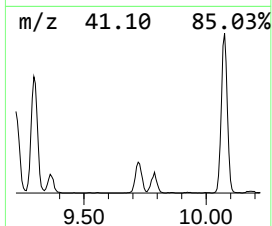
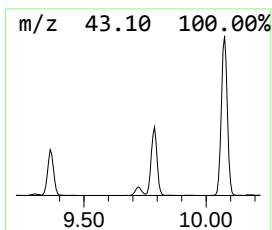
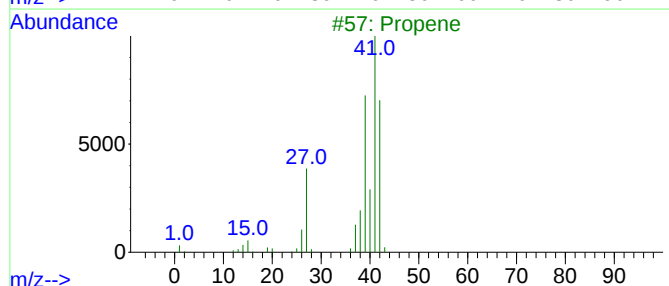
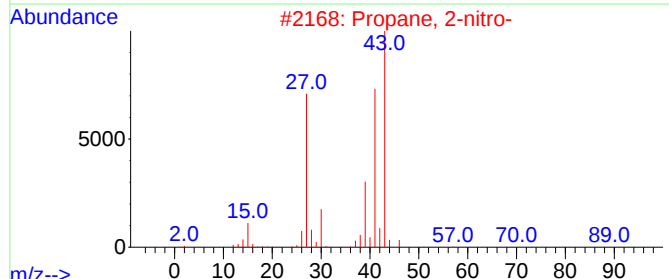
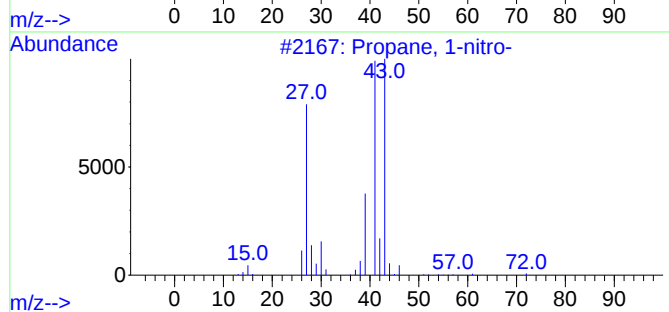
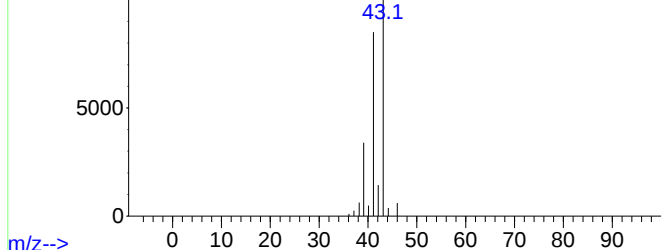
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.721	6.49 ug/l	44881	1,4-Difluorobenzene	8.697

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1-nitro-	89	C3H7NO2	000108-03-2	83
2			Propane, 2-nitro-	89	C3H7NO2	000079-46-9	64
3			Propene	42	C3H6	000115-07-1	9
4			Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	4
5			Hydrogen azide	43	HN3	007782-79-8	4

Abundance Scan 1296 (9.721 min): VY003950.D\data.ms (-1289) (-)



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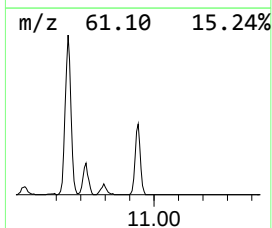
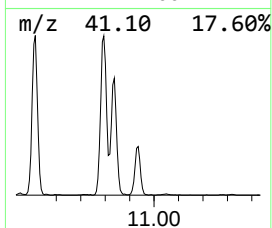
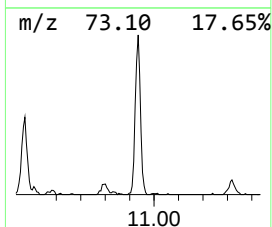
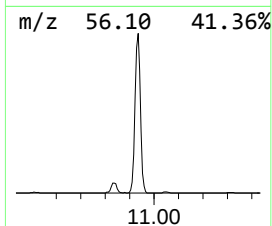
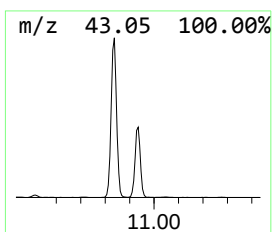
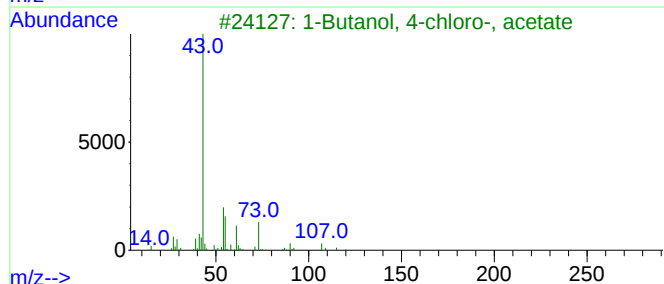
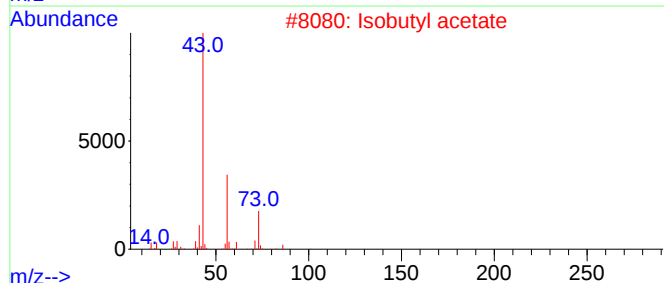
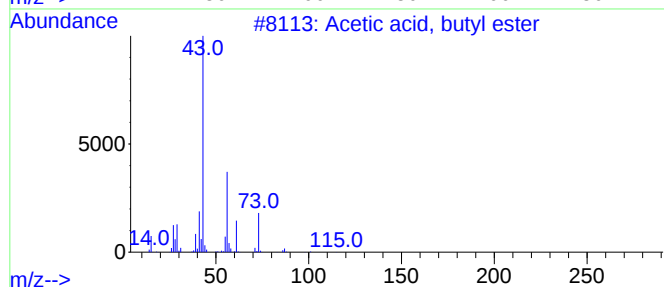
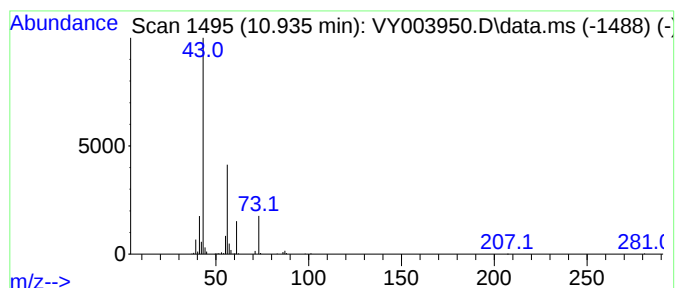
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y012721S.M
Quant Title : SW846 8260

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

Peak Number 2 Acetic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.935	10.78 ug/l	223806	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	39
3			1-Butanol, 4-chloro-, acetate	150	C6H11ClO2	006962-92-1	17
4			Isobutylamine	73	C4H11N	000078-81-9	9
5			2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9



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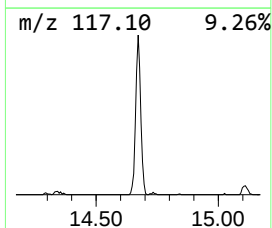
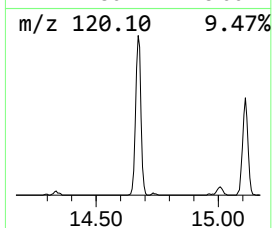
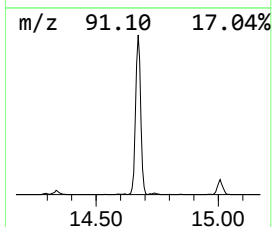
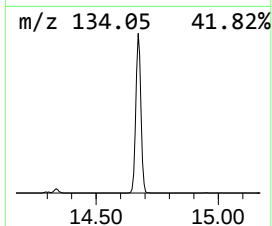
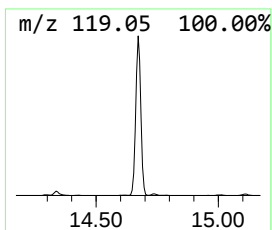
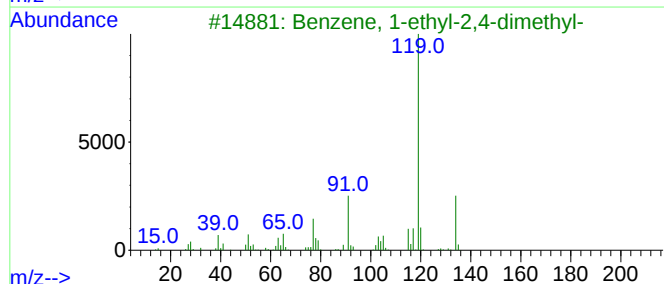
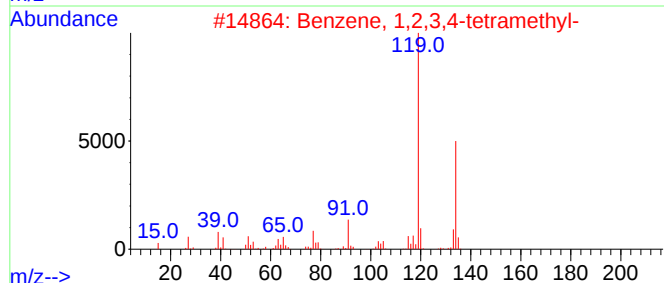
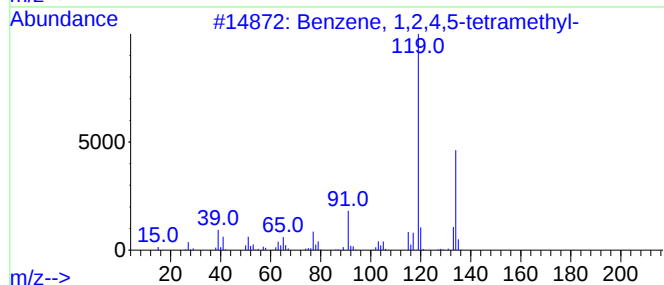
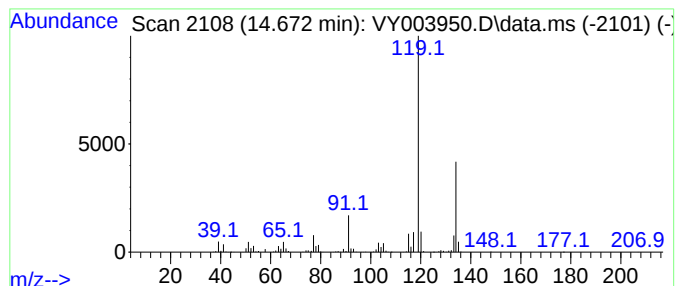
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.672	34.90 ug/l	796385	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	94
4			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	94
5			o-Cymene	134	C10H14	000527-84-4	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1-nitro-	9.721	6.5	ug/l	44881	2	8.697	345514	50.0
Acetic acid, bu...	10.935	10.8	ug/l	223806	3	11.496	1037590	50.0
Benzene, 1,2,4,...	14.672	34.9	ug/l	796385	4	13.428	1141040	50.0