

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
 Data File : VU045016.D
 Acq On : 30 Sep 2021 01:06
 Operator : SY/MD
 Sample : VU0929WBSD02
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VU0929WBSD02

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_U\Method\82U092821W.M
 Title : SW846 8260

Signal : TIC: VU045016.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.385	7	14	32	rVB	67471	73512	3.78%	0.208%
2	1.520	49	56	68	rVB	73540	82305	4.23%	0.233%
3	1.604	75	82	90	rBV	82815	91959	4.73%	0.261%
4	1.684	99	107	116	rBV	54508	62645	3.22%	0.178%
5	1.832	146	153	169	rVB	63206	76732	3.95%	0.218%
6	1.916	171	179	193	rVB	52920	74618	3.84%	0.212%
7	2.128	235	245	265	rVB	113948	176041	9.05%	0.499%
8	2.379	312	323	338	rVB	96014	141914	7.30%	0.402%
9	2.488	345	357	368	rBV	18436	29285	1.51%	0.083%
10	2.578	371	385	394	rBV2	214504	378416	19.46%	1.073%
11	2.629	394	401	418	rVB	126042	212275	10.92%	0.602%
12	2.719	418	429	441	rBV	38896	67166	3.45%	0.190%
13	2.793	441	452	468	rVB	83231	144613	7.44%	0.410%
14	2.925	472	493	497	rBV	109351	210136	10.81%	0.596%
15	3.047	518	531	557	rVB	106592	210439	10.82%	0.597%
16	3.199	557	578	601	rBV2	50753	135063	6.94%	0.383%
17	3.318	601	615	621	rVV	190247	385734	19.83%	1.094%
18	3.359	622	628	657	rVB2	224157	511457	26.30%	1.450%
19	3.874	771	788	800	rBV	76568	179800	9.25%	0.510%
20	3.961	800	815	861	rVB2	302467	1059954	54.50%	3.005%
21	4.671	1018	1036	1041	rBV	184042	413689	21.27%	1.173%
22	4.777	1058	1069	1085	rBV2	103338	305464	15.71%	0.866%
23	4.977	1116	1131	1144	rBV2	155021	338233	17.39%	0.959%
24	5.054	1144	1155	1184	rVB3	210651	683702	35.16%	1.939%
25	5.295	1213	1230	1245	rBV2	186883	566323	29.12%	1.606%
26	5.378	1245	1256	1272	rVV3	370084	876084	45.05%	2.484%
27	5.462	1272	1282	1291	rVV	112482	226875	11.67%	0.643%
28	5.526	1291	1302	1325	rVB	206461	438207	22.53%	1.242%
29	5.706	1342	1358	1369	rBV	196831	408760	21.02%	1.159%
30	5.780	1369	1381	1405	rVV3	237774	600789	30.89%	1.703%
31	5.915	1409	1423	1445	rVV	117841	233991	12.03%	0.663%
32	6.253	1512	1528	1548	rBV	407022	765043	39.34%	2.169%
33	6.546	1606	1619	1635	rBV	143138	265401	13.65%	0.753%
34	6.768	1671	1688	1716	rBV4	196135	619511	31.86%	1.757%
35	6.922	1721	1736	1742	rBV	89061	163838	8.42%	0.465%
36	6.964	1742	1749	1763	rVV2	171250	301503	15.50%	0.855%

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Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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37	7.044	1763	1774	1783	rVV	119231	209069	10.75%	0.593%
38	7.108	1784	1794	1817	rVB	116978	239358	12.31%	0.679%
39	7.369	1862	1875	1891	rBV	36189	69886	3.59%	0.198%
40	7.465	1892	1905	1925	rVB	303007	503889	25.91%	1.429%
41	7.610	1937	1950	1967	rBV	142960	243750	12.53%	0.691%
42	7.796	1990	2008	2027	rBV	712607	1247952	64.17%	3.538%
43	7.899	2027	2040	2052	rVV	645705	1111150	57.14%	3.150%
44	7.973	2052	2063	2087	rVB	296796	501419	25.78%	1.422%
45	8.214	2122	2138	2152	rBV	141019	234416	12.05%	0.665%
46	8.337	2164	2176	2186	rBV	172588	271956	13.98%	0.771%
47	8.404	2186	2197	2209	rVB	168374	282759	14.54%	0.802%
48	8.558	2231	2245	2264	rBV2	225250	607772	31.25%	1.723%
49	8.690	2273	2286	2312	rBV	558502	942663	48.47%	2.673%
50	8.835	2313	2331	2348	rVV2	190193	449044	23.09%	1.273%
51	8.928	2348	2360	2380	rVB	81033	138675	7.13%	0.393%
52	9.420	2499	2513	2520	rBV	601208	1069070	54.97%	3.031%
53	9.539	2538	2550	2554	rBV	172330	277426	14.27%	0.787%
54	9.574	2554	2561	2584	rVB	339432	540983	27.82%	1.534%
55	9.697	2584	2599	2619	rBV	657202	1065094	54.77%	3.020%
56	10.108	2713	2727	2744	rBV5	516772	1027022	52.81%	2.912%
57	10.295	2769	2785	2787	rBV	88036	112550	5.79%	0.319%
58	10.324	2788	2794	2818	rVB	206685	336573	17.31%	0.954%
59	10.488	2830	2845	2855	rBV	366868	571748	29.40%	1.621%
60	10.549	2855	2864	2879	rVV	122633	196679	10.11%	0.558%
61	10.636	2879	2891	2917	rVB	489181	765852	39.38%	2.171%
62	10.787	2924	2938	2945	rBV	407370	663465	34.12%	1.881%
63	10.828	2945	2951	2966	rVV2	214709	464941	23.91%	1.318%
64	10.909	2966	2976	2989	rVV	371046	565688	29.09%	1.604%
65	10.989	2989	3001	3015	rVV	314146	488341	25.11%	1.385%
66	11.095	3021	3034	3052	rVB4	612487	1048260	53.90%	2.972%
67	11.426	3122	3137	3144	rBV2	473520	824737	42.41%	2.338%
68	11.472	3144	3151	3168	rVB	368045	574566	29.54%	1.629%
69	11.645	3188	3205	3221	rBV	372901	581219	29.89%	1.648%
70	11.748	3226	3237	3244	rVV	270634	418515	21.52%	1.187%
71	11.812	3244	3257	3282	rVB4	711219	1944779	100.00%	5.514%
72	12.214	3367	3382	3400	rBV2	594205	923497	47.49%	2.618%
73	12.478	3453	3464	3477	rVB2	170708	279024	14.35%	0.791%
74	12.999	3611	3626	3647	rBV2	85043	147743	7.60%	0.419%
75	13.449	3747	3766	3782	rBV	341948	520257	26.75%	1.475%
76	13.844	3877	3889	3909	rVB	201719	315882	16.24%	0.896%

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ALS Vial : 35 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VU0929WBSD02

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	14.024	3933	3945	3955	rBV2	140515	216687	11.14%	0.614%
78	14.089	3955	3965	3981	rVB	277641	441899	22.72%	1.253%
79	14.333	4029	4041	4055	rBV	199878	321491	16.53%	0.912%

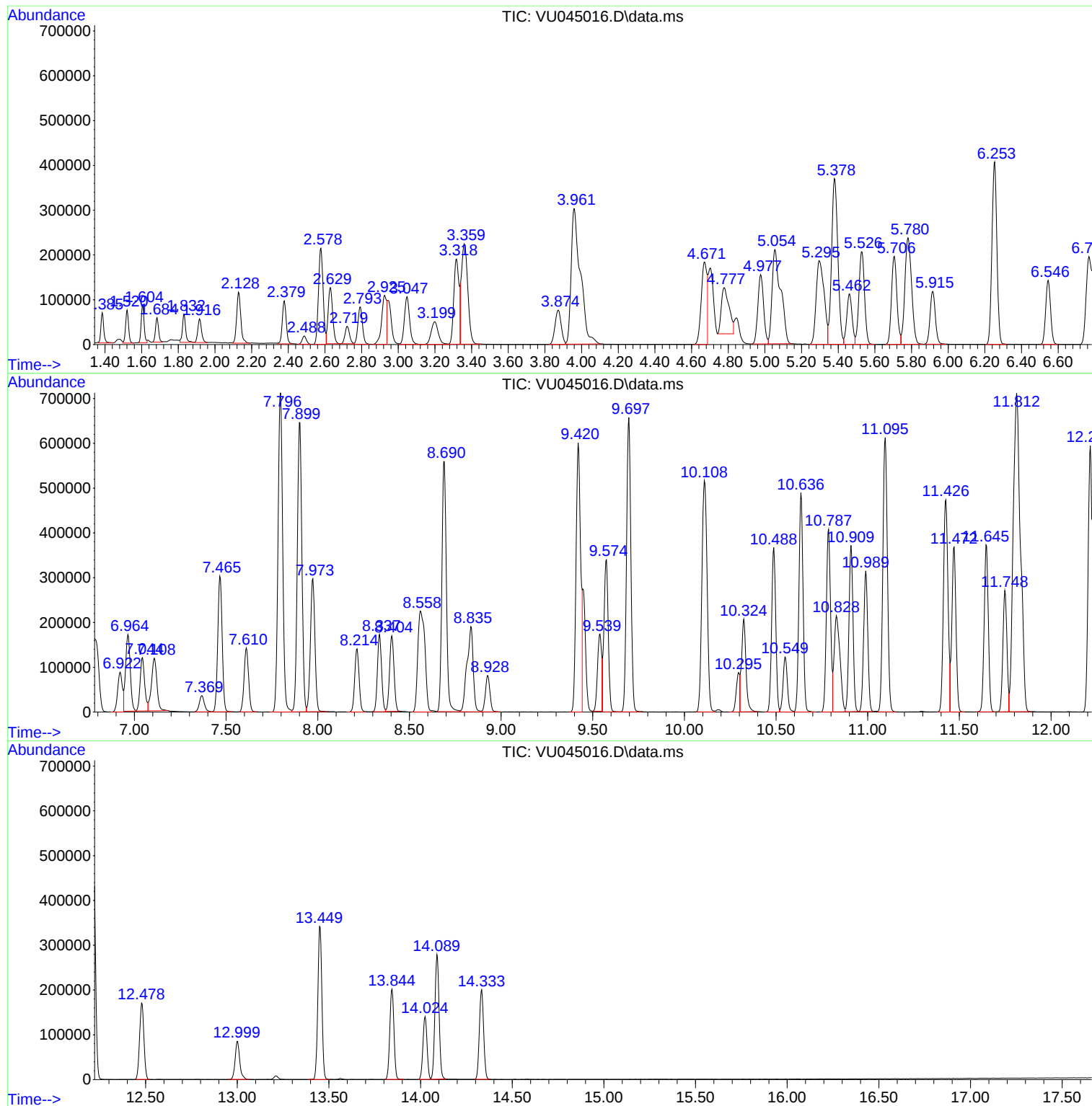
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Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092921\
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VU0929WBSD02

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Operator : SY/MD
Sample : VU0929WBSD02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 35 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VU0929WBSD02

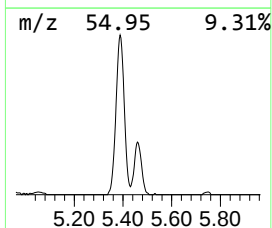
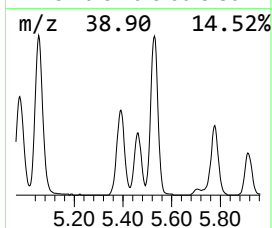
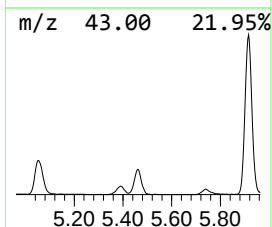
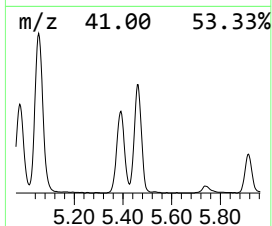
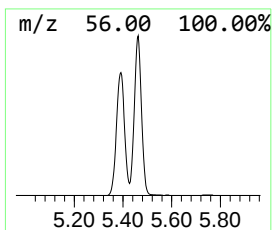
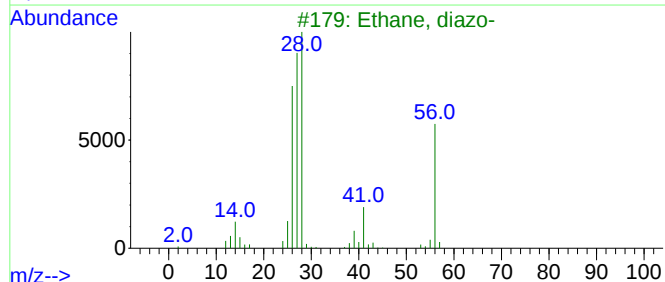
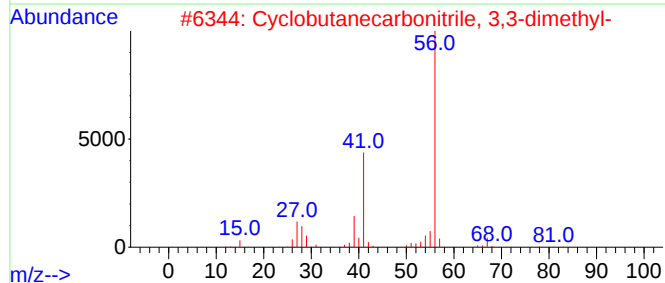
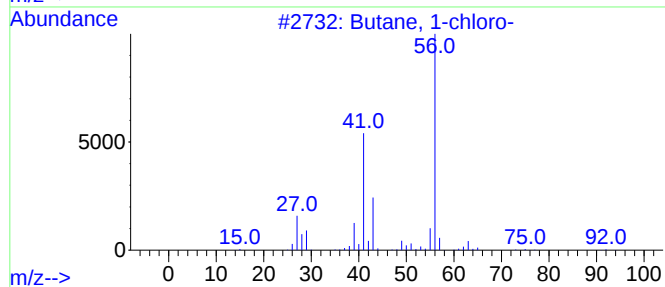
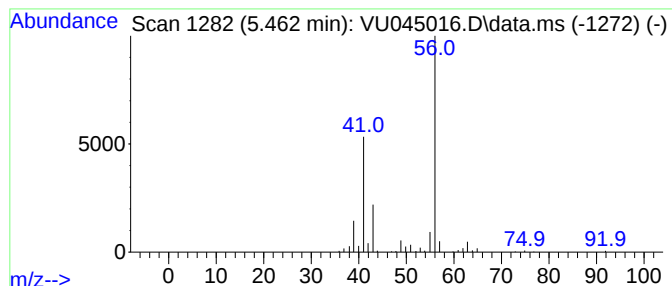
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 1-chloro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.462	12.95 ug/l	226875	Pentafluorobenzene	5.375

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 1-chloro-	92	C4H9Cl	000109-69-3	91
2			Cyclobutanecarbonitrile, 3,3-dimethyl-	109	C7H11N	053783-86-1	72
3			Ethane, diazo-	56	C2H4N2	001117-96-0	45
4			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	39
5			Cyclobutane, ethyl-	84	C6H12	004806-61-5	39



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ALS Vial : 35 Sample Multiplier: 1

Instrument :
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ClientSampleId :
VU0929WBSD02

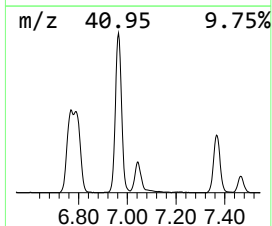
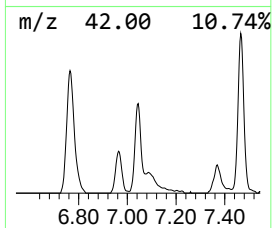
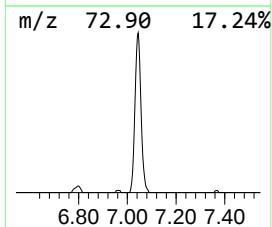
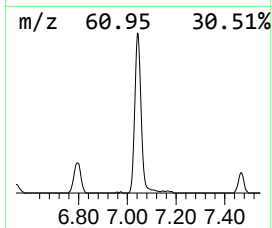
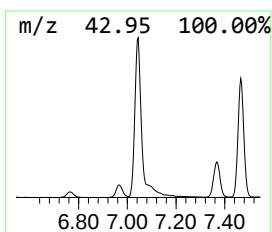
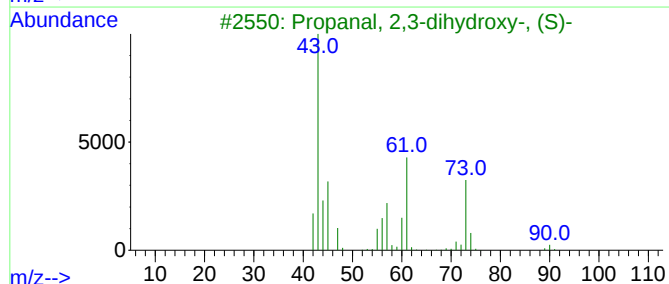
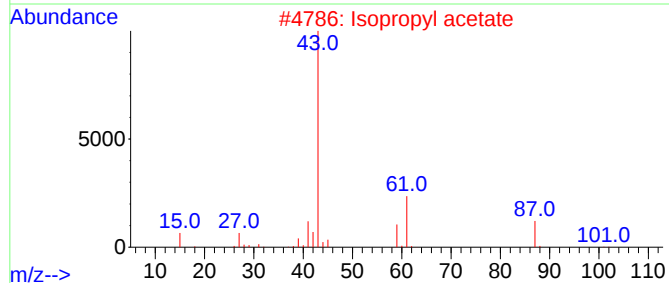
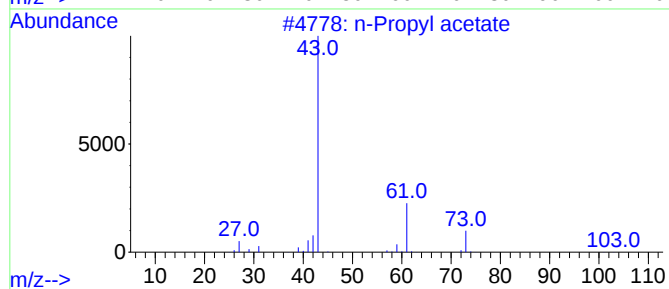
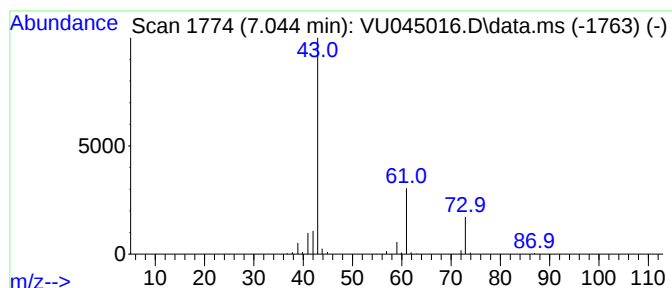
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.044	13.66 ug/l	209069	1,4-Difluorobenzene	6.253

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Propyl acetate	102	C5H10O2	000109-60-4	83
2			Isopropyl acetate	102	C5H10O2	000108-21-4	36
3			Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	36
4			Isobutyl acetate	116	C6H12O2	000110-19-0	9
5			1-Butanamine	73	C4H11N	000109-73-9	7



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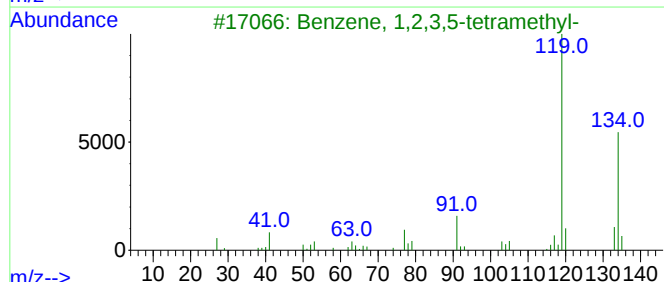
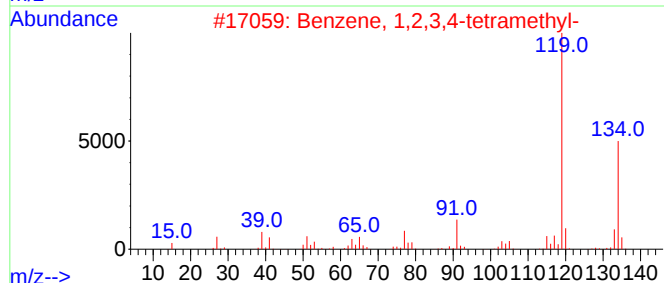
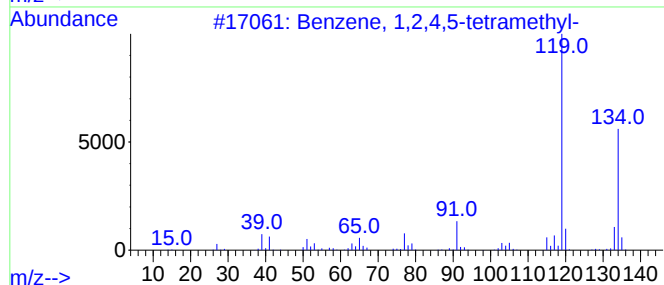
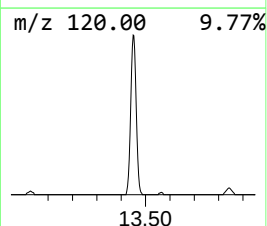
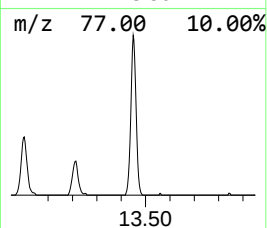
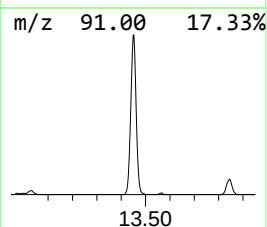
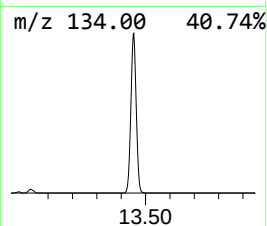
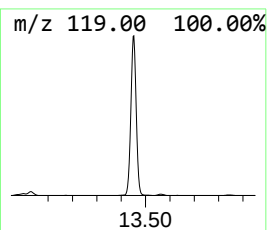
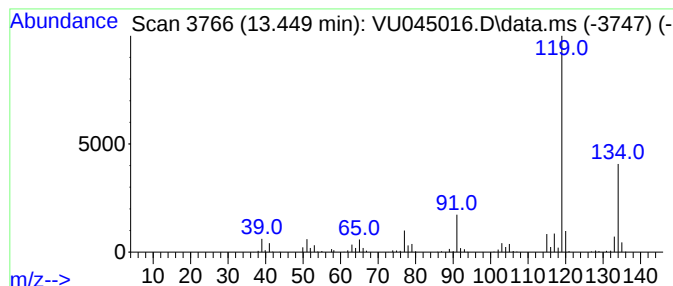
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092821W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.449	13.38 ug/l	520257	1,4-Dichlorobenzene-d4	11.816

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, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
4			o-Cymene	134	C10H14	000527-84-4	95
5			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	94



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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 1-chloro-	5.462	12.9	ug/l	226875	1	5.375	876084	50.0
n-Propyl acetate	7.044	13.7	ug/l	209069	2	6.253	765043	50.0
Benzene, 1,2,4,...	13.449	13.4	ug/l	520257	4	11.816	1944780	50.0