

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU111318\
 Data File : VU028096.D
 Acq On : 13 Nov 2018 16:54
 Operator : MD/SY
 Sample : J5921-02
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 SP-TANK1-N29675

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\82U110218W.M

Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.286	28	35	52	rBV	869663	807007	36.88%	3.008%
2	1.386	60	66	77	rBV	27669	29413	1.34%	0.110%
3	1.473	87	93	101	rBV	28957	28828	1.32%	0.107%
4	2.321	344	357	381	rBV	674527	1072982	49.04%	4.000%
5	2.453	387	398	421	rVB	47555	93032	4.25%	0.347%
6	2.836	506	517	536	rVB2	26400	61028	2.79%	0.227%
7	3.000	554	568	589	rVB2	164132	360762	16.49%	1.345%
8	3.997	860	878	889	rBV6	9232	25282	1.16%	0.094%
9	4.093	895	908	927	rVB6	11208	31465	1.44%	0.117%
10	4.263	948	961	994	rVB	208240	514161	23.50%	1.917%
11	4.636	1051	1077	1113	rBV	916725	2188058	100.00%	8.156%
12	4.884	1134	1154	1170	rBV	220398	500927	22.89%	1.867%
13	4.984	1171	1185	1209	rVB	370436	831827	38.02%	3.101%
14	5.308	1271	1286	1300	rBV	260113	548036	25.05%	2.043%
15	5.392	1300	1312	1330	rVB	218156	472716	21.60%	1.762%
16	5.787	1421	1435	1452	rBV	134283	284481	13.00%	1.060%
17	5.887	1452	1466	1497	rVB	576462	1141626	52.18%	4.256%
18	6.029	1497	1510	1538	rBV	63680	138352	6.32%	0.516%
19	6.267	1568	1584	1596	rBV3	16621	35009	1.60%	0.131%
20	6.421	1616	1632	1653	rBV2	68568	146985	6.72%	0.548%
21	6.826	1737	1758	1771	rBV3	19716	52230	2.39%	0.195%
22	7.373	1920	1928	1941	rVB3	15756	28687	1.31%	0.107%
23	7.463	1943	1956	1974	rBV2	56208	110254	5.04%	0.411%
24	7.566	1974	1988	2000	rVV	937141	1621163	74.09%	6.043%
25	7.636	2000	2010	2023	rVV	891687	1533412	70.08%	5.716%
26	7.704	2023	2031	2043	rVV2	49781	97582	4.46%	0.364%
27	7.768	2044	2051	2068	rVB3	17018	31269	1.43%	0.117%
28	7.865	2068	2081	2092	rBV4	18943	40258	1.84%	0.150%
29	7.955	2101	2109	2122	rVB3	26006	49419	2.26%	0.184%
30	8.167	2164	2175	2186	rVV	42555	77743	3.55%	0.290%
31	8.231	2186	2195	2214	rVB2	43073	76987	3.52%	0.287%
32	8.366	2227	2237	2251	rBV2	88744	157768	7.21%	0.588%
33	8.482	2264	2273	2289	rVB5	27801	64533	2.95%	0.241%
34	8.958	2409	2421	2422	rBV2	28463	38098	1.74%	0.142%

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35	9.032	2437	2444	2451	rBV3	21504	41016	1.87%	0.153%
36	9.090	2451	2462	2473	rBV	792571	1251023	57.18%	4.663%
37	9.218	2494	2502	2504	rBV4	24276	29320	1.34%	0.109%
38	9.254	2505	2513	2521	rVV2	155459	251163	11.48%	0.936%
39	9.373	2539	2550	2563	rVB	1252458	2043714	93.40%	7.618%
40	9.453	2563	2575	2583	rBV3	70279	172398	7.88%	0.643%
41	9.601	2609	2621	2636	rBV2	50722	102529	4.69%	0.382%
42	9.726	2648	2660	2665	rBV9	12607	24072	1.10%	0.090%
43	9.778	2665	2676	2686	rBV	834363	1319995	60.33%	4.921%
44	9.919	2711	2720	2734	rBV	123912	203670	9.31%	0.759%
45	10.067	2753	2766	2779	rVB5	54154	133148	6.09%	0.496%
46	10.144	2780	2790	2806	rVB8	47823	112956	5.16%	0.421%
47	10.225	2806	2815	2824	rBV4	18311	31278	1.43%	0.117%
48	10.308	2825	2841	2855	rBV	638987	1093900	49.99%	4.078%
49	10.392	2857	2867	2869	rBV6	31802	48931	2.24%	0.182%
50	10.488	2890	2897	2908	rBV5	51076	108581	4.96%	0.405%
51	10.575	2918	2924	2934	rVB3	60503	101808	4.65%	0.380%
52	10.681	2942	2957	2972	rBV	250421	537943	24.59%	2.005%
53	10.771	2978	2985	3002	rVB2	186585	332460	15.19%	1.239%
54	10.897	3018	3024	3032	rVB7	38326	58267	2.66%	0.217%
55	10.971	3033	3047	3057	rBV4	177537	360783	16.49%	1.345%
56	11.080	3072	3081	3088	rBV3	31596	56213	2.57%	0.210%
57	11.147	3092	3102	3114	rVV	612280	936486	42.80%	3.491%
58	11.257	3127	3136	3148	rBV3	88999	155044	7.09%	0.578%
59	11.421	3174	3187	3197	rBV	201744	376962	17.23%	1.405%
60	11.482	3197	3206	3217	rBV	721504	1113780	50.90%	4.152%
61	11.572	3225	3234	3242	rBV	218384	311283	14.23%	1.160%
62	11.765	3281	3294	3315	rBV3	119438	339424	15.51%	1.265%
63	11.880	3322	3330	3336	rBV7	63241	104531	4.78%	0.390%
64	12.028	3370	3376	3379	rBV4	31582	39903	1.82%	0.149%
65	12.061	3382	3386	3398	rVB3	92708	129871	5.94%	0.484%
66	12.141	3399	3411	3417	rBV6	51864	115897	5.30%	0.432%
67	12.183	3418	3424	3437	rVB5	56330	92041	4.21%	0.343%
68	12.250	3440	3445	3451	rVB2	32616	39153	1.79%	0.146%
69	12.295	3453	3459	3468	rVB6	31398	51190	2.34%	0.191%
70	12.356	3472	3478	3486	rBV3	28300	37167	1.70%	0.139%
71	12.459	3500	3510	3524	rBV10	39126	108213	4.95%	0.403%

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72	12.649	3563	3569	3576	rVB	29123	39329	1.80%	0.147%
73	12.704	3579	3586	3595	rVB	49792	82198	3.76%	0.306%
74	12.961	3662	3666	3674	rVB	25654	32354	1.48%	0.121%
75	13.122	3708	3716	3726	rVB3	77292	120779	5.52%	0.450%
76	13.192	3732	3738	3748	rVB3	38132	56033	2.56%	0.209%
77	13.298	3764	3771	3785	rVB8	31404	67077	3.07%	0.250%
78	13.517	3832	3839	3846	rBV6	27487	45002	2.06%	0.168%
79	13.665	3878	3885	3895	rVB2	55487	81914	3.74%	0.305%
80	13.742	3900	3909	3921	rVB	209684	321789	14.71%	1.200%
81	13.861	3941	3946	3967	rVB3	40597	99155	4.53%	0.370%
82	14.292	4074	4080	4089	rVB3	18409	26670	1.22%	0.099%
83	14.408	4107	4116	4133	rBV3	28146	54125	2.47%	0.202%
84	14.726	4208	4215	4224	rBV2	21296	31322	1.43%	0.117%
85	14.877	4255	4262	4281	rVB4	33811	65699	3.00%	0.245%
86	15.064	4313	4320	4332	rVB5	26686	45321	2.07%	0.169%

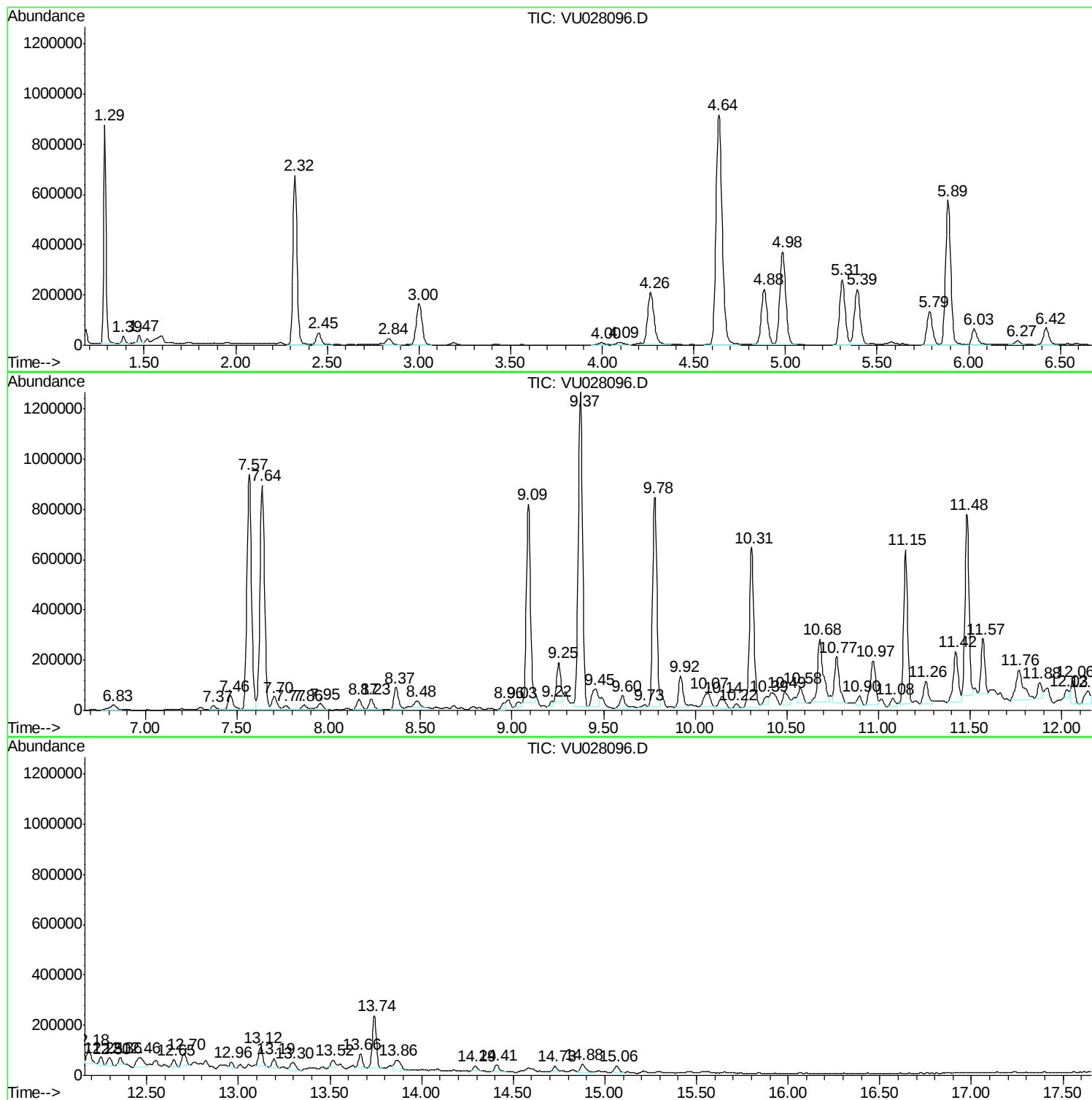
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\82U110218W.M
Quant Title : SW846 8260

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



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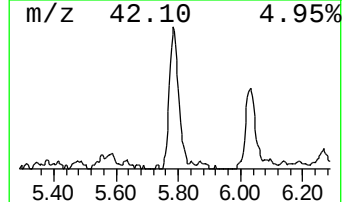
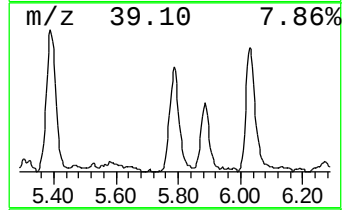
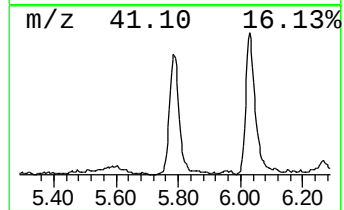
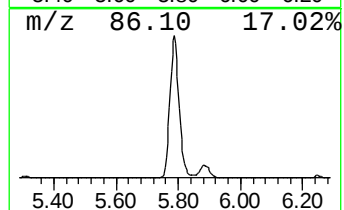
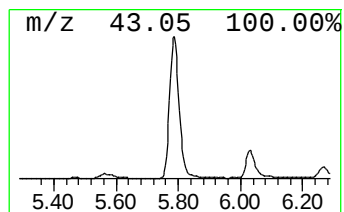
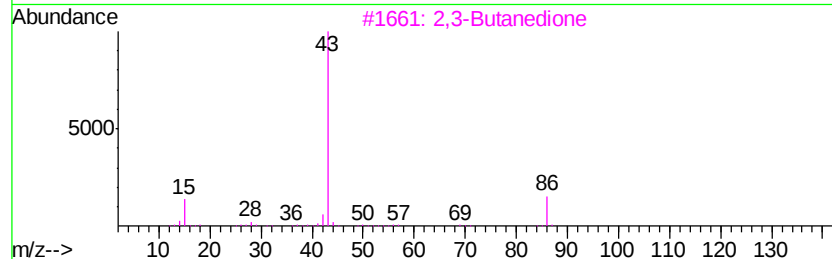
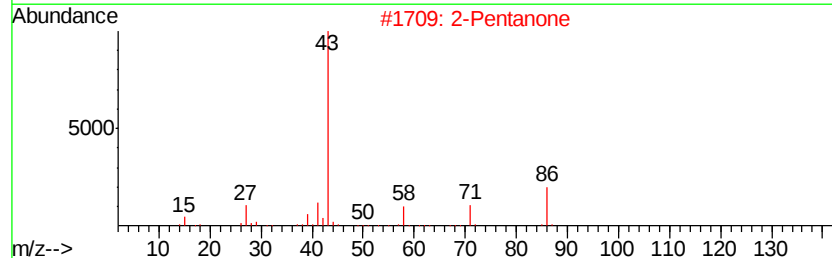
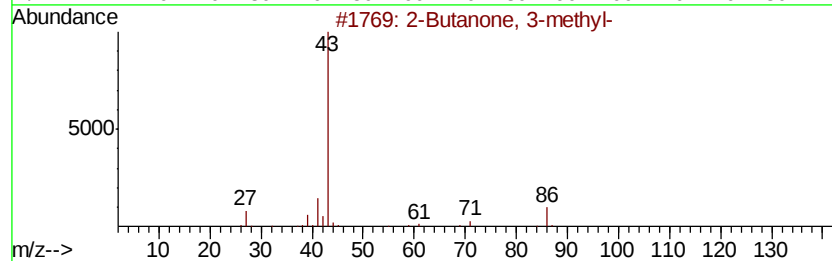
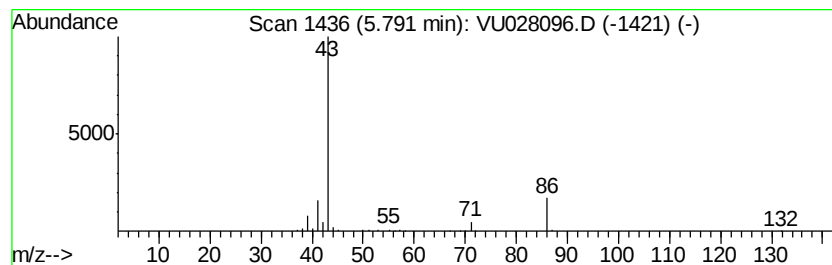
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\82U110218W.M
Quant Title : SW846 8260

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

Peak Number 2 2-Butanone, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.79	12.46 ug/l	284481	1,4-Difluorobenzene	5.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	72
2		2-Pentanone	86	C5H10O	000107-87-9	64
3		2,3-Butanedione	86	C4H6O2	000431-03-8	53
4		2-Pentanone, 3-ethyl-	114	C7H14O	006137-03-7	9
5		Acetic acid ethenyl ester	86	C4H6O2	000108-05-4	7



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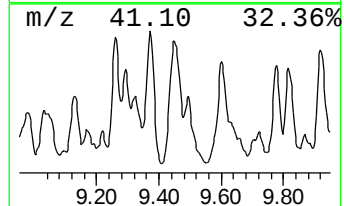
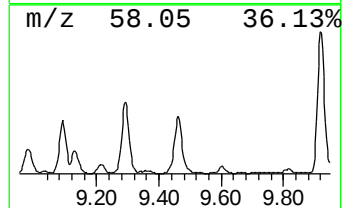
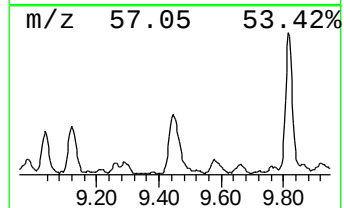
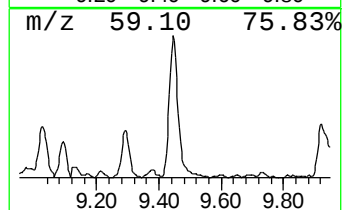
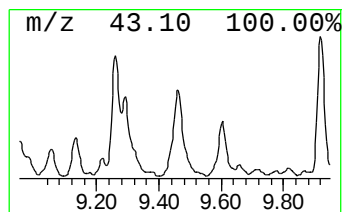
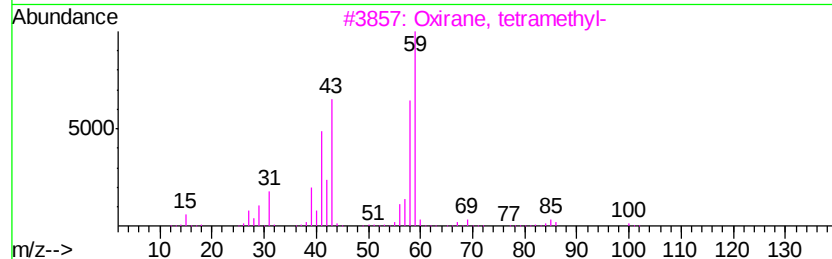
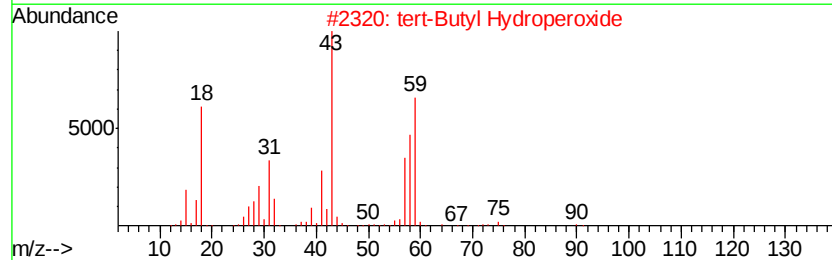
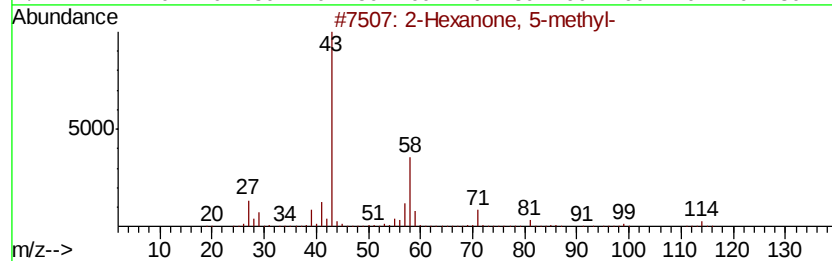
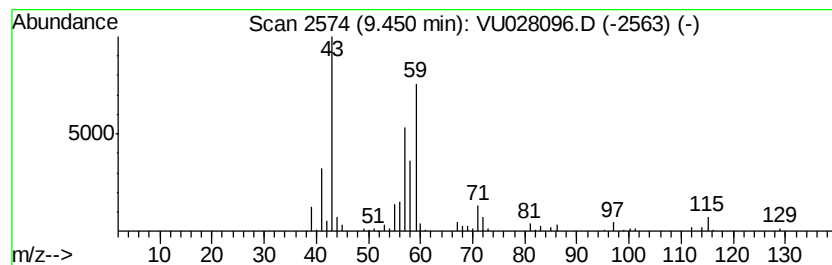
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown9.45 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.45	6.89 ug/l	172398	Chlorobenzene-d5	9.09

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	43
2			tert-Butyl Hydroperoxide	90	C4H10O2	000075-91-2	42
3			Oxirane, tetramethyl-	100	C6H12O	005076-20-0	38
4			2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	32
5			2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	28



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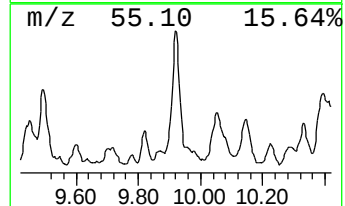
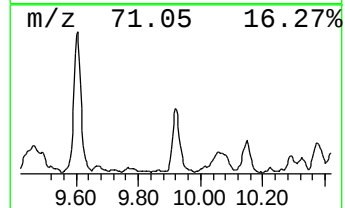
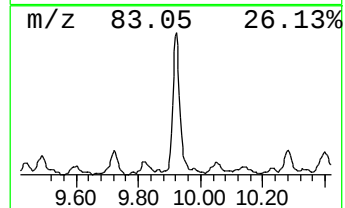
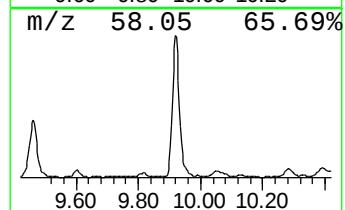
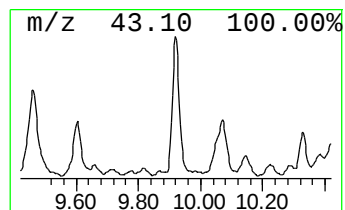
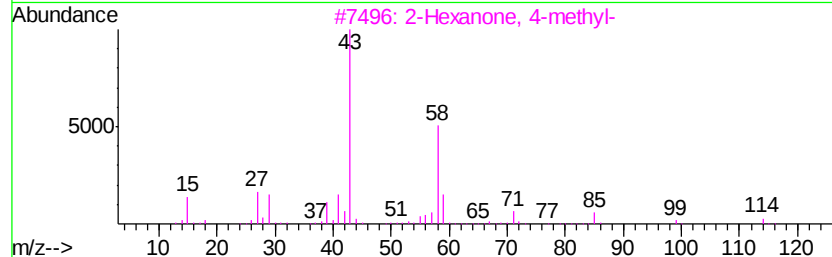
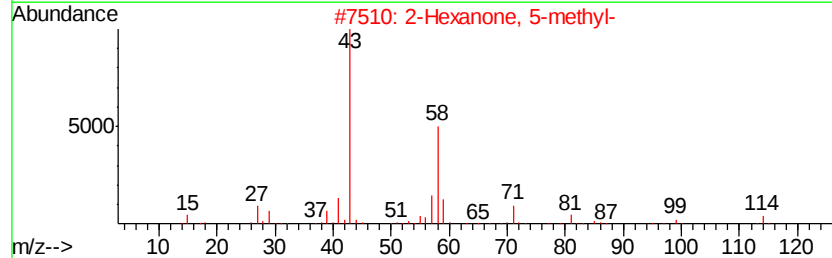
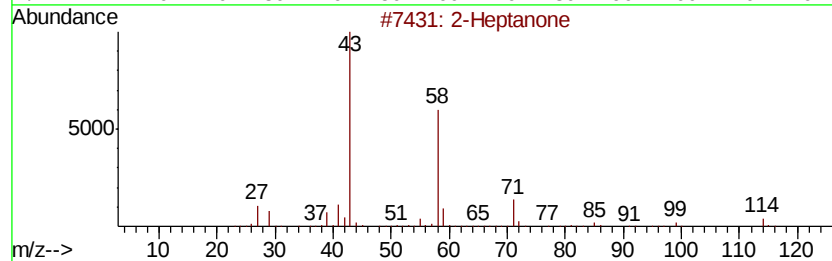
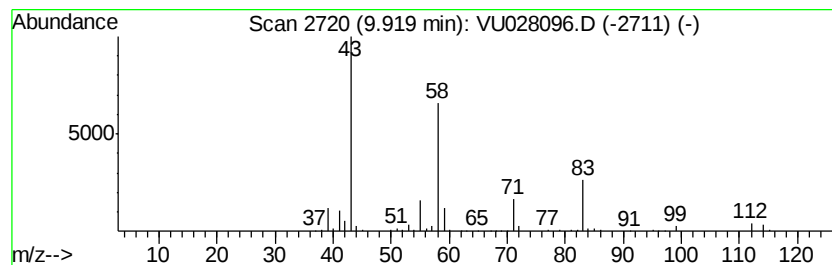
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\82U110218W.M
Quant Title : SW846 8260

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

Peak Number 4 2-Heptanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.92	8.14 ug/l	203670	Chlorobenzene-d5	9.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Heptanone	114	C7H14O	000110-43-0	64
2		2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	59
3		2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	42
4		2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	33
5		2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	32



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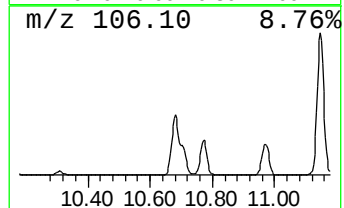
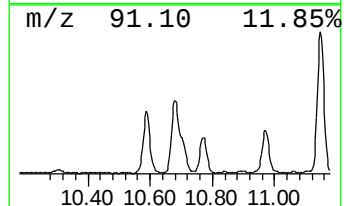
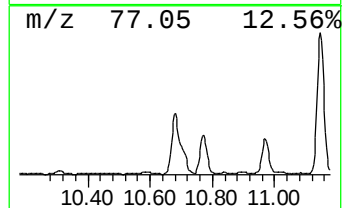
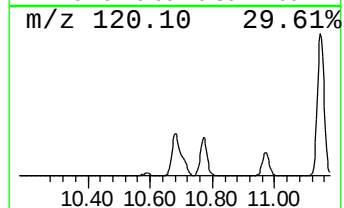
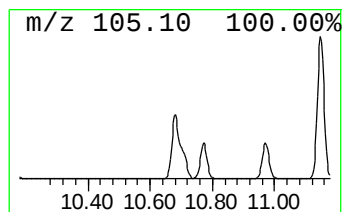
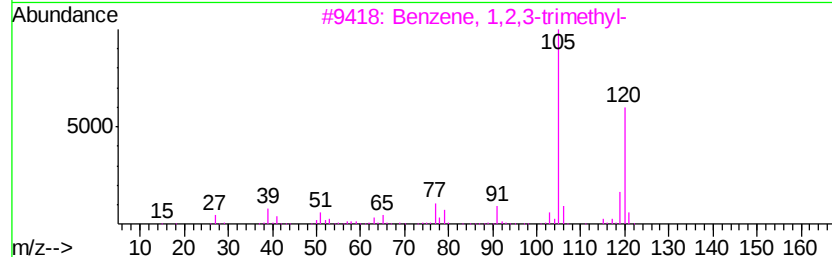
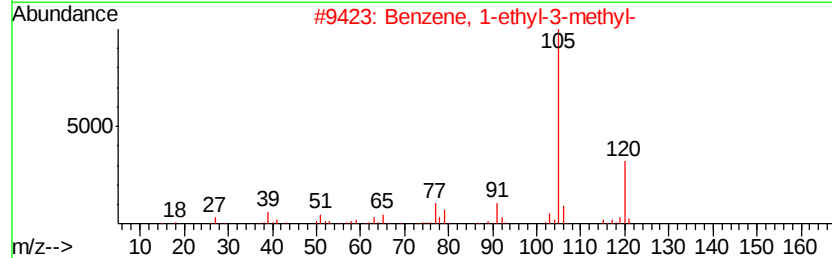
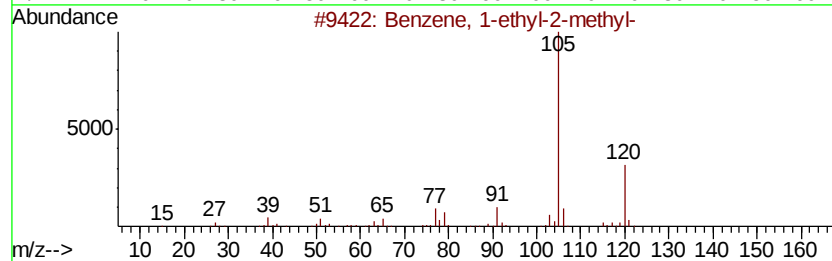
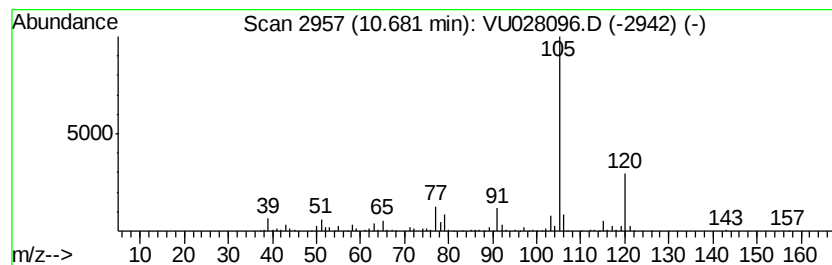
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.68	24.15 ug/l	537943	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU111318\
Data File : VU028096.D
Acq On : 13 Nov 2018 16:54
Operator : MD/SY
Sample : J5921-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 17 Sample Multiplier: 1

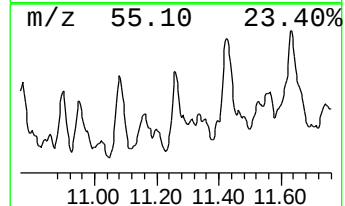
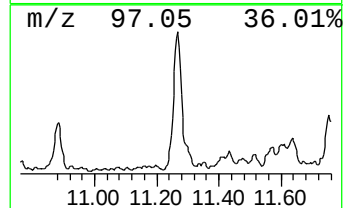
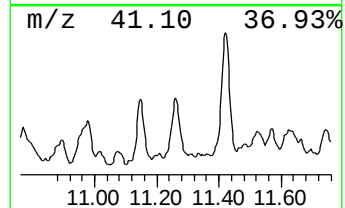
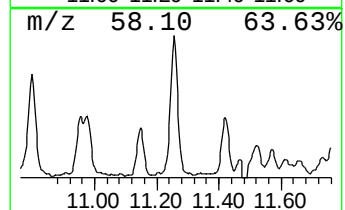
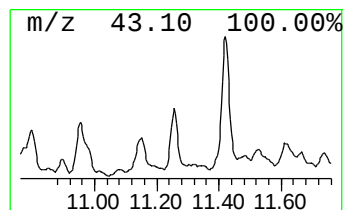
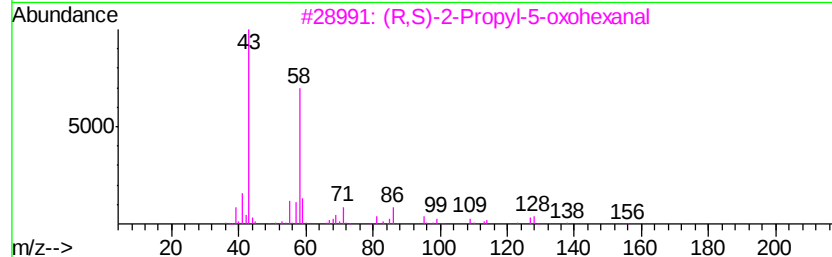
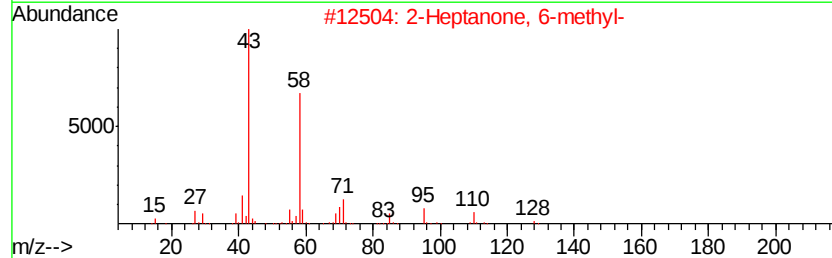
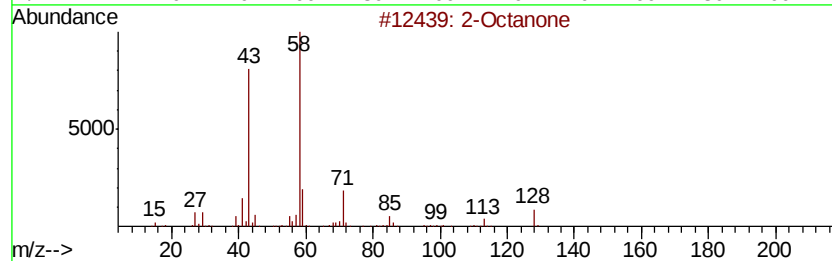
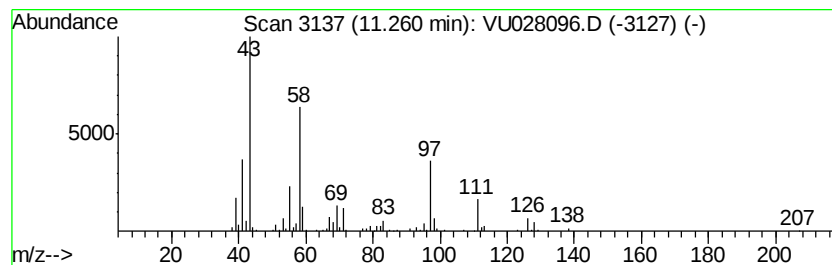
Instrument :
MSVOA_U
ClientSampleId :
SP-TANK1-N29675

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\82U110218W.M
Quant Title : SW846 8260

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

Peak Number 7 unknown11.26 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.26	6.96 ug/l	155044	1,4-Dichlorobenzene-d4	11.48	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanone	128	C8H16O	000111-13-7	46
2	2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	43
3	(R,S)-2-Propyl-5-oxohexanal	156	C9H16O2	1000109-76-5	25
4	2-Heptanone	114	C7H14O	000110-43-0	23
5	N,N'-Diethyl-1,6-hexanediamine	172	C10H24N2	013093-05-5	17



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU111318\
Data File : VU028096.D
Acq On : 13 Nov 2018 16:54
Operator : MD/SY
Sample : J5921-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
SP-TANK1-N29675

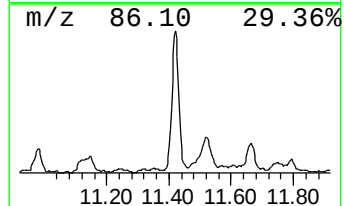
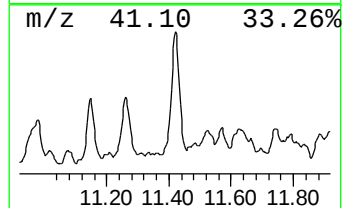
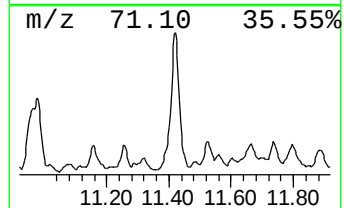
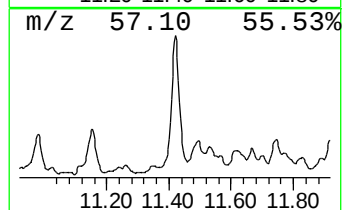
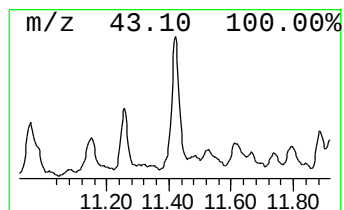
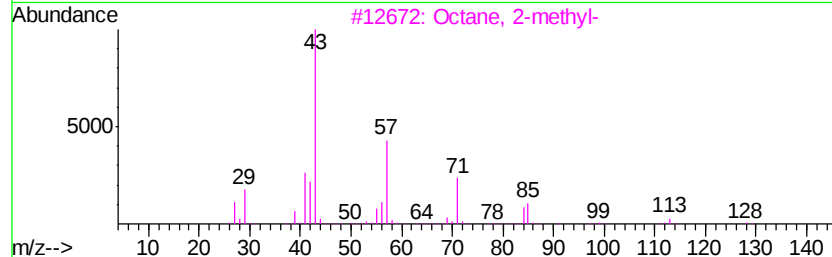
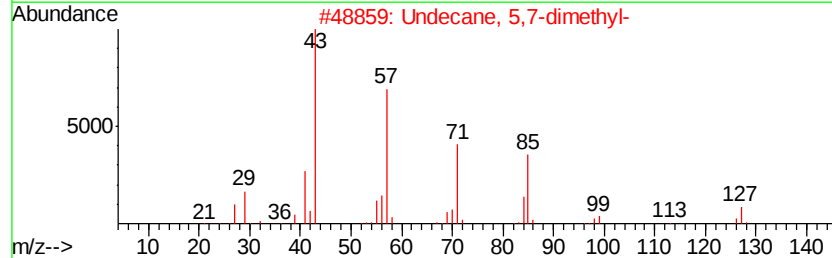
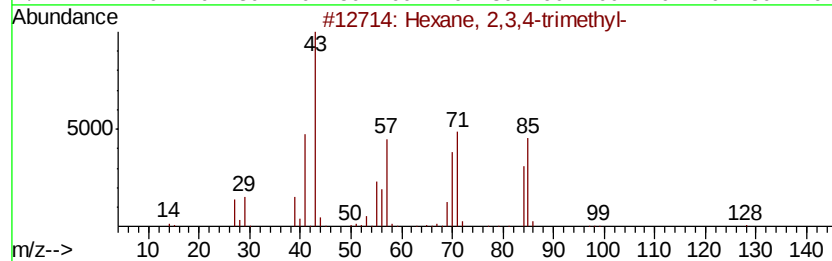
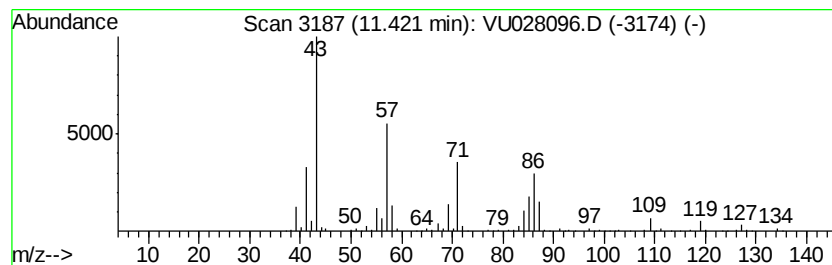
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Quant Title : SW846 8260

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

Peak Number 8 unknown11.42 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.42	16.92 ug/l	376962	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	43
2		Undecane, 5,7-dimethyl-	184	C13H28	017312-83-3	37
3		Octane, 2-methyl-	128	C9H20	003221-61-2	32
4		Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	32
5		Hexadecane	226	C16H34	000544-76-3	27



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU111318\
Data File : VU028096.D
Acq On : 13 Nov 2018 16:54
Operator : MD/SY
Sample : J5921-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 17 Sample Multiplier: 1

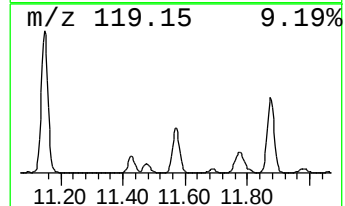
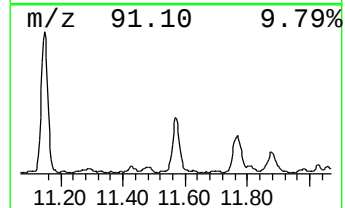
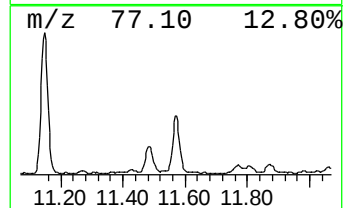
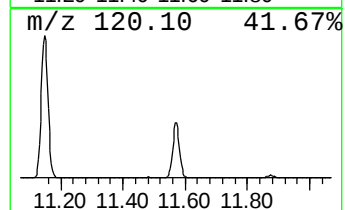
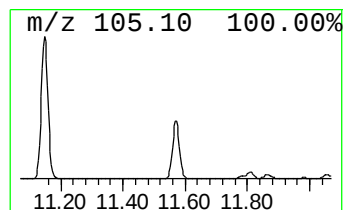
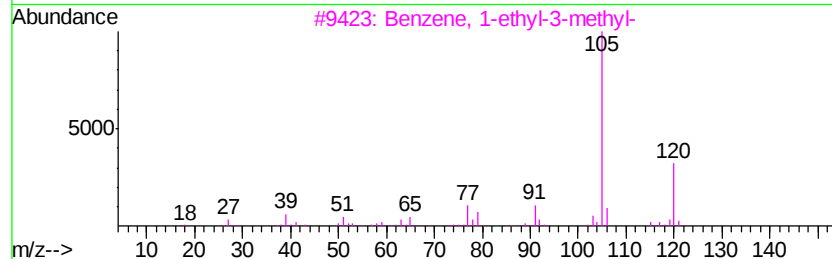
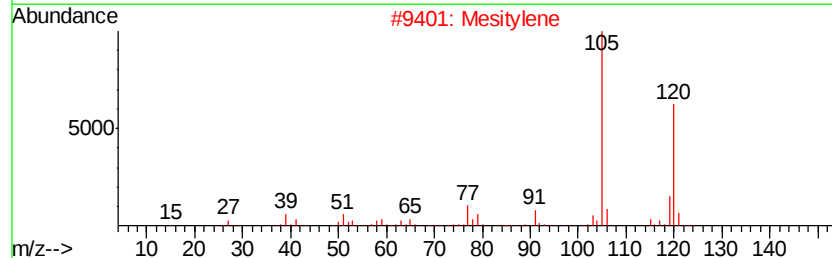
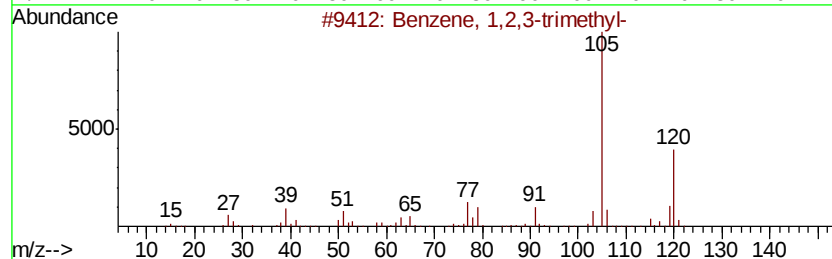
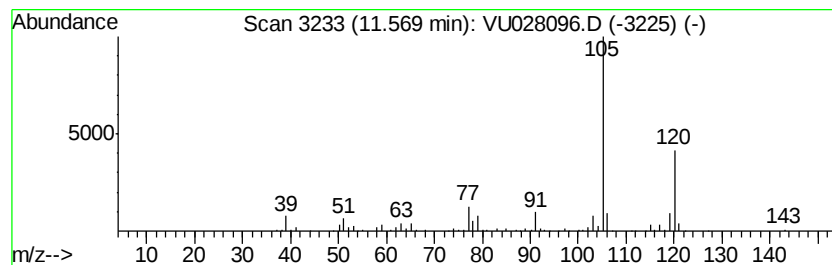
Instrument :
MSVOA_U
ClientSampleId :
SP-TANK1-N29675

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\82U110218W.M
Quant Title : SW846 8260

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

Peak Number 9 Benzene, 1,2,3-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.57	13.97 ug/l	311283	1,4-Dichlorobenzene-d4	11.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzene, 1,2,3-trimethyl-	120 C9H12	000526-73-8 95
2		Mesitylene	120 C9H12	000108-67-8 94
3		Benzene, 1-ethyl-3-methyl-	120 C9H12	000620-14-4 91
4		Benzene, 1,2,4-trimethyl-	120 C9H12	000095-63-6 91
5		Benzene, 1-ethyl-2-methyl-	120 C9H12	000611-14-3 90



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU111318\
Data File : VU028096.D
Acq On : 13 Nov 2018 16:54
Operator : MD/SY
Sample : J5921-02
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
SP-TANK1-N29675

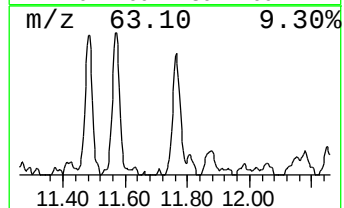
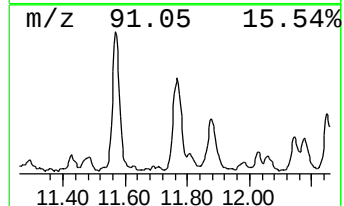
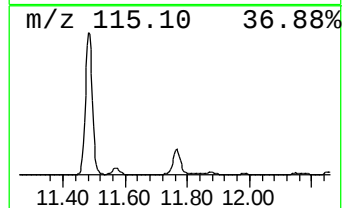
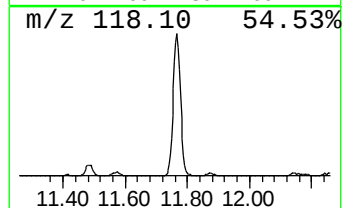
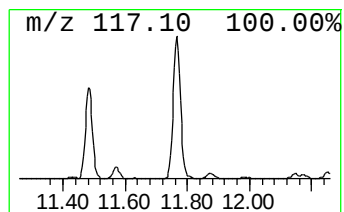
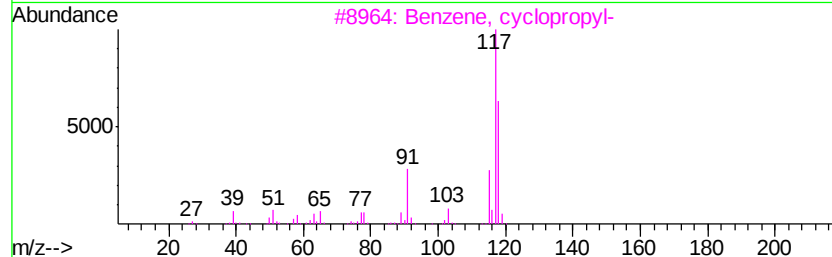
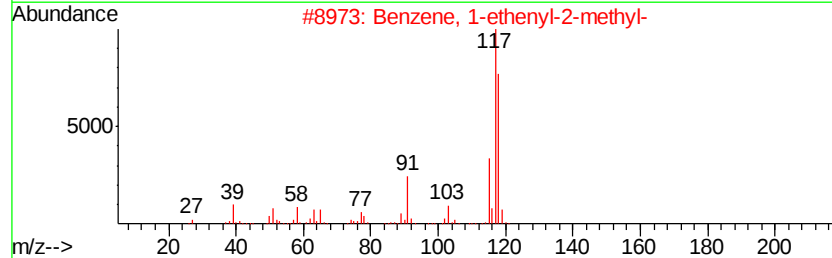
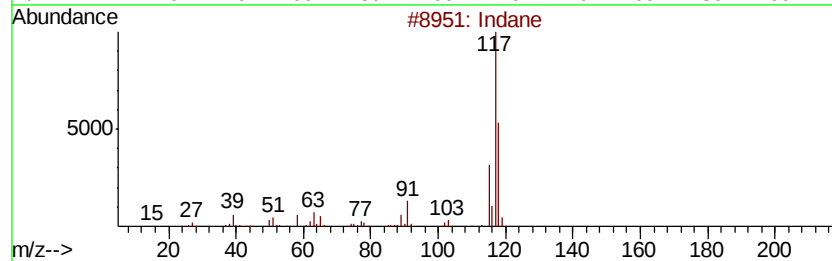
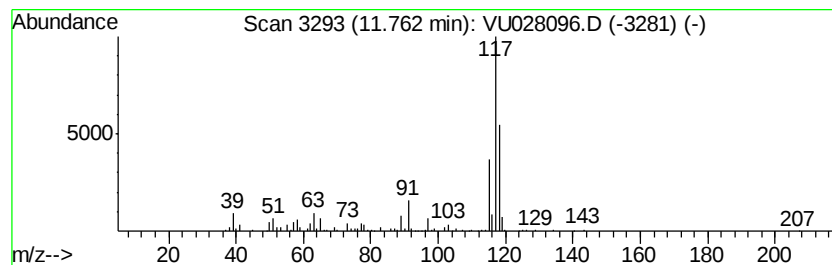
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\82U110218W.M
Quant Title : SW846 8260

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

Peak Number 10 Indane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.76	15.24 ug/l	339424	1,4-Dichlorobenzene-d4	11.48

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane		118	C9H10	000496-11-7	95
2	Benzene, 1-ethenyl-2-methyl-		118	C9H10	000611-15-4	81
3	Benzene, cyclopropyl-		118	C9H10	000873-49-4	81
4	Tetracyclo[3.3.1.0(2,8).0(4,6)]-	...	118	C9H10	1000191-13-7	81
5	Benzene, 2-propenyl-		118	C9H10	000300-57-2	74



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU111318\
Data File : VU028096.D
Acq On : 13 Nov 2018 16:54
Operator : MD/SY
Sample : J5921-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
SP-TANK1-N29675

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\82U110218W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown9.45	9.45	6.9	ug/l	172398	3	9.09	1251020	50.0
2-Heptanone	9.92	8.1	ug/l	203670	3	9.09	1251020	50.0
Benzene, 1-ethyl-...	10.68	24.1	ug/l	537943	4	11.48	1113780	50.0
unknown11.26	11.26	7.0	ug/l	155044	4	11.48	1113780	50.0
unknown11.42	11.42	16.9	ug/l	376962	4	11.48	1113780	50.0
Benzene, 1,2,3-tr...	11.57	14.0	ug/l	311283	4	11.48	1113780	50.0
Indane	11.76	15.2	ug/l	339424	4	11.48	1113780	50.0