

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092521\
 Data File : VU044850.D
 Acq On : 25 Sep 2021 20:28
 Operator : SY/MD
 Sample : M3875-15
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 20882

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % 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\82U092421W.M
 Title : SW846 8260

Signal : TIC: VU044850.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.495	34	48	74	rBV	435701	2002488	64.21%	11.922%
2	2.546	364	375	388	rBV	39224	62975	2.02%	0.375%
3	2.630	388	401	412	rBV	474436	815408	26.15%	4.855%
4	2.687	412	419	432	rVB	84200	143224	4.59%	0.853%
5	2.797	432	453	466	rBV3	74355	235171	7.54%	1.400%
6	3.051	518	532	563	rVB	1628883	3118626	100.00%	18.568%
7	3.186	564	574	592	rVB4	17945	44066	1.41%	0.262%
8	4.707	1033	1047	1071	rVB	70437	160740	5.15%	0.957%
9	5.295	1214	1230	1243	rBV2	154302	326008	10.45%	1.941%
10	5.379	1243	1256	1273	rVB	262459	534703	17.15%	3.184%
11	5.707	1342	1358	1375	rBV	193089	397325	12.74%	2.366%
12	6.157	1479	1498	1513	rBV2	17108	41279	1.32%	0.246%
13	6.253	1514	1528	1549	rVV	398828	742300	23.80%	4.420%
14	6.771	1677	1689	1706	rBV	38890	71695	2.30%	0.427%
15	7.793	1995	2007	2021	rBV2	32401	56964	1.83%	0.339%
16	7.903	2024	2041	2055	rBV	610765	1052010	33.73%	6.263%
17	7.973	2055	2063	2074	rVB	27659	48161	1.54%	0.287%
18	8.555	2232	2244	2263	rBV	326951	549868	17.63%	3.274%
19	8.690	2276	2286	2303	rVB	22128	37845	1.21%	0.225%
20	9.420	2501	2513	2534	rBV	556908	907950	29.11%	5.406%
21	9.575	2549	2561	2570	rBV2	70818	118422	3.80%	0.705%
22	10.237	2755	2767	2782	rBV	38453	62417	2.00%	0.372%
23	10.494	2835	2847	2860	rBV2	19587	32229	1.03%	0.192%
24	10.636	2878	2891	2915	rVV	430412	681257	21.84%	4.056%
25	11.304	3081	3099	3109	rBV3	20643	41343	1.33%	0.246%
26	11.472	3135	3151	3164	rBV4	56629	135371	4.34%	0.806%
27	11.613	3189	3195	3202	rBV2	24367	36839	1.18%	0.219%
28	11.748	3215	3237	3246	rBV	123538	215002	6.89%	1.280%
29	11.816	3246	3258	3274	rVB	601097	1009677	32.38%	6.011%
30	11.915	3275	3289	3304	rBV	152278	285475	9.15%	1.700%
31	12.060	3321	3334	3368	rBV	614972	1096082	35.15%	6.526%
32	12.459	3447	3458	3467	rBV2	39717	64098	2.06%	0.382%
33	12.529	3467	3480	3507	rVB	363325	592188	18.99%	3.526%
34	12.845	3568	3578	3607	rVB	235627	402076	12.89%	2.394%
35	13.433	3752	3761	3776	rVB	54118	78963	2.53%	0.470%
36	13.742	3839	3857	3869	rBV2	51023	91153	2.92%	0.543%

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Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % 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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37	13.812	3869	3879	3885	rVV2	53961	97692	3.13%	0.582%
38	13.848	3886	3890	3909	rVV5	50828	100240	3.21%	0.597%
39	14.037	3937	3949	3961	rBV	138519	225605	7.23%	1.343%
40	15.404	4362	4374	4386	rBV	55581	80982	2.60%	0.482%

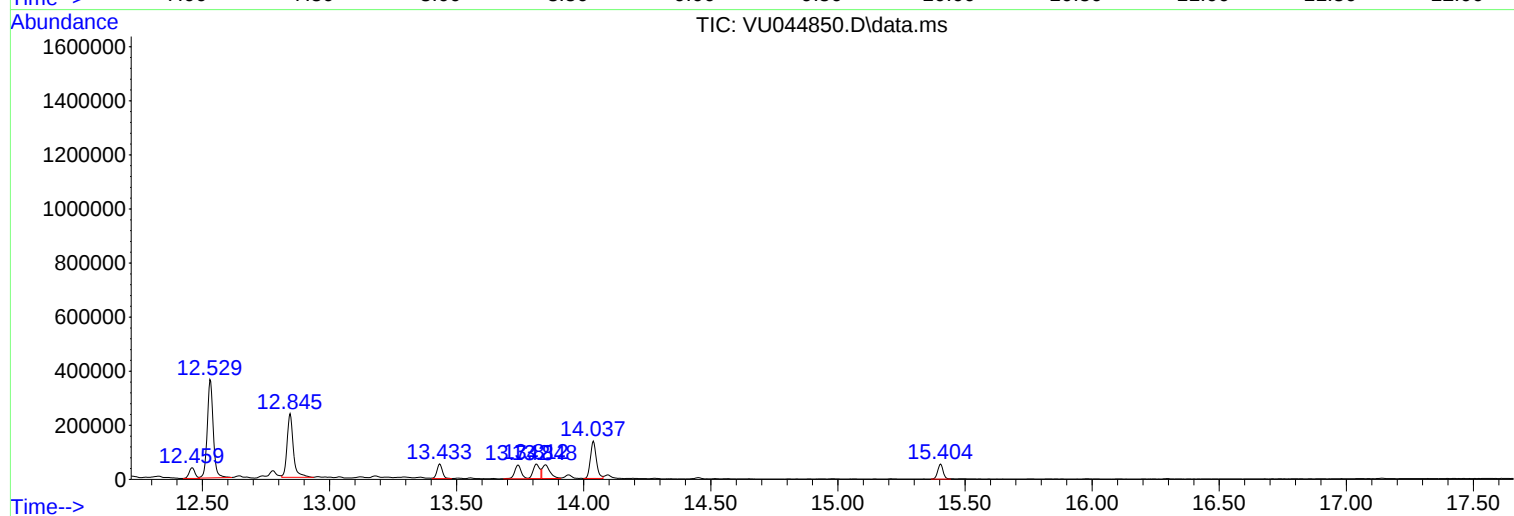
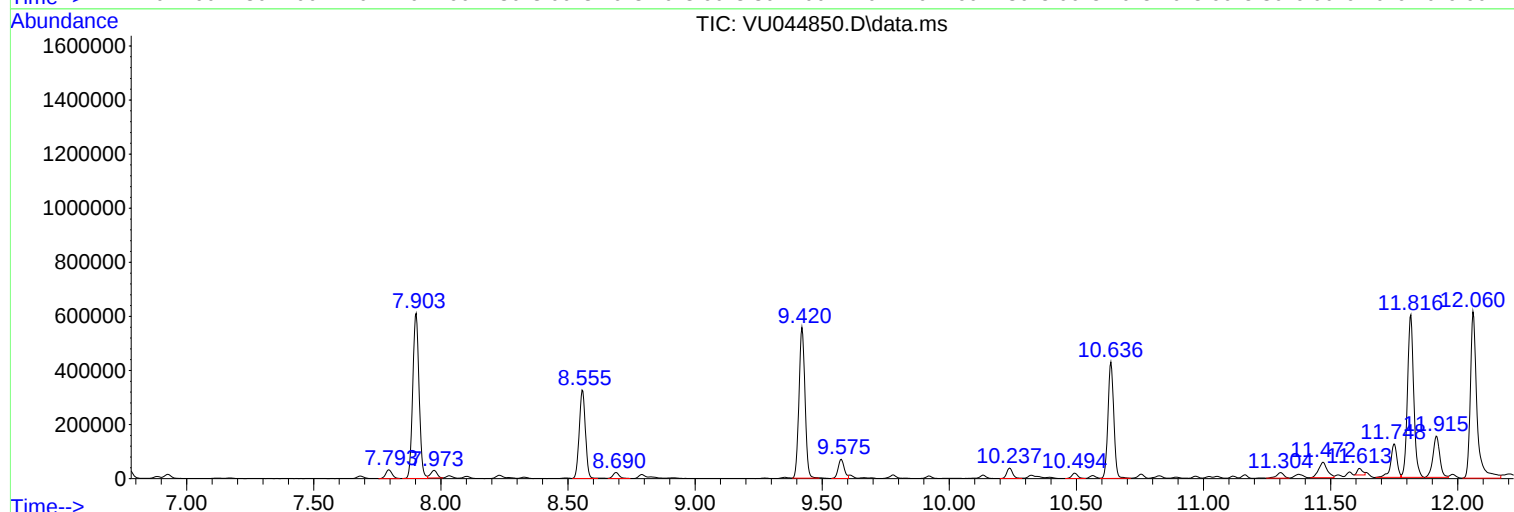
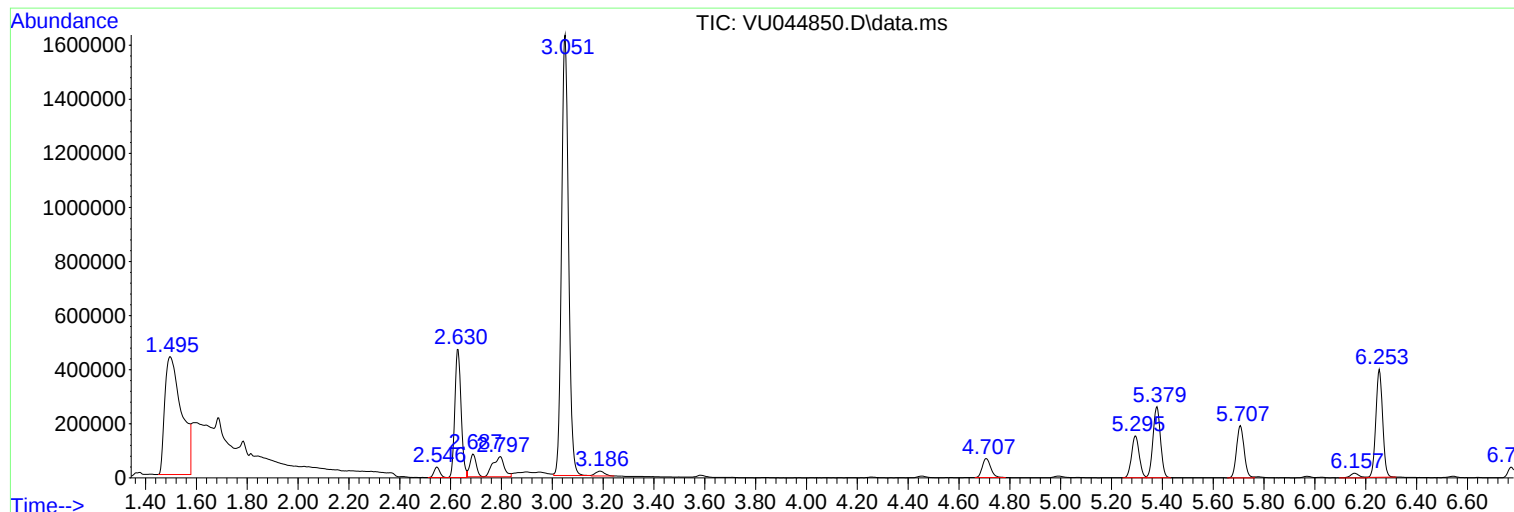
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

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



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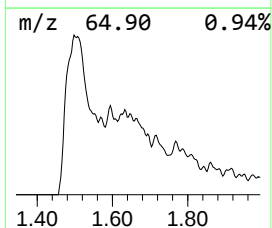
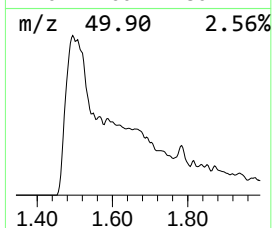
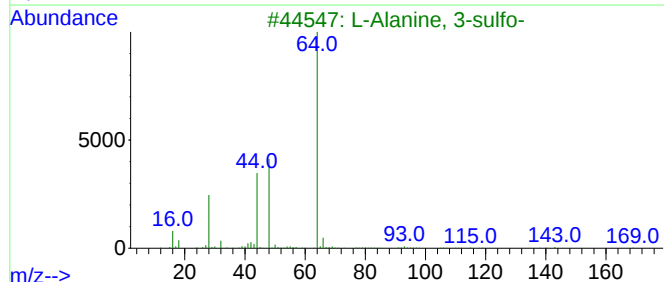
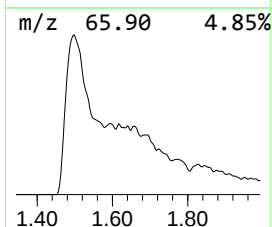
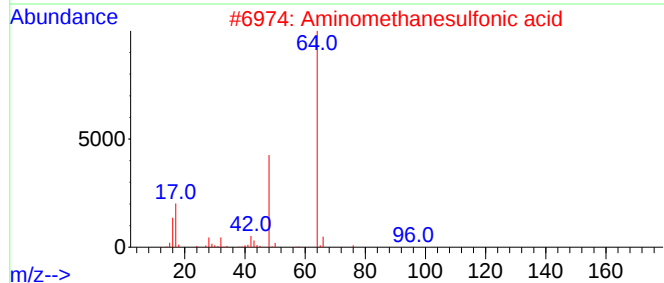
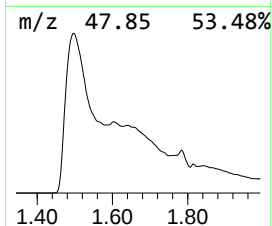
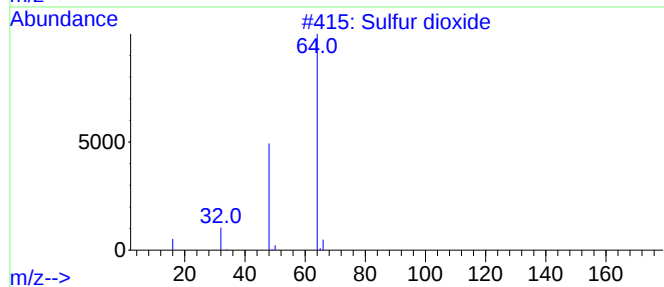
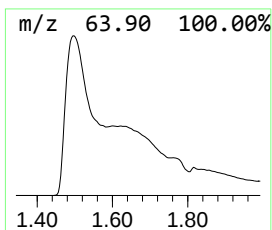
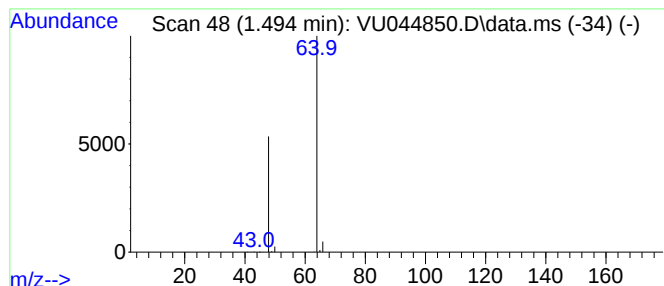
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.494	187.25 ug/l	2002490	Pentafluorobenzene	5.379

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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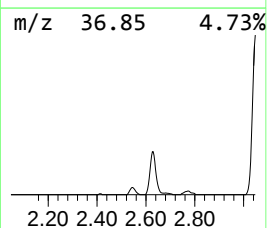
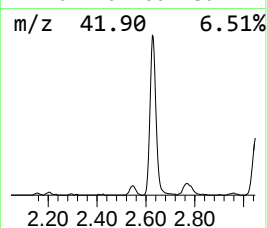
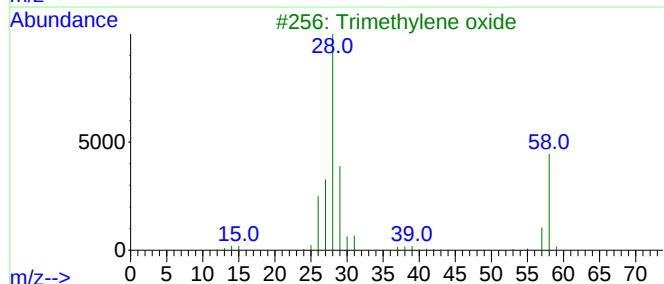
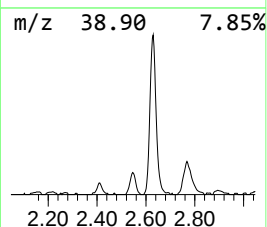
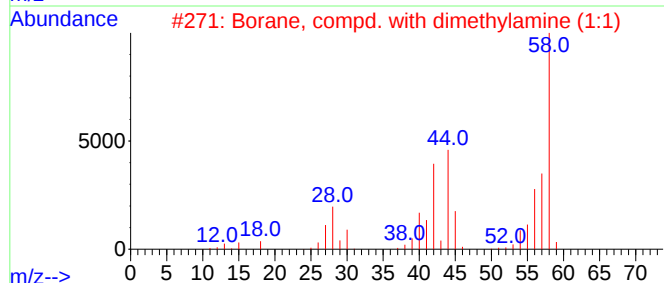
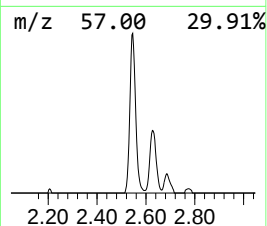
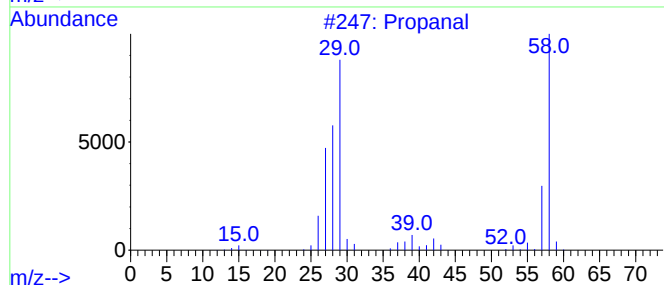
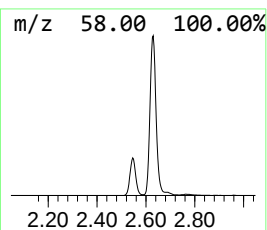
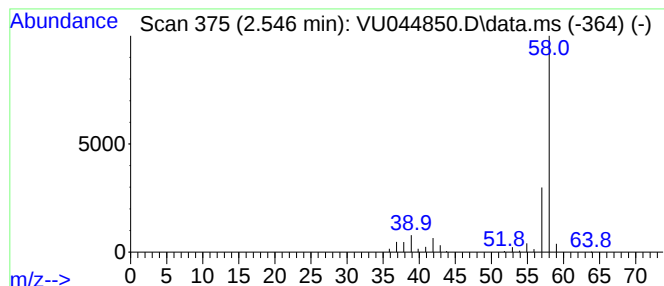
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.546	5.89 ug/l	62975	Pentafluorobenzene	5.379

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal	58	C3H6O	000123-38-6	78
2			Borane, compd. with dimethylamin...	59	C2H10BN	000074-94-2	9
3			Trimethylene oxide	58	C3H6O	000503-30-0	9
4			.alpha.-Pinene, 10-(dimethylamin...	193	C13H23N	015063-97-5	9
5			Propylene oxide	58	C3H6O	000075-56-9	7



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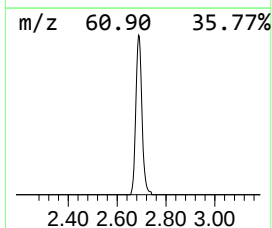
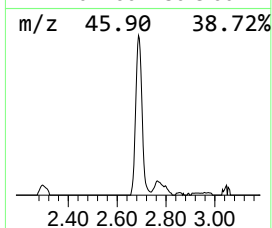
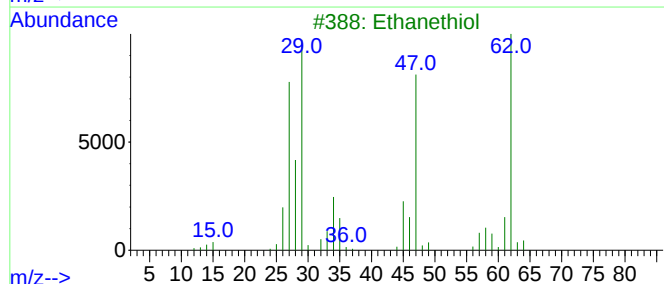
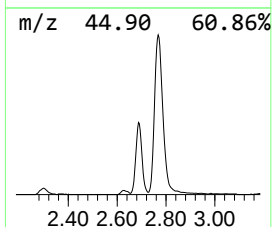
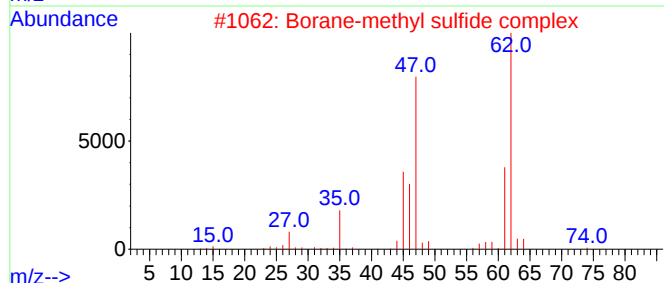
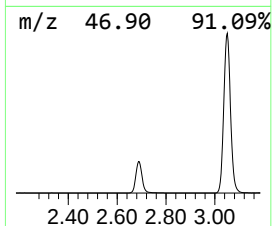
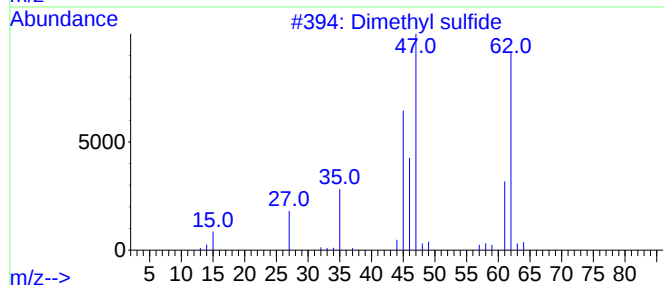
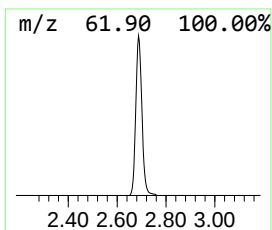
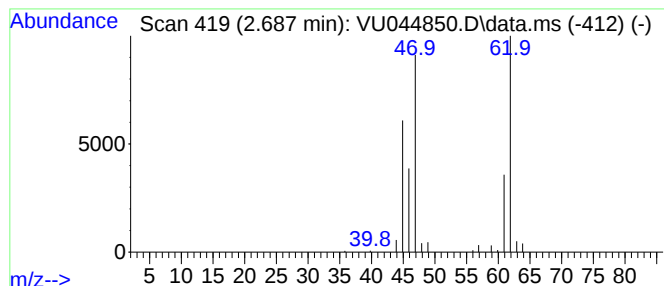
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 3 Dimethyl sulfide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.687	13.39 ug/l	143224	Pentafluorobenzene	5.379

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl sulfide	62	C2H6S	000075-18-3	94
2			Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	90
3			Ethanethiol	62	C2H6S	000075-08-1	72
4			Ethene, chloro-	62	C2H3Cl	000075-01-4	9
5			Boric acid	62	BH3O3	010043-35-3	5



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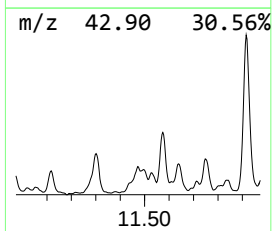
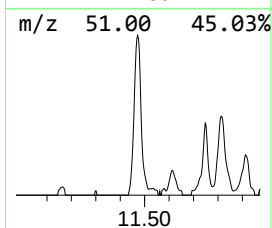
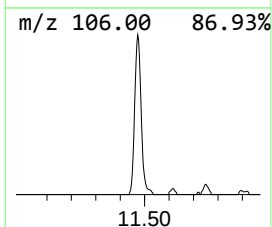
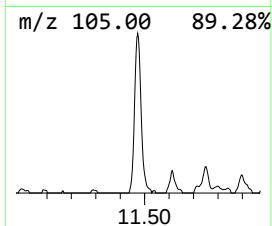
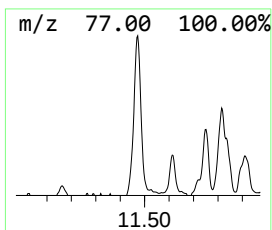
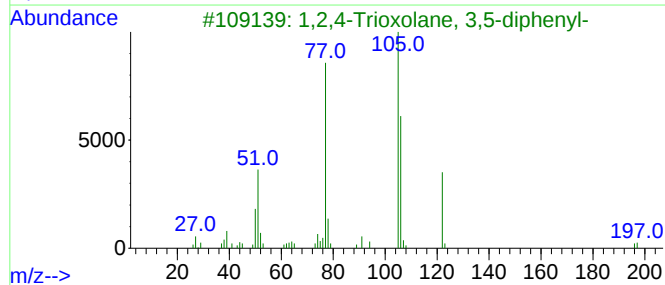
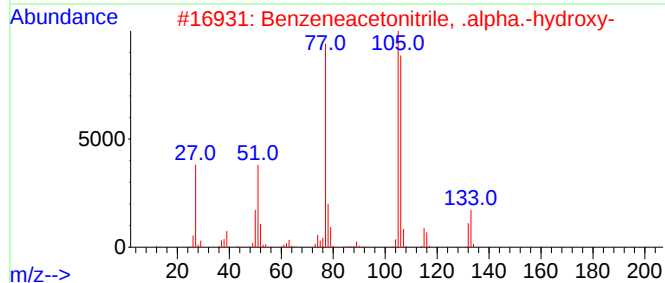
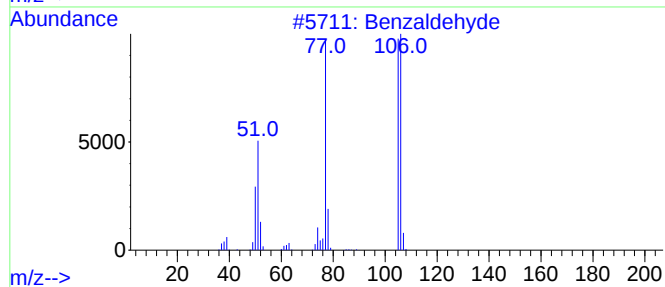
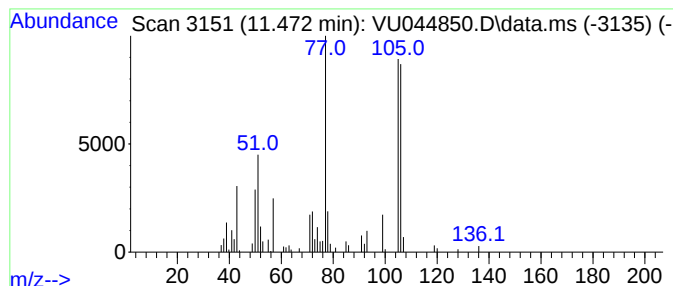
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Benzeneacetonitrile, .alpha... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.472	6.70 ug/l	135371	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzaldehyde	106	C7H6O	000100-52-7	96
2			Benzeneacetonitrile, .alpha.-hyd...	133	C8H7NO	000532-28-5	64
3			1,2,4-Trioxolane, 3,5-diphenyl-	228	C14H12O3	023888-15-5	53
4			Ethanone, 2-hydroxy-1-phenyl-	136	C8H8O2	000582-24-1	47
5			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47



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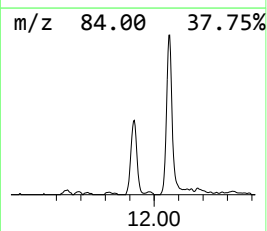
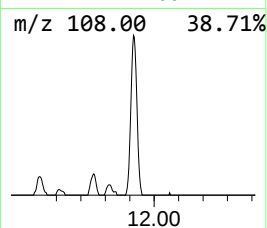
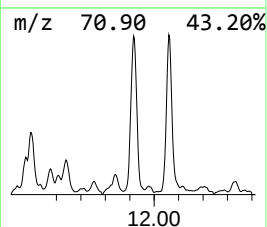
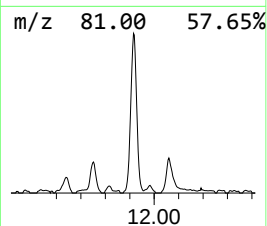
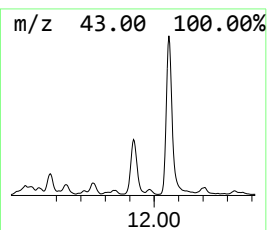
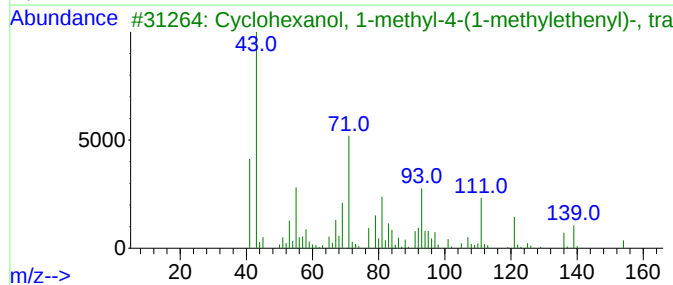
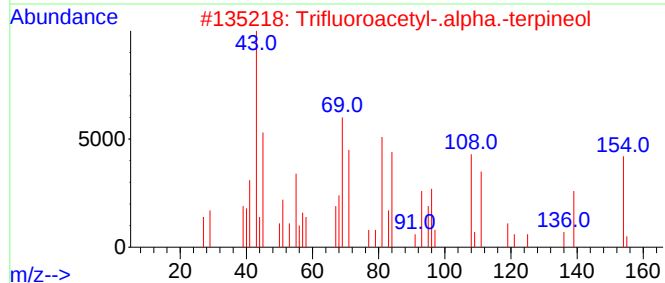
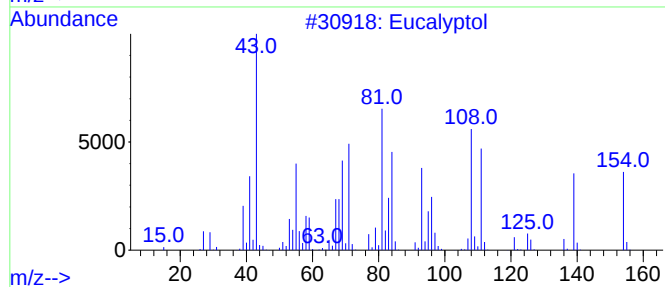
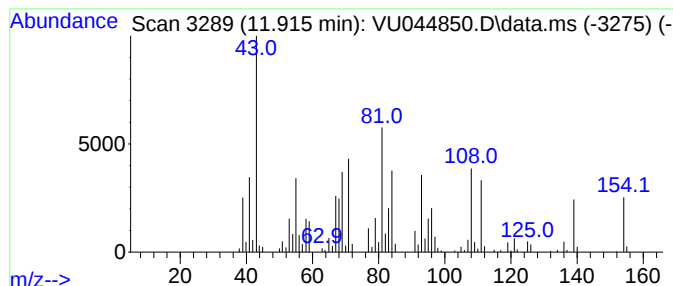
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

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

Peak Number 5 Eucalyptol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.915	14.14 ug/l	285475	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	98
2			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	64
3			Cyclohexanol, 1-methyl-4-(1-meth...	154	C10H18O	007299-40-3	32
4			1-Hepten-6-one, 2-methyl-	126	C8H14O	010408-15-8	27
5			Bicyclo[3.3.0]octan-3-one, 6-hyd...	154	C9H14O2	1005239-70-2	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092521\
Data File : VU044850.D
Acq On : 25 Sep 2021 20:28
Operator : SY/MD
Sample : M3875-15
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
20882

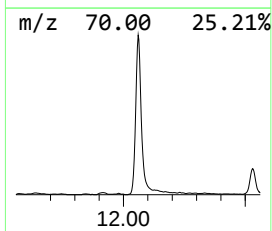
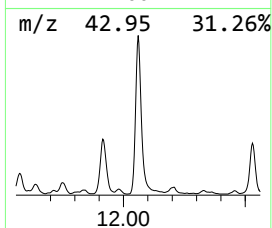
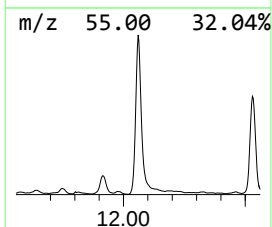
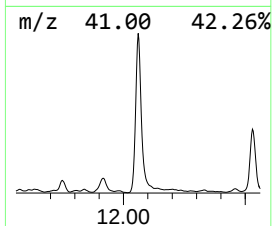
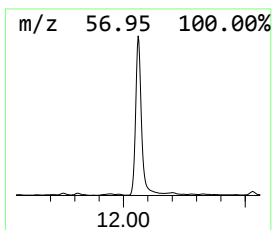
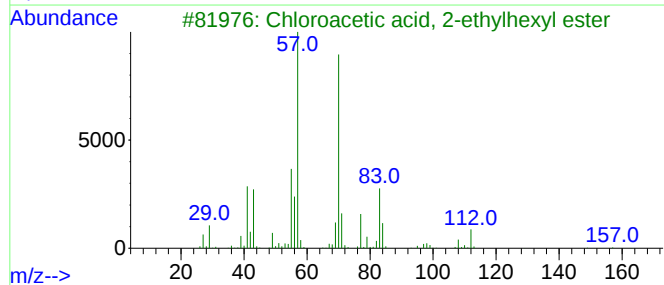
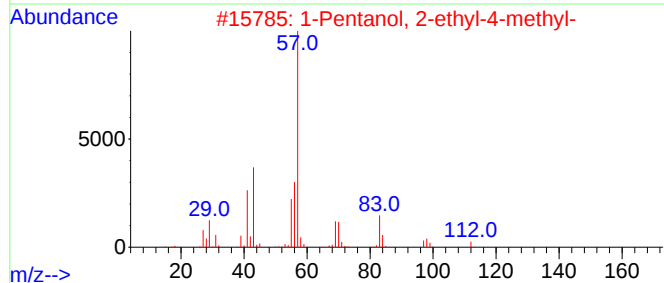
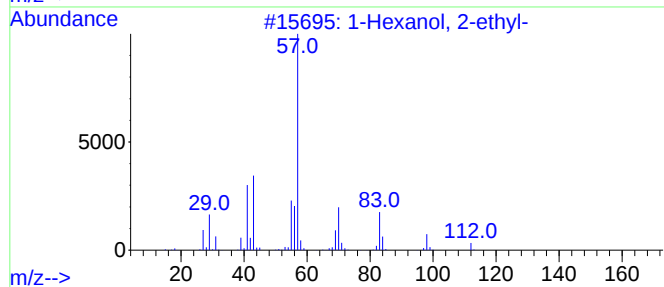
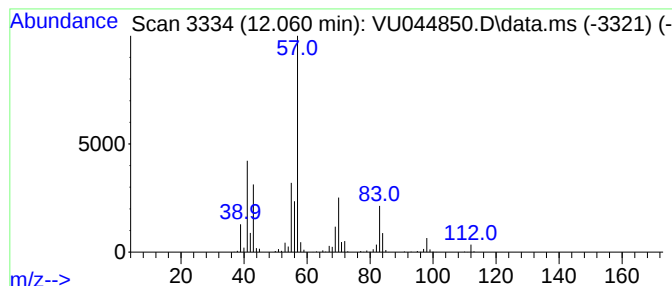
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Quant Title : SW846 8260

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

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.060	54.28 ug/l	1096080	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3			Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	53
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092521\
Data File : VU044850.D
Acq On : 25 Sep 2021 20:28
Operator : SY/MD
Sample : M3875-15
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
20882

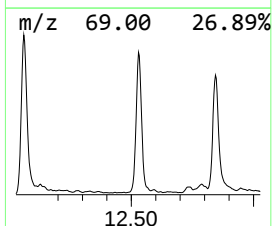
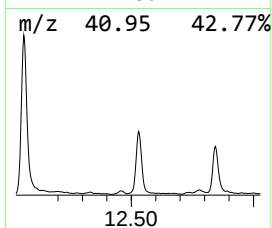
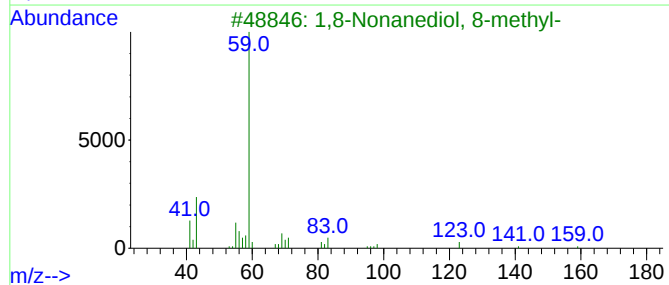
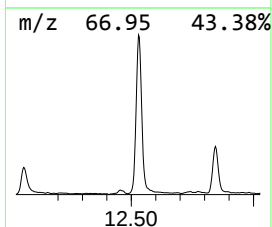
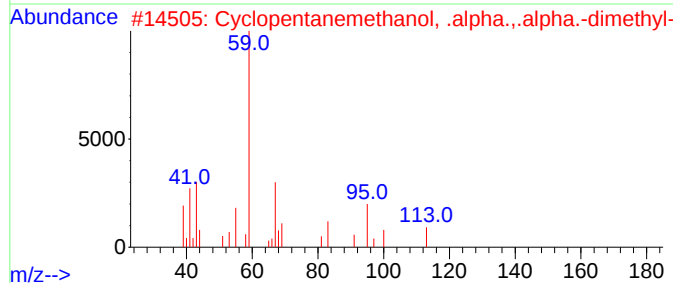
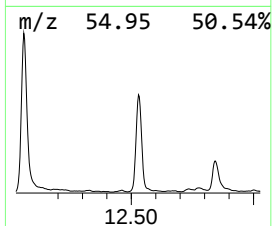
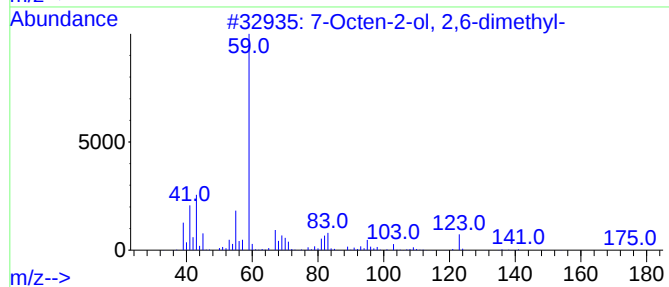
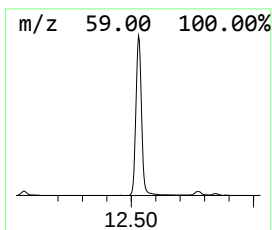
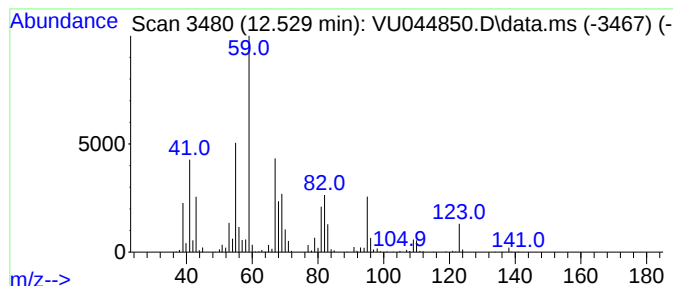
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Quant Title : SW846 8260

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

Peak Number 7 7-Octen-2-ol, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.529	29.33 ug/l	592188	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	59
2			Cyclopentanemethanol, .alpha.,.a...	128	C8H16O	001462-06-2	42
3			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	35
4			1,7-Octanediol, 3,7-dimethyl-	174	C10H22O2	000107-74-4	32
5			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092521\
Data File : VU044850.D
Acq On : 25 Sep 2021 20:28
Operator : SY/MD
Sample : M3875-15
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

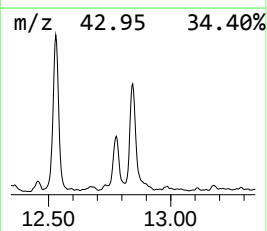
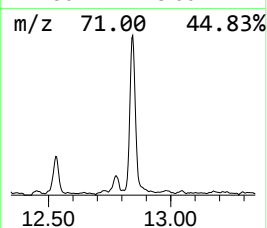
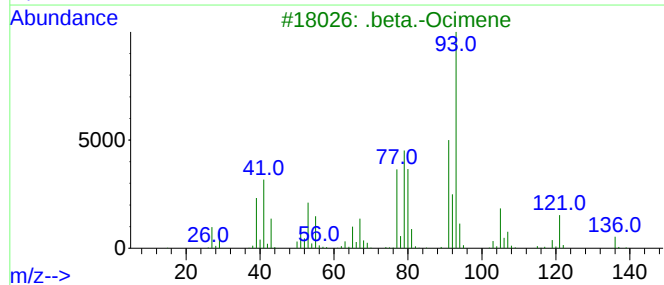
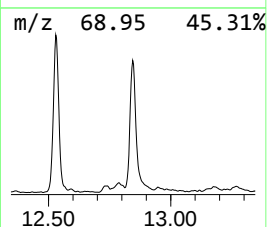
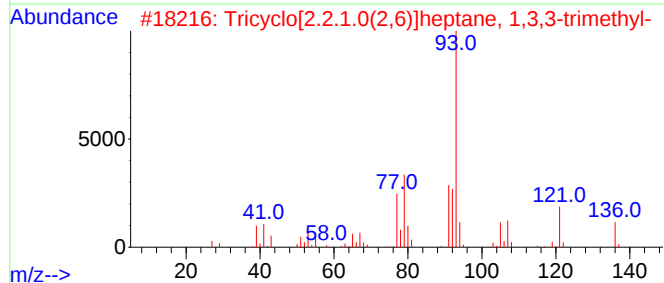
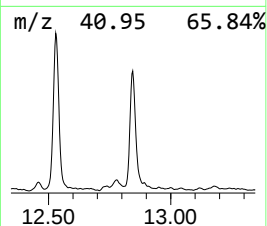
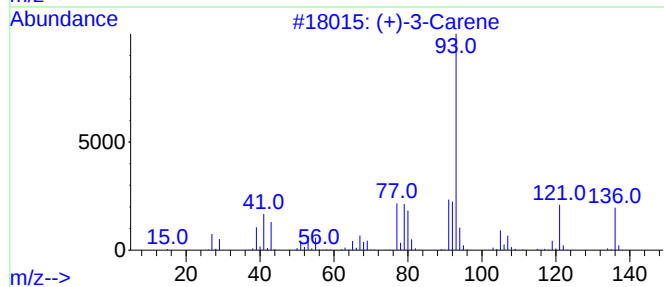
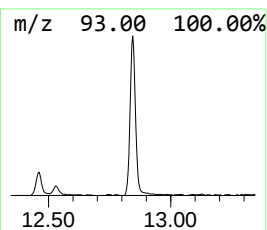
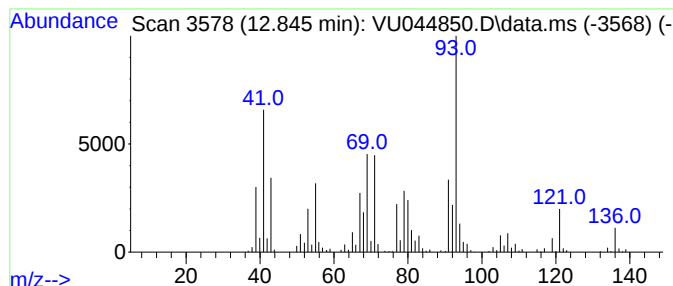
Instrument :
MSVOA_U
ClientSampleId :
20882

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

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

Peak Number 8 (+)-3-Carene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.845	19.91 ug/l	402076	1,4-Dichlorobenzene-d4	11.816	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-3-Carene	136	C10H16	000498-15-7	93
2	Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000488-97-1	90
3	.beta.-Ocimene	136	C10H16	013877-91-3	76
4	Butanoic acid, 3-methyl-, 1-ethe...	238	C15H26O2	001118-27-0	74
5	3-Carene	136	C10H16	013466-78-9	70



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092521\
Data File : VU044850.D
Acq On : 25 Sep 2021 20:28
Operator : SY/MD
Sample : M3875-15
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
20882

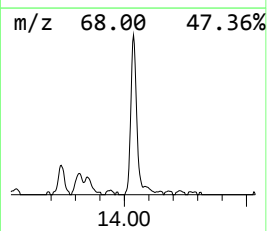
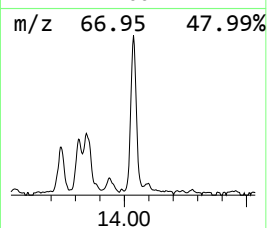
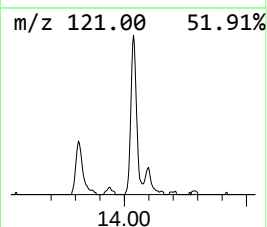
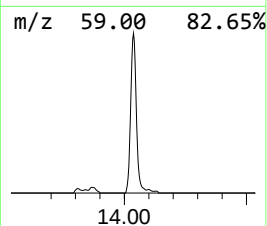
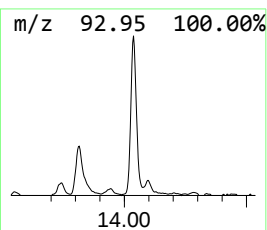
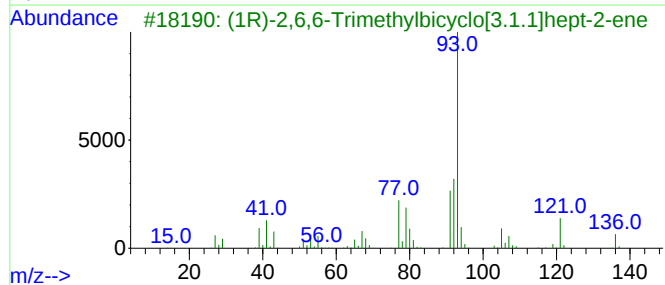
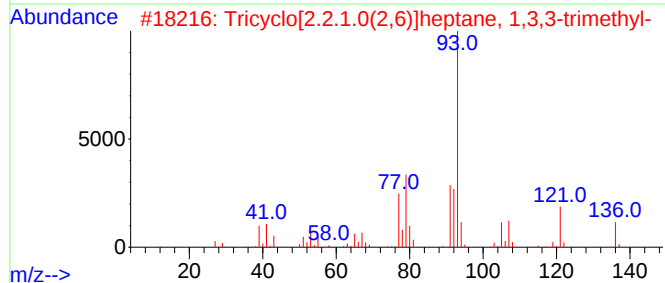
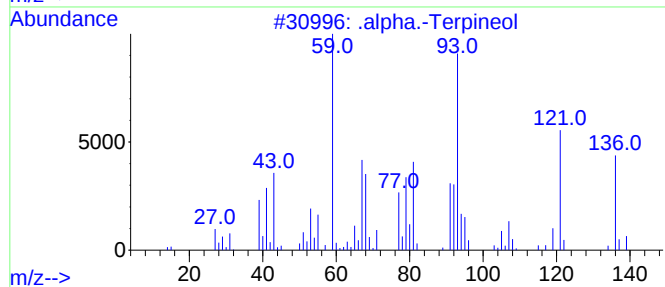
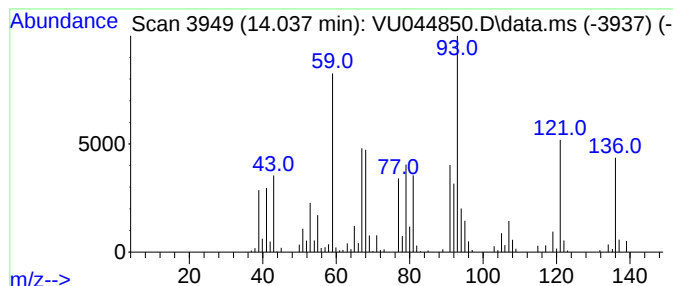
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

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

Peak Number 9 .alpha.-Terpineol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.037	11.17 ug/l	225605	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.alpha.-Terpineol	154	C10H18O	000098-55-5	91
2			Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000488-97-1	70
3			(1R)-2,6,6-Trimethylbicyclo[3.1...	136	C10H16	007785-70-8	59
4			1,3-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-86-5	50
5			Cyclohexene, 1-methyl-4-(1-methy...	136	C10H16	000586-62-9	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092521\
Data File : VU044850.D
Acq On : 25 Sep 2021 20:28
Operator : SY/MD
Sample : M3875-15
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
20882

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.494	187.3	ug/l	2002490	1	5.379	534703	50.0
Propanal	2.546	5.9	ug/l	62975	1	5.379	534703	50.0
Dimethyl sulfide	2.687	13.4	ug/l	143224	1	5.379	534703	50.0
Benzeneacetone...	11.472	6.7	ug/l	135371	4	11.816	1009680	50.0
Eucalyptol	11.915	14.1	ug/l	285475	4	11.816	1009680	50.0
1-Hexanol, 2-ethyl...	12.060	54.3	ug/l	1096080	4	11.816	1009680	50.0
7-Octen-2-ol, 2-methyl...	12.529	29.3	ug/l	592188	4	11.816	1009680	50.0
(+)-3-Carene	12.845	19.9	ug/l	402076	4	11.816	1009680	50.0
.alpha.-Terpineol	14.037	11.2	ug/l	225605	4	11.816	1009680	50.0