

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU053122\
 Data File : VU048738.D
 Acq On : 31 May 2022 14:21
 Operator : SY/MD
 Sample : N3067-01
 Misc : 1.03g/10.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 33686

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\82U052622W.M
 Title : SW846 8260

Signal : TIC: VU048738.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.459	28	37	92	rBV	249774	761494	47.30%	6.093%
2	2.957	493	503	518	rBV2	10684	23246	1.44%	0.186%
3	3.179	553	572	589	rBV	27999	72645	4.51%	0.581%
4	4.726	1041	1053	1083	rBV2	19616	61206	3.80%	0.490%
5	5.289	1212	1228	1240	rBV	209129	490479	30.46%	3.925%
6	5.366	1240	1252	1271	rVB	408913	882976	54.84%	7.065%
7	5.700	1341	1356	1380	rBV	243144	538539	33.45%	4.309%
8	5.977	1427	1442	1456	rBV4	17034	41392	2.57%	0.331%
9	6.247	1510	1526	1550	rBV	565745	1148914	71.36%	9.193%
10	7.896	2026	2039	2058	rBV	805153	1448977	89.99%	11.594%
11	7.993	2058	2069	2086	rVB4	10222	24393	1.52%	0.195%
12	9.420	2498	2513	2541	rBV	768821	1439418	89.40%	11.518%
13	10.639	2878	2892	2909	rBV	602542	1035584	64.32%	8.286%
14	11.118	3028	3041	3052	rVB7	12956	23629	1.47%	0.189%
15	11.472	3140	3151	3159	rBV3	12730	20018	1.24%	0.160%
16	11.816	3244	3258	3278	rBV	995322	1610067	100.00%	12.883%
17	11.919	3278	3290	3304	rVB2	164524	277060	17.21%	2.217%
18	12.066	3325	3336	3343	rBV3	23256	45746	2.84%	0.366%
19	12.777	3545	3557	3561	rBV3	49035	82668	5.13%	0.661%
20	12.806	3561	3566	3582	rVB3	62033	118959	7.39%	0.952%
21	12.899	3584	3595	3609	rBV2	173815	344296	21.38%	2.755%
22	13.044	3632	3640	3647	rBV5	54226	98383	6.11%	0.787%
23	13.172	3673	3680	3686	rBV4	42713	65592	4.07%	0.525%
24	13.214	3686	3693	3700	rBV4	79481	128507	7.98%	1.028%
25	13.365	3731	3740	3753	rBV2	31578	58578	3.64%	0.469%
26	13.639	3816	3825	3843	rVB8	21675	47752	2.97%	0.382%
27	13.738	3846	3856	3875	rVB2	64256	114199	7.09%	0.914%
28	14.005	3924	3939	3953	rBV	199397	331391	20.58%	2.652%
29	14.089	3954	3965	3984	rVB	107907	197193	12.25%	1.578%
30	14.214	3996	4004	4010	rBV7	15396	26213	1.63%	0.210%
31	14.256	4010	4017	4035	rVB5	25894	51338	3.19%	0.411%
32	14.533	4094	4103	4111	rBV4	15575	23835	1.48%	0.191%
33	14.658	4131	4142	4158	rBV2	48708	96652	6.00%	0.773%
34	14.925	4215	4225	4235	rBV	177673	280654	17.43%	2.246%
35	14.986	4240	4244	4253	rVV7	28875	44913	2.79%	0.359%
36	15.041	4257	4261	4272	rVB7	11849	19086	1.19%	0.153%

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M

Title : SW846 8260

37	15.224	4311	4318	4331	rVB	58467	96628	6.00%	0.773%
38	15.410	4366	4376	4392	rVB2	81688	135280	8.40%	1.082%
39	15.690	4456	4463	4475	rVB8	9915	17342	1.08%	0.139%
40	15.954	4533	4545	4557	rBV	25915	47001	2.92%	0.376%
41	16.262	4631	4641	4650	rBV4	14771	29864	1.85%	0.239%
42	16.410	4678	4687	4695	rBV4	28509	45565	2.83%	0.365%
43	17.098	4892	4901	4915	rBV3	27261	49690	3.09%	0.398%

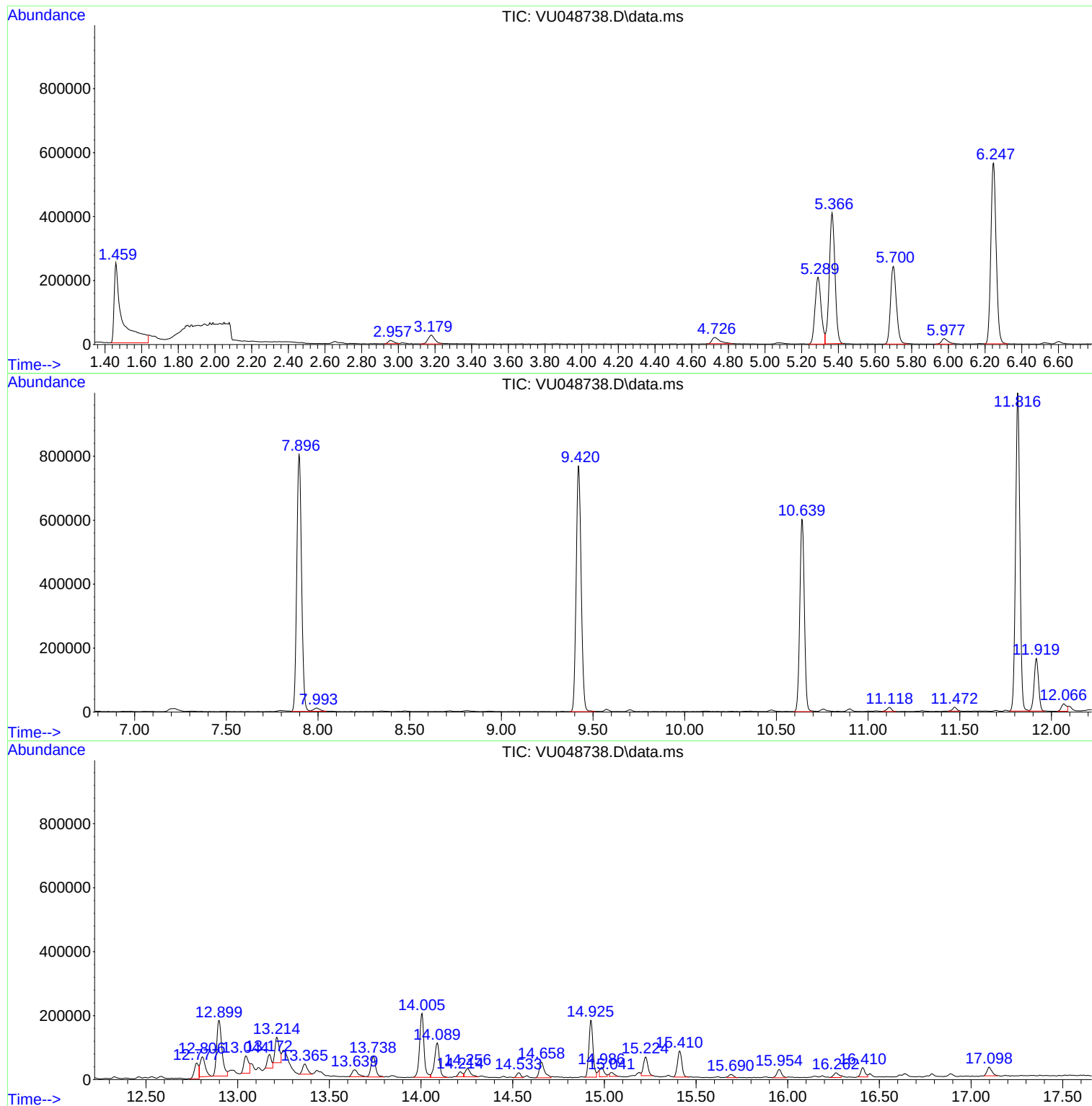
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

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



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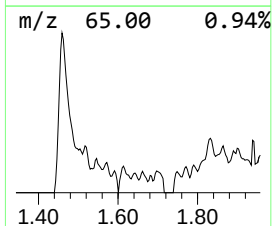
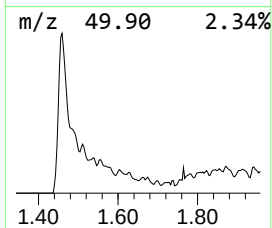
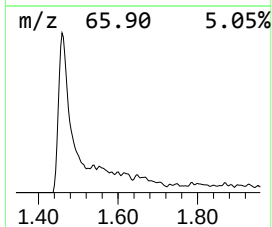
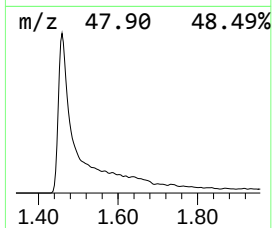
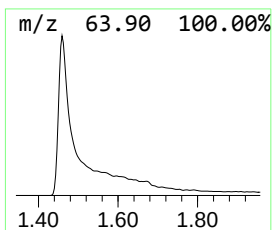
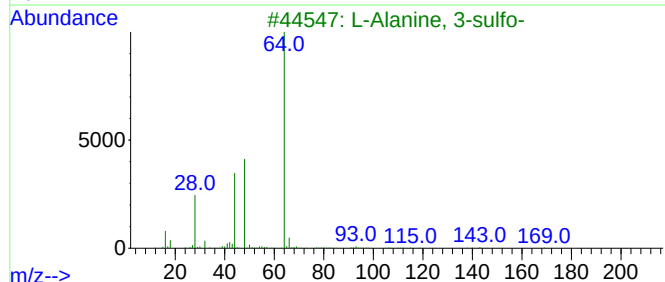
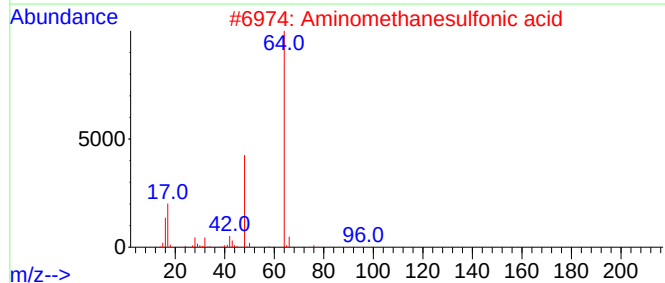
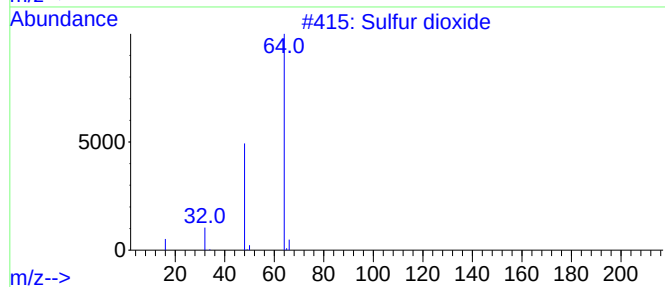
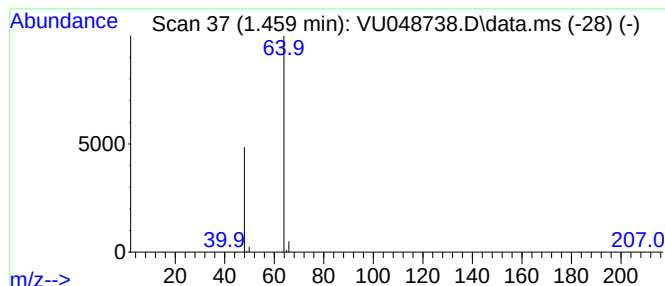
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

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.
1.459	43.12 ug/l	761494	Pentafluorobenzene	5.366

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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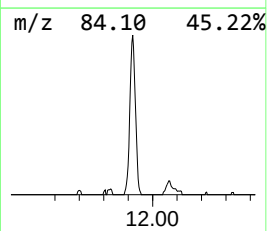
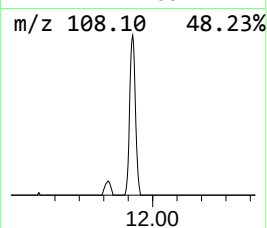
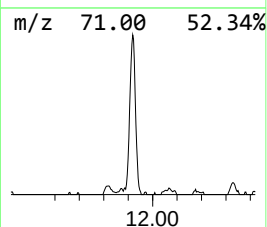
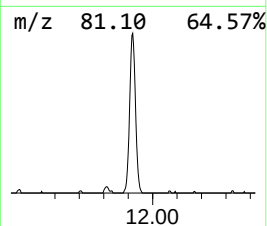
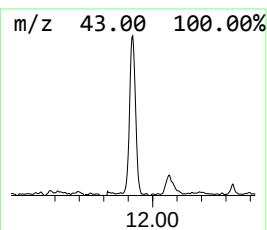
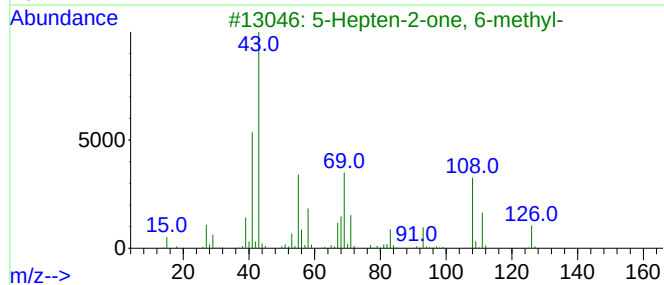
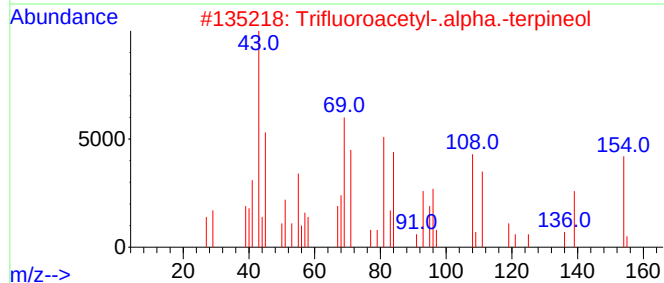
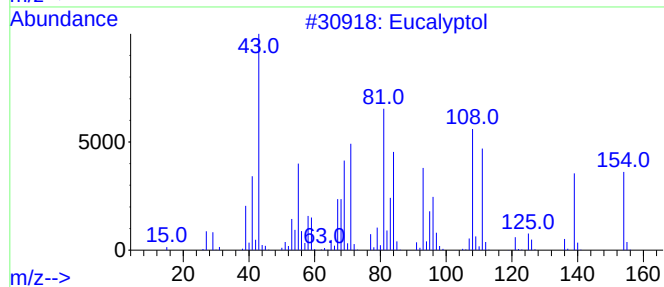
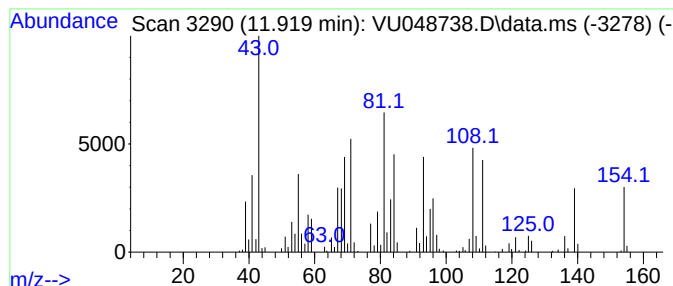
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Eucalyptol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.919	8.60 ug/l	277060	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eucalyptol	154	C10H18O	000470-82-6	97
2			Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	72
3			5-Hepten-2-one, 6-methyl-	126	C8H14O	000110-93-0	30
4			4-Isopropyl-1-methylcyclohex-2-enol	154	C10H18O	000619-62-5	27
5			1-Methyl-3-(1'-methylcyclopropyl-...	136	C10H16	103240-53-5	15



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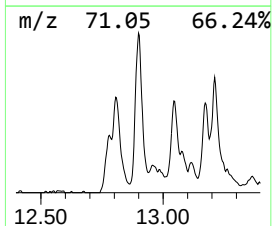
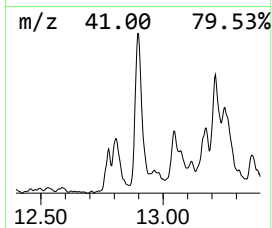
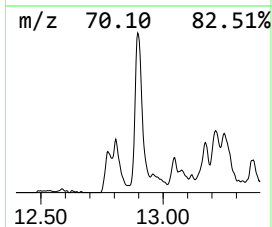
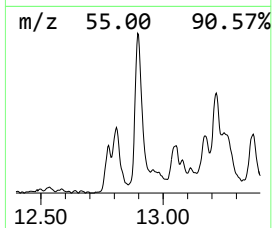
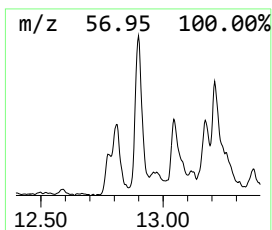
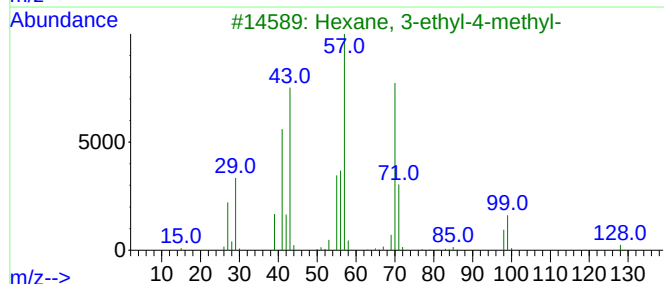
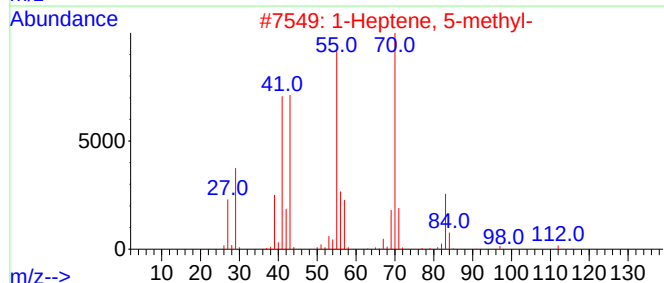
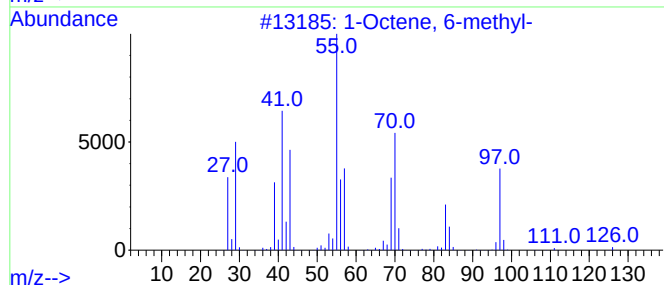
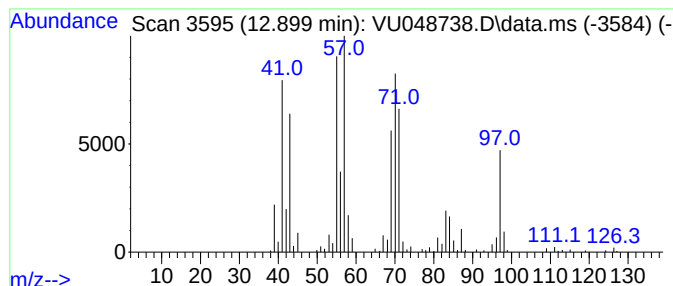
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Quant Title : SW846 8260

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

Peak Number 3 1-Octene, 6-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.899	10.69 ug/l	344296	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octene, 6-methyl-	126	C9H18	013151-10-5	53
2			1-Heptene, 5-methyl-	112	C8H16	013151-04-7	47
3			Hexane, 3-ethyl-4-methyl-	128	C9H20	003074-77-9	43
4			1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	43
5			Cyclohexane, (1,1-dimethylpropyl)-	154	C11H22	031797-64-5	43



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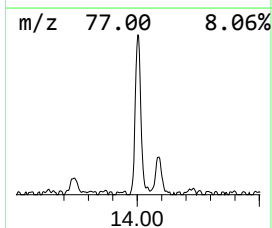
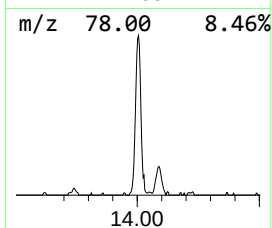
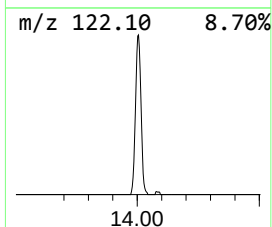
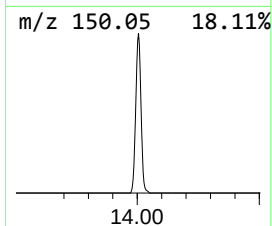
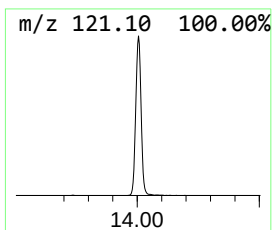
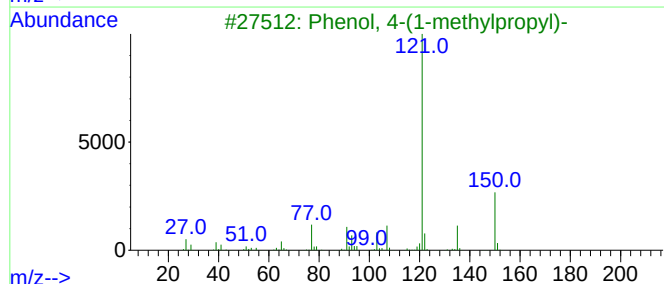
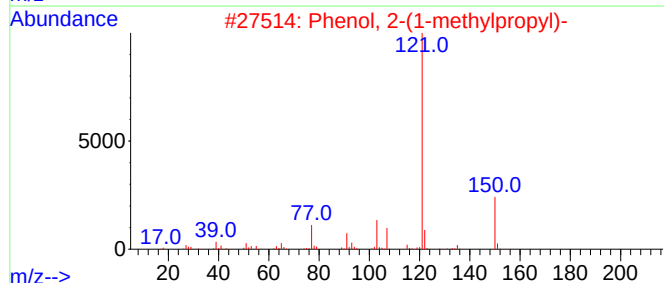
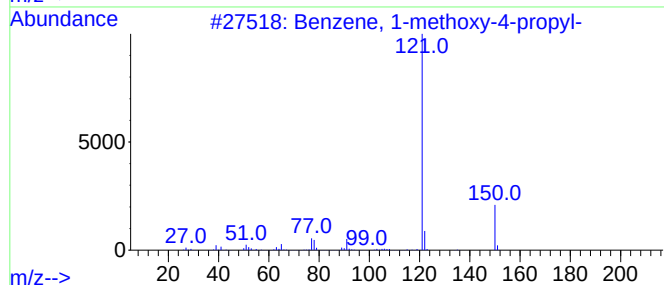
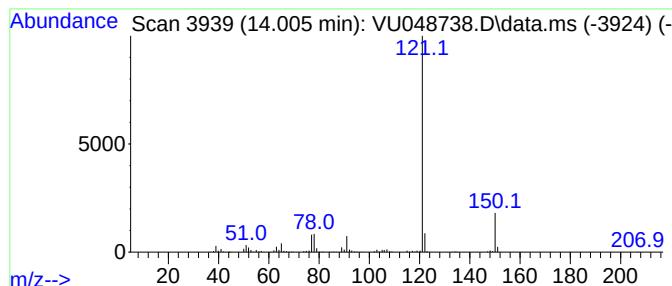
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1-methoxy-4-propyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.005	10.29 ug/l	331391	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methoxy-4-propyl-	150	C10H14O	000104-45-0	90
2			Phenol, 2-(1-methylpropyl)-	150	C10H14O	000089-72-5	86
3			Phenol, 4-(1-methylpropyl)-	150	C10H14O	000099-71-8	78
4			Fenobucarb	207	C12H17NO2	003766-81-2	78
5			2-Methyl-6-propylphenol	150	C10H14O	003520-52-3	78



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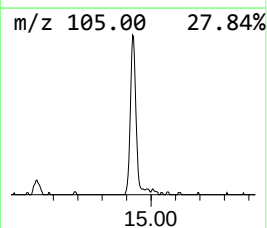
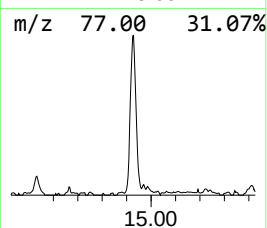
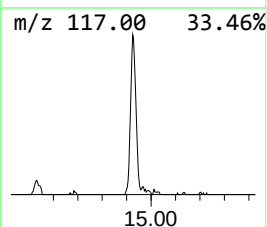
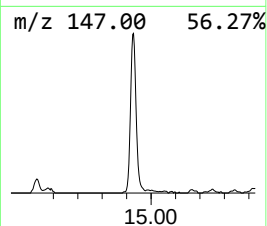
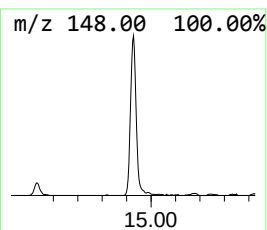
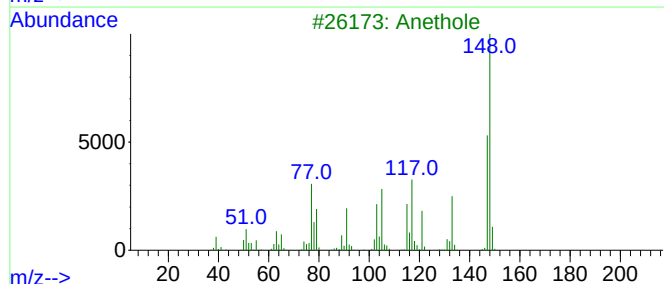
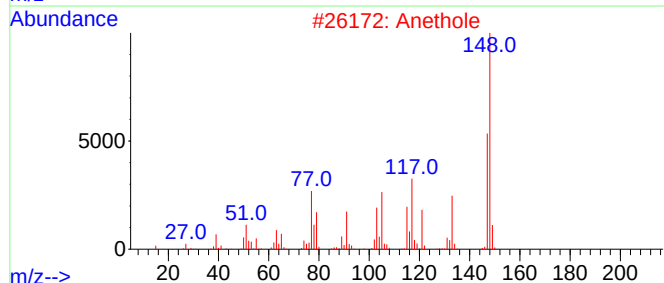
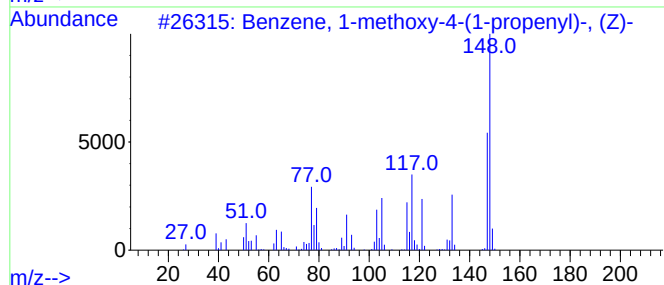
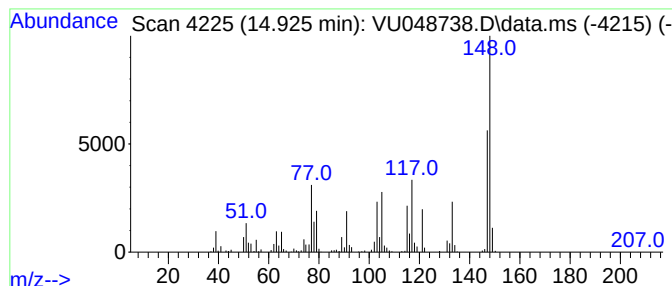
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-methoxy-4-(1-pro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.925	8.72 ug/l	280654	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methoxy-4-(1-propenyl...	148	C10H12O	025679-28-1	98
2			Anethole	148	C10H12O	000104-46-1	98
3			Anethole	148	C10H12O	004180-23-8	98
4			Estragole	148	C10H12O	000140-67-0	91
5			2-Isopropylbenzaldehyde	148	C10H12O	006502-22-3	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU053122\
Data File : VU048738.D
Acq On : 31 May 2022 14:21
Operator : SY/MD
Sample : N3067-01
Misc : 1.03g/10.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
33686

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U052622W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.459	43.1	ug/l	761494	1	5.366	882976	50.0
Eucalyptol	11.919	8.6	ug/l	277060	4	11.816	1610070	50.0
1-Octene, 6-met...	12.899	10.7	ug/l	344296	4	11.816	1610070	50.0
Benzene, 1-meth...	14.005	10.3	ug/l	331391	4	11.816	1610070	50.0
Benzene, 1-meth...	14.925	8.7	ug/l	280654	4	11.816	1610070	50.0