

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV111219\
 Data File : VV013591.D
 Acq On : 12 Nov 2019 16:08
 Operator : SY/MD
 Sample : K5797-03
 Misc : 25.0mL/MSVOA V/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AM0

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

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_V\METHOD\SOMVTR110819WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.113	4	7	12	rVB	20545	15435	1.11%	0.113%
2	1.222	37	41	46	rVB	37213	33826	2.43%	0.247%
3	1.296	58	64	81	rBV2	485934	540986	38.92%	3.949%
4	1.576	144	151	162	rVB	116018	136101	9.79%	0.993%
5	2.123	311	321	331	rBV	174471	248131	17.85%	1.811%
6	3.737	803	823	847	rBV2	505906	1390121	100.00%	10.146%
7	4.000	885	905	959	rBV3	92546	636298	45.77%	4.644%
8	4.393	1010	1027	1047	rBV	217880	522578	37.59%	3.814%
9	4.704	1111	1124	1142	rVB4	48062	119936	8.63%	0.875%
10	5.084	1227	1242	1271	rBV2	458031	1051131	75.61%	7.672%
11	5.656	1404	1420	1443	rBV	438460	870318	62.61%	6.352%
12	6.113	1548	1562	1583	rBV	279601	562719	40.48%	4.107%
13	6.582	1692	1708	1719	rBV	585923	1214209	87.35%	8.862%
14	7.026	1832	1846	1859	rBV2	131453	238575	17.16%	1.741%
15	7.354	1935	1948	1965	rBV	432115	747885	53.80%	5.459%
16	7.662	2033	2044	2055	rBV	77502	137807	9.91%	1.006%
17	7.981	2126	2143	2150	rBV4	14136	30817	2.22%	0.225%
18	8.138	2178	2192	2219	rBV	658044	1336481	96.14%	9.755%
19	8.286	2233	2238	2252	rVB8	30349	56122	4.04%	0.410%
20	8.891	2414	2426	2449	rBV	675135	1088130	78.28%	7.942%
21	9.852	2715	2725	2735	rVB8	15509	26558	1.91%	0.194%
22	10.257	2832	2851	2864	rBV	237673	374085	26.91%	2.730%
23	10.415	2891	2900	2911	rVB4	19276	33534	2.41%	0.245%
24	10.820	3015	3026	3039	rVB2	18755	33549	2.41%	0.245%
25	11.289	3161	3172	3193	rVB	605144	946256	68.07%	6.907%
26	11.569	3251	3259	3273	rBV4	27008	47860	3.44%	0.349%
27	11.666	3278	3289	3306	rVV	541256	846832	60.92%	6.181%
28	11.997	3385	3392	3400	rBV2	10140	16404	1.18%	0.120%
29	12.389	3505	3514	3522	rBV7	18847	26770	1.93%	0.195%
30	13.794	3936	3951	3961	rBV2	98336	161764	11.64%	1.181%
31	14.373	4121	4131	4143	rBV3	26091	47209	3.40%	0.345%
32	15.161	4367	4376	4385	rBV3	14084	23670	1.70%	0.173%
33	16.228	4700	4708	4717	rVB6	25300	36822	2.65%	0.269%
34	17.144	4985	4993	5008	rBV	66738	101879	7.33%	0.744%

LSC Area Percent Report

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 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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Title : TRACE VOA SOM01.0

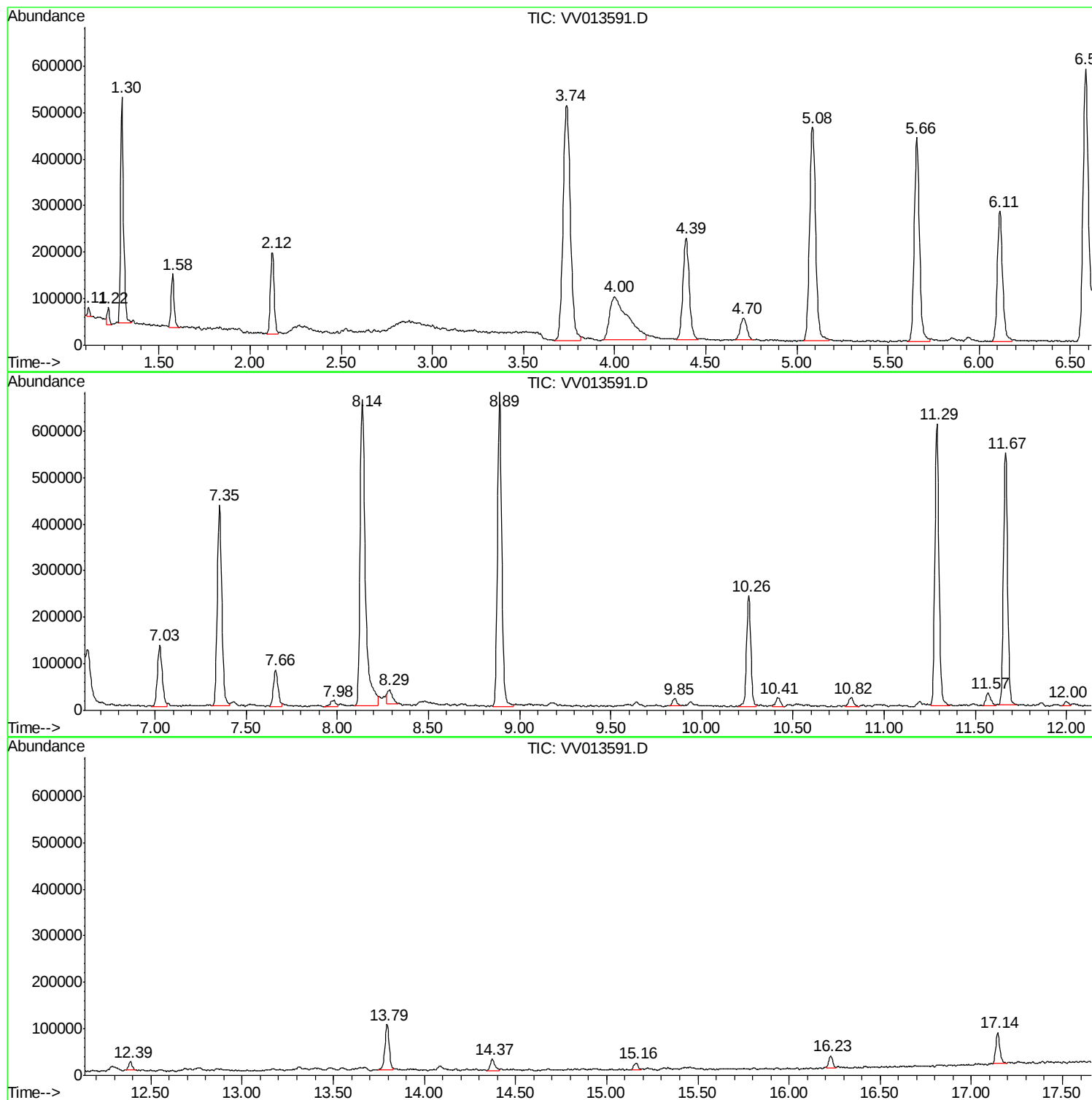
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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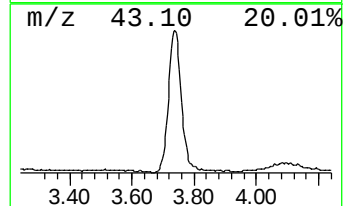
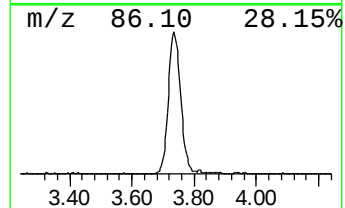
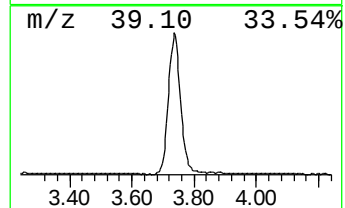
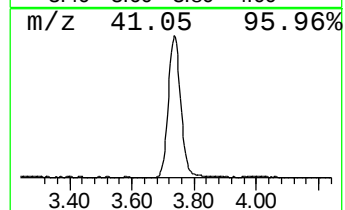
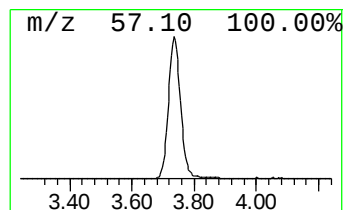
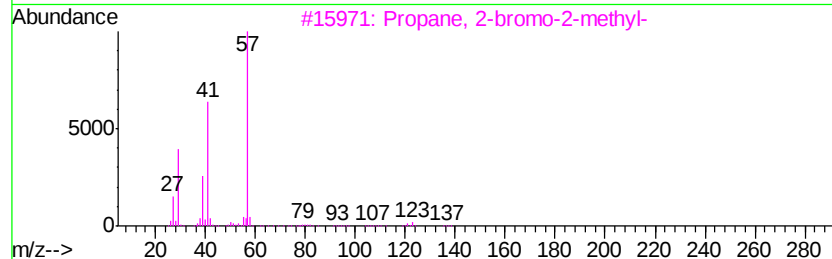
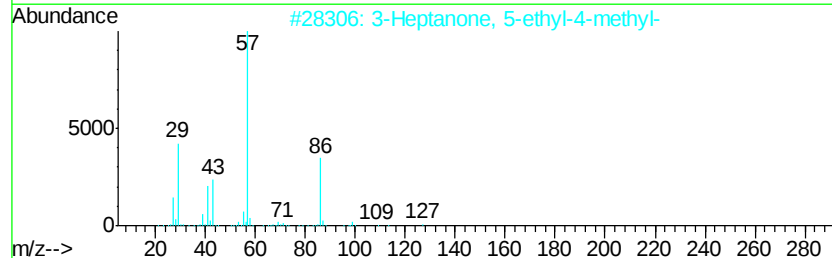
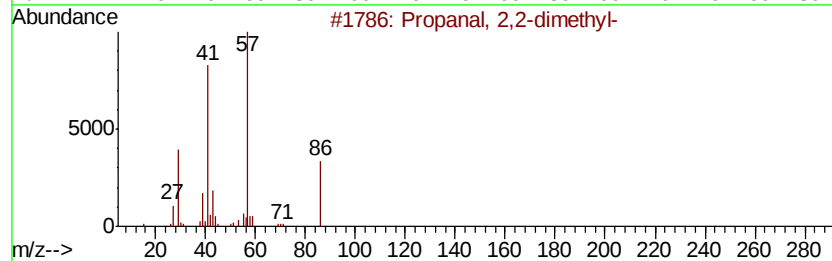
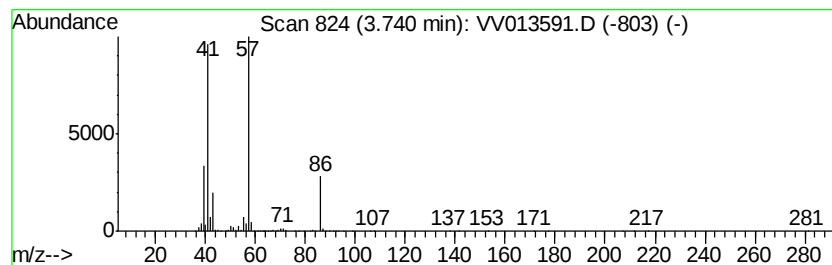
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR110819WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Propanal, 2,2-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.74	7.99 ug/L	1390120	1,4-Difluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	64
2		3-Heptanone, 5-ethyl-4-methyl-	156	C10H20O	027607-63-2	53
3		Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	47
4		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	47
5		Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	45



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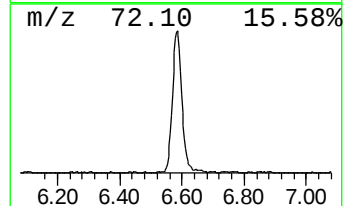
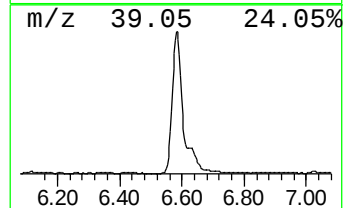
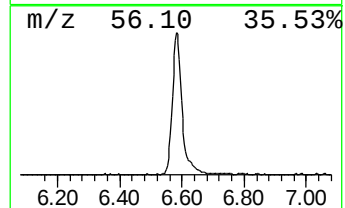
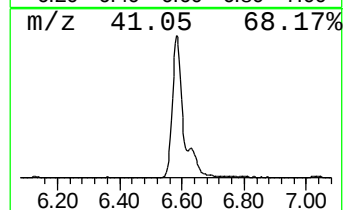
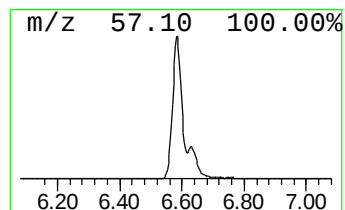
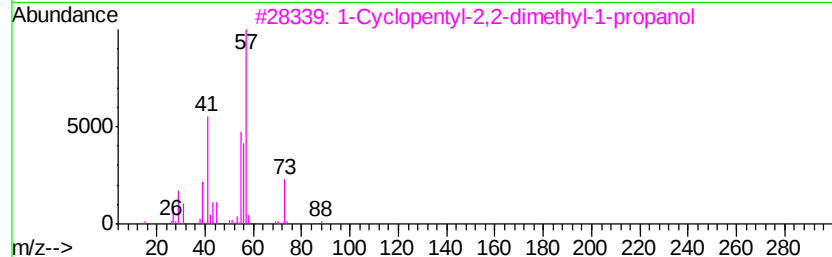
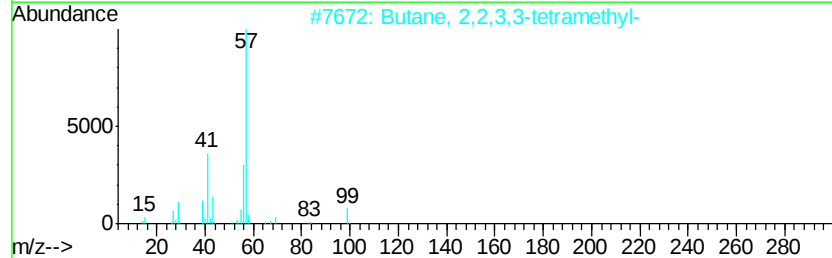
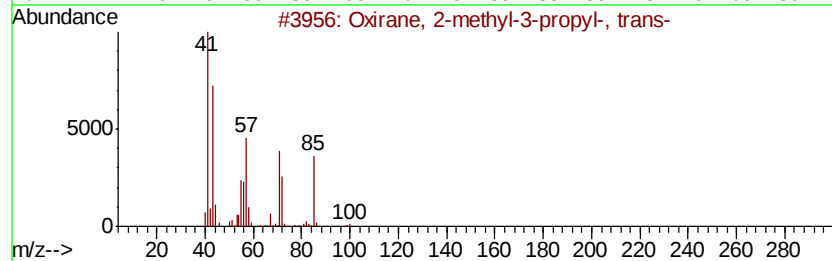
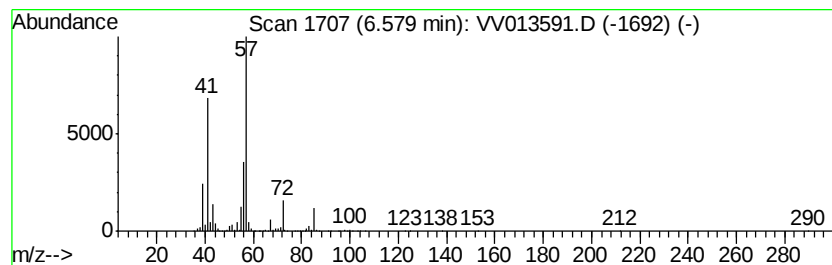
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR110819WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	6.98 ug/L	1214210	1,4-Difluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxirane, 2-methyl-3-propyl-, trans-	100	C6H12O	006124-91-0	43
2		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	38
3		1-Cyclopentyl-2,2-dimethyl-1-propanol	156	C10H20O	337966-85-5	38
4		1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	38
5		Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	38



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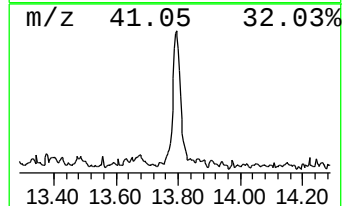
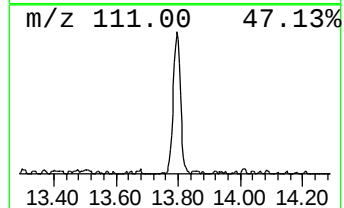
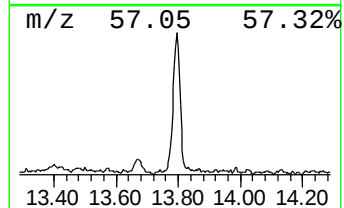
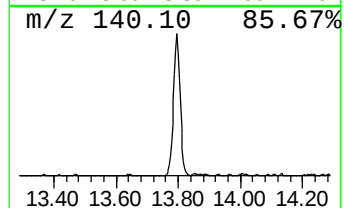
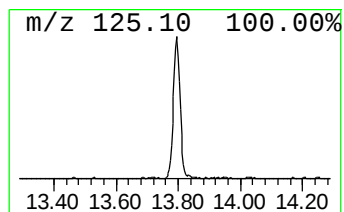
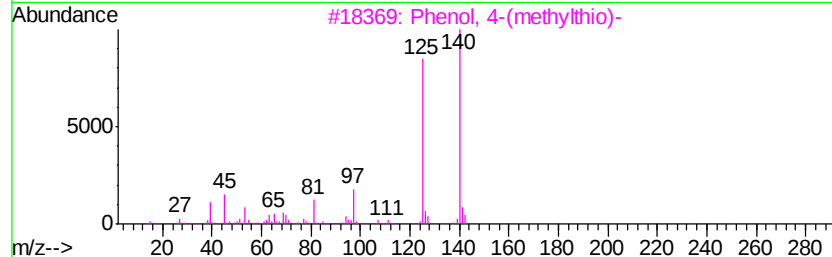
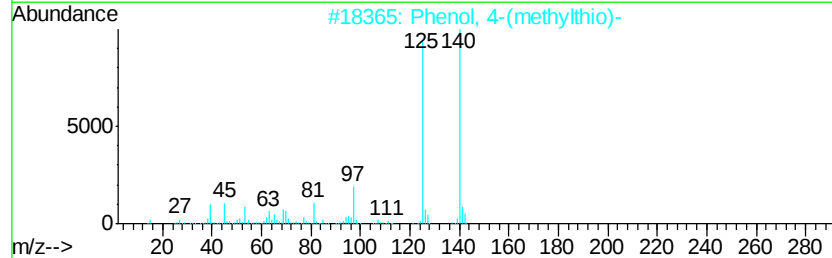
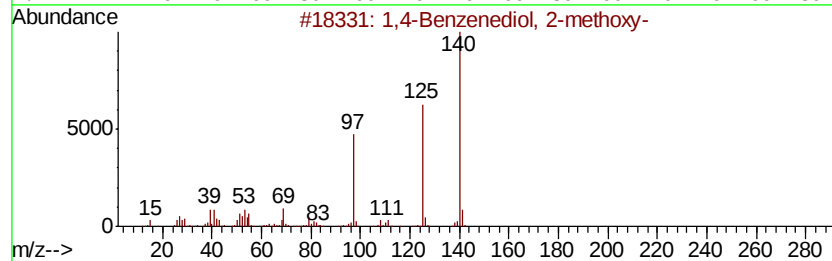
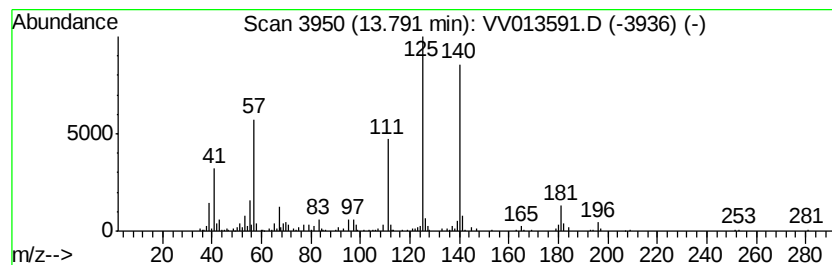
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 1,4-Benzenediol, 2-methoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	0.85 ug/L	161764	1,4-Dichlorobenzene-d4	11.29

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Benzenediol, 2-methoxy-	140	C7H8O3	000824-46-4	53
2		Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	53
3		Phenol, 4-(methylthio)-	140	C7H8OS	001073-72-9	53
4		Benzenethiol, 2-methoxy-	140	C7H8OS	007217-59-6	53
5		Benzenethiol, 4-methoxy-	140	C7H8OS	000696-63-9	43



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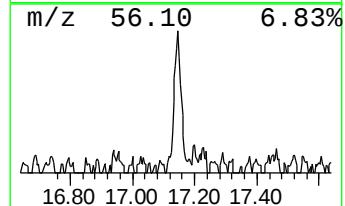
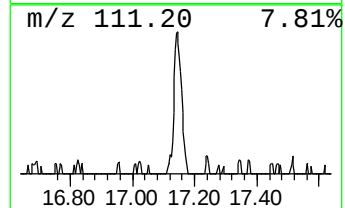
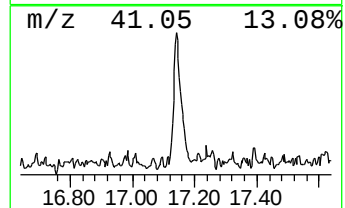
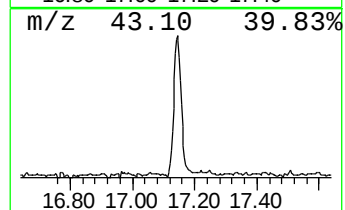
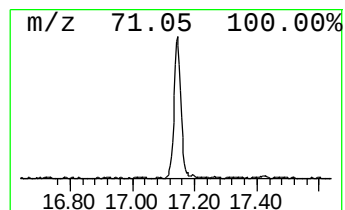
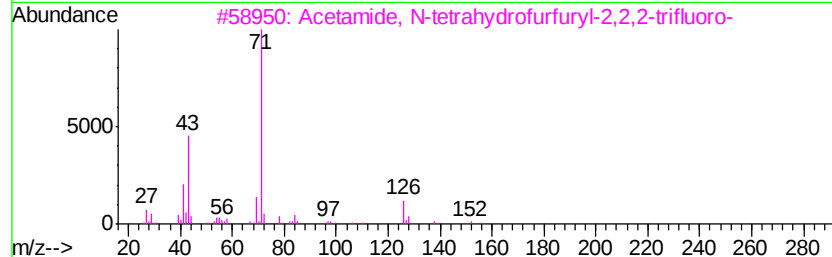
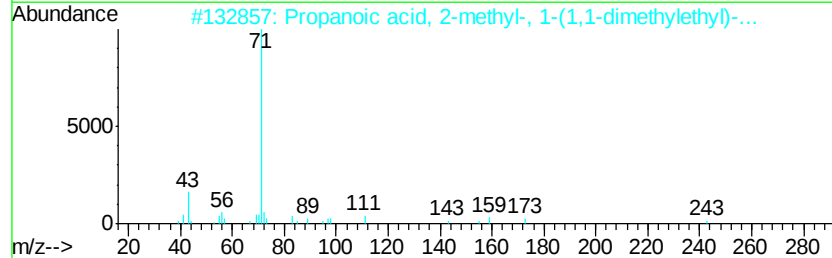
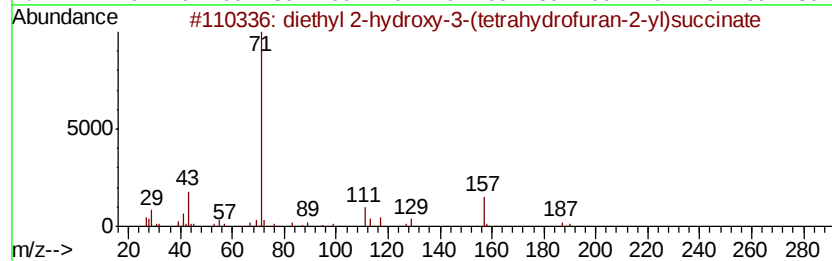
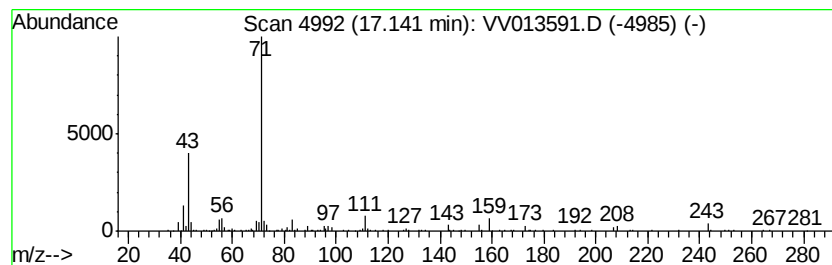
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 diethyl 2-hydroxy-3-(tetrah... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.14	0.54 ug/L	101879	1,4-Dichlorobenzene-d4	11.29

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		diethyl 2-hydroxy-3-(tetrahydrofuran-2-yl)succinate	260	C12H20O6	1000365-67-1	59
2		Propanoic acid, 2-methyl-, 1-(1,1-dimethylethyl)-...	286	C16H30O4	074381-40-1	56
3		Acetamide, N-tetrahydrofurfuryl-2,2,2-trifluoro-	197	C7H10F3NO2	1000307-30-7	53
4		Furan, 2-butyltetrahydro-	128	C8H16O	001004-29-1	53
5		Oxalic acid, decyl neopentyl ester	300	C17H32O4	1000309-73-4	45



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanal, 2,2-dim...	3.74	8.0	ug/L	1390120	1	5.66	870318	5.0
unknown-01	6.58	7.0	ug/L	1214210	1	5.66	870318	5.0
1,4-Benzenediol, ...	13.79	0.8	ug/L	161764	3	11.29	946256	5.0
diethyl 2-hydroxy...	17.14	0.5	ug/L	101879	3	11.29	946256	5.0