

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051220\
 Data File : VU038127.D
 Acq On : 12 May 2020 16:22
 Operator : JC/MD
 Sample : L2570-04
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFSP4

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_U\METHOD\SOMUTR050720WMA.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	1.613	74	85	94	rBV	201880	229869	10.79%	1.418%
2	1.932	175	184	195	rVB	174269	220415	10.35%	1.359%
3	2.591	378	389	403	rVB	287161	463124	21.75%	2.856%
4	3.218	574	584	601	rVB	17471	39208	1.84%	0.242%
5	4.687	1022	1041	1099	rBV3	269752	1072799	50.38%	6.616%
6	5.102	1152	1170	1197	rBV2	262971	582029	27.33%	3.589%
7	5.758	1351	1374	1408	rBV2	560523	1506691	70.75%	9.291%
8	6.279	1521	1536	1559	rBV	448564	863499	40.55%	5.325%
9	6.536	1601	1616	1638	rBV	40961	99809	4.69%	0.615%
10	6.719	1657	1673	1692	rBV	350104	688246	32.32%	4.244%
11	6.832	1697	1708	1723	rVB6	12729	27654	1.30%	0.171%
12	7.591	1929	1944	1963	rBV	178495	317151	14.89%	1.956%
13	7.922	2029	2047	2077	rBV	673526	1213996	57.01%	7.486%
14	8.202	2117	2134	2151	rBV	118374	205885	9.67%	1.270%
15	8.510	2221	2230	2242	rVB	14461	25240	1.19%	0.156%
16	8.658	2260	2276	2316	rBV	1091991	2129572	100.00%	13.133%
17	9.436	2505	2518	2545	rBV	646512	1169956	54.94%	7.215%
18	9.710	2592	2603	2613	rBV2	28545	48845	2.29%	0.301%
19	9.777	2613	2624	2645	rVB	109372	191992	9.02%	1.184%
20	10.115	2719	2729	2748	rVB4	16691	30719	1.44%	0.189%
21	10.584	2858	2875	2887	rBV4	28833	53888	2.53%	0.332%
22	10.771	2921	2933	2949	rVB	282898	447764	21.03%	2.761%
23	10.896	2958	2972	2982	rBV3	54652	94606	4.44%	0.583%
24	11.404	3122	3130	3140	rVB3	23216	36699	1.72%	0.226%
25	11.645	3191	3205	3227	rBV3	62302	137577	6.46%	0.848%
26	11.825	3248	3261	3277	rBV	691810	1155122	54.24%	7.123%
27	11.906	3278	3286	3297	rVV8	18014	43702	2.05%	0.269%
28	11.957	3298	3302	3316	rVB5	13592	26241	1.23%	0.162%
29	12.105	3332	3348	3356	rBV2	39164	77296	3.63%	0.477%
30	12.205	3366	3379	3399	rBV2	713517	1293433	60.74%	7.976%
31	12.555	3478	3488	3505	rVB	72625	122364	5.75%	0.755%
32	12.841	3570	3577	3588	rVB5	18417	34561	1.62%	0.213%
33	13.070	3643	3648	3659	rVB7	24587	36477	1.71%	0.225%
34	13.478	3765	3775	3790	rVB8	43220	88341	4.15%	0.545%

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35	13.629	3810	3822	3842	rBV7	86183	208459	9.79%	1.286%
36	13.880	3890	3900	3909	rBV4	42511	80405	3.78%	0.496%
37	13.983	3924	3932	3937	rBV8	21905	38590	1.81%	0.238%
38	14.028	3942	3946	3954	rVB4	27579	37288	1.75%	0.230%
39	14.227	3997	4008	4021	rBV3	51294	92801	4.36%	0.572%
40	14.597	4114	4123	4135	rVB	139596	223777	10.51%	1.380%
41	15.031	4250	4258	4259	rBV5	22195	29092	1.37%	0.179%
42	15.118	4276	4285	4296	rVB4	129380	224613	10.55%	1.385%
43	15.259	4322	4329	4338	rVB2	43651	65173	3.06%	0.402%
44	15.314	4341	4346	4358	rVB5	18182	28491	1.34%	0.176%
45	15.404	4368	4374	4383	rVV4	21696	33879	1.59%	0.209%
46	15.455	4386	4390	4400	rVB3	17738	23576	1.11%	0.145%
47	15.851	4508	4513	4523	rVB	28024	42127	1.98%	0.260%
48	16.044	4566	4573	4584	rVB2	38634	58548	2.75%	0.361%
49	16.147	4599	4605	4625	rVB2	66386	119880	5.63%	0.739%
50	16.365	4668	4673	4682	rVB4	17705	24564	1.15%	0.151%
51	16.844	4812	4822	4835	rBV4	60025	109959	5.16%	0.678%

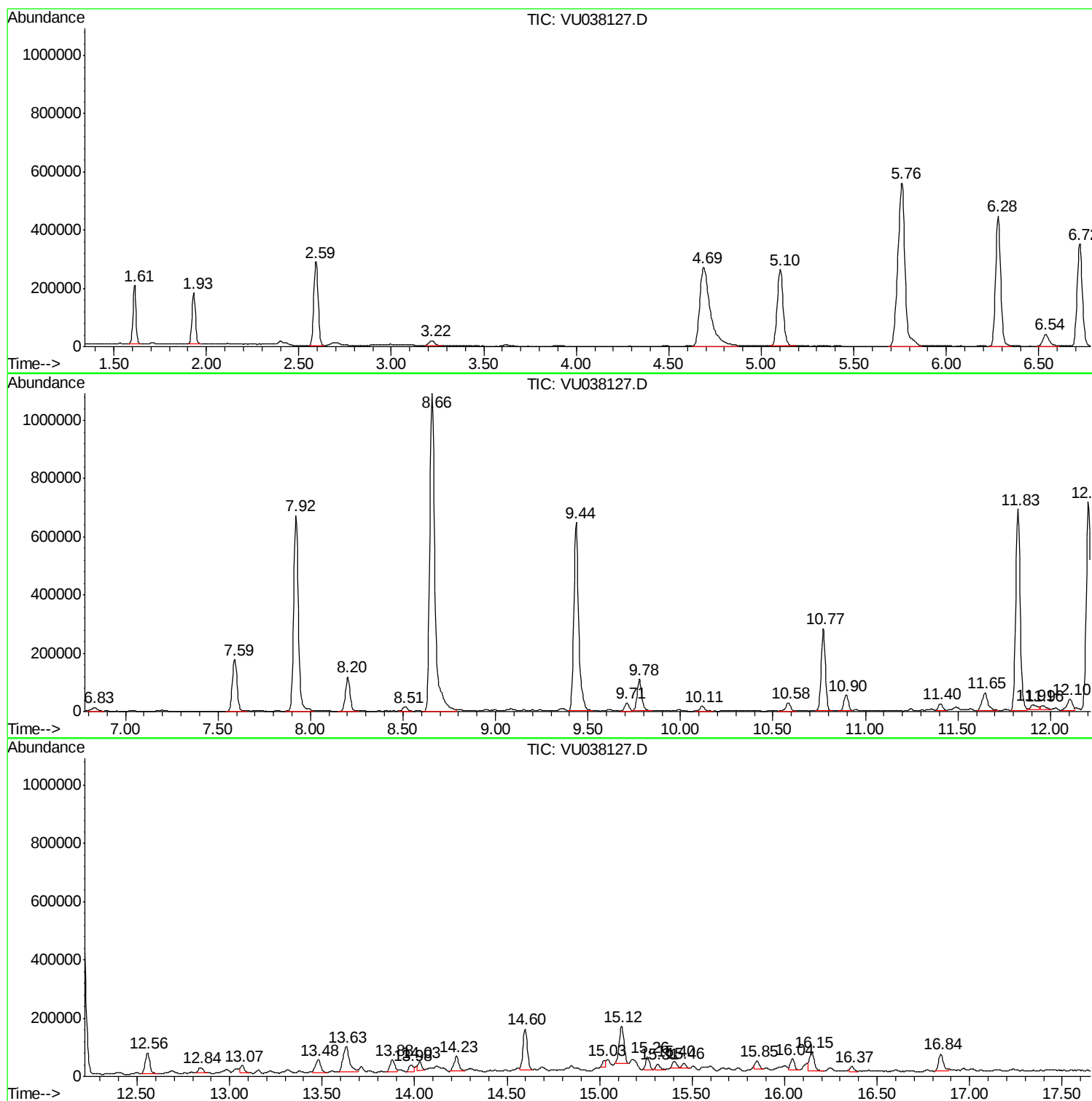
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Instrument :
MSVOA_U
ClientSampled :
BFSP4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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



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MSVOA_U
ClientSampleId :
BFSP4

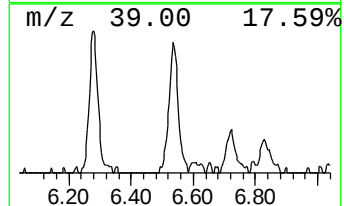
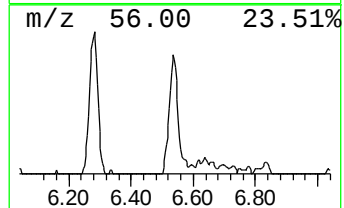
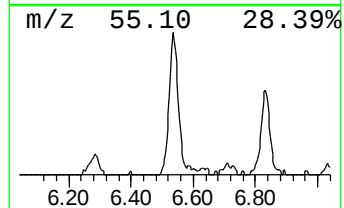
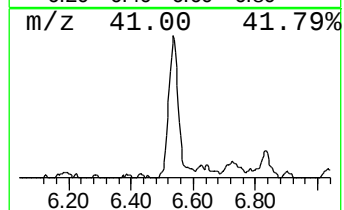
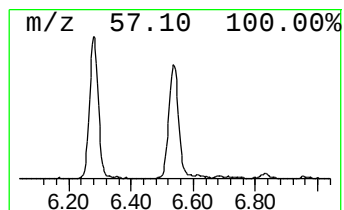
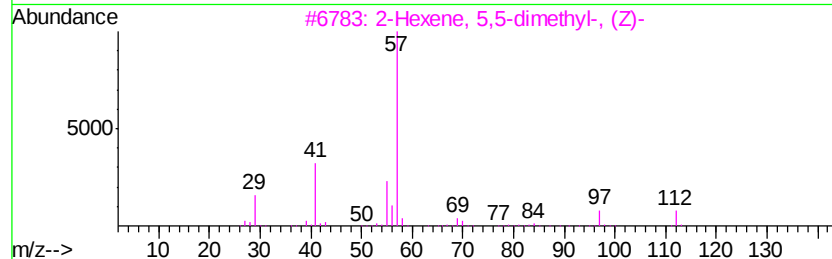
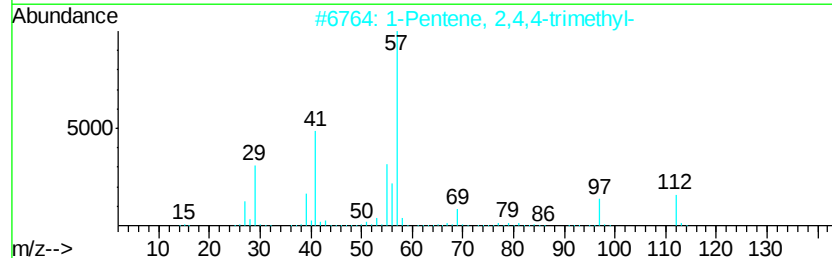
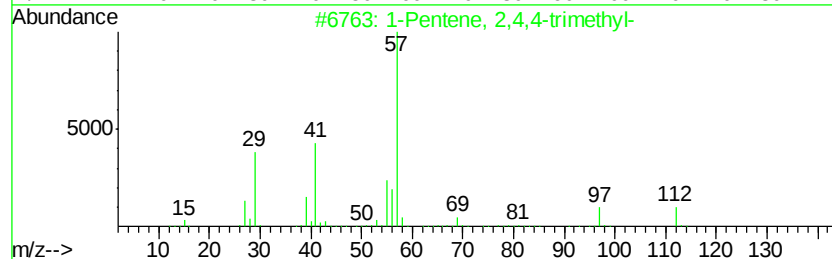
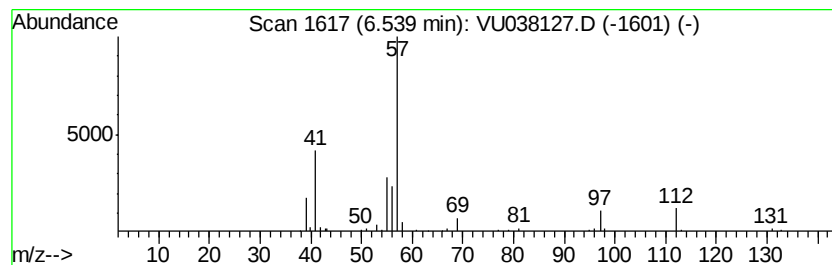
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 1-Pentene, 2,4,4-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	0.58 ug/L	99809	1,4-Difluorobenzene	6.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-39-1	81
2			1-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-39-1	81
3			2-Hexene, 5,5-dimethyl-, (Z)-	112	C8H16	039761-61-0	58
4			2,4,4-Trimethyl-1-pentanol	130	C8H18O	016325-63-6	53
5			1-Pentene, 2,4,4-trimethyl-	112	C8H16	000107-39-1	46



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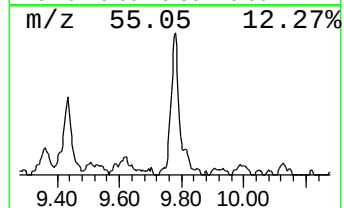
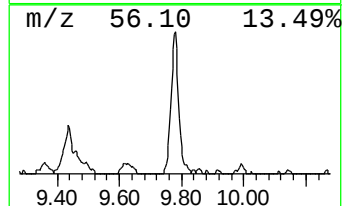
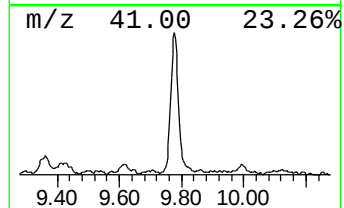
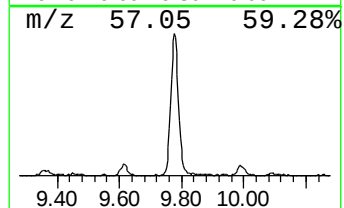
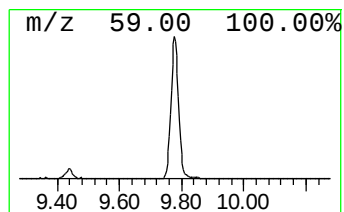
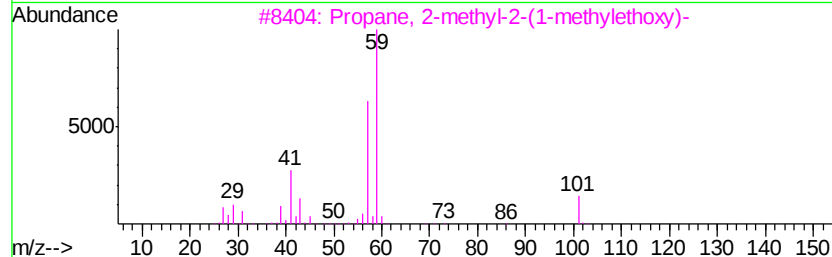
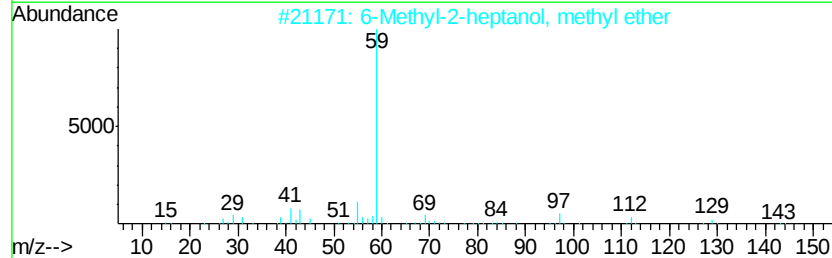
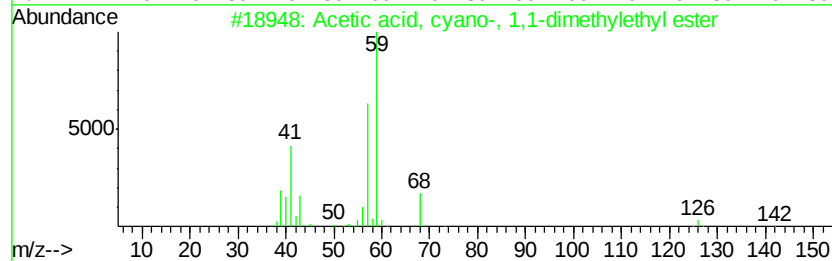
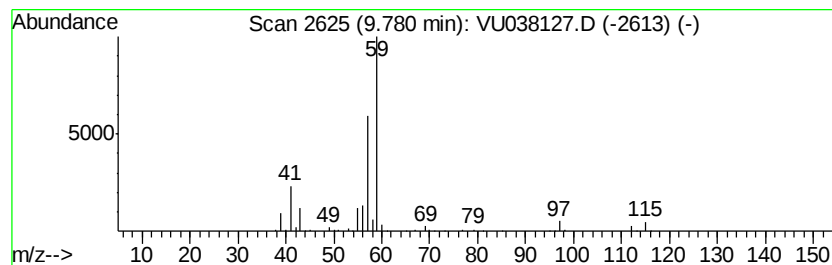
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 Acetic acid, cyano-, 1,1-di... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.78	0.82 ug/L	191992	Chlorobenzene-d5	9.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	56
2		6-Methyl-2-heptanol, methyl ether	144	C9H20O	1000365-52-0	39
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	39
4		2-Hexanol, 2,3-dimethyl-	130	C8H18O	019550-03-9	38
5		Butane, 2-methoxy-3-methyl-	102	C6H14O	062016-49-3	36



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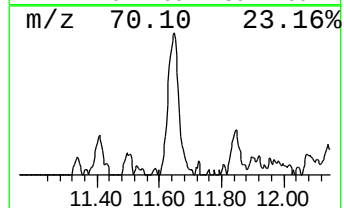
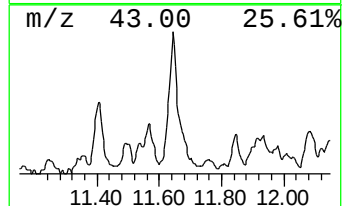
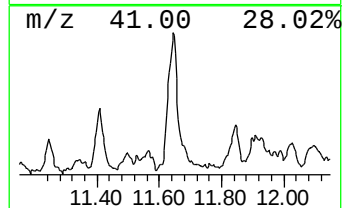
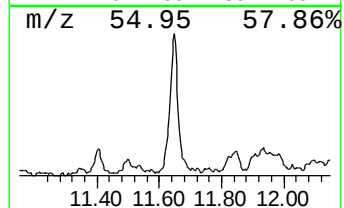
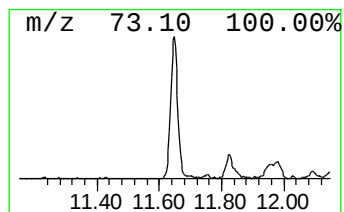
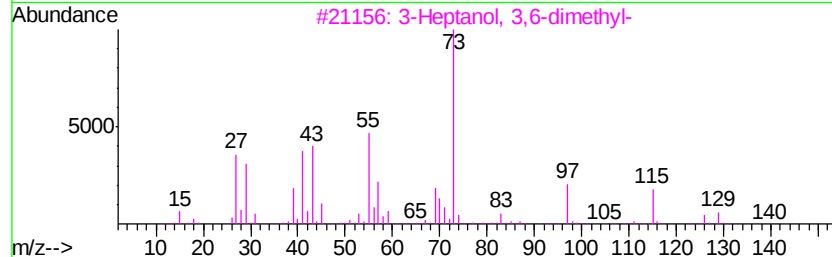
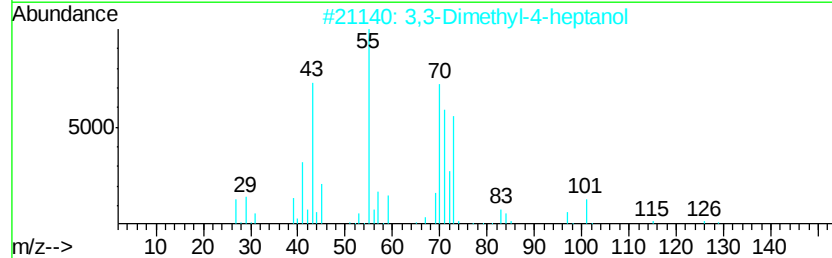
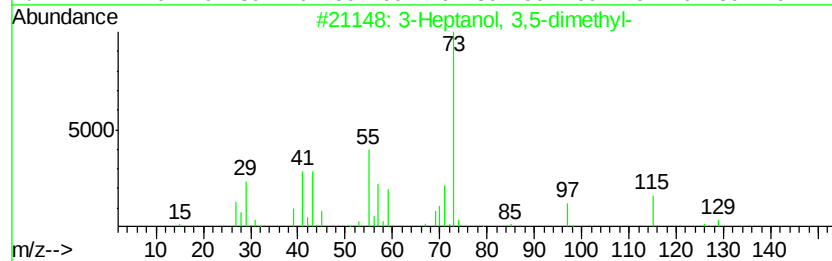
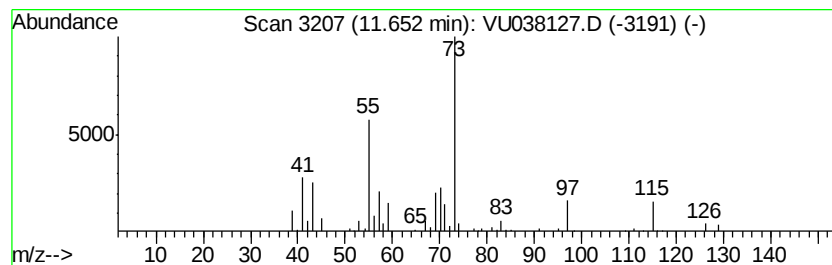
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 3-Heptanol, 3,5-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.65	0.60 ug/L	137577	1,4-Dichlorobenzene-d4	11.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Heptanol, 3,5-dimethyl-	144	C9H20O	019549-74-7	50
2			3,3-Dimethyl-4-heptanol	144	C9H20O	019549-78-1	23
3			3-Heptanol, 3,6-dimethyl-	144	C9H20O	001573-28-0	16
4			(SS)- or (RR)-4-methyl-2,3-penta...	118	C6H14O2	006464-40-0	10
5			Morpholine, 2,6-dimethyl-	115	C6H13NO	000141-91-3	10



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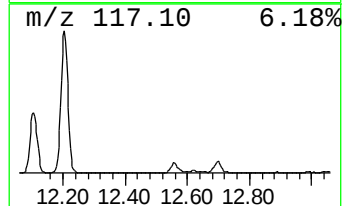
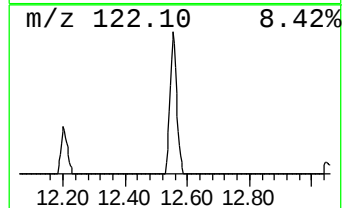
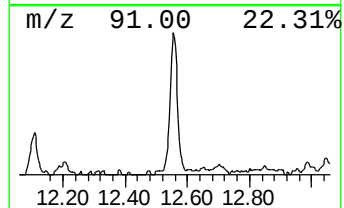
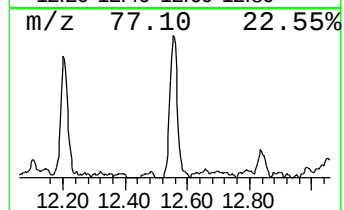
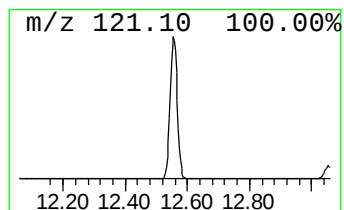
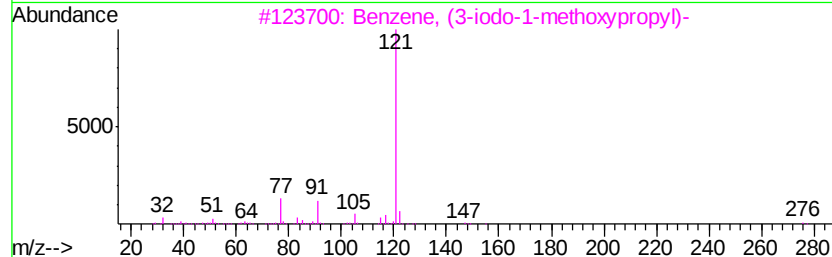
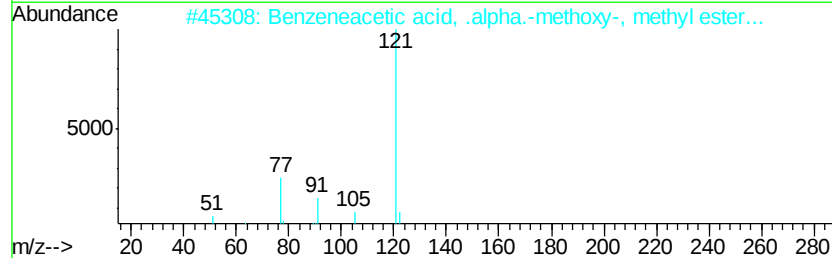
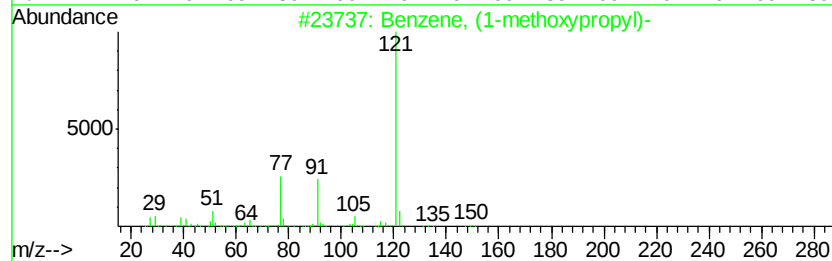
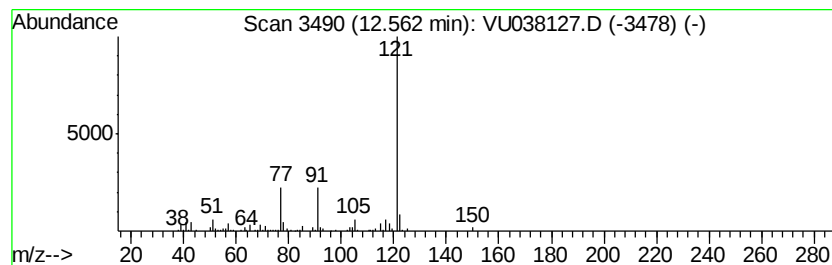
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzene, (1-methoxypropyl)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.56	0.53 ug/L	122364	1,4-Dichlorobenzene-d4	11.83

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzene, (1-methoxypropyl)-	150	C10H14O	059588-12-4	87
2		Benzeneacetic acid, .alpha.-meth...	180	C10H12O3	056143-21-6	64
3		Benzene, (3-iodo-1-methoxypropyl)-	276	C10H13IO	1000327-31-9	64
4		Benzeneacetic acid, .alpha.-meth...	180	C10H12O3	056143-21-6	64
5		Benzene, (3-iodo-1-methoxybutyl)-	290	C11H15IO	1000327-38-8	56



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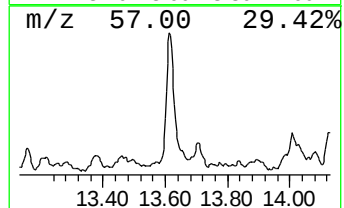
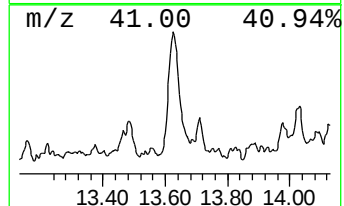
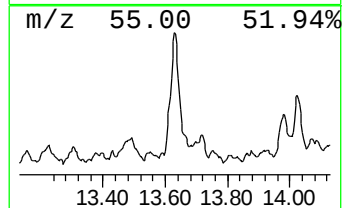
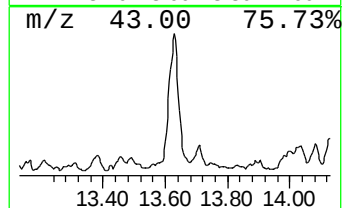
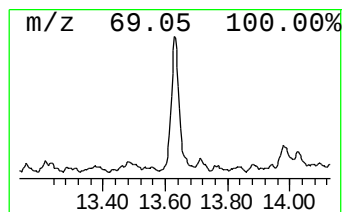
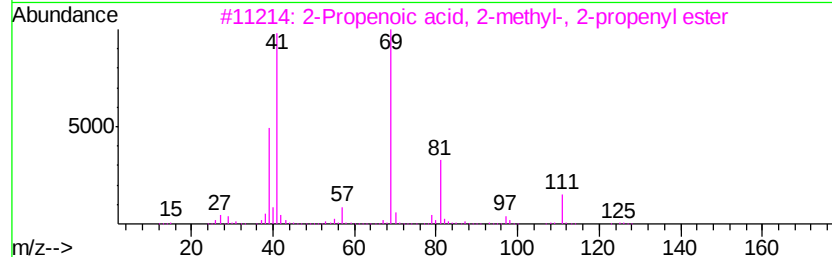
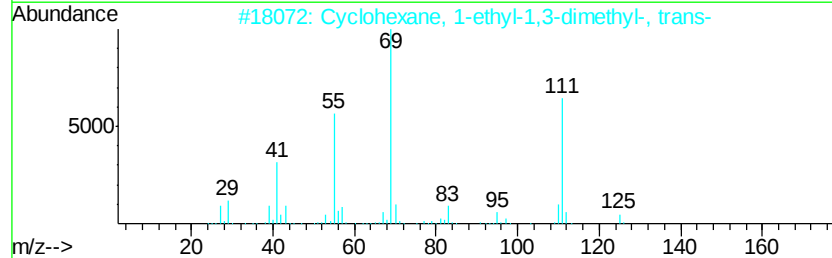
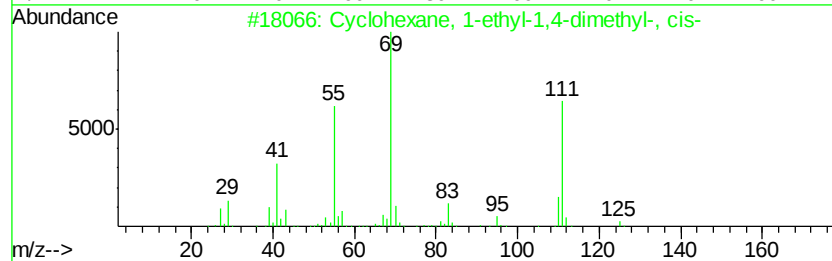
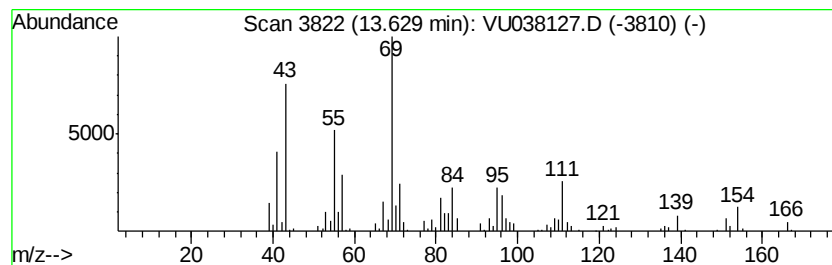
Instrument :
MSVOA_U
ClientSampleId :
BFSP4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 (DEL) Alkane: Cyclic13.63 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.63	0.90 ug/L	208459	1,4-Dichlorobenzene-d4	11.83	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-1,4-dimethy...	140	C10H20	062238-30-6	43
2	Cyclohexane, 1-ethyl-1,3-dimethy...	140	C10H20	062238-29-3	38
3	2-Propenoic acid, 2-methyl-, 2-p...	126	C7H10O2	000096-05-9	38
4	Cyclohexane, 1-ethyl-1,3-dimethy...	140	C10H20	062238-31-7	38
5	4-Methyl-2-hexene,c&t	98	C7H14	003404-55-5	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051220\
Data File : VU038127.D
Acq On : 12 May 2020 16:22
Operator : JC/MD
Sample : L2570-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFSP4

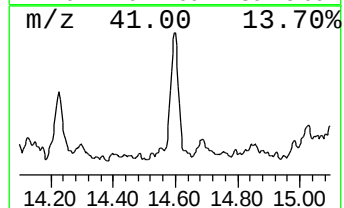
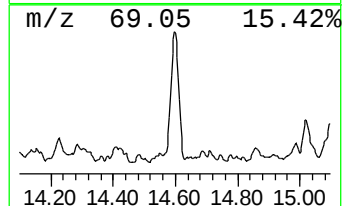
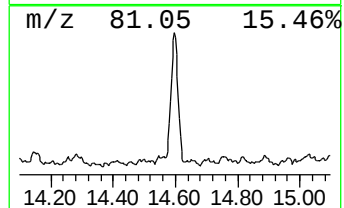
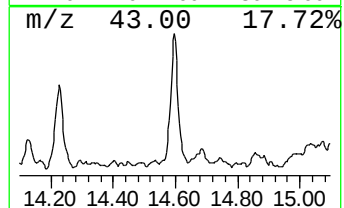
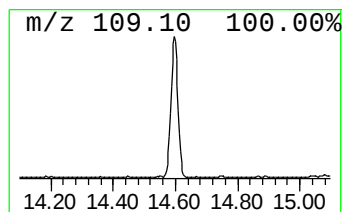
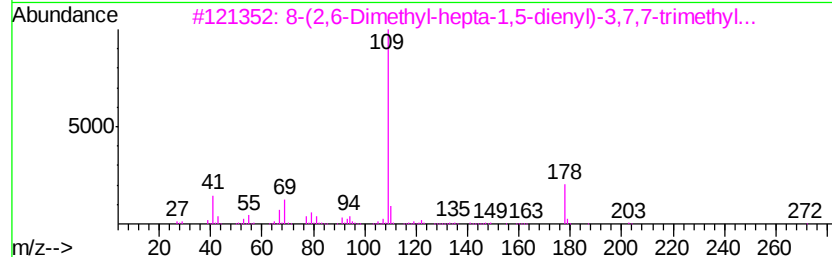
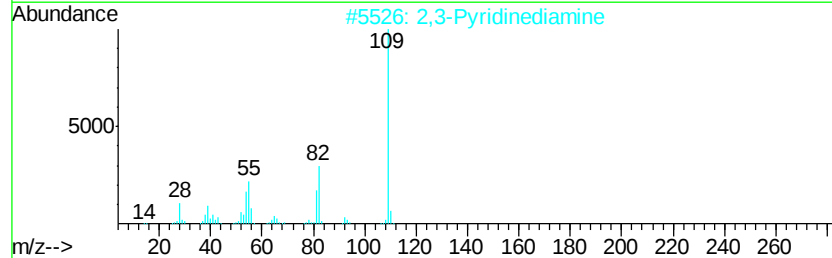
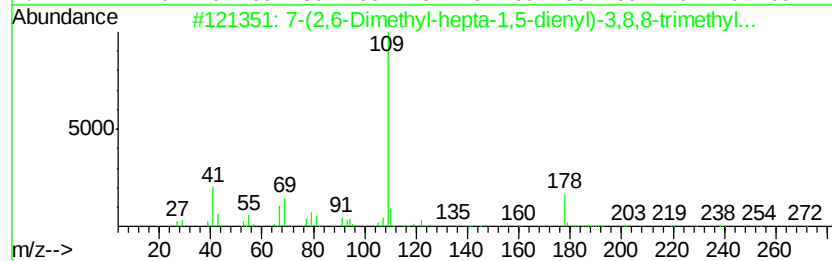
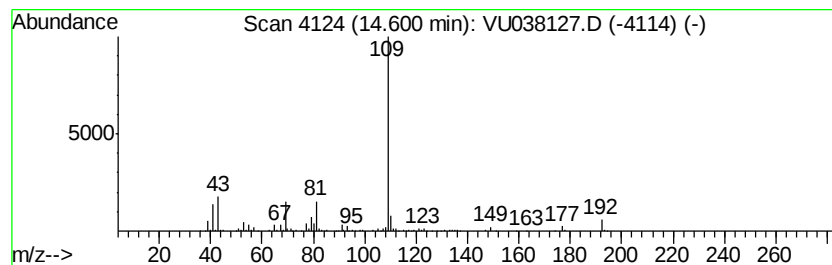
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 7-(2,6-Dimethyl-hepta-1,5-d... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	0.97 ug/L	223777	1,4-Dichlorobenzene-d4	11.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	7-(2,6-Dimethyl-hepta-1,5-dienyl...	272	C20H32	1000190-62-8	64
2		2,3-Pyridinediamine	109	C5H7N3	000452-58-4	58
3		8-(2,6-Dimethyl-hepta-1,5-dienyl...	272	C20H32	113725-56-7	50
4		Pyridine, 3-methoxy-	109	C6H7NO	007295-76-3	40
5		1,2-Benzenediol, 0-(ethoxycarbon...	264	C13H12O6	1000329-71-6	39



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051220\
Data File : VU038127.D
Acq On : 12 May 2020 16:22
Operator : JC/MD
Sample : L2570-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFSP4

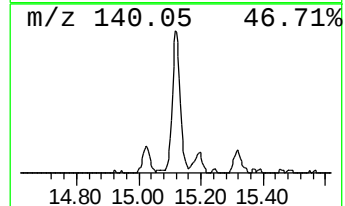
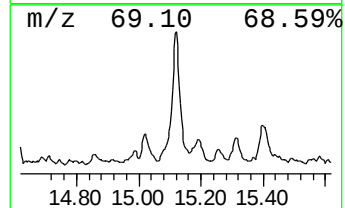
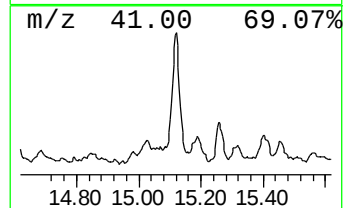
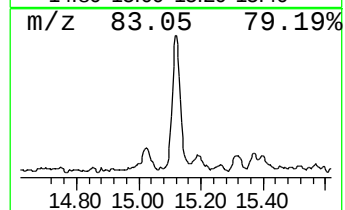
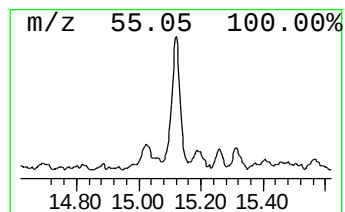
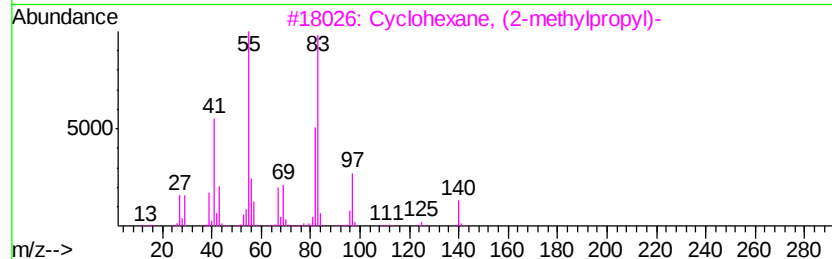
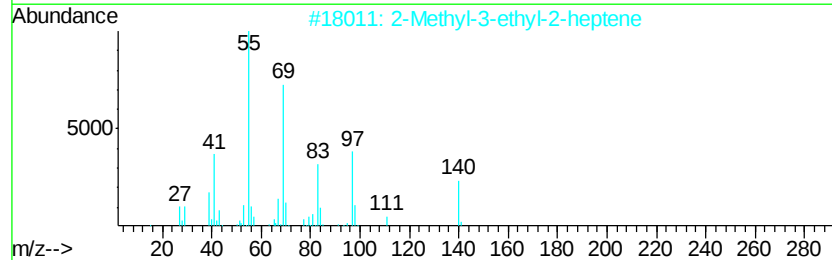
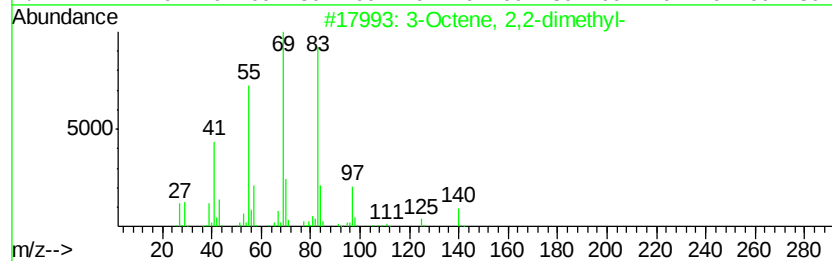
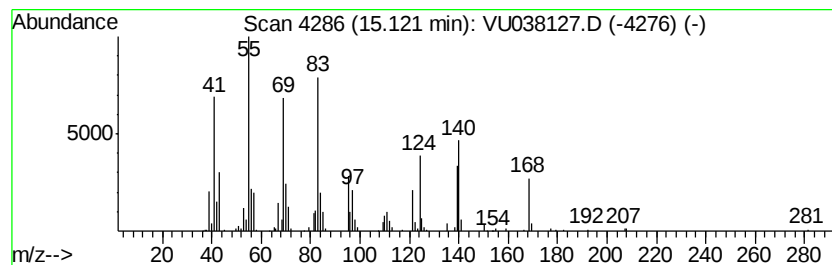
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.12	0.97 ug/L	224613	1,4-Dichlorobenzene-d4	11.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Octene, 2,2-dimethyl-	140	C10H20	086869-76-3	49
2			2-Methyl-3-ethyl-2-heptene	140	C10H20	019780-61-1	46
3			Cyclohexane, (2-methylpropyl)-	140	C10H20	001678-98-4	46
4			1,3-Cyclohexanedione, 5,5-dimethyl-	140	C8H12O2	000126-81-8	43
5			2,3-Dimethyl-2-octene	140	C10H20	019781-18-1	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051220\
Data File : VU038127.D
Acq On : 12 May 2020 16:22
Operator : JC/MD
Sample : L2570-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFSP4

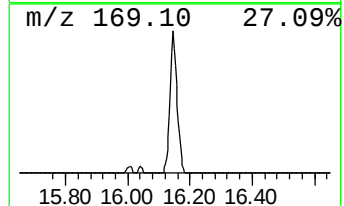
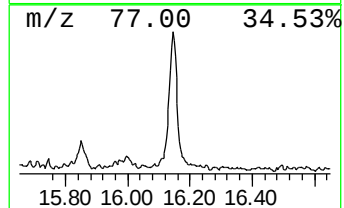
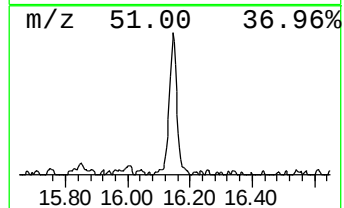
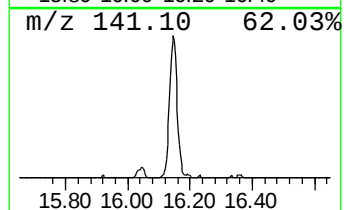
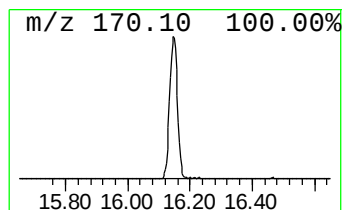
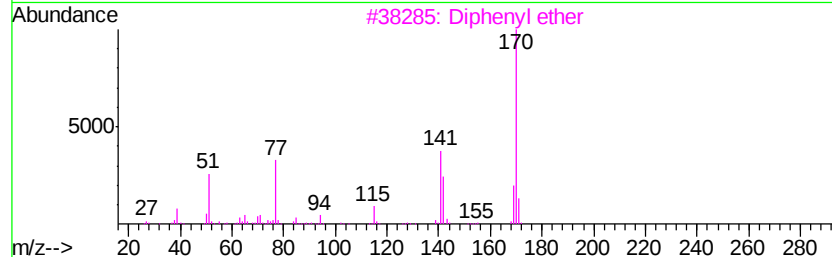
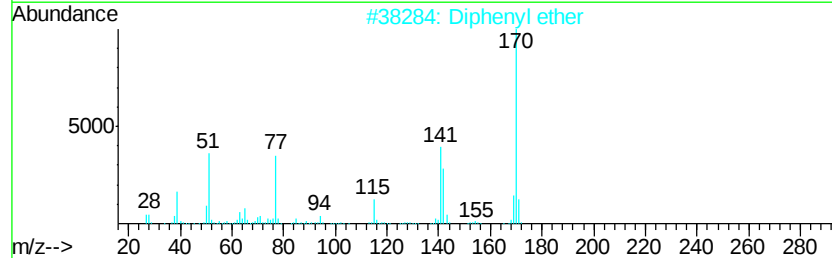
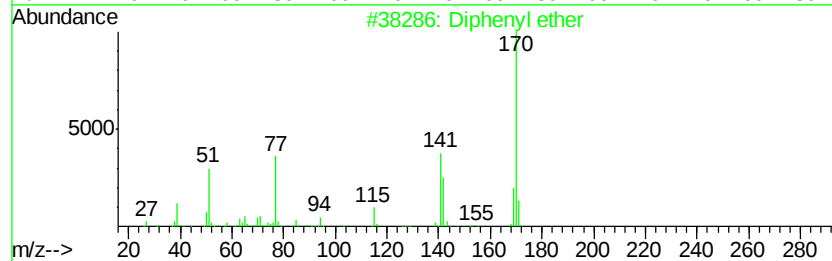
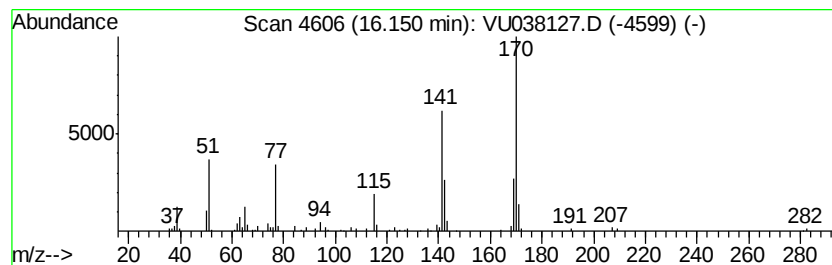
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 9 Diphenyl ether Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.15	0.52 ug/L	119880	1,4-Dichlorobenzene-d4	11.83

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diphenyl ether	170	C12H10O	000101-84-8	90	
2	Diphenyl ether	170	C12H10O	000101-84-8	87	
3	Diphenyl ether	170	C12H10O	000101-84-8	81	
4	Spiro[cyclopropane-1,1'(4'H)-nap...	170	C12H10O	033498-24-7	76	
5	Diphenyl ether	170	C12H10O	000101-84-8	64	



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051220\
Data File : VU038127.D
Acq On : 12 May 2020 16:22
Operator : JC/MD
Sample : L2570-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFSP4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR050720WMA.M
Quant Title : TRACE VOA SOM01.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Pentene, 2,4,4-...	6.54	0.6	ug/L	99809	1	6.28	863499	5.0
Acetic acid, cyan...	9.78	0.8	ug/L	191992	2	9.44	1169960	5.0
3-Heptanol, 3,5-d...	11.65	0.6	ug/L	137577	3	11.83	1155120	5.0
Benzene, (1-metho...	12.56	0.5	ug/L	122364	3	11.83	1155120	5.0
(DEL) Alkane: Cyc...	13.63	0.9	ug/L	208459	3	11.83	1155120	5.0
7-(2,6-Dimethyl-h...	14.60	1.0	ug/L	223777	3	11.83	1155120	5.0
(DEL) Alkane: Str...	15.12	1.0	ug/L	224613	3	11.83	1155120	5.0
Diphenyl ether	16.15	0.5	ug/L	119880	3	11.83	1155120	5.0