

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV062420\
 Data File : VV017081.D
 Acq On : 24 Jun 2020 19:05
 Operator : SY/MD
 Sample : L3105-05
 Misc : 25.0mL/MSVOA V/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BFXK8

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\SOMVTR061720WMA.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	3	7	16	rVB	152524	140942	4.68%	0.668%
2	1.322	62	72	90	rBV	2021391	2111096	70.15%	10.004%
3	1.579	145	152	165	rVB	57646	67742	2.25%	0.321%
4	2.129	311	323	337	rBV3	182203	318536	10.58%	1.509%
5	2.550	433	454	467	rBV	118049	294472	9.79%	1.395%
6	2.782	511	526	544	rBV	473757	924853	30.73%	4.383%
7	3.061	597	613	627	rBV2	97408	198184	6.59%	0.939%
8	3.212	641	660	686	rBV	610104	1281890	42.60%	6.074%
9	3.788	815	839	861	rBV	1113830	2828883	94.00%	13.405%
10	3.939	868	886	921	rBV2	1213221	3009415	100.00%	14.261%
11	4.100	921	936	968	rVB	526130	1340350	44.54%	6.351%
12	4.380	1006	1023	1045	rBV2	114406	322046	10.70%	1.526%
13	4.634	1085	1102	1114	rBV	201704	505320	16.79%	2.395%
14	4.704	1114	1124	1143	rVB2	138334	341389	11.34%	1.618%
15	5.074	1220	1239	1248	rBV3	236380	570395	18.95%	2.703%
16	5.126	1249	1255	1279	rVB2	143554	331420	11.01%	1.570%
17	5.643	1402	1416	1437	rBV2	218166	448057	14.89%	2.123%
18	5.942	1497	1509	1526	rBV	39483	79893	2.65%	0.379%
19	6.097	1543	1557	1576	rBV2	133253	273434	9.09%	1.296%
20	7.010	1825	1841	1860	rBV	71320	130353	4.33%	0.618%
21	7.338	1931	1943	1958	rBV	282960	491534	16.33%	2.329%
22	7.643	2026	2038	2052	rBV2	43367	79583	2.64%	0.377%
23	7.862	2095	2106	2122	rBV2	67399	116693	3.88%	0.553%
24	8.109	2172	2183	2206	rBV	285020	483202	16.06%	2.290%
25	8.322	2240	2249	2265	rVB	29132	48318	1.61%	0.229%
26	8.900	2408	2429	2453	rBV2	918445	2000549	66.48%	9.480%
27	9.566	2621	2636	2655	rBV	169238	276888	9.20%	1.312%
28	9.952	2746	2756	2770	rVB2	42522	69248	2.30%	0.328%
29	10.238	2835	2845	2859	rVB	98399	153544	5.10%	0.728%
30	11.203	3131	3145	3156	rBV	84429	136229	4.53%	0.646%
31	11.270	3156	3166	3184	rVV3	347170	772170	25.66%	3.659%
32	11.357	3184	3193	3205	rVB	109362	167760	5.57%	0.795%
33	11.646	3271	3283	3303	rBV2	319225	598818	19.90%	2.838%
34	13.286	3780	3793	3804	rBV3	22747	41182	1.37%	0.195%

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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

35	13.527	3857	3868	3879	rBV2	39865	65682	2.18%	0.311%
36	16.736	4857	4866	4875	rBV2	54867	82995	2.76%	0.393%

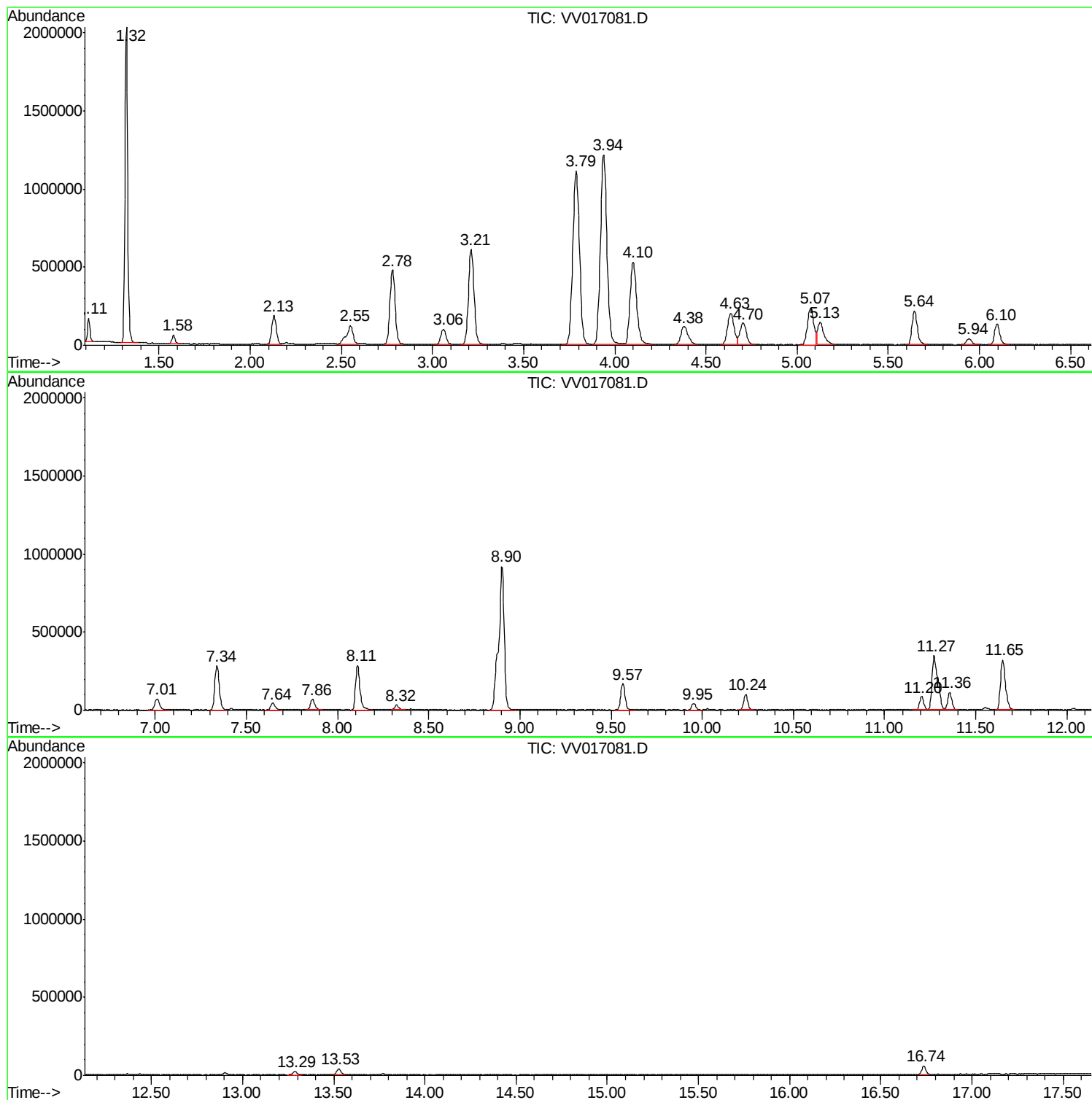
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Quant Title : TRACE VOA SOM01.0

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



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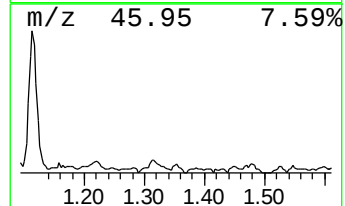
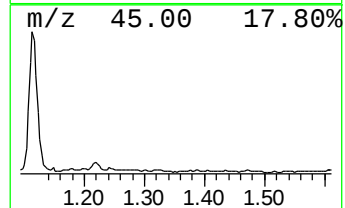
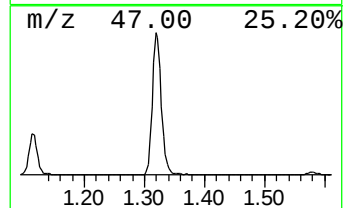
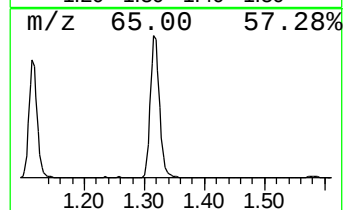
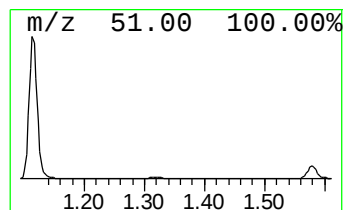
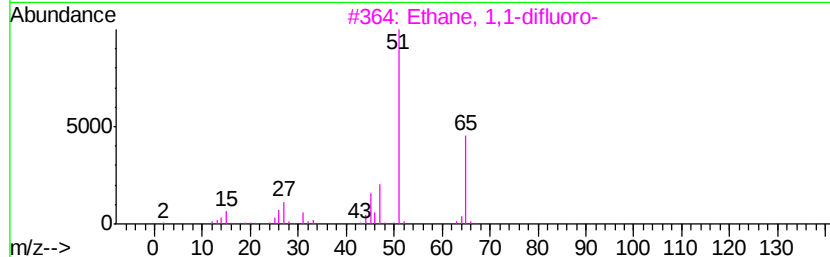
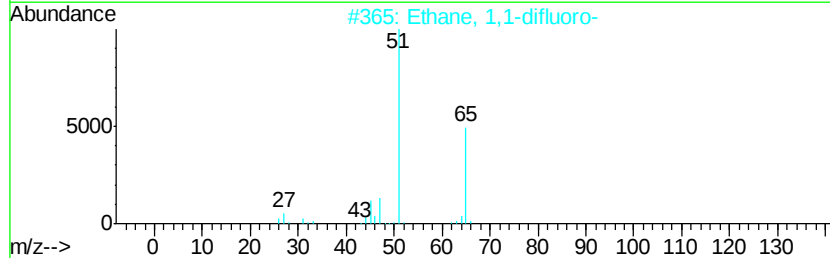
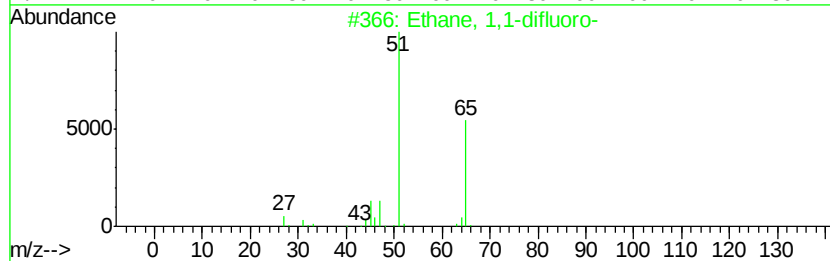
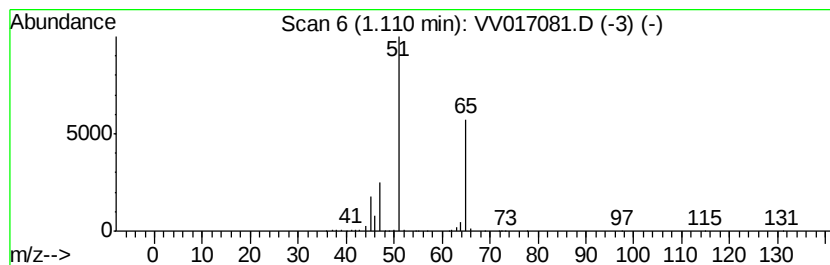
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Ethane, 1,1-difluoro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.11	1.57 ug/L	140942	1,4-Difluorobenzene	5.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	90	
2	Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	83	
3	Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	83	
4	Propiolonitrile	51	C3HN	001070-71-9	3	
5	Propane, 2,2-difluoro-	80	C3H6F2	000420-45-1	2	



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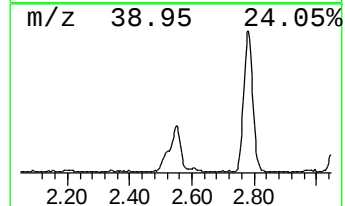
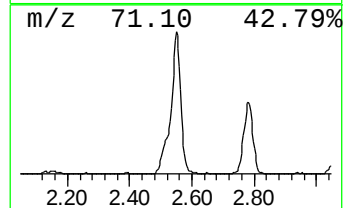
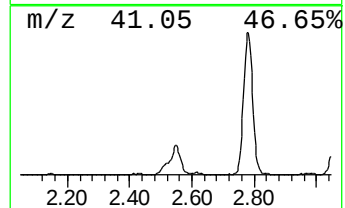
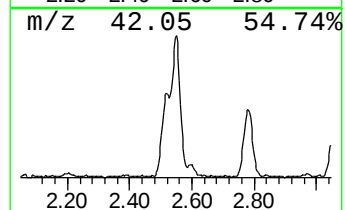
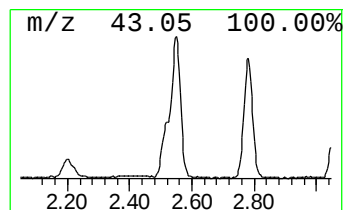
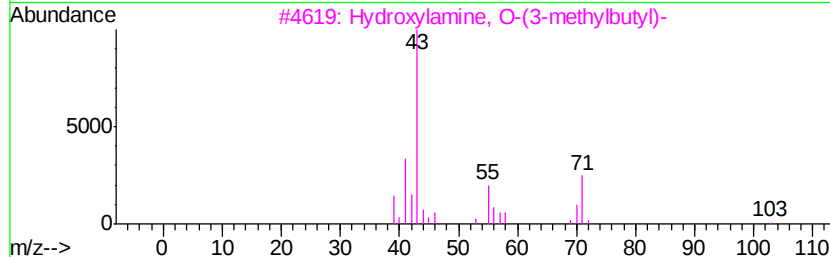
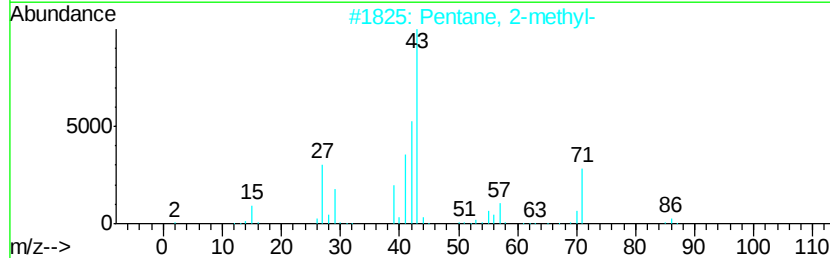
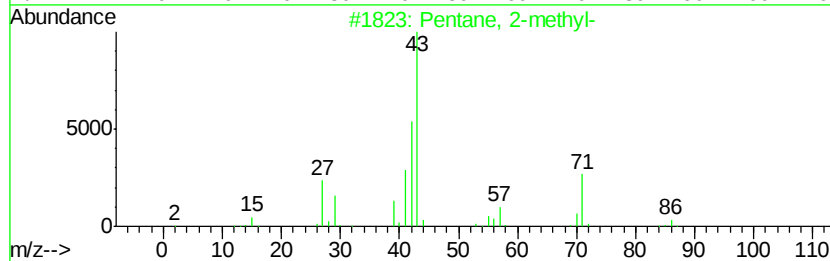
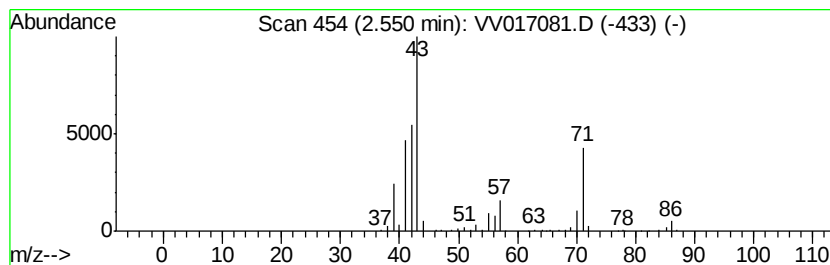
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.55	3.29 ug/L	294472	1,4-Difluorobenzene	5.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	91
3			Hydroxylamine, O-(3-methylbutyl)-	103	C5H13NO	019411-65-5	50
4			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	50
5			Pentane, 2-bromo-	150	C5H11Br	000107-81-3	50



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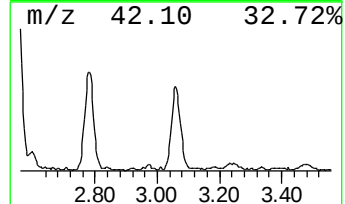
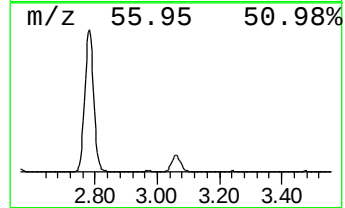
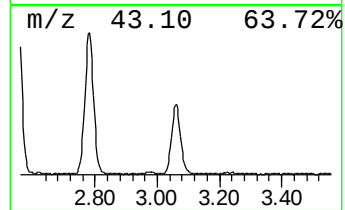
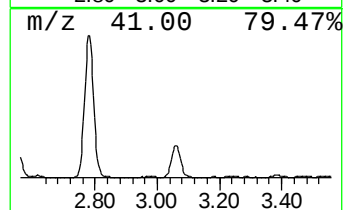
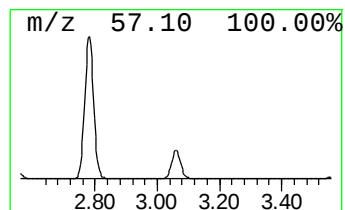
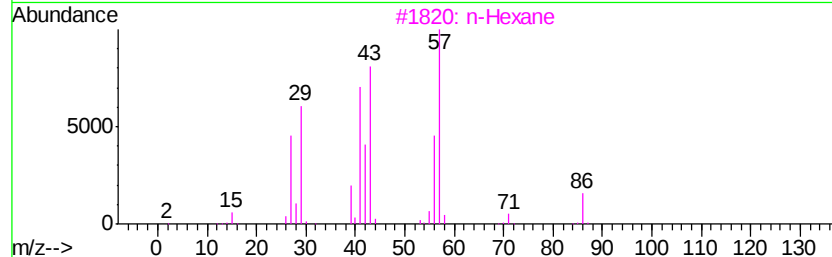
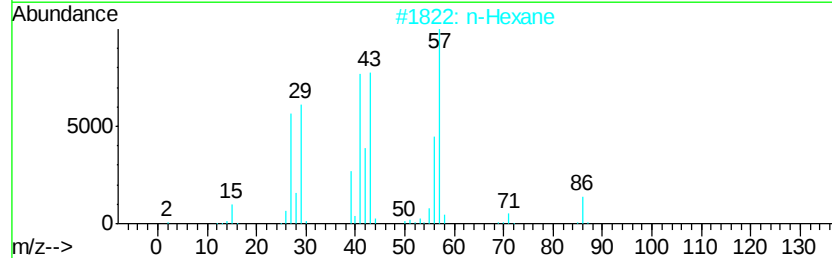
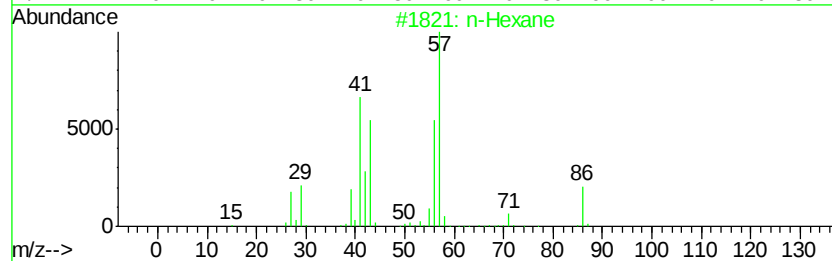
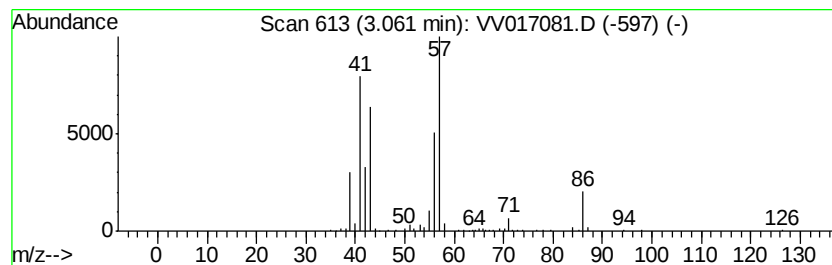
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.06	2.21 ug/L	198184	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexane	86	C6H14	000110-54-3	87
2		n-Hexane	86	C6H14	000110-54-3	64
3		n-Hexane	86	C6H14	000110-54-3	59
4		2(3H)-Furanone, dihydro-3-methyl-	100	C5H8O2	001679-47-6	47
5		Butanal, 2-methyl-	86	C5H10O	000096-17-3	43



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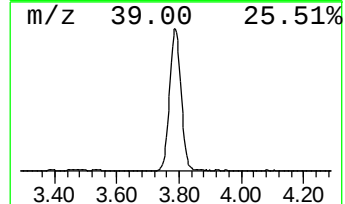
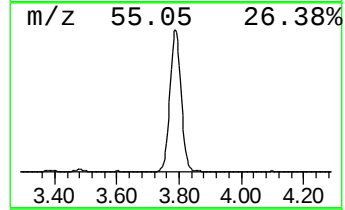
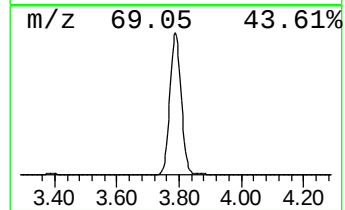
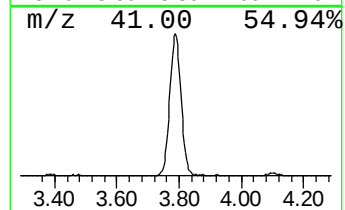
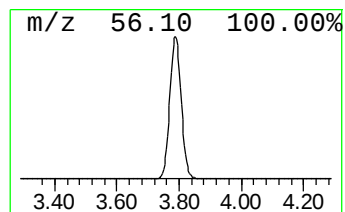
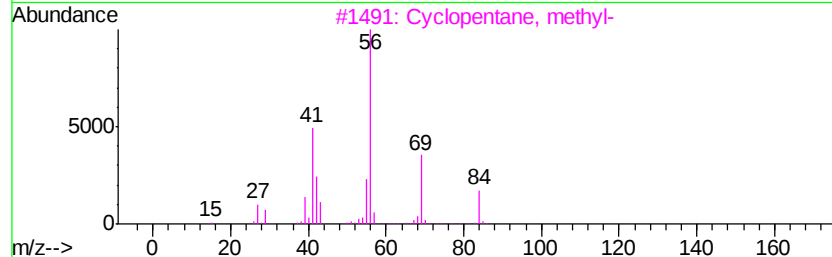
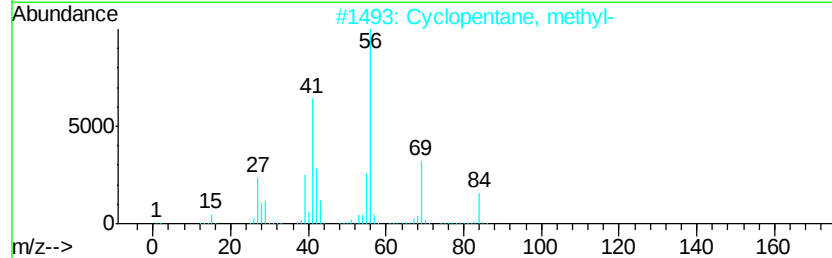
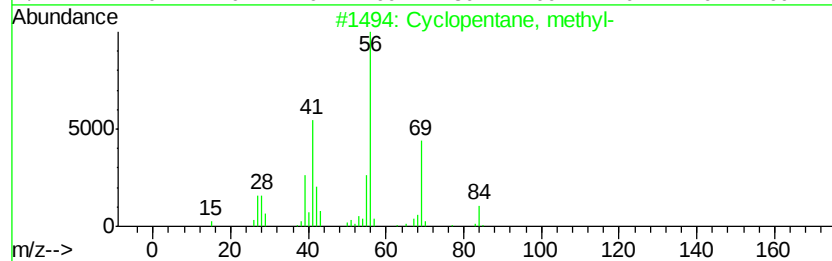
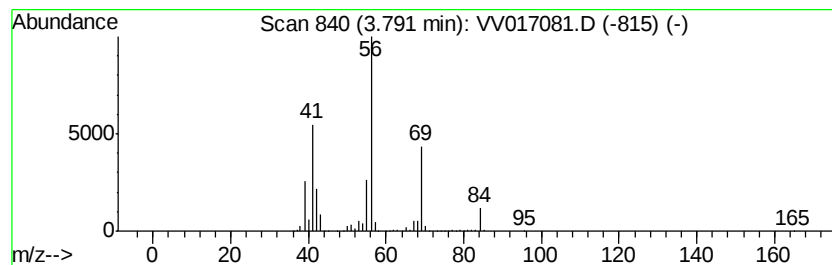
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 (DEL) Alkane: Cyclic3.79 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.79	31.57 ug/L	2828880	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2		Cyclopentane, methyl-	84	C6H12	000096-37-7	91
3		Cyclopentane, methyl-	84	C6H12	000096-37-7	86
4		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
5		Cyclohexane	84	C6H12	000110-82-7	78



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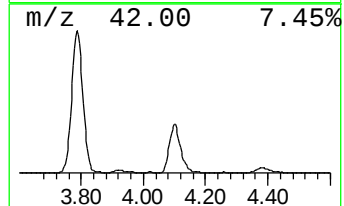
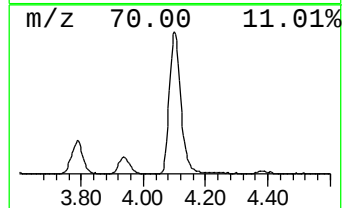
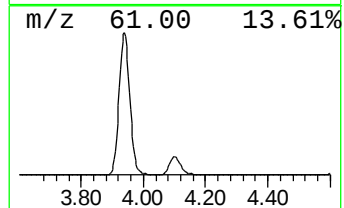
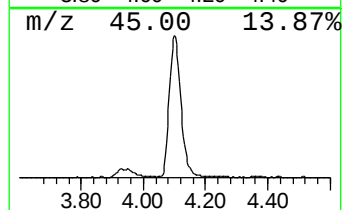
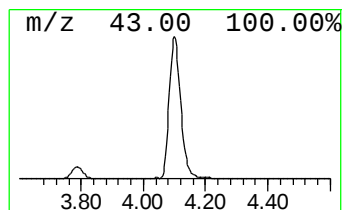
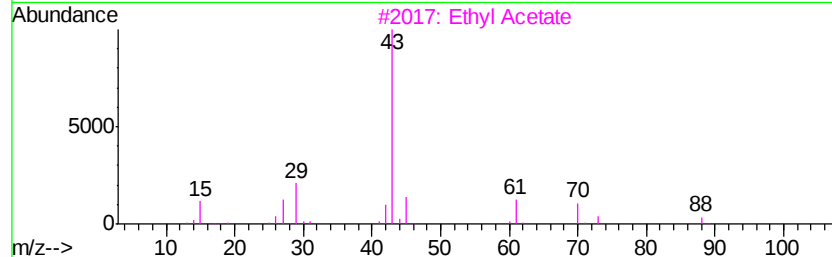
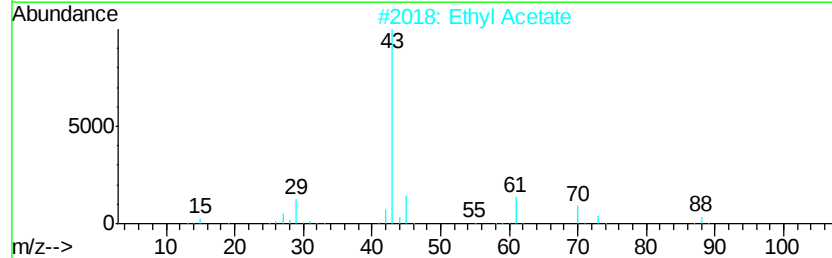
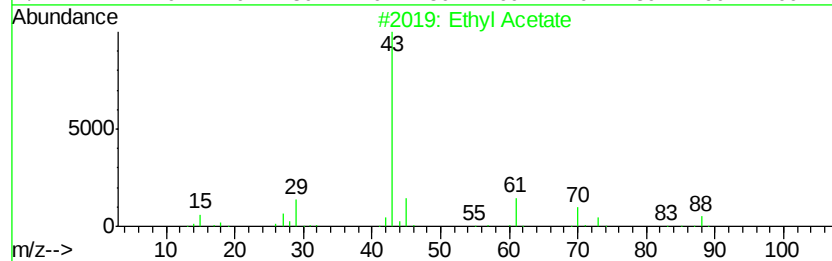
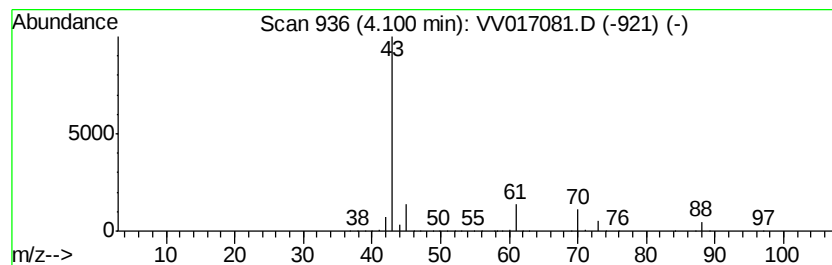
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Ethyl Acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.10	14.96 ug/L	1340350	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethyl Acetate	88	C4H8O2	000141-78-6	91
2		Ethyl Acetate	88	C4H8O2	000141-78-6	86
3		Ethyl Acetate	88	C4H8O2	000141-78-6	86
4		Ethyl Acetate	88	C4H8O2	000141-78-6	64
5		CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	53



Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV062420\
Data File : VV017081.D
Acq On : 24 Jun 2020 19:05
Operator : SY/MD
Sample : L3105-05
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BFXK8

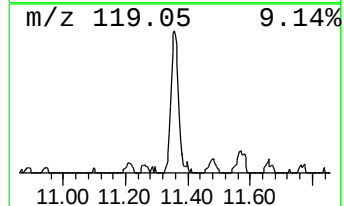
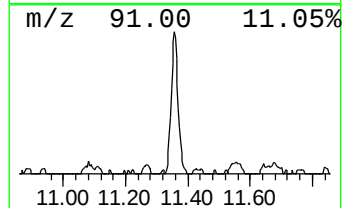
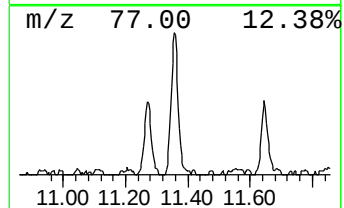
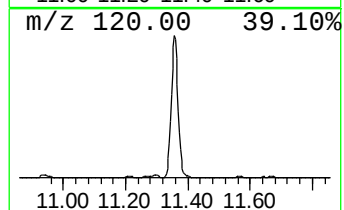
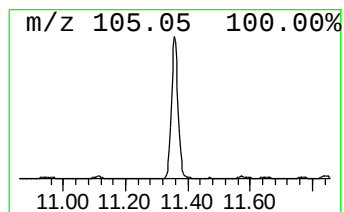
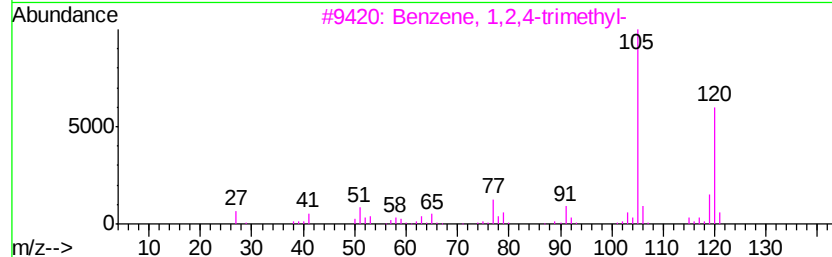
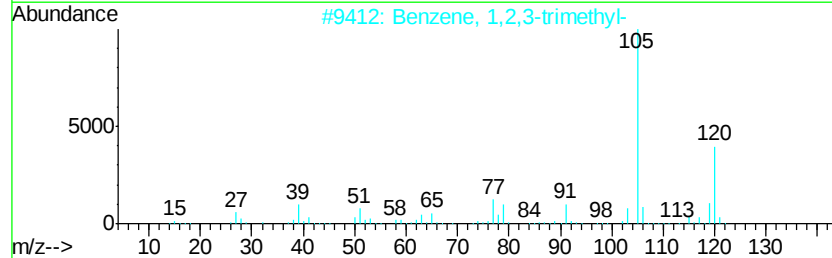
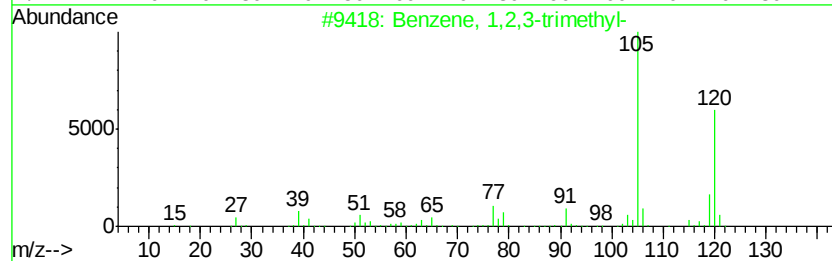
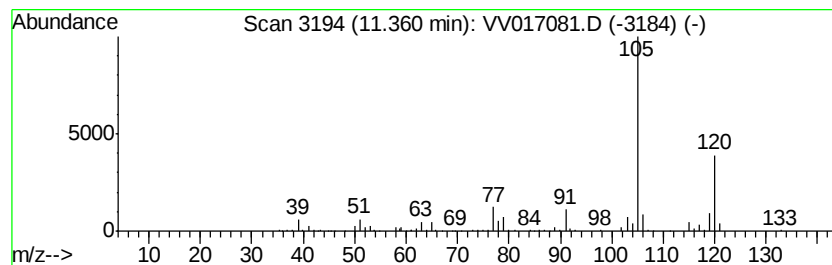
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 Benzene, 1,2,3-trimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.36	1.09 ug/L	167760	1,4-Dichlorobenzene-d4	11.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	94
3		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4		Mesitylene	120	C9H12	000108-67-8	91
5		Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV062420\
Data File : VV017081.D
Acq On : 24 Jun 2020 19:05
Operator : SY/MD
Sample : L3105-05
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BFXK8

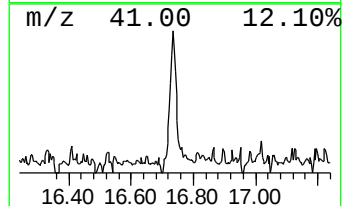
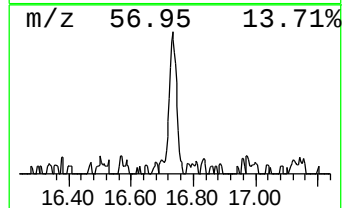
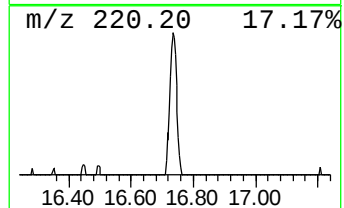
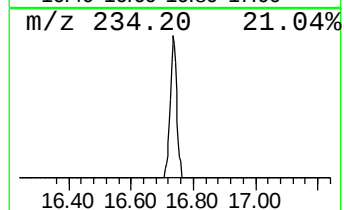
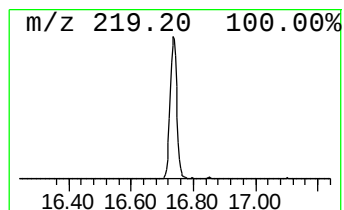
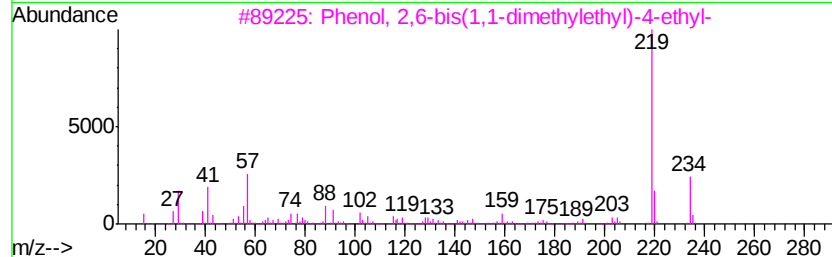
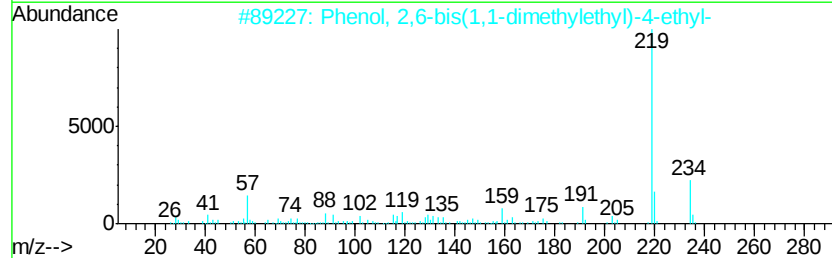
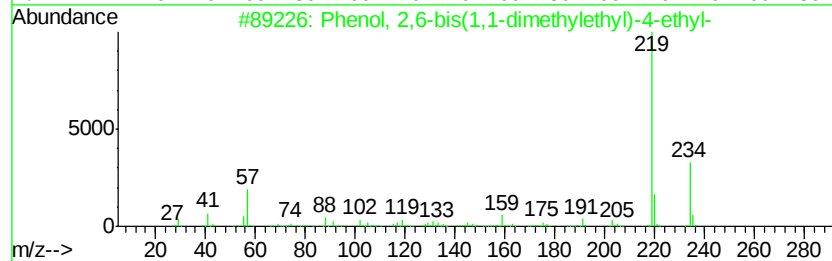
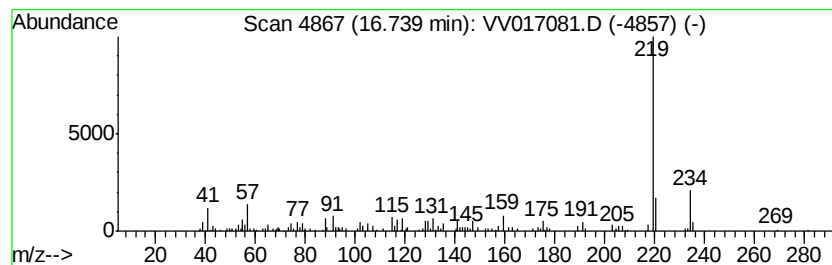
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR061720WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.74	0.54 ug/L	82995	1,4-Dichlorobenzene-d4	11.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	94
2		Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	93
3		Phenol, 2,6-bis(1,1-dimethylethy...	234	C16H26O	004130-42-1	93
4		3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	93
5		3,5-di-tert-Butyl-4-hydroxybenza...	234	C15H22O2	001620-98-0	93



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV062420\
 Data File : VV017081.D
 Acq On : 24 Jun 2020 19:05
 Operator : SY/MD
 Sample : L3105-05
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BFXK8

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR061720WMA.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
Ethane, 1,1-diflu...	1.11	1.6	ug/L	140942	1	5.64	448057	5.0
(DEL) Alkane: Str...	2.55	3.3	ug/L	294472	1	5.64	448057	5.0
(DEL) Alkane: Str...	3.06	2.2	ug/L	198184	1	5.64	448057	5.0
(DEL) Alkane: Cyc...	3.79	31.6	ug/L	2828880	1	5.64	448057	5.0
Ethyl Acetate	4.10	15.0	ug/L	1340350	1	5.64	448057	5.0
Benzene, 1,2,3-tr...	11.36	1.1	ug/L	167760	3	11.27	772170	5.0
Phenol, 2,6-bis(1...	16.74	0.5	ug/L	82995	3	11.27	772170	5.0