

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV060120\
 Data File : VV016402.D
 Acq On : 01 Jun 2020 11:10
 Operator : SY/MD
 Sample : L2826-06
 Misc : 25.0mL/MSVOA V/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 CWKB9

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\SOMVTR053020WMA.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	1.319	61	71	77	rBV3	72759	89778	12.09%	2.173%
2	1.476	81	120	146	rVV2	170617	742680	100.00%	17.979%
3	1.579	147	152	167	rVB	43215	67641	9.11%	1.637%
4	1.817	219	226	246	rVB	110132	151216	20.36%	3.661%
5	2.048	291	298	311	rVV3	12591	21142	2.85%	0.512%
6	2.122	312	321	334	rVB	77131	115863	15.60%	2.805%
7	2.778	515	525	549	rVB	70807	125877	16.95%	3.047%
8	3.058	601	612	625	rVB2	11956	24373	3.28%	0.590%
9	3.942	869	887	928	rBV3	114254	338037	45.52%	8.183%
10	4.380	1003	1023	1051	rBV2	56497	154641	20.82%	3.744%
11	5.074	1223	1239	1268	rBV2	129405	306365	41.25%	7.416%
12	5.515	1364	1376	1391	rBV3	11412	23724	3.19%	0.574%
13	5.643	1401	1416	1436	rBV	104129	203615	27.42%	4.929%
14	5.939	1498	1508	1528	rBV2	25917	50941	6.86%	1.233%
15	6.097	1544	1557	1584	rBV2	69565	146616	19.74%	3.549%
16	6.325	1619	1628	1636	rBV6	6365	13595	1.83%	0.329%
17	6.373	1637	1643	1665	rVB	8097	20274	2.73%	0.491%
18	7.010	1831	1841	1858	rBV2	33803	59627	8.03%	1.443%
19	7.338	1932	1943	1960	rBV	143107	246547	33.20%	5.968%
20	7.521	1988	2000	2001	rBV6	5461	9527	1.28%	0.231%
21	7.588	2013	2021	2030	rBV3	18183	28584	3.85%	0.692%
22	7.646	2031	2039	2054	rVB	21104	37765	5.08%	0.914%
23	8.116	2174	2185	2211	rBV	167954	299161	40.28%	7.242%
24	8.264	2223	2231	2252	rVB2	29085	48803	6.57%	1.181%
25	8.875	2409	2421	2447	rBV	145189	249476	33.59%	6.039%
26	9.518	2609	2621	2631	rBV2	11173	23440	3.16%	0.567%
27	9.833	2708	2719	2728	rBV5	10805	17977	2.42%	0.435%
28	10.238	2835	2845	2859	rBV	44634	70744	9.53%	1.713%
29	10.739	2994	3001	3010	rVB2	15884	23028	3.10%	0.557%
30	10.961	3059	3070	3083	rBV2	11752	19445	2.62%	0.471%
31	11.174	3127	3136	3146	rBV3	6054	8961	1.21%	0.217%
32	11.270	3155	3166	3182	rBV	116709	178515	24.04%	4.321%
33	11.556	3244	3255	3269	rBV	20434	37497	5.05%	0.908%
34	11.646	3272	3283	3300	rVB	97533	153886	20.72%	3.725%

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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	12.370	3499	3508	3521	rBV5	7844	13290	1.79%	0.322%
36	12.871	3649	3664	3671	rBV6	3471	8242	1.11%	0.200%

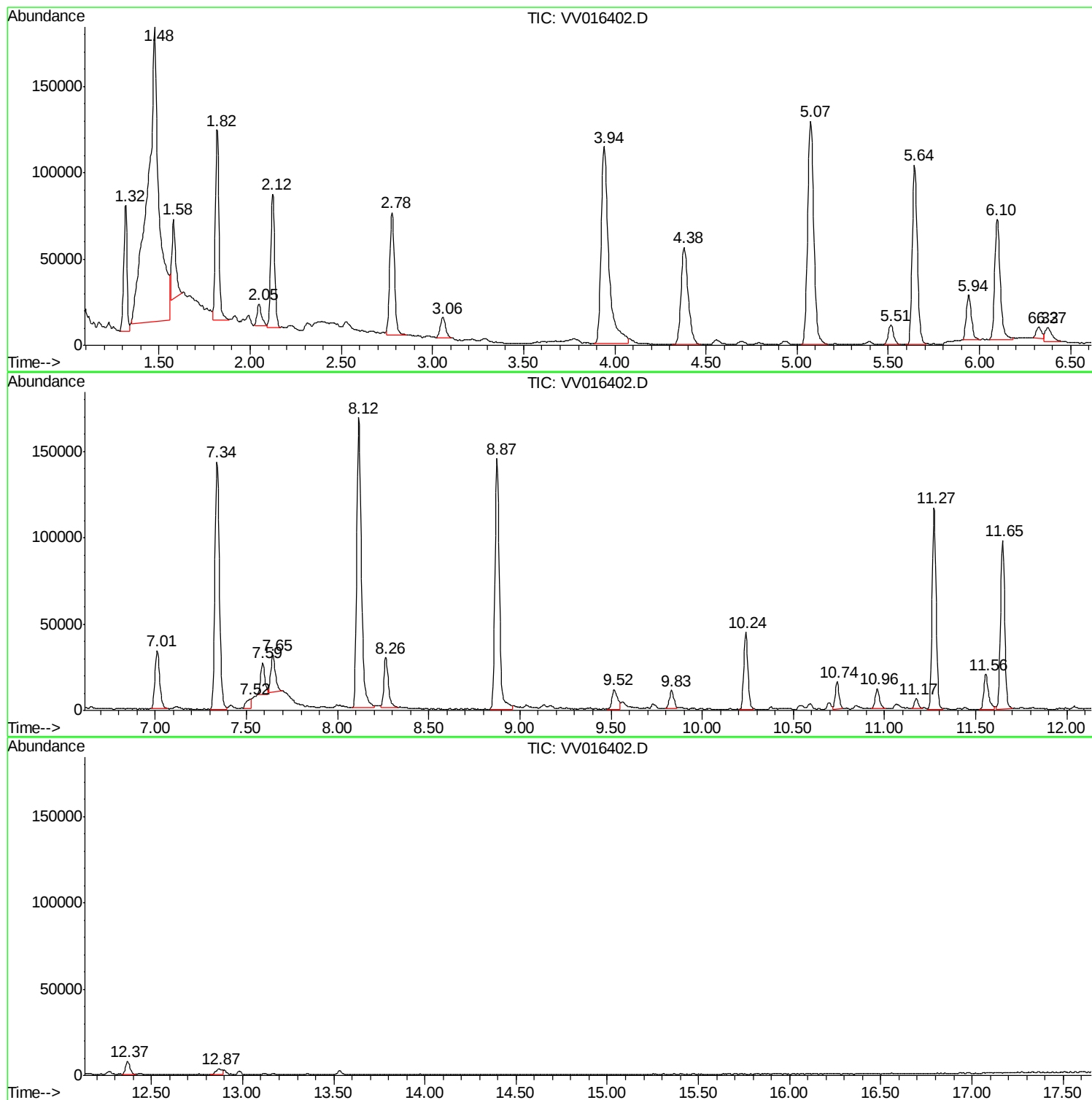
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Quant Title : TRACE VOA SOM01.0

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



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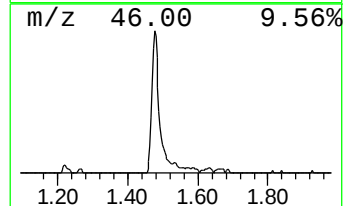
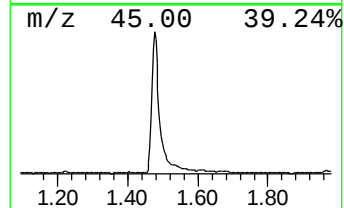
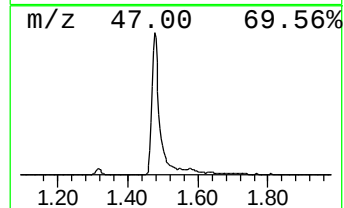
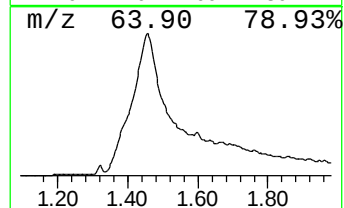
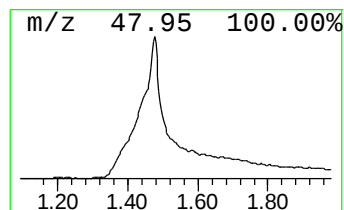
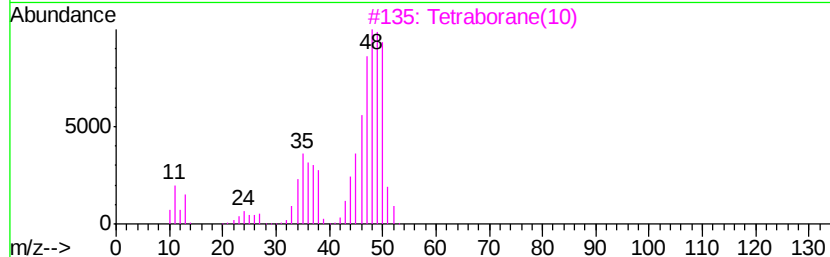
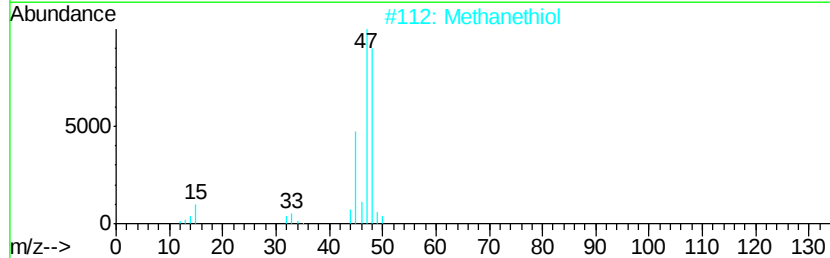
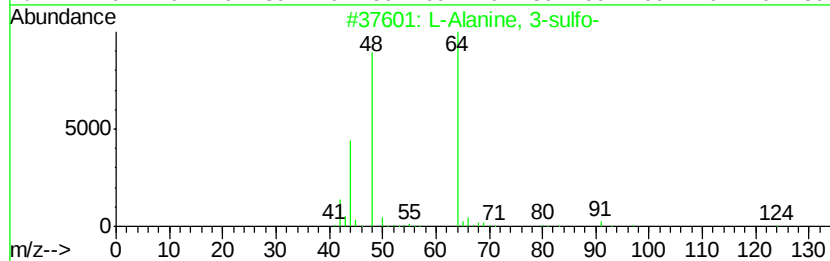
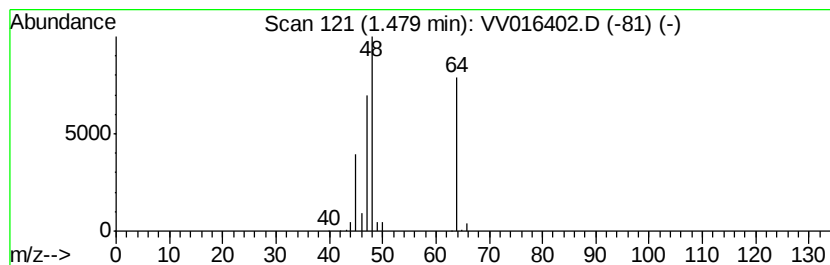
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.48	18.24 ug/L	742680	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	39
2		Methanethiol	48	CH4S	000074-93-1	10
3		Tetraborane(10)	54	B4H10	018283-93-7	9
4		Taurine	125	C2H7NO3S	000107-35-7	9
5		Methanethiol	48	CH4S	000074-93-1	7



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ClientSampleId :
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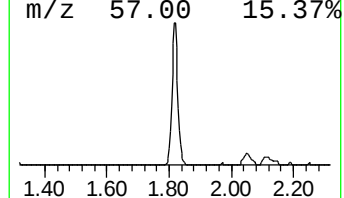
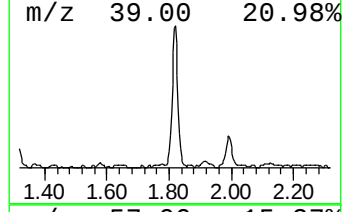
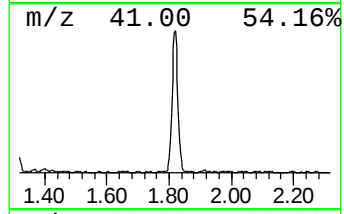
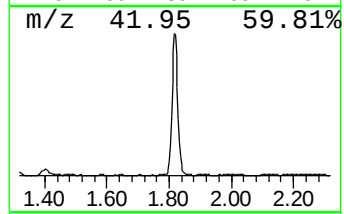
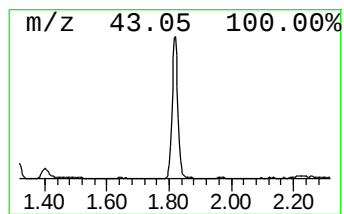
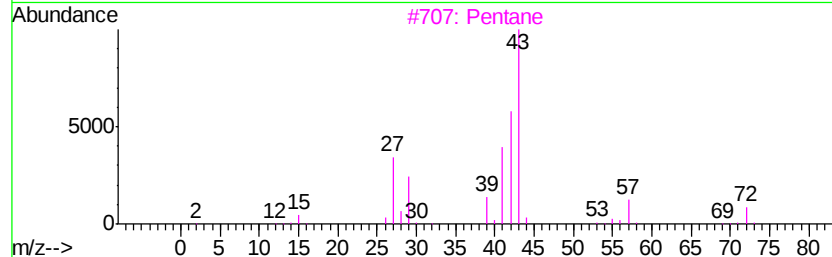
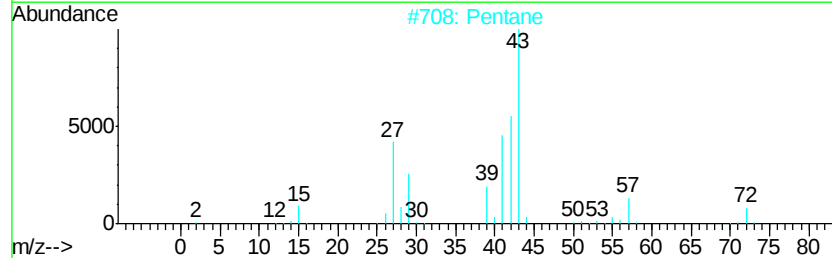
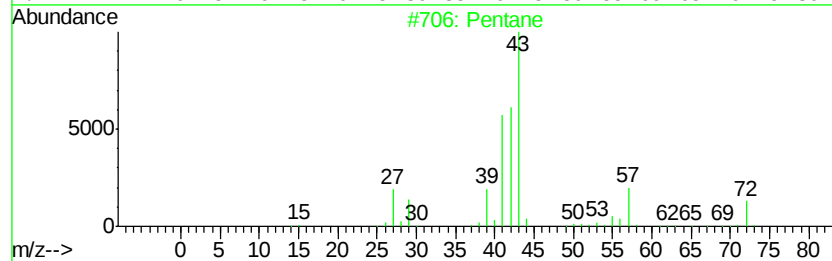
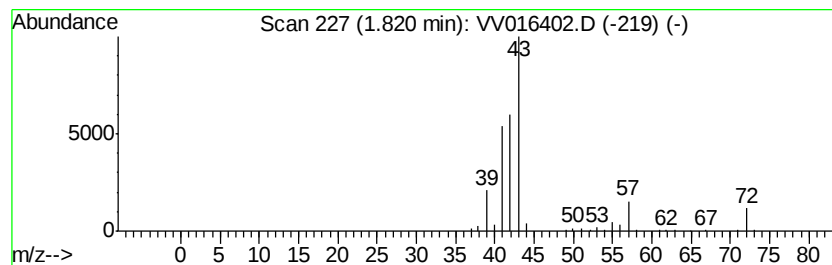
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR053020WMA.M
Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.82	3.71 ug/L	151216	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane	72	C5H12	000109-66-0	91
2		Pentane	72	C5H12	000109-66-0	86
3		Pentane	72	C5H12	000109-66-0	86
4		Pentane	72	C5H12	000109-66-0	86
5		Butane, 2-methyl-	72	C5H12	000078-78-4	50



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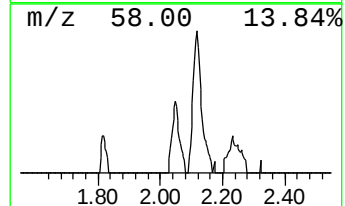
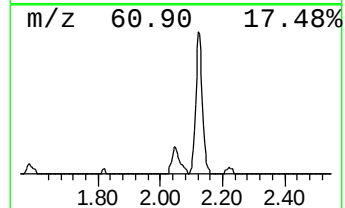
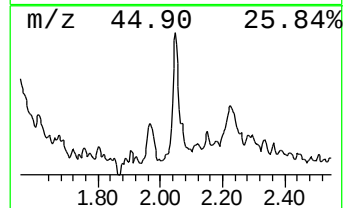
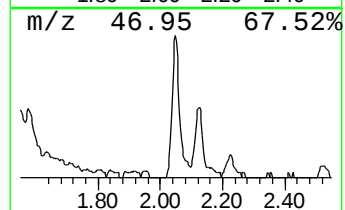
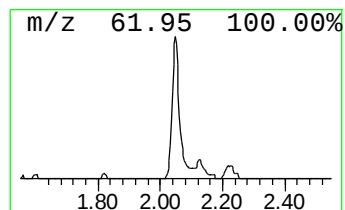
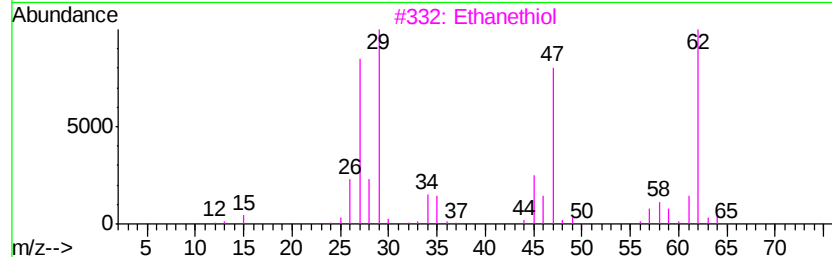
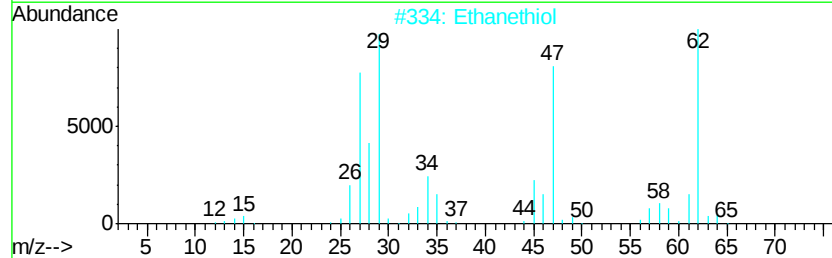
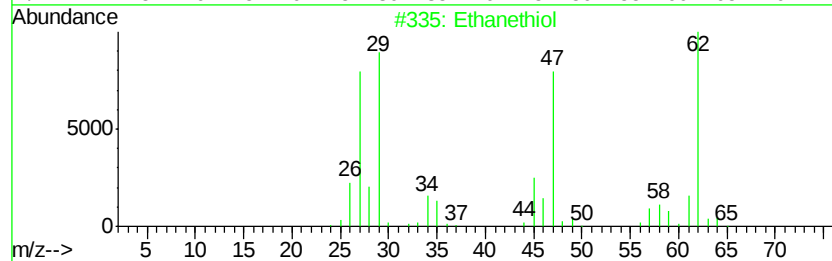
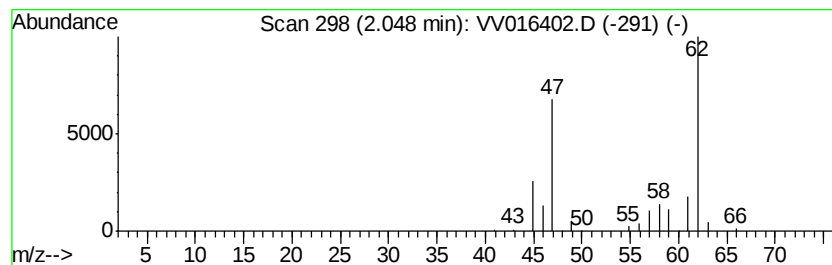
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR053020WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 Ethanethiol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.05	0.52 ug/L	21142	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanethiol	62	C2H6S	000075-08-1	87
2		Ethanethiol	62	C2H6S	000075-08-1	87
3		Ethanethiol	62	C2H6S	000075-08-1	87
4		Ethanethiol	62	C2H6S	000075-08-1	86
5		Ethanethiol	62	C2H6S	000075-08-1	86



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Instrument :
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ClientSampleId :
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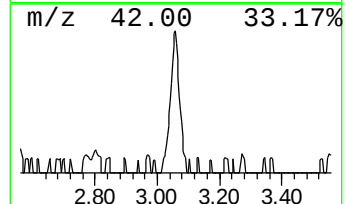
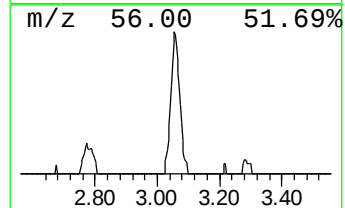
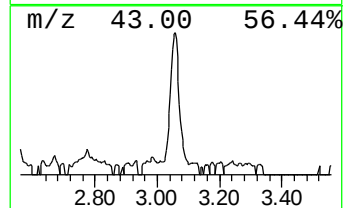
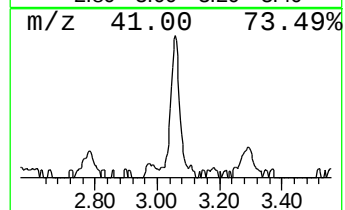
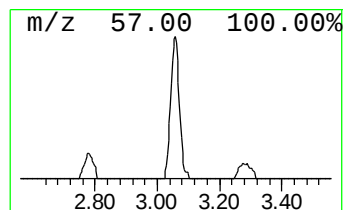
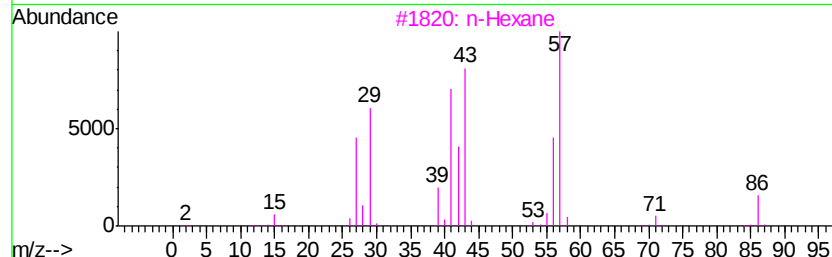
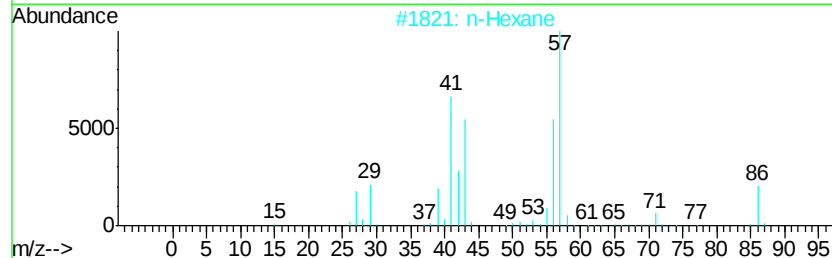
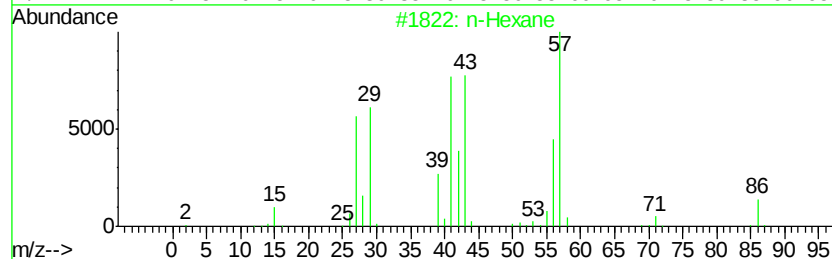
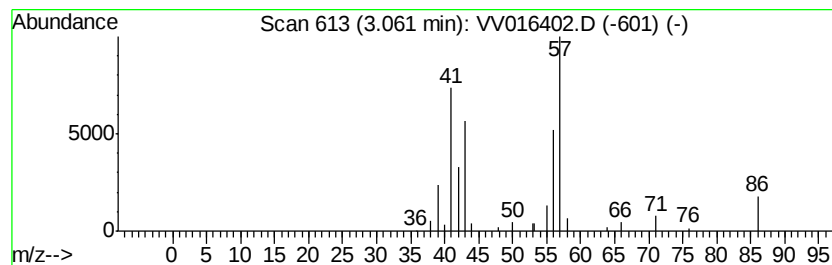
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.06	0.60 ug/L	24373	1,4-Difluorobenzene	5.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexane	86	C6H14	000110-54-3	80
2		n-Hexane	86	C6H14	000110-54-3	80
3		n-Hexane	86	C6H14	000110-54-3	72
4		Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	40
5		3-Buten-1-ol, 3-methyl-	86	C5H10O	000763-32-6	38



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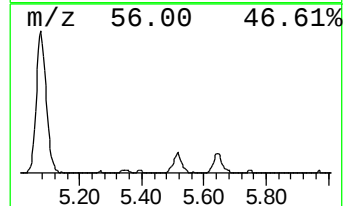
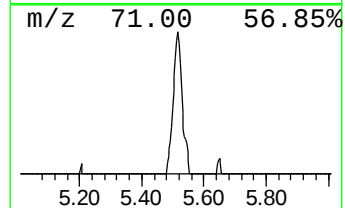
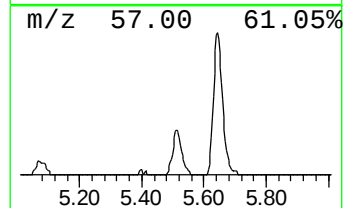
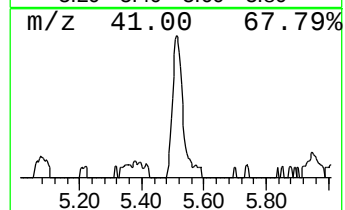
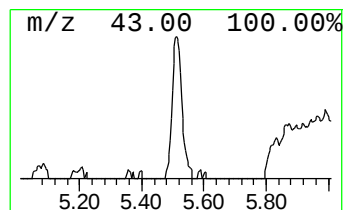
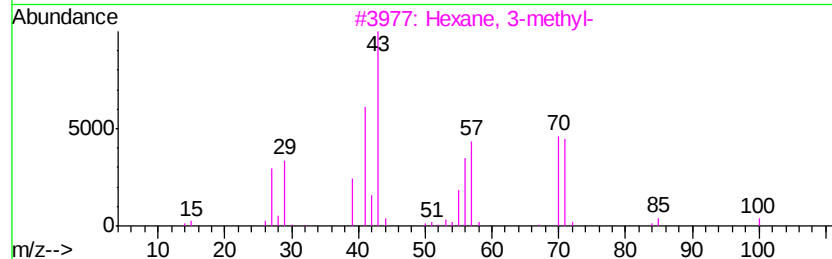
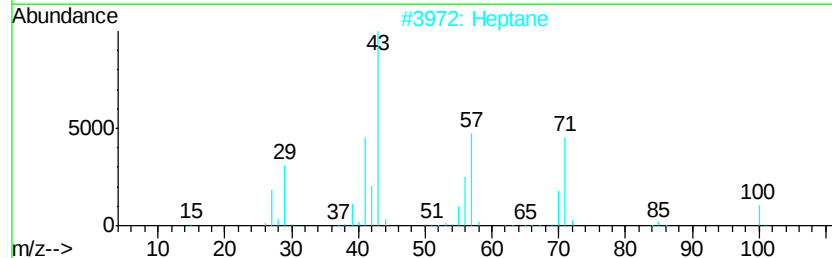
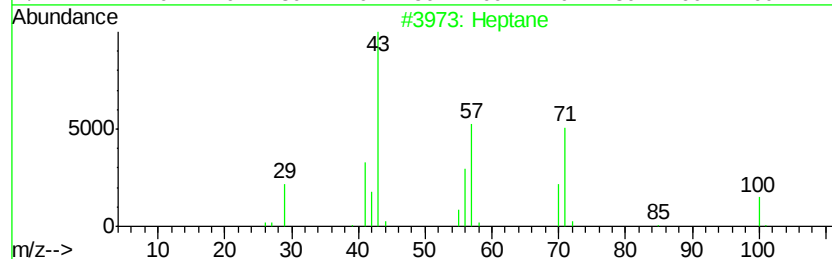
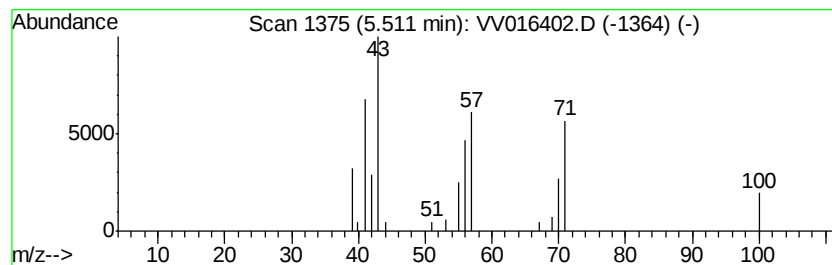
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR053020WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.51	0.58 ug/L	23724	1,4-Difluorobenzene	5.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane		100	C7H16	000142-82-5	59
2	Heptane		100	C7H16	000142-82-5	43
3	Hexane, 3-methyl-		100	C7H16	000589-34-4	40
4	Heptane		100	C7H16	000142-82-5	40
5	Heptane		100	C7H16	000142-82-5	38



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Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
CWKB9

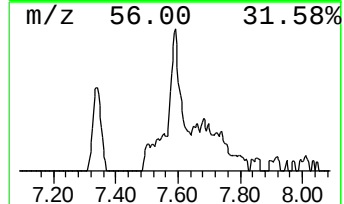
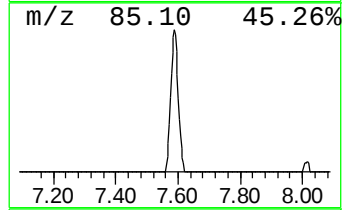
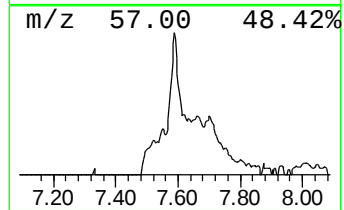
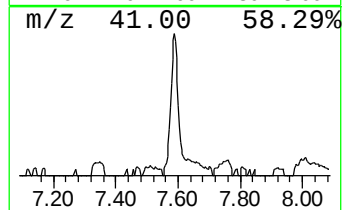
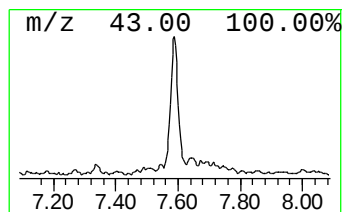
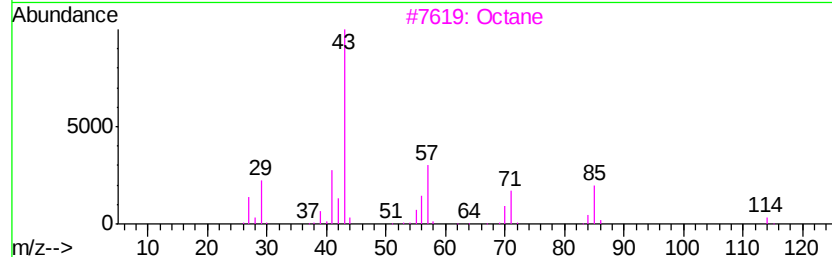
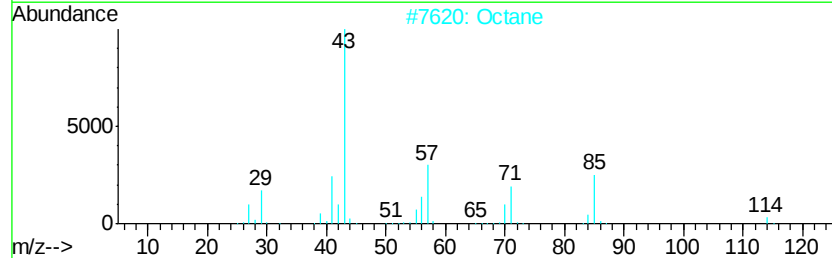
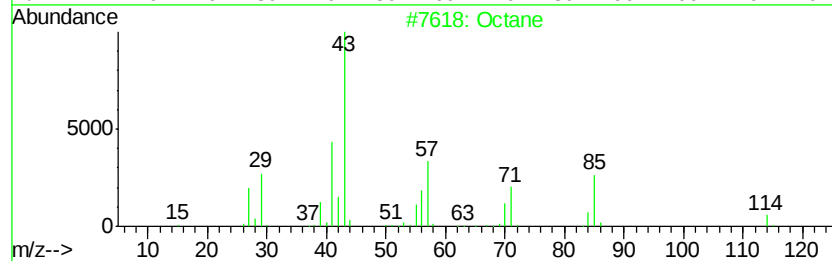
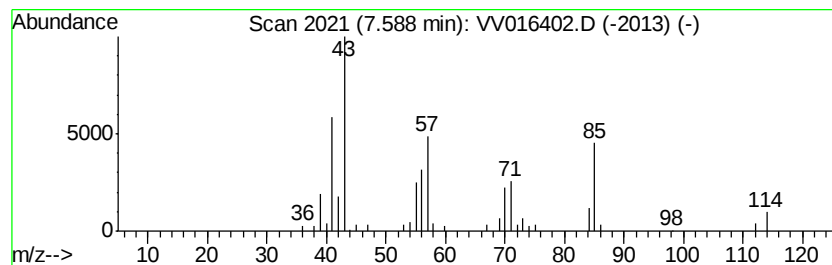
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	0.57 ug/L	28584	Chlorobenzene-d5	8.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane			114	C8H18	000111-65-9	76
2	Octane			114	C8H18	000111-65-9	68
3	Octane			114	C8H18	000111-65-9	64
4	Heptane, 2,4-dimethyl-			128	C9H20	002213-23-2	50
5	Hexane, 3-ethyl-			114	C8H18	000619-99-8	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV060120\
 Data File : VV016402.D
 Acq On : 01 Jun 2020 11:10
 Operator : SY/MD
 Sample : L2826-06
 Misc : 25.0mL/MSVOA V/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 CWKB9

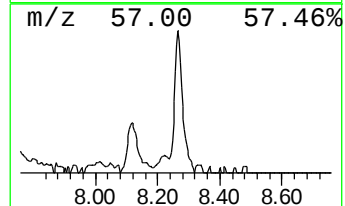
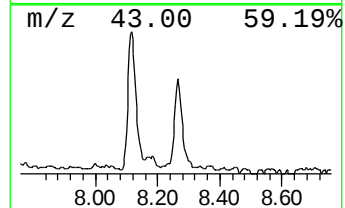
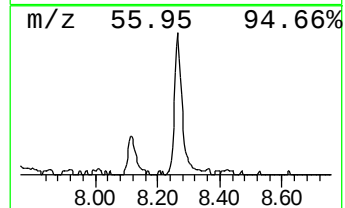
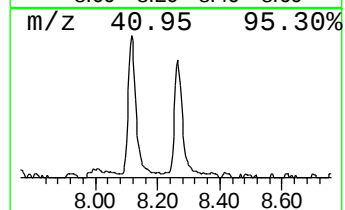
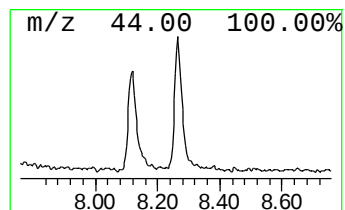
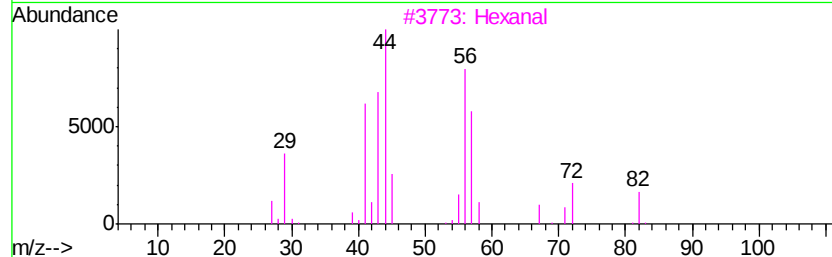
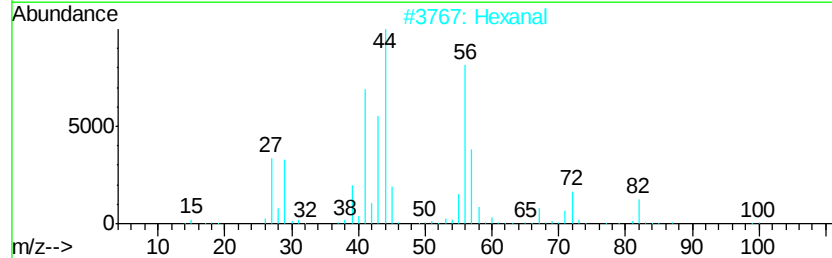
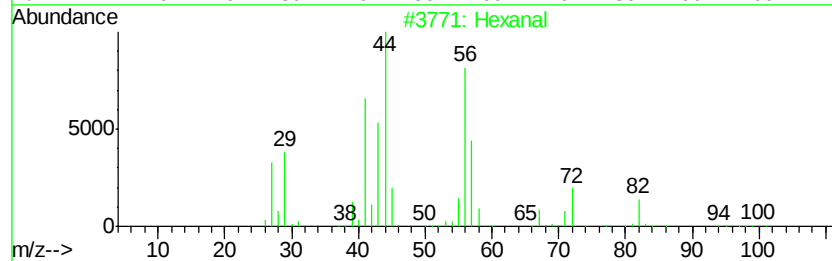
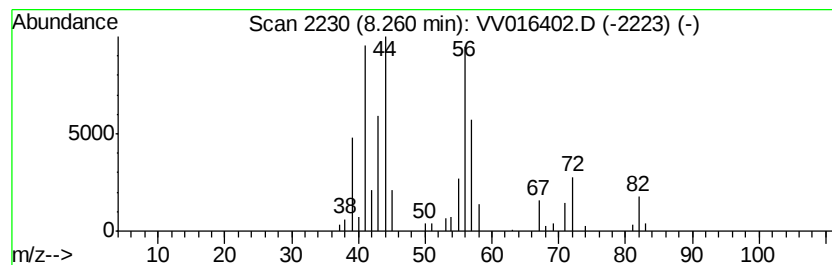
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 Quant Title : TRACE VOA SOM01.0

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

 Peak Number 8 Hexanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.26	0.98 ug/L	48803	Chlorobenzene-d5	8.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanal	100	C6H12O	000066-25-1	72
2		Hexanal	100	C6H12O	000066-25-1	64
3		Hexanal	100	C6H12O	000066-25-1	64
4		Hexanal	100	C6H12O	000066-25-1	59
5		2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	32



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV060120\
Data File : VV016402.D
Acq On : 01 Jun 2020 11:10
Operator : SY/MD
Sample : L2826-06
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
CWKB9

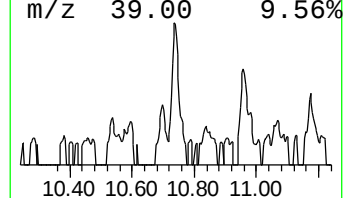
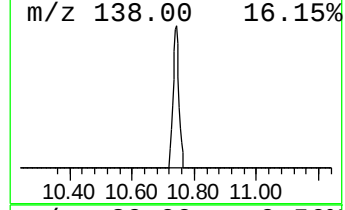
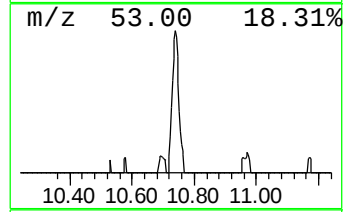
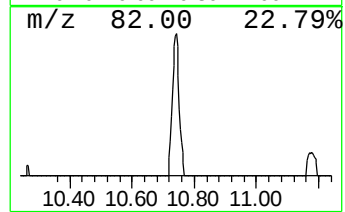
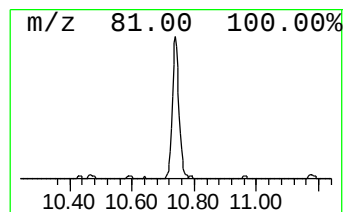
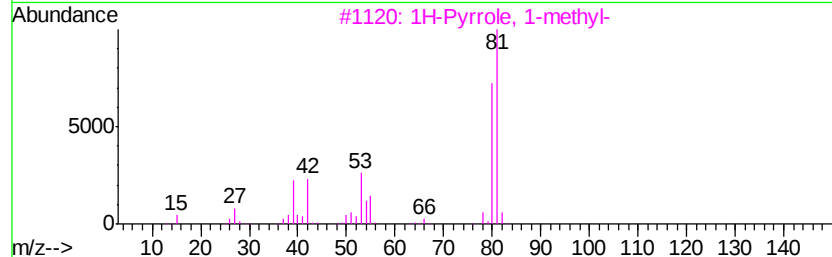
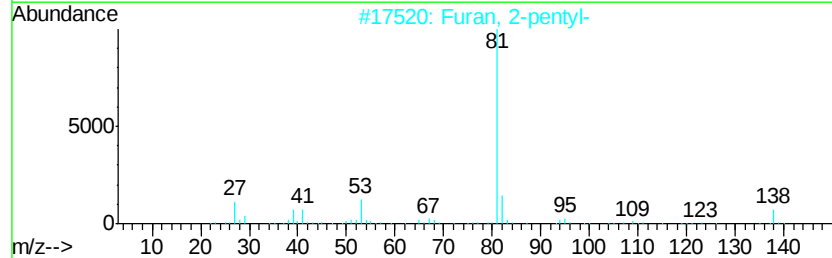
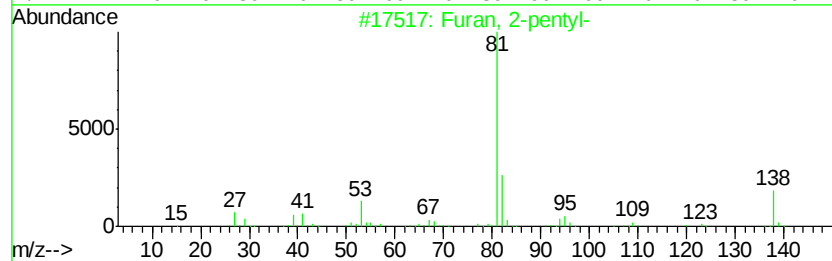
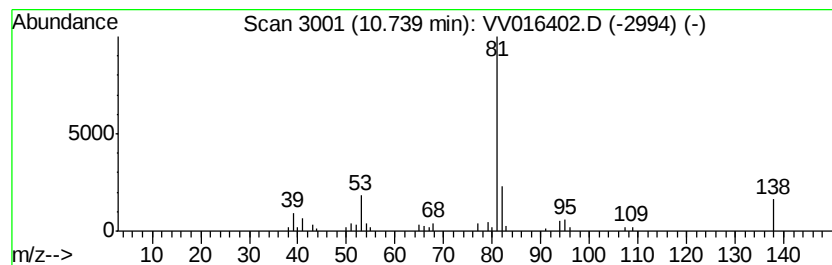
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 9 Furan, 2-pentyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.74	0.64 ug/L	23028	1,4-Dichlorobenzene-d4	11.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, 2-pentyl-		138	C9H14O	003777-69-3	90
2	Furan, 2-pentyl-		138	C9H14O	003777-69-3	64
3	1H-Pyrrole, 1-methyl-		81	C5H7N	000096-54-8	52
4	2-n-Butyl furan		124	C8H12O	004466-24-4	50
5	2-n-Butyl furan		124	C8H12O	004466-24-4	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV060120\
Data File : VV016402.D
Acq On : 01 Jun 2020 11:10
Operator : SY/MD
Sample : L2826-06
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
CWKB9

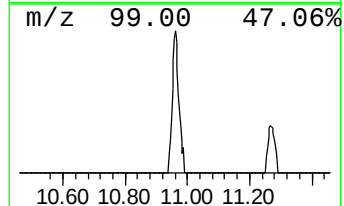
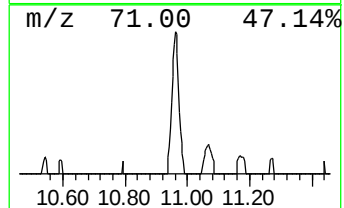
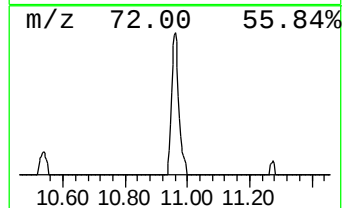
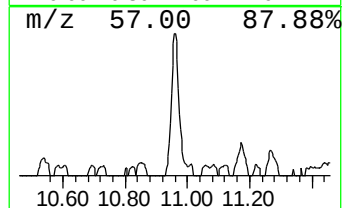
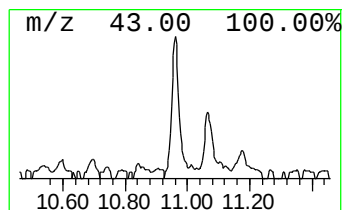
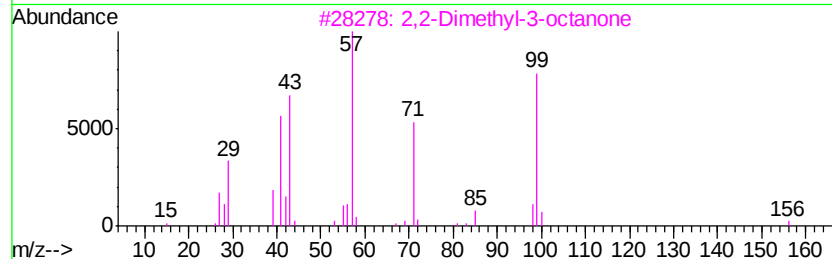
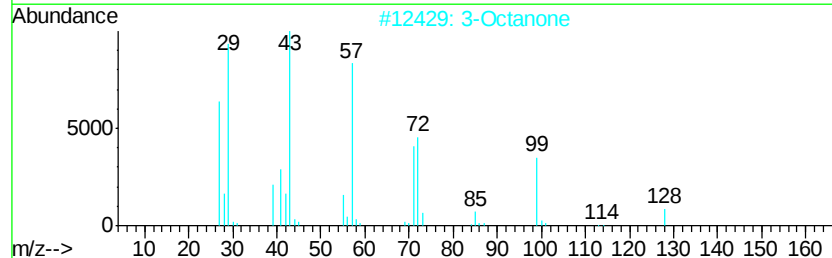
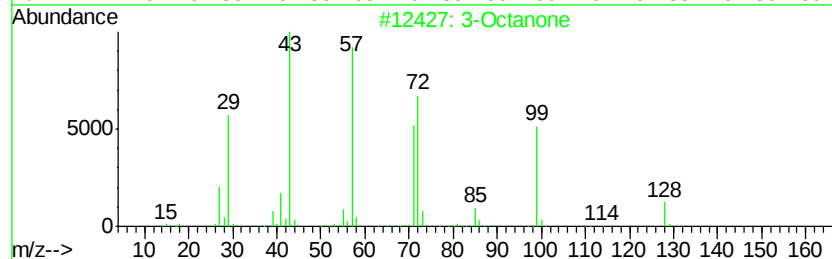
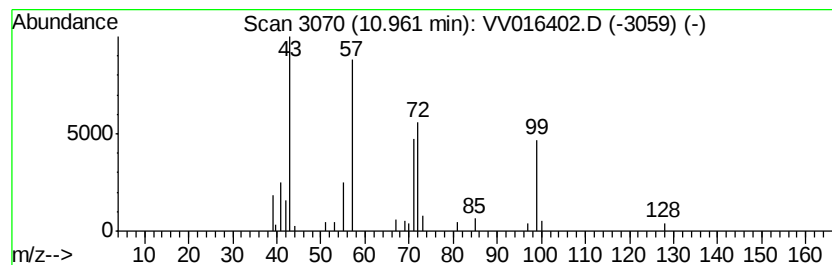
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 10 3-Octanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.96	0.54 ug/L	19445	1,4-Dichlorobenzene-d4	11.27

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Octanone	128	C8H16O	000106-68-3	64
2			3-Octanone	128	C8H16O	000106-68-3	59
3			2,2-Dimethyl-3-octanone	156	C10H20O	005340-64-7	50
4			Butanal, 2-ethyl-	100	C6H12O	000097-96-1	43
5			3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	40



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA V\DATA\VV060120\
Data File : VV016402.D
Acq On : 01 Jun 2020 11:10
Operator : SY/MD
Sample : L2826-06
Misc : 25.0mL/MSVOA V/WATER
ALS Vial : 6 Sample Multiplier: 1

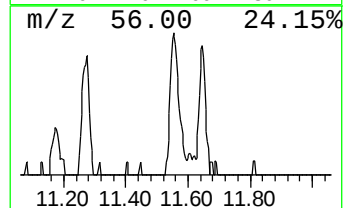
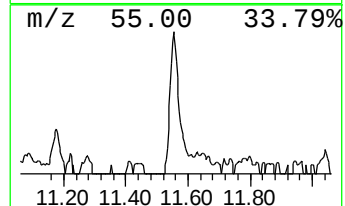
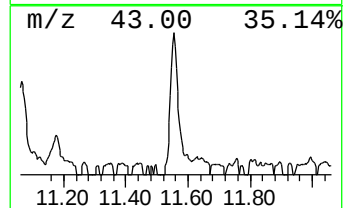
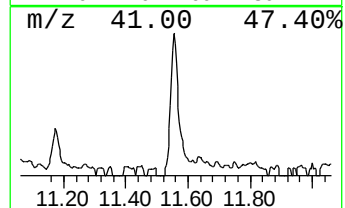
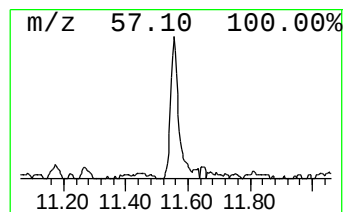
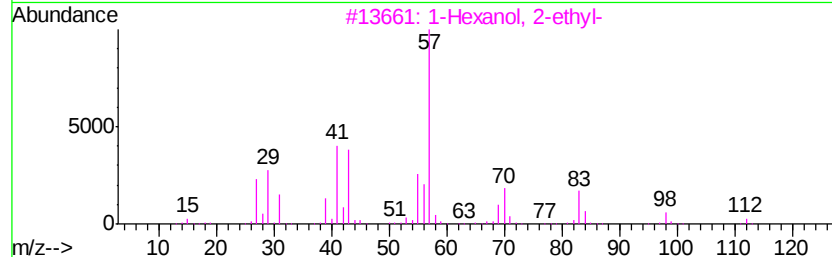
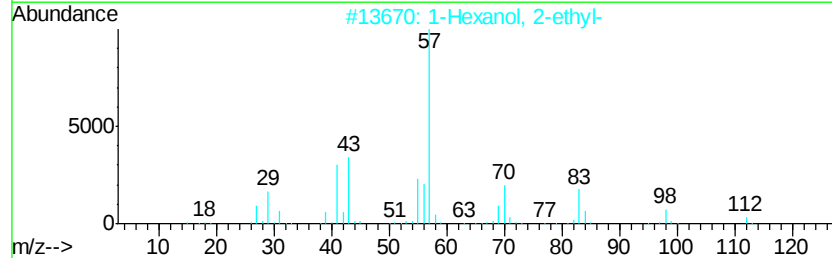
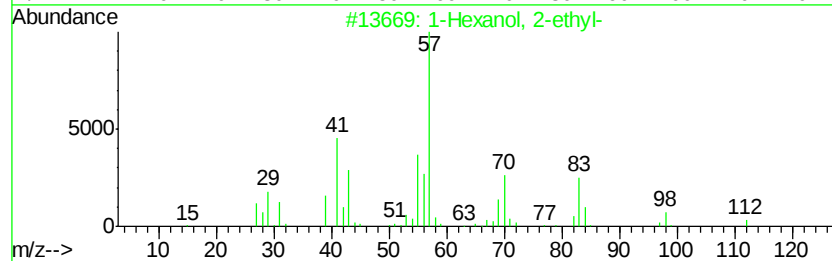
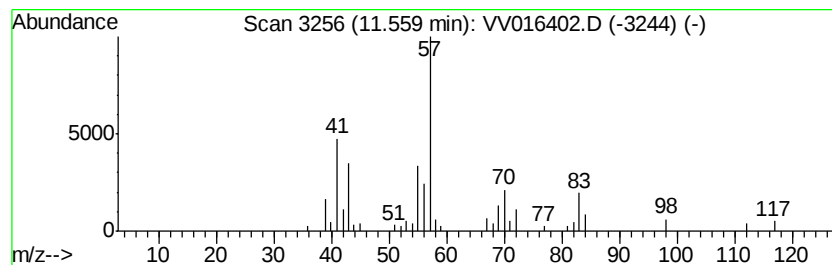
Instrument :
MSVOA_V
ClientSampleId :
CWKB9

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR053020WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 11 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.56	1.05 ug/L	37497	1,4-Dichlorobenzene-d4	11.27
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Hexanol, 2-ethyl-	130 C8H18O	000104-76-7	80
2	1-Hexanol, 2-ethyl-	130 C8H18O	000104-76-7	72
3	1-Hexanol, 2-ethyl-	130 C8H18O	000104-76-7	72
4	1-Isobutoxy-2-ethylhexane	186 C12H26O	1000139-90-3	56
5	1-Hexanol, 2-ethyl-	130 C8H18O	000104-76-7	50



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV060120\
 Data File : VV016402.D
 Acq On : 01 Jun 2020 11:10
 Operator : SY/MD
 Sample : L2826-06
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 CWKB9

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVTR053020WMA.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
unknown-01	1.48	18.2	ug/L	742680	1	5.64	203615	5.0
(DEL) Alkane: Str...	1.82	3.7	ug/L	151216	1	5.64	203615	5.0
Ethanethiol	2.05	0.5	ug/L	21142	1	5.64	203615	5.0
(DEL) Alkane: Str...	3.06	0.6	ug/L	24373	1	5.64	203615	5.0
(DEL) Alkane: Str...	5.51	0.6	ug/L	23724	1	5.64	203615	5.0
(DEL) Alkane: Str...	7.59	0.6	ug/L	28584	2	8.87	249476	5.0
Hexanal	8.26	1.0	ug/L	48803	2	8.87	249476	5.0
Furan, 2-pentyl-	10.74	0.6	ug/L	23028	3	11.27	178515	5.0
3-Octanone	10.96	0.5	ug/L	19445	3	11.27	178515	5.0
1-Hexanol, 2-ethyl-	11.56	1.1	ug/L	37497	3	11.27	178515	5.0