

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062420\
 Data File : VU039089.D
 Acq On : 25 Jun 2020 02:35
 Operator : SY/MD
 Sample : L3110-05
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F9F20

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\SOMUTR062320WMA.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	1.372	4	10	21	rBV	43335	44385	1.20%	0.215%
2	1.613	75	85	94	rVV2	179168	203595	5.50%	0.985%
3	1.665	94	101	110	rVB	165586	193693	5.23%	0.937%
4	1.932	175	184	196	rBV	129149	163873	4.43%	0.793%
5	2.012	201	209	219	rVB	33256	48638	1.31%	0.235%
6	2.594	372	390	393	rBV	252288	371755	10.05%	1.799%
7	3.073	523	539	562	rBV	156610	347051	9.38%	1.680%
8	3.398	621	640	672	rBV	1601266	3700575	100.00%	17.911%
9	4.337	914	932	949	rBV5	23813	64380	1.74%	0.312%
10	4.472	954	974	995	rVV	238021	608389	16.44%	2.945%
11	4.674	1017	1037	1088	rBV2	259814	831304	22.46%	4.023%
12	5.102	1153	1170	1182	rBV	217925	480945	13.00%	2.328%
13	5.169	1182	1191	1208	rVB3	42542	103007	2.78%	0.499%
14	5.494	1277	1292	1311	rVB4	106045	240981	6.51%	1.166%
15	5.758	1353	1374	1401	rBV2	456955	1215520	32.85%	5.883%
16	5.931	1405	1428	1453	rVV	1247764	2773966	74.96%	13.426%
17	6.279	1522	1536	1560	rVB	379449	705354	19.06%	3.414%
18	6.719	1657	1673	1699	rBV	284498	612349	16.55%	2.964%
19	6.832	1699	1708	1717	rVV3	36721	71123	1.92%	0.344%
20	6.890	1717	1726	1737	rVV3	83974	158731	4.29%	0.768%
21	6.951	1737	1745	1757	rVB2	27312	50743	1.37%	0.246%
22	7.095	1774	1790	1803	rBV6	28115	58875	1.59%	0.285%
23	7.282	1829	1848	1863	rBV	442435	844722	22.83%	4.088%
24	7.404	1870	1886	1907	rBV	307917	609047	16.46%	2.948%
25	7.591	1930	1944	1955	rBV	151019	272830	7.37%	1.320%
26	7.857	2016	2027	2035	rBV3	36479	68170	1.84%	0.330%
27	7.922	2035	2047	2060	rVV	521585	893846	24.15%	4.326%
28	8.201	2123	2134	2144	rBV	93491	161370	4.36%	0.781%
29	8.655	2259	2275	2303	rBV	947174	1699701	45.93%	8.227%
30	8.806	2314	2322	2332	rVB5	22979	39115	1.06%	0.189%
31	9.436	2504	2518	2532	rBV	514490	854351	23.09%	4.135%
32	10.771	2920	2933	2950	rBV	242956	392724	10.61%	1.901%
33	11.700	3212	3222	3233	rBV3	35141	52046	1.41%	0.252%
34	11.822	3246	3260	3278	rBV	497770	785477	21.23%	3.802%

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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

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062320WMA.M
Title : TRACE VOA SOM01.0

35	12.205	3366	3379	3396	rbV	503989	817646	22.10%	3.957%
36	12.909	3587	3598	3612	rbV2	78093	120959	3.27%	0.585%

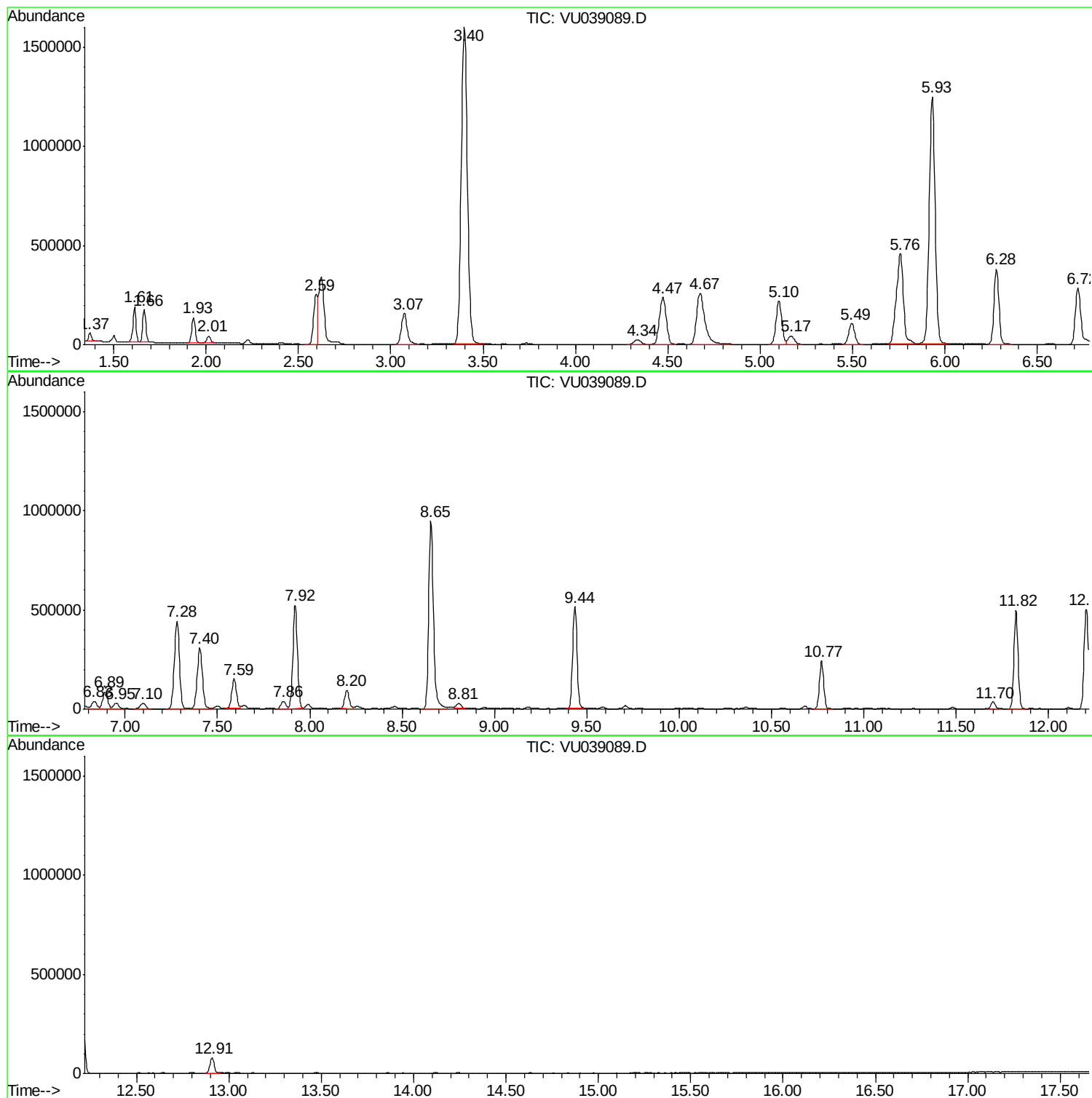
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062320WMA.M
Quant Title : TRACE VOA SOM01.0

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



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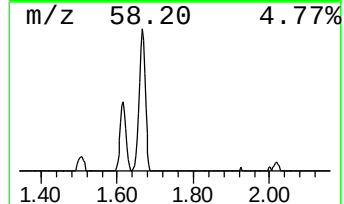
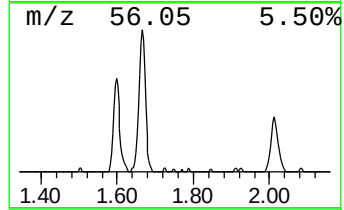
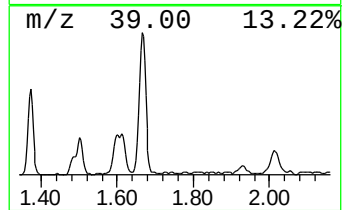
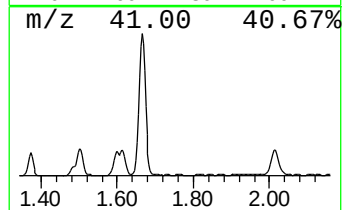
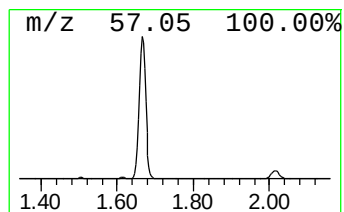
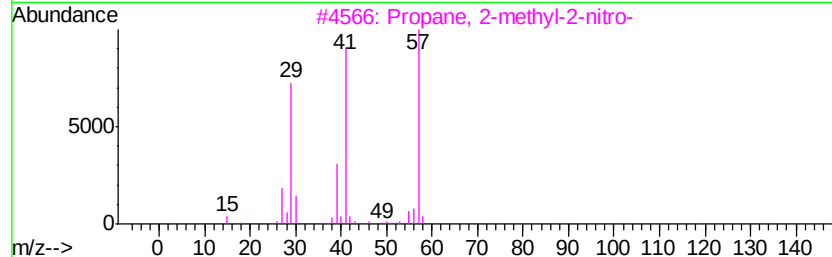
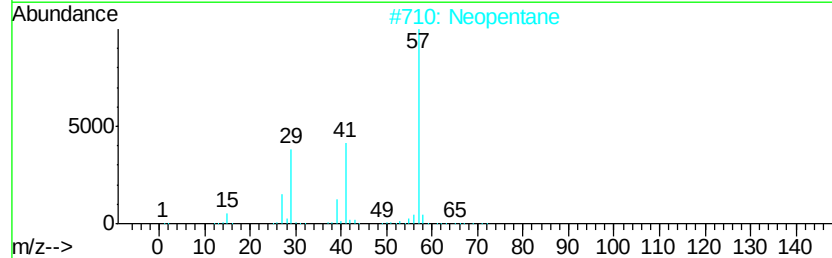
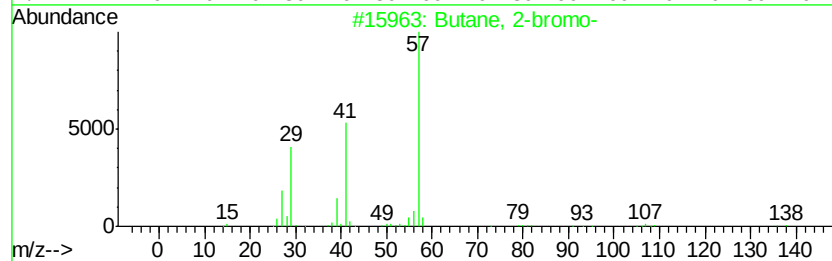
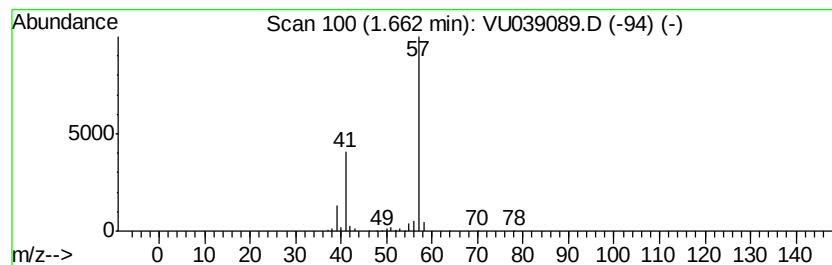
Instrument :
MSVOA_U
ClientSampleId :
F9F20

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062320WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 Butane, 2-bromo- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.66	1.37 ug/L	193693	1,4-Difluorobenzene	6.28	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-bromo-	136	C4H9Br	000078-76-2	83
2	Neopentane	72	C5H12	000463-82-1	72
3	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	64
4	Butane, 2-bromo-	136	C4H9Br	000078-76-2	40
5	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	36



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Instrument :
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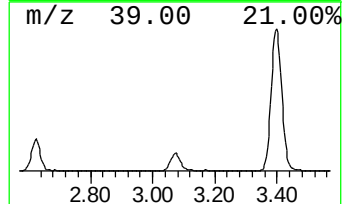
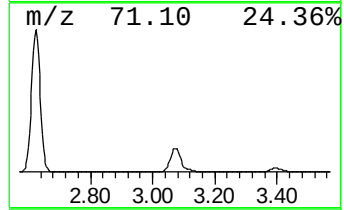
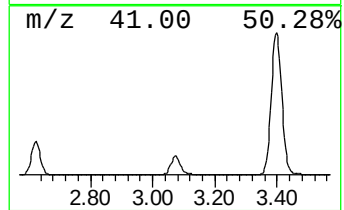
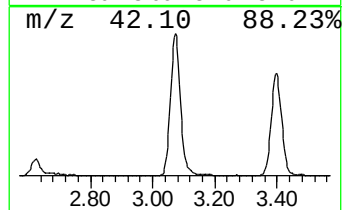
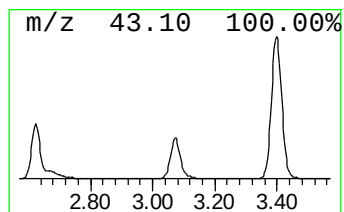
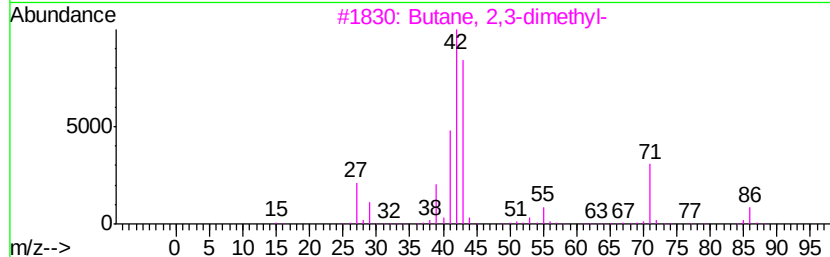
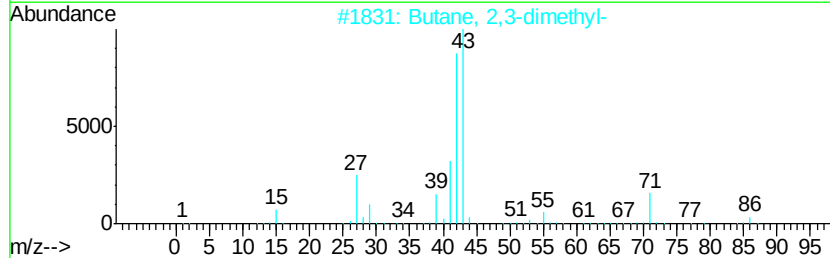
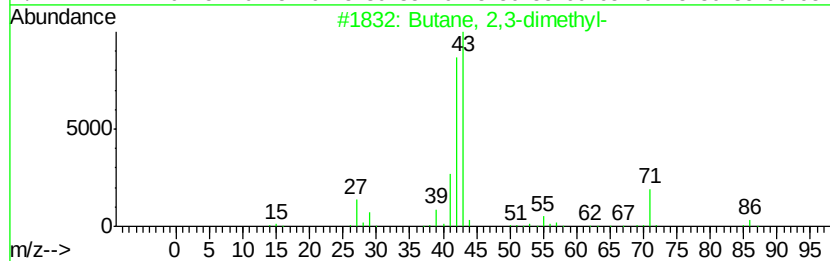
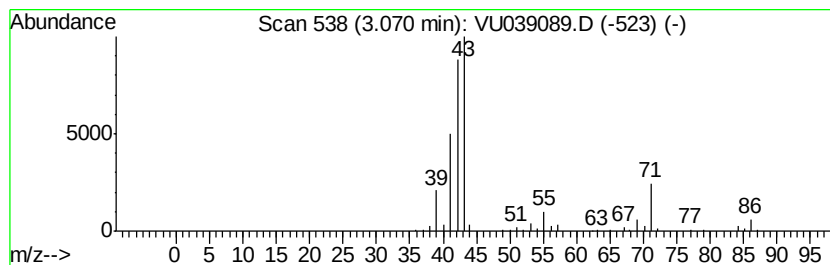
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.07	2.46 ug/L	347051	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
2		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
3		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	80
4		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	52
5		Pentane	72	C5H12	000109-66-0	33



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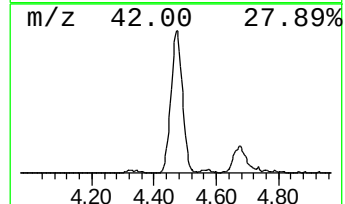
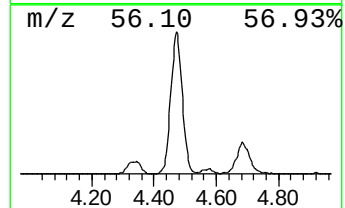
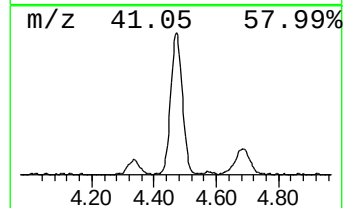
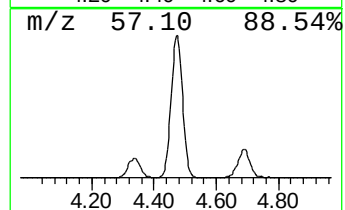
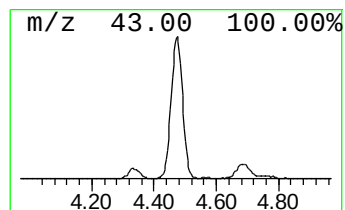
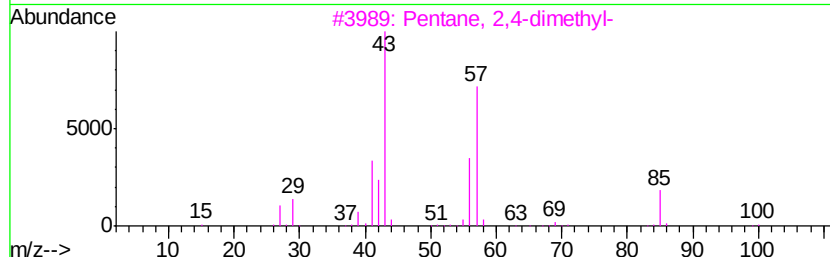
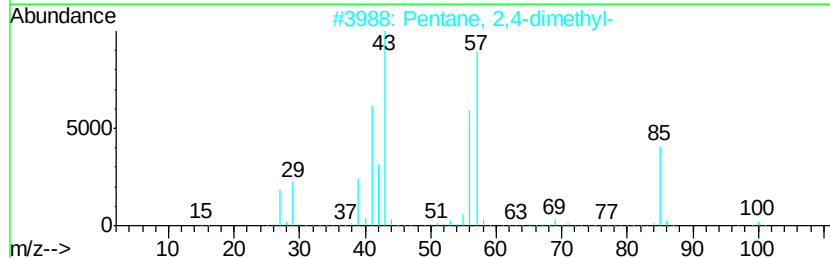
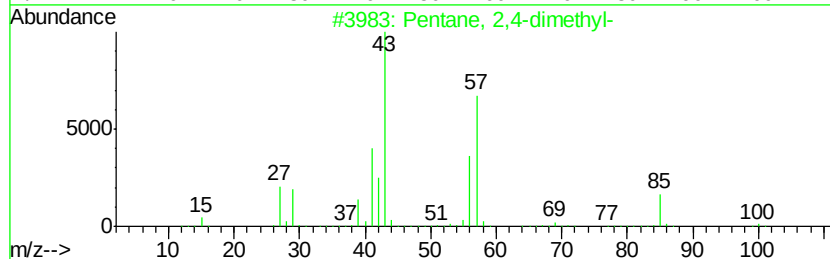
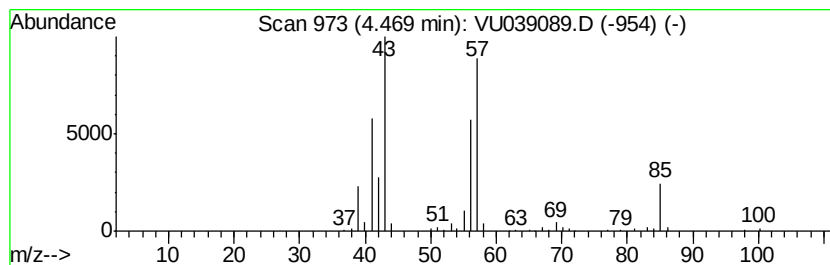
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062320WMA.M
Quant Title : TRACE VOA SOM01.0

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.
4.47	4.31 ug/L	608389	1,4-Difluorobenzene	6.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,4-dimethyl-			100	C7H16	000108-08-7	90
2	Pentane, 2,4-dimethyl-			100	C7H16	000108-08-7	83
3	Pentane, 2,4-dimethyl-			100	C7H16	000108-08-7	72
4	Heptane, 3-methyl-			114	C8H18	000589-81-1	72
5	Butane, 2,2,3-trimethyl-			100	C7H16	000464-06-2	59



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

Instrument :
MSVOA_U
ClientSampled :
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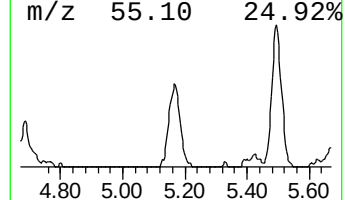
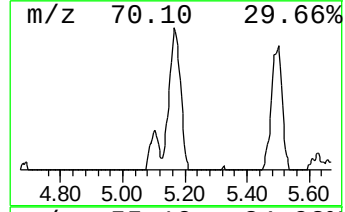
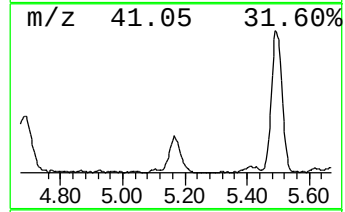
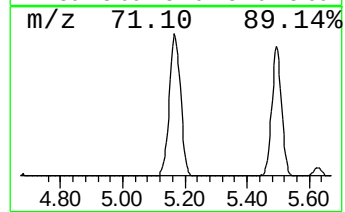
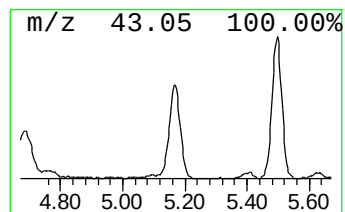
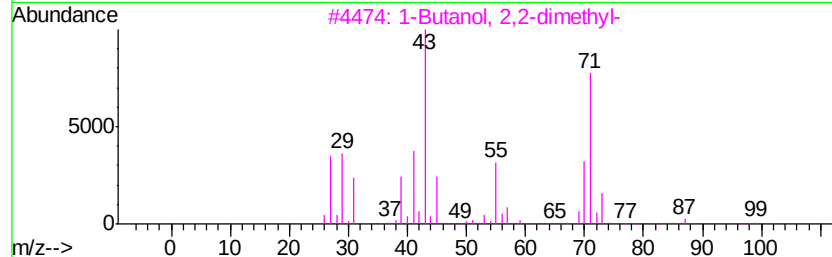
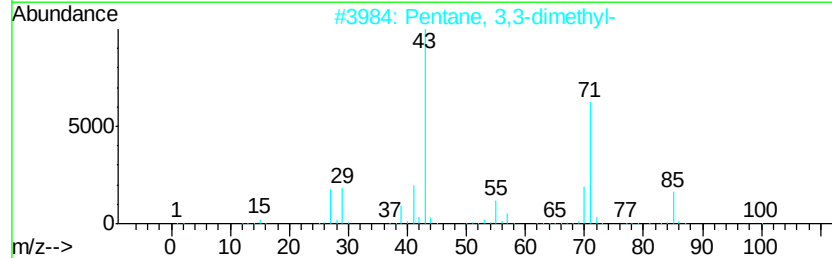
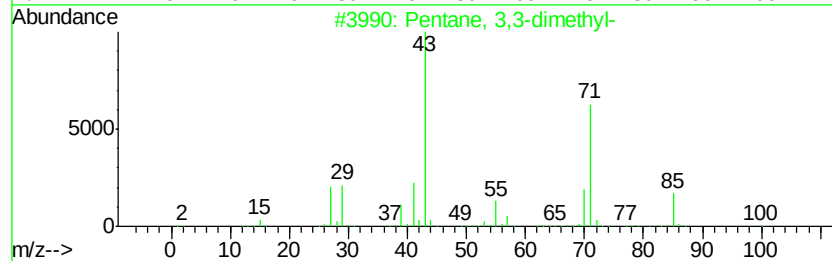
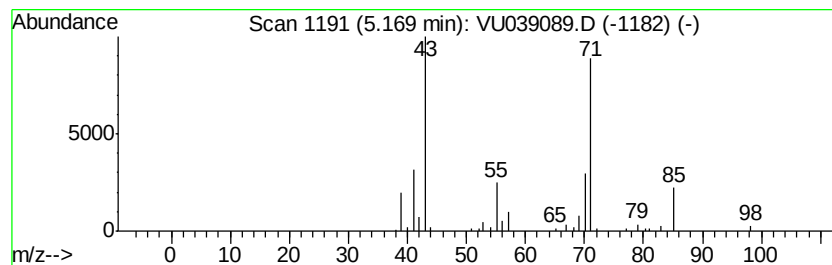
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	0.73 ug/L	103007	1,4-Difluorobenzene	6.28

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	78	
2	Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	78	
3	1-Butanol, 2,2-dimethyl-	102	C6H14O	001185-33-7	50	
4	1-Butanol, 2,2-dimethyl-	102	C6H14O	001185-33-7	50	
5	1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	38	



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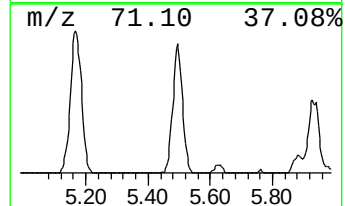
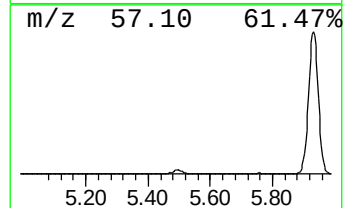
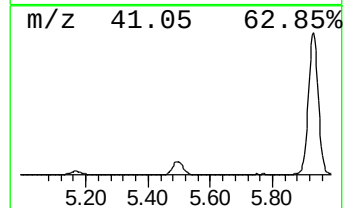
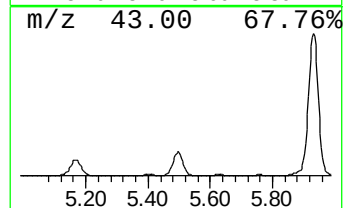
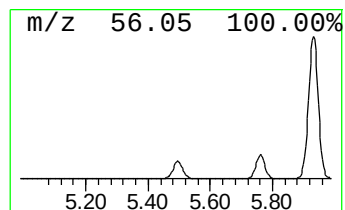
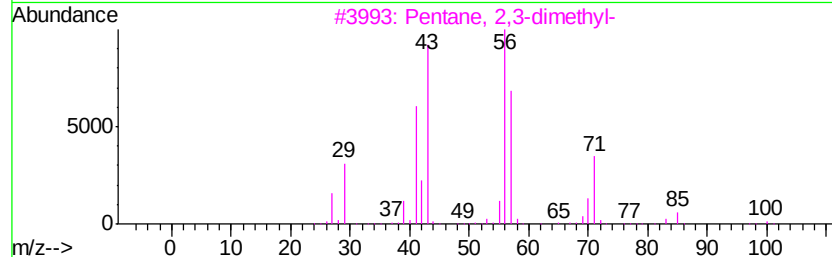
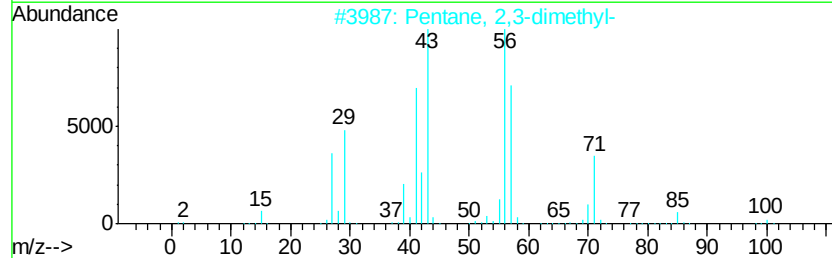
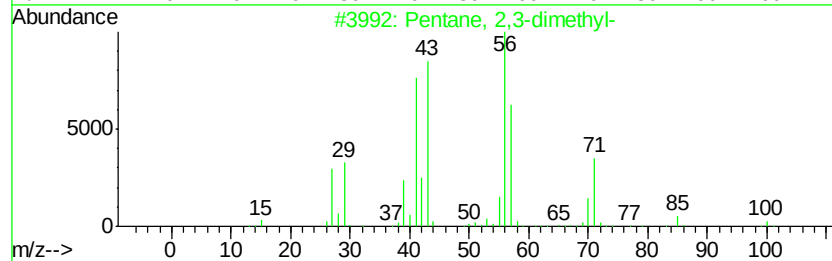
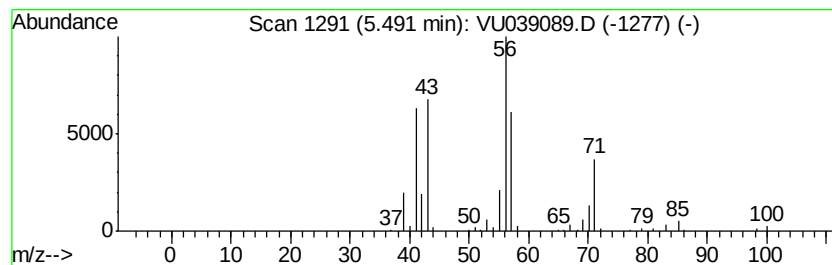
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062320WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.49	1.71 ug/L	240981	1,4-Difluorobenzene	6.28

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91	
2	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	90	
3	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	86	
4	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	72	
5	(Z)-2-Heptene	98	C7H14	006443-92-1	59	



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU062420\
Data File : VU039089.D
Acq On : 25 Jun 2020 02:35
Operator : SY/MD
Sample : L3110-05
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F9F20

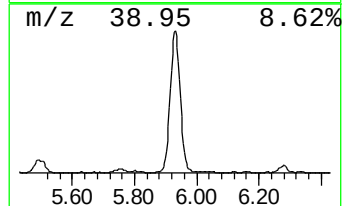
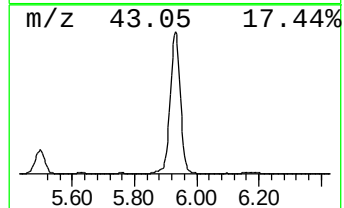
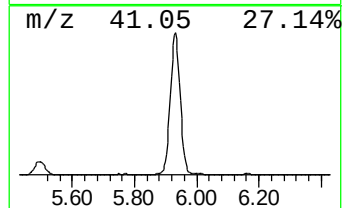
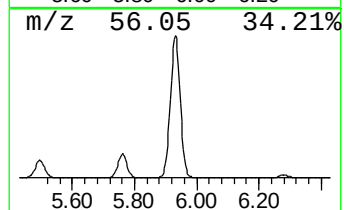
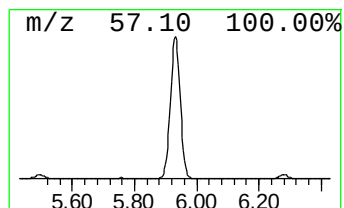
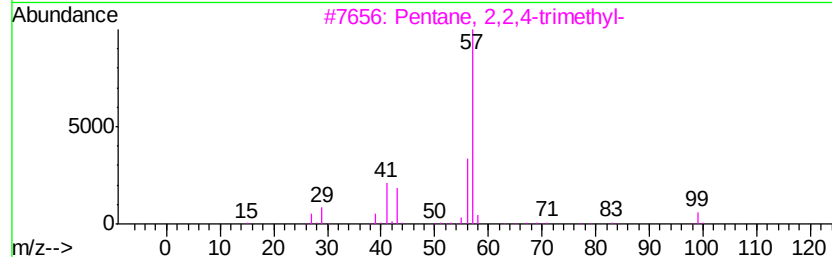
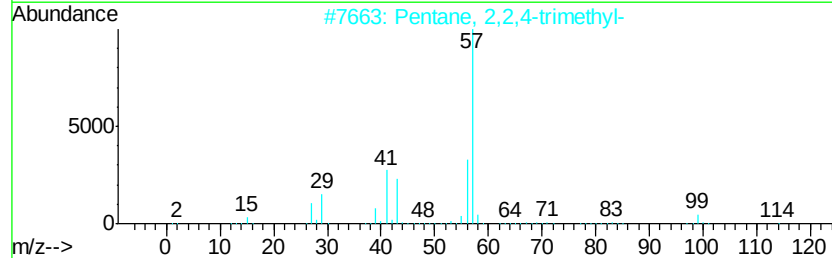
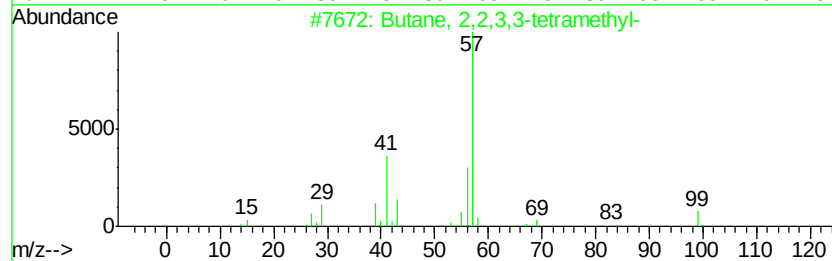
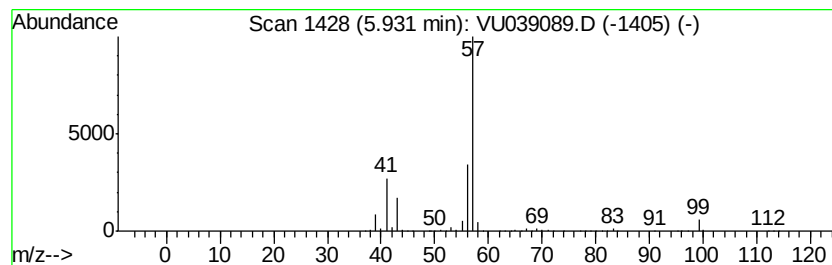
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.93	19.66 ug/L	2773970	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
2		Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
3		Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
4		Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
5		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU062420\
Data File : VU039089.D
Acq On : 25 Jun 2020 02:35
Operator : SY/MD
Sample : L3110-05
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

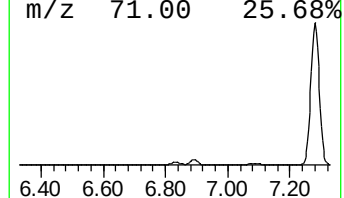
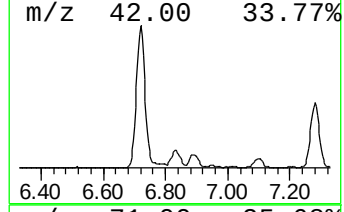
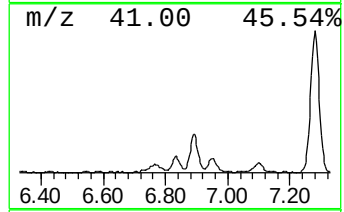
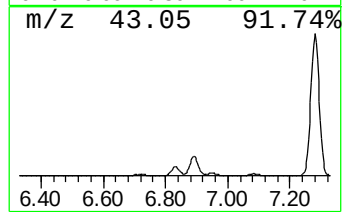
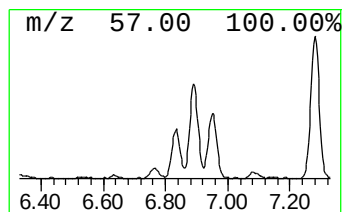
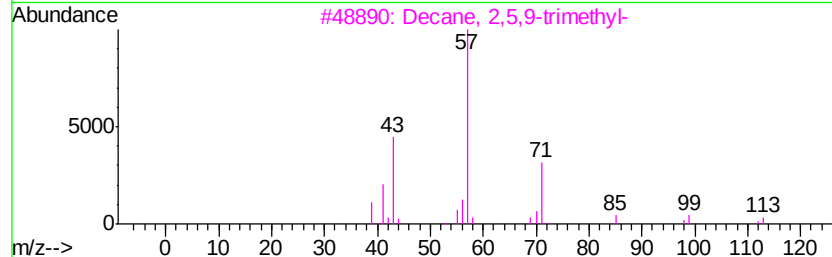
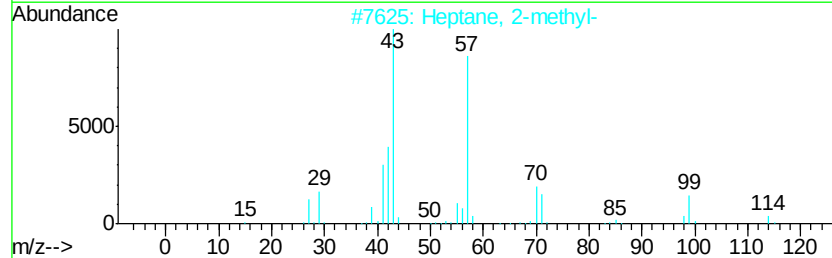
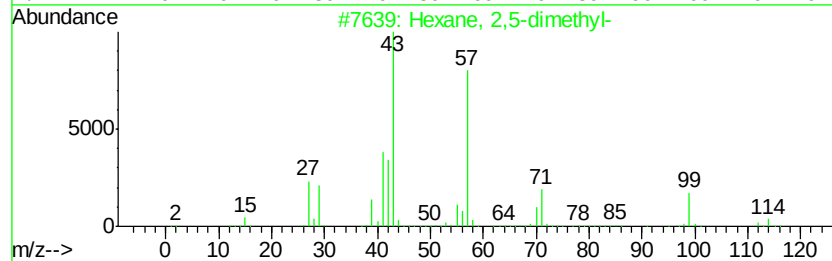
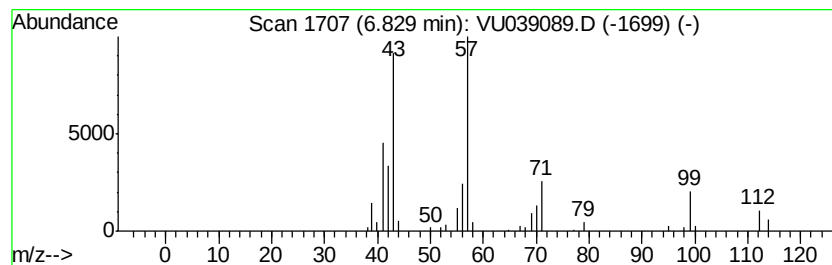
Instrument :
MSVOA_U
ClientSampleId :
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.83	0.50 ug/L	71123	1,4-Difluorobenzene	6.28	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	83
2	Heptane, 2-methyl-	114	C8H18	000592-27-8	64
3	Decane, 2,5,9-trimethyl-	184	C13H28	062108-22-9	50
4	Heptane, 2-methyl-	114	C8H18	000592-27-8	50
5	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	47



Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU062420\
Data File : VU039089.D
Acq On : 25 Jun 2020 02:35
Operator : SY/MD
Sample : L3110-05
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

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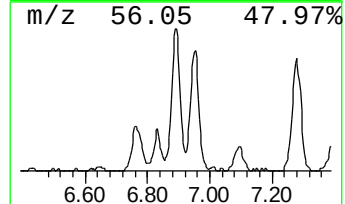
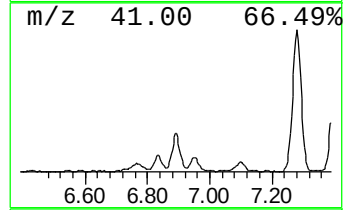
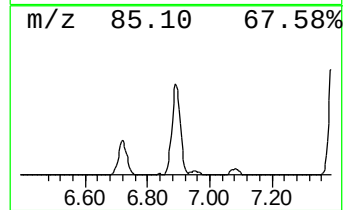
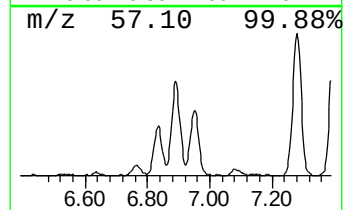
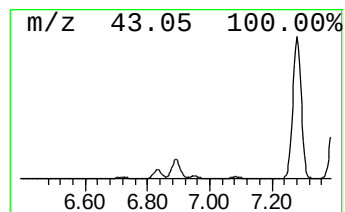
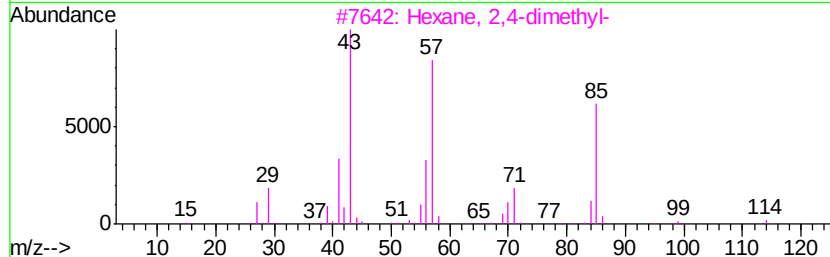
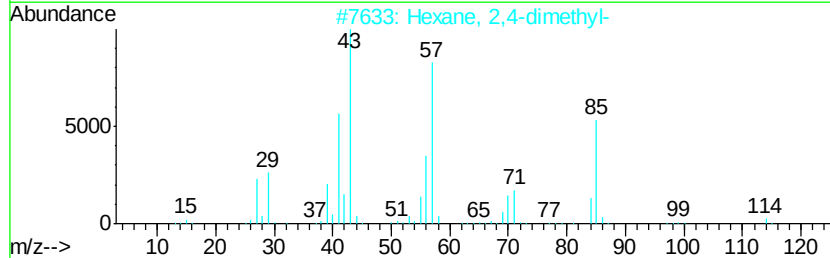
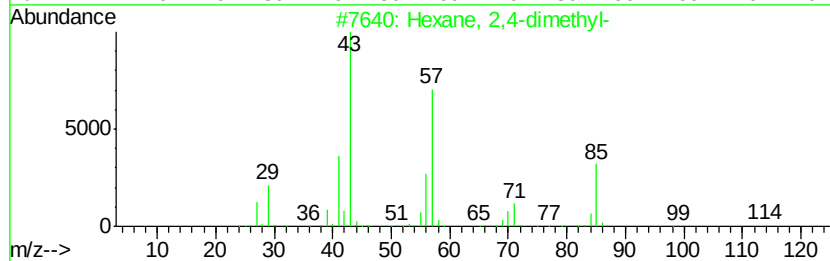
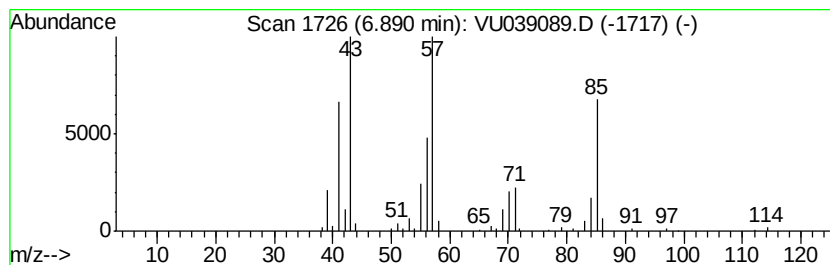
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.89	1.13 ug/L	158731	1,4-Difluorobenzene	6.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	91
2			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	83
3			Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	72
4			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	59
5			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU062420\
Data File : VU039089.D
Acq On : 25 Jun 2020 02:35
Operator : SY/MD
Sample : L3110-05
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

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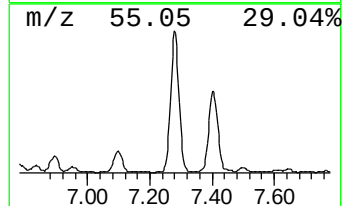
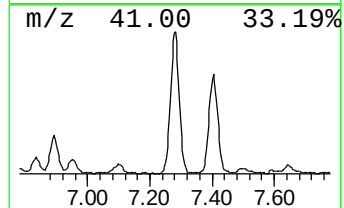
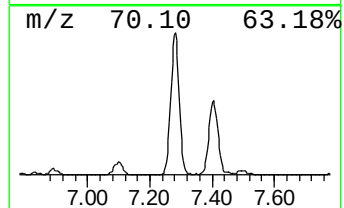
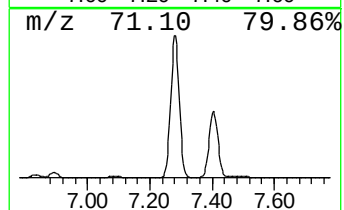
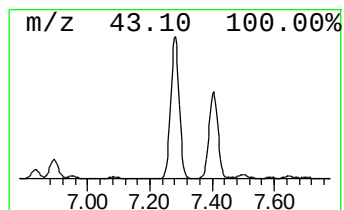
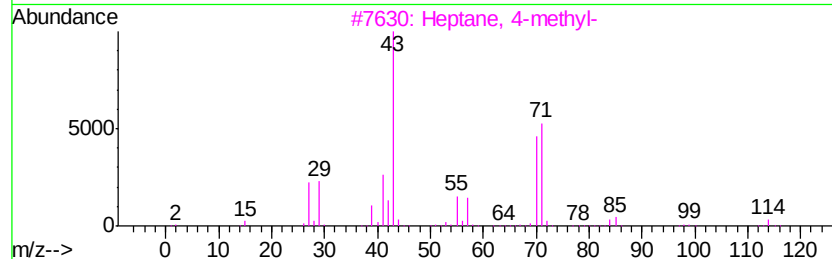
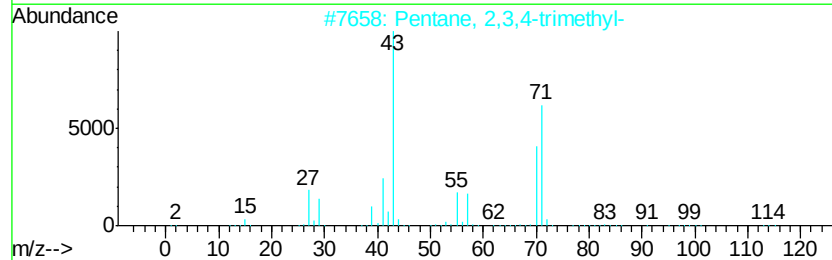
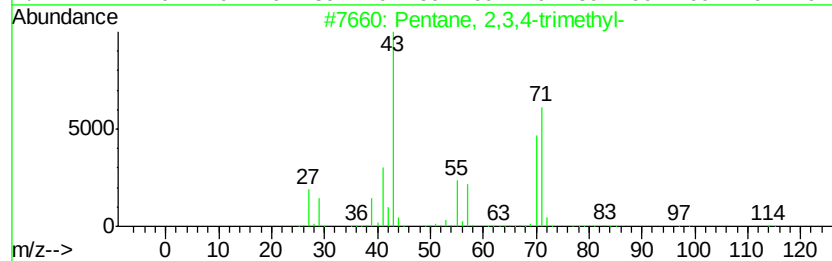
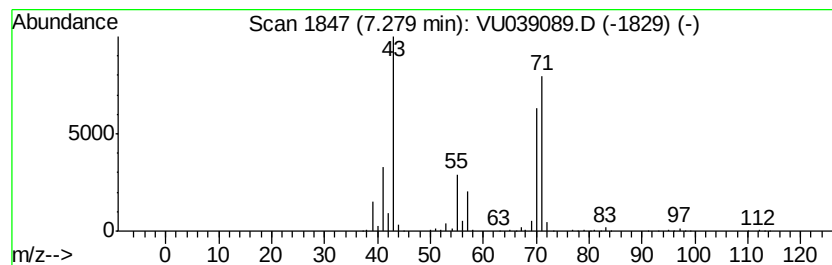
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 9 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.28	5.99 ug/L	844722	1,4-Difluorobenzene	6.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	86
3			Heptane, 4-methyl-	114	C8H18	000589-53-7	83
4			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	83
5			Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	83



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU062420\
Data File : VU039089.D
Acq On : 25 Jun 2020 02:35
Operator : SY/MD
Sample : L3110-05
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

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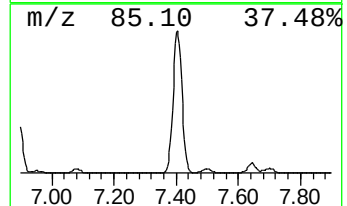
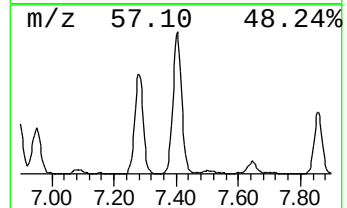
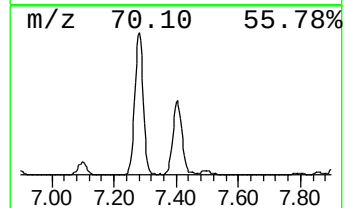
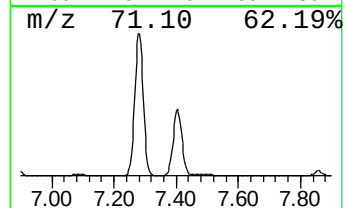
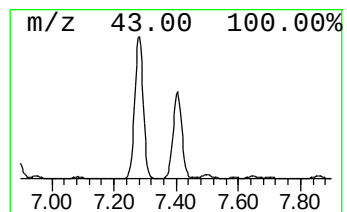
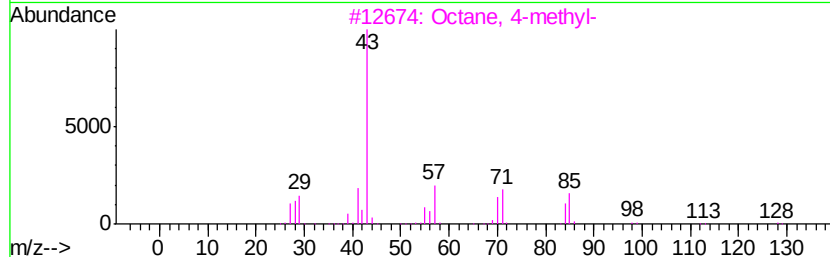
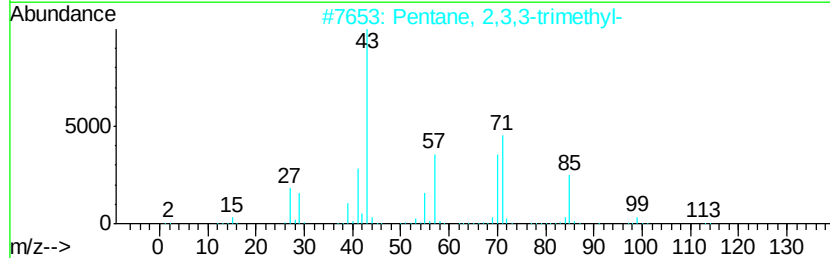
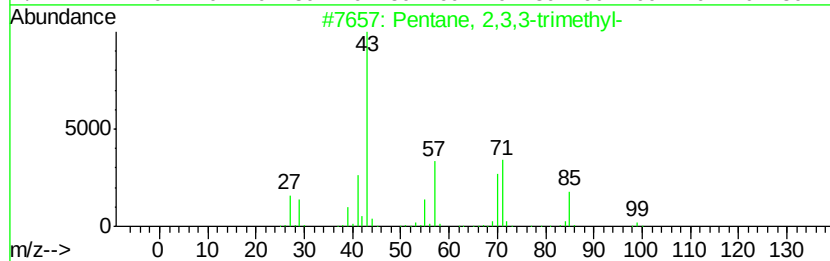
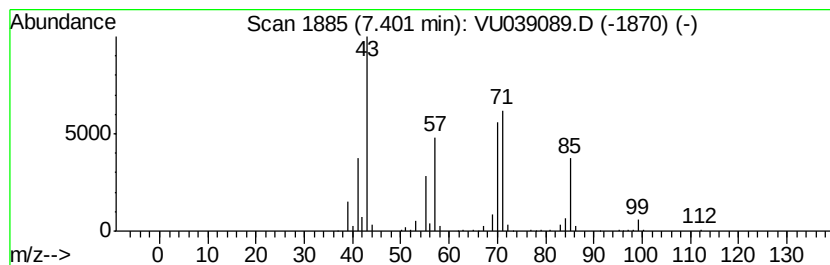
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 10 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.40	4.32 ug/L	609047	1,4-Difluorobenzene	6.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	83
2			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	72
3			Octane, 4-methyl-	128	C9H20	002216-34-4	64
4			Hexane, 3-methyl-	100	C7H16	000589-34-4	64
5			Hexane, 3-methyl-	100	C7H16	000589-34-4	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU062420\
Data File : VU039089.D
Acq On : 25 Jun 2020 02:35
Operator : SY/MD
Sample : L3110-05
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 1 Sample Multiplier: 1

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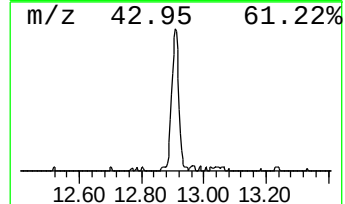
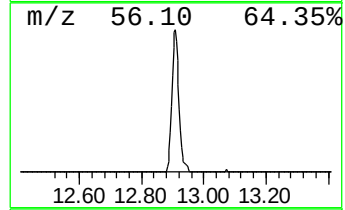
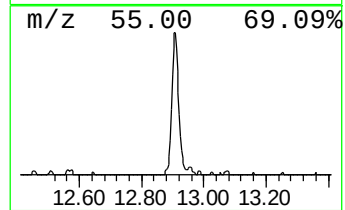
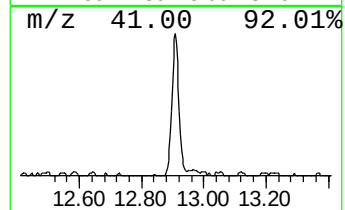
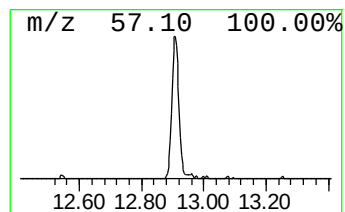
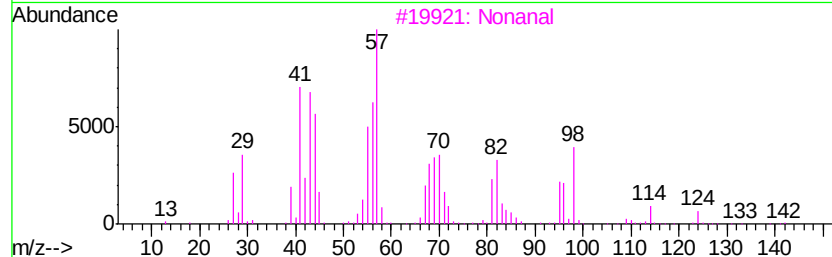
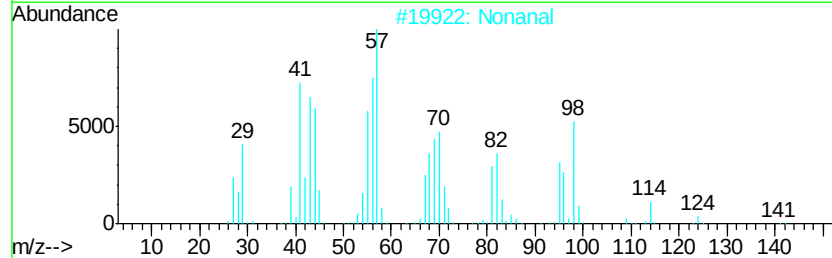
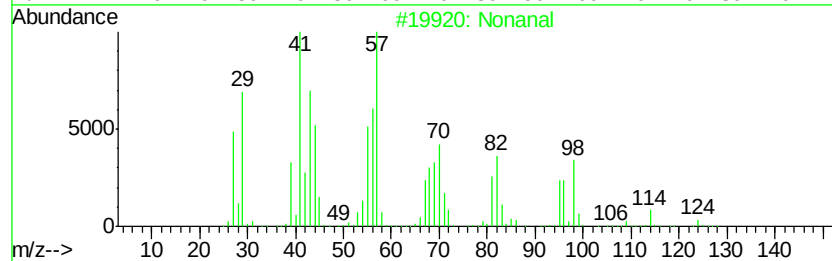
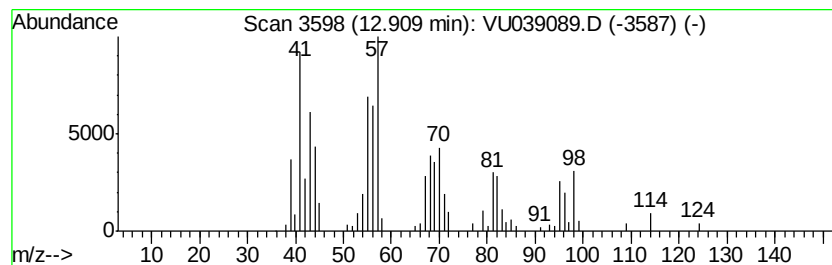
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 12 Nonanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.91	0.77 ug/L	120959	1,4-Dichlorobenzene-d4	11.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonanal	142	C9H18O	000124-19-6	83
2		Nonanal	142	C9H18O	000124-19-6	72
3		Nonanal	142	C9H18O	000124-19-6	72
4		2-Propen-1-amine, N-2-propenyl-	97	C6H11N	000124-02-7	35
5		Heptane, 4-chloro-	134	C7H15Cl	000998-95-8	27



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU062420\
 Data File : VU039089.D
 Acq On : 25 Jun 2020 02:35
 Operator : SY/MD
 Sample : L3110-05
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F9F20

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR062320WMA.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
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(DEL) Alkane: Str...	3.07	2.5	ug/L	347051	1	6.28	705354	5.0
(DEL) Alkane: Str...	4.47	4.3	ug/L	608389	1	6.28	705354	5.0
(DEL) Alkane: Str...	5.17	0.7	ug/L	103007	1	6.28	705354	5.0
(DEL) Alkane: Str...	5.49	1.7	ug/L	240981	1	6.28	705354	5.0
(DEL) Alkane: Str...	5.93	19.7	ug/L	2773970	1	6.28	705354	5.0
(DEL) Alkane: Str...	6.83	0.5	ug/L	71123	1	6.28	705354	5.0
(DEL) Alkane: Str...	6.89	1.1	ug/L	158731	1	6.28	705354	5.0
(DEL) Alkane: Str...	7.28	6.0	ug/L	844722	1	6.28	705354	5.0
(DEL) Alkane: Str...	7.40	4.3	ug/L	609047	1	6.28	705354	5.0
Nonanal	12.91	0.8	ug/L	120959	3	11.82	785477	5.0