

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV100322\
 Data File : VV028306.D
 Acq On : 04 Oct 2022 02:29
 Operator : SY/MD
 Sample : N4866-19
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 EXFR3

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_V\Method\SFAMVTR100322WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VV028306.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.105	14	20	38	rVB	223271	210697	6.02%	1.256%
2	1.211	46	53	69	rBV	354625	303336	8.67%	1.808%
3	1.301	73	81	90	rBV	1954919	1930741	55.15%	11.510%
4	1.388	98	108	135	rBV2	36747	134327	3.84%	0.801%
5	1.561	156	162	173	rVB	95057	107880	3.08%	0.643%
6	1.629	173	183	202	rVB	2853365	3500573	100.00%	20.869%
7	1.799	230	236	247	rVB	41926	56388	1.61%	0.336%
8	2.101	321	330	355	rVB	208266	365242	10.43%	2.177%
9	2.487	436	450	463	rBV3	17856	40509	1.16%	0.242%
10	2.571	463	476	501	rVB	599469	1071443	30.61%	6.388%
11	3.754	826	844	861	rBV3	84600	219441	6.27%	1.308%
12	3.905	881	891	933	rBV	49583	230988	6.60%	1.377%
13	4.342	1010	1027	1054	rBV2	126558	326703	9.33%	1.948%
14	4.670	1108	1129	1150	rBV	179102	451387	12.89%	2.691%
15	5.040	1227	1244	1249	rBV2	325882	665175	19.00%	3.966%
16	5.092	1250	1260	1287	rVV	1373484	3056753	87.32%	18.223%
17	5.214	1288	1298	1315	rVB3	26599	67032	1.91%	0.400%
18	5.612	1408	1422	1441	rBV	214287	444583	12.70%	2.650%
19	6.066	1549	1563	1590	rBV	170325	354499	10.13%	2.113%
20	6.985	1837	1849	1875	rBV	71779	140088	4.00%	0.835%
21	7.310	1939	1950	1970	rBV	338448	605221	17.29%	3.608%
22	7.622	2038	2047	2065	rBV2	41584	77547	2.22%	0.462%
23	8.088	2181	2192	2224	rBV	317355	654515	18.70%	3.902%
24	8.847	2417	2428	2456	rBV	318985	547920	15.65%	3.267%
25	10.214	2841	2853	2868	rBV2	129050	207394	5.92%	1.236%
26	11.246	3163	3174	3200	rBV	315884	494623	14.13%	2.949%
27	11.619	3279	3290	3310	rBV	319609	508825	14.54%	3.033%

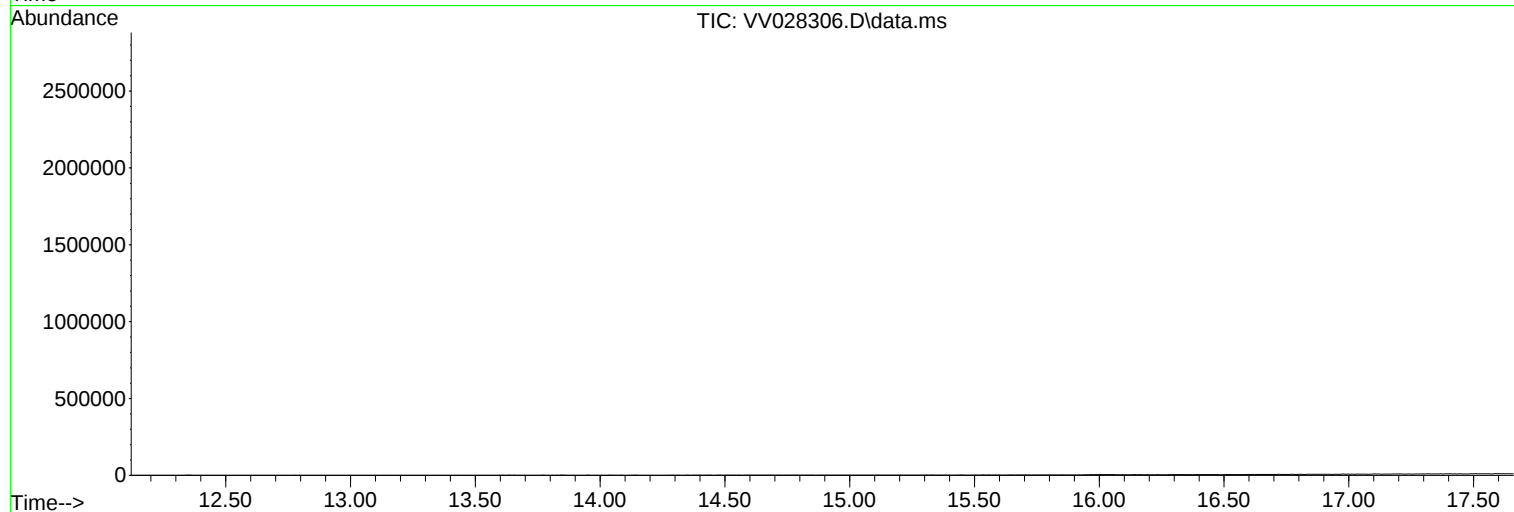
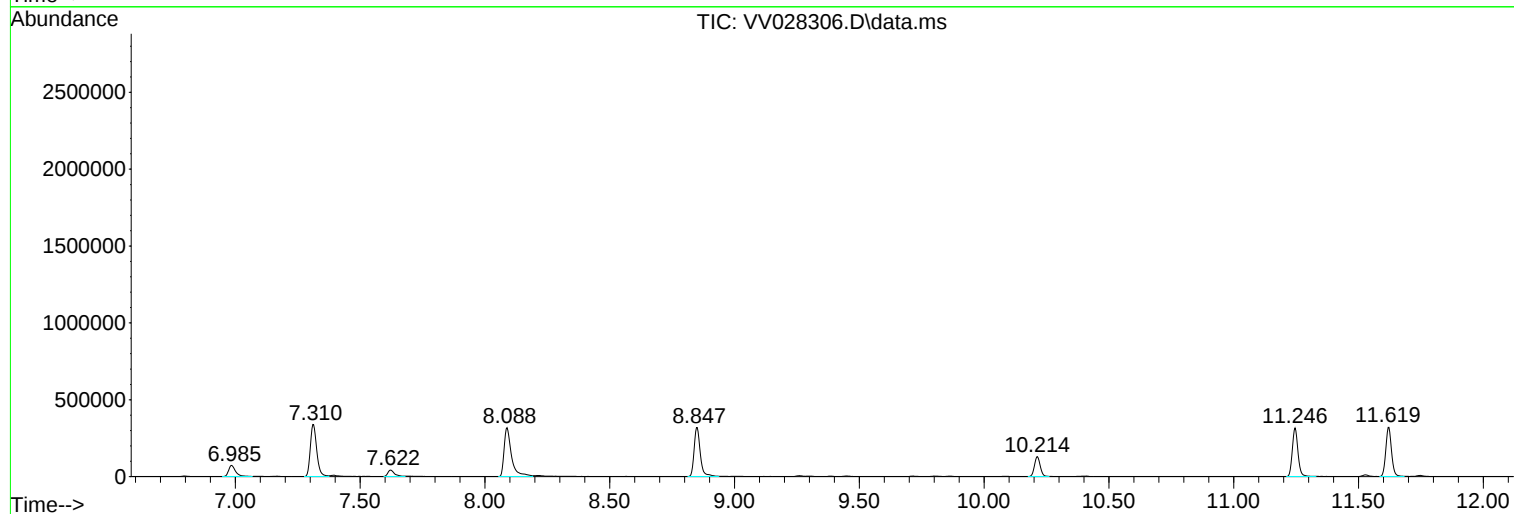
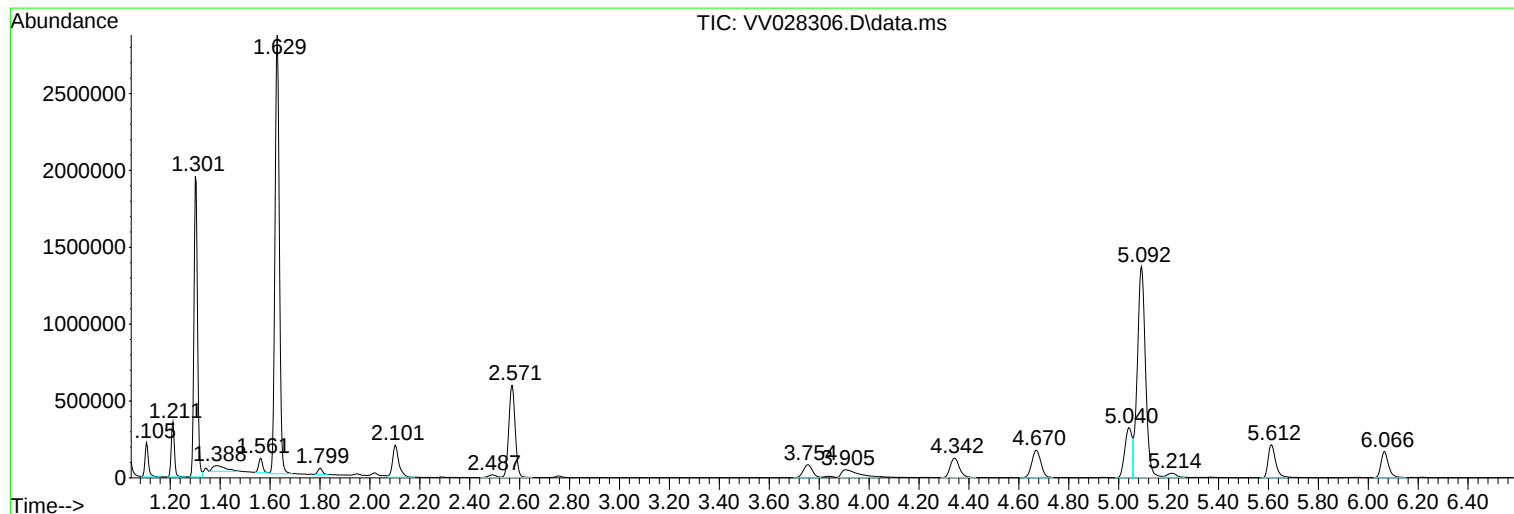
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR100322WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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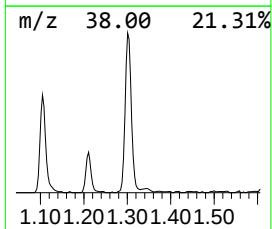
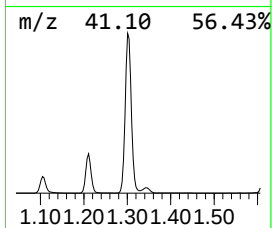
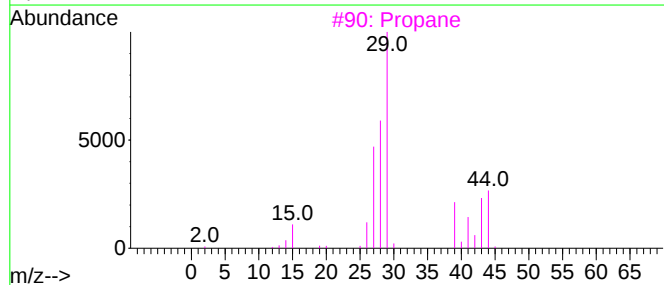
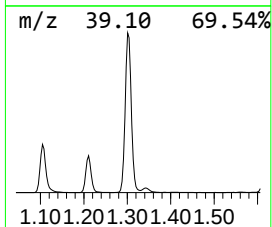
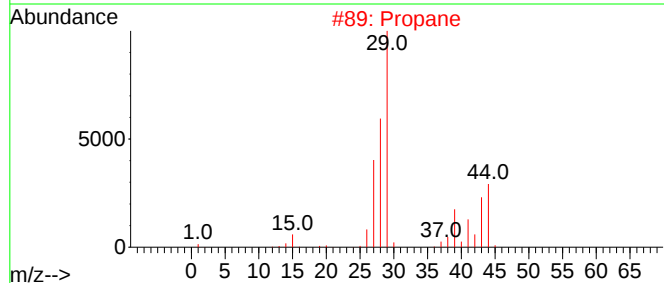
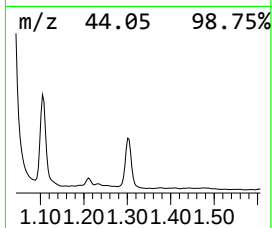
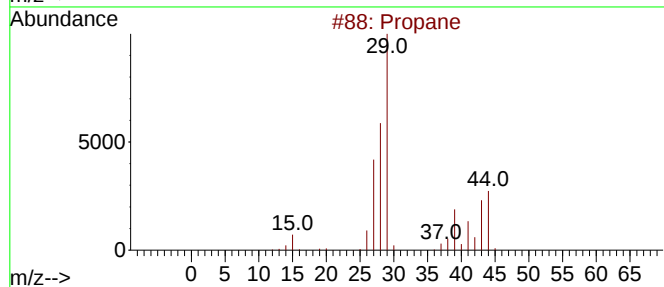
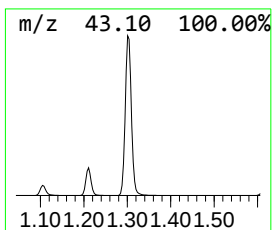
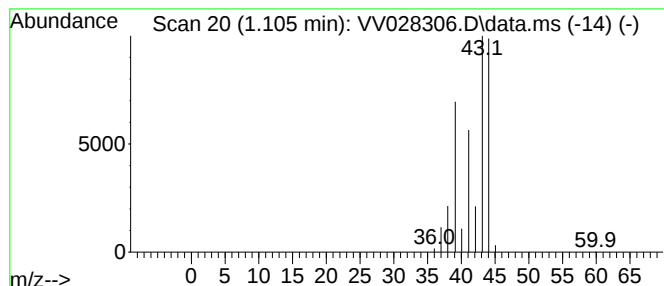
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR100322WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.105	2.37 ug/L	210697	1,4-Difluorobenzene	5.612

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane	44	C3H8	000074-98-6	90
2			Propane	44	C3H8	000074-98-6	83
3			Propane	44	C3H8	000074-98-6	9
4			Propene	42	C3H6	000115-07-1	9
5			Ethylene oxide	44	C2H4O	000075-21-8	5



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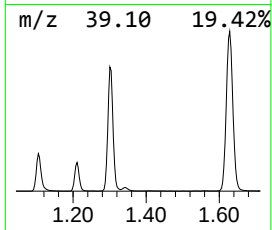
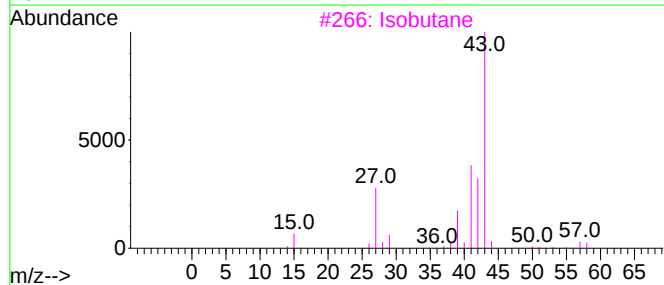
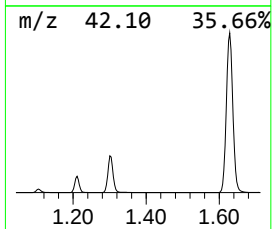
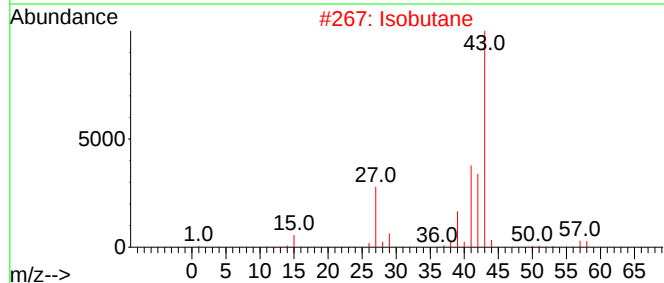
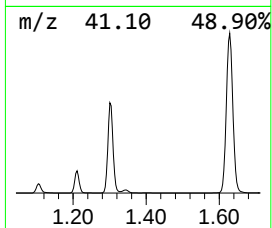
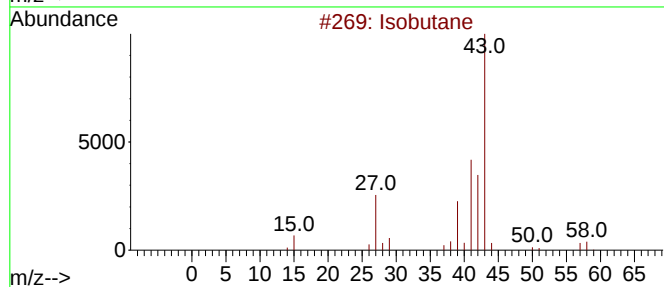
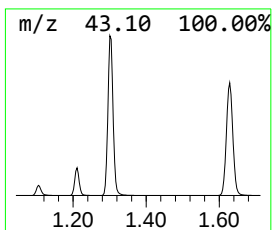
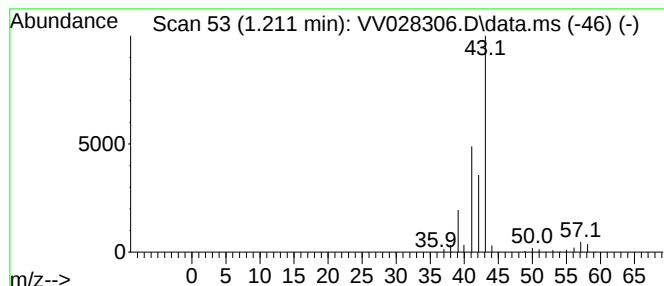
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR100322WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.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.
1.211	3.41 ug/L	303336	1,4-Difluorobenzene	5.612

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isobutane	58	C4H10	000075-28-5	72
2		Isobutane	58	C4H10	000075-28-5	72
3		Isobutane	58	C4H10	000075-28-5	64
4		Isobutane	58	C4H10	000075-28-5	64
5		Isobutane	58	C4H10	000075-28-5	45



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ALS Vial : 42 Sample Multiplier: 1

Instrument :
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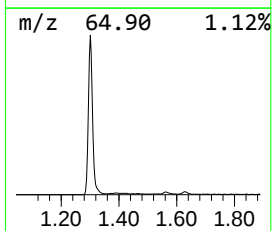
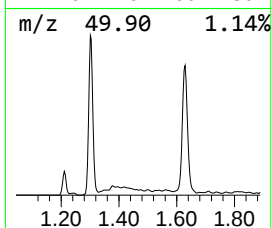
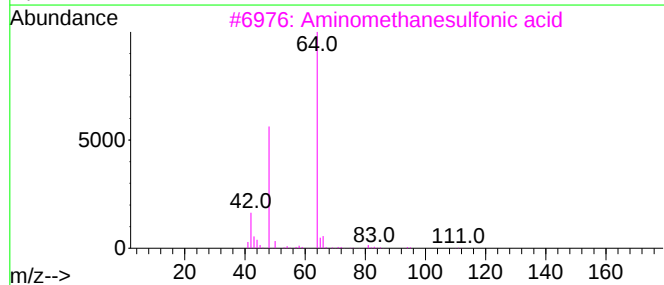
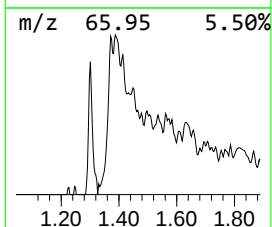
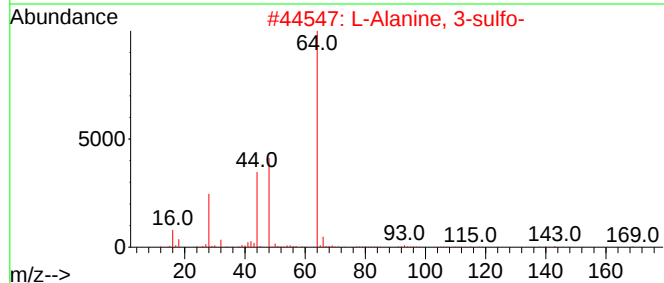
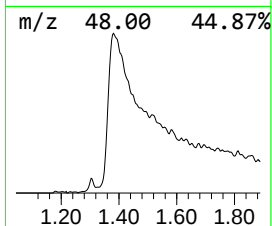
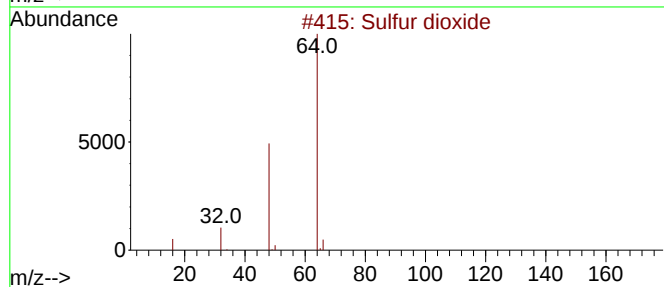
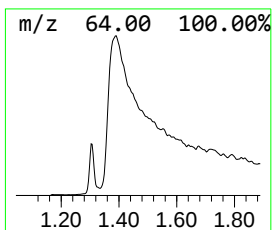
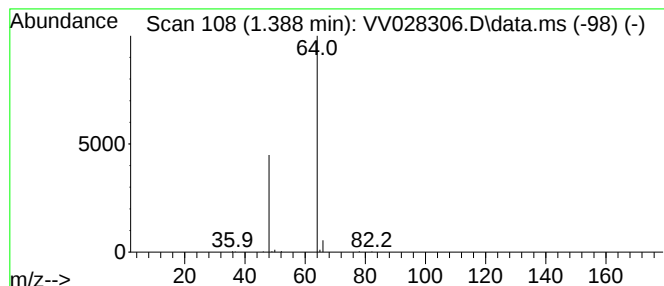
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR100322WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Sulfur dioxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.388	1.51 ug/L	134327	1,4-Difluorobenzene	5.612

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	9



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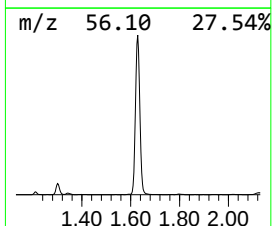
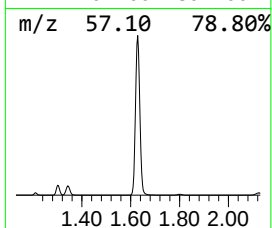
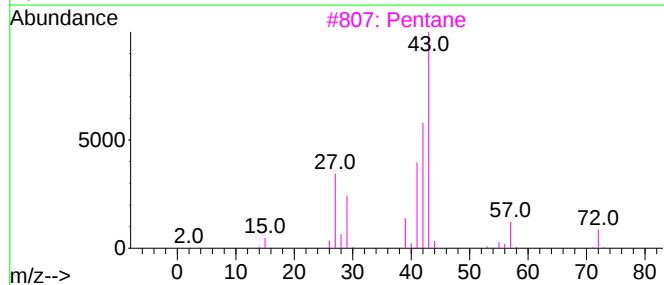
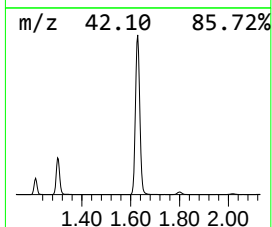
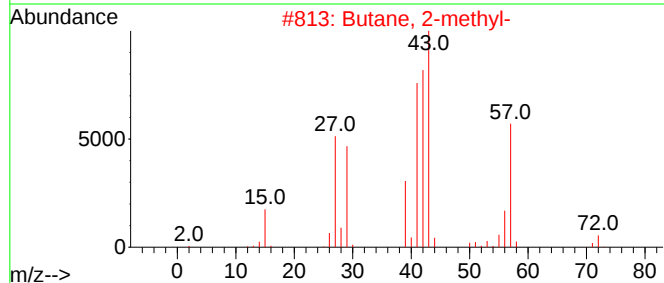
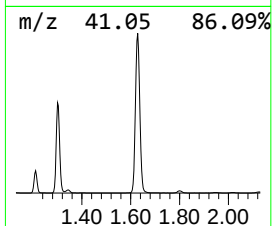
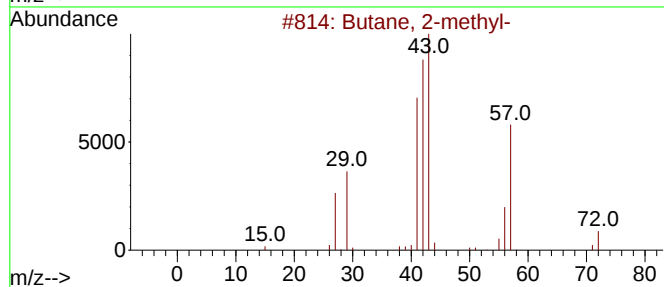
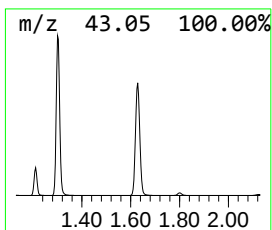
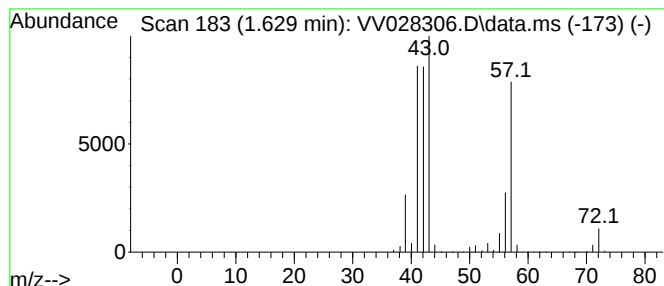
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.629	39.37 ug/L	3500570	1,4-Difluorobenzene	5.612	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	87
2	Butane, 2-methyl-	72	C5H12	000078-78-4	86
3	Pentane	72	C5H12	000109-66-0	42
4	Pentane	72	C5H12	000109-66-0	38
5	1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	36



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Instrument :
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ClientSampleId :
EXFR3

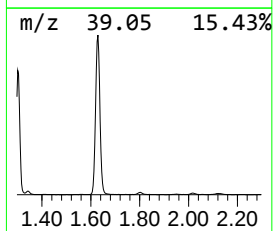
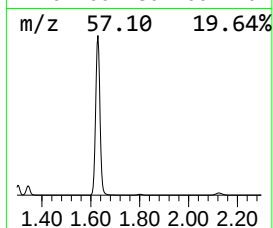
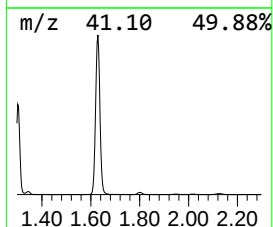
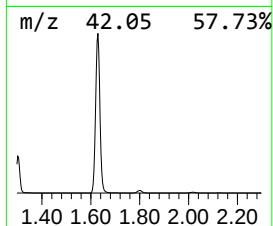
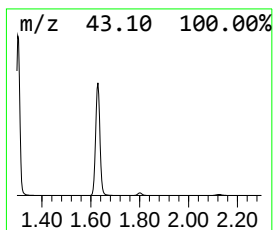
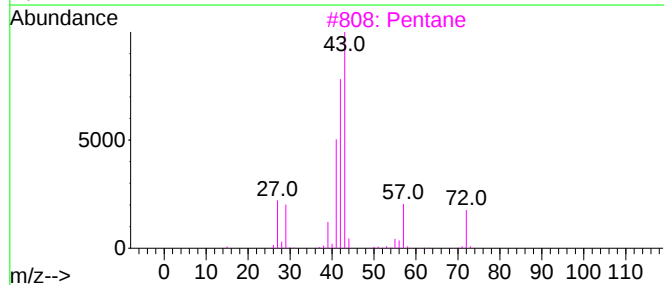
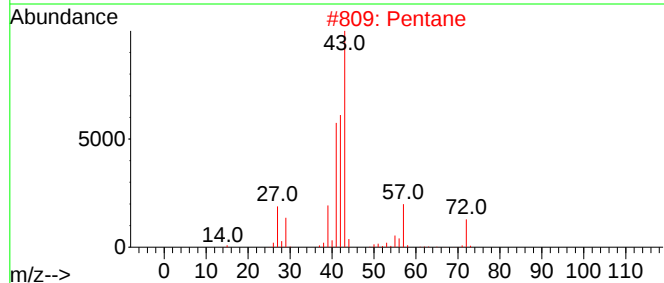
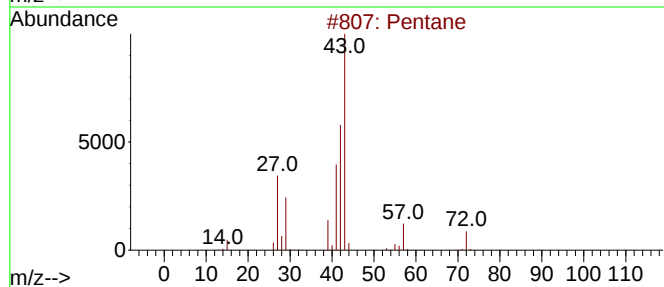
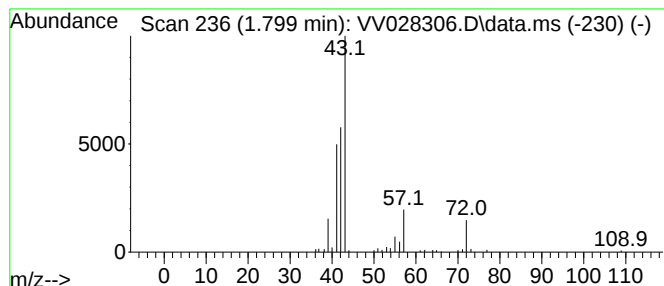
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
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Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.799	0.63 ug/L	56388	1,4-Difluorobenzene	5.612

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane			72	C5H12	000109-66-0	90
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	Pentane			72	C5H12	000109-66-0	86



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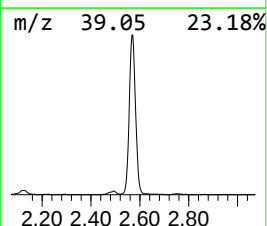
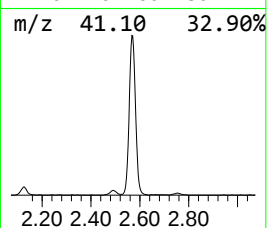
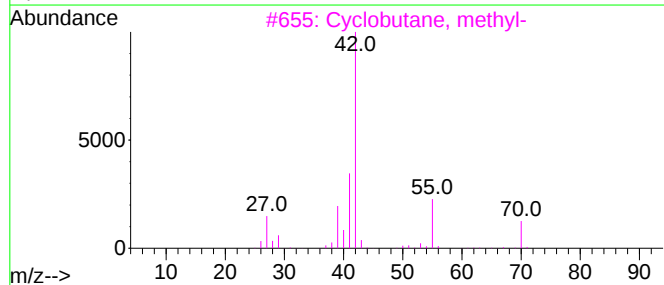
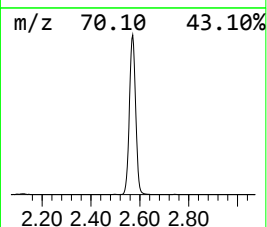
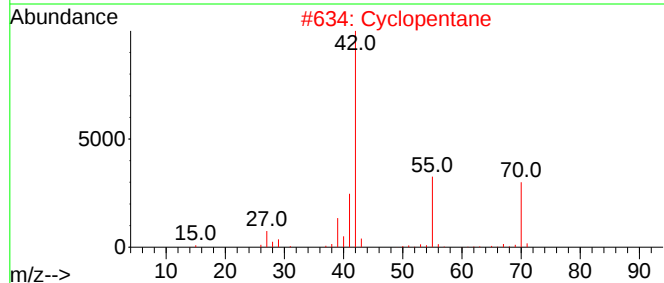
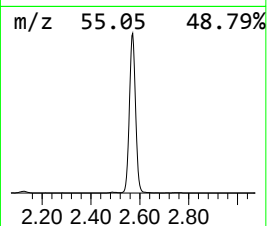
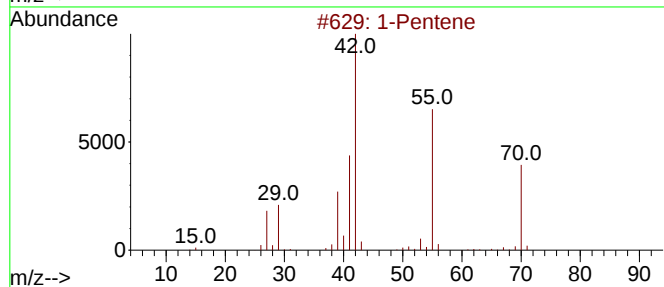
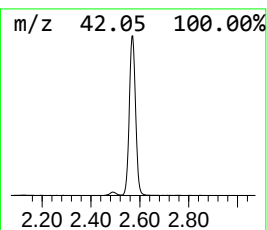
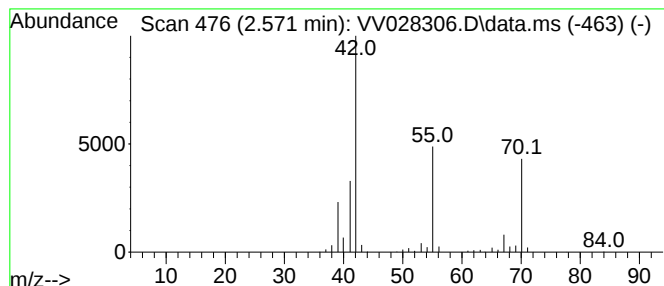
Instrument :
MSVOA_V
ClientSampleId :
EXFR3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR100322WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.571	12.05 ug/L	1071440	1,4-Difluorobenzene	5.612	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene	70	C5H10	000109-67-1	90
2	Cyclopentane	70	C5H10	000287-92-3	86
3	Cyclobutane, methyl-	70	C5H10	000598-61-8	78
4	Cyclobutane, methyl-	70	C5H10	000598-61-8	78
5	Cyclopentane	70	C5H10	000287-92-3	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV100322\
Data File : VV028306.D
Acq On : 04 Oct 2022 02:29
Operator : SY/MD
Sample : N4866-19
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EXFR3

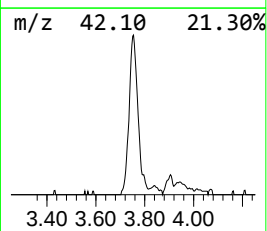
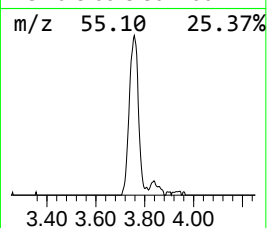
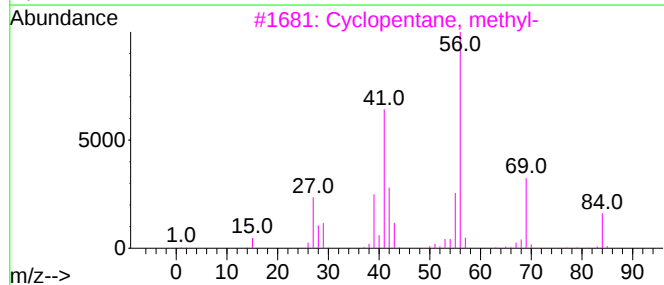
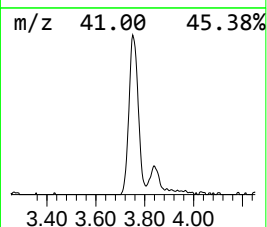
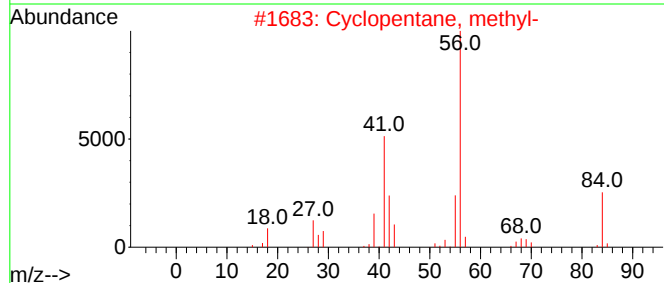
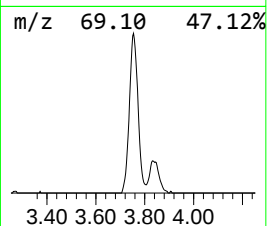
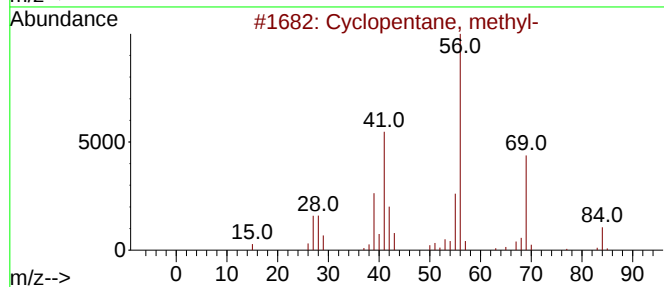
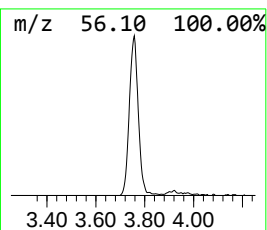
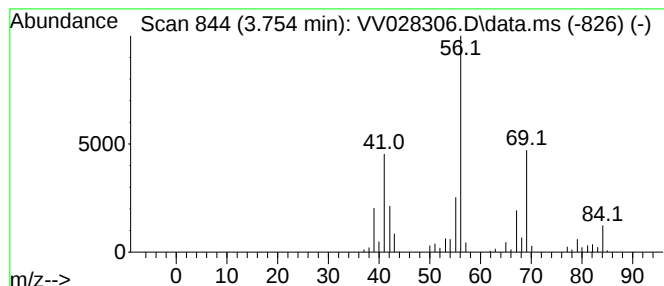
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 (DEL) Alkane: Cyclic3.754 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.754	2.47 ug/L	219441	1,4-Difluorobenzene	5.612

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	81
2		Cyclopentane, methyl-	84	C6H12	000096-37-7	64
3		Cyclopentane, methyl-	84	C6H12	000096-37-7	64
4		Cyclohexane	84	C6H12	000110-82-7	64
5		Cyclopentane, methyl-	84	C6H12	000096-37-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV100322\
Data File : VV028306.D
Acq On : 04 Oct 2022 02:29
Operator : SY/MD
Sample : N4866-19
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EXFR3

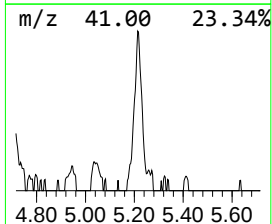
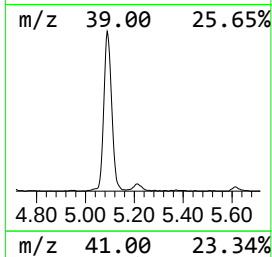
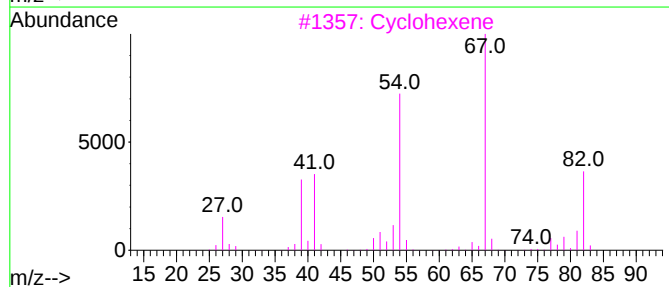
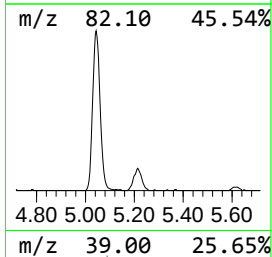
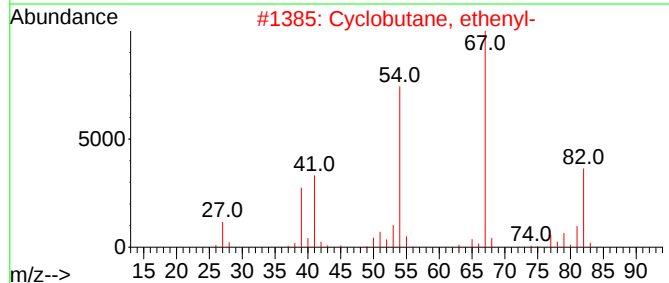
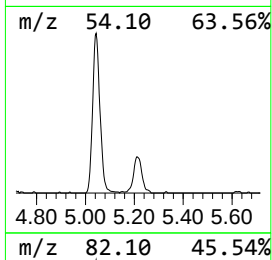
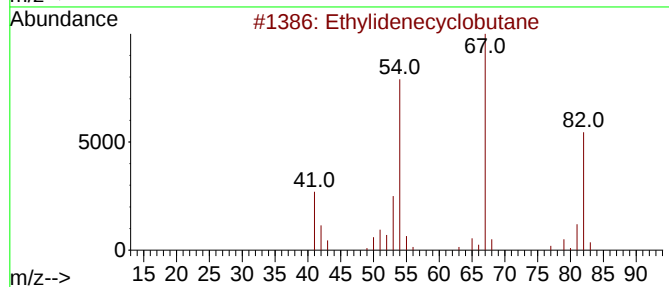
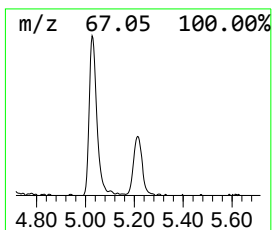
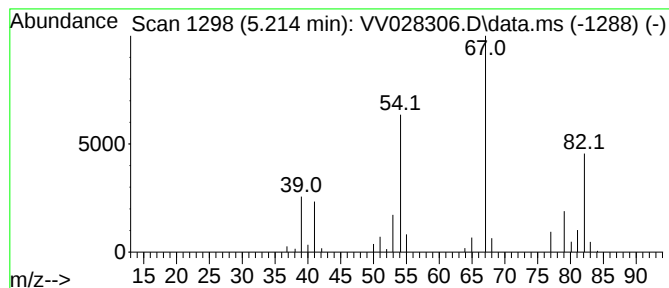
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Ethylidenecyclobutane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.214	0.75 ug/L	67032	1,4-Difluorobenzene	5.612

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethylidenecyclobutane	82	C6H10	001528-21-8	90
2			Cyclobutane, ethenyl-	82	C6H10	002597-49-1	87
3			Cyclohexene	82	C6H10	000110-83-8	80
4			Cyclohexene	82	C6H10	000110-83-8	80
5			Cyclohexene	82	C6H10	000110-83-8	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV100322\
Data File : VV028306.D
Acq On : 04 Oct 2022 02:29
Operator : SY/MD
Sample : N4866-19
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EXFR3

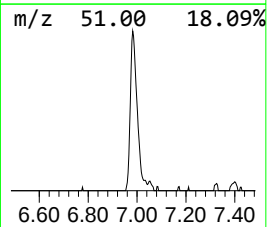
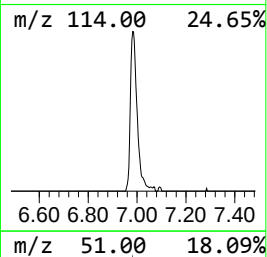
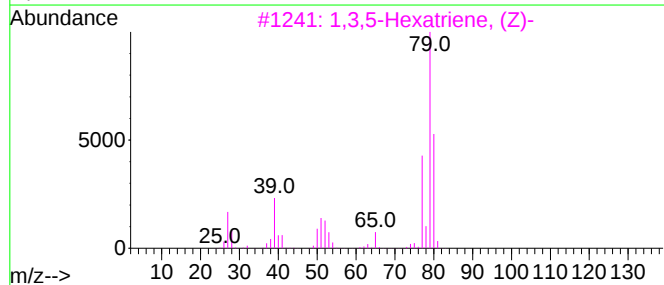
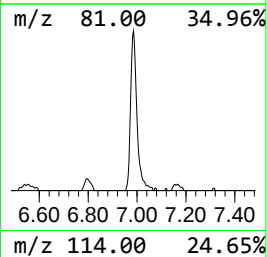
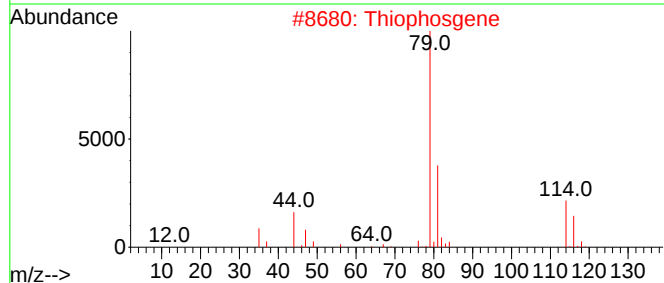
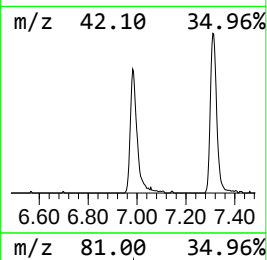
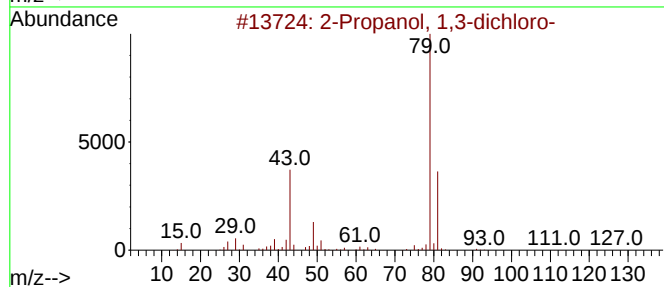
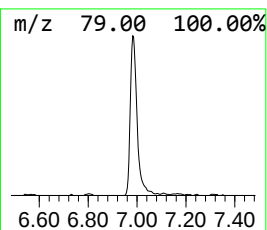
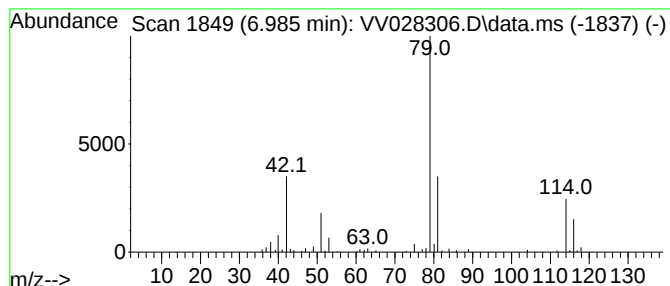
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.985	1.58 ug/L	140088	1,4-Difluorobenzene	5.612

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propanol, 1,3-dichloro-	128	C3H6Cl2O	000096-23-1	47
2		Thiophosgene	114	CCl2S	000463-71-8	45
3		1,3,5-Hexatriene, (Z)-	80	C6H8	002612-46-6	38
4		1,3-Cyclohexadiene	80	C6H8	000592-57-4	38
5		2-Propanol, 1,3-dichloro-	128	C3H6Cl2O	000096-23-1	28



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV100322\
Data File : VV028306.D
Acq On : 04 Oct 2022 02:29
Operator : SY/MD
Sample : N4866-19
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EXFR3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR100322WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	1.105	2.4	ug/L	210697	1	5.612	444583	5.0
(DEL) Alkane: S...	1.211	3.4	ug/L	303336	1	5.612	444583	5.0
Sulfur dioxide	1.388	1.5	ug/L	134327	1	5.612	444583	5.0
(DEL) Alkane: S...	1.629	39.4	ug/L	3500570	1	5.612	444583	5.0
(DEL) Alkane: S...	1.799	0.6	ug/L	56388	1	5.612	444583	5.0
(DEL) Alkane: S...	2.571	12.1	ug/L	1071440	1	5.612	444583	5.0
(DEL) Alkane: C...	3.754	2.5	ug/L	219441	1	5.612	444583	5.0
Ethylidenecyclo...	5.214	0.8	ug/L	67032	1	5.612	444583	5.0
unknown-01	6.985	1.6	ug/L	140088	1	5.612	444583	5.0