

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092722\
 Data File : VV028145.D
 Acq On : 27 Sep 2022 17:29
 Operator : SY/MD
 Sample : N4856-06
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 F5H33

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\SFAMVTR092222WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VV028145.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.301	73	81	92	rVB	177871	178380	4.09%	1.436%
2	1.394	100	110	131	rBV	115026	409826	9.40%	3.299%
3	1.561	156	162	173	rVB	85394	103430	2.37%	0.833%
4	1.629	174	183	202	rVB	482879	604532	13.87%	4.867%
5	2.102	321	330	345	rVB2	160489	256366	5.88%	2.064%
6	2.182	345	355	380	rVB	21161	65472	1.50%	0.527%
7	2.491	439	451	464	rBV	66405	135351	3.10%	1.090%
8	2.568	465	475	493	rVB	125523	226069	5.19%	1.820%
9	2.754	517	533	568	rBV2	2121598	4359975	100.00%	35.102%
10	3.899	876	889	929	rVB3	295624	824054	18.90%	6.634%
11	4.343	1008	1027	1057	rBV2	116199	312871	7.18%	2.519%
12	5.040	1228	1244	1274	rBV2	251492	691791	15.87%	5.570%
13	5.236	1293	1305	1315	rBV5	18552	45581	1.05%	0.367%
14	5.613	1409	1422	1449	rBV	199949	422661	9.69%	3.403%
15	5.915	1503	1516	1535	rBV2	38954	87459	2.01%	0.704%
16	6.063	1549	1562	1592	rBV	149492	328916	7.54%	2.648%
17	6.770	1770	1782	1798	rBV6	20646	51060	1.17%	0.411%
18	6.986	1832	1849	1866	rBV2	69065	136747	3.14%	1.101%
19	7.310	1940	1950	1970	rVB	260395	455105	10.44%	3.664%
20	7.622	2039	2047	2065	rVB	38604	73119	1.68%	0.589%
21	7.838	2105	2114	2133	rVB	31264	55483	1.27%	0.447%
22	8.085	2180	2191	2205	rBV	382476	664665	15.24%	5.351%
23	8.850	2418	2429	2443	rBV	301503	490399	11.25%	3.948%
24	10.214	2841	2853	2868	rVB	121649	191519	4.39%	1.542%
25	11.246	3162	3174	3192	rBV	316372	495904	11.37%	3.992%
26	11.622	3280	3291	3309	rBV	291664	466268	10.69%	3.754%
27	12.297	3491	3501	3512	rVB3	28881	48336	1.11%	0.389%
28	14.226	4091	4101	4110	rBV	32476	48336	1.11%	0.389%
29	14.574	4199	4209	4221	rBV	89267	141765	3.25%	1.141%
30	16.175	4699	4707	4719	rVB4	31826	49554	1.14%	0.399%

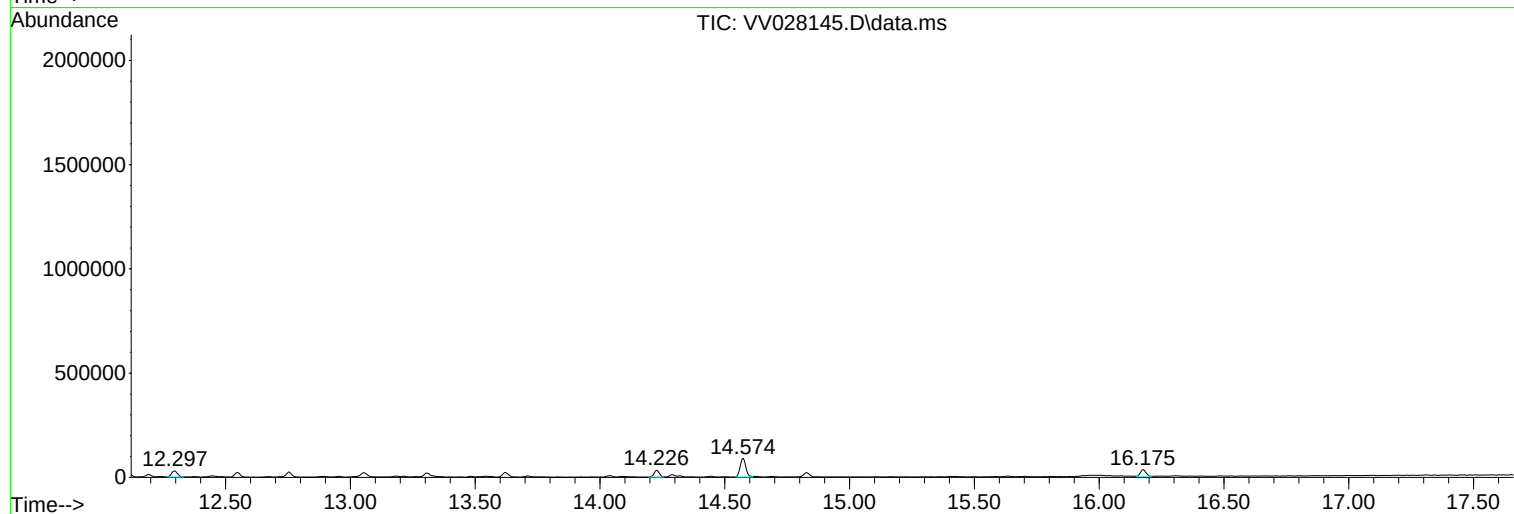
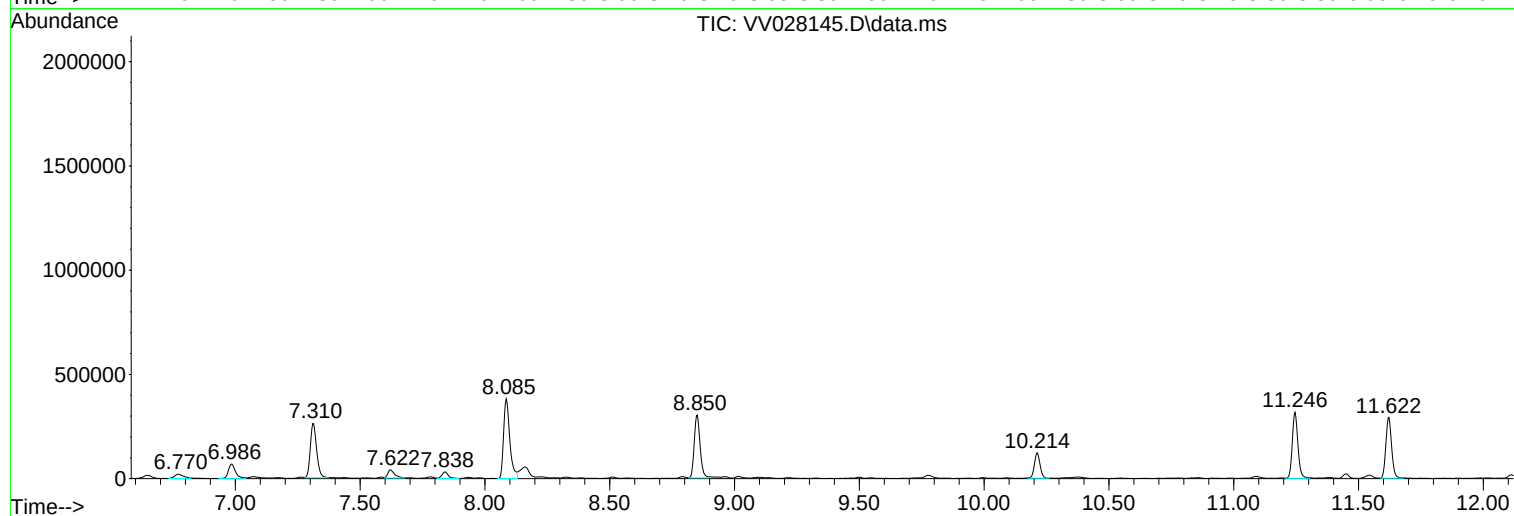
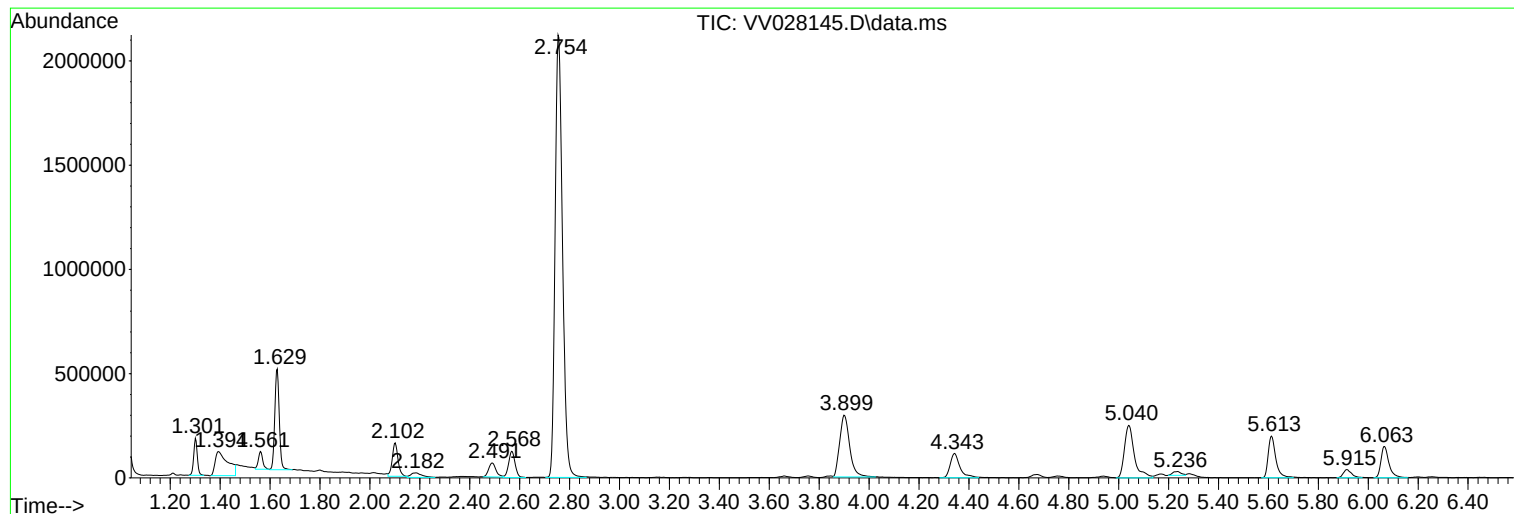
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092222WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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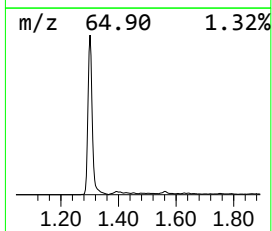
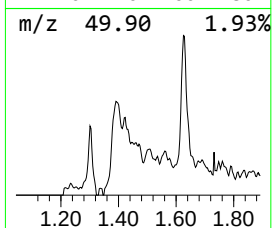
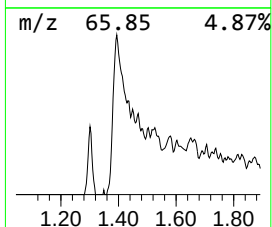
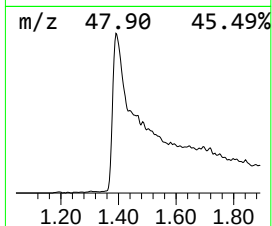
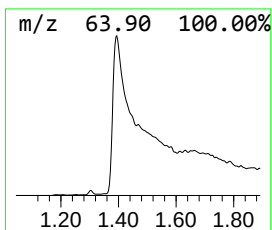
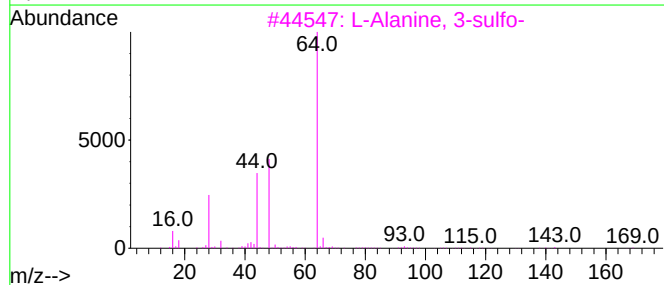
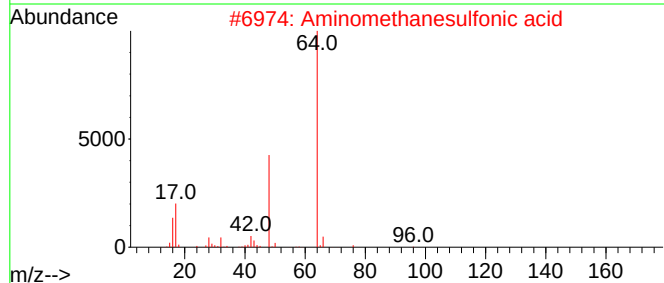
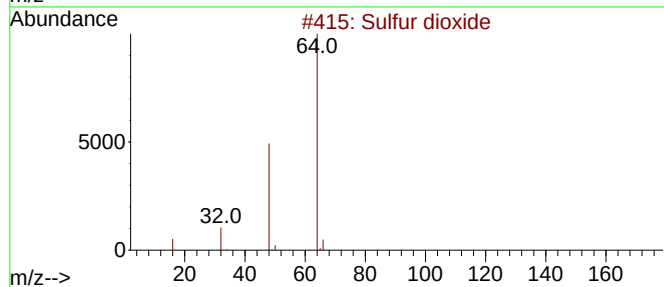
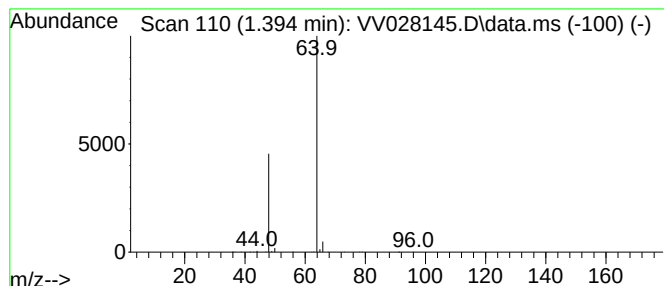
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.394	4.85 ug/L	409826	1,4-Difluorobenzene	5.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Sulfur dioxide	64	O2S	007446-09-5	5
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	5



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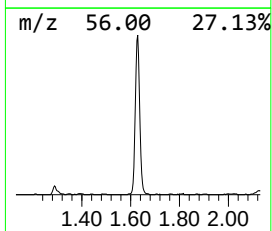
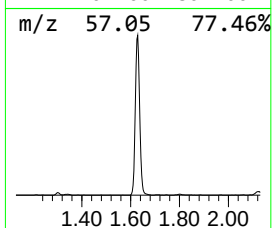
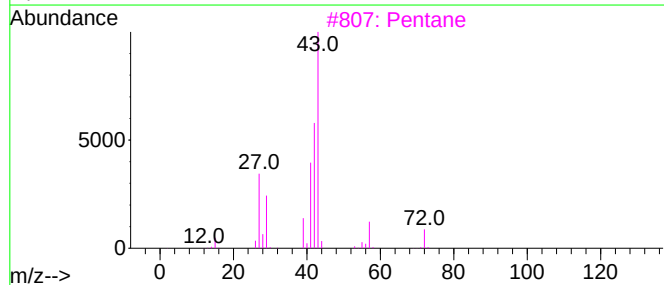
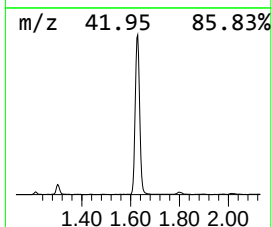
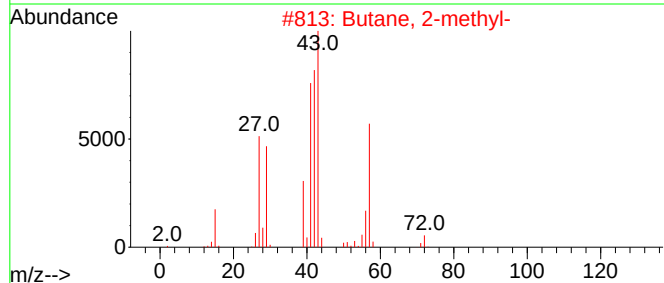
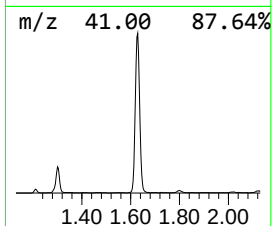
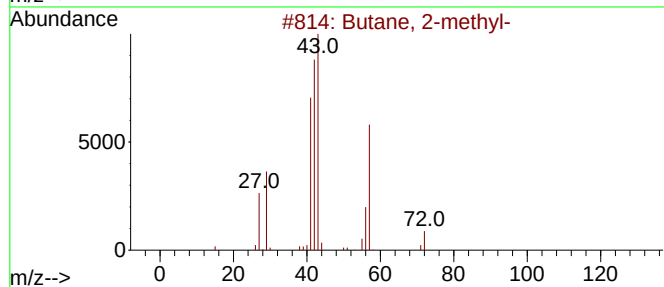
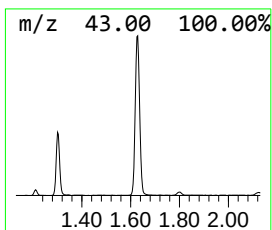
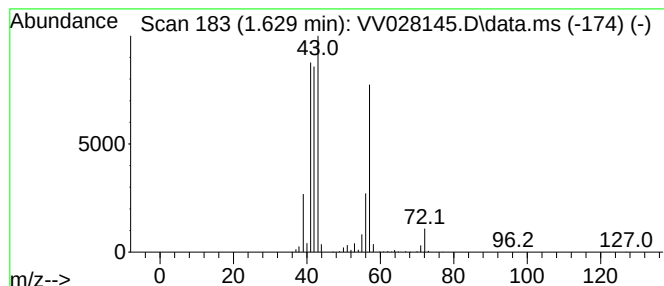
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092222WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.629	7.15 ug/L	604532	1,4-Difluorobenzene	5.613

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	3-Buten-1-ol			72	C4H8O	000627-27-0	37



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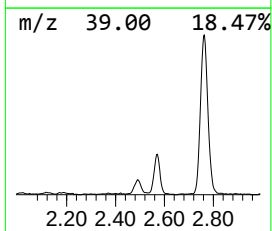
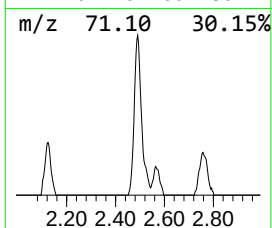
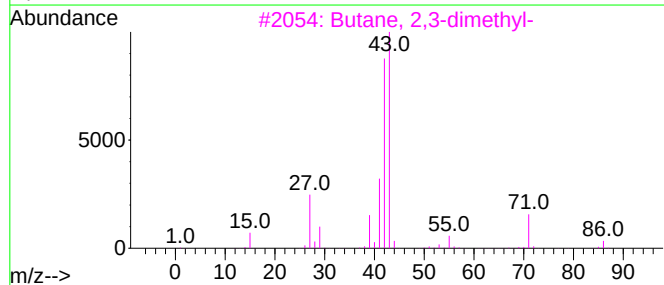
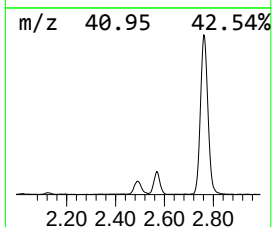
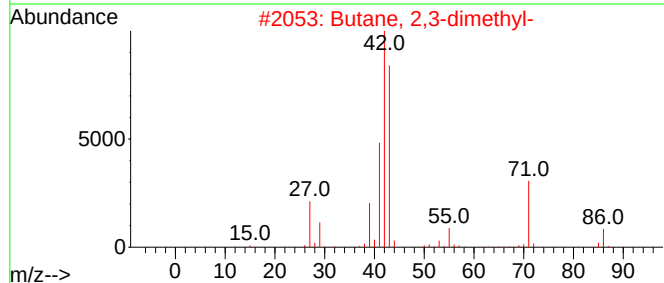
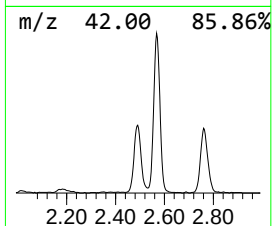
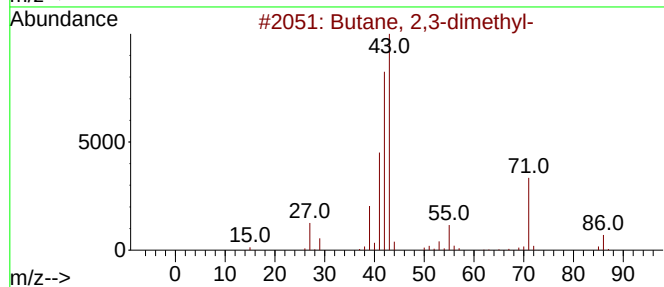
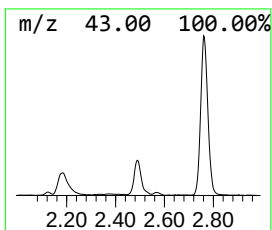
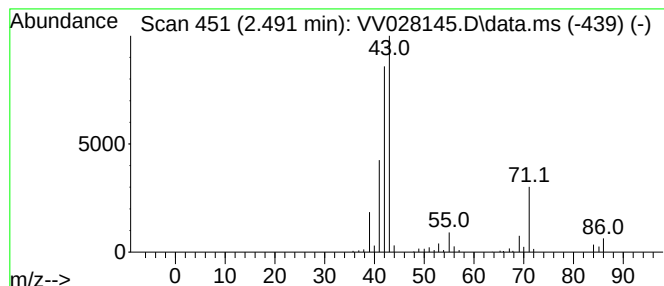
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092222WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.491	1.60 ug/L	135351	1,4-Difluorobenzene	5.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	90
2			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	72
3			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	72
4			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	64
5			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	64



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ALS Vial : 18 Sample Multiplier: 1

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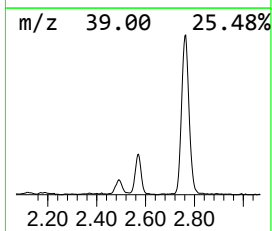
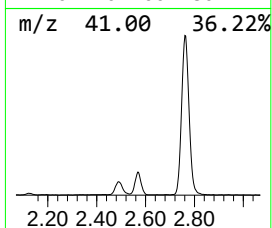
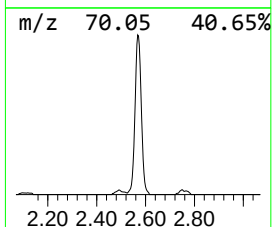
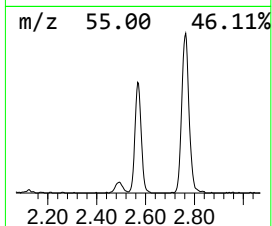
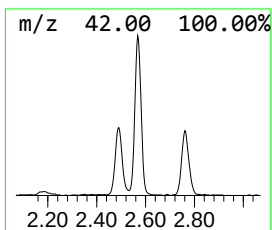
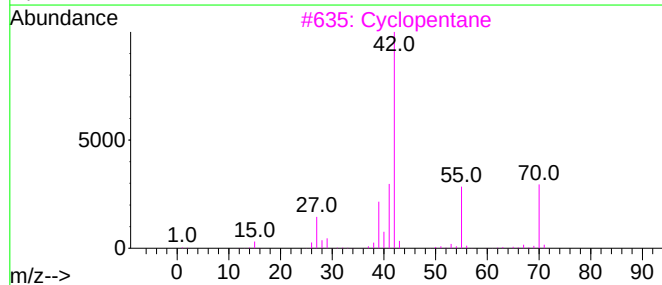
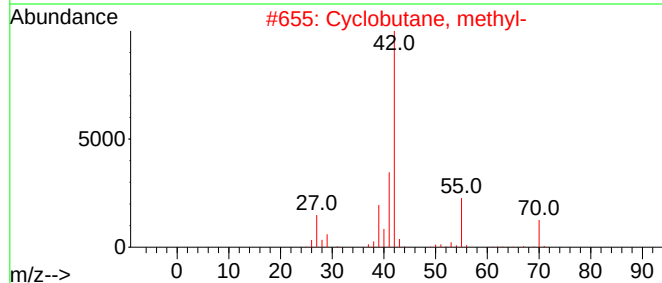
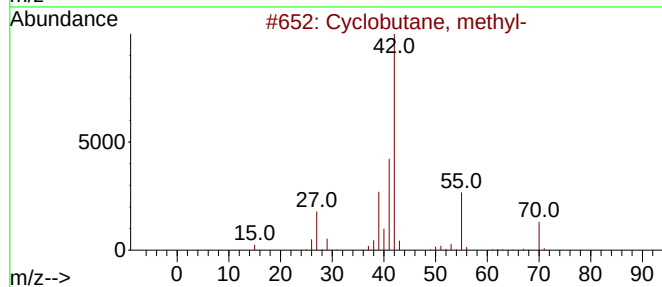
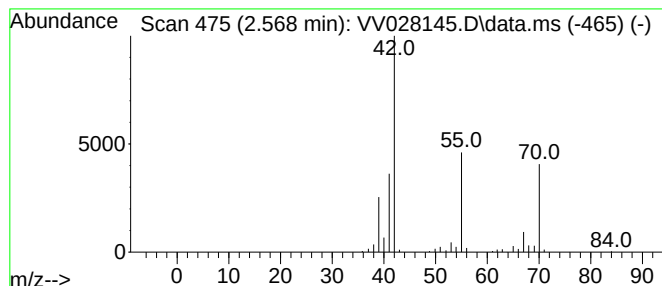
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 (DEL) Alkane: Cyclic2.568 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.568	2.67 ug/L	226069	1,4-Difluorobenzene	5.613

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclobutane, methyl-	70	C5H10	000598-61-8	86
2		Cyclobutane, methyl-	70	C5H10	000598-61-8	78
3		Cyclopentane	70	C5H10	000287-92-3	72
4		1-Pentene	70	C5H10	000109-67-1	59
5		Cyclopentane	70	C5H10	000287-92-3	56



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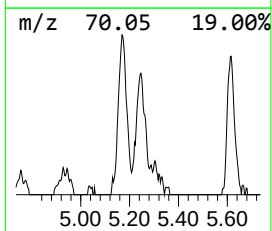
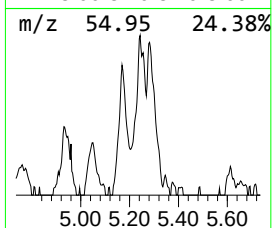
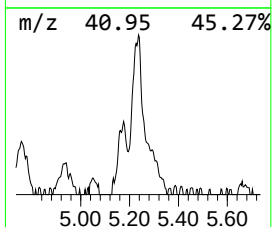
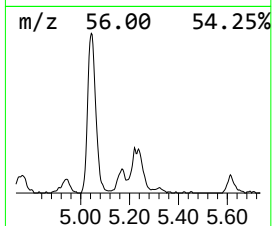
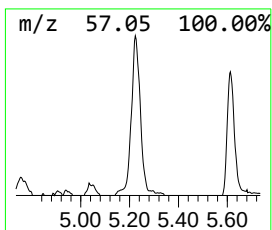
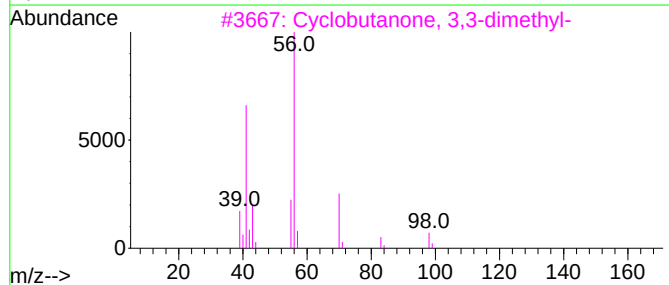
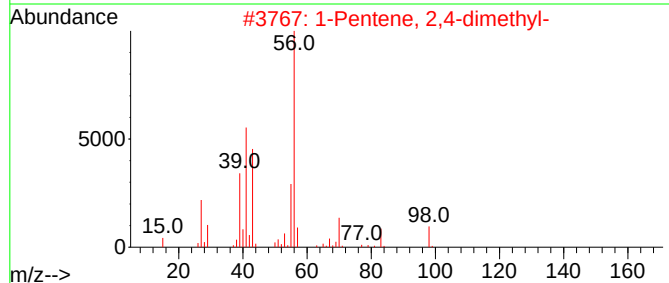
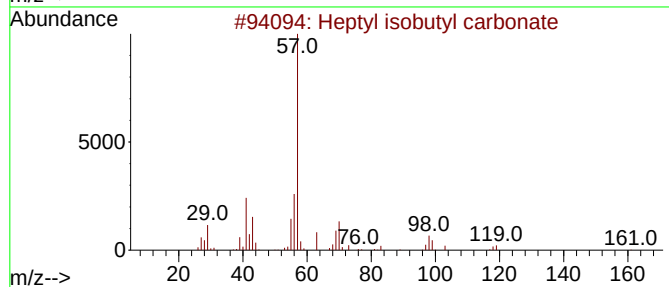
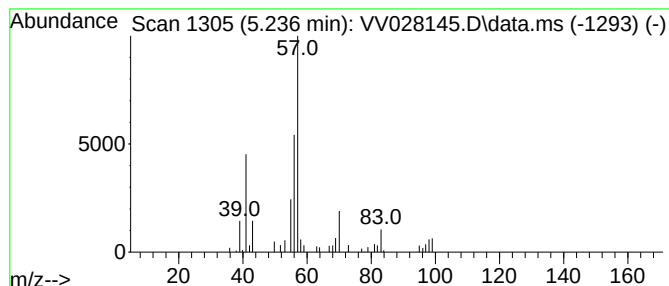
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Heptyl isobutyl carbonate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.236	0.54 ug/L	45581	1,4-Difluorobenzene	5.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	50
2			1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	49
3			Cyclobutanone, 3,3-dimethyl-	98	C6H10O	001192-33-2	47
4			1-Hexene, 4-methyl-	98	C7H14	003769-23-1	43
5			Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	43



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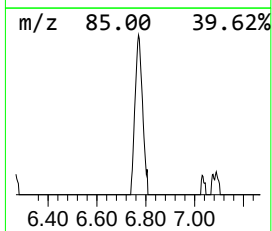
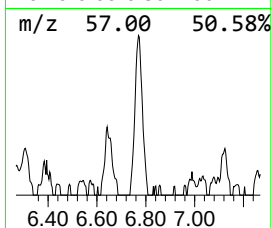
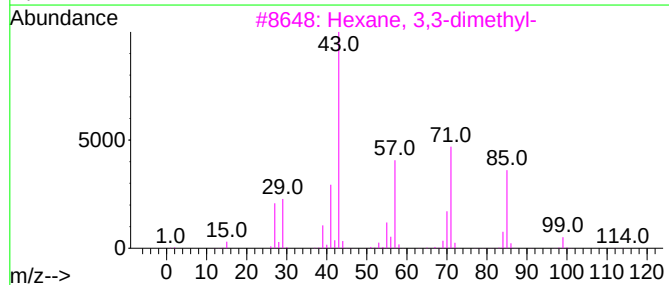
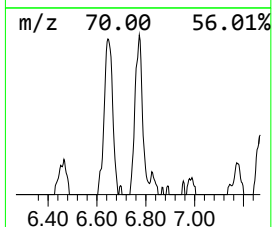
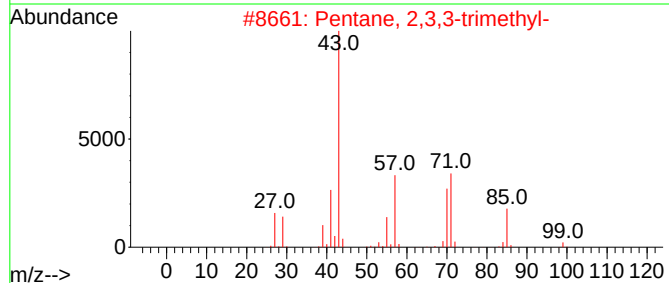
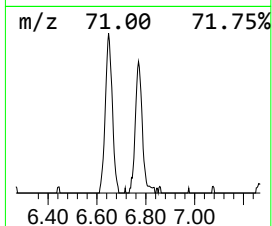
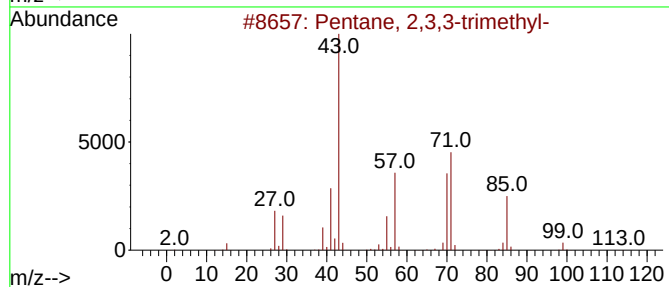
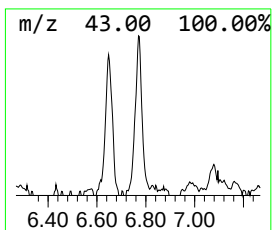
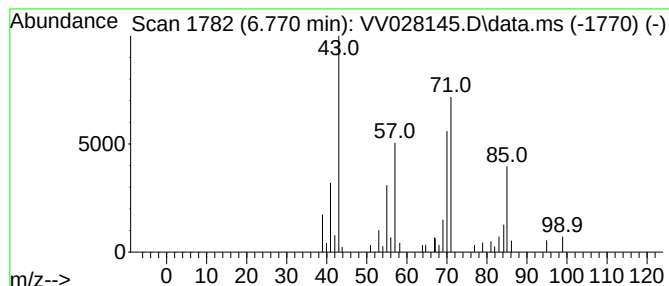
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.770	0.60 ug/L	51060	1,4-Difluorobenzene	5.613

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	72
2		Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	64
3		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
4		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
5		Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092722\
Data File : VV028145.D
Acq On : 27 Sep 2022 17:29
Operator : SY/MD
Sample : N4856-06
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F5H33

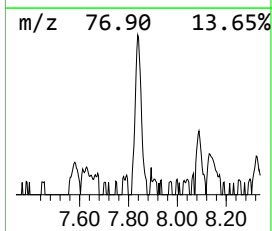
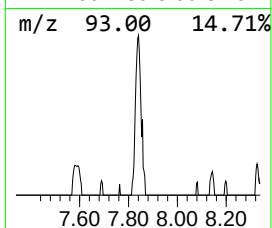
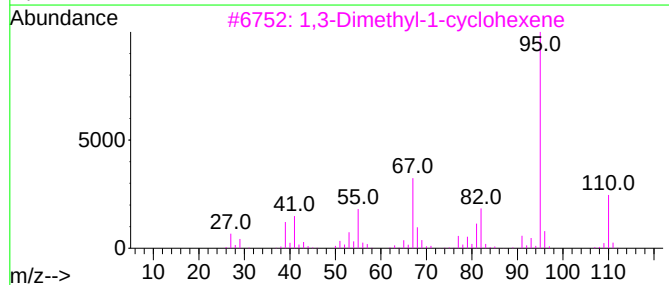
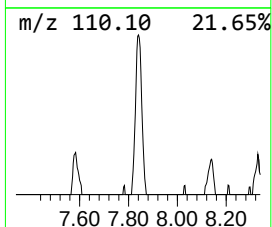
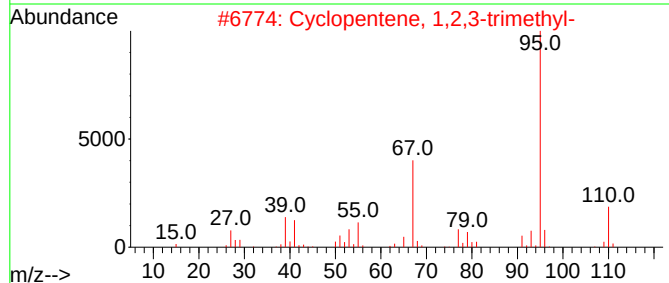
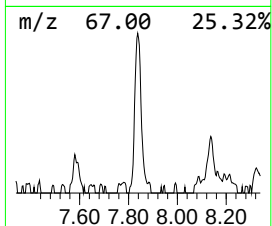
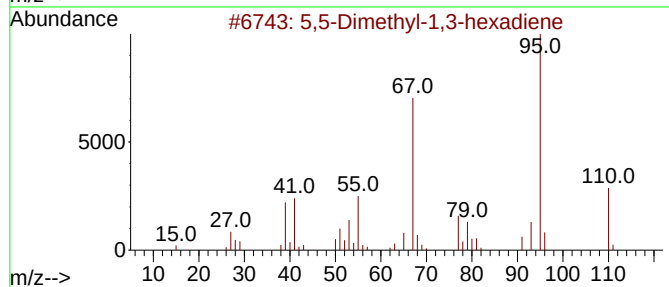
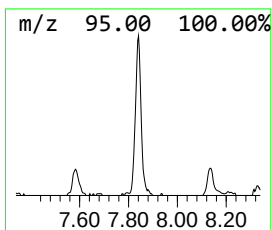
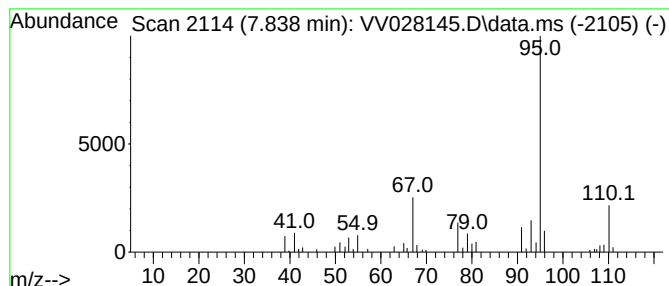
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 5,5-Dimethyl-1,3-hexadiene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.838	0.57 ug/L	55483	Chlorobenzene-d5	8.850

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	90
2			Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	87
3			1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	80
4			5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	72
5			5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092722\
Data File : VV028145.D
Acq On : 27 Sep 2022 17:29
Operator : SY/MD
Sample : N4856-06
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F5H33

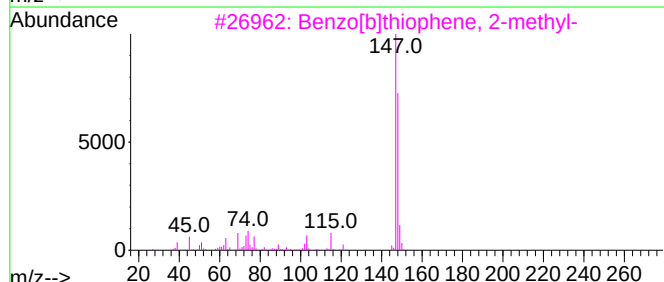
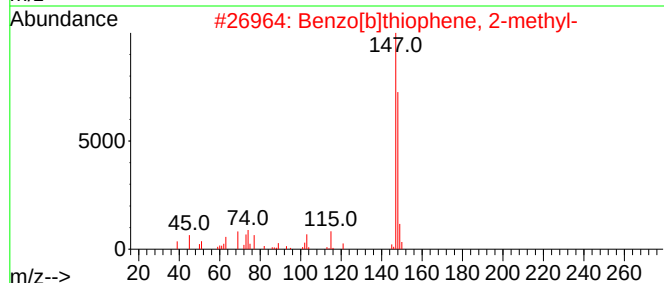
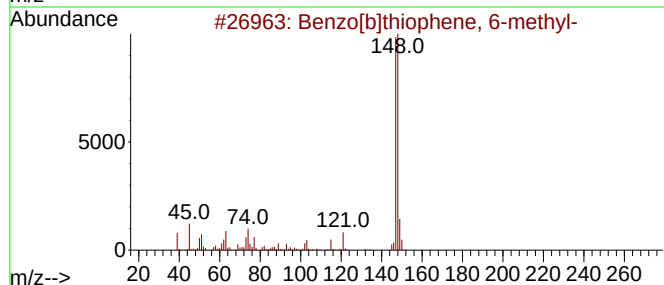
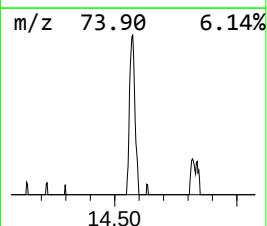
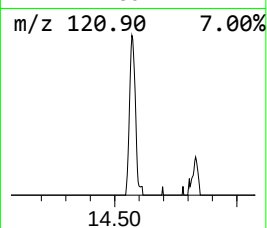
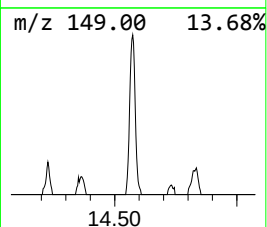
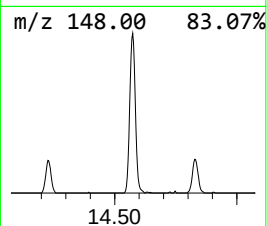
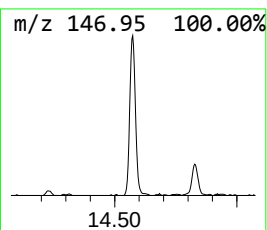
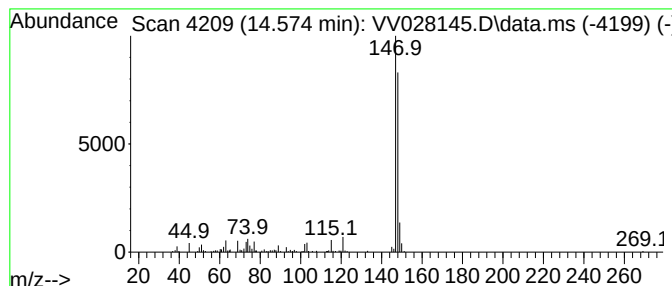
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 9 Benzo[b]thiophene, 6-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.574	1.43 ug/L	141765	1,4-Dichlorobenzene-d4	11.246

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[b]thiophene, 6-methyl-	148	C9H8S	016587-47-6	94
2			Benzo[b]thiophene, 2-methyl-	148	C9H8S	001195-14-8	91
3			Benzo[b]thiophene, 2-methyl-	148	C9H8S	001195-14-8	91
4			Benzo[b]thiophene, 4-methyl-	148	C9H8S	014315-11-8	91
5			3-Methylbenzothiophene	148	C9H8S	001455-18-1	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092722\
Data File : VV028145.D
Acq On : 27 Sep 2022 17:29
Operator : SY/MD
Sample : N4856-06
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F5H33

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092222WMA.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
Sulfur dioxide	1.394	4.8	ug/L	409826	1	5.613	422661	5.0
(DEL) Alkane: S...	1.629	7.2	ug/L	604532	1	5.613	422661	5.0
(DEL) Alkane: S...	2.491	1.6	ug/L	135351	1	5.613	422661	5.0
(DEL) Alkane: C...	2.568	2.7	ug/L	226069	1	5.613	422661	5.0
Heptyl isobutyl...	5.236	0.5	ug/L	45581	1	5.613	422661	5.0
(DEL) Alkane: S...	6.770	0.6	ug/L	51060	1	5.613	422661	5.0
5,5-Dimethyl-1,...	7.838	0.6	ug/L	55483	2	8.850	490399	5.0
Benzo[b]thiophe...	14.574	1.4	ug/L	141765	3	11.246	495904	5.0