

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110322\
 Data File : VU051735.D
 Acq On : 03 Nov 2022 15:50
 Operator : JC/MD
 Sample : N5407-01
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW4Y1

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\SFAMUTR102822WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU051735.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.359	3	6	22	rVB2	159728	156789	7.98%	0.738%
2	1.472	33	41	49	rBV	157104	301279	15.33%	1.419%
3	1.552	51	66	69	rVV	110195	310141	15.78%	1.460%
4	1.584	70	76	95	rVB3	327969	612319	31.15%	2.883%
5	1.729	117	121	131	rVB	104255	127523	6.49%	0.600%
6	1.787	132	139	151	rBV	724844	903402	45.96%	4.254%
7	2.244	276	281	293	rVB	58604	80724	4.11%	0.380%
8	2.469	344	351	369	rVB2	27812	46915	2.39%	0.221%
9	2.565	370	381	390	rBV	122358	192987	9.82%	0.909%
10	2.629	390	401	409	rVV	394111	683085	34.75%	3.216%
11	2.684	409	418	434	rVV	718931	1230712	62.61%	5.795%
12	2.784	434	449	478	rVB2	436546	1211331	61.63%	5.704%
13	3.044	516	530	555	rBV	388277	740351	37.67%	3.486%
14	3.867	761	786	801	rBV	341419	816707	41.55%	3.846%
15	3.961	801	815	837	rVB2	112743	310477	15.80%	1.462%
16	4.623	1010	1021	1036	rBV	117467	290470	14.78%	1.368%
17	4.703	1036	1046	1071	rVB	142918	336685	17.13%	1.585%
18	4.986	1121	1134	1146	rBV	144354	357347	18.18%	1.683%
19	5.060	1148	1157	1183	rVB	147812	345815	17.59%	1.628%
20	5.726	1341	1364	1376	rBV2	274033	733439	37.31%	3.453%
21	5.835	1393	1398	1412	rVB3	14007	25702	1.31%	0.121%
22	6.153	1487	1497	1513	rBV2	25061	57671	2.93%	0.272%
23	6.247	1513	1526	1544	rBV	227971	444865	22.63%	2.095%
24	6.366	1554	1563	1577	rVB3	25363	52018	2.65%	0.245%
25	6.690	1651	1664	1675	rBV	166432	321424	16.35%	1.513%
26	6.768	1676	1688	1707	rVB2	57865	136237	6.93%	0.641%
27	7.115	1781	1796	1804	rBV4	34011	71318	3.63%	0.336%
28	7.163	1806	1811	1821	rVB2	20125	35801	1.82%	0.169%
29	7.565	1924	1936	1951	rBV	76938	140580	7.15%	0.662%
30	7.677	1960	1971	1992	rBV	26229	57236	2.91%	0.270%
31	7.793	1993	2007	2027	rBV3	360554	1041173	52.97%	4.903%
32	7.896	2028	2039	2052	rVV	336773	610524	31.06%	2.875%
33	7.967	2052	2061	2073	rVV	139508	253966	12.92%	1.196%
34	8.028	2073	2080	2093	rVB	29510	53644	2.73%	0.253%
35	8.179	2114	2127	2133	rBV2	52484	89099	4.53%	0.420%
36	8.221	2133	2140	2162	rVB	121774	234753	11.94%	1.105%

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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37	8.475	2208	2219	2232	rVB4	22071	45622	2.32%	0.215%
38	8.629	2256	2267	2279	rBV	415178	733974	37.34%	3.456%
39	8.893	2341	2349	2365	rVB3	16417	31241	1.59%	0.147%
40	9.041	2387	2395	2406	rVB4	12542	21129	1.07%	0.099%
41	9.414	2500	2511	2529	rVV	352016	597447	30.39%	2.813%
42	9.568	2550	2559	2567	rBV3	22576	39892	2.03%	0.188%
43	9.690	2581	2597	2609	rVV	63175	109174	5.55%	0.514%
44	10.099	2715	2724	2729	rBV	24961	36506	1.86%	0.172%
45	10.230	2756	2765	2777	rBV2	36132	59852	3.04%	0.282%
46	10.359	2792	2805	2813	rBV2	26442	55440	2.82%	0.261%
47	10.751	2917	2927	2940	rVB2	186289	311731	15.86%	1.468%
48	10.890	2961	2970	2987	rVB	37257	67112	3.41%	0.316%
49	11.111	3027	3039	3046	rBV9	13576	33832	1.72%	0.159%
50	11.211	3062	3070	3085	rBV4	16356	30401	1.55%	0.143%
51	11.359	3107	3116	3129	rVB	26305	48300	2.46%	0.227%
52	11.465	3138	3149	3162	rVB	23519	41049	2.09%	0.193%
53	11.568	3169	3181	3189	rBV5	16305	32063	1.63%	0.151%
54	11.645	3190	3205	3214	rVV5	35777	78789	4.01%	0.371%
55	11.809	3243	3256	3274	rVV	428449	709968	36.12%	3.343%
56	11.893	3275	3282	3299	rVB3	12905	23857	1.21%	0.112%
57	12.053	3320	3332	3356	rBV	1097696	1965618	100.00%	9.255%
58	12.189	3365	3374	3395	rVB	371199	635542	32.33%	2.993%
59	12.304	3403	3410	3420	rBV	28843	46179	2.35%	0.217%
60	12.533	3471	3481	3511	rBV	572804	1016213	51.70%	4.785%
61	12.944	3600	3609	3624	rVB	96298	163408	8.31%	0.769%
62	13.288	3707	3716	3731	rVB4	54153	97495	4.96%	0.459%
63	13.446	3758	3765	3776	rVV5	15148	26081	1.33%	0.123%
64	13.513	3777	3786	3802	rVB2	69026	116714	5.94%	0.550%
65	13.732	3845	3854	3864	rBV3	49129	83547	4.25%	0.393%
66	13.835	3879	3886	3899	rVB10	26318	49932	2.54%	0.235%
67	13.934	3910	3917	3936	rVB5	25610	53254	2.71%	0.251%
68	14.031	3938	3947	3958	rBV3	90889	154449	7.86%	0.727%
69	14.278	4016	4024	4036	rVB3	14429	25643	1.30%	0.121%
70	14.420	4058	4068	4081	rBV	58392	93617	4.76%	0.441%
71	14.725	4157	4163	4177	rVB4	13000	21127	1.07%	0.099%
72	16.516	4709	4720	4732	rBV2	68439	122506	6.23%	0.577%
73	16.764	4788	4797	4811	rBV8	23527	44372	2.26%	0.209%

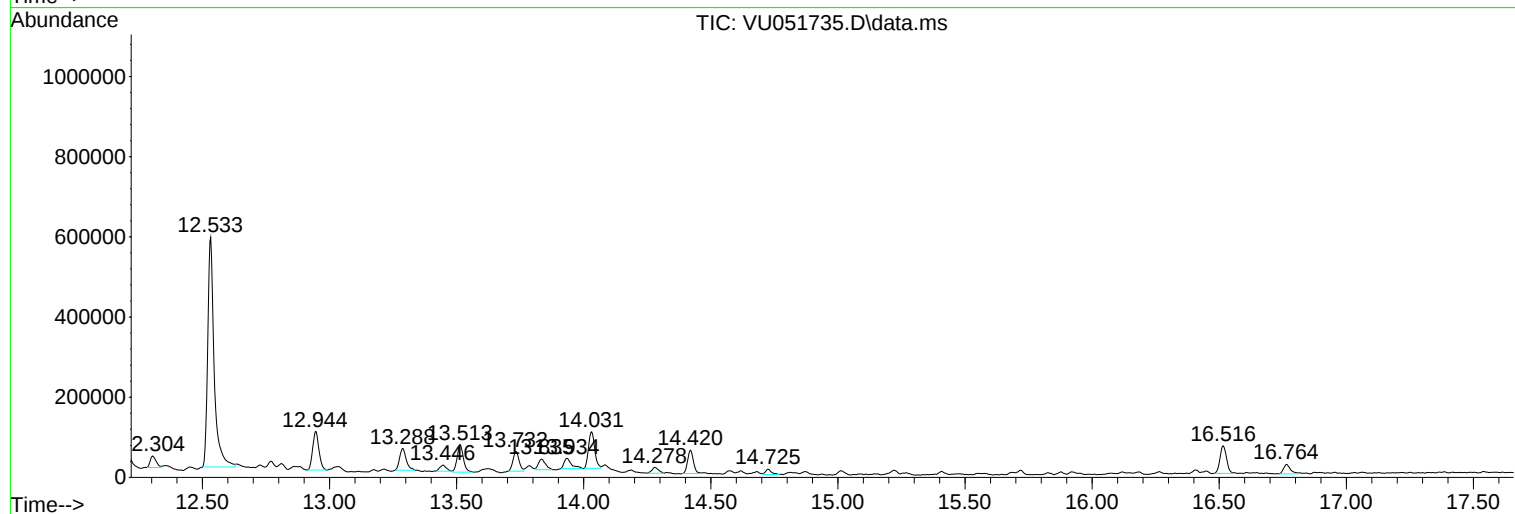
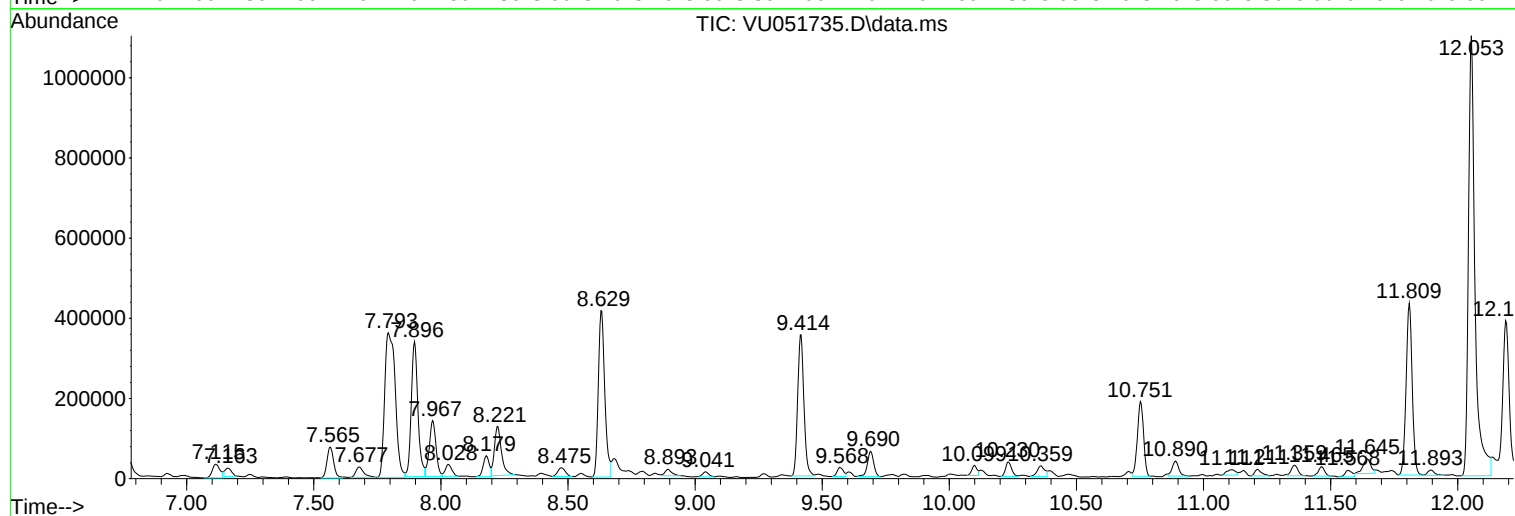
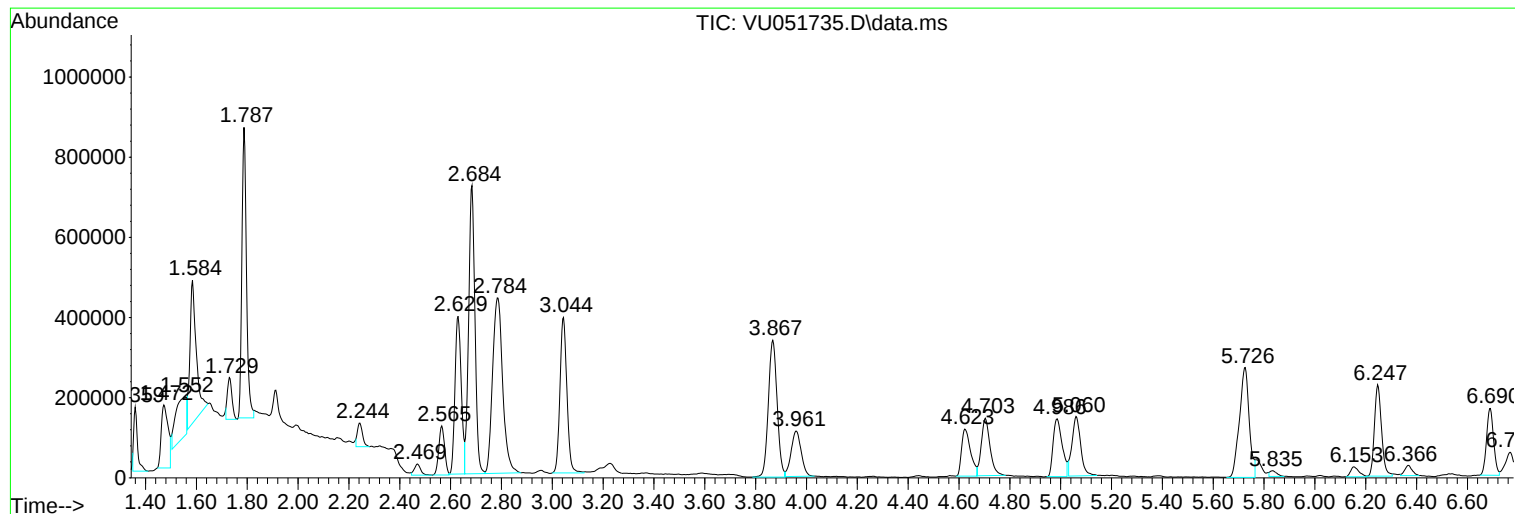
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Instrument :
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ClientSampleId :
EW4Y1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4Y1

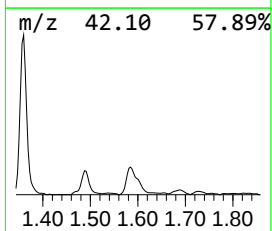
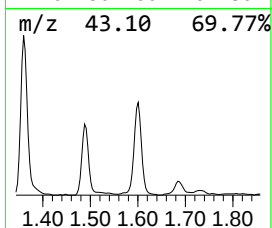
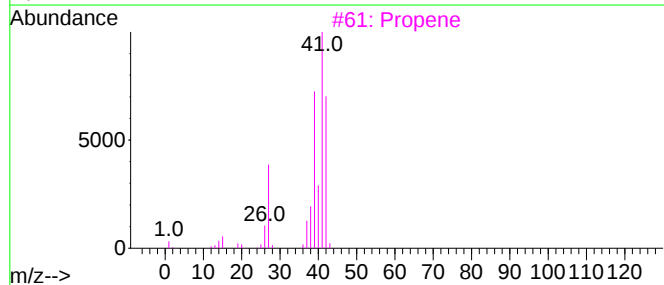
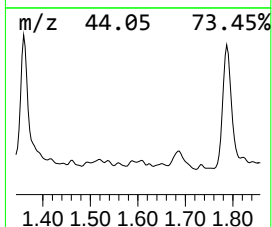
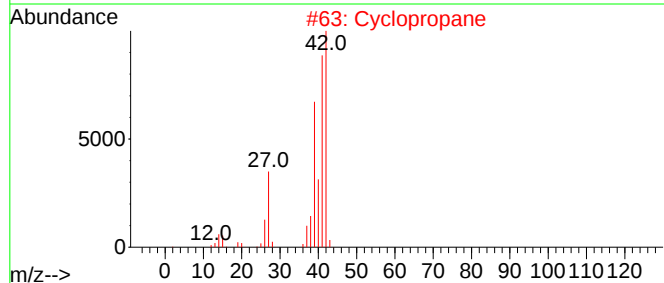
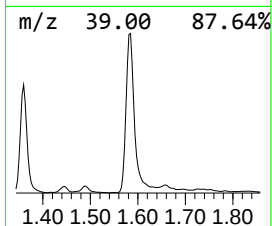
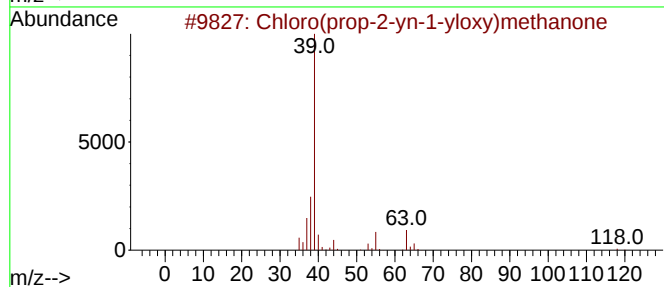
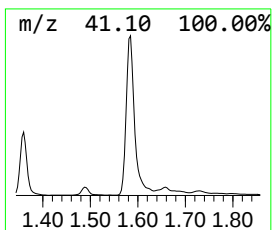
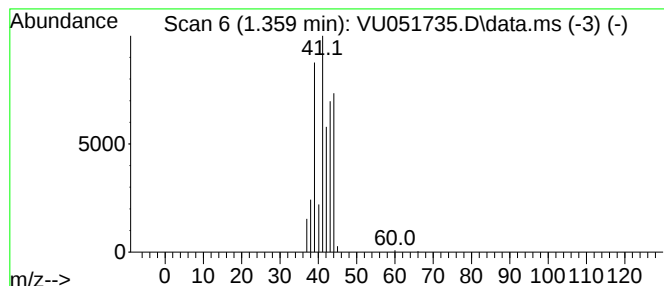
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 unknown-01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.359	1.76 ug/L	156789	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Chloro(prop-2-yn-1-yloxy)methanone	118	C4H3ClO2	035718-08-2	9
2			Cyclopropane	42	C3H6	000075-19-4	9
3			Propene	42	C3H6	000115-07-1	9
4			Cyclopropane	42	C3H6	000075-19-4	9
5			2-Oxetanone, 4-methyl-	86	C4H6O2	003068-88-0	9



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Instrument :
MSVOA_U
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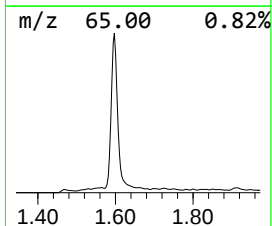
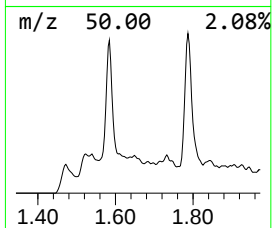
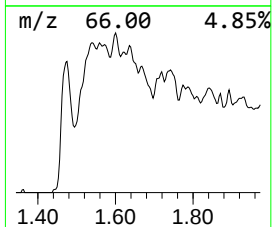
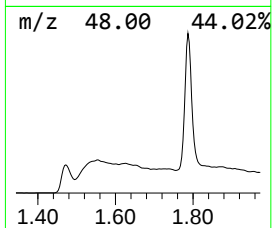
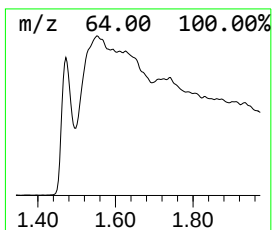
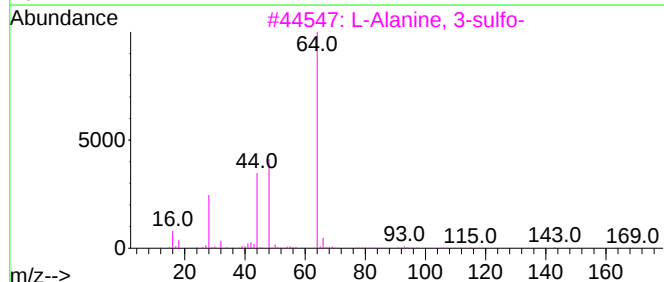
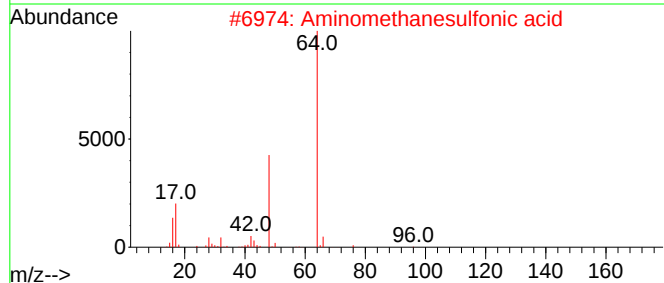
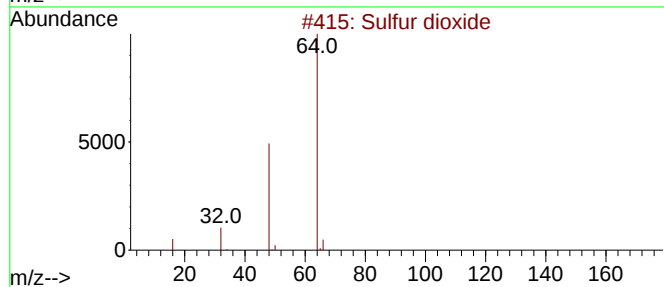
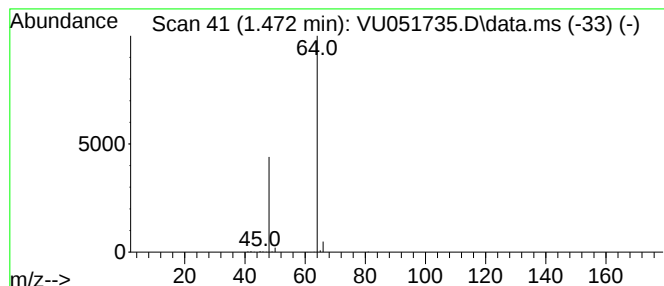
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Sulfur dioxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.472	3.39 ug/L	301279	1,4-Difluorobenzene	6.247

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	4



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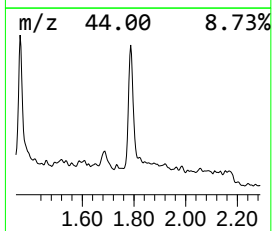
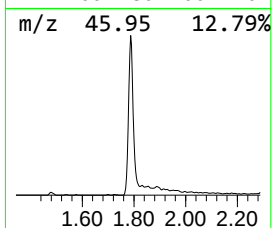
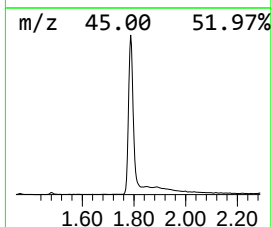
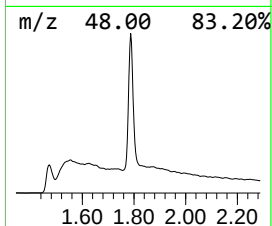
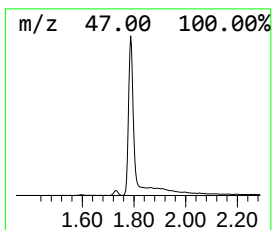
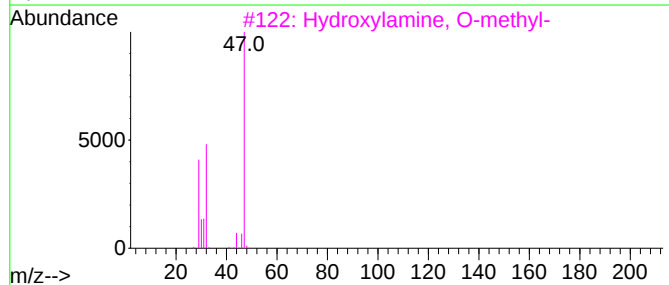
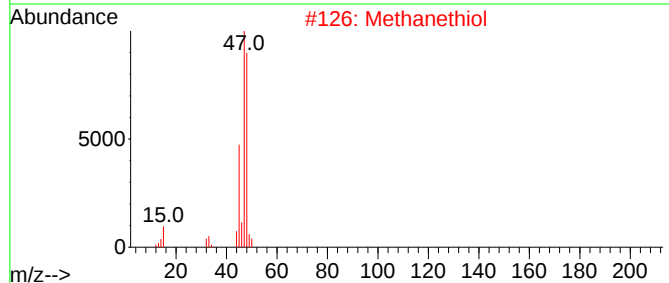
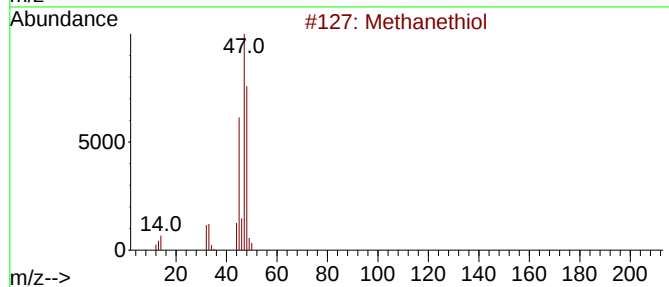
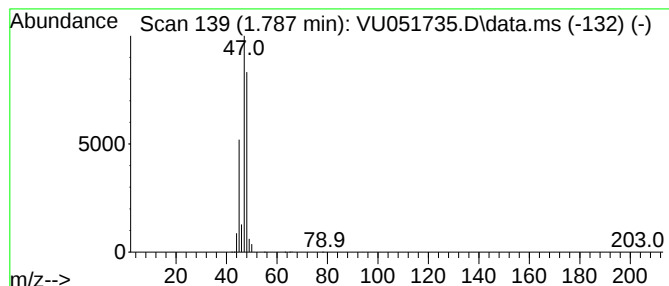
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Methanethiol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.787	10.15 ug/L	903402	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanethiol	48	CH4S	000074-93-1	90
2			Methanethiol	48	CH4S	000074-93-1	90
3			Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
4			Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
5			Methane, nitroso-	45	CH3NO	000865-40-7	5



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MSVOA_U
ClientSampleId :
EW4Y1

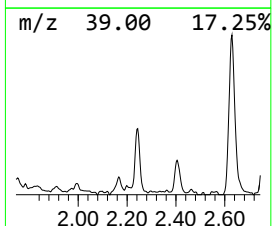
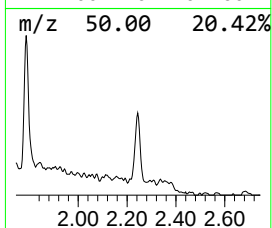
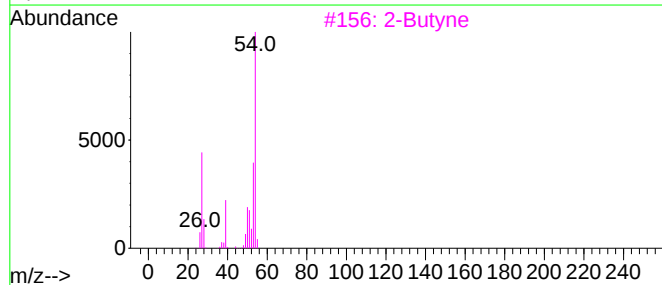
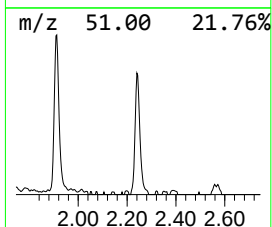
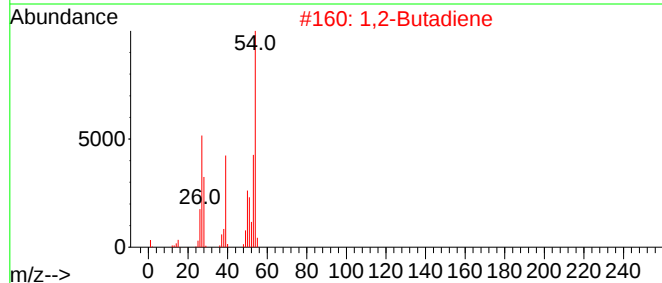
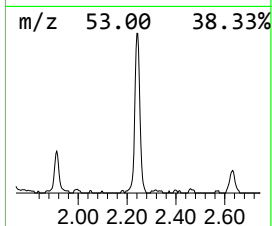
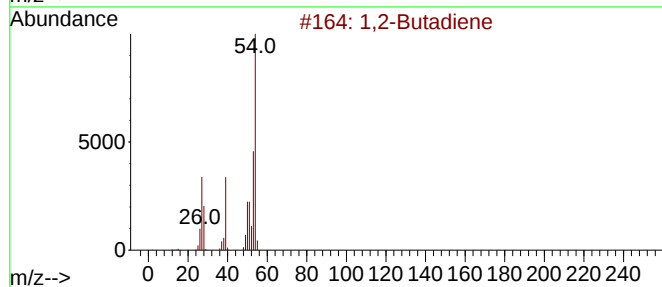
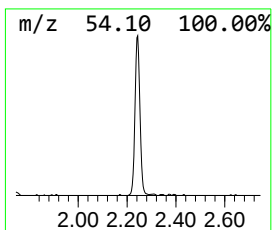
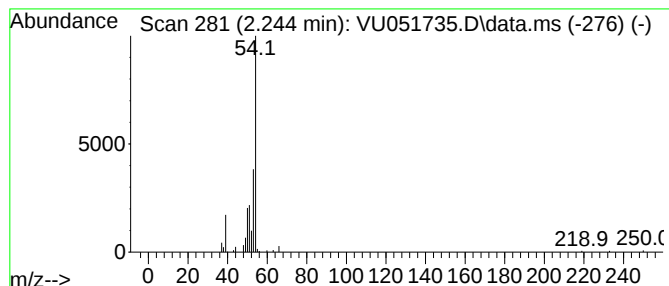
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 1,2-Butadiene Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.244	0.91 ug/L	80724	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Butadiene	54	C4H6	000590-19-2	86
2			1,2-Butadiene	54	C4H6	000590-19-2	86
3			2-Butyne	54	C4H6	000503-17-3	86
4			1,2-Butadiene	54	C4H6	000590-19-2	78
5			2-Butyne	54	C4H6	000503-17-3	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110322\
Data File : VU051735.D
Acq On : 03 Nov 2022 15:50
Operator : JC/MD
Sample : N5407-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4Y1

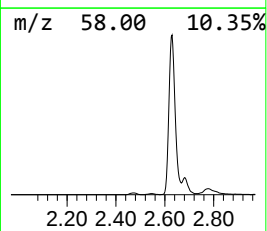
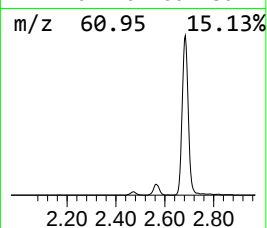
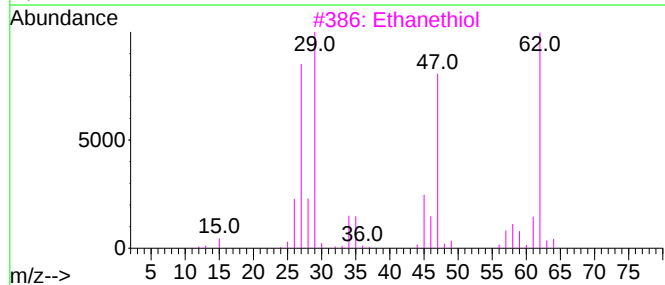
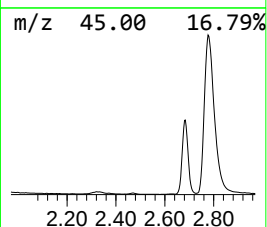
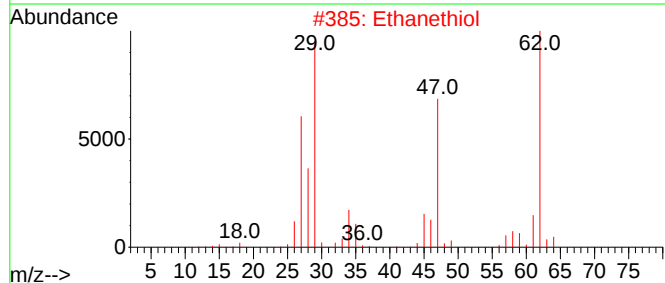
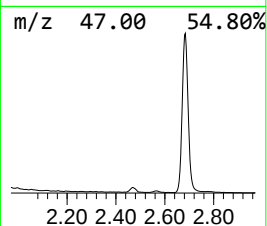
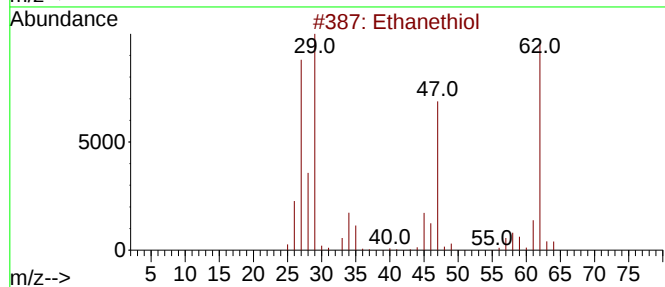
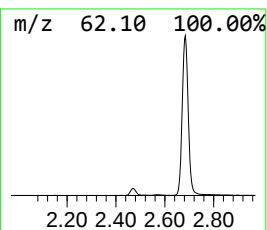
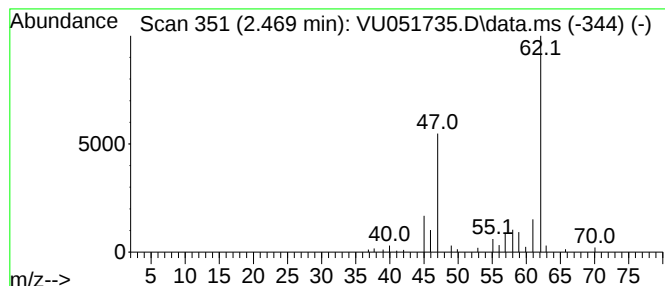
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Ethanethiol Concentration Rank 25

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.469	0.53 ug/L	46915	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanethiol			62	C2H6S	000075-08-1	91
2	Ethanethiol			62	C2H6S	000075-08-1	91
3	Ethanethiol			62	C2H6S	000075-08-1	90
4	Ethanethiol			62	C2H6S	000075-08-1	83
5	Peroxide, dimethyl			62	C2H6O2	000690-02-8	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110322\
Data File : VU051735.D
Acq On : 03 Nov 2022 15:50
Operator : JC/MD
Sample : N5407-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4Y1

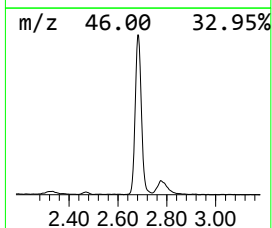
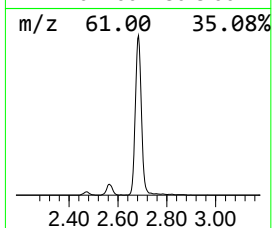
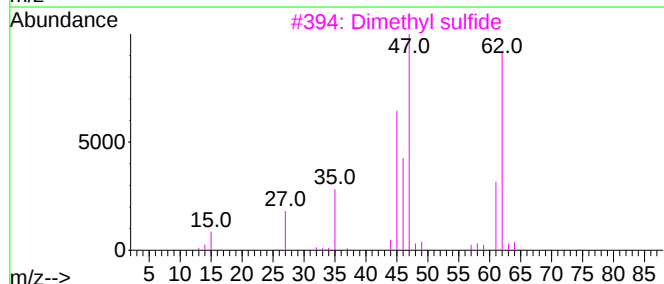
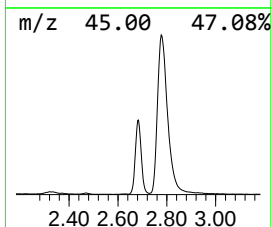
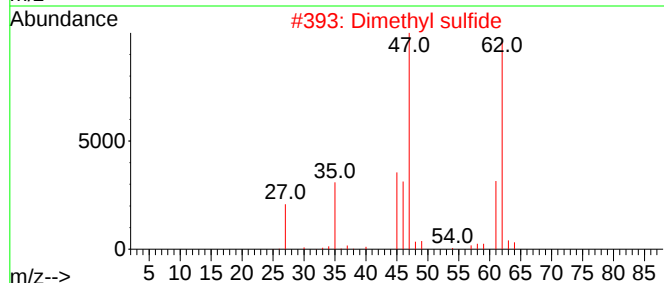
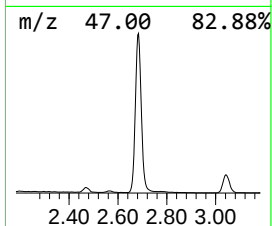
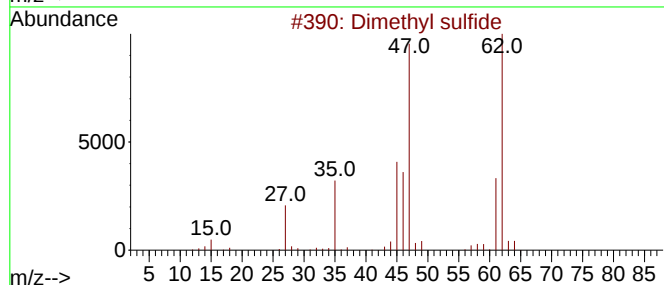
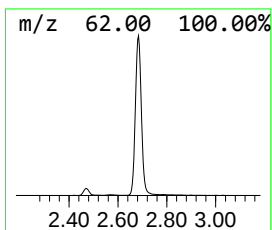
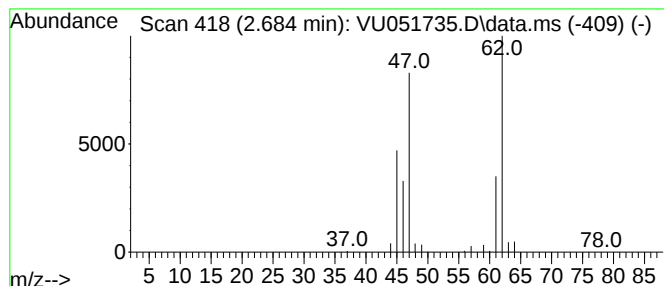
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 Dimethyl sulfide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.684	13.83 ug/L	1230710	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl sulfide	62	C2H6S	000075-18-3	94
2			Dimethyl sulfide	62	C2H6S	000075-18-3	91
3			Dimethyl sulfide	62	C2H6S	000075-18-3	91
4			Dimethyl sulfide	62	C2H6S	000075-18-3	91
5			Dimethyl sulfide	62	C2H6S	000075-18-3	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110322\
Data File : VU051735.D
Acq On : 03 Nov 2022 15:50
Operator : JC/MD
Sample : N5407-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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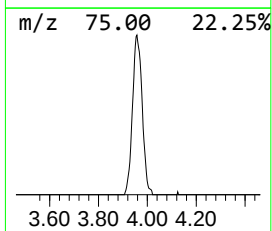
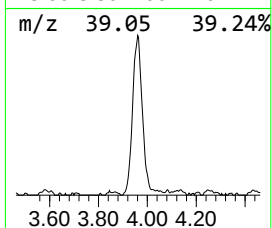
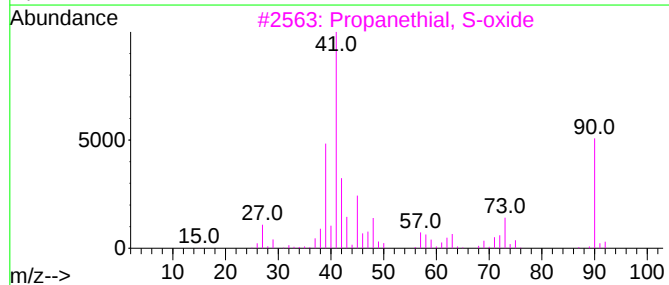
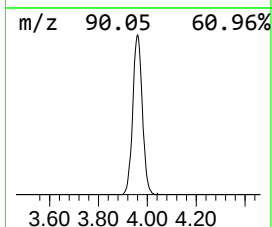
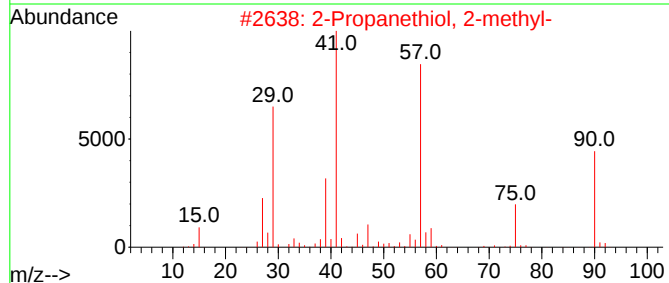
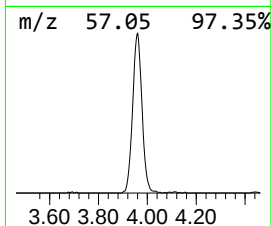
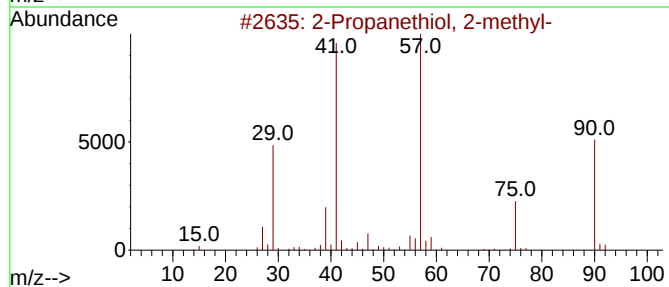
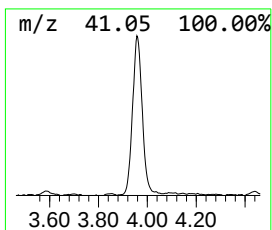
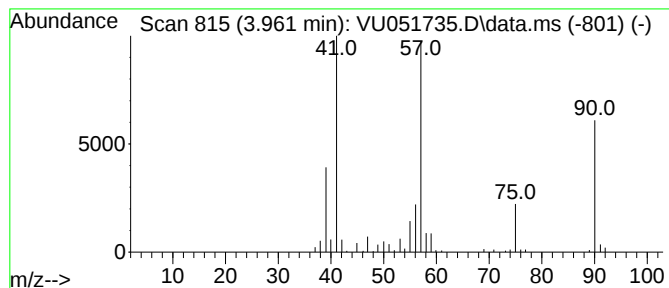
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 2-Propanethiol, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.961	3.49 ug/L	310477	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	50
2			2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	49
3			Propanethial, S-oxide	90	C3H6OS	032157-29-2	47
4			2-Butanethiol	90	C4H10S	000513-53-1	38
5			2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110322\
Data File : VU051735.D
Acq On : 03 Nov 2022 15:50
Operator : JC/MD
Sample : N5407-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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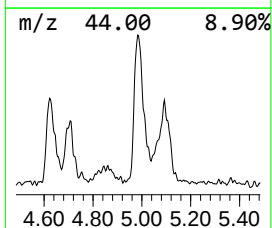
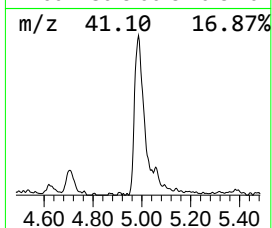
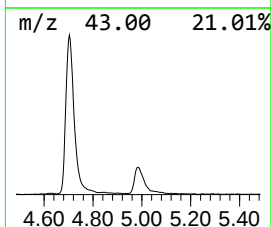
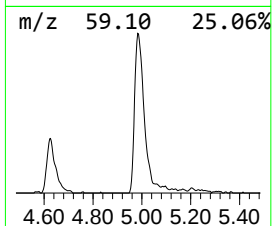
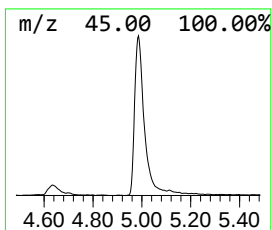
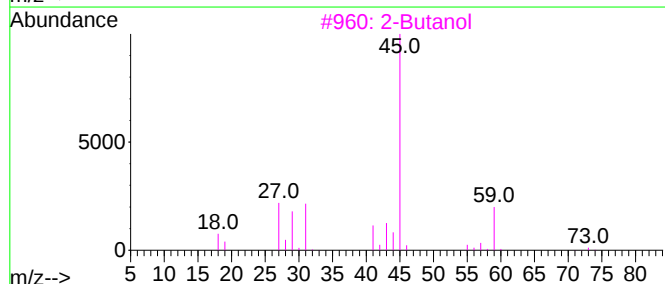
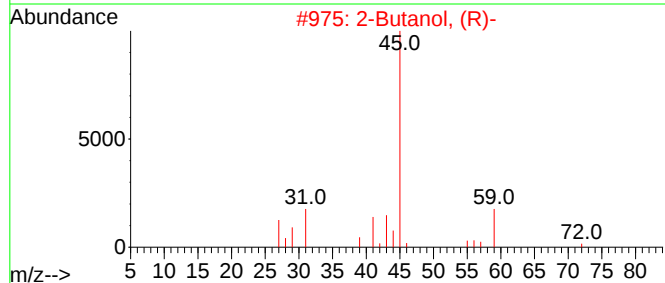
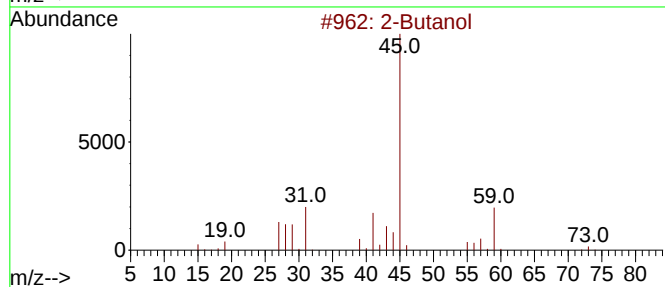
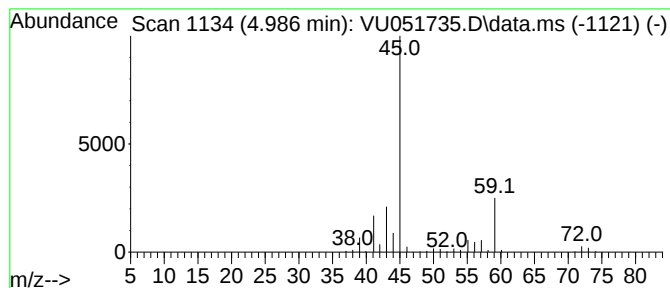
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 9 2-Butanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.986	4.02 ug/L	357347	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol	74	C4H10O	000078-92-2	83
2	2-Butanol, (R)-	74	C4H10O	014898-79-4	83
3	2-Butanol	74	C4H10O	000078-92-2	78
4	2-Butanol	74	C4H10O	000078-92-2	72
5	2-Butanol, (R)-	74	C4H10O	014898-79-4	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110322\
Data File : VU051735.D
Acq On : 03 Nov 2022 15:50
Operator : JC/MD
Sample : N5407-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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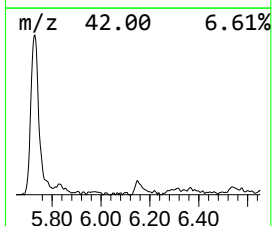
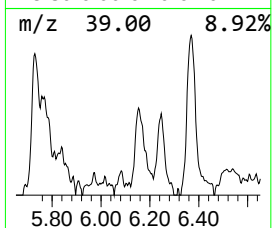
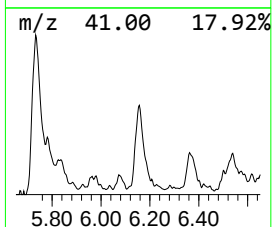
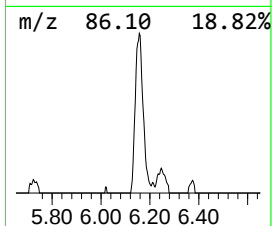
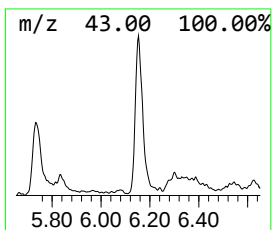
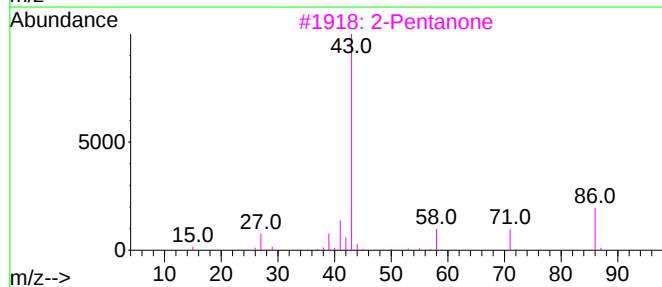
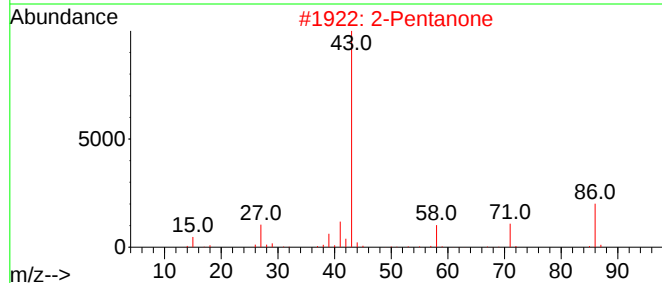
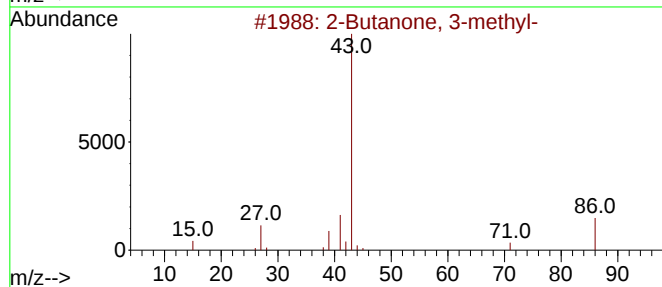
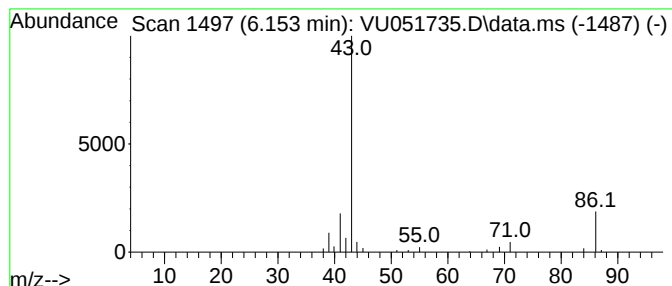
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 10 2-Butanone, 3-methyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.153	0.65 ug/L	57671	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3-methyl-			86	C5H10O	000563-80-4	59
2	2-Pentanone			86	C5H10O	000107-87-9	53
3	2-Pentanone			86	C5H10O	000107-87-9	53
4	Acetic acid ethenyl ester			86	C4H6O2	000108-05-4	42
5	2-Pentanone			86	C5H10O	000107-87-9	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110322\
Data File : VU051735.D
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Operator : JC/MD
Sample : N5407-01
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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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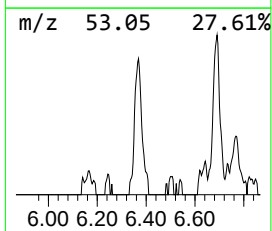
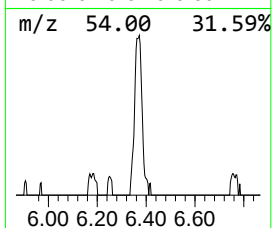
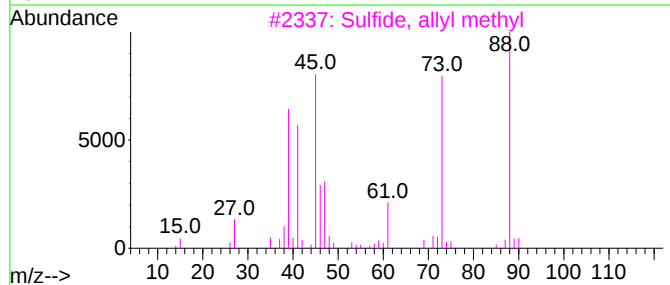
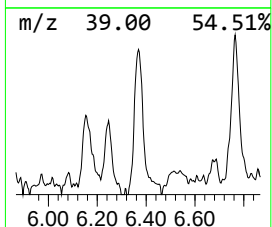
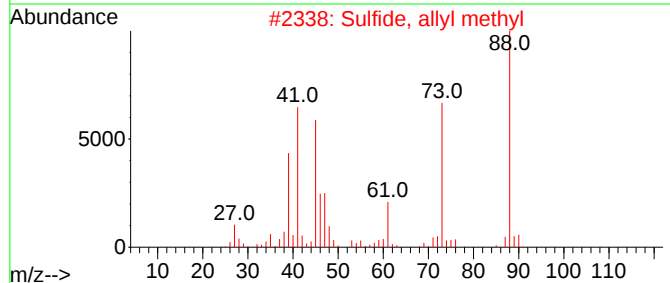
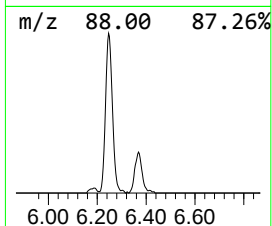
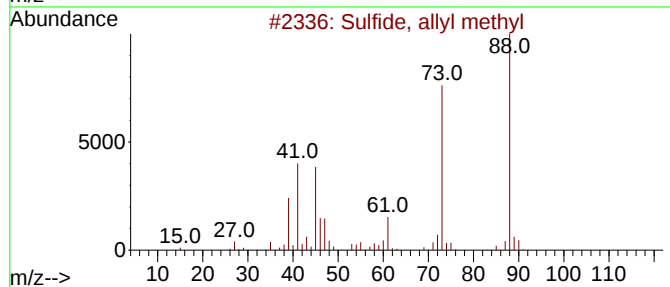
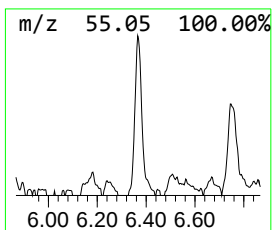
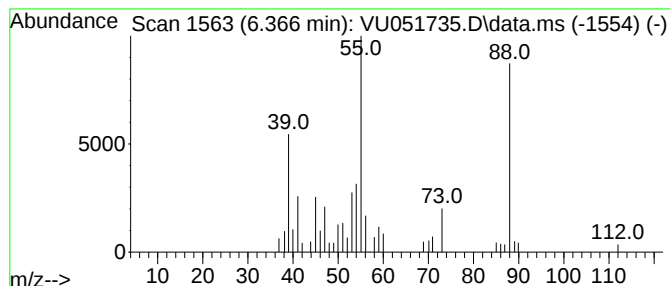
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 11 unknown-02 Concentration Rank 23

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.366	0.58 ug/L	52018	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfide, allyl methyl	88	C4H8S	010152-76-8	49
2			Sulfide, allyl methyl	88	C4H8S	010152-76-8	43
3			Sulfide, allyl methyl	88	C4H8S	010152-76-8	38
4			Methyl-4-deoxy-2-O-methyl.beta.l...	204	C8H12O6	1000312-10-0	38
5			2,2-Dimethylthiirane	88	C4H8S	003772-13-2	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110322\
Data File : VU051735.D
Acq On : 03 Nov 2022 15:50
Operator : JC/MD
Sample : N5407-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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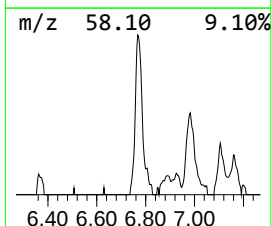
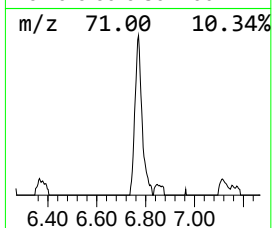
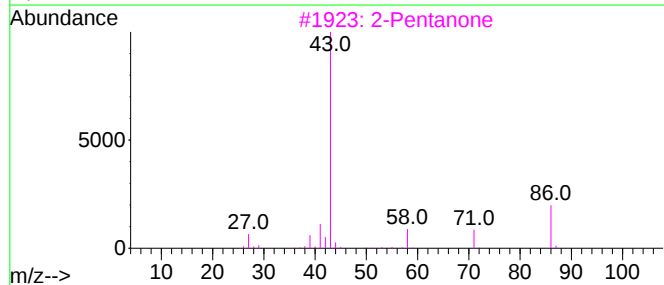
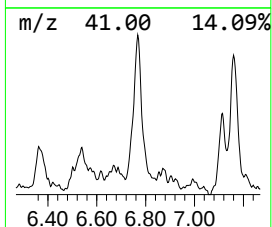
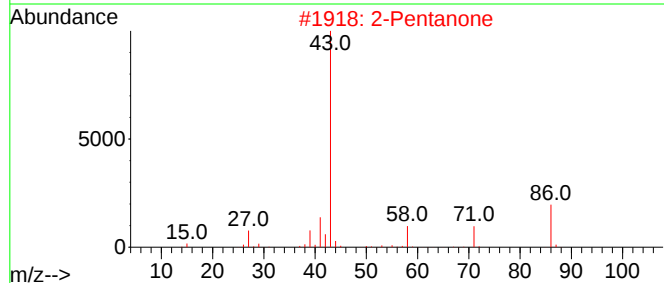
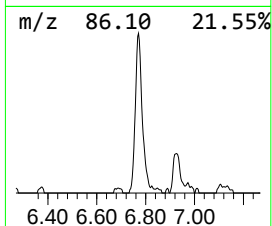
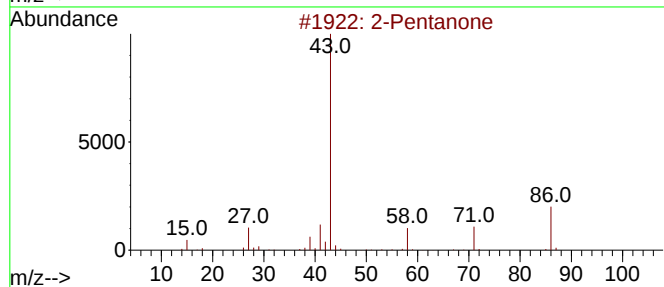
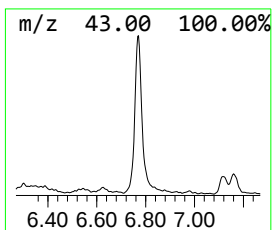
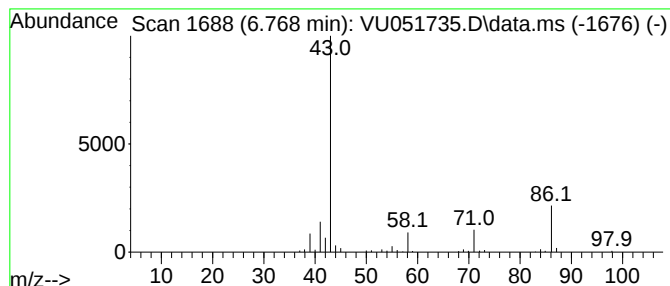
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 12 2-Pentanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.768	1.53 ug/L	136237	1,4-Difluorobenzene	6.247

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone	86	C5H10O	000107-87-9	87
2		2-Pentanone	86	C5H10O	000107-87-9	83
3		2-Pentanone	86	C5H10O	000107-87-9	80
4		2-Pentanone	86	C5H10O	000107-87-9	64
5		2-Pentanone	86	C5H10O	000107-87-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110322\
Data File : VU051735.D
Acq On : 03 Nov 2022 15:50
Operator : JC/MD
Sample : N5407-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4Y1

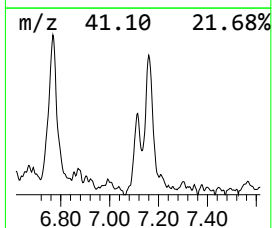
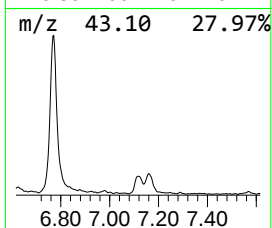
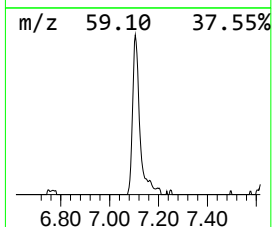
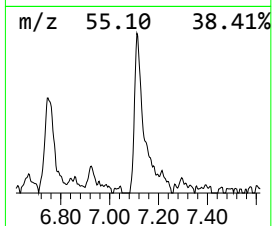
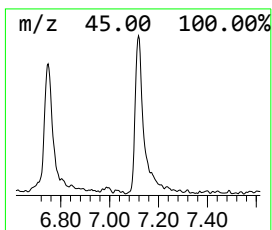
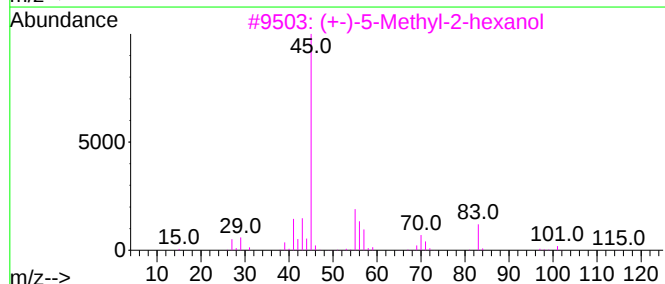
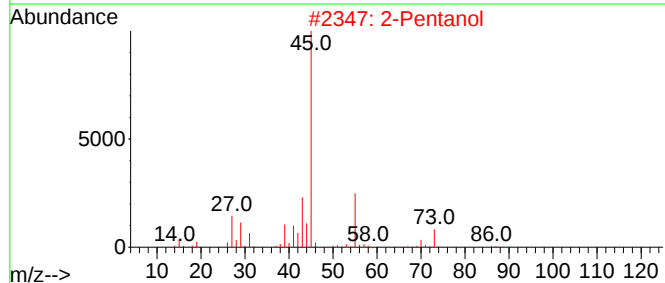
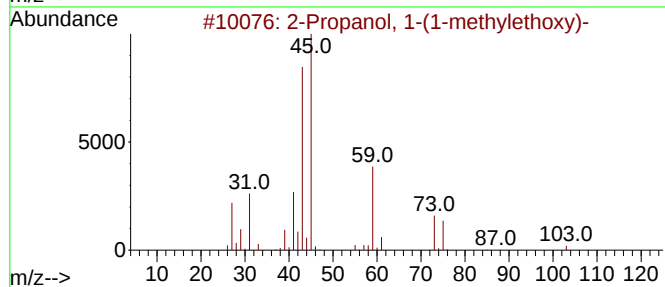
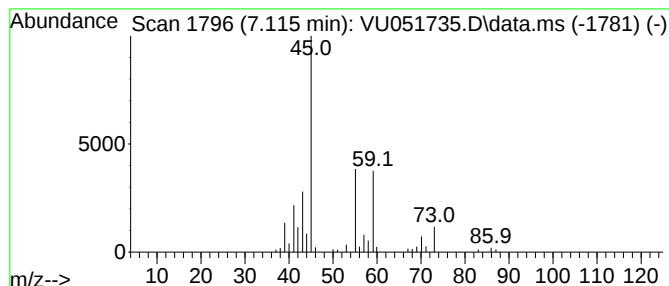
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 13 2-Propanol, 1-(1-methyletho... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.115	0.80 ug/L	71318	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(1-methylethoxy)-		118	C6H14O2		003944-36-3	50
2	2-Pentanol		88	C5H12O		006032-29-7	45
3	(+)-5-Methyl-2-hexanol		116	C7H16O		111768-09-3	40
4	4-Penten-2-ol		86	C5H10O		000625-31-0	38
5	Formic acid, 3-methylbut-2-yl ester		116	C6H12O2		1010367-95-2	36



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110322\
Data File : VU051735.D
Acq On : 03 Nov 2022 15:50
Operator : JC/MD
Sample : N5407-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4Y1

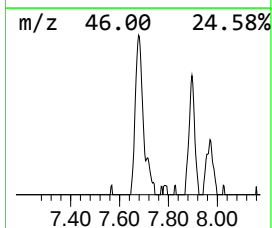
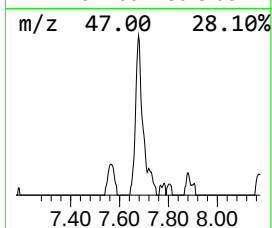
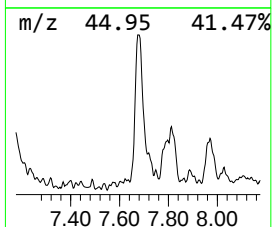
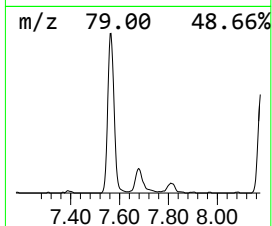
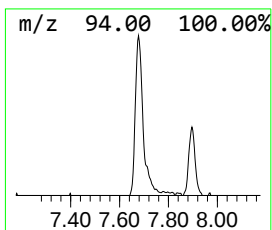
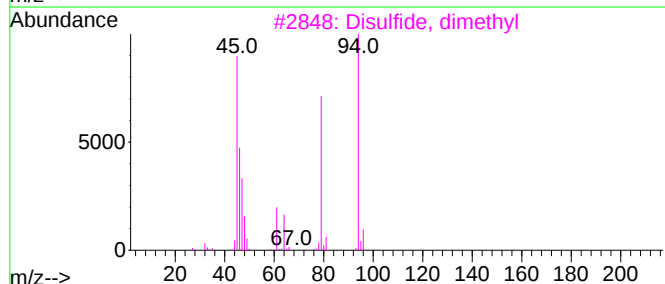
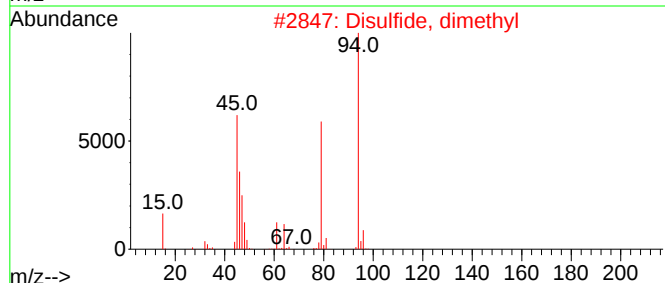
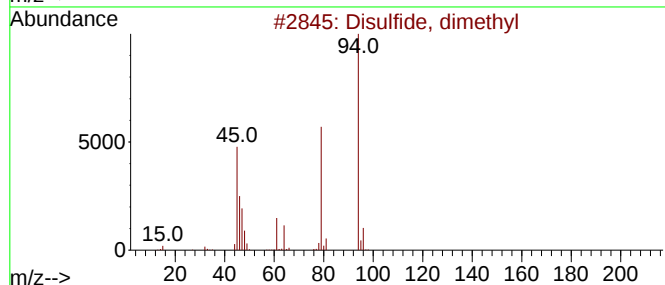
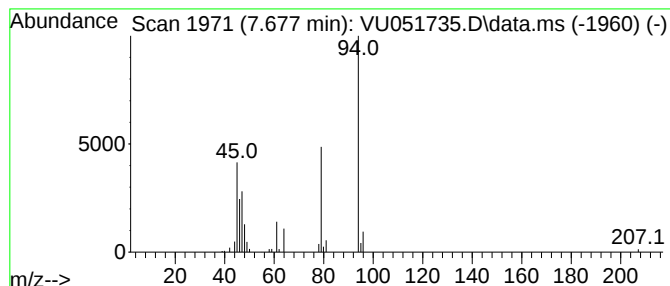
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 15 Disulfide, dimethyl Concentration Rank 21

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.677	0.64 ug/L	57236	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Disulfide, dimethyl	94	C2H6S2	000624-92-0	97
2			Disulfide, dimethyl	94	C2H6S2	000624-92-0	94
3			Disulfide, dimethyl	94	C2H6S2	000624-92-0	91
4			Disulfide, dimethyl	94	C2H6S2	000624-92-0	91
5			Disulfide, dimethyl	94	C2H6S2	000624-92-0	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110322\
Data File : VU051735.D
Acq On : 03 Nov 2022 15:50
Operator : JC/MD
Sample : N5407-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4Y1

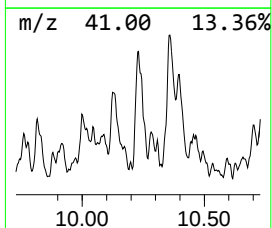
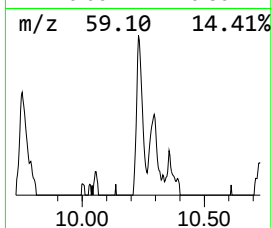
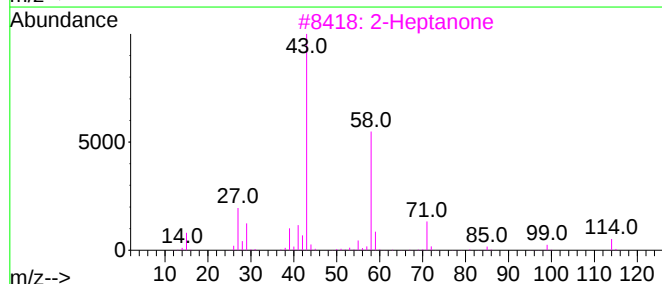
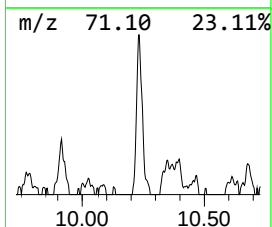
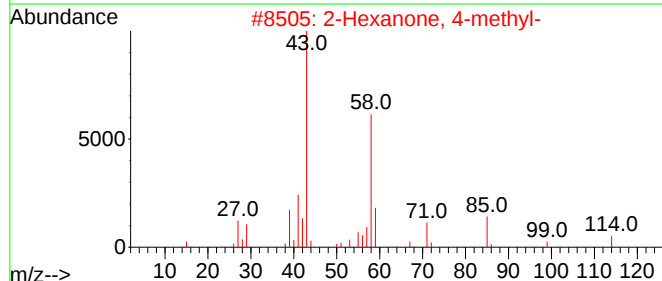
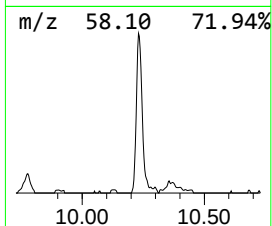
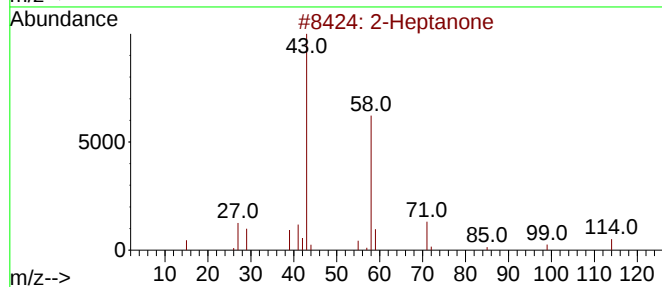
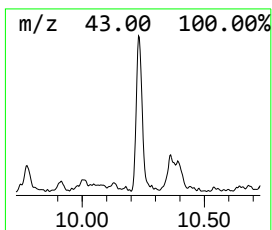
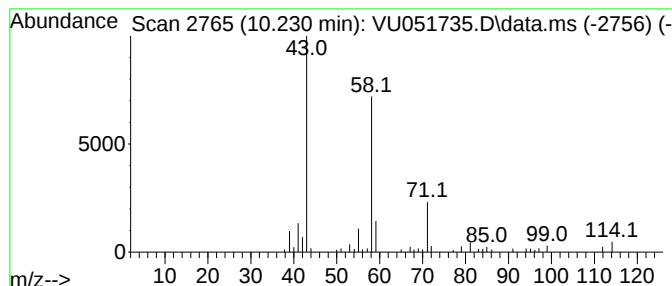
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 16 2-Heptanone Concentration Rank 26

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.230	0.50 ug/L	59852	Chlorobenzene-d5	9.414

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Heptanone	114	C7H14O	000110-43-0	87
2		2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	72
3		2-Heptanone	114	C7H14O	000110-43-0	72
4		2-Heptanone	114	C7H14O	000110-43-0	72
5		2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110322\
Data File : VU051735.D
Acq On : 03 Nov 2022 15:50
Operator : JC/MD
Sample : N5407-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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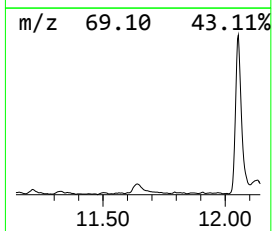
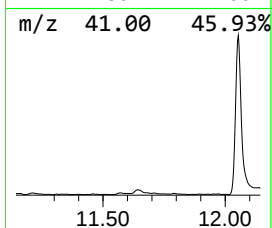
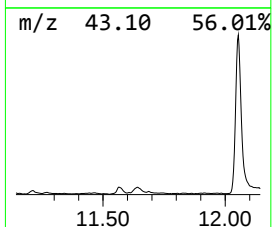
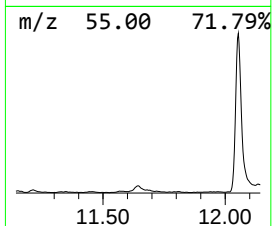
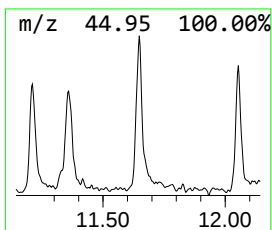
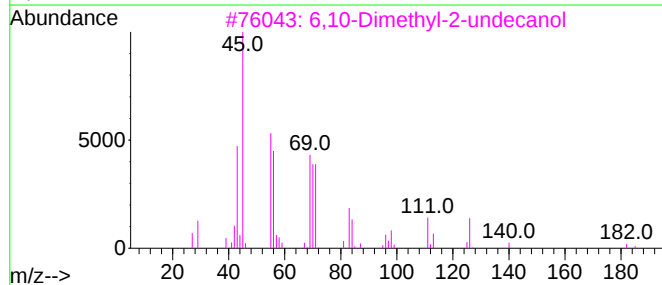
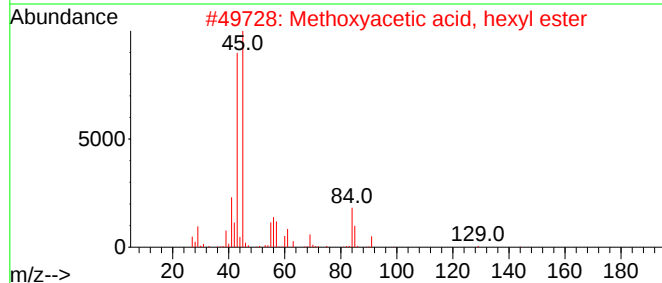
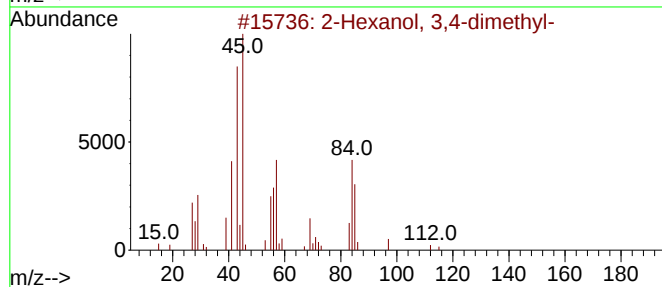
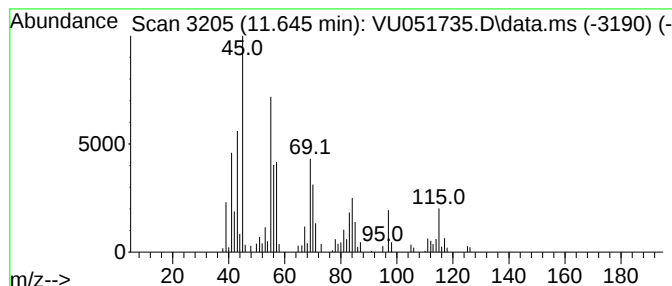
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 17 2-Hexanol, 3,4-dimethyl- Concentration Rank 24

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.645	0.55 ug/L	78789	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hexanol, 3,4-dimethyl-	130	C8H18O	019550-05-1	58
2			Methoxyacetic acid, hexyl ester	174	C9H18O3	145747-16-6	53
3			6,10-Dimethyl-2-undecanol	200	C13H28O	1000432-19-5	53
4			2-Heptanol, 6-methyl-	130	C8H18O	004730-22-7	50
5			2-Heptanol, 5-methyl-	130	C8H18O	054630-50-1	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110322\
Data File : VU051735.D
Acq On : 03 Nov 2022 15:50
Operator : JC/MD
Sample : N5407-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4Y1

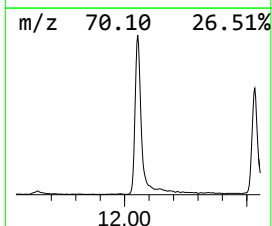
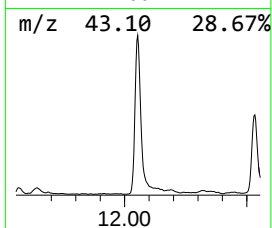
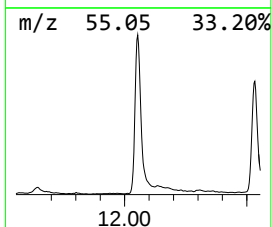
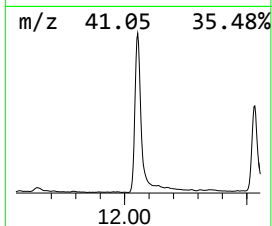
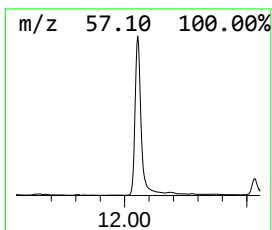
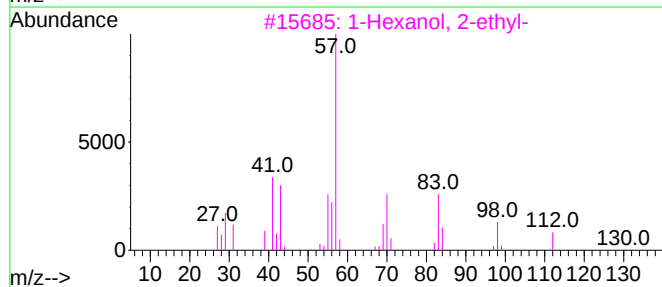
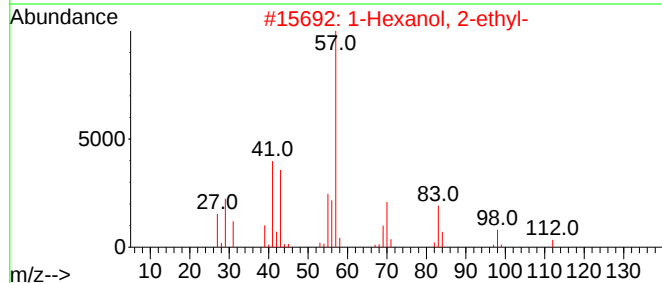
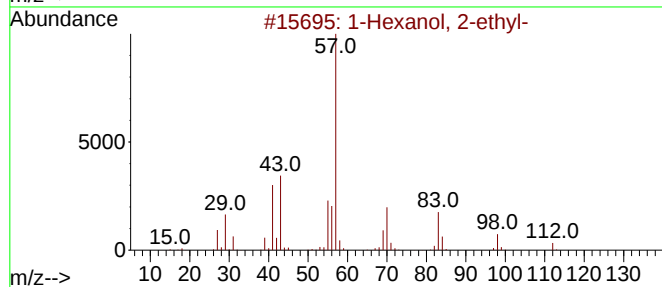
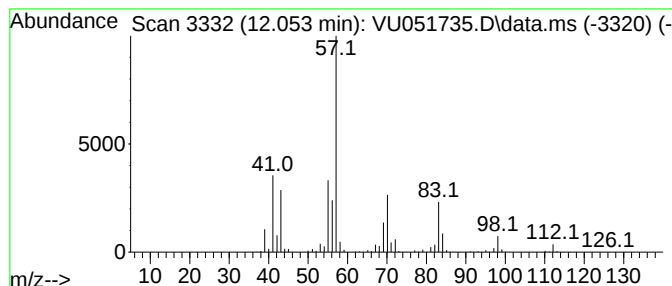
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 18 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.054	13.84 ug/L	1965620	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110322\
Data File : VU051735.D
Acq On : 03 Nov 2022 15:50
Operator : JC/MD
Sample : N5407-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4Y1

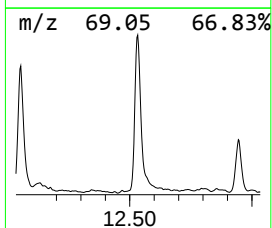
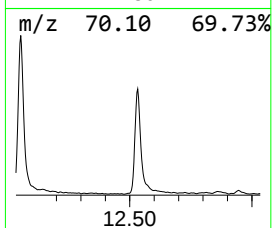
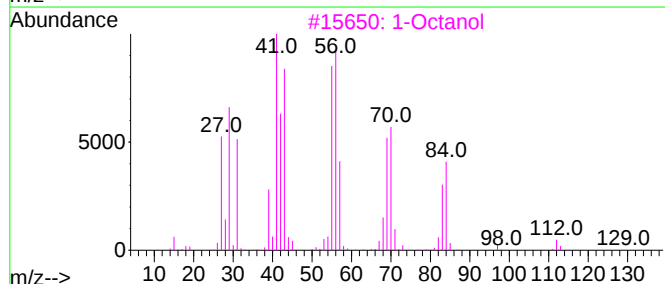
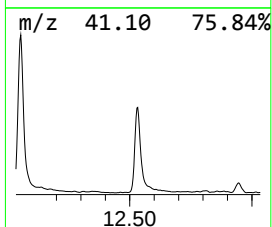
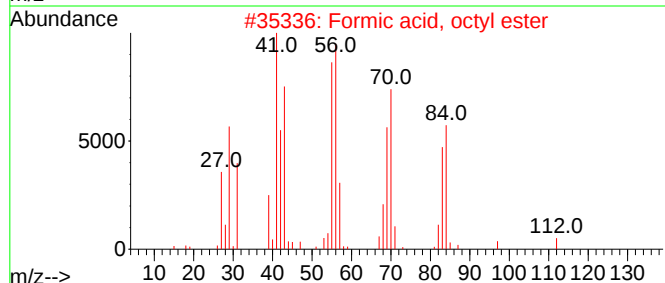
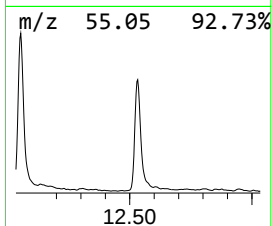
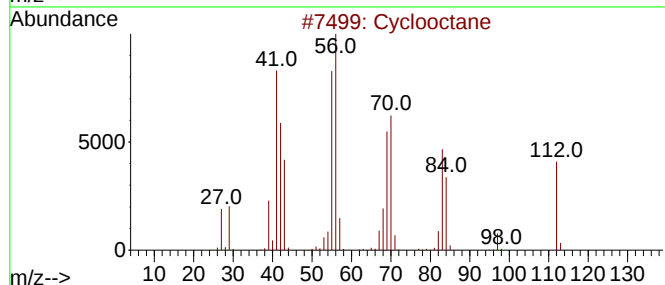
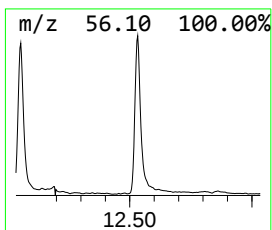
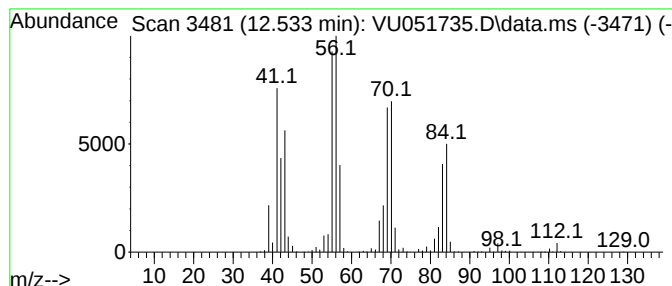
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 19 (DEL) Alkane: Cyclic12.533 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.533	7.16 ug/L	1016210	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclooctane	112	C8H16	000292-64-8	90
2			Formic acid, octyl ester	158	C9H18O2	000112-32-3	90
3			1-Octanol	130	C8H18O	000111-87-5	90
4			1-Octanol	130	C8H18O	000111-87-5	90
5			1-Octanol	130	C8H18O	000111-87-5	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110322\
Data File : VU051735.D
Acq On : 03 Nov 2022 15:50
Operator : JC/MD
Sample : N5407-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4Y1

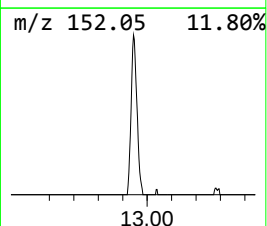
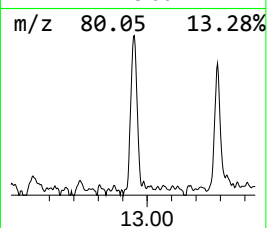
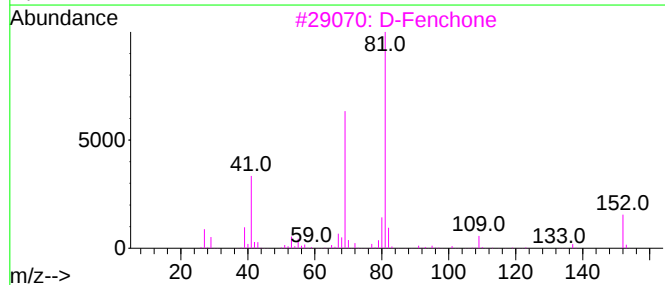
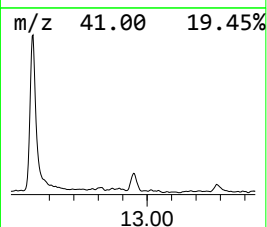
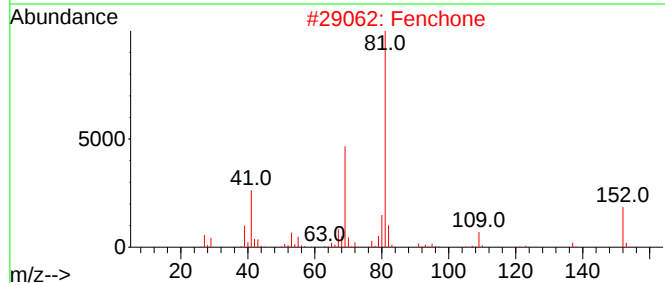
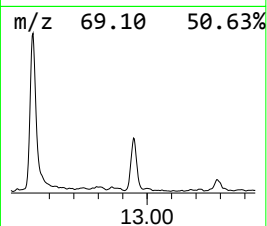
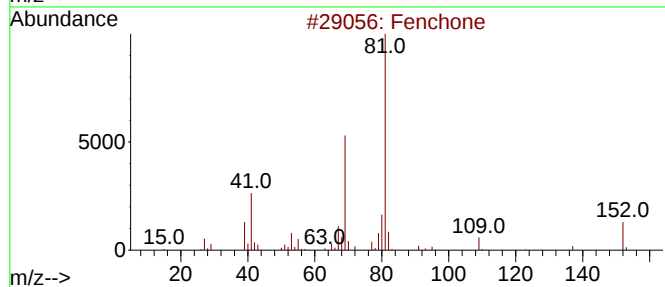
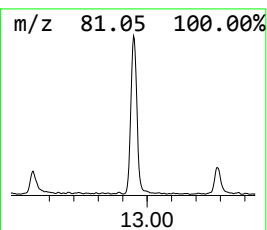
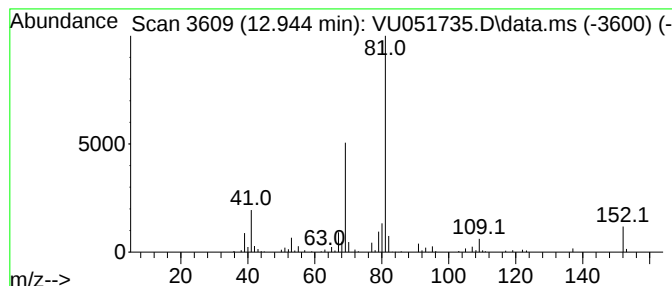
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 20 Fenchone Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.944	1.15 ug/L	163408	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fenchone	152	C10H16O	001195-79-5	91
2			Fenchone	152	C10H16O	001195-79-5	91
3			D-Fenchone	152	C10H16O	004695-62-9	90
4			L-Fenchone	152	C10H16O	007787-20-4	90
5			Fenchone	152	C10H16O	001195-79-5	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110322\
Data File : VU051735.D
Acq On : 03 Nov 2022 15:50
Operator : JC/MD
Sample : N5407-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4Y1

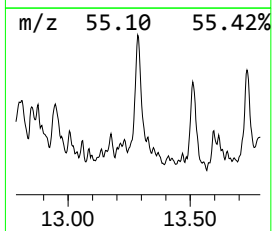
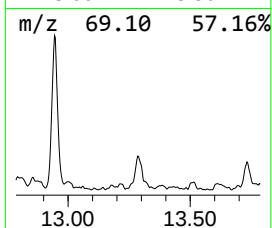
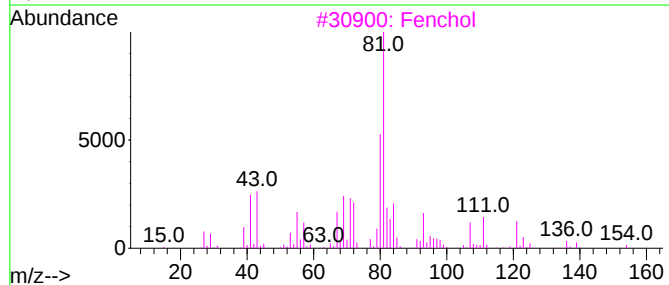
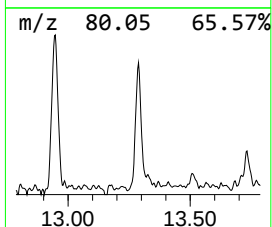
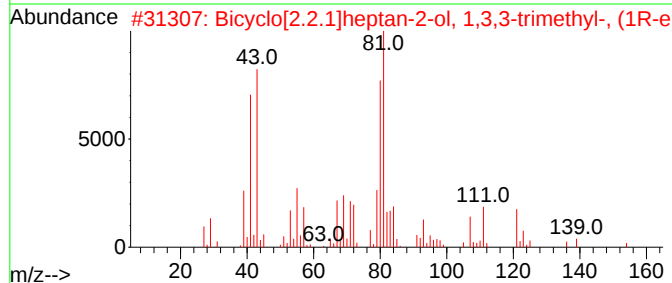
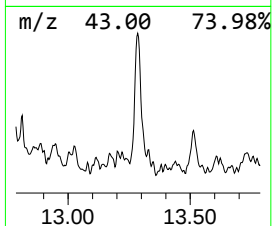
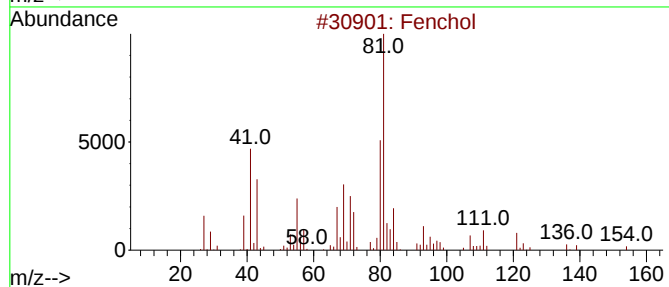
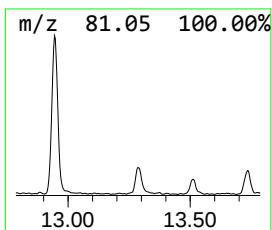
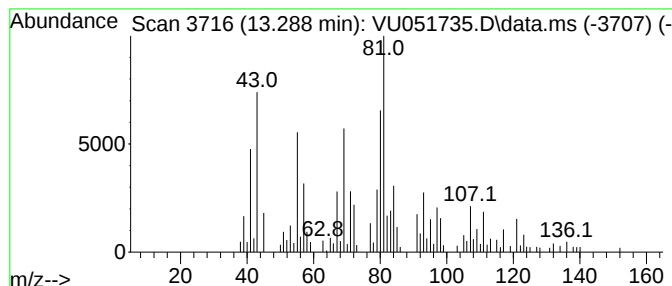
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 21 Fenchol Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.288	0.69 ug/L	97495	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fenchol	154	C10H18O	001632-73-1	64
2			Bicyclo[2.2.1]heptan-2-ol, 1,3,3...	154	C10H18O	002217-02-9	59
3			Fenchol	154	C10H18O	001632-73-1	59
4			Fenchol	154	C10H18O	001632-73-1	59
5			Fenchol	154	C10H18O	001632-73-1	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110322\
Data File : VU051735.D
Acq On : 03 Nov 2022 15:50
Operator : JC/MD
Sample : N5407-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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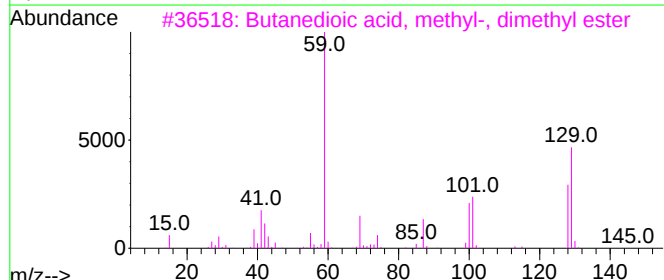
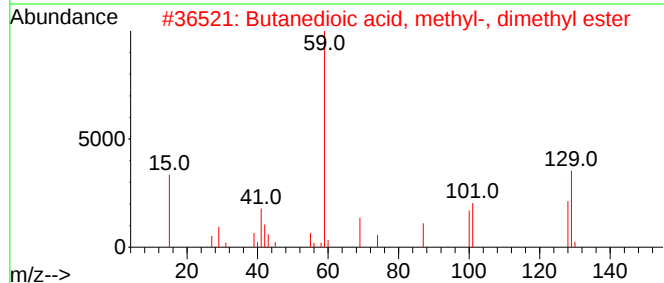
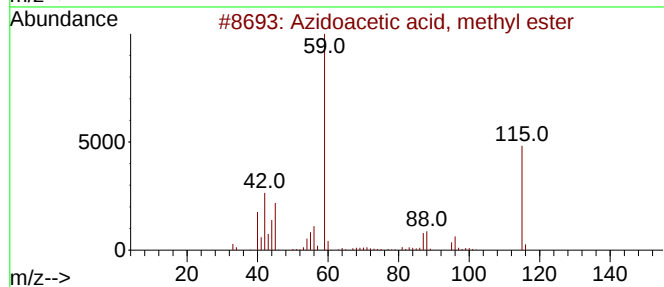
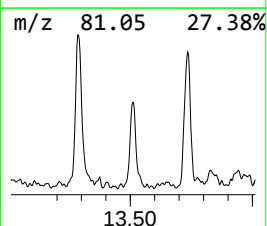
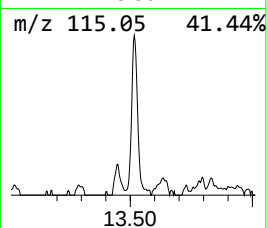
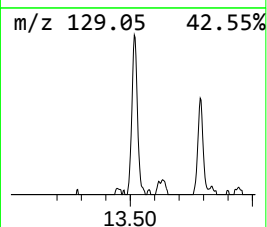
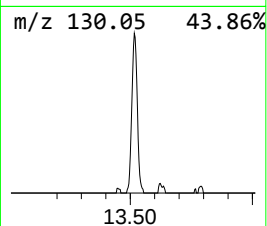
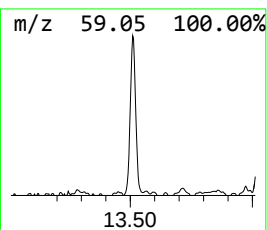
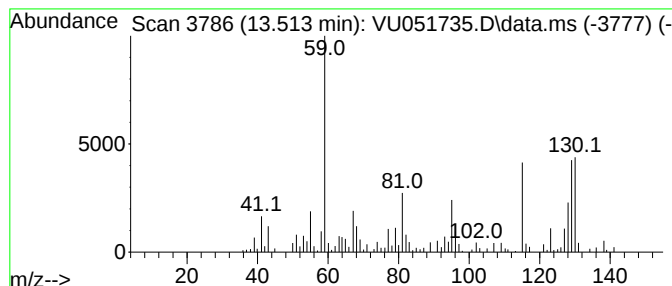
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 22 unknown-03 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.513	0.82 ug/L	116714	1,4-Dichlorobenzene-d4	11.809

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Azidoacetic acid, methyl ester	115	C3H5N3O2	1000316-94-5	35
2		Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	32
3		Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	23
4		Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	000498-81-7	22
5		Cyclohexanemethanol, .alpha.,.al...	156	C10H20O	005114-00-1	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110322\
Data File : VU051735.D
Acq On : 03 Nov 2022 15:50
Operator : JC/MD
Sample : N5407-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4Y1

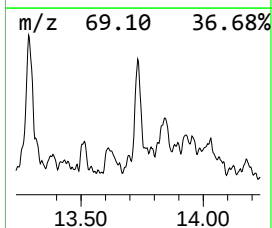
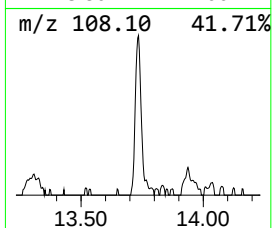
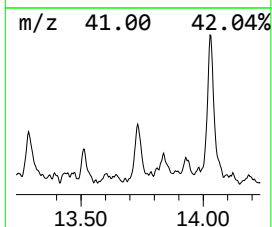
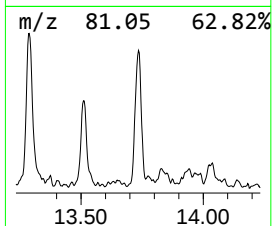
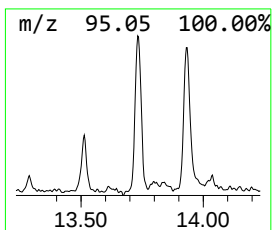
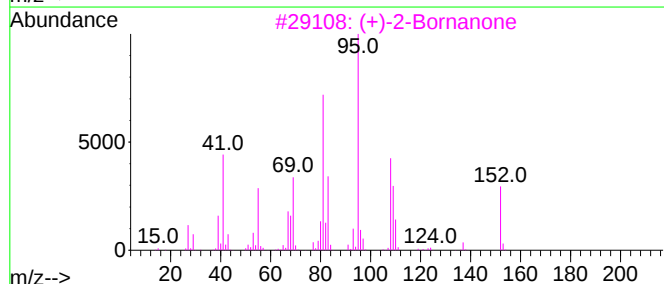
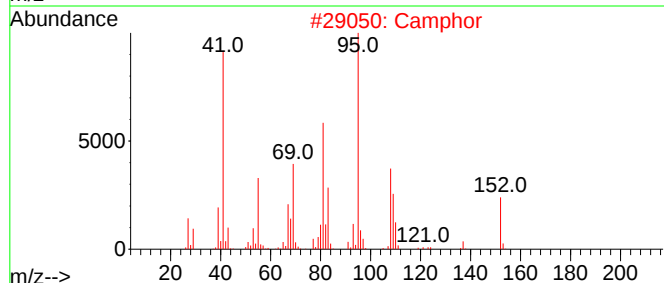
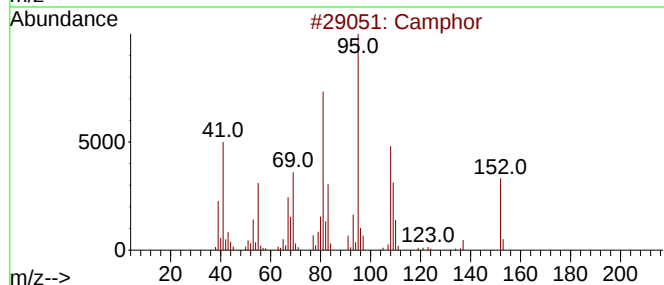
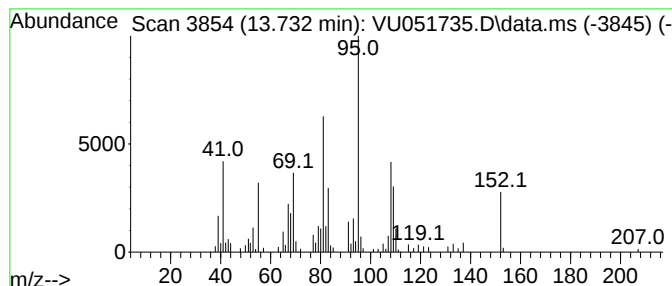
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 23 Camphor Concentration Rank 22

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.732	0.59 ug/L	83547	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Camphor	152	C10H16O	000076-22-2	95
2			Camphor	152	C10H16O	000076-22-2	95
3			(+)-2-Bornanone	152	C10H16O	000464-49-3	95
4			(+)-2-Bornanone	152	C10H16O	000464-49-3	95
5			Camphor	152	C10H16O	000076-22-2	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110322\
Data File : VU051735.D
Acq On : 03 Nov 2022 15:50
Operator : JC/MD
Sample : N5407-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4Y1

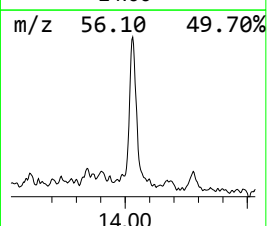
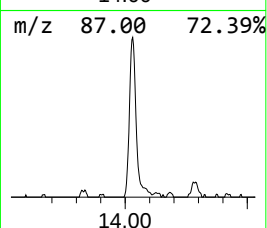
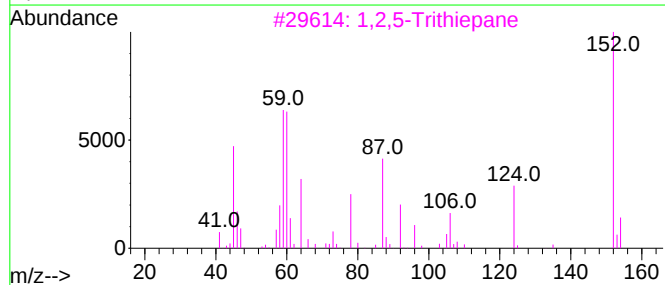
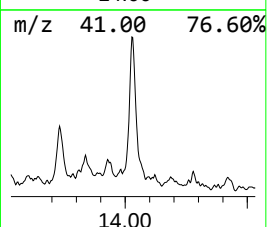
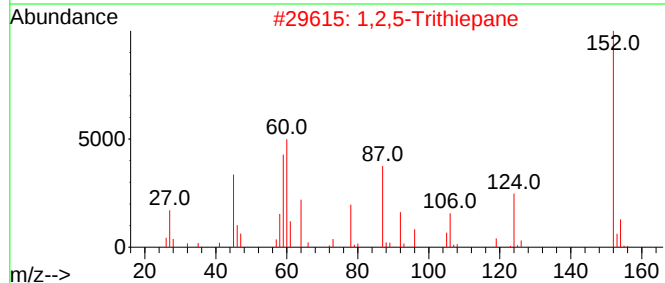
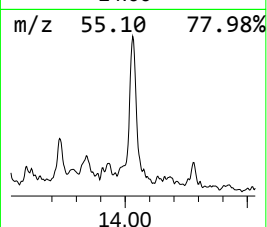
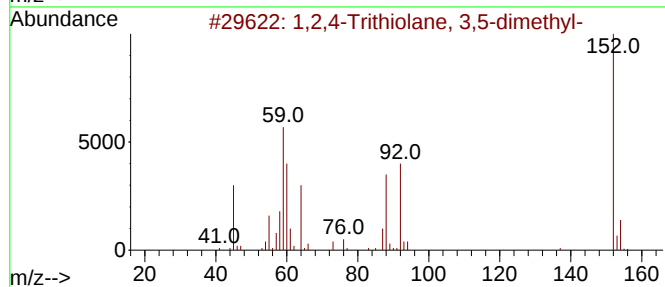
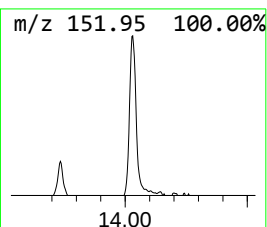
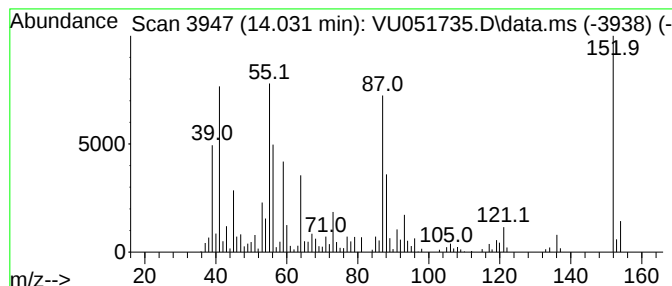
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 24 unknown-04 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.031	1.09 ug/L	154449	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2,4-Trithiolane, 3,5-dimethyl-	152	C4H8S3	023654-92-4	38
2			1,2,5-Trithiepane	152	C4H8S3	006576-93-8	38
3			1,2,5-Trithiepane	152	C4H8S3	006576-93-8	25
4			Ethane, isothiocyanato-	87	C3H5NS	000542-85-8	18
5			Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	12



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110322\
Data File : VU051735.D
Acq On : 03 Nov 2022 15:50
Operator : JC/MD
Sample : N5407-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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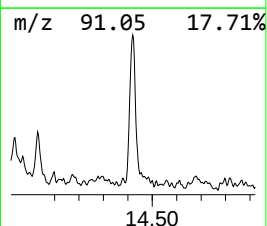
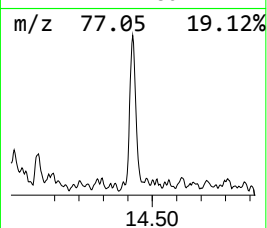
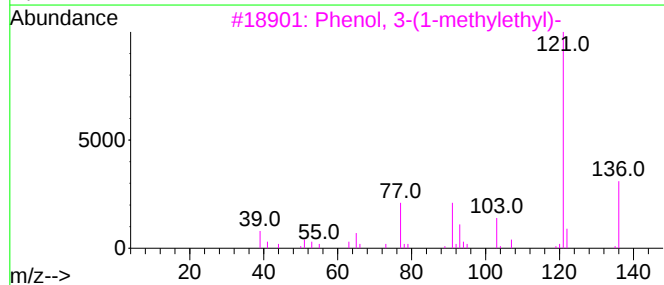
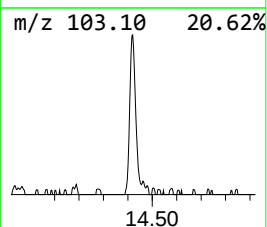
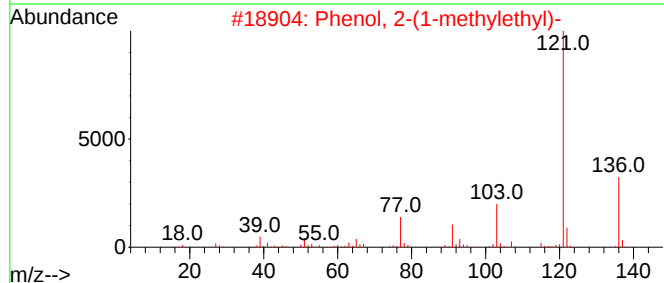
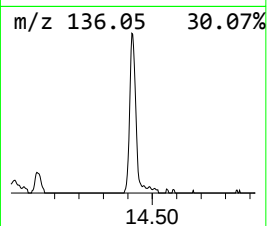
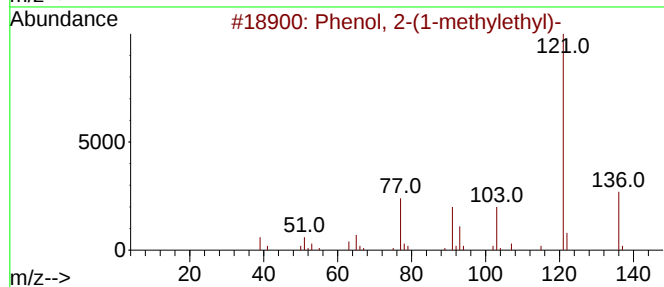
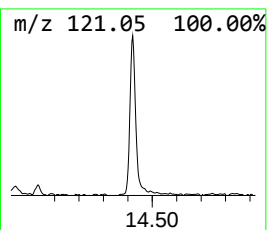
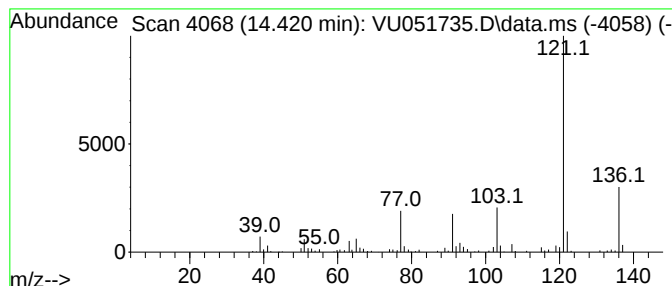
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 25 Phenol, 2-(1-methylethyl)- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.420	0.66 ug/L	93617	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-(1-methylethyl)-	136	C9H12O	000088-69-7	94
2			Phenol, 2-(1-methylethyl)-	136	C9H12O	000088-69-7	91
3			Phenol, 3-(1-methylethyl)-	136	C9H12O	000618-45-1	90
4			p-Cumenol	136	C9H12O	000099-89-8	90
5			Phenol, 2-(1-methylethyl)-	136	C9H12O	000088-69-7	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110322\
Data File : VU051735.D
Acq On : 03 Nov 2022 15:50
Operator : JC/MD
Sample : N5407-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4Y1

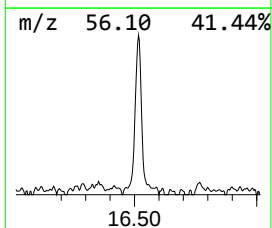
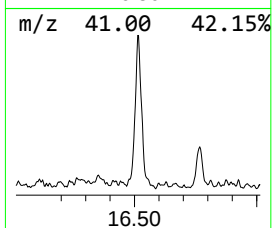
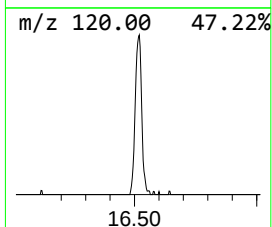
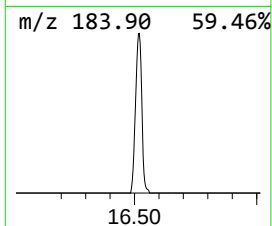
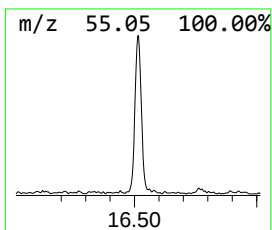
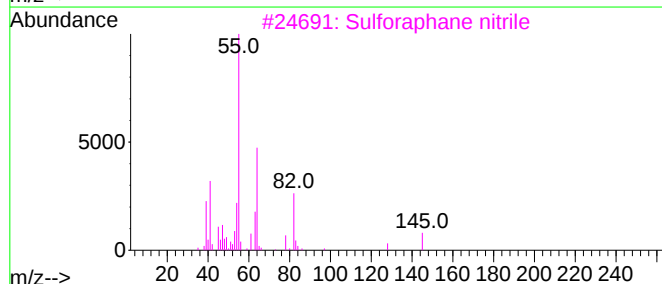
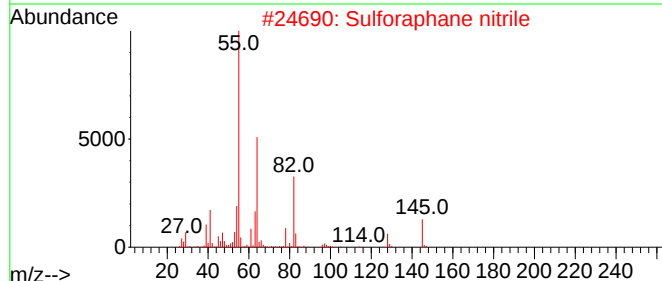
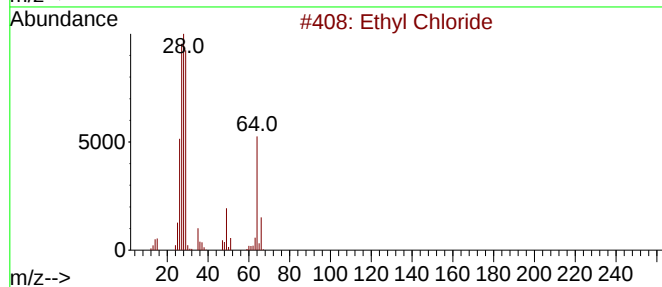
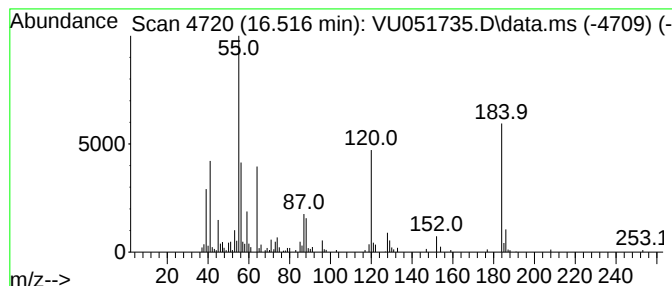
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 26 unknown-05 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.516	0.86 ug/L	122506	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl Chloride	64	C2H5Cl	000075-00-3	35
2			Sulforaphane nitrile	145	C6H11NOS	061121-66-2	32
3			Sulforaphane nitrile	145	C6H11NOS	061121-66-2	23
4			3H-1,2-Benzodithiole-3-thione	184	C7H4S3	003354-42-5	10
5			3H-1,2-Benzodithiole-3-thione	184	C7H4S3	003354-42-5	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110322\
 Data File : VU051735.D
 Acq On : 03 Nov 2022 15:50
 Operator : JC/MD
 Sample : N5407-01
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW4Y1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.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
unknown-01	1.359	1.8	ug/L	156789	1	6.247	444865	5.0
Sulfur dioxide	1.472	3.4	ug/L	301279	1	6.247	444865	5.0
Methanethiol	1.787	10.2	ug/L	903402	1	6.247	444865	5.0
1,2-Butadiene	2.244	0.9	ug/L	80724	1	6.247	444865	5.0
Ethanethiol	2.469	0.5	ug/L	46915	1	6.247	444865	5.0
Dimethyl sulfide	2.684	13.8	ug/L	1230710	1	6.247	444865	5.0
2-Propanethiol,...	3.961	3.5	ug/L	310477	1	6.247	444865	5.0
2-Butanol	4.986	4.0	ug/L	357347	1	6.247	444865	5.0
2-Butanone, 3-m...	6.153	0.7	ug/L	57671	1	6.247	444865	5.0
unknown-02	6.366	0.6	ug/L	52018	1	6.247	444865	5.0
2-Pentanone	6.768	1.5	ug/L	136237	1	6.247	444865	5.0
2-Propanol, 1-(...	7.115	0.8	ug/L	71318	1	6.247	444865	5.0
Disulfide, dime...	7.677	0.6	ug/L	57236	1	6.247	444865	5.0
2-Heptanone	10.230	0.5	ug/L	59852	2	9.414	597447	5.0
2-Hexanol, 3,4-...	11.645	0.6	ug/L	78789	3	11.809	709968	5.0
1-Hexanol, 2-et...	12.054	13.8	ug/L	1965620	3	11.809	709968	5.0
(DEL) Alkane: C...	12.533	7.2	ug/L	1016210	3	11.809	709968	5.0
Fenchone	12.944	1.1	ug/L	163408	3	11.809	709968	5.0
Fenchol	13.288	0.7	ug/L	97495	3	11.809	709968	5.0
unknown-03	13.513	0.8	ug/L	116714	3	11.809	709968	5.0
Camphor	13.732	0.6	ug/L	83547	3	11.809	709968	5.0
unknown-04	14.031	1.1	ug/L	154449	3	11.809	709968	5.0
Phenol, 2-(1-me...	14.420	0.7	ug/L	93617	3	11.809	709968	5.0
unknown-05	16.516	0.9	ug/L	122506	3	11.809	709968	5.0