

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121724\
 Data File : VU062419.D
 Acq On : 18 Dec 2024 05:09
 Operator : MD/SY
 Sample : P5309-07
 Misc : 25mL/MSVOA_U/WATER
 ALS Vial : 49 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0CF8

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR120924WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU062419.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.390	23	31	51	rVB	91503	99409	14.47%	1.898%
2	1.528	65	74	83	rBV	10548	10449	1.52%	0.199%
3	1.628	96	105	121	rBV4	153976	252762	36.80%	4.825%
4	1.705	122	129	141	rVV	46926	54418	7.92%	1.039%
5	1.782	142	153	166	rVB	79746	98247	14.30%	1.876%
6	1.968	202	211	224	rVB	29059	40711	5.93%	0.777%
7	2.136	253	263	278	rBV	147365	211794	30.84%	4.043%
8	2.203	278	284	293	rVV2	14225	20270	2.95%	0.387%
9	2.300	305	314	326	rVV	41411	61394	8.94%	1.172%
10	2.370	327	336	346	rVB	11245	16982	2.47%	0.324%
11	2.467	356	366	377	rBV2	12603	20665	3.01%	0.395%
12	2.621	403	414	429	rVB	67453	111157	16.18%	2.122%
13	3.586	702	714	723	rBV7	5347	11804	1.72%	0.225%
14	3.650	723	734	750	rVB5	5556	12717	1.85%	0.243%
15	3.891	801	809	821	rBV8	7049	15677	2.28%	0.299%
16	3.968	821	833	849	rVB7	8946	25364	3.69%	0.484%
17	4.245	908	919	931	rVB6	6107	13509	1.97%	0.258%
18	4.621	1024	1036	1047	rBV2	22457	46085	6.71%	0.880%
19	4.714	1050	1065	1082	rBV	308641	686818	100.00%	13.112%
20	5.113	1176	1189	1205	rBV	67244	150130	21.86%	2.866%
21	5.804	1385	1404	1415	rBV2	135804	322558	46.96%	6.158%
22	6.094	1481	1494	1510	rBV	27806	55091	8.02%	1.052%
23	6.312	1550	1562	1582	rBV	117970	219004	31.89%	4.181%
24	6.598	1637	1651	1672	rBV2	202500	611438	89.02%	11.673%
25	6.743	1686	1696	1728	rVB	86889	186162	27.10%	3.554%
26	7.598	1951	1962	1980	rBV2	38088	66619	9.70%	1.272%
27	7.923	2051	2063	2080	rBV	143276	269018	39.17%	5.136%
28	8.126	2116	2126	2140	rBV2	9499	16587	2.42%	0.317%
29	8.203	2140	2150	2163	rVB3	22015	36007	5.24%	0.687%
30	8.441	2211	2224	2234	rBV3	15505	25802	3.76%	0.493%
31	8.656	2278	2291	2323	rBV3	125470	271200	39.49%	5.177%
32	8.807	2332	2338	2356	rVB4	5752	11446	1.67%	0.219%
33	9.335	2495	2502	2517	rVB5	6740	12259	1.78%	0.234%
34	9.425	2517	2530	2557	rBV	152461	300753	43.79%	5.741%
35	9.717	2612	2621	2634	rVB8	4065	8323	1.21%	0.159%
36	10.020	2707	2715	2723	rBV5	8626	13258	1.93%	0.253%

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Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.1 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR120924WMA.M
 Title : TRACE VOA SFAM1.0

37	10.113	2736	2744	2755	rBV10	3890	7646	1.11%	0.146%
38	10.576	2878	2888	2899	rBV4	5735	9825	1.43%	0.188%
39	10.753	2930	2943	2959	rBV	57544	92263	13.43%	1.761%
40	11.685	3223	3233	3246	rVB6	9513	15663	2.28%	0.299%
41	11.807	3260	3271	3286	rBV	166354	274366	39.95%	5.238%
42	12.055	3338	3348	3371	rBV2	32455	69899	10.18%	1.334%
43	12.187	3378	3389	3404	rBV	158676	260284	37.90%	4.969%
44	12.878	3594	3604	3616	rBV2	51545	78834	11.48%	1.505%
45	13.974	3932	3945	3955	rBV3	27617	43588	6.35%	0.832%

Sum of corrected areas: 5238255

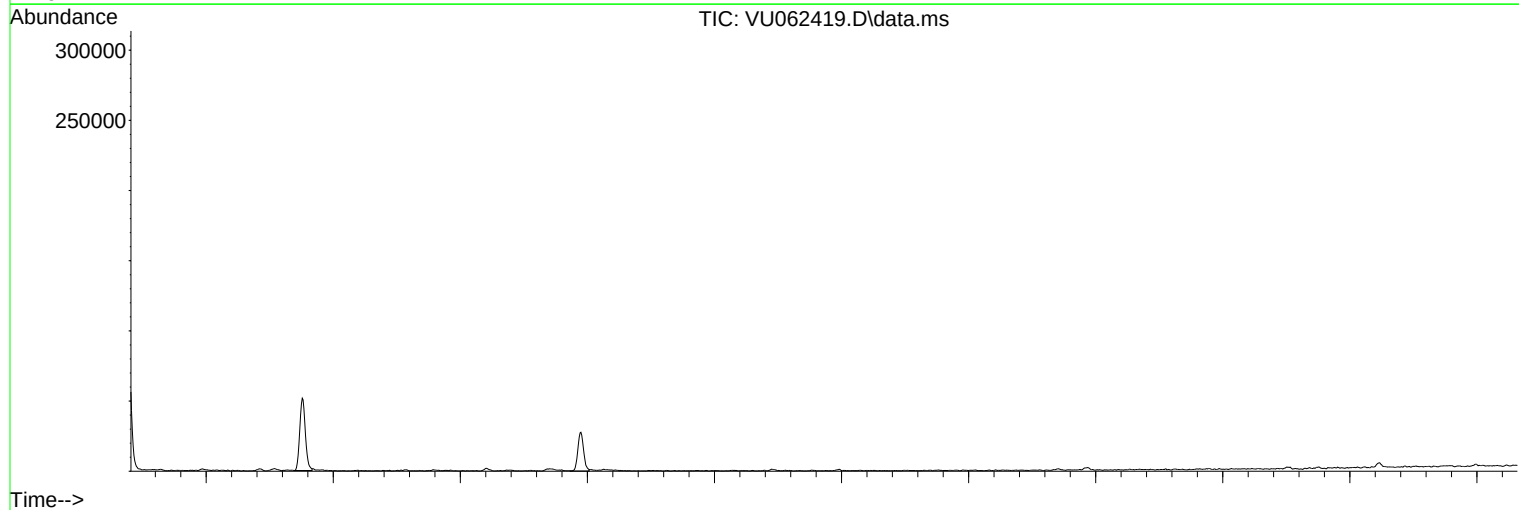
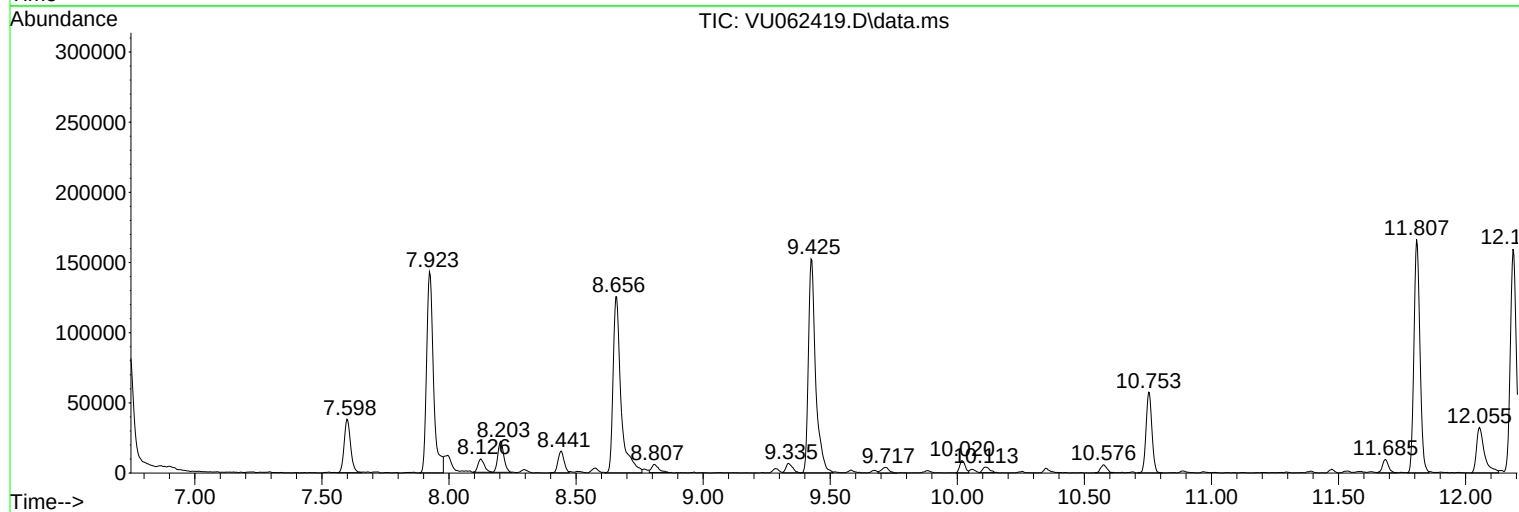
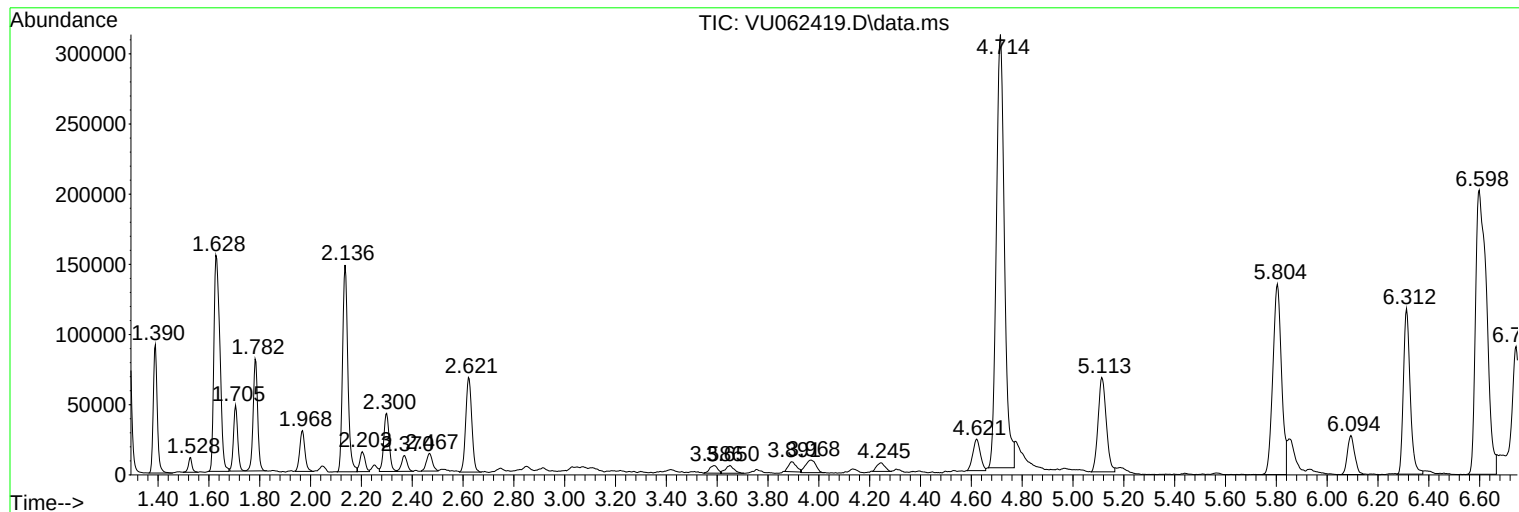
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR120924WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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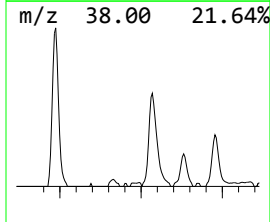
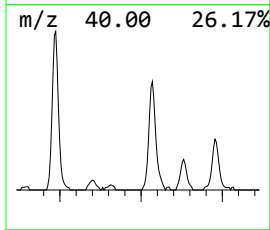
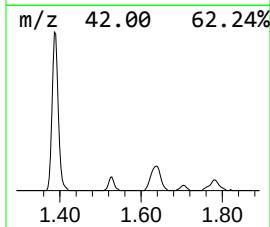
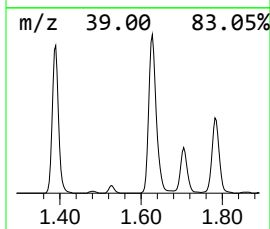
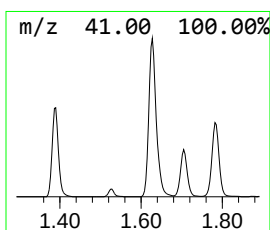
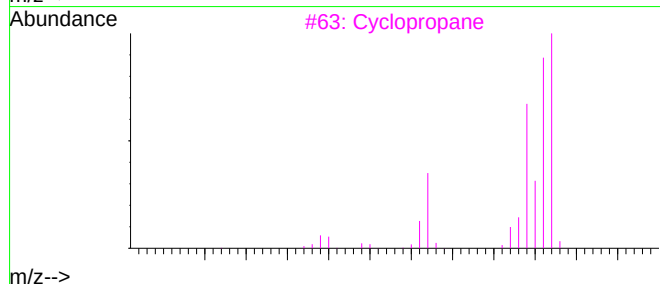
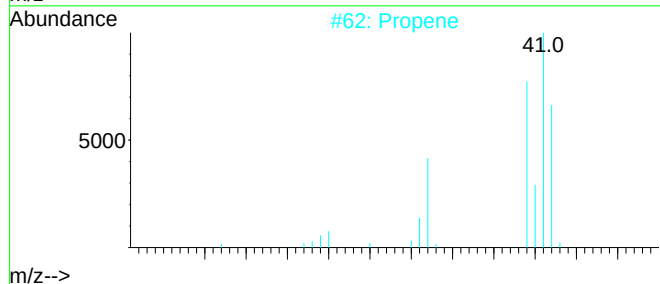
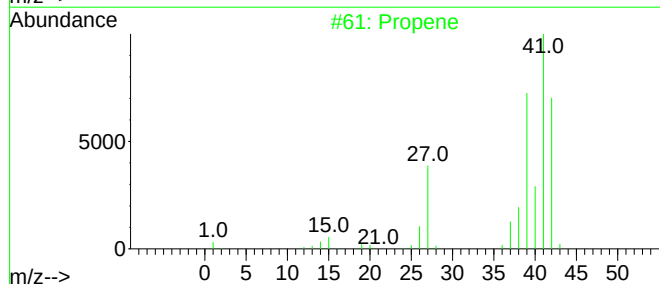
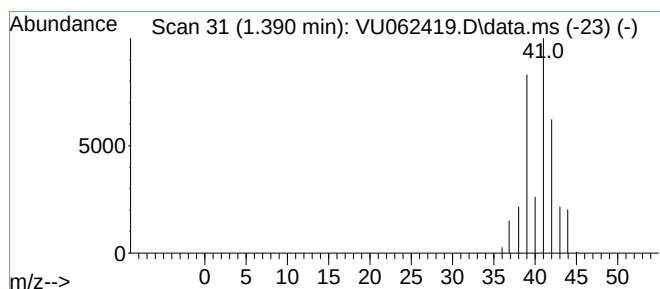
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
1.390	2.27 ug/L	99409	1,4-Difluorobenzene	6.312	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	90
2	Propene	42	C3H6	000115-07-1	42
3	Cyclopropane	42	C3H6	000075-19-4	40
4	Cyclopropene	40	C3H4	002781-85-3	10
5	2-Oxetanone, 4-methyl-	86	C4H6O2	003068-88-0	9



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ClientSampleId :
C0CF8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR120924WMA.M
Quant Title : TRACE VOA SFAM1.0

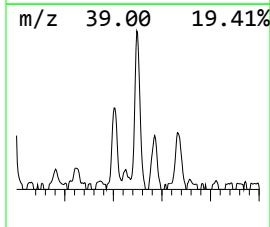
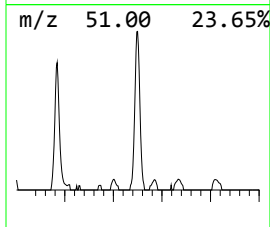
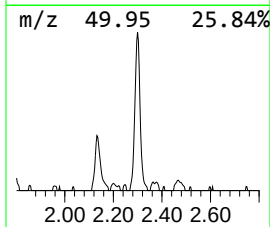
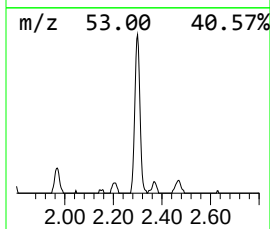
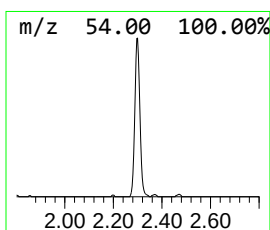
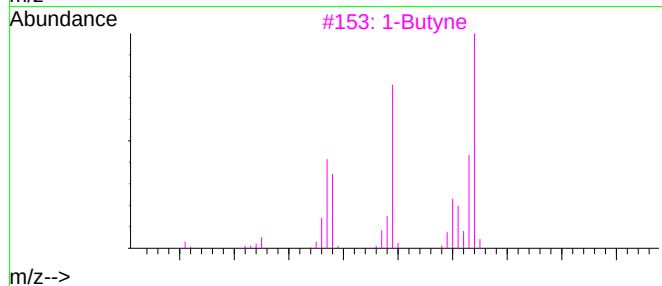
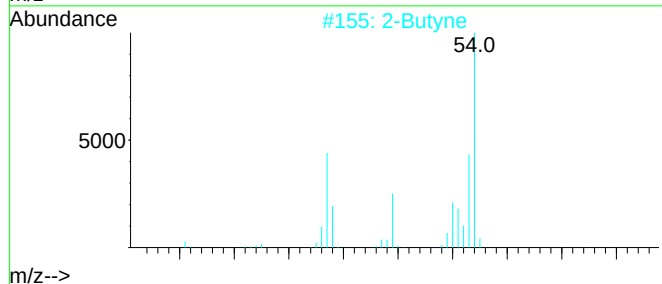
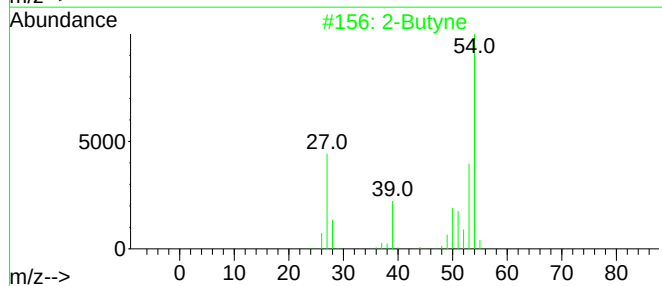
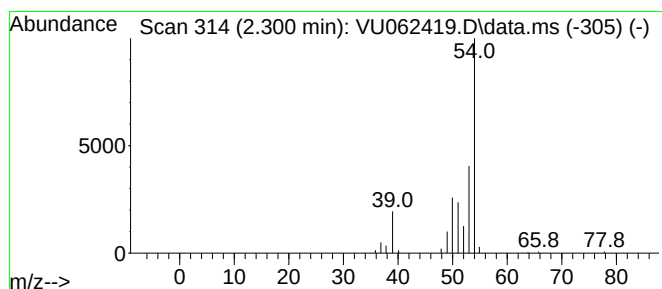
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Butyne Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.300	1.40 ug/L	61394	1,4-Difluorobenzene	6.312

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butyne	54	C4H6	000503-17-3	86
2	2-Butyne	54	C4H6	000503-17-3	86
3	1-Butyne	54	C4H6	000107-00-6	86
4	1,2-Butadiene	54	C4H6	000590-19-2	86
5	1,2-Butadiene	54	C4H6	000590-19-2	86



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Misc : 25mL/MSVOA_U/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
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ClientSampleId :
C0CF8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR120924WMA.M
Quant Title : TRACE VOA SFAM1.0

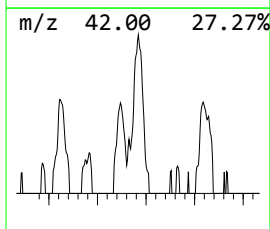
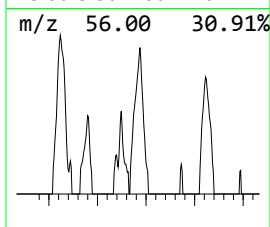
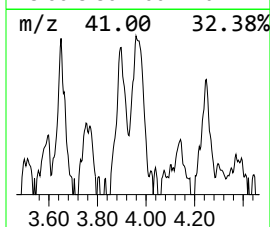
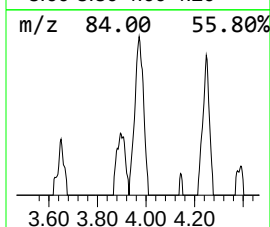
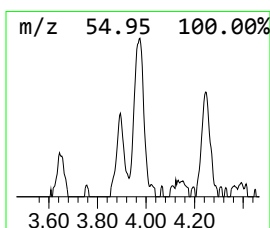
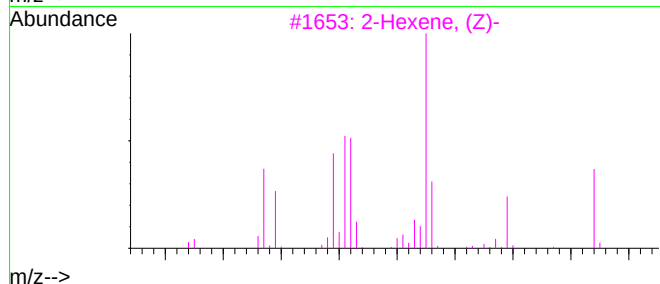
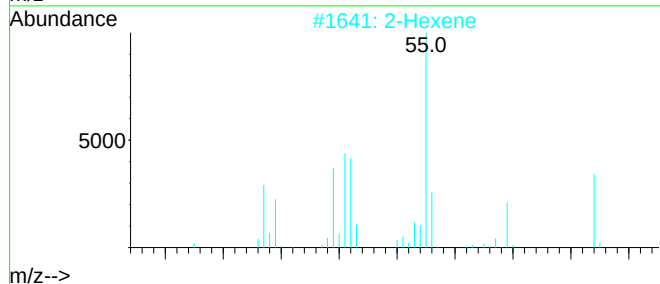
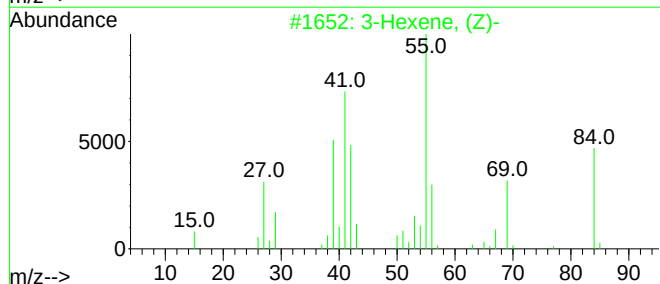
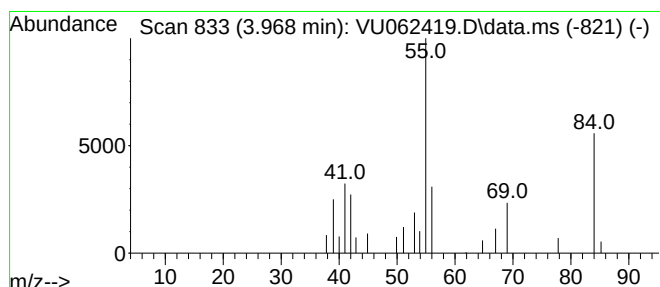
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.968	0.58 ug/L	25364	1,4-Difluorobenzene	6.312

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexene, (Z)-	84	C6H12	007642-09-3	87
2	2-Hexene	84	C6H12	000592-43-8	72
3	2-Hexene, (Z)-	84	C6H12	007688-21-3	72
4	3-Hexene, (Z)-	84	C6H12	007642-09-3	64
5	2-Hexene, (E)-	84	C6H12	004050-45-7	64



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR120924WMA.M
Quant Title : TRACE VOA SFAM1.0

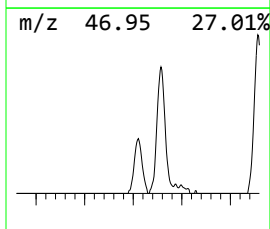
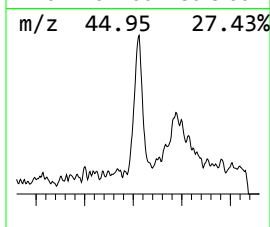
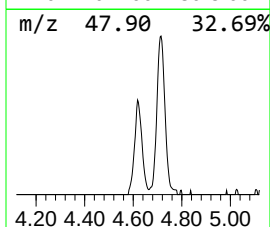
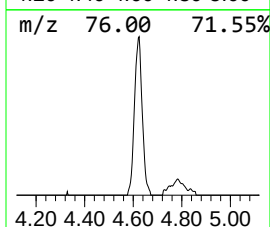
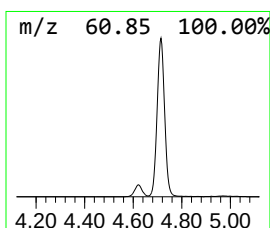
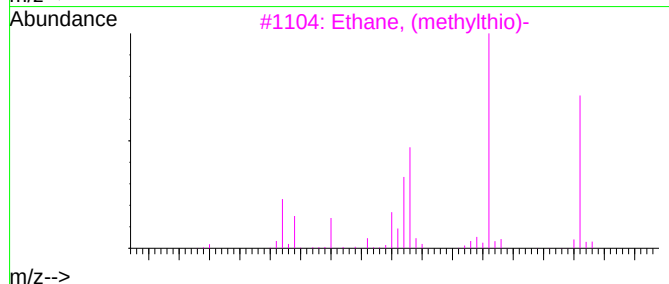
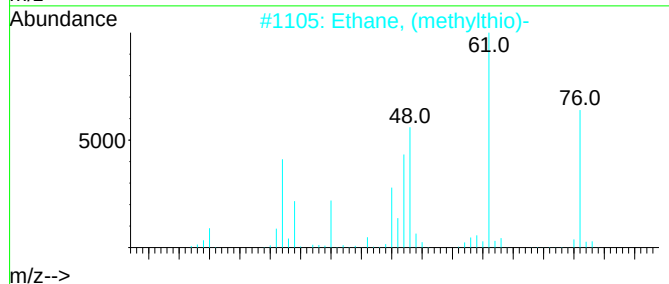
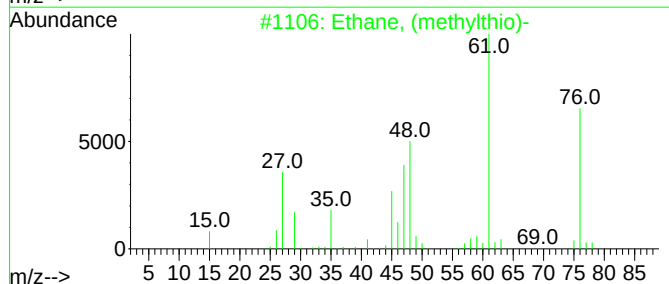
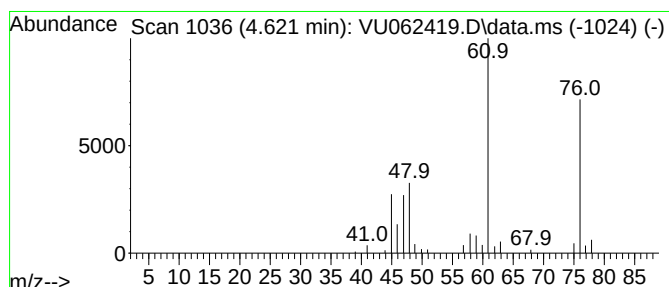
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 6 Ethane, (methylthio)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.621	1.05 ug/L	46085	1,4-Difluorobenzene	6.312

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethane, (methylthio)-	76	C3H8S	000624-89-5	90
2	Ethane, (methylthio)-	76	C3H8S	000624-89-5	90
3	Ethane, (methylthio)-	76	C3H8S	000624-89-5	90
4	Ethane, (methylthio)-	76	C3H8S	000624-89-5	87
5	Trimethylphosphine	76	C3H9P	000594-09-2	74



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR120924WMA.M
Quant Title : TRACE VOA SFAM1.0

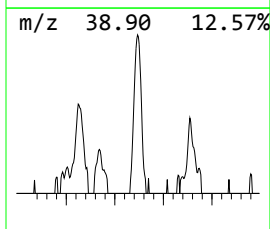
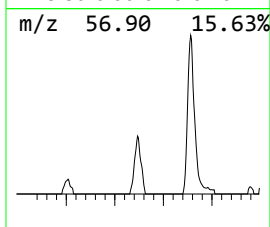
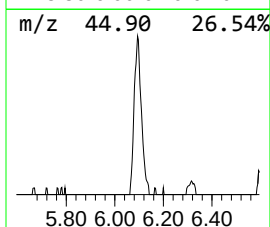
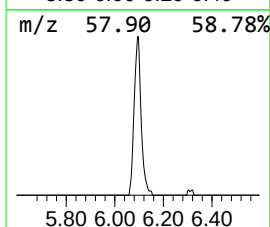
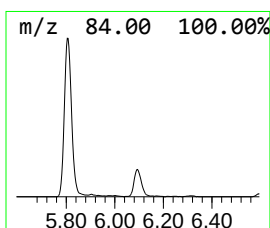
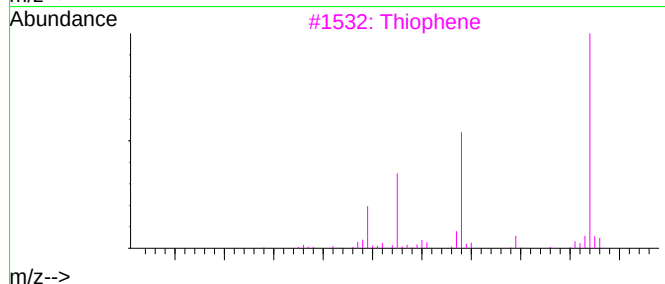
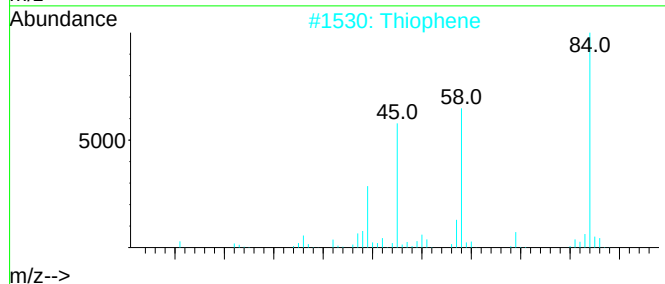
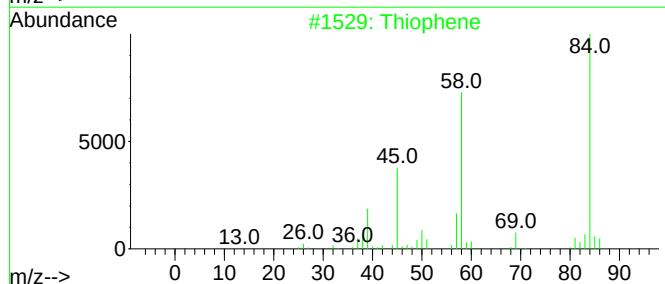
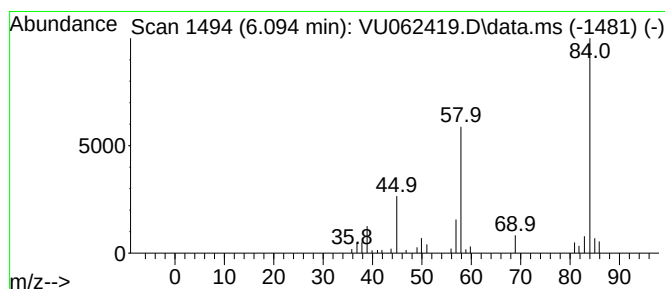
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 7 Thiophene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.094	1.26 ug/L	55091	1,4-Difluorobenzene	6.312

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene	84	C4H4S	000110-02-1	91
2	Thiophene	84	C4H4S	000110-02-1	91
3	Thiophene	84	C4H4S	000110-02-1	87
4	Thiophene	84	C4H4S	000110-02-1	83
5	4H-1,2,4-Triazol-4-amine	84	C2H4N4	000584-13-4	37



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121724\
Data File : VU062419.D
Acq On : 18 Dec 2024 05:09
Operator : MD/SY
Sample : P5309-07
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0CF8

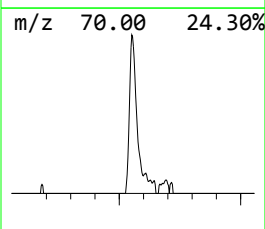
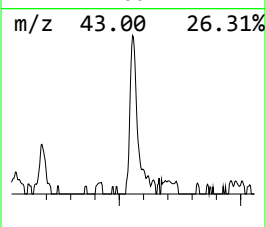
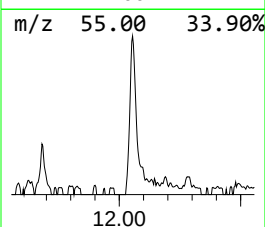
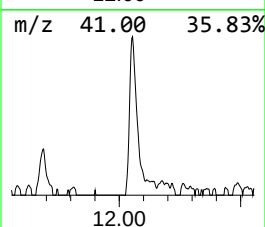
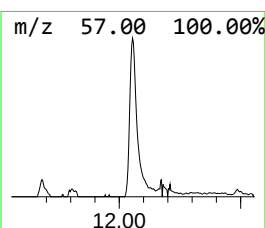
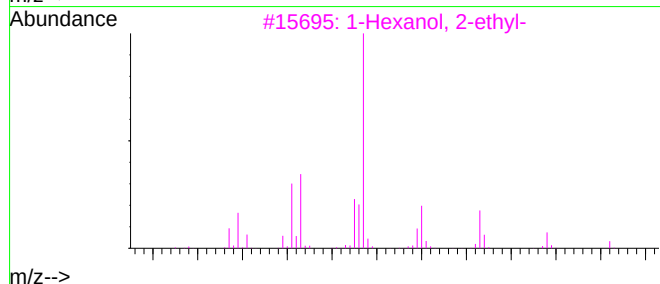
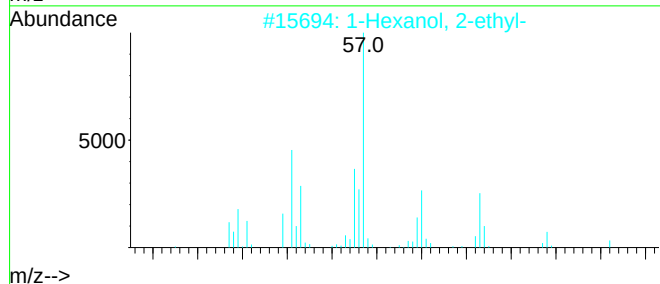
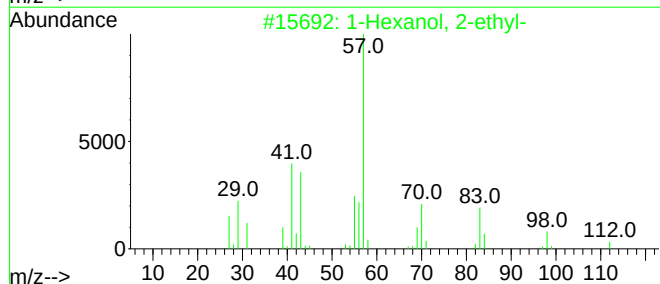
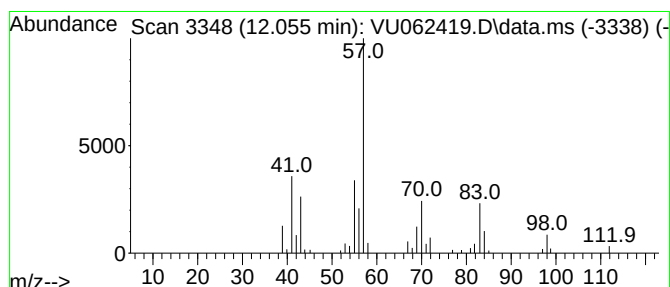
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.055	1.27 ug/L	69899	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121724\
Data File : VU062419.D
Acq On : 18 Dec 2024 05:09
Operator : MD/SY
Sample : P5309-07
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0CF8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR120924WMA.M
Quant Title : TRACE VOA SFAM1.0

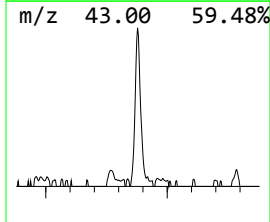
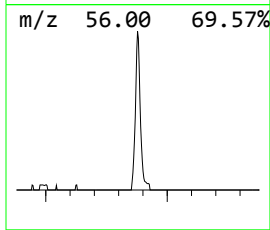
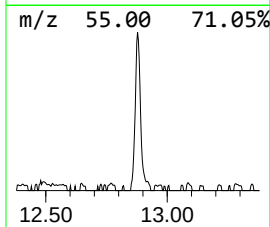
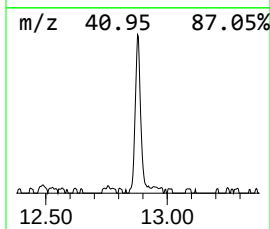
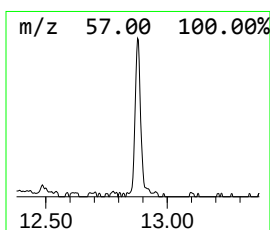
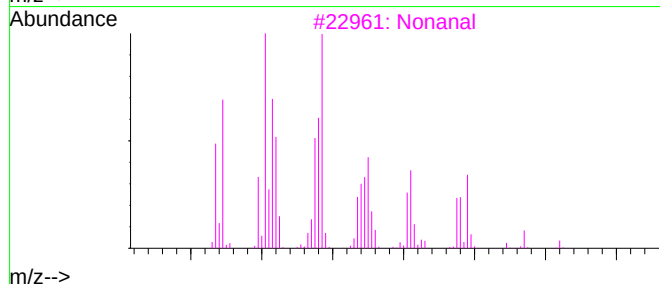
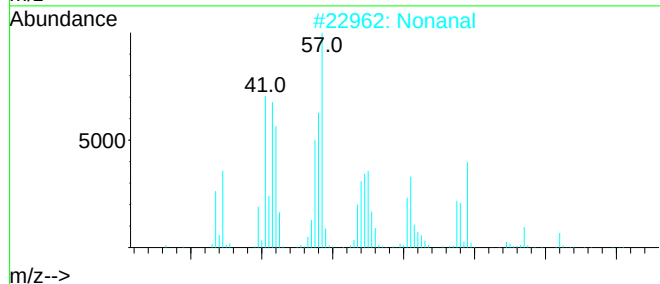
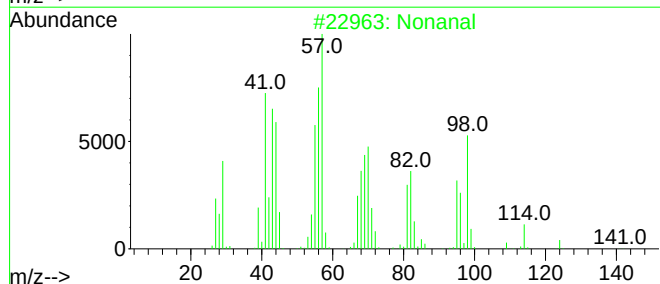
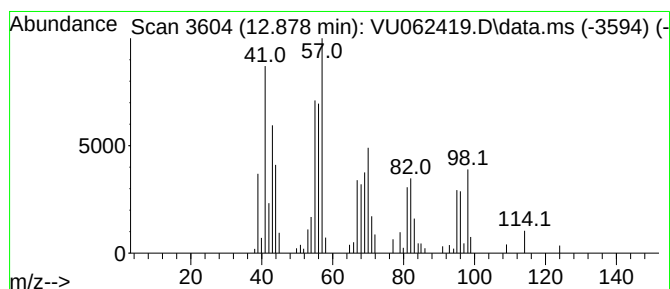
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 10 Nonanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.878	1.44 ug/L	78834	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanal	142	C9H18O	000124-19-6	87
2	Nonanal	142	C9H18O	000124-19-6	80
3	Nonanal	142	C9H18O	000124-19-6	80
4	Cycloheptane	98	C7H14	000291-64-5	43
5	Cycloheptane	98	C7H14	000291-64-5	41



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121724\
Data File : VU062419.D
Acq On : 18 Dec 2024 05:09
Operator : MD/SY
Sample : P5309-07
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0CF8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR120924WMA.M
Quant Title : TRACE VOA SFAM1.0

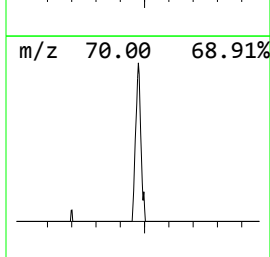
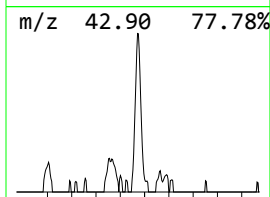
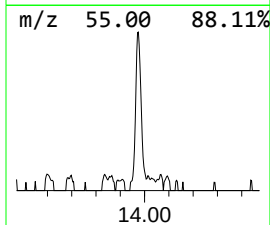
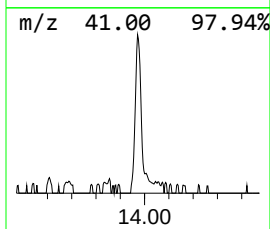
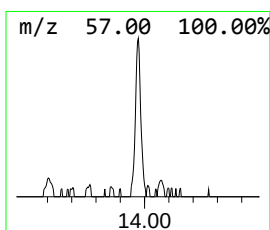
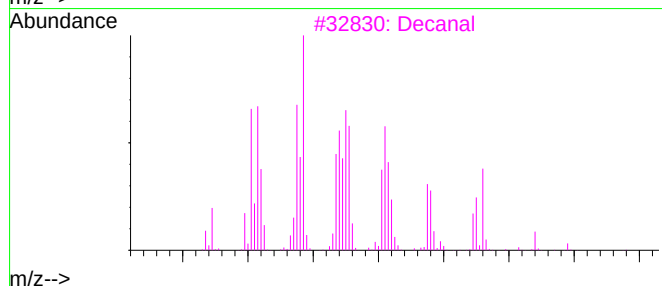
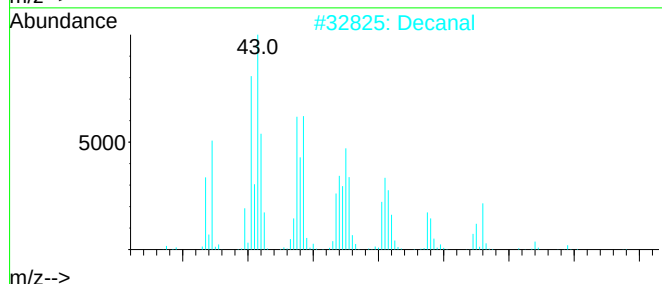
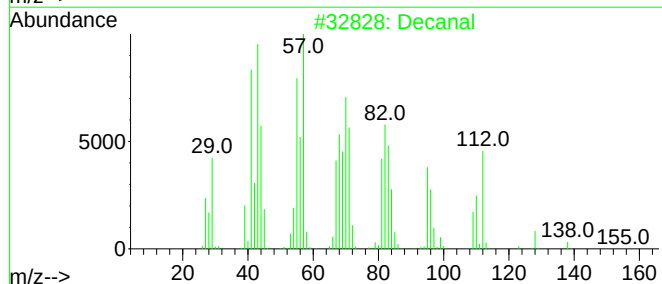
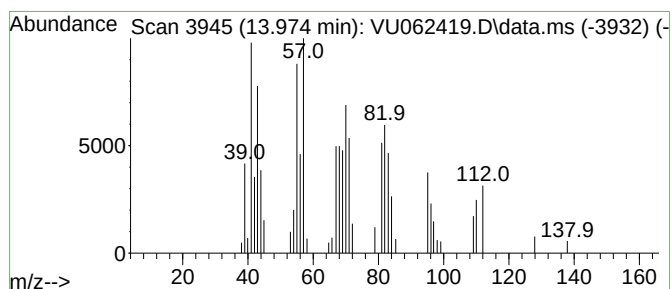
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 11 Decanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.974	0.79 ug/L	43588	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanal	156	C10H20O	000112-31-2	91
2	Decanal	156	C10H20O	000112-31-2	91
3	Decanal	156	C10H20O	000112-31-2	91
4	Decanal	156	C10H20O	000112-31-2	87
5	Decanal	156	C10H20O	000112-31-2	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121724\
Data File : VU062419.D
Acq On : 18 Dec 2024 05:09
Operator : MD/SY
Sample : P5309-07
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 49 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0CF8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR120924WMA.M
Quant Title : TRACE VOA SFAM1.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	1.390	2.3	ug/L	99409	1	6.312	219004	5.0
2-Butyne	2.300	1.4	ug/L	61394	1	6.312	219004	5.0
(DEL) Alkane: S...	3.968	0.6	ug/L	25364	1	6.312	219004	5.0
Ethane, (methyl...	4.621	1.1	ug/L	46085	1	6.312	219004	5.0
Thiophene	6.094	1.3	ug/L	55091	1	6.312	219004	5.0
1-Hexanol, 2-et...	12.055	1.3	ug/L	69899	3	11.807	274366	5.0
Nonanal	12.878	1.4	ug/L	78834	3	11.807	274366	5.0
Decanal	13.974	0.8	ug/L	43588	3	11.807	274366	5.0