LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070824\
Data File : VU059885.D
Acq On : 08 Jul 2024 15:55
Operator : MD/SY
Sample : P3137-18DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
YDZG7DL

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\SFAMUTR061724WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VU059885.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.358	15	21	31	rBV3	8978	11616	1.85%	0.115%
2	1.599	84	96	109	rBV2	234104	317173	50.51%	3.136%
3	1.653	110	113	119	rVB	7895	7463	1.19%	0.074%
4	1.727	131	136	143	rVB2	6451	7057	1.12%	0.070%
5	1.907	183	192	208	rBV	51341	73204	11.66%	0.724%
6	2.457	357	363	373	rVB2	7016	11275	1.80%	0.111%
7	2.557	382	394	408	rBV	91723	149671	23.83%	1.480%
8	2.641	411	420	429	rBV	4292	8784	1.40%	0.087%
9	2.788	456	466	479	rBV2	4465	7301	1.16%	0.072%
10	3.039	532	544	558	rBV2	24088	47495	7.56%	0.470%
11	3.206	581	596	597	rBV2	9615	15898	2.53%	0.157%
12	3.348	629	640	654	rVB3	12847	27168	4.33%	0.269%
13	3.859	783	799	821	rBV	127657	306598	48.82%	3.031%
14	4.657	1015	1047	1075	rBV2	139682	471463	75.07%	4.662%
15	5.055	1150	1171	1199	rBV	98710	227032	36.15%	2.245%
16	5.718	1357	1377	1407	rBV2	189347	513420	81.76%	5.076%
17	5.965	1444	1454	1470	rBV7	4602	9297	1.48%	0.092%
18	6.242	1525	1540	1564	rBV	195943	379930	60.50%	3.757%
19	6.538	1620	1632	1653	rBV3	58870	116574	18.56%	1.153%
20	6.682	1664	1677	1698	rBV	121263	239966	38.21%	2.373%
21	6.994	1763	1774	1788	rBV6	9074	20400	3.25%	0.202%
22	7.161	1814	1826	1846	rVB4	7460	16275	2.59%	0.161%
23	7.566	1937	1952	1972	rBV3	128683	259201	41.27%	2.563%
24	7.711	1985	1997	2007	rVB3	8848	16247	2.59%	0.161%
25	7.894	2041	2054	2071	rBV	224006	396988	63.22%	3.925%
26	7.968	2071	2077	2090	rVB2	6541	12264	1.95%	0.121%
27	8.177	2127	2142	2161	rVB	34769	61822	9.84%	0.611%
28	8.306	2168	2182	2199	rBV	242276	417496	66.48%	4.128%
29	8.480	2223	2236	2250	rBV	65119	115097	18.33%	1.138%
30	8.627	2267	2282	2303	rBV	305697	575398	91.63%	5.689%
31	9.084	2412	2424	2439	rBV2	38205	68797	10.96%	0.680%
32	9.190	2445	2457	2471	rBV2	64248	105303	16.77%	1.041%
33	9.328	2490	2500	2514	rVV9	9647	19542	3.11%	0.193%
34	9.412	2514	2526	2553	rBV	303491	514707	81.96%	5.089%
35	9.570	2565	2575	2581	rBV	8101	12808	2.04%	0.127%
36	9.820	2642	2653	2661	rBV8	6162	11188	1.78%	0.111%

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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
YDZG7DL

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\SFAMUTR061724WMA.M
Title : TRACE VOA SFAM1.0

37	9.875	2661	2670	2684	rVB2	72953	118114	18.81%	1.168%
38	9.981	2686	2703	2716	rBV4	49196	103683	16.51%	1.025%
39	10.071	2720	2731	2739	rBV5	6019	12239	1.95%	0.121%
40	10.270	2783	2793	2802	rBV8	7651	14014	2.23%	0.139%
41	10.332	2802	2812	2835	rVV5	35208	90674	14.44%	0.897%
42	10.496	2845	2863	2874	rBV	265051	452406	72.04%	4.473%
43	10.602	2884	2896	2900	rBV2	8572	13685	2.18%	0.135%
44	10.640	2900	2908	2928	rVB3	35910	65161	10.38%	0.644%
45	10.750	2928	2942	2963	rVB	113592	191659	30.52%	1.895%
46	10.888	2977	2985	2992	rBV6	9364	14997	2.39%	0.148%
47	10.926	2992	2997	3006	rVB5	6955	11162	1.78%	0.110%
48	11.007	3013	3022	3033	rVB2	17683	28862	4.60%	0.285%
49	11.084	3033	3046	3063	rBV4	31625	62945	10.02%	0.622%
50	11.248	3079	3097	3112	rBV9	26295	75829	12.07%	0.750%
51	11.319	3114	3119	3130	rVB8	10753	15221	2.42%	0.150%
52	11.396	3133	3143	3153	rBV10	4820	8611	1.37%	0.085%
53	11.496	3162	3174	3184	rBV3	56907	97548	15.53%	0.964%
54	11.557	3184	3193	3208	rVV4	32289	60033	9.56%	0.594%
55	11.650	3208	3222	3238	rVV2	119727	243363	38.75%	2.406%
56	11.730	3239	3247	3254	rVV7	17849	34916	5.56%	0.345%
57	11.807	3254	3271	3289	rVB	329177	627990	100.00%	6.209%
58	11.907	3293	3302	3309	rBV8	18402	29010	4.62%	0.287%
59	11.968	3311	3321	3325	rVV2	33088	55454	8.83%	0.548%
60	12.013	3325	3335	3348	rVB5	109088	241220	38.41%	2.385%
61	12.148	3366	3377	3382	rBV	124957	199350	31.74%	1.971%
62	12.187	3382	3389	3412	rVB	247490	511841	81.50%	5.061%
63	12.309	3412	3427	3433	rBV5	50375	101714	16.20%	1.006%
64	12.357	3434	3442	3454	rVB7	46513	105224	16.76%	1.040%
65	12.438	3454	3467	3480	rBV3	35028	71312	11.36%	0.705%
66	12.557	3492	3504	3513	rBV8	15487	39232	6.25%	0.388%
67	12.624	3515	3525	3536	rVB5	43760	77762	12.38%	0.769%
68	12.695	3544	3547	3561	rVB5	7831	14231	2.27%	0.141%
69	12.769	3563	3570	3576	rBV7	5940	8234	1.31%	0.081%
70	12.817	3576	3585	3601	rVB3	49634	87064	13.86%	0.861%
71	12.942	3604	3624	3633	rBV5	29014	71353	11.36%	0.705%
72	13.084	3658	3668	3677	rVV7	23317	41842	6.66%	0.414%
73	13.296	3727	3734	3742	rVB5	18239	28035	4.46%	0.277%
74	13.466	3777	3787	3797	rBV7	5549	10127	1.61%	0.100%
75	13.614	3817	3833	3840	rBV7	17136	40061	6.38%	0.396%
76	13.730	3861	3869	3879	rVB9	13606	23729	3.78%	0.235%

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ClientSampleId :
YDZG7DL

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
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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Title : TRACE VOA SFAM1.0

77	13.891	3911	3919	3927	rBV4	16771	26811	4.27%	0.265%
78	14.013	3952	3957	3969	rVB10	7926	12723	2.03%	0.126%
79	14.110	3979	3987	3993	rBV4	14191	20887	3.33%	0.207%
80	14.155	3993	4001	4021	rVB4	41298	77239	12.30%	0.764%
81	14.241	4022	4028	4033	rBV4	6060	8338	1.33%	0.082%
82	14.347	4051	4061	4070	rBV3	37212	58953	9.39%	0.583%
83	14.486	4094	4104	4118	rVB3	7355	17009	2.71%	0.168%
84	14.576	4121	4132	4142	rBV2	63170	110531	17.60%	1.093%
85	14.901	4224	4233	4236	rBV9	4345	7701	1.23%	0.076%
86	15.032	4266	4274	4286	rVB10	7755	13494	2.15%	0.133%
87	15.470	4401	4410	4417	rVB	6833	10950	1.74%	0.108%
88	15.518	4417	4425	4431	rBV4	14690	20227	3.22%	0.200%
89	15.563	4431	4439	4450	rVB4	29397	49424	7.87%	0.489%
90	15.688	4468	4478	4486	rBV4	3671	7770	1.24%	0.077%

Sum of corrected areas: 10113882

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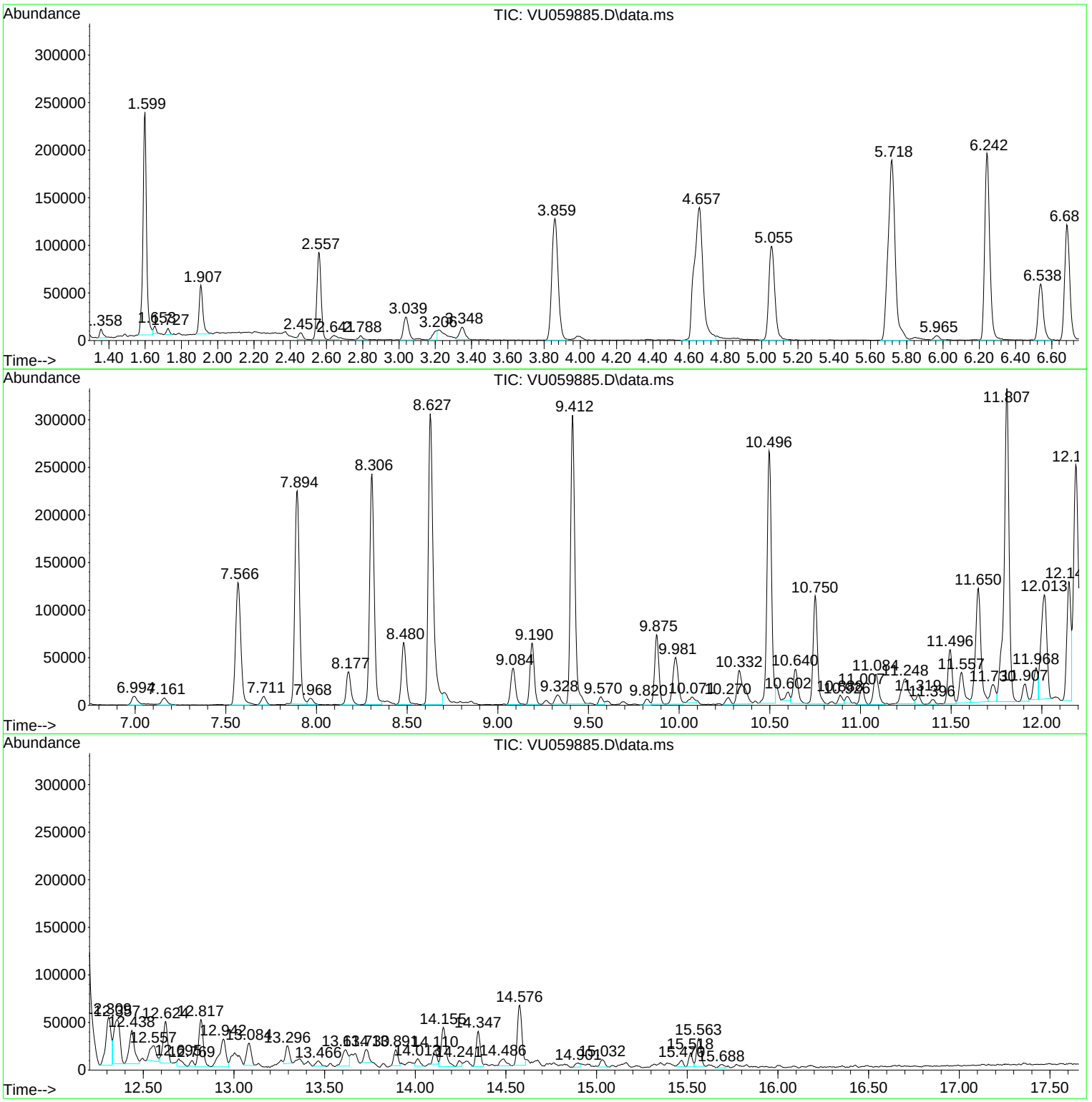
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
YDZG7DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070824\
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Instrument :
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ClientSampleId :
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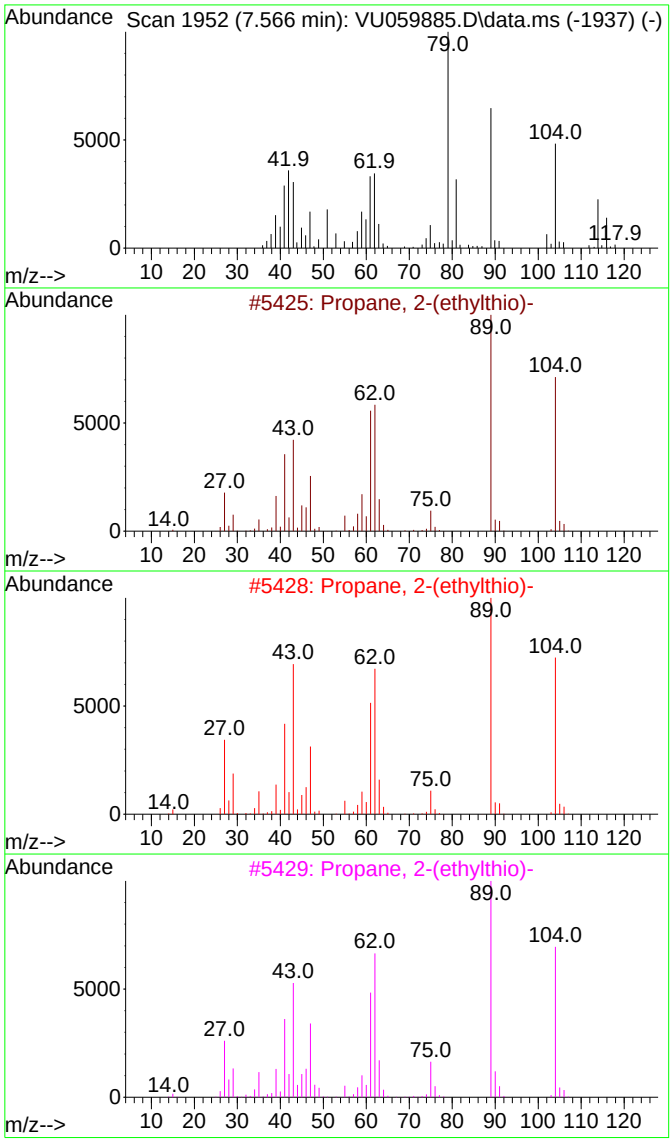
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

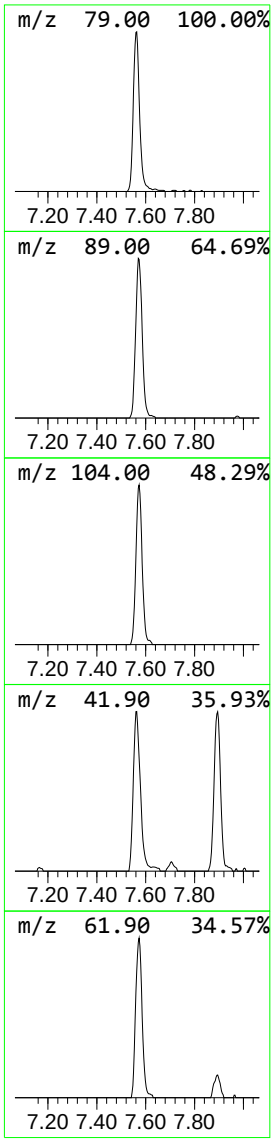
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Propane, 2-(ethylthio)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.566	3.41 ug/L	259201	1,4-Difluorobenzene	6.242

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-(ethylthio)-	104	C5H12S	005145-99-3	92
2	Propane, 2-(ethylthio)-	104	C5H12S	005145-99-3	90
3	Propane, 2-(ethylthio)-	104	C5H12S	005145-99-3	37
4	Thiophosgene	114	CCl2S	000463-71-8	25
5	Ethanethiol	62	C2H6S	000075-08-1	14





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Acq On : 08 Jul 2024 15:55
Operator : MD/SY
Sample : P3137-18DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
YDZG7DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

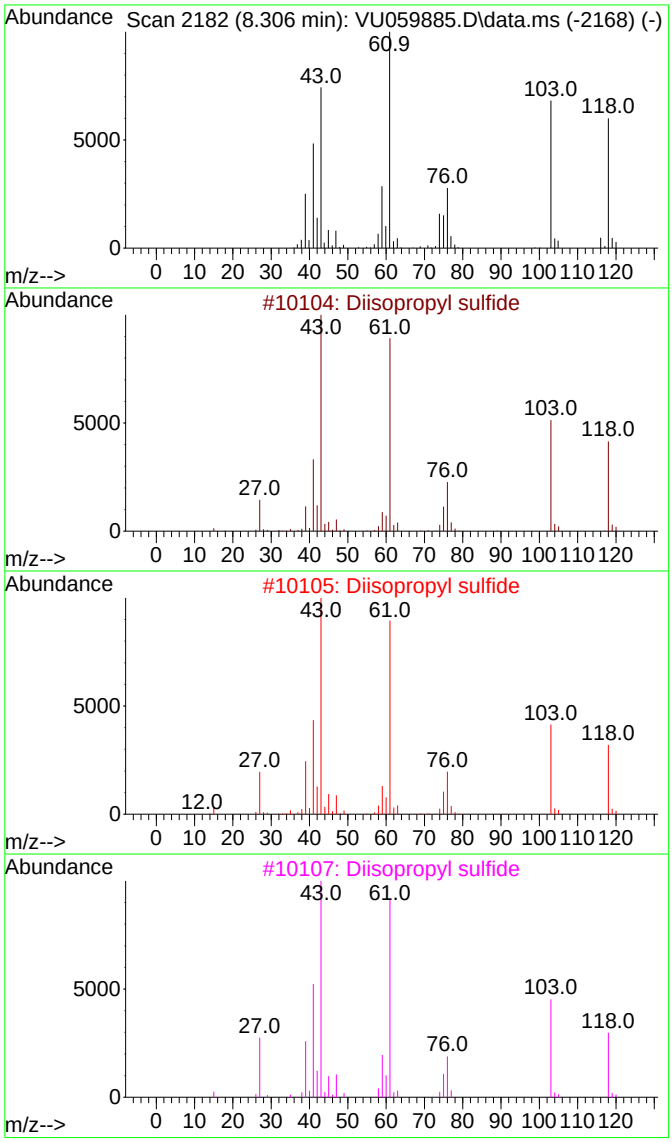
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

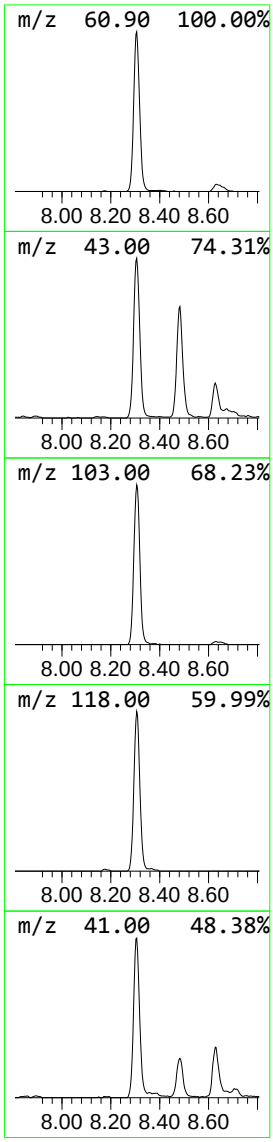
****

Peak Number 2 Diisopropyl sulfide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.306	4.06 ug/L	417496	Chlorobenzene-d5	9.412

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diisopropyl sulfide	118	C6H14S	000625-80-9	93
2	Diisopropyl sulfide	118	C6H14S	000625-80-9	90
3	Diisopropyl sulfide	118	C6H14S	000625-80-9	90
4	Diisopropyl sulfide	118	C6H14S	000625-80-9	78
5	Ethanethioic acid, S-(1-methylet...	118	C5H10OS	000926-73-8	30





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ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
YDZG7DL

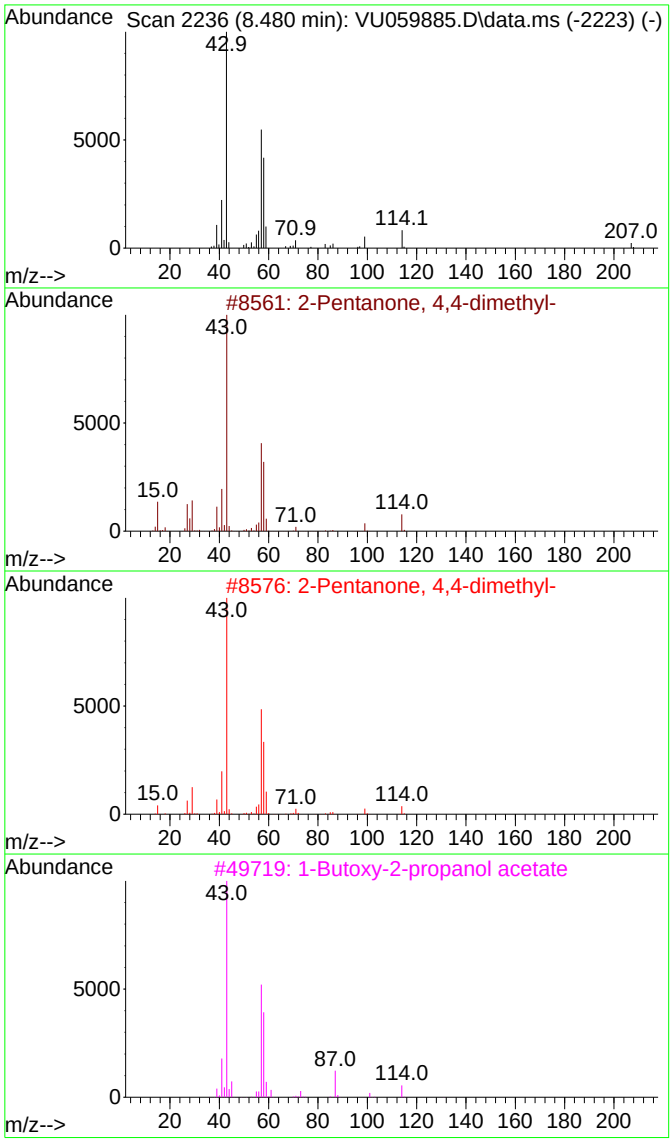
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

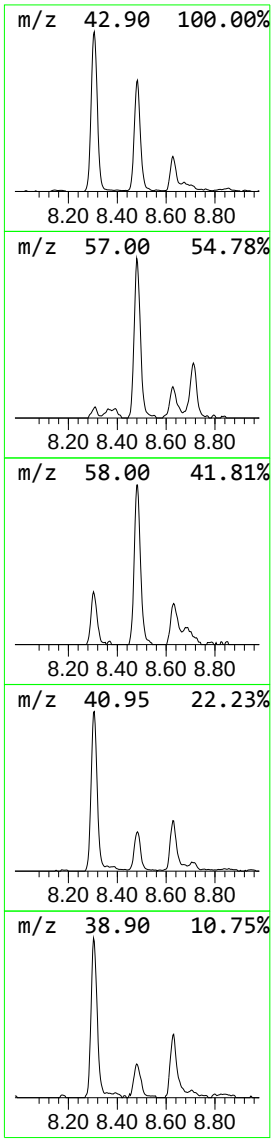
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.480	1.12 ug/L	115097	Chlorobenzene-d5	9.412

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	90
2	2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	87
3	1-Butoxy-2-propanol acetate	174	C9H18O3	085409-76-3	72
4	2-Heptanone	114	C7H14O	000110-43-0	72
5	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	64





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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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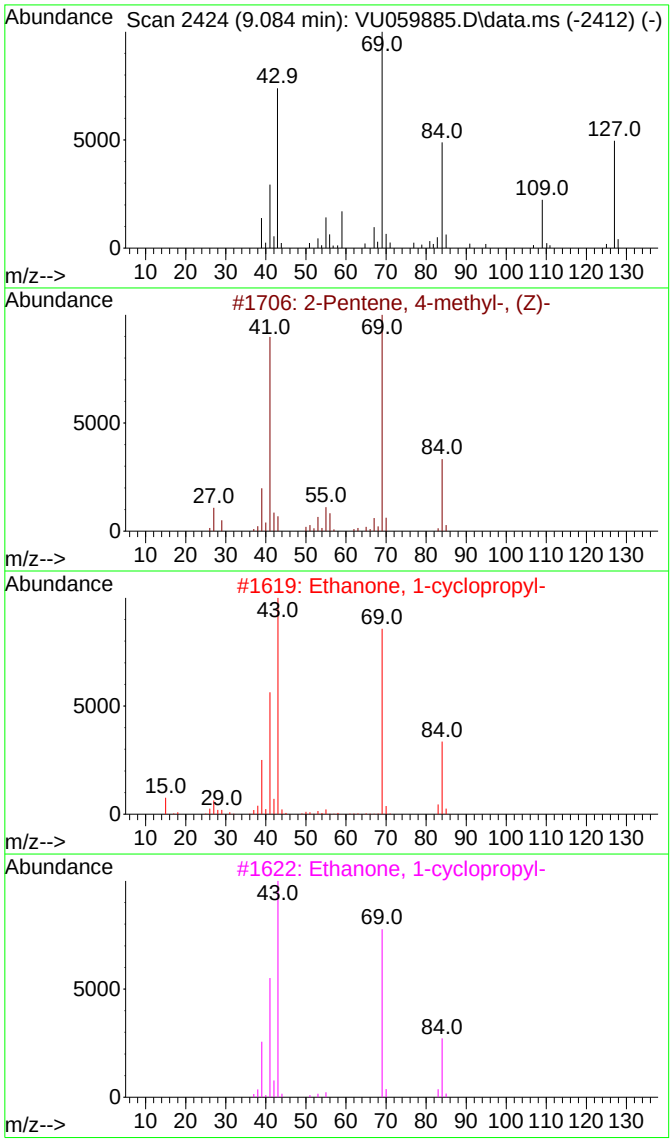
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

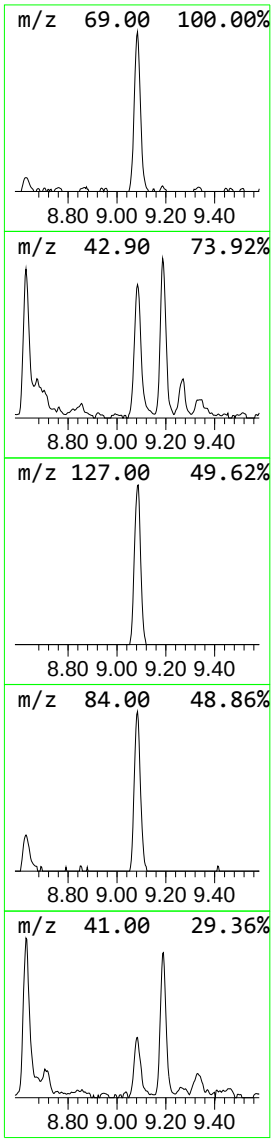
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.084	0.67 ug/L	68797	Chlorobenzene-d5	9.412

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, 4-methyl-, (Z)-	84	C6H12	000691-38-3	49
2	Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	47
3	Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	47
4	Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	43
5	1H-Pyrazole, 4,5-dihydro-5-methyl-	84	C4H8N2	001568-20-3	38





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ALS Vial : 16 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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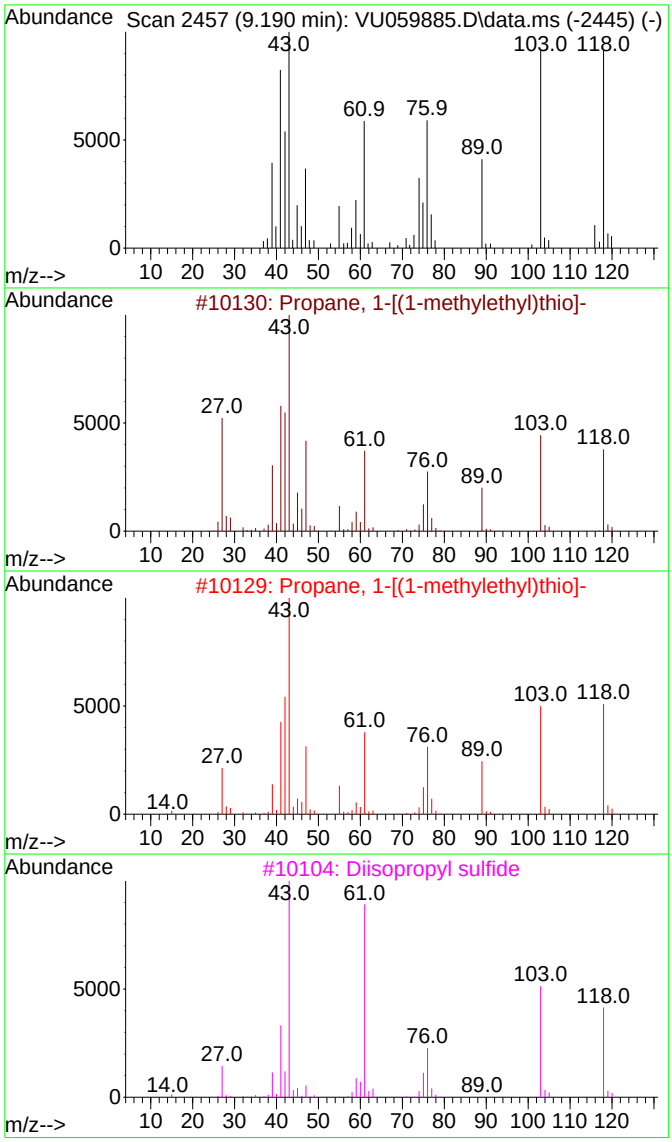
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

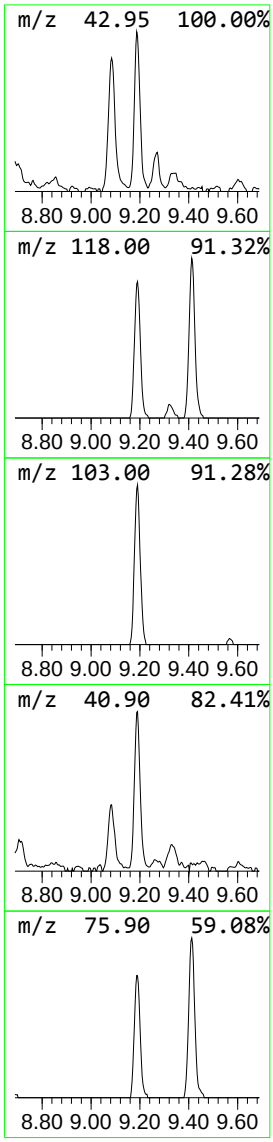
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Propane, 1-[(1-methylethyl)... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.190	1.02 ug/L	105303	Chlorobenzene-d5	9.412

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1-[(1-methylethyl)thio]-	118	C6H14S	005008-73-1	96
2	Propane, 1-[(1-methylethyl)thio]-	118	C6H14S	005008-73-1	96
3	Diisopropyl sulfide	118	C6H14S	000625-80-9	52
4	Diisopropyl sulfide	118	C6H14S	000625-80-9	49
5	Acetamide, N-(aminothioxomethyl)-	118	C3H6N2OS	000591-08-2	43





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ClientSampleId :
YDZG7DL

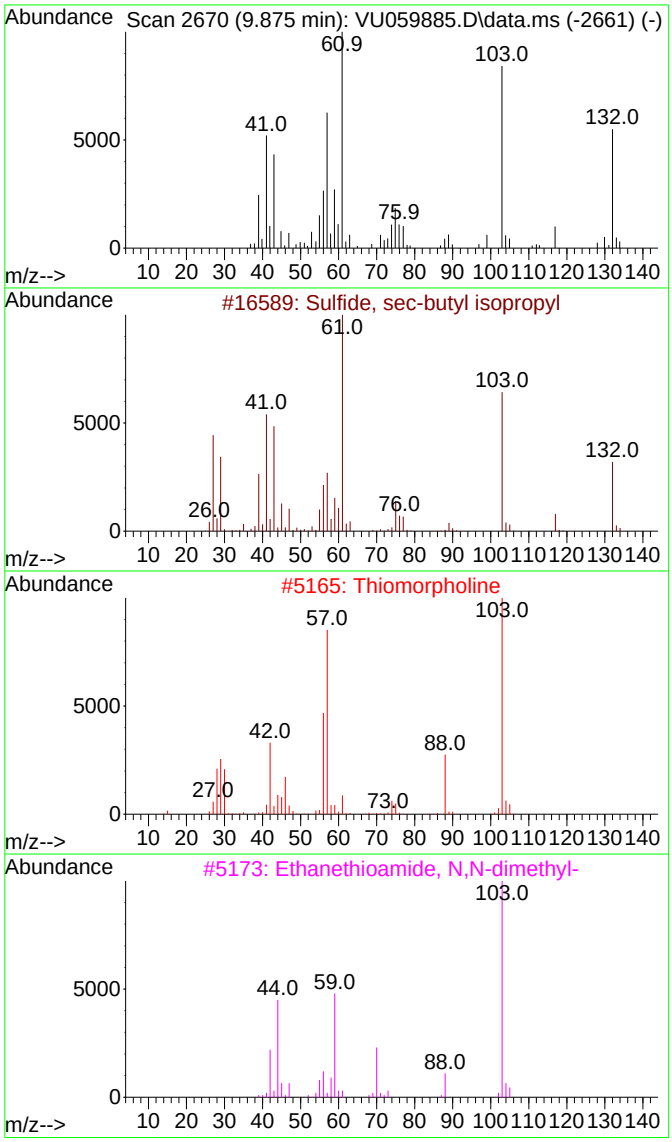
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

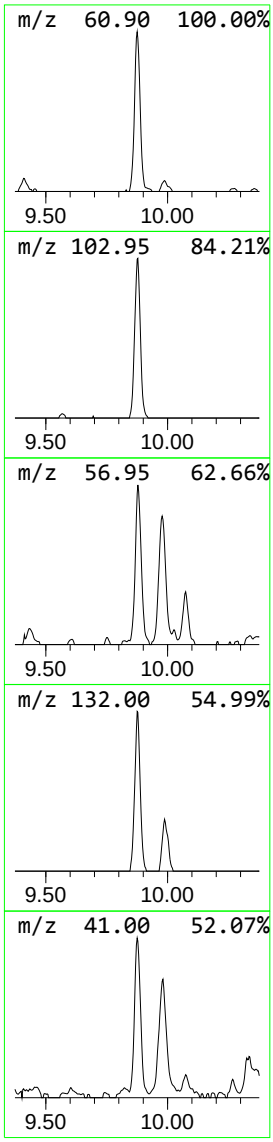
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Sulfide, sec-butyl isopropyl Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.875	1.15 ug/L	118114	Chlorobenzene-d5	9.412

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfide, sec-butyl isopropyl	132	C7H16S	022438-36-4	87
2	Thiomorpholine	103	C4H9NS	000123-90-0	27
3	Ethanethioamide, N,N-dimethyl-	103	C4H9NS	000631-67-4	27
4	Propane, 2,2-bis(ethylthio)-	164	C7H16S2	014252-45-0	22
5	Ethanol, TMS derivative	118	C5H14OSi	001825-62-3	16





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Data File : VU059885.D
Acq On : 08 Jul 2024 15:55
Operator : MD/SY
Sample : P3137-18DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
YDZG7DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

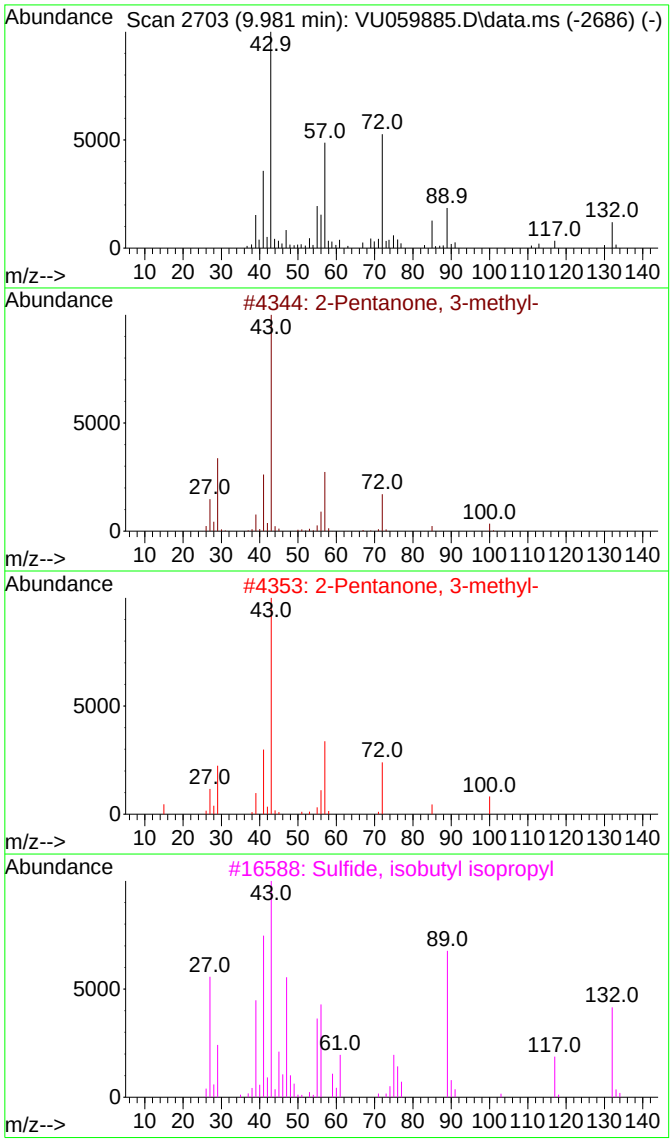
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

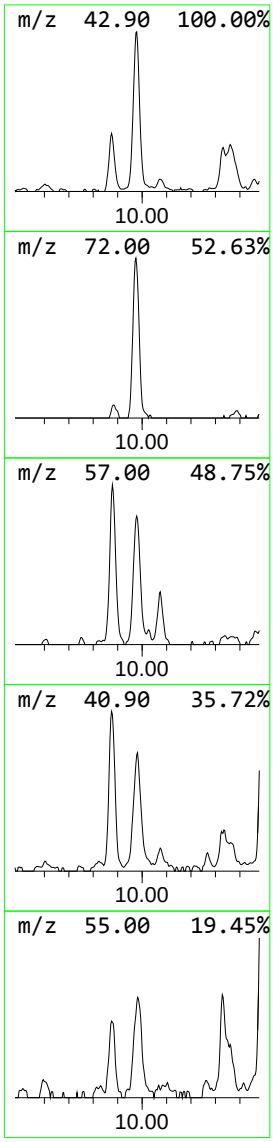
****

Peak Number 7 unknown-01 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.981	1.01 ug/L	103683	Chlorobenzene-d5	9.412

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	43
2	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	43
3	Sulfide, isobutyl isopropyl	132	C7H16S	010359-65-6	38
4	3,5-Dimethyl-2-octanone	156	C10H20O	019781-14-7	37
5	2-Hexanone, 3,4-dimethyl-	128	C8H16O	019550-10-8	37





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Data File : VU059885.D
Acq On : 08 Jul 2024 15:55
Operator : MD/SY
Sample : P3137-18DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
YDZG7DL

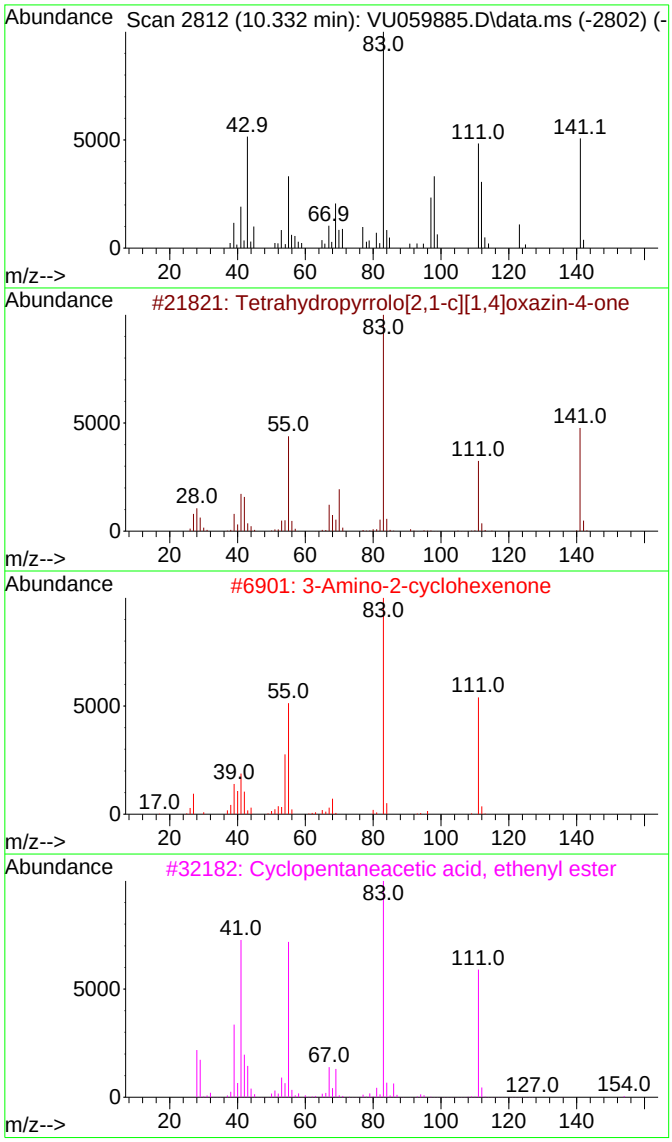
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

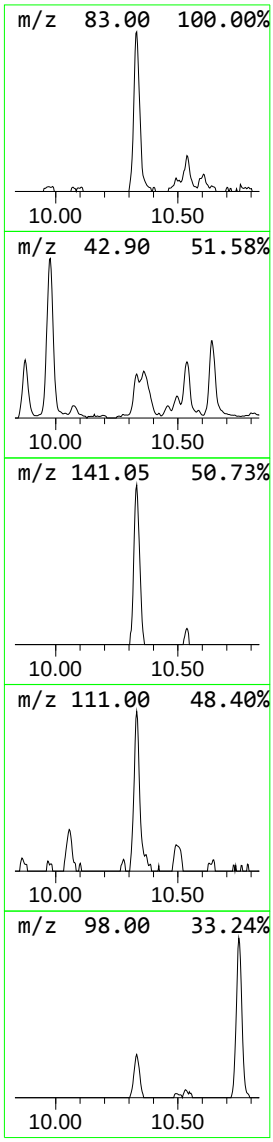
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Tetrahydropyrrolo[2,1-c][1,... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.332	0.88 ug/L	90674	Chlorobenzene-d5	9.412

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetrahydropyrrolo[2,1-c][1,4]oxa...	141	C7H11NO2	101250-37-7	50
2	3-Amino-2-cyclohexenone	111	C6H9NO	005220-49-5	43
3	Cyclopentaneacetic acid, ethenyl...	154	C9H14O2	045955-66-6	38
4	trans-4,4-Dimethyl-2-hexene	112	C8H16	019550-83-5	35
5	2-Pyrazoline, 4-ethyl-1-methyl-	112	C6H12N2	022581-42-6	35





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Data File : VU059885.D
Acq On : 08 Jul 2024 15:55
Operator : MD/SY
Sample : P3137-18DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
YDZG7DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

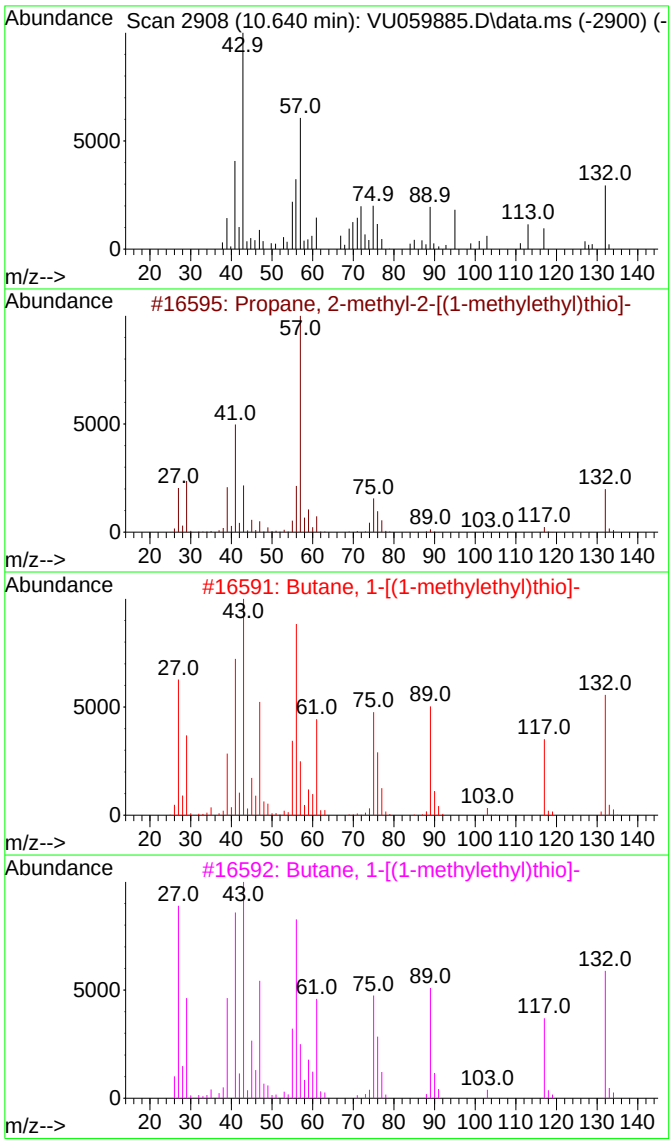
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

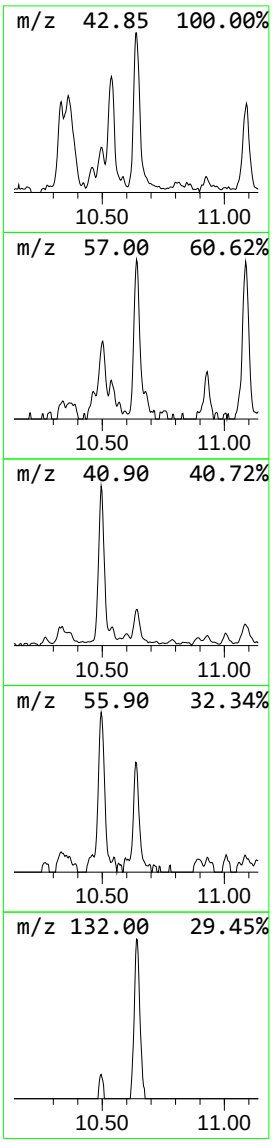
****

Peak Number 10 unknown-02 Concentration Rank 22

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.640	0.52 ug/L	65161	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-methyl-2-[(1-methylet...	132	C7H16S	044657-76-3	38
2	Butane, 1-[(1-methylethyl)thio]-	132	C7H16S	007309-43-5	37
3	Butane, 1-[(1-methylethyl)thio]-	132	C7H16S	007309-43-5	37
4	Butane, 1-(propylthio)-	132	C7H16S	001613-46-3	25
5	t-Butyl n-propyl sulfide	132	C7H16S	1000343-63-5	25





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Data File : VU059885.D
Acq On : 08 Jul 2024 15:55
Operator : MD/SY
Sample : P3137-18DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
YDZG7DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

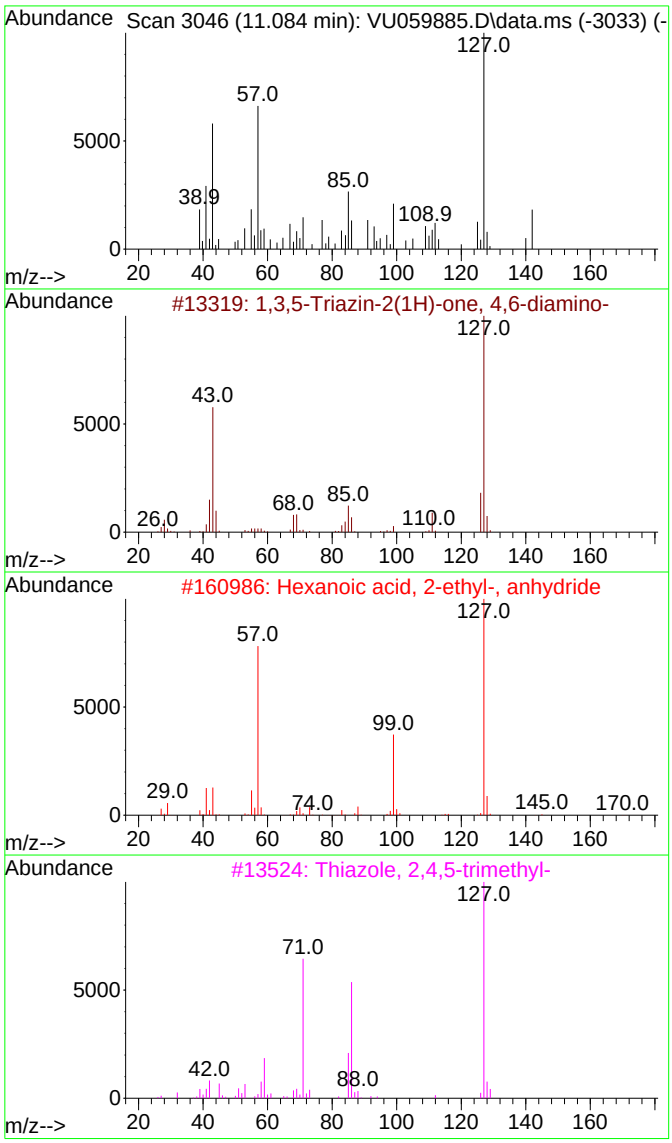
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

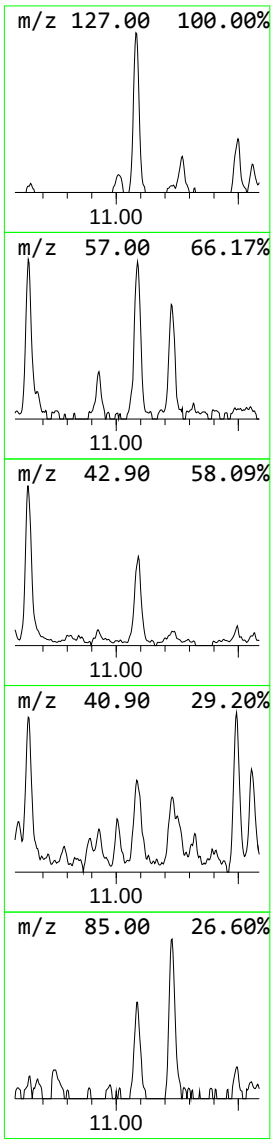
****

Peak Number 11 unknown-03 Concentration Rank 23

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.084	0.50 ug/L	62945	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazin-2(1H)-one, 4,6-dia...	127	C3H5N5O	000645-92-1	43
2	Hexanoic acid, 2-ethyl-, anhydride	270	C16H30O3	036765-89-6	43
3	Thiazole, 2,4,5-trimethyl-	127	C6H9NS	013623-11-5	43
4	2-Fluoro-5-methoxypyridine	127	C6H6FNO	136888-79-4	38
5	1,3,5-Triazin-2(1H)-one, 4,6-dia...	127	C3H5N5O	000645-92-1	38





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Data File : VU059885.D
Acq On : 08 Jul 2024 15:55
Operator : MD/SY
Sample : P3137-18DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
YDZG7DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

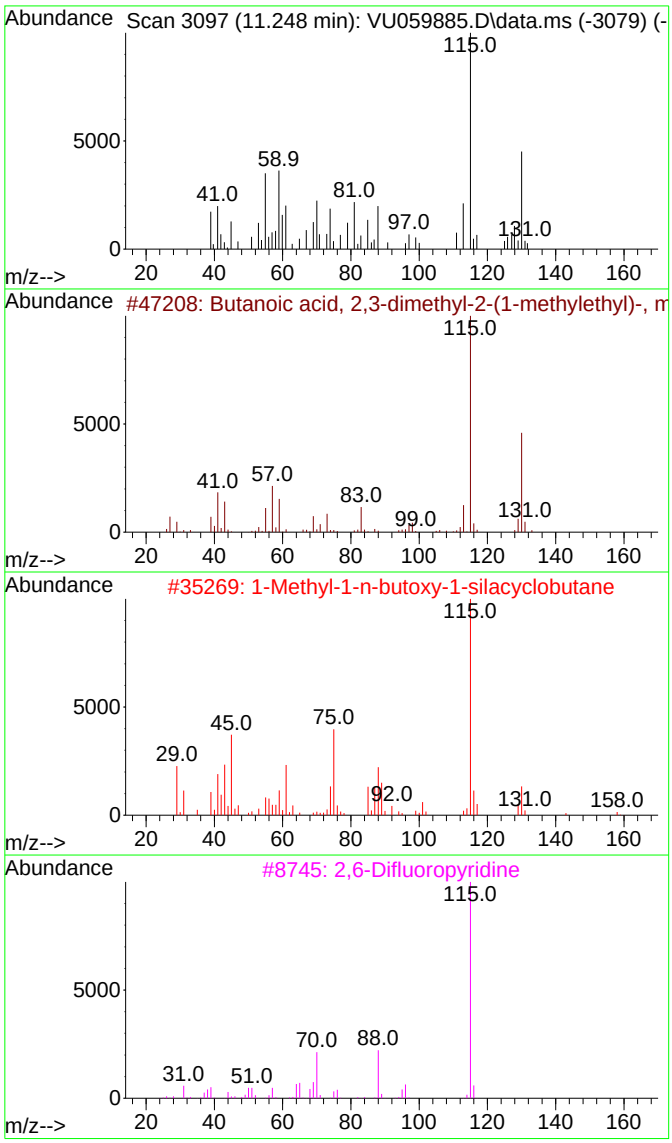
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

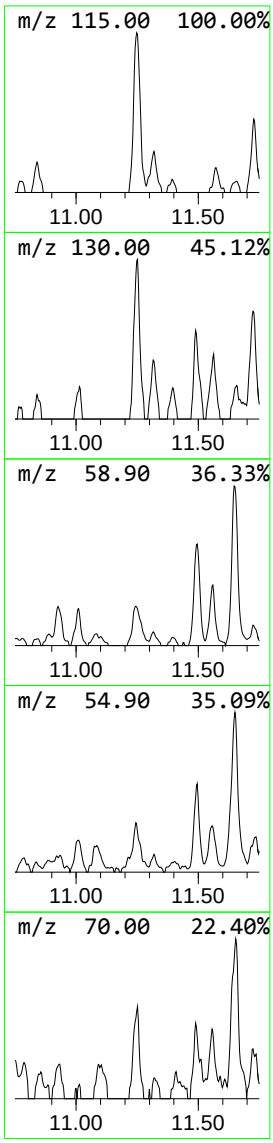
****

Peak Number 12 unknown-04 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.248	0.60 ug/L	75829	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 2,3-dimethyl-2-(1...	172	C10H20O2	055519-33-0	38
2	1-Methyl-1-n-butoxy-1-silacyclob...	158	C8H18OSi	1000216-91-6	37
3	2,6-Difluoropyridine	115	C5H3F2N	001513-65-1	35
4	Silane, ethenylethoxydimethyl-	130	C6H14OSi	005356-83-2	32
5	3-Dimethyl(dichloromethyl)silylo...	198	C6H12Cl2OSi	1000279-98-7	32





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Data File : VU059885.D
Acq On : 08 Jul 2024 15:55
Operator : MD/SY
Sample : P3137-18DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
YDZG7DL

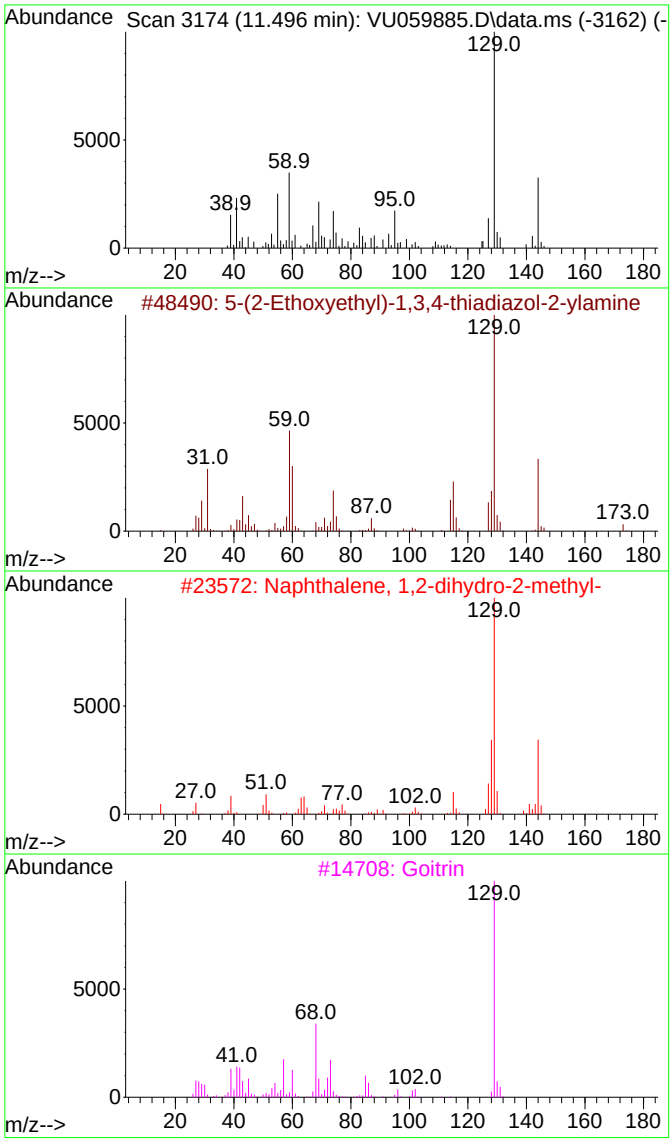
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

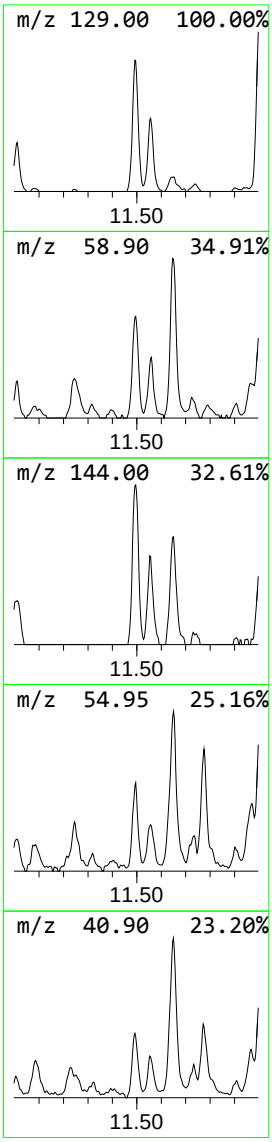
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 5-(2-Ethoxyethyl)-1,3,4-thi... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.496	0.78 ug/L	97548	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-(2-Ethoxyethyl)-1,3,4-thiadiaz...	173	C6H11N3OS	299936-83-7	72
2	Naphthalene, 1,2-dihydro-2-methyl-	144	C11H12	021564-79-4	53
3	Goitrin	129	C5H7NOS	000500-12-9	43
4	1,3-Disilacyclobutane, 1,1,3,3-t...	144	C6H16Si2	001627-98-1	42
5	1H-Indene, 1,1-dimethyl-	144	C11H12	018636-55-0	38





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Data File : VU059885.D
Acq On : 08 Jul 2024 15:55
Operator : MD/SY
Sample : P3137-18DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
YDZG7DL

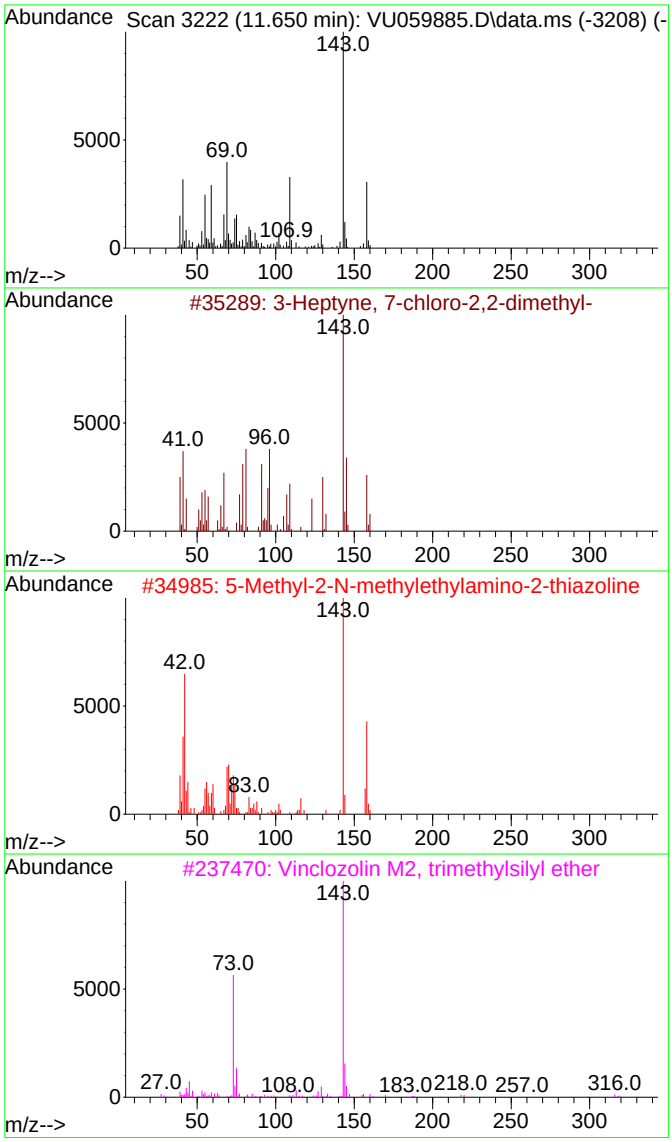
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

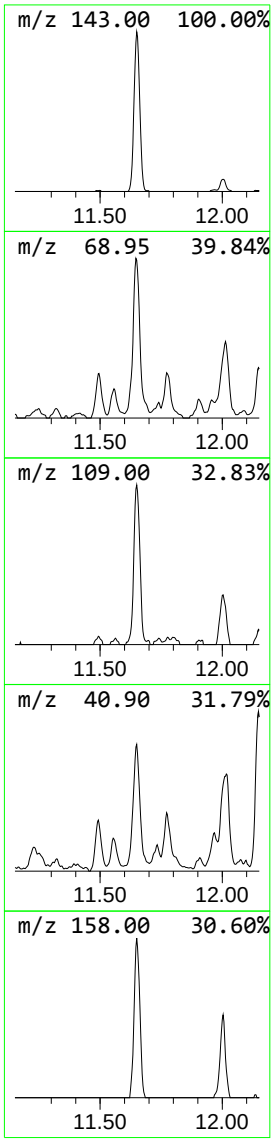
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 14 3-Heptyne, 7-chloro-2,2-dim... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.650	1.94 ug/L	243363	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptyne, 7-chloro-2,2-dimethyl-	158	C9H15Cl	055402-10-3	59
2	5-Methyl-2-N-methylethylamino-2-...	158	C7H14N2S	077158-37-3	53
3	Vinclozolin M2, trimethylsilyl e...	331	C14H19Cl2NO2Si	1010395-60-7	47
4	4(1H)-Pyrimidinone, 6-amino-2,3-...	143	C4H5N3OS	001004-40-6	47
5	tert-Butyldimethylsilyl methacry...	200	C10H20O2Si	1000385-80-8	43





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Data File : VU059885.D
Acq On : 08 Jul 2024 15:55
Operator : MD/SY
Sample : P3137-18DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
YDZG7DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

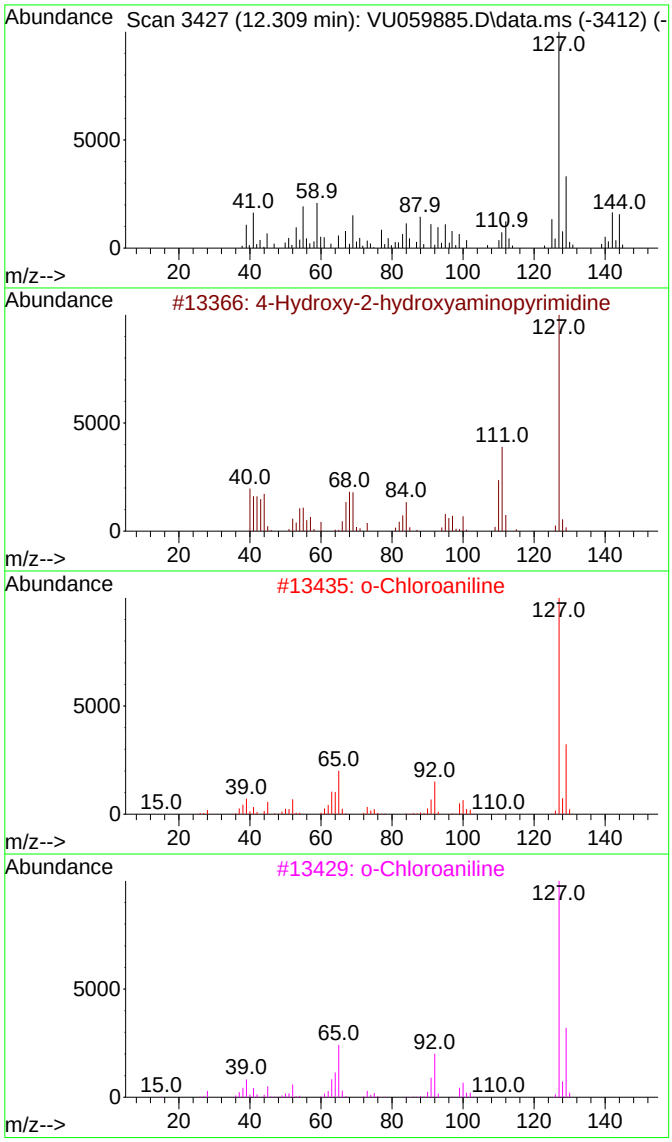
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

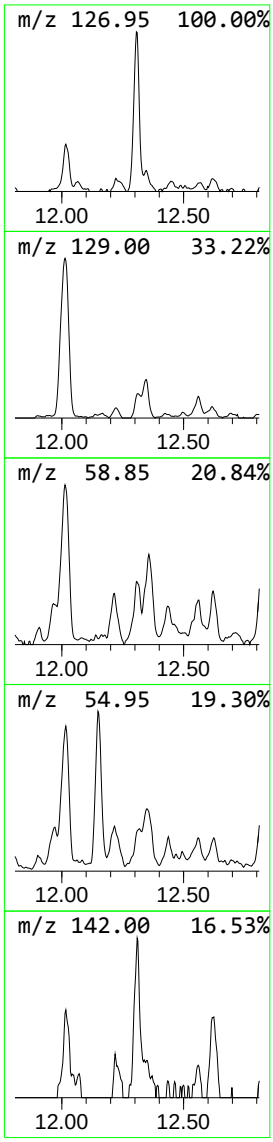
****

Peak Number 16 unknown-05 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.309	0.81 ug/L	101714	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Hydroxy-2-hydroxyaminopyrimidine	127	C4H5N3O2	1000111-25-4	46
2	o-Chloroaniline	127	C6H6ClN	000095-51-2	43
3	o-Chloroaniline	127	C6H6ClN	000095-51-2	43
4	4-(Chloromethyl)pyridine	127	C6H6ClN	010445-91-7	43
5	p-Chloroaniline	127	C6H6ClN	000106-47-8	43





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Data File : VU059885.D
Acq On : 08 Jul 2024 15:55
Operator : MD/SY
Sample : P3137-18DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
YDZG7DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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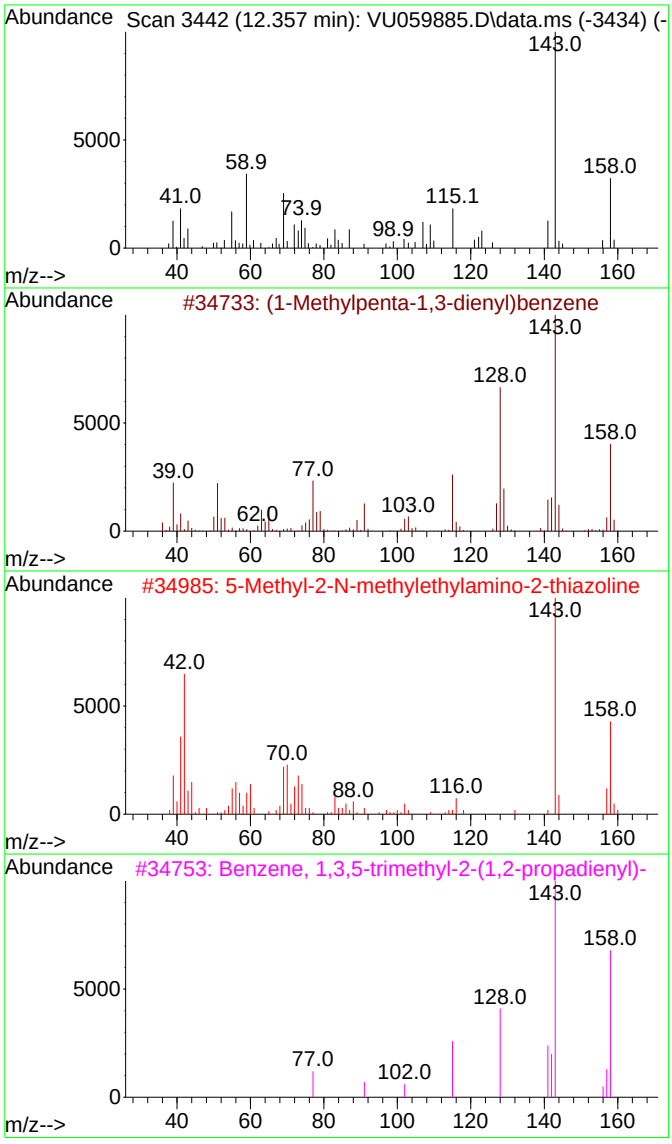
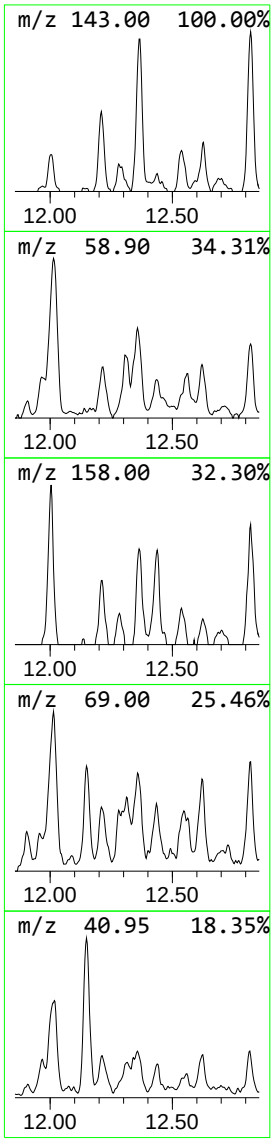
Peak Number 17 unknown-06 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.357	0.84 ug/L	105224	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1-Methylpenta-1,3-dienyl)benzene	158	C12H14	116669-49-9	40
2	5-Methyl-2-N-methylethylamino-2-...	158	C7H14N2S	077158-37-3	40
3	Benzene, 1,3,5-trimethyl-2-(1,2-...	158	C12H14	029555-07-5	32
4	Quinoline, 6-methyl-	143	C10H9N	000091-62-3	25
5	Glutaric acid, di(2-(2-methoxyet...	416	C23H44O6	1000358-49-9	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070824\
Data File : VU059885.D
Acq On : 08 Jul 2024 15:55
Operator : MD/SY
Sample : P3137-18DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
YDZG7DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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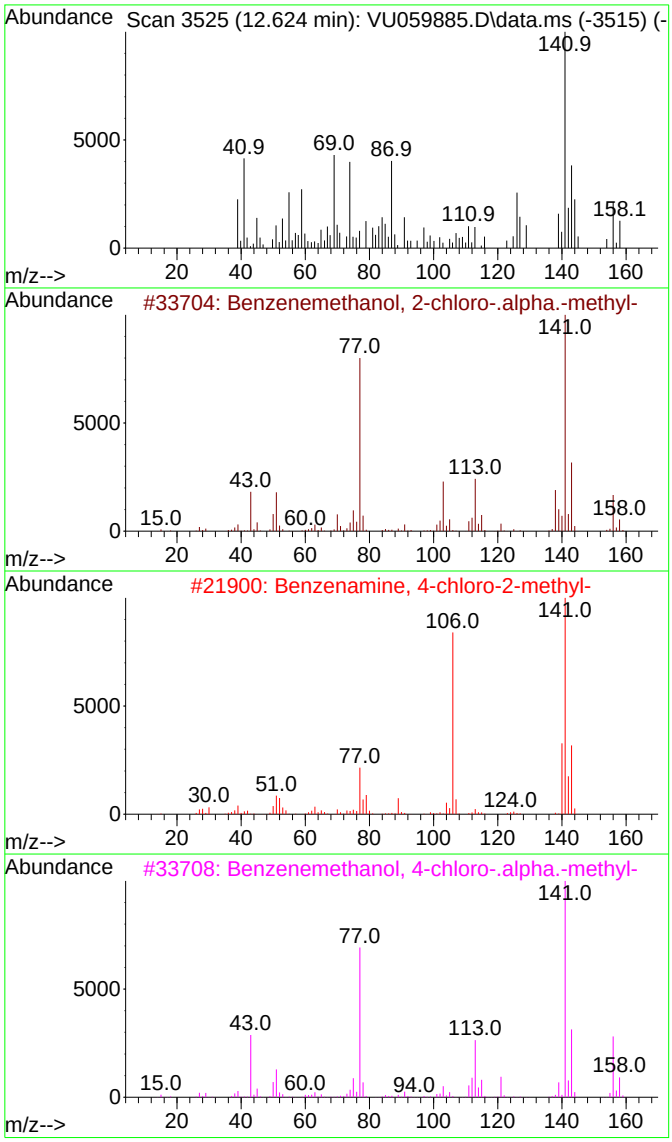
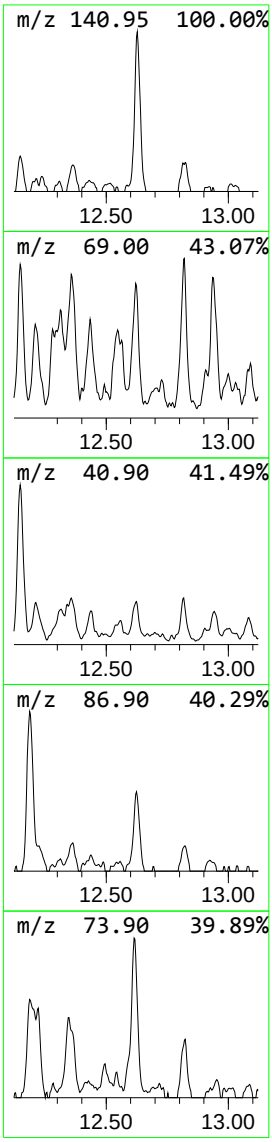
Peak Number 19 unknown-07 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.624	0.62 ug/L	77762	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenemethanol, 2-chloro-.alpha...	156	C8H9ClO	013524-04-4	43
2	Benzenamine, 4-chloro-2-methyl-	141	C7H8ClN	000095-69-2	35
3	Benzenemethanol, 4-chloro-.alpha...	156	C8H9ClO	003391-10-4	35
4	3-Chloro-2,6-dimethylpyridine	141	C7H8ClN	002405-06-3	35
5	Silane, trimethyl-2-thienyl-	156	C7H12SSi	018245-28-8	27





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Data File : VU059885.D
Acq On : 08 Jul 2024 15:55
Operator : MD/SY
Sample : P3137-18DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
YDZG7DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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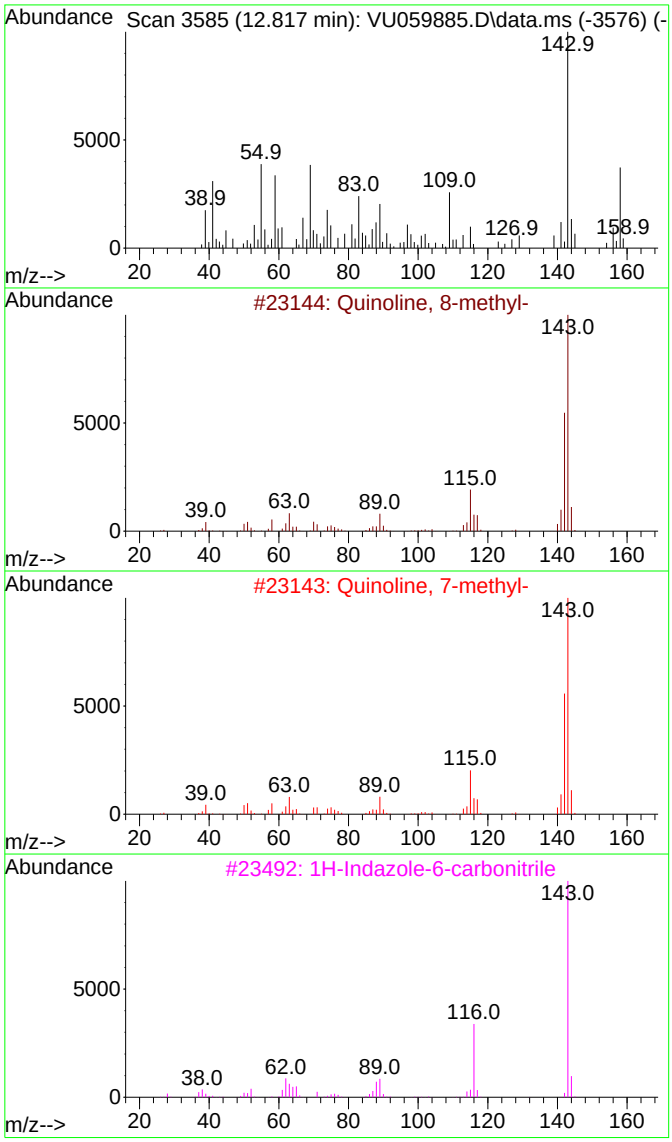
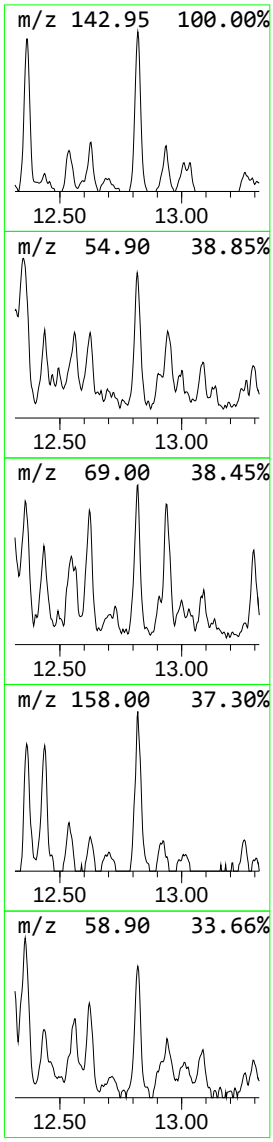
Peak Number 20 unknown-08 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.817	0.69 ug/L	87064	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Quinoline, 8-methyl-	143	C10H9N	000611-32-5	47
2	Quinoline, 7-methyl-	143	C10H9N	000612-60-2	43
3	1H-Indazole-6-carbonitrile	143	C8H5N3	141290-59-7	38
4	3-Aminophthalonitrile	143	C8H5N3	058632-96-5	38
5	1,2-Benzenedicarbonitrile, 4-amino-	143	C8H5N3	056765-79-8	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070824\
Data File : VU059885.D
Acq On : 08 Jul 2024 15:55
Operator : MD/SY
Sample : P3137-18DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
YDZG7DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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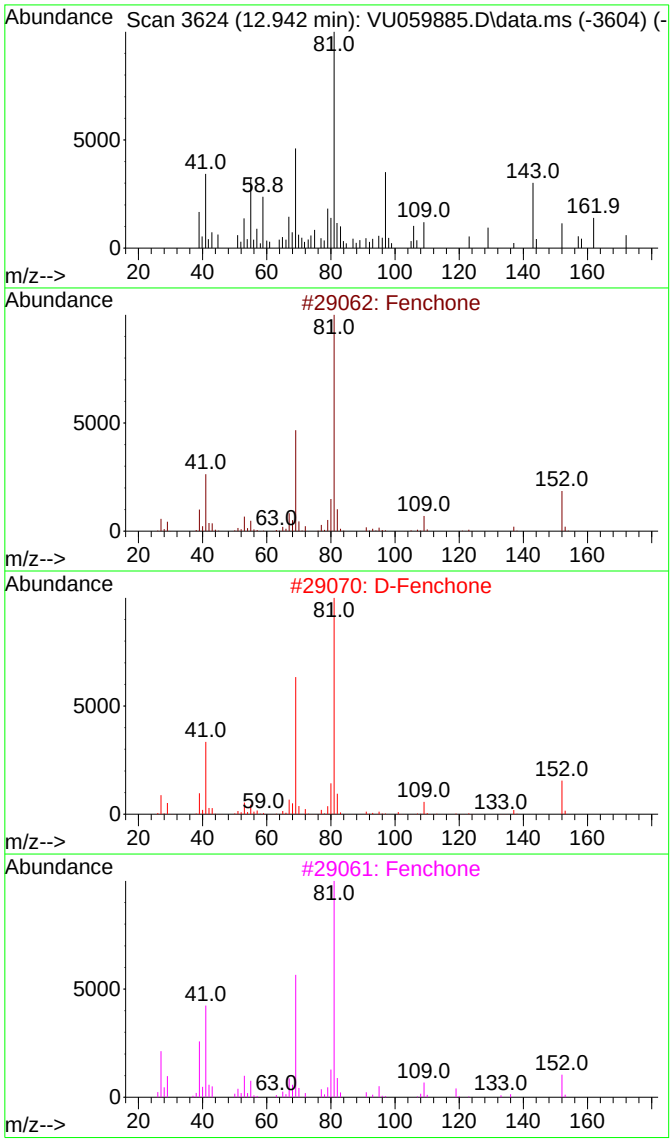
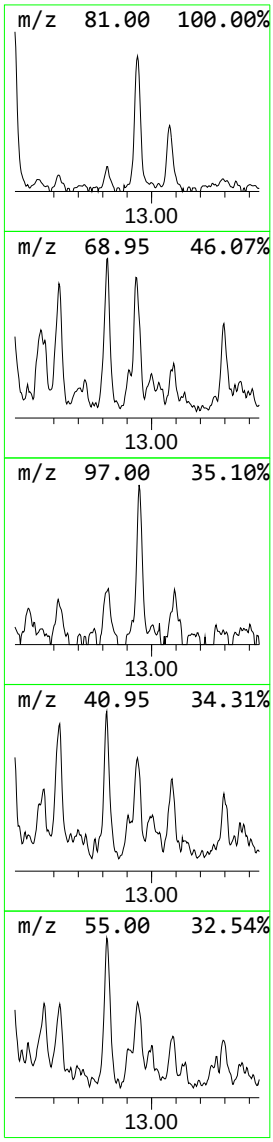
Peak Number 21 Fenchone Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.942	0.57 ug/L	71353	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fenchone	152	C10H16O	001195-79-5	50
2	D-Fenchone	152	C10H16O	004695-62-9	43
3	Fenchone	152	C10H16O	001195-79-5	43
4	L-Fenchone	152	C10H16O	007787-20-4	41
5	L-Fenchone	152	C10H16O	007787-20-4	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070824\
Data File : VU059885.D
Acq On : 08 Jul 2024 15:55
Operator : MD/SY
Sample : P3137-18DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
YDZG7DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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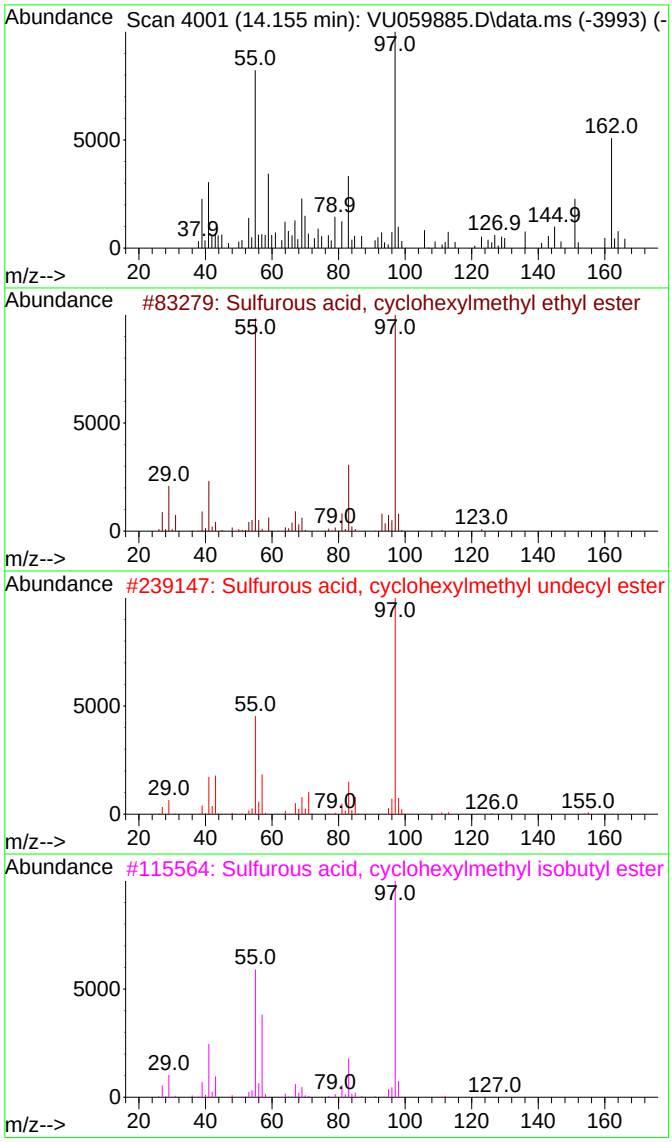
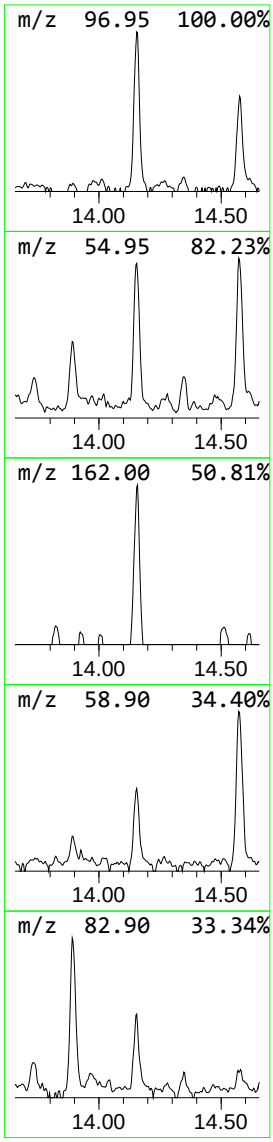
Peak Number 22 unknown-09 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.155	0.61 ug/L	77239	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, cyclohexylmethyl...	206	C9H18O3S	1000309-21-2	43
2	Sulfurous acid, cyclohexylmethyl...	332	C18H36O3S	1000309-21-9	43
3	Sulfurous acid, cyclohexylmethyl...	234	C11H22O3S	1000309-21-3	43
4	Sulfurous acid, butyl cyclohexyl...	234	C11H22O3S	1000309-21-4	43
5	Propanedinitrile, cyclohexyl(2-m...	244	C16H24N2	074764-55-9	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070824\
Data File : VU059885.D
Acq On : 08 Jul 2024 15:55
Operator : MD/SY
Sample : P3137-18DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
YDZG7DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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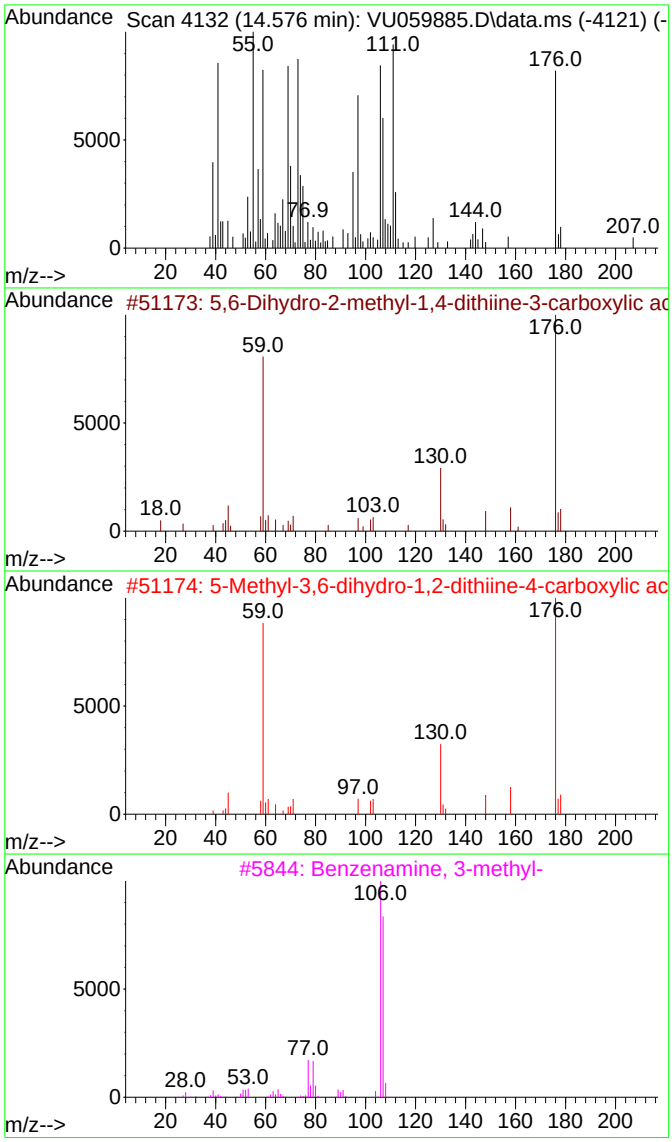
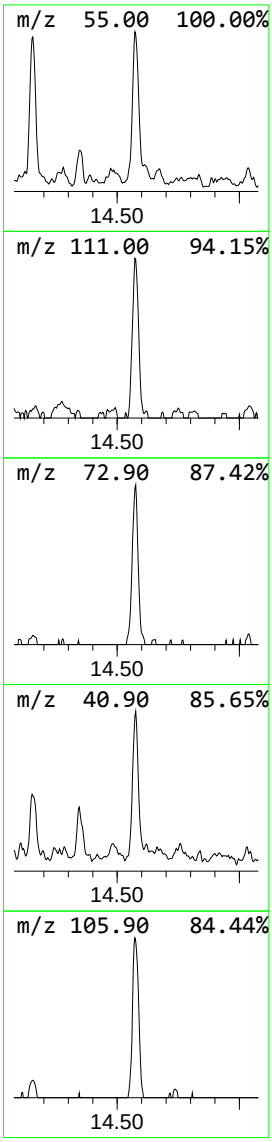
Peak Number 23 unknown-10 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.576	0.88 ug/L	110531	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,6-Dihydro-2-methyl-1,4-dithiin...	176	C6H8O2S2	035756-29-7	20
2	5-Methyl-3,6-dihydro-1,2-dithiin...	176	C6H8O2S2	959252-25-6	20
3	Benzenamine, 3-methyl-	107	C7H9N	000108-44-1	11
4	3-Bromo-2-hydroxy-2-cyclopenten-...	176	C5H5BrO2	003019-83-8	11
5	3-Heptene, 2-methyl-	112	C8H16	017618-76-7	11





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070824\
Data File : VU059885.D
Acq On : 08 Jul 2024 15:55
Operator : MD/SY
Sample : P3137-18DL 10X
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
YDZG7DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane, 2-(eth...	7.566	3.4	ug/L	259201	1	6.242	379930	5.0
Diisopropyl sul...	8.306	4.1	ug/L	417496	2	9.412	514707	5.0
2-Pentanone, 4,...	8.480	1.1	ug/L	115097	2	9.412	514707	5.0
(DEL) Alkane: S...	9.084	0.7	ug/L	68797	2	9.412	514707	5.0
Propane, 1-[(1-...	9.190	1.0	ug/L	105303	2	9.412	514707	5.0
Sulfide, sec-bu...	9.875	1.1	ug/L	118114	2	9.412	514707	5.0
unknown-01	9.981	1.0	ug/L	103683	2	9.412	514707	5.0
Tetrahydropyrro...	10.332	0.9	ug/L	90674	2	9.412	514707	5.0
unknown-02	10.640	0.5	ug/L	65161	3	11.807	627990	5.0
unknown-03	11.084	0.5	ug/L	62945	3	11.807	627990	5.0
unknown-04	11.248	0.6	ug/L	75829	3	11.807	627990	5.0
5-(2-Ethoxyethy...	11.496	0.8	ug/L	97548	3	11.807	627990	5.0
3-Heptyne, 7-ch...	11.650	1.9	ug/L	243363	3	11.807	627990	5.0
unknown-05	12.309	0.8	ug/L	101714	3	11.807	627990	5.0
unknown-06	12.357	0.8	ug/L	105224	3	11.807	627990	5.0
unknown-07	12.624	0.6	ug/L	77762	3	11.807	627990	5.0
unknown-08	12.817	0.7	ug/L	87064	3	11.807	627990	5.0
Fenchone	12.942	0.6	ug/L	71353	3	11.807	627990	5.0
unknown-09	14.155	0.6	ug/L	77239	3	11.807	627990	5.0
unknown-10	14.576	0.9	ug/L	110531	3	11.807	627990	5.0