

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070121\
 Data File : VU044289.D
 Acq On : 01 Jul 2021 16:26
 Operator : SY/MD
 Sample : M2905-22
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBK40

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\SFAMUTR062121WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU044289.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.539	52	62	63	rBV4	4306	6866	1.11%	0.106%
2	1.604	75	82	92	rBV	47251	52994	8.54%	0.821%
3	1.919	174	180	191	rVB	47640	59874	9.65%	0.927%
4	2.575	368	384	401	rBV	90006	151113	24.36%	2.341%
5	4.459	957	970	984	rBV4	8383	21810	3.52%	0.338%
6	4.642	1010	1027	1063	rBV	74287	243283	39.23%	3.769%
7	5.073	1143	1161	1178	rBV	92493	204785	33.02%	3.172%
8	5.732	1345	1366	1389	rBV3	182936	481645	77.66%	7.461%
9	6.256	1516	1529	1554	rVB	177741	333735	53.81%	5.170%
10	6.700	1653	1667	1683	rBV	118087	229038	36.93%	3.548%
11	7.571	1925	1938	1955	rBV	62106	110608	17.83%	1.713%
12	7.799	2002	2009	2024	rVB2	4083	7227	1.17%	0.112%
13	7.906	2029	2042	2058	rBV	231832	406145	65.49%	6.291%
14	7.976	2058	2064	2076	rVB3	4196	7240	1.17%	0.112%
15	8.185	2117	2129	2155	rBV	40663	77031	12.42%	1.193%
16	8.642	2255	2271	2300	rBV	316086	620209	100.00%	9.607%
17	9.423	2491	2514	2539	rBV	247955	419505	67.64%	6.498%
18	10.764	2920	2931	2944	rVB	95346	152544	24.60%	2.363%
19	11.018	2998	3010	3022	rVB5	7733	16458	2.65%	0.255%
20	11.098	3026	3035	3046	rVV5	10045	16566	2.67%	0.257%
21	11.166	3049	3056	3066	rVV8	4994	8215	1.32%	0.127%
22	11.237	3069	3078	3091	rVV2	15263	23497	3.79%	0.364%
23	11.471	3141	3151	3164	rVB	11099	19065	3.07%	0.295%
24	11.561	3168	3179	3188	rBV2	7957	13928	2.25%	0.216%
25	11.645	3188	3205	3220	rBV	74178	119295	19.23%	1.848%
26	11.815	3244	3258	3278	rVB3	286250	545865	88.01%	8.456%
27	11.986	3303	3311	3322	rBV3	10149	15440	2.49%	0.239%
28	12.050	3323	3331	3339	rVB3	6266	9877	1.59%	0.153%
29	12.102	3339	3347	3356	rBV7	6411	10576	1.71%	0.164%
30	12.198	3364	3377	3390	rBV	247639	410124	66.13%	6.353%
31	12.487	3450	3467	3476	rBV2	32296	67354	10.86%	1.043%
32	12.719	3531	3539	3548	rVB2	5995	11734	1.89%	0.182%
33	12.835	3561	3575	3581	rBV10	5384	11639	1.88%	0.180%
34	12.947	3601	3610	3616	rBV9	6129	9319	1.50%	0.144%
35	12.992	3616	3624	3629	rBV2	13650	22836	3.68%	0.354%
36	13.108	3649	3660	3667	rBV5	9785	18036	2.91%	0.279%

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Integrator: RTE

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Filtering: 5

Sampling : 1

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Stop Thrs : 0

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

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
 Title : TRACE VOA SFAM1.0

37	13.240	3696	3701	3715	rVB5	3361	6761	1.09%	0.105%
38	13.343	3723	3733	3742	rBV3	16490	30614	4.94%	0.474%
39	13.410	3744	3754	3765	rVB	81384	126961	20.47%	1.967%
40	13.520	3782	3788	3804	rVB	11319	19912	3.21%	0.308%
41	13.738	3850	3856	3864	rBV8	4543	6875	1.11%	0.106%
42	13.938	3909	3918	3922	rBV5	8638	13323	2.15%	0.206%
43	13.979	3923	3931	3941	rVB7	21361	40751	6.57%	0.631%
44	14.089	3958	3965	3975	rVB4	13705	22596	3.64%	0.350%
45	14.153	3977	3985	3993	rBV3	18949	31347	5.05%	0.486%
46	14.327	4031	4039	4047	rBV8	9911	15614	2.52%	0.242%
47	14.378	4048	4055	4071	rVB7	11666	22226	3.58%	0.344%
48	14.536	4098	4104	4113	rBV10	4755	6482	1.05%	0.100%
49	14.584	4113	4119	4127	rVB3	7006	8869	1.43%	0.137%
50	14.655	4135	4141	4150	rBV3	4488	7765	1.25%	0.120%
51	14.712	4150	4159	4168	rVV	24503	43087	6.95%	0.667%
52	14.757	4169	4173	4180	rVB4	8546	11364	1.83%	0.176%
53	14.851	4196	4202	4210	rVB10	4847	6883	1.11%	0.107%
54	14.960	4227	4236	4245	rBV2	14900	25298	4.08%	0.392%
55	15.134	4282	4290	4298	rBV7	14633	25402	4.10%	0.393%
56	15.188	4298	4307	4315	rVV3	48221	82491	13.30%	1.278%
57	15.227	4315	4319	4328	rVB2	12950	18178	2.93%	0.282%
58	15.410	4366	4376	4385	rBV	116239	185002	29.83%	2.866%
59	15.564	4408	4424	4435	rVB4	11335	27372	4.41%	0.424%
60	15.658	4443	4453	4459	rBV2	28128	47901	7.72%	0.742%
61	15.751	4473	4482	4491	rBV2	13884	25445	4.10%	0.394%
62	15.809	4495	4500	4505	rVB3	7659	10035	1.62%	0.155%
63	16.002	4552	4560	4570	rVB6	12038	19984	3.22%	0.310%
64	16.072	4574	4582	4584	rBV6	5995	7425	1.20%	0.115%
65	16.111	4586	4594	4614	rVB3	42046	91050	14.68%	1.410%
66	16.198	4615	4621	4629	rBV9	4943	8481	1.37%	0.131%
67	16.269	4637	4643	4653	rVB3	5623	8015	1.29%	0.124%
68	16.394	4672	4682	4696	rBV6	16973	43028	6.94%	0.667%
69	16.671	4763	4768	4774	rBV8	6501	8244	1.33%	0.128%
70	16.818	4802	4814	4828	rVB7	17270	38015	6.13%	0.589%
71	16.944	4840	4853	4863	rBV6	11308	22928	3.70%	0.355%
72	17.018	4866	4876	4890	rBV	224168	341395	55.05%	5.288%
73	17.166	4915	4922	4935	rVB9	9930	16974	2.74%	0.263%
74	17.236	4937	4944	4950	rBV6	8322	11616	1.87%	0.180%
75	17.442	5000	5008	5024	rVB6	14028	34353	5.54%	0.532%

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ClientSampleId :
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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\SFAMUTR062121WMA.M
Title : TRACE VOA SFAM1.0

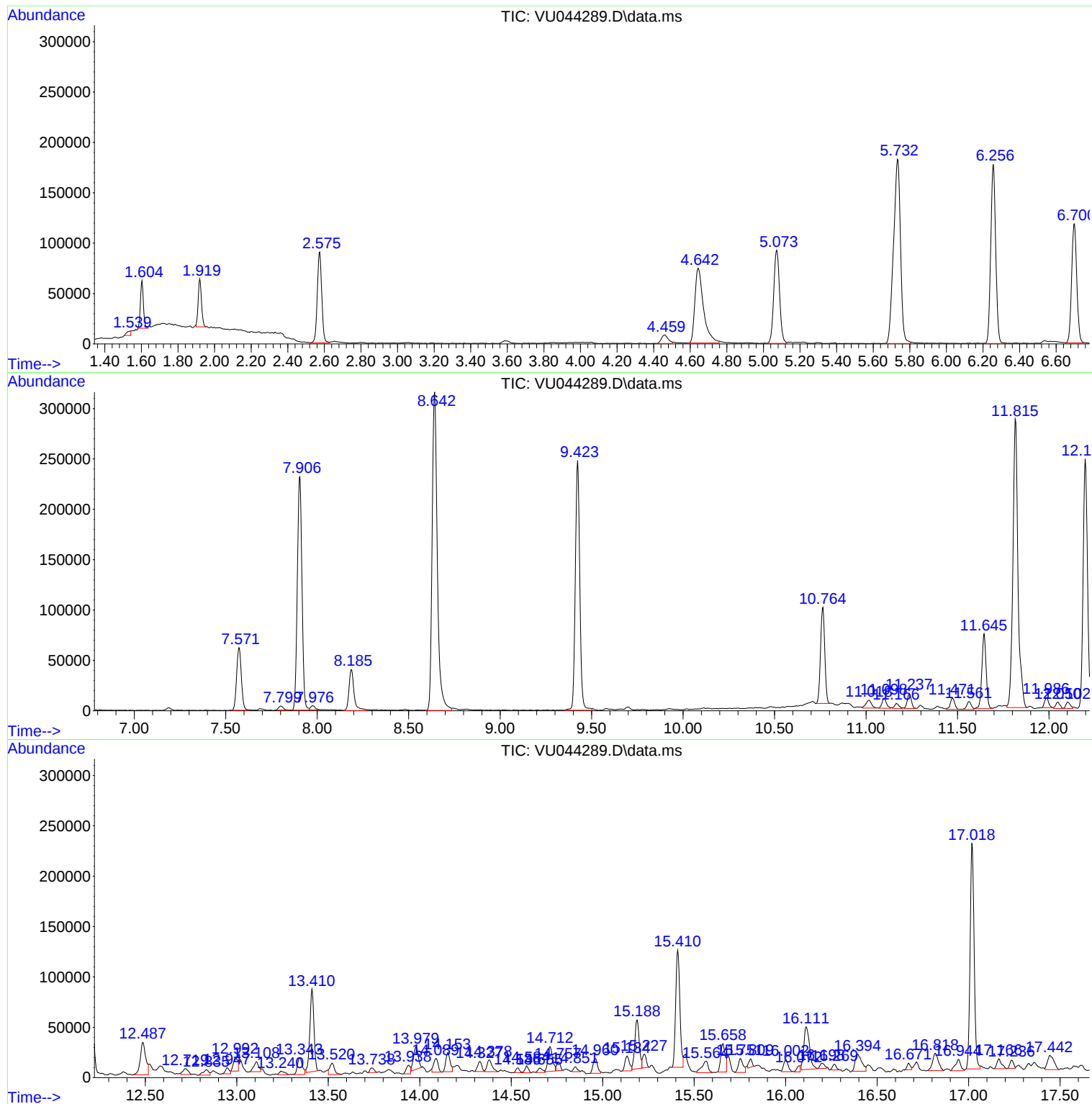
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Operator : SY/MD
Sample : M2905-22
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBK40

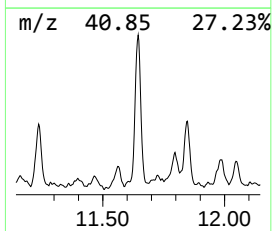
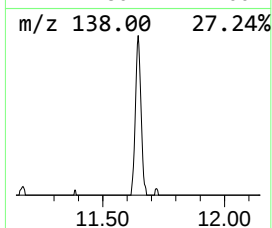
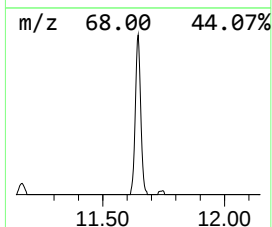
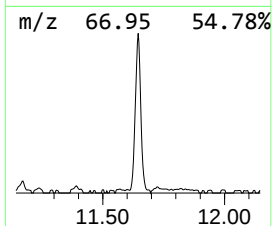
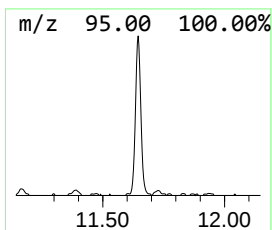
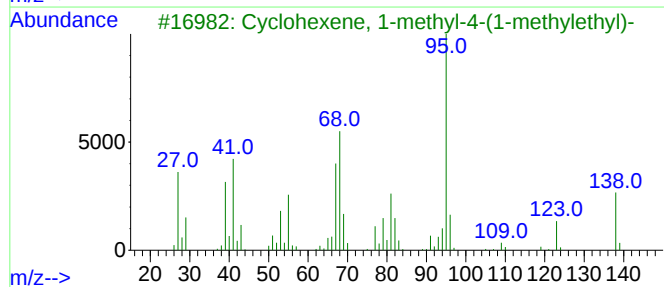
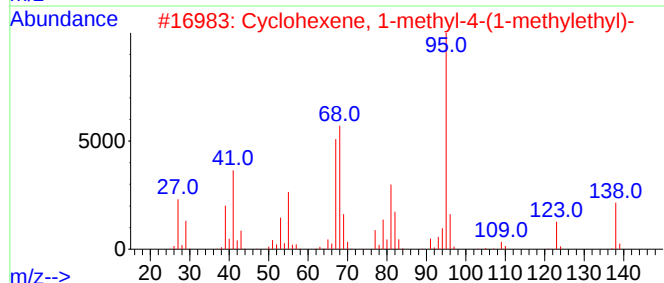
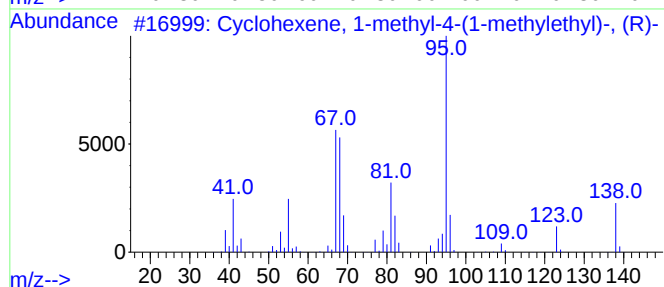
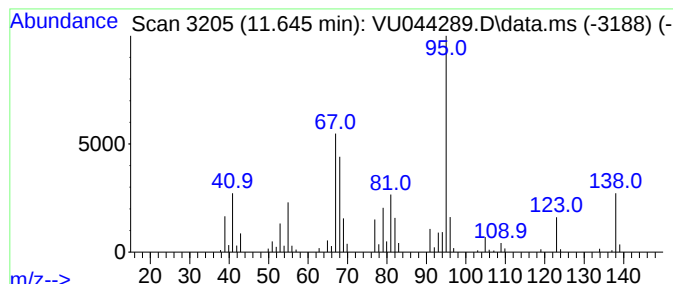
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclohexene, 1-methyl-4-(1-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.645	1.09 ug/L	119295	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene, 1-methyl-4-(1-methy...	138	C10H18	001195-31-9	95
2			Cyclohexene, 1-methyl-4-(1-methy...	138	C10H18	005502-88-5	93
3			Cyclohexene, 1-methyl-4-(1-methy...	138	C10H18	005502-88-5	91
4			Cyclohexene, 1-methyl-4-(1-methy...	138	C10H18	001195-31-9	91
5			Cyclohexene, 3-methyl-6-(1-methy...	138	C10H18	005256-65-5	87



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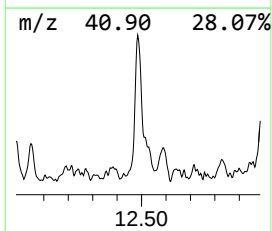
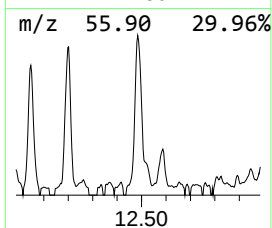
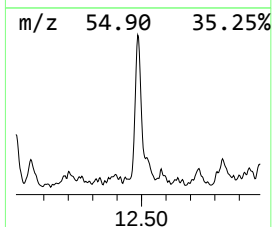
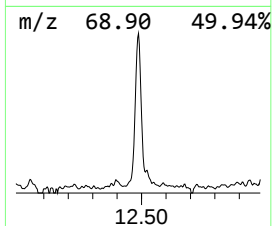
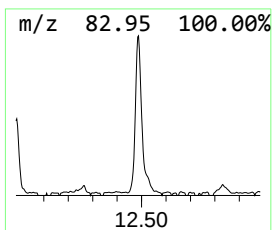
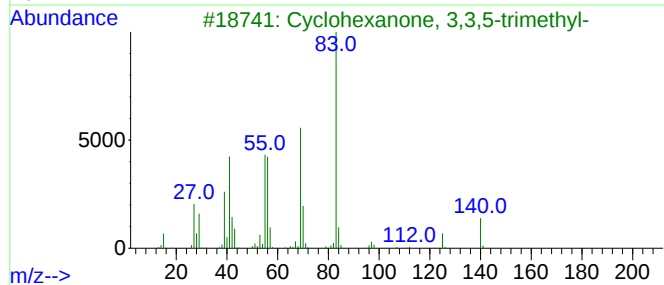
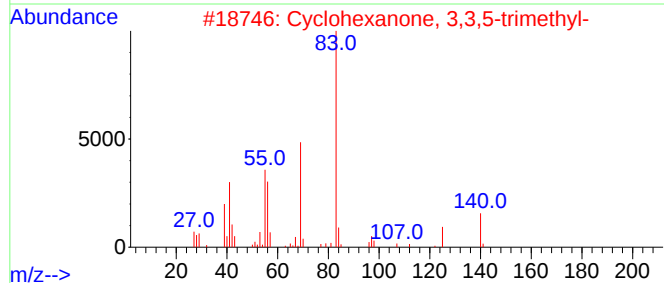
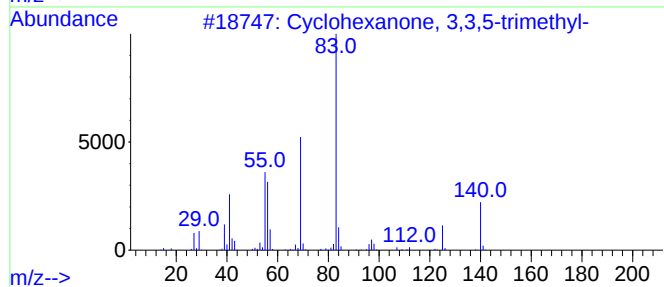
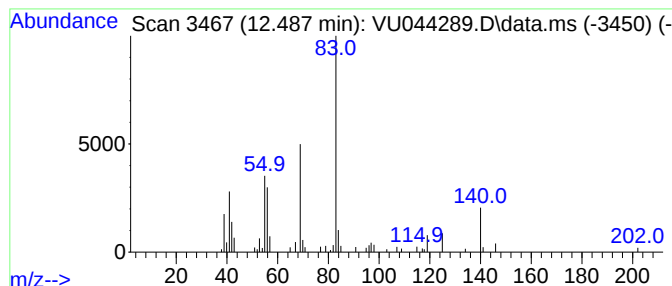
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Cyclohexanone, 3,3,5-trimet... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.487	0.62 ug/L	67354	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	94
2			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	91
3			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	91
4			Cyclohexane, butyl-	140	C10H20	001678-93-9	64
5			1,4-Pentadien-3-ol	84	C5H8O	000922-65-6	53



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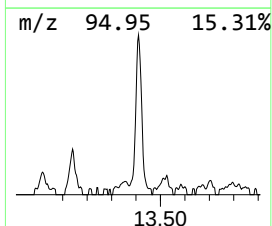
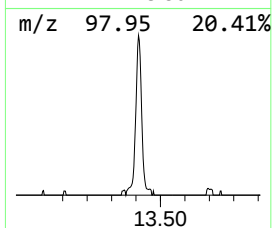
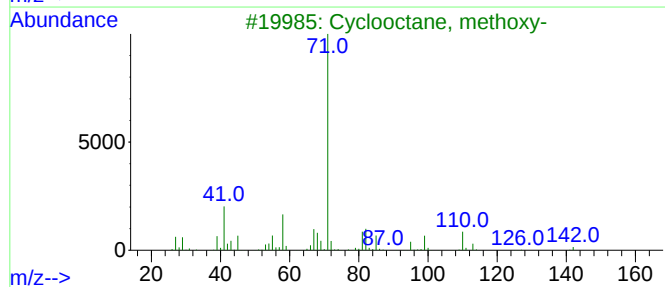
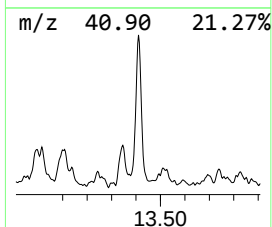
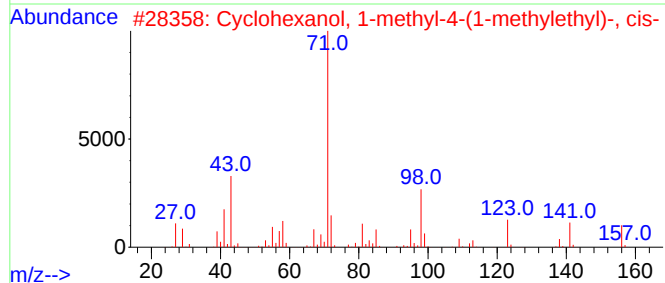
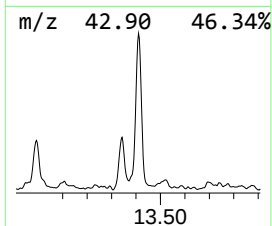
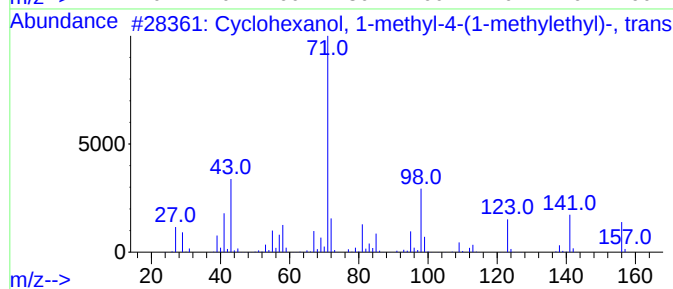
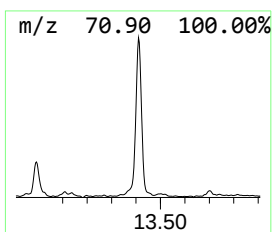
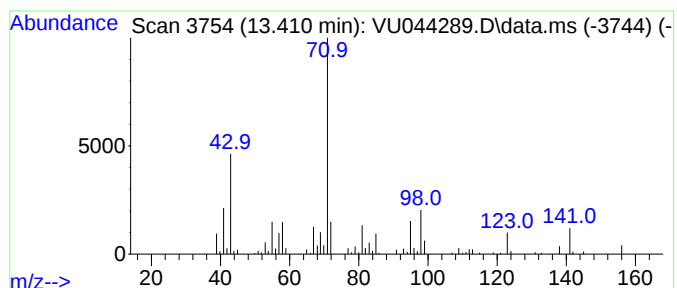
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyclohexanol, 1-methyl-4-(1... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.410	1.16 ug/L	126961	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanol, 1-methyl-4-(1-meth...	156	C10H20O	003901-93-7	91
2			Cyclohexanol, 1-methyl-4-(1-meth...	156	C10H20O	003901-95-9	87
3			Cyclooctane, methoxy-	142	C9H18O	013213-32-6	49
4			3-Cyclopentylpropionic acid, 2-t...	226	C13H22O3	1000293-46-9	47
5			1-Hexadecen-3-ol, 3,5,11,15-tetr...	296	C20H40O	1000262-55-5	47



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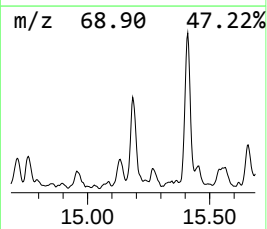
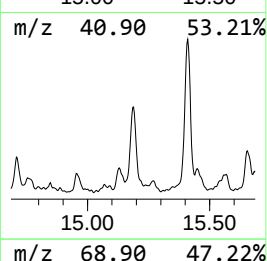
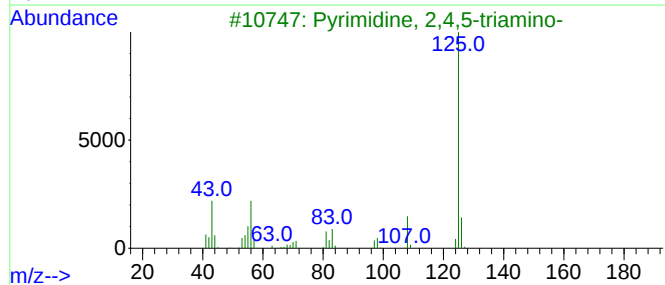
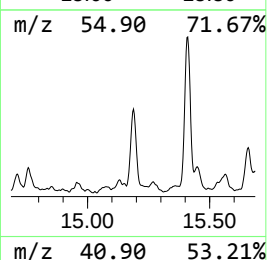
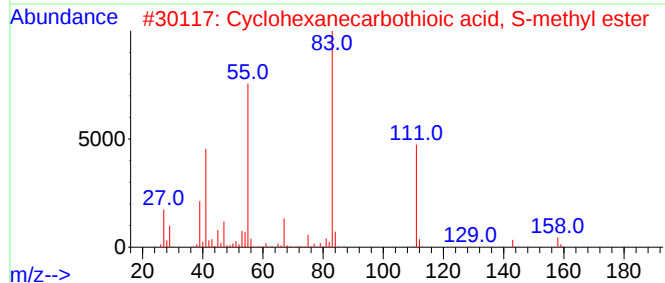
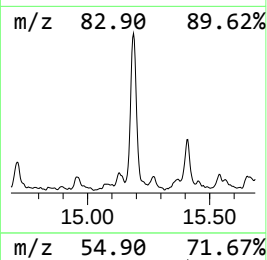
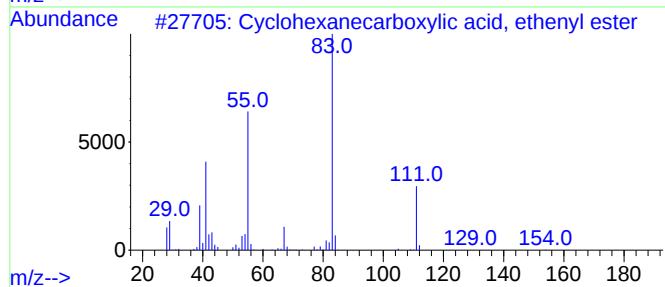
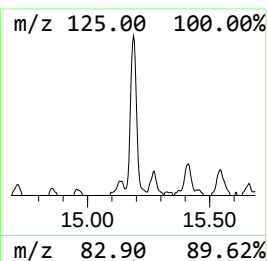
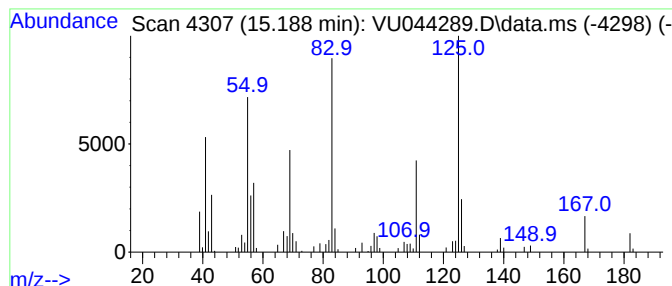
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.188	0.76 ug/L	82491	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanecarboxylic acid, ethe...	154	C9H14O2	004840-76-0	35
2			Cyclohexanecarbothioic acid, S-m...	158	C8H14OS	035377-82-3	35
3			Pyrimidine, 2,4,5-triamino-	125	C4H7N5	003546-50-7	35
4			t-Butyl cyclohexaneperoxycarboxy...	200	C11H20O3	020396-49-0	35
5			Cyclohexane, propyl-	126	C9H18	001678-92-8	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070121\
Data File : VU044289.D
Acq On : 01 Jul 2021 16:26
Operator : SY/MD
Sample : M2905-22
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBK40

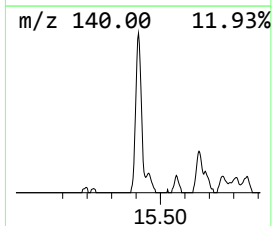
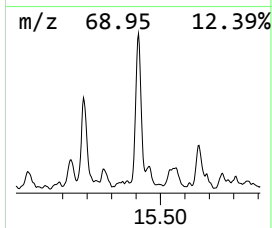
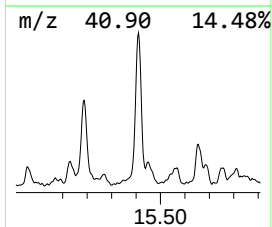
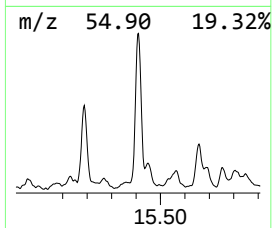
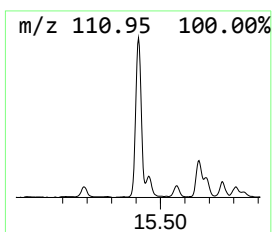
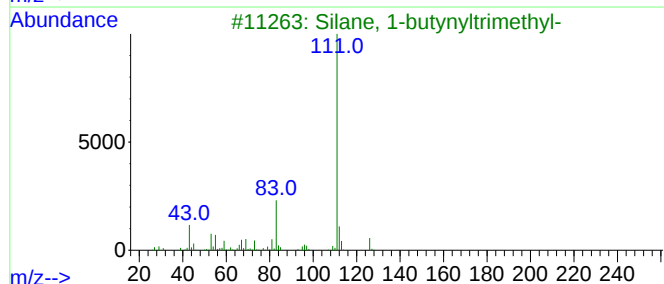
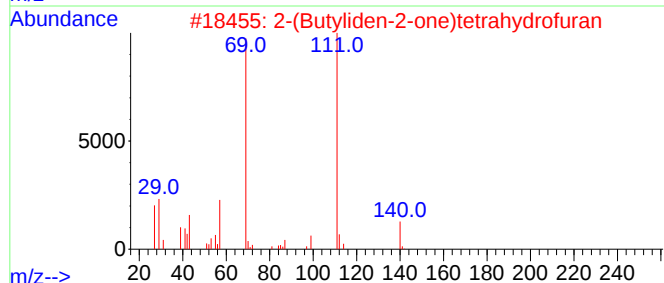
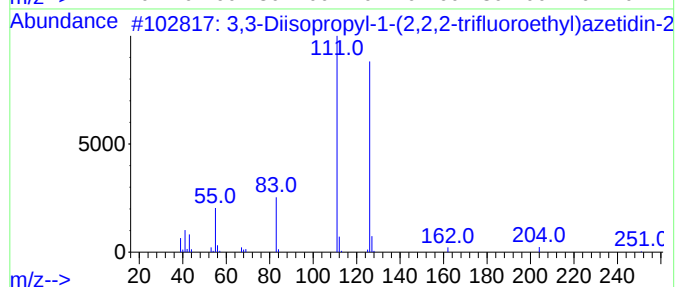
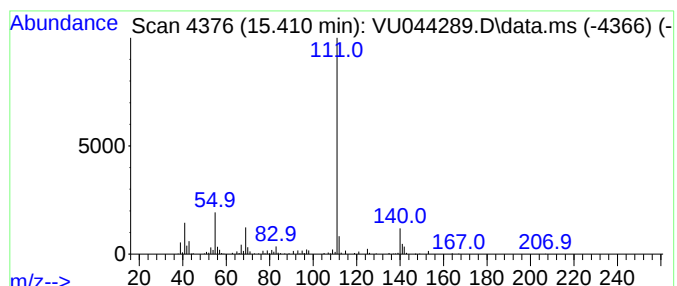
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 3,3-Diisopropyl-1-(2,2,2-tr... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.410	1.69 ug/L	185002	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,3-Diisopropyl-1-(2,2,2-trifluo...	251	C11H16F3NO2	1000305-99-5	53
2			2-(Butyliden-2-one)tetrahydrofuran	140	C8H12O2	343270-50-8	45
3			Silane, 1-butylnyltrimethyl-	126	C7H14Si	062108-37-6	42
4			2-Thiophenecarboxylic acid, 2-me...	186	C8H10O3S	1000330-98-8	40
5			2H-Pyran-2-carboxaldehyde, 3,4-d...	140	C8H12O2	001920-21-4	39



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070121\
Data File : VU044289.D
Acq On : 01 Jul 2021 16:26
Operator : SY/MD
Sample : M2905-22
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBK40

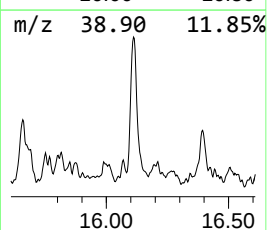
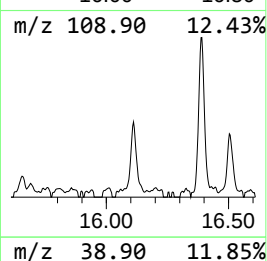
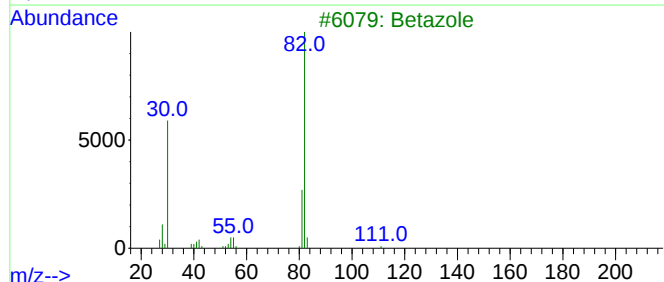
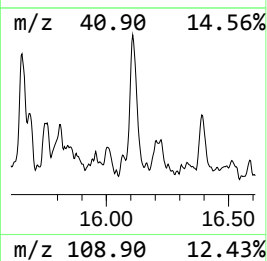
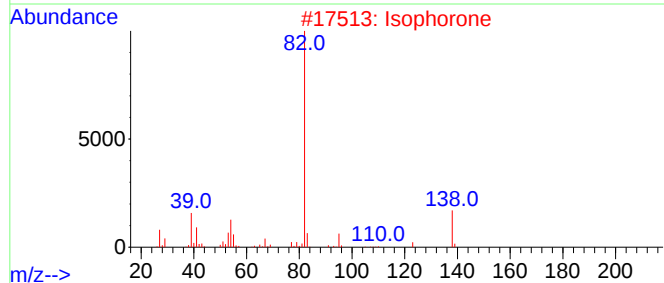
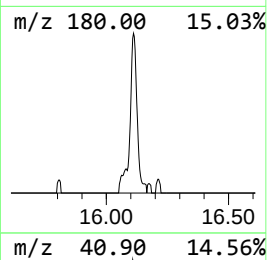
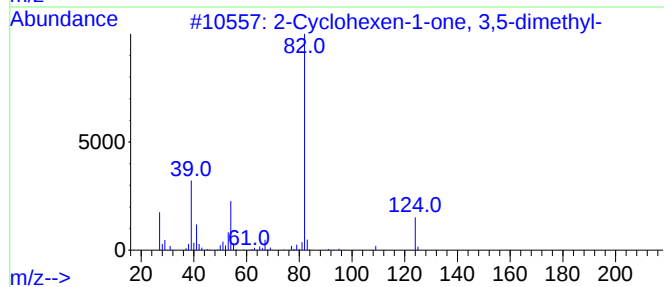
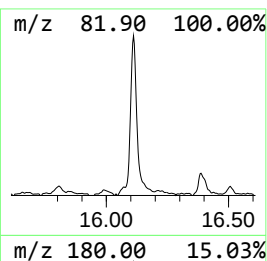
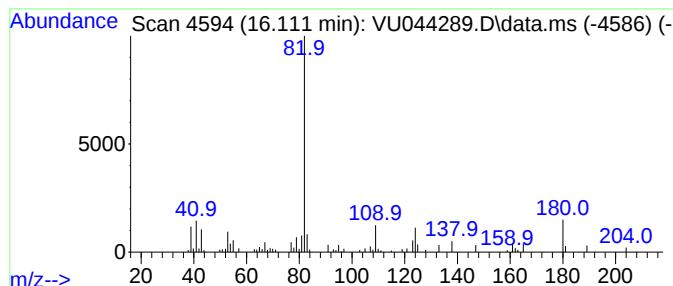
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 2-Cyclohexen-1-one, 3,5-dim... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.111	0.83 ug/L	91050	1,4-Dichlorobenzene-d4	11.819

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Cyclohexen-1-one, 3,5-dimethyl-	124	C8H12O	001123-09-7	53
2		Isophorone	138	C9H14O	000078-59-1	47
3		Betazole	111	C5H9N3	000105-20-4	43
4		2-Cyclohexen-1-one, 3,5-dimethyl-	124	C8H12O	001123-09-7	40
5		2-Cyclohexen-1-one, 3,5-dimethyl-	124	C8H12O	001123-09-7	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070121\
Data File : VU044289.D
Acq On : 01 Jul 2021 16:26
Operator : SY/MD
Sample : M2905-22
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBK40

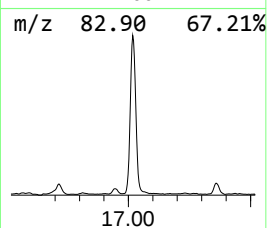
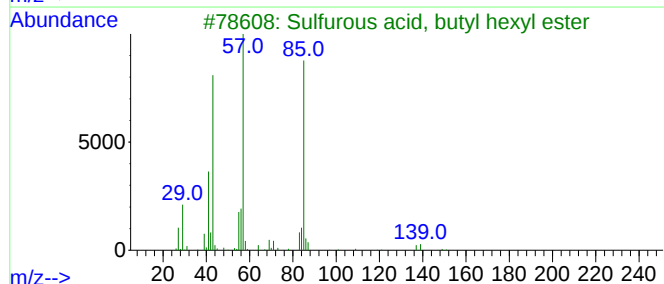
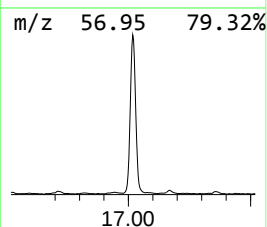
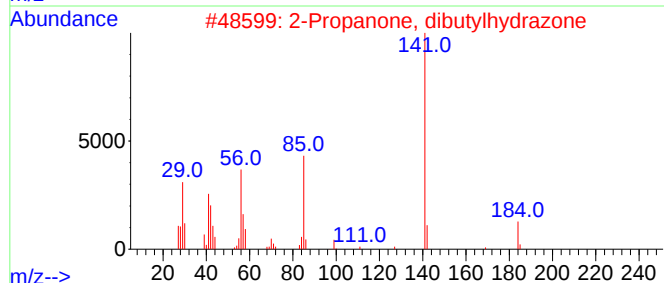
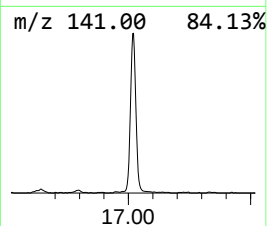
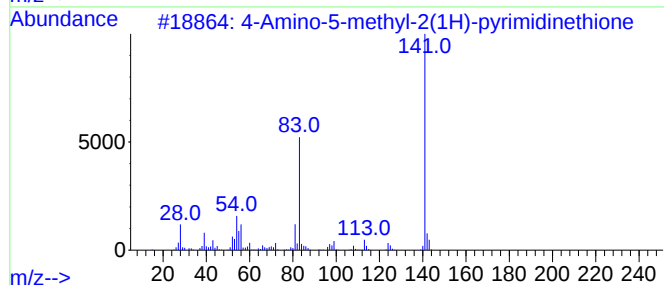
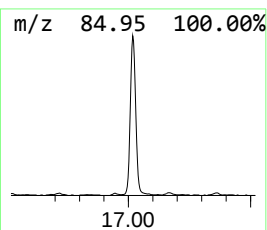
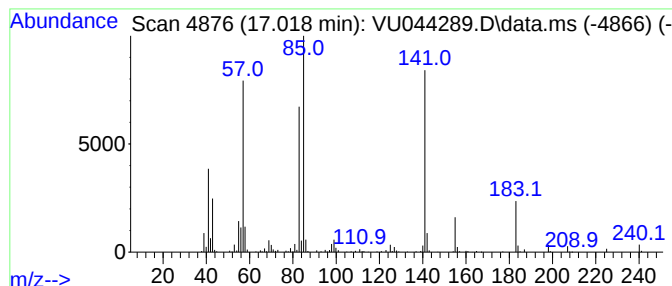
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 unknown-02 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.018	3.13 ug/L	341395	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Amino-5-methyl-2(1H)-pyrimidin...	141	C5H7N3S	007390-56-9	35
2			2-Propanone, dibutylhydrazone	184	C11H24N2	067660-52-0	27
3			Sulfurous acid, butyl hexyl ester	222	C10H22O3S	1000309-17-3	27
4			2-Methylbutanoic anhydride	186	C10H18O3	001468-39-9	22
5			2,5-Difluorobenzoic acid, 5-tetr...	354	C21H32F2O2	1000338-48-1	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070121\
Data File : VU044289.D
Acq On : 01 Jul 2021 16:26
Operator : SY/MD
Sample : M2905-22
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBK40

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR062121WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclohexene, 1-...	11.645	1.1	ug/L	119295	3	11.819	545865	5.0
Cyclohexanone, ...	12.487	0.6	ug/L	67354	3	11.819	545865	5.0
Cyclohexanol, 1...	13.410	1.2	ug/L	126961	3	11.819	545865	5.0
unknown-01	15.188	0.8	ug/L	82491	3	11.819	545865	5.0
3,3-Diisopropyl...	15.410	1.7	ug/L	185002	3	11.819	545865	5.0
2-Cyclohexen-1-...	16.111	0.8	ug/L	91050	3	11.819	545865	5.0
unknown-02	17.018	3.1	ug/L	341395	3	11.819	545865	5.0