

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121222\
 Data File : VU052349.D
 Acq On : 12 Dec 2022 13:49
 Operator : JC/MD
 Sample : N5922-03
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0B20

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\SFAMUTR111822WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU052349.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	23	rVB2	134192	144111	13.14%	1.483%
2	1.491	41	47	53	rBV	13841	14487	1.32%	0.149%
3	1.601	70	81	95	rVB3	184468	245193	22.35%	2.522%
4	1.694	103	110	116	rBV	10132	14089	1.28%	0.145%
5	1.732	116	122	131	rVB2	18270	24290	2.21%	0.250%
6	1.916	170	179	196	rBV	109052	150599	13.73%	1.549%
7	1.999	197	205	212	rVV4	12741	16367	1.49%	0.168%
8	2.160	246	255	262	rBV3	13934	20005	1.82%	0.206%
9	2.208	262	270	278	rVB	12549	17214	1.57%	0.177%
10	2.568	367	382	396	rBV	209396	347995	31.73%	3.580%
11	2.655	397	409	430	rVB2	9355	30663	2.80%	0.315%
12	2.797	442	453	466	rBV	7709	14028	1.28%	0.144%
13	3.048	520	531	550	rVB	31537	66896	6.10%	0.688%
14	3.183	561	573	586	rBV	16481	39400	3.59%	0.405%
15	3.591	687	700	712	rBV10	4577	11074	1.01%	0.114%
16	4.462	950	971	984	rBV9	5272	17981	1.64%	0.185%
17	4.636	1005	1025	1064	rBV	171235	601348	54.82%	6.186%
18	4.806	1065	1078	1109	rVB	102010	258187	23.54%	2.656%
19	5.060	1142	1157	1177	rBV	180109	396024	36.10%	4.074%
20	5.723	1341	1363	1399	rBV2	362479	969457	88.38%	9.973%
21	6.247	1512	1526	1545	rBV	318756	612937	55.88%	6.305%
22	6.687	1646	1663	1682	rBV	230084	449994	41.02%	4.629%
23	7.163	1801	1811	1832	rVB3	19284	40071	3.65%	0.412%
24	7.562	1923	1935	1958	rBV2	103558	184890	16.86%	1.902%
25	7.896	2024	2039	2056	rBV	415550	728440	66.41%	7.494%
26	8.176	2115	2126	2142	rBV	64273	110484	10.07%	1.137%
27	8.633	2254	2268	2307	rBV2	527781	1096897	100.00%	11.284%
28	8.787	2307	2316	2329	rVB4	13395	25599	2.33%	0.263%
29	9.414	2497	2511	2532	rBV	466491	774574	70.62%	7.968%
30	10.751	2910	2927	2944	rBV	196397	323445	29.49%	3.327%
31	11.041	3008	3017	3031	rBV6	6916	11448	1.04%	0.118%
32	11.684	3207	3217	3233	rVB7	11135	18129	1.65%	0.186%
33	11.809	3242	3256	3279	rBV	429254	681073	62.09%	7.006%
34	12.057	3320	3333	3353	rBV	86096	164127	14.96%	1.688%
35	12.189	3362	3374	3399	rVB	424385	691916	63.08%	7.118%
36	12.883	3577	3590	3601	rBV3	24345	39042	3.56%	0.402%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121222\
Data File : VU052349.D
Acq On : 12 Dec 2022 13:49
Operator : JC/MD
Sample : N5922-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0B20

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\SFAMUTR111822WMA.M
Title : TRACE VOA SFAM1.0

37	13.205	3679	3690	3702	rBV3	38194	63035	5.75%	0.648%
38	15.690	4454	4463	4474	rBV8	10735	16878	1.54%	0.174%
39	16.677	4762	4770	4780	rBV5	15032	21714	1.98%	0.223%
40	16.883	4823	4834	4846	rBV	176969	266690	24.31%	2.744%

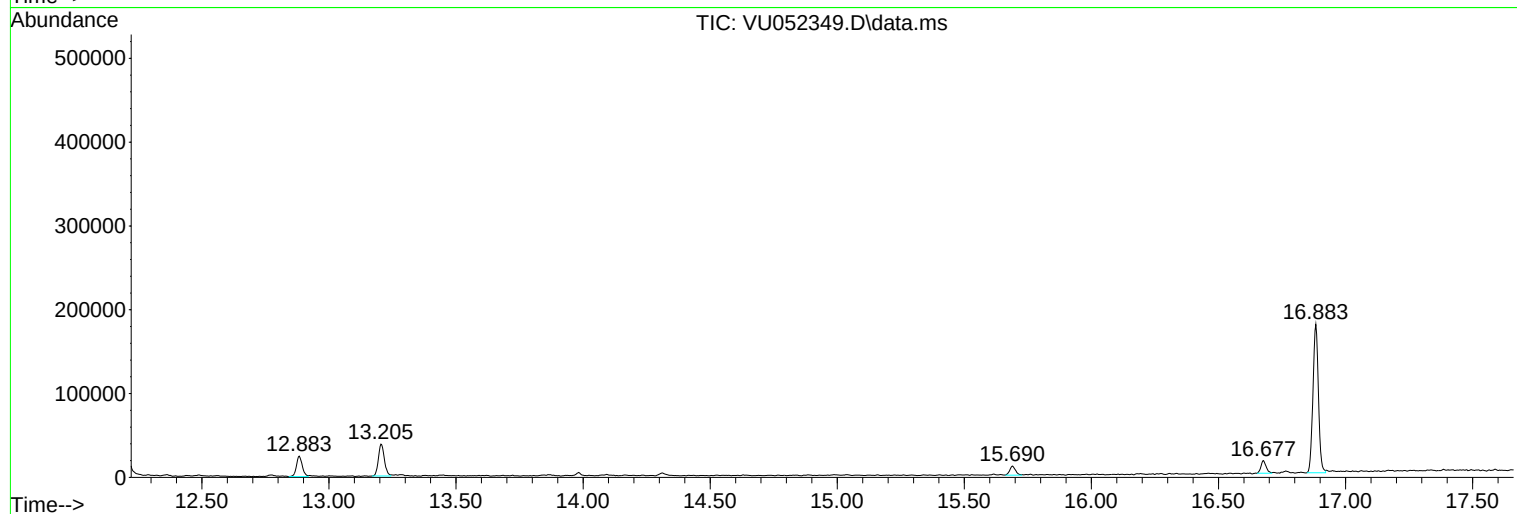
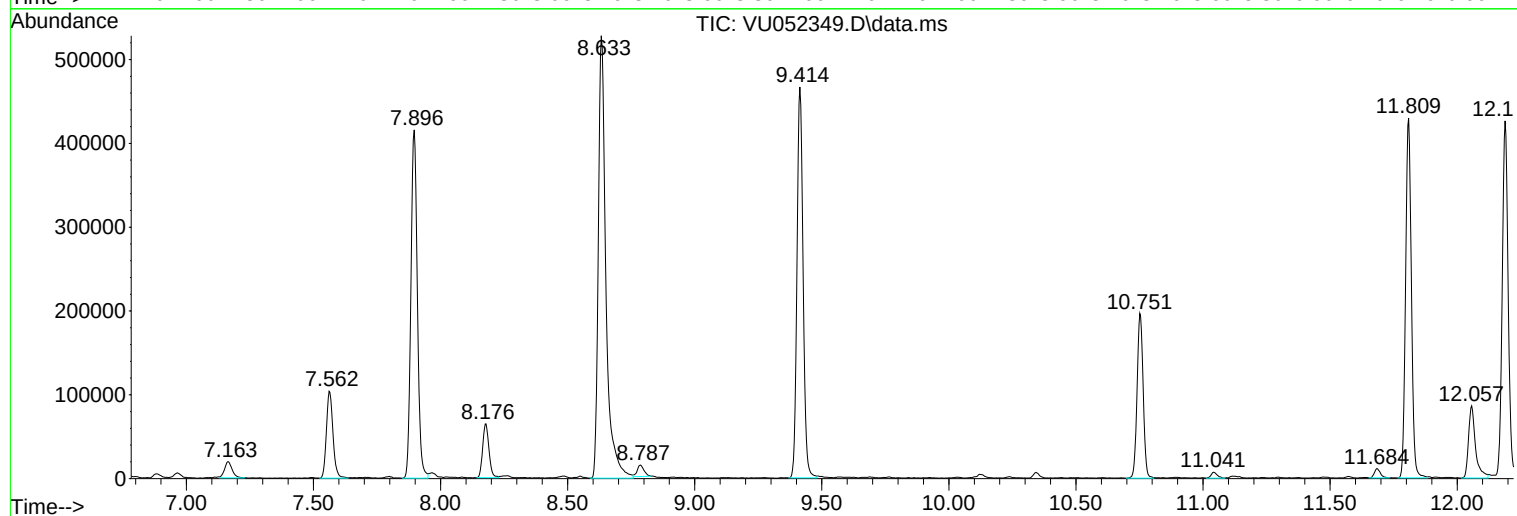
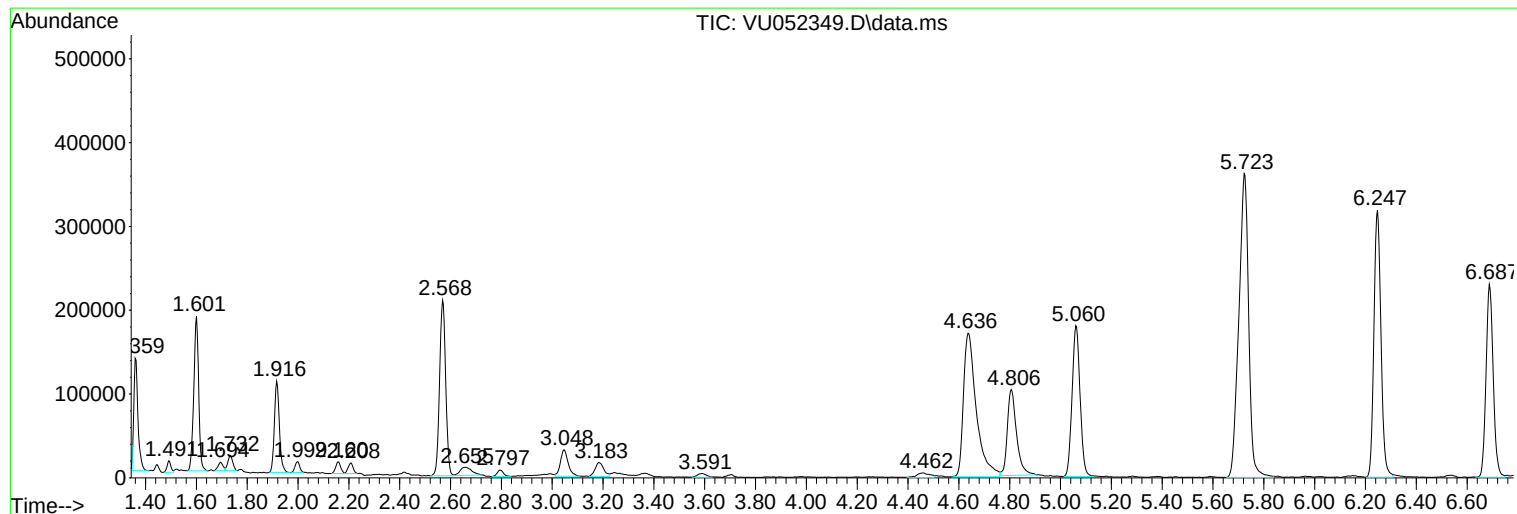
Sum of corrected areas: 9720791

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121222\
Data File : VU052349.D
Acq On : 12 Dec 2022 13:49
Operator : JC/MD
Sample : N5922-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0B20

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.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\VU121222\
Data File : VU052349.D
Acq On : 12 Dec 2022 13:49
Operator : JC/MD
Sample : N5922-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
COB20

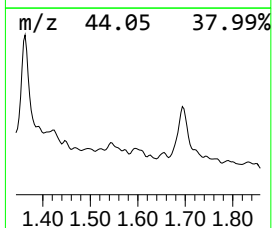
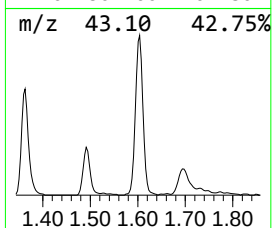
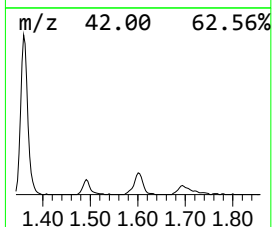
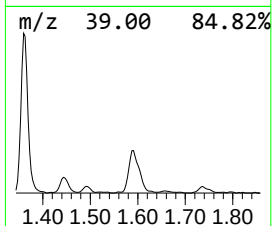
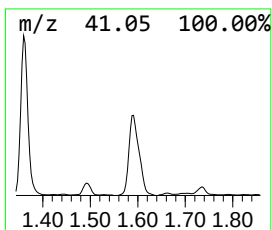
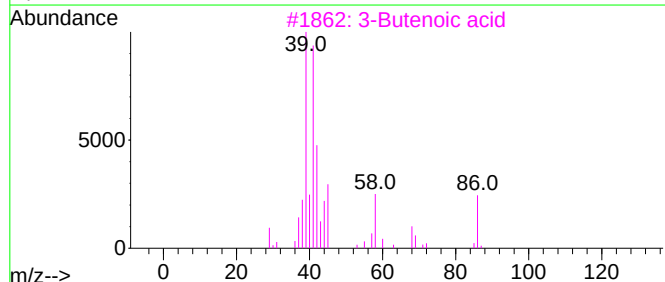
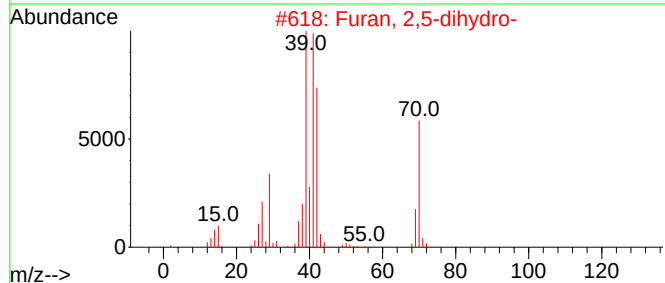
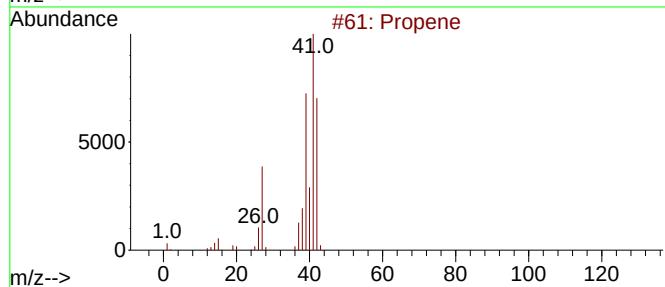
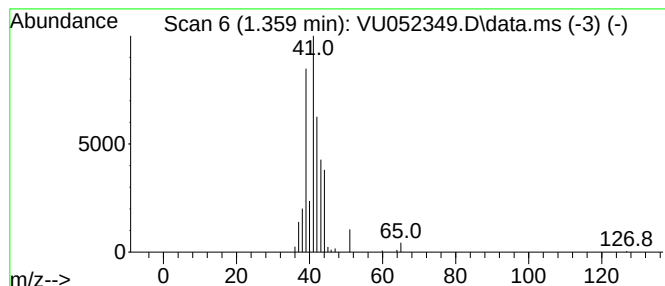
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.359	1.18 ug/L	144111	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	86
2			Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	78
3			3-Butenoic acid	86	C4H6O2	000625-38-7	74
4			Cyclopropanecarboxylic acid	86	C4H6O2	001759-53-1	74
5			2-Butenal, (E)-	70	C4H6O	000123-73-9	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121222\
Data File : VU052349.D
Acq On : 12 Dec 2022 13:49
Operator : JC/MD
Sample : N5922-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0B20

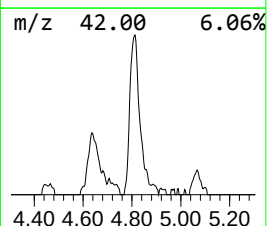
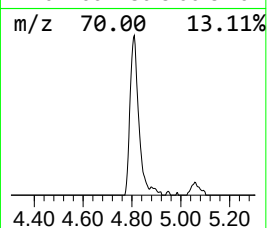
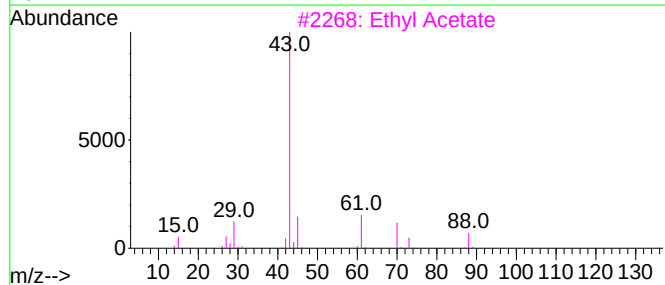
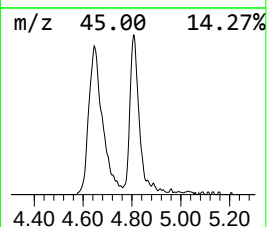
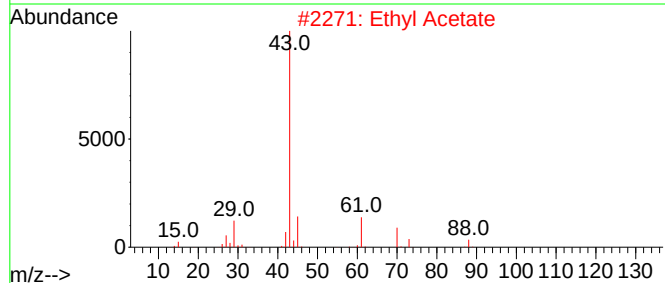
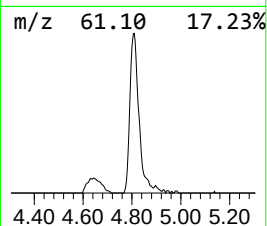
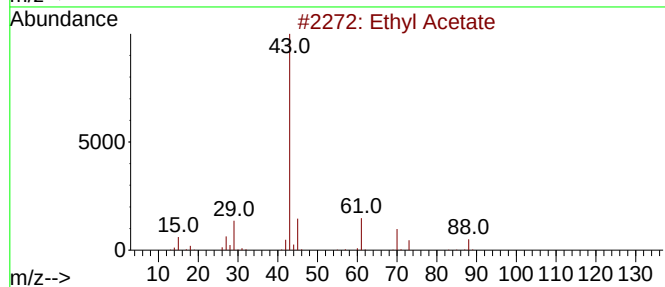
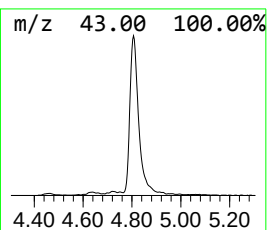
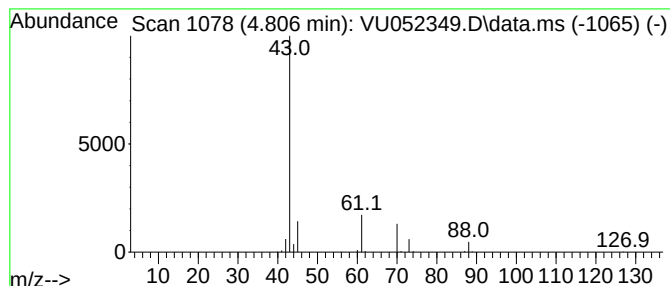
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Ethyl Acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.806	2.11 ug/L	258187	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl Acetate	88	C4H8O2	000141-78-6	90
2			Ethyl Acetate	88	C4H8O2	000141-78-6	86
3			Ethyl Acetate	88	C4H8O2	000141-78-6	83
4			Ethyl Acetate	88	C4H8O2	000141-78-6	50
5			CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121222\
Data File : VU052349.D
Acq On : 12 Dec 2022 13:49
Operator : JC/MD
Sample : N5922-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0B20

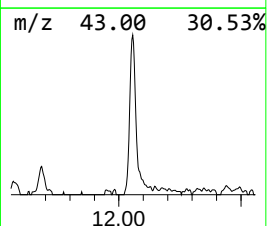
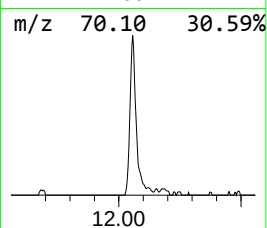
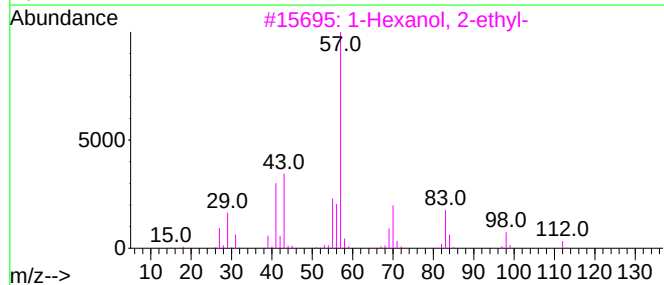
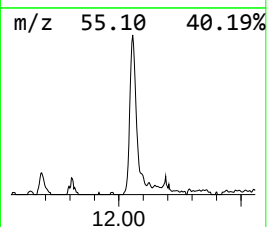
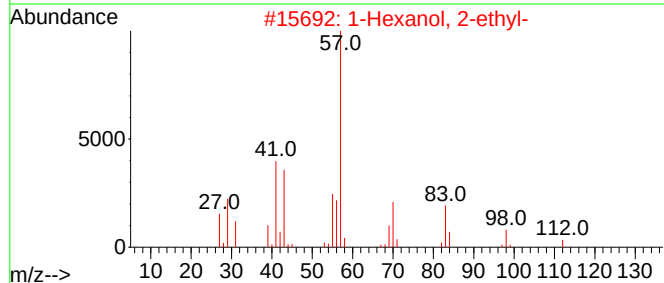
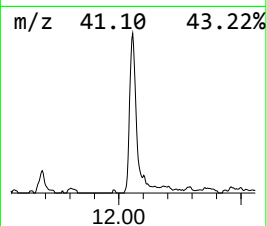
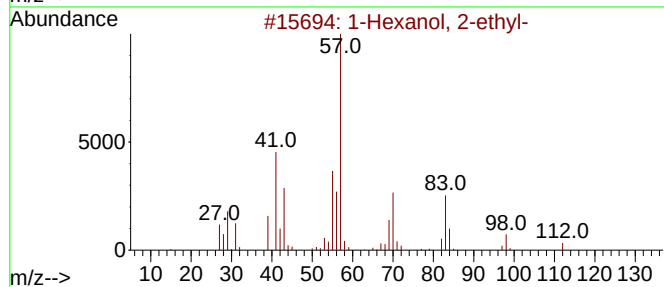
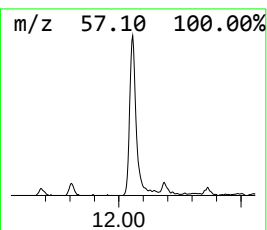
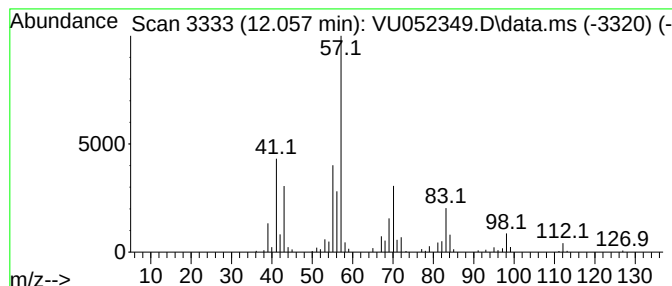
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.057	1.20 ug/L	164127	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	86
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121222\
Data File : VU052349.D
Acq On : 12 Dec 2022 13:49
Operator : JC/MD
Sample : N5922-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0B20

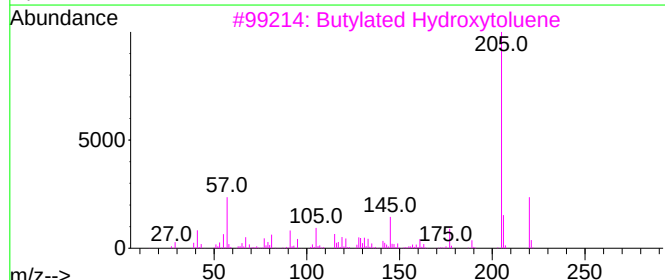
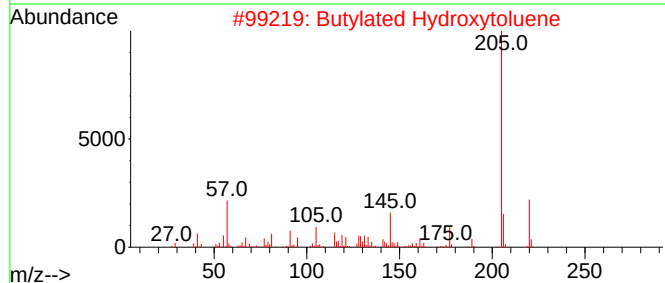
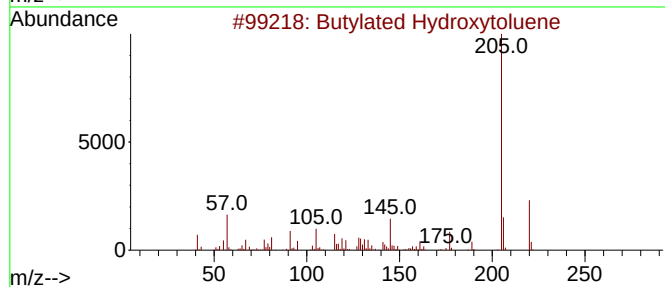
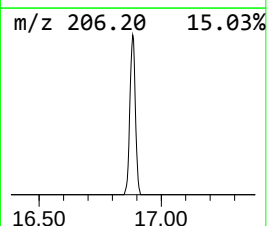
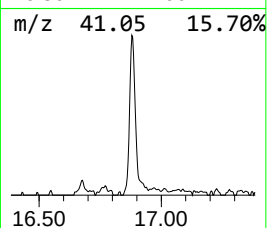
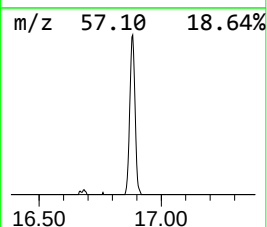
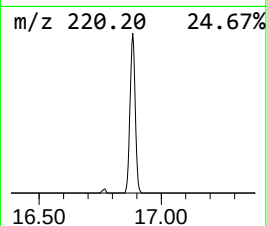
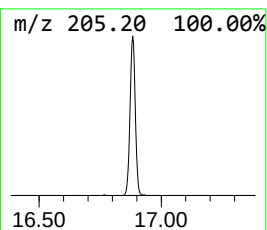
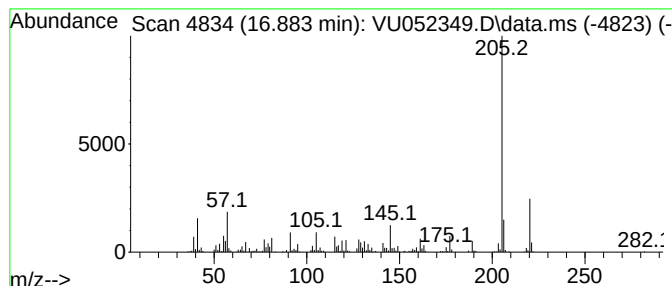
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Butylated Hydroxytoluene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.883	1.96 ug/L	266690	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	99
2			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	99
3			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
4			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	96
5			Ethyl 4-oxo-2-phenylpentanoate	220	C13H16O3	1000427-11-2	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121222\
Data File : VU052349.D
Acq On : 12 Dec 2022 13:49
Operator : JC/MD
Sample : N5922-03
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0B20

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.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...	1.359	1.2	ug/L	144111	1	6.247	612937	5.0
Ethyl Acetate	4.806	2.1	ug/L	258187	1	6.247	612937	5.0
1-Hexanol, 2-et...	12.057	1.2	ug/L	164127	3	11.809	681073	5.0
Butylated Hydro...	16.883	2.0	ug/L	266690	3	11.809	681073	5.0