

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU103122\
 Data File : VU051644.D
 Acq On : 01 Nov 2022 05:22
 Operator : JC/MD
 Sample : N5319-08
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHAA1

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.1

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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

Peak separation: 5

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

Signal : TIC: VU051644.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.375	310	322	342	rVB	3598465	5247477	3.77%	1.146%
2	3.989	806	824	852	rVB	2821114	7140032	5.13%	1.559%
3	4.530	974	992	1012	rBV	1074337	2839854	2.04%	0.620%
4	4.661	1012	1033	1076	rVB2	955877	2826543	2.03%	0.617%
5	5.780	1345	1381	1438	rBV2	49124545	113035263	81.19%	24.688%
6	7.980	2048	2065	2119	rVB3	65178161	139214668	100.00%	30.406%
7	9.446	2500	2521	2546	rBV	11328907	19138144	13.75%	4.180%
8	9.568	2546	2559	2582	rVV	12901286	20536323	14.75%	4.485%
9	9.697	2583	2599	2636	rVB2	48502979	80692781	57.96%	17.624%
10	10.099	2710	2724	2756	rVB	17245390	26886538	19.31%	5.872%
11	10.481	2826	2843	2855	rBV	890571	1438093	1.03%	0.314%
12	10.902	2956	2974	2990	rBV	1441240	2777940	2.00%	0.607%
13	10.996	2990	3003	3010	rBV	3045037	5270720	3.79%	1.151%
14	11.086	3022	3031	3048	rVB	1823068	2783017	2.00%	0.608%
15	11.288	3084	3094	3117	rVB	1809419	2809845	2.02%	0.614%
16	11.465	3137	3149	3168	rVB	7742923	11441367	8.22%	2.499%
17	11.893	3272	3282	3295	rVB	2392290	3695109	2.65%	0.807%
18	12.092	3327	3344	3362	rBV2	1226953	2261016	1.62%	0.494%
19	12.192	3362	3375	3398	rVB5	859035	2269961	1.63%	0.496%
20	12.478	3448	3464	3484	rBV3	1348283	3556447	2.55%	0.777%
21	12.857	3574	3582	3600	rVB2	1208820	1988497	1.43%	0.434%

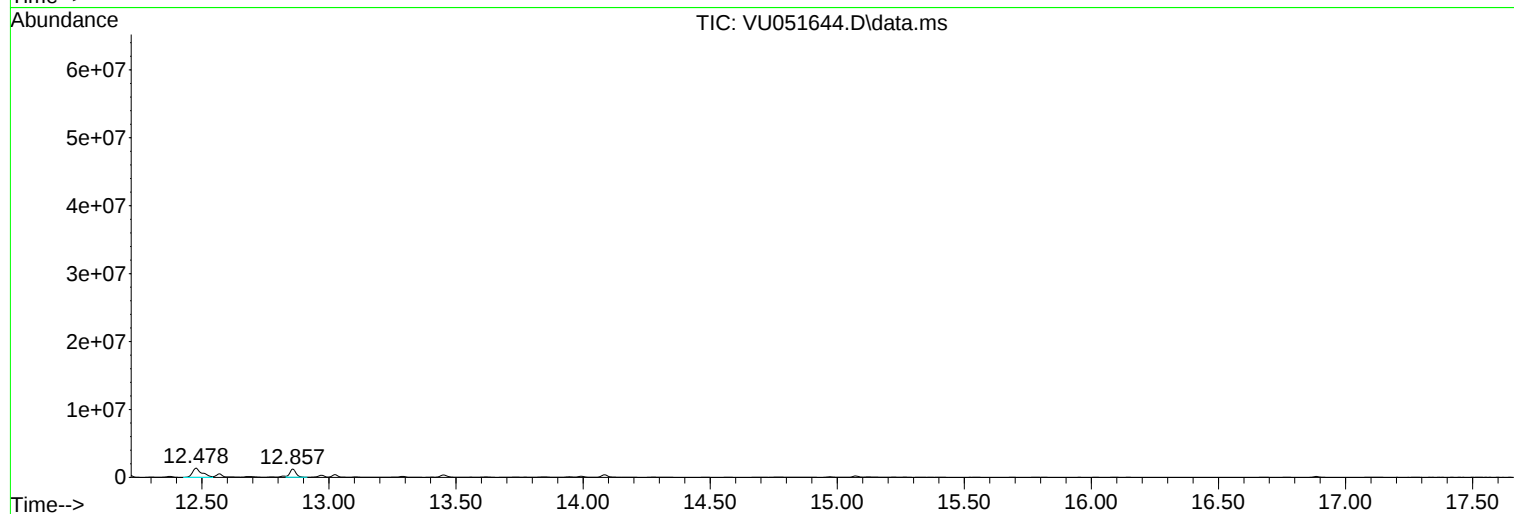
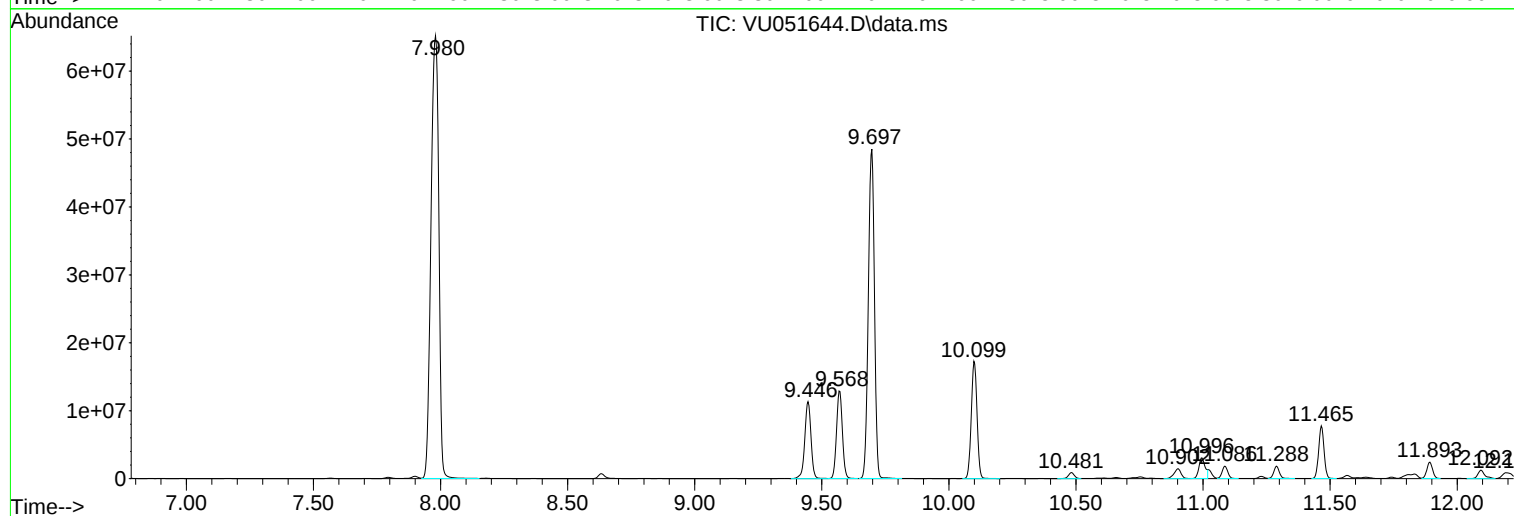
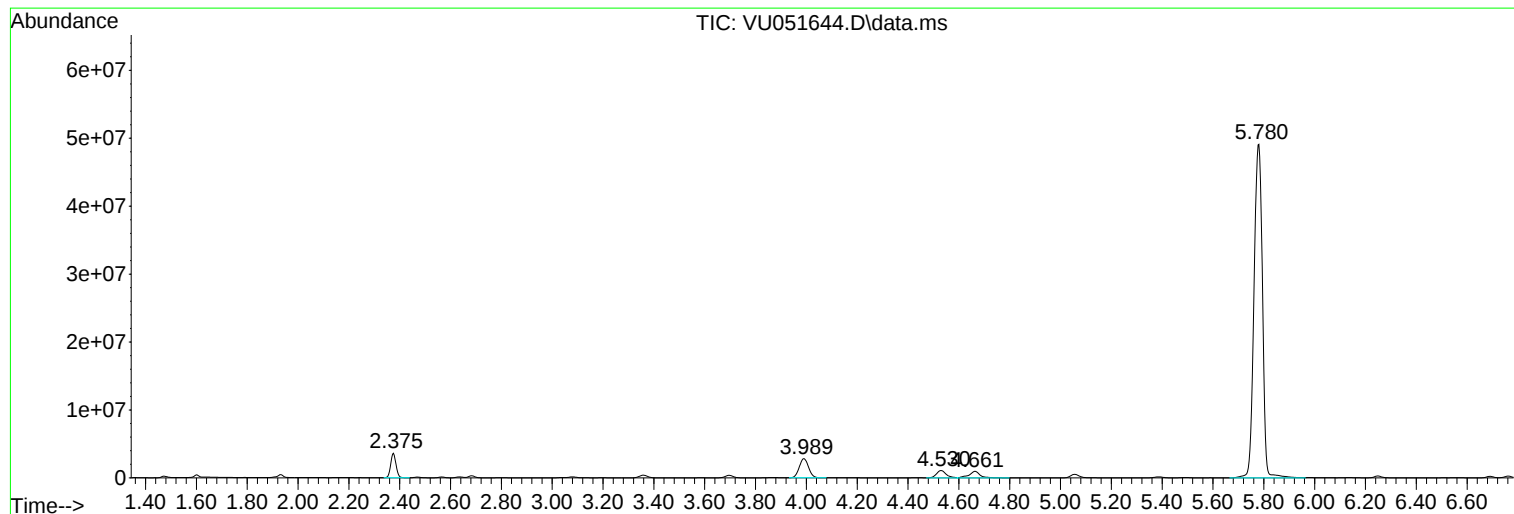
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ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHAA1

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

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



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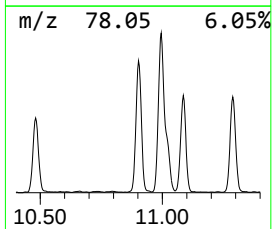
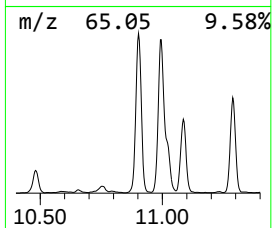
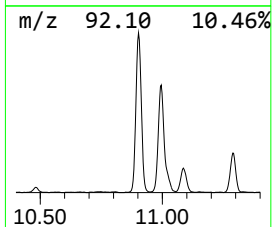
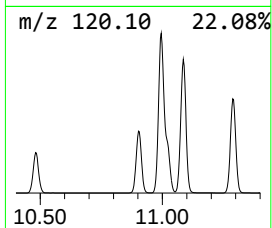
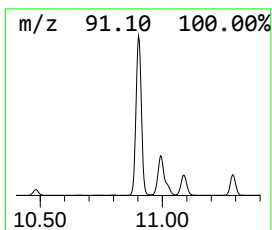
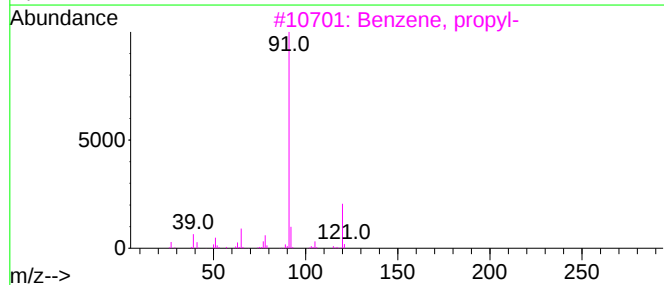
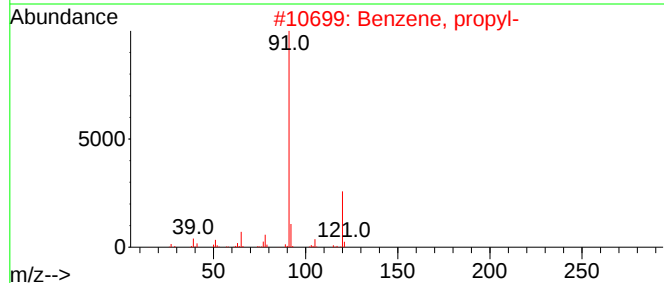
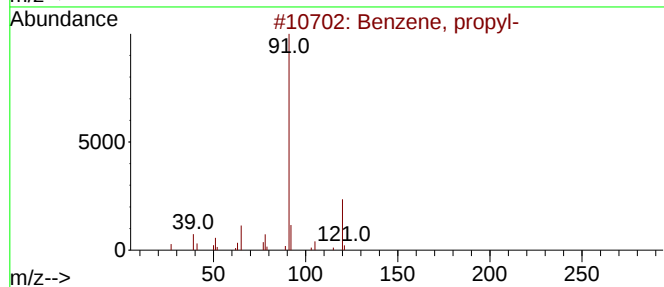
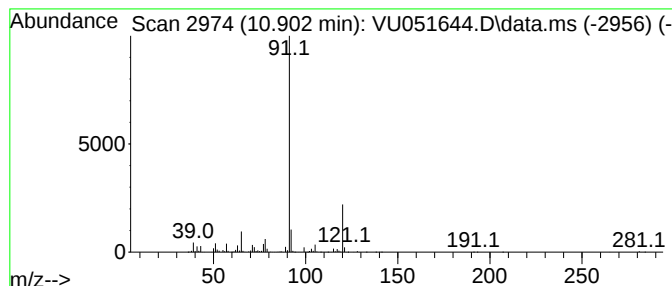
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Benzene, propyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.902	3.76 ug/L	2777940	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, propyl-	120	C9H12	000103-65-1	93
2			Benzene, propyl-	120	C9H12	000103-65-1	87
3			Benzene, propyl-	120	C9H12	000103-65-1	87
4			N-Butylbenzylamine	163	C11H17N	002403-22-7	64
5			N-Isobutyl(phenyl)methanesulfona...	227	C11H17NO2S	144615-94-1	64



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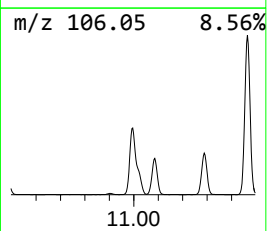
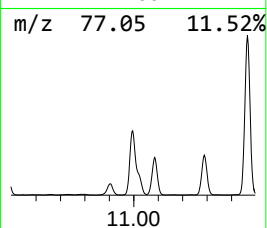
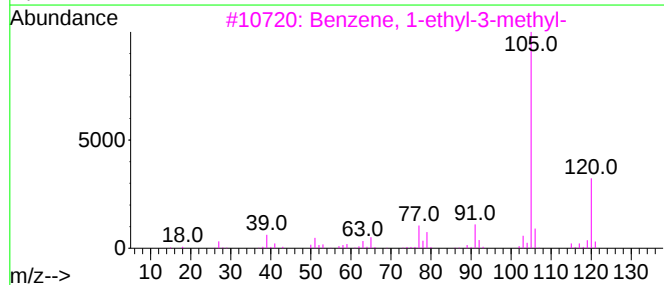
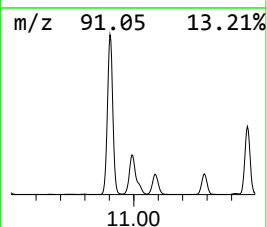
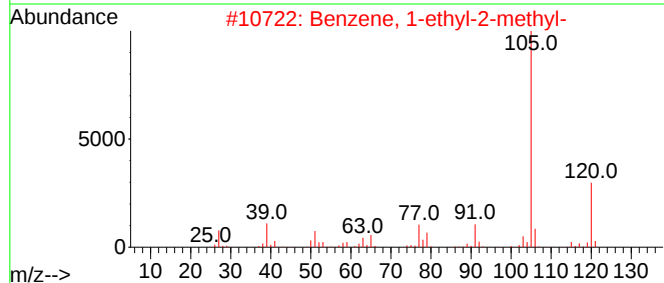
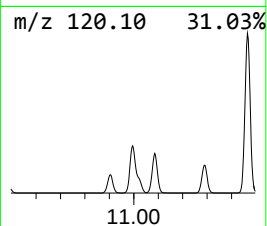
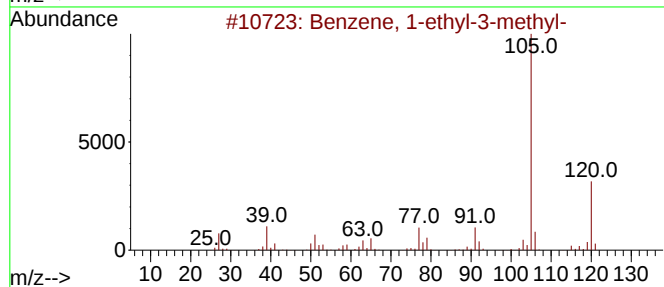
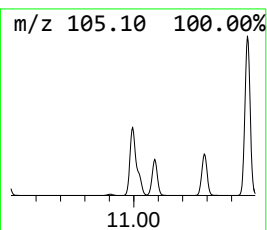
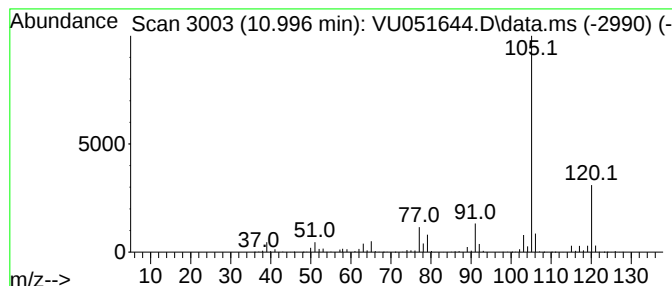
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Benzene, 1-ethyl-3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.996	7.13 ug/L	5270720	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
4			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



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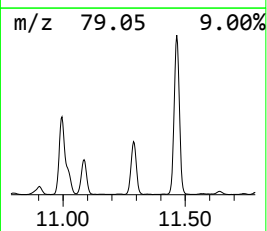
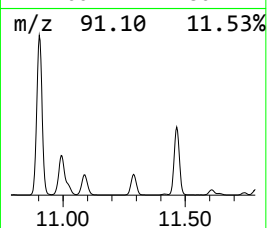
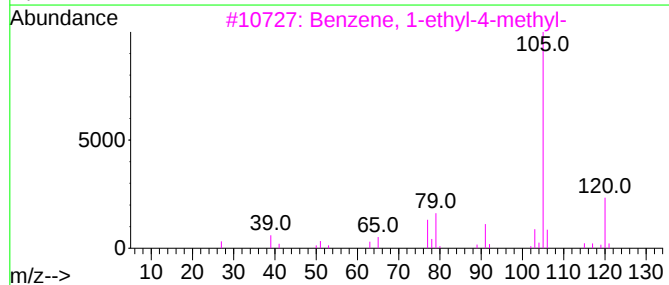
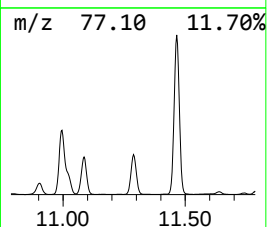
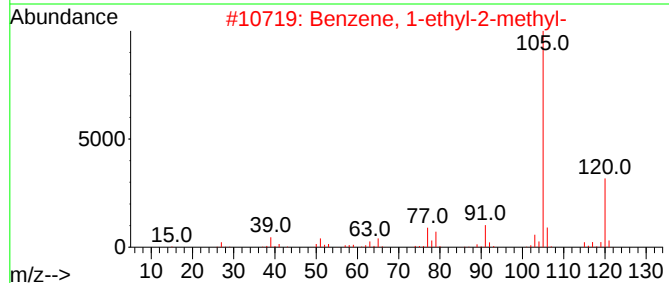
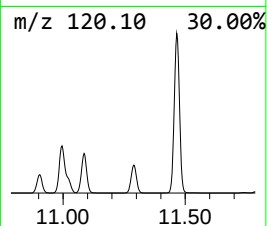
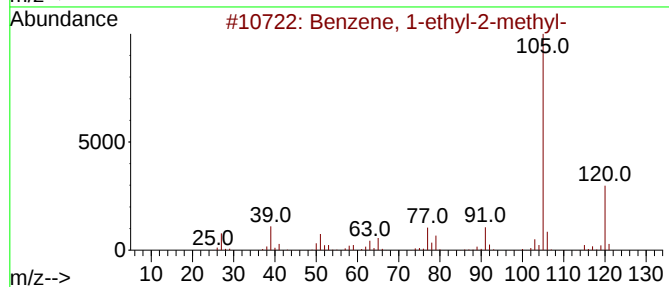
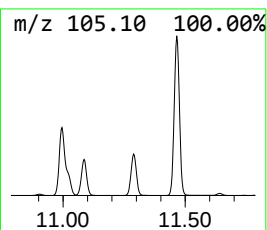
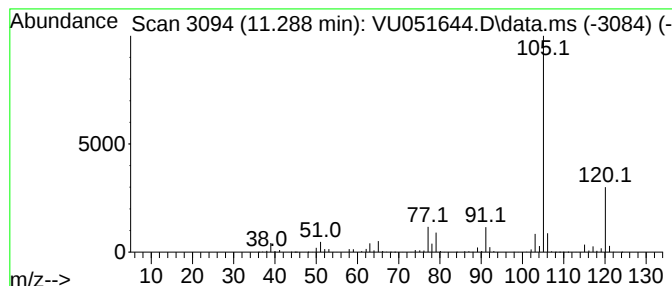
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.288	3.80 ug/L	2809850	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	93
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90
5			Mesitylene	120	C9H12	000108-67-8	90



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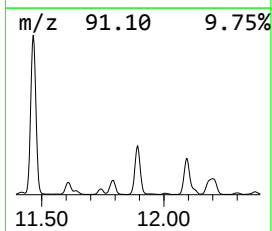
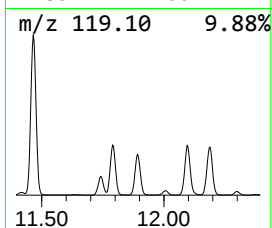
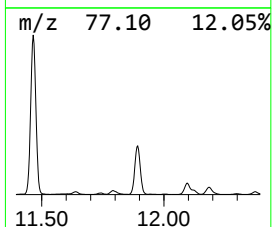
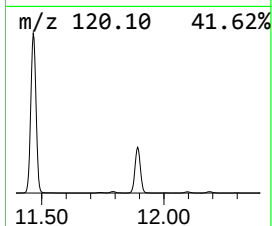
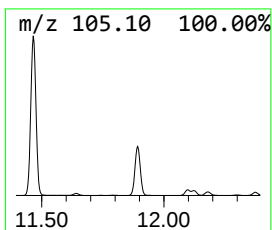
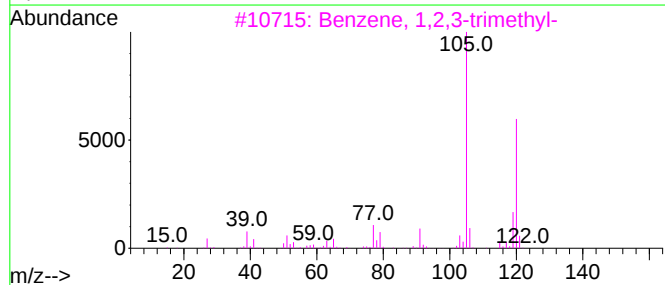
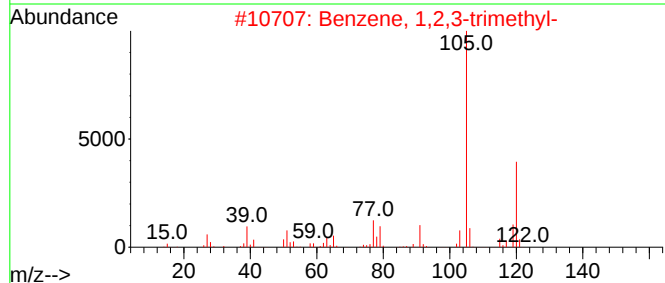
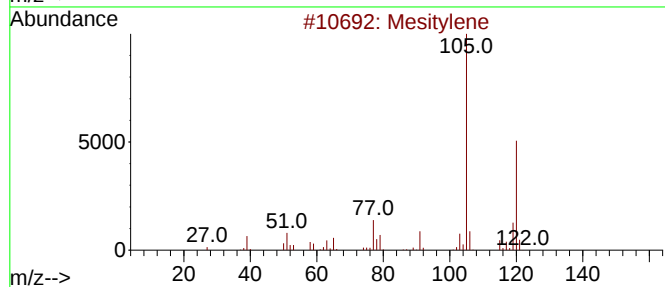
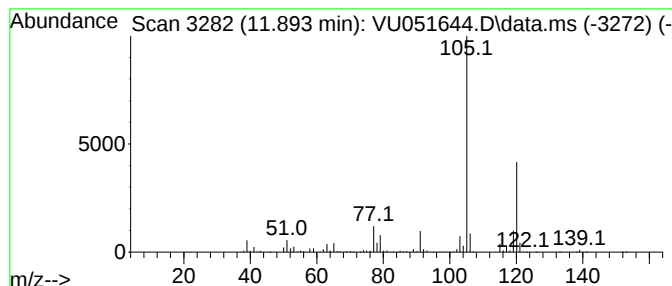
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1,2,3-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.893	5.00 ug/L	3695110	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	97
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
4			Mesitylene	120	C9H12	000108-67-8	94
5			Mesitylene	120	C9H12	000108-67-8	91



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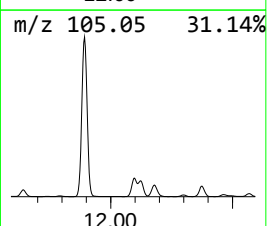
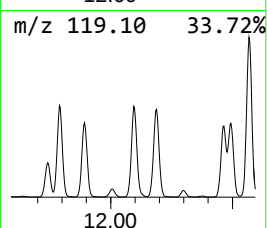
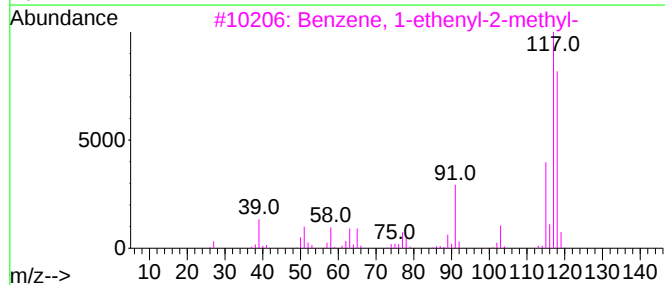
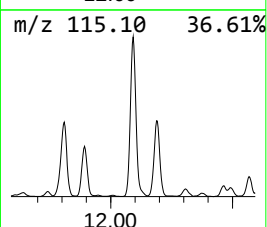
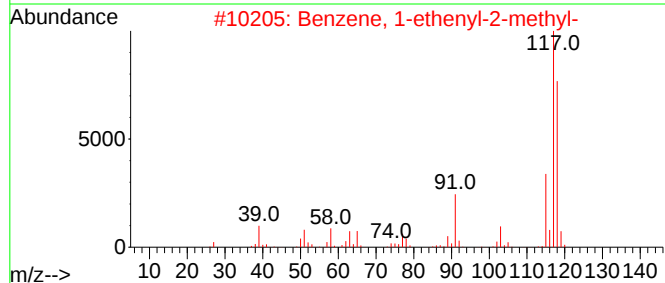
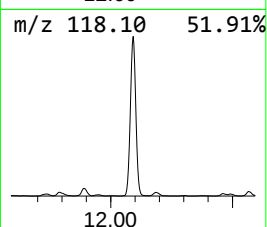
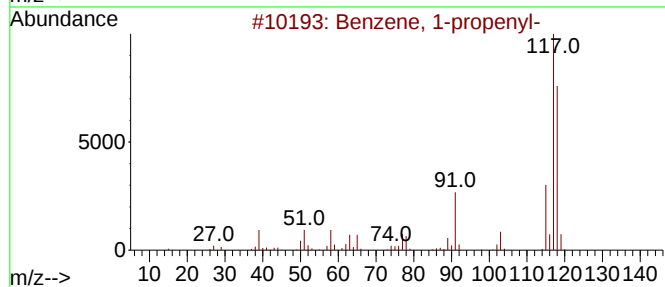
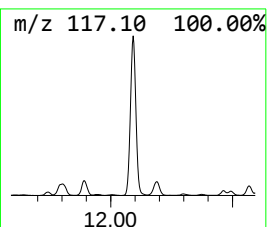
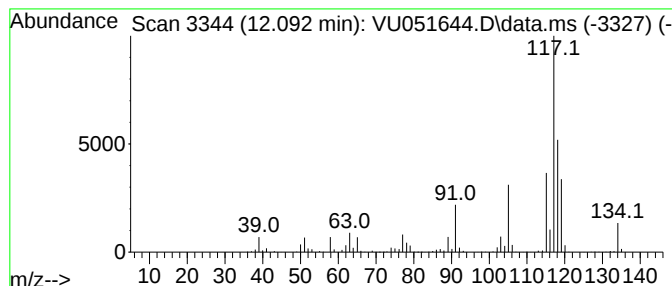
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Benzene, 1-propenyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.092	3.06 ug/L	2261020	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-propenyl-	118	C9H10	000637-50-3	92
2			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	91
3			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	86
4			Indane	118	C9H10	000496-11-7	64
5			Deltacyclene	118	C9H10	007785-10-6	64



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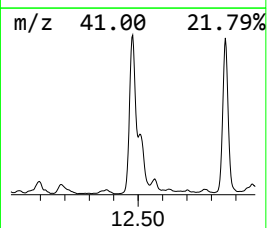
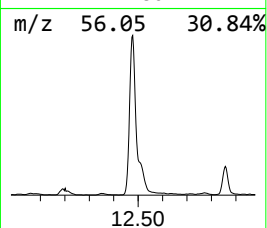
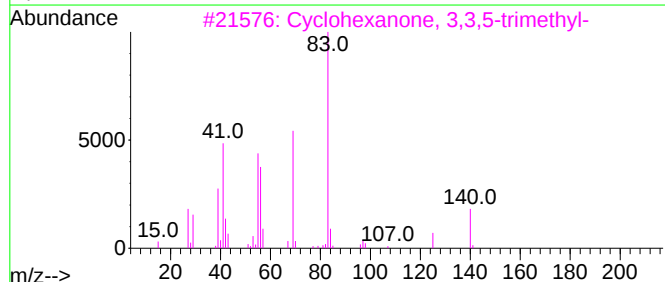
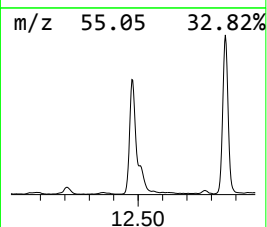
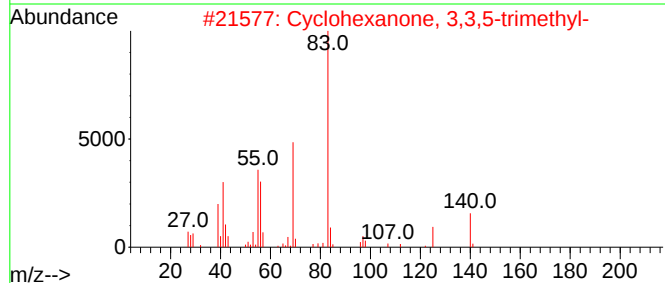
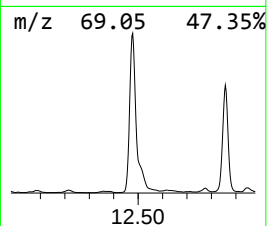
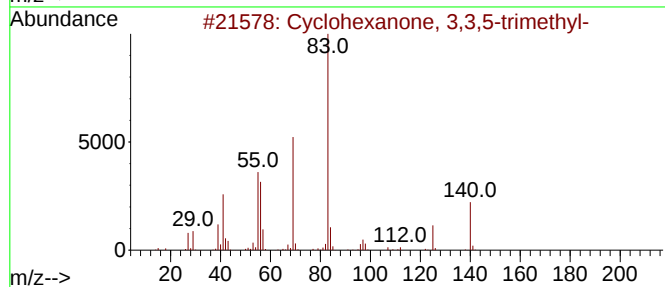
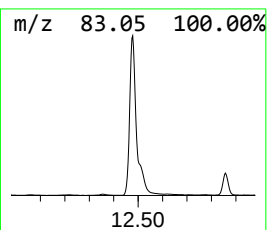
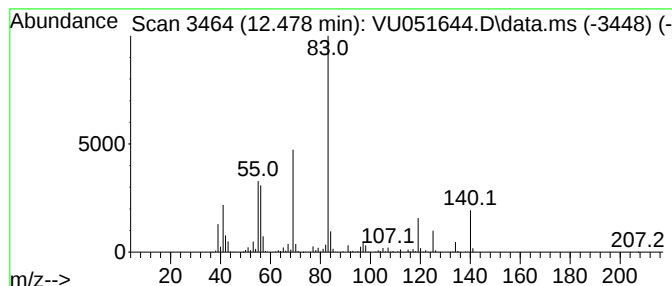
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Cyclohexanone, 3,3,5-trimet... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.478	4.81 ug/L	3556450	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	96
2			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	93
3			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	90
4			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	90
5			1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU103122\
Data File : VU051644.D
Acq On : 01 Nov 2022 05:22
Operator : JC/MD
Sample : N5319-08
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHAA1

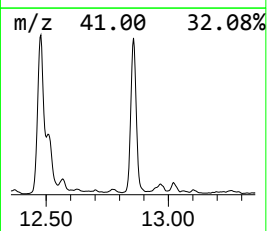
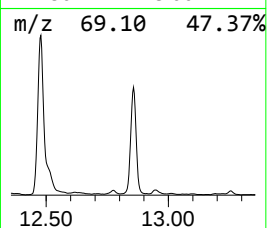
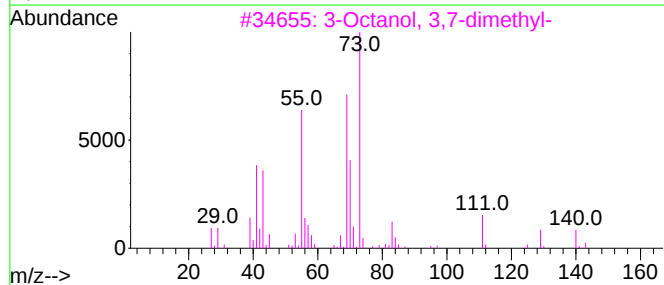
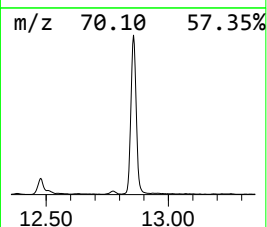
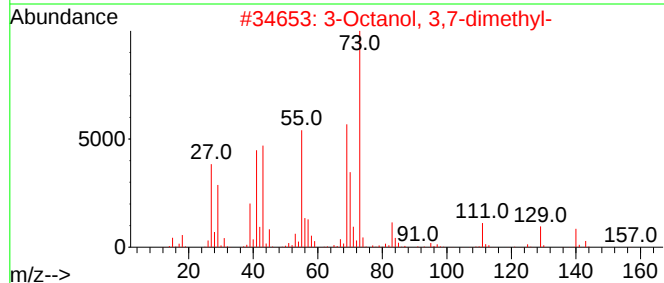
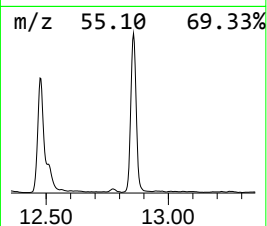
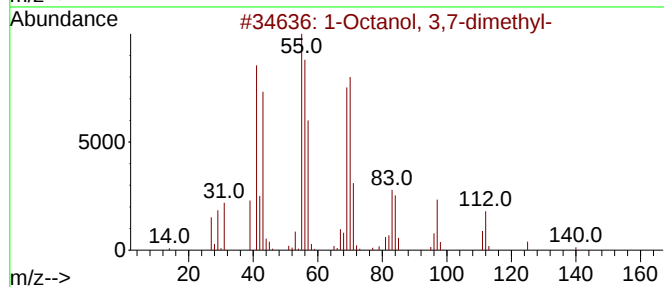
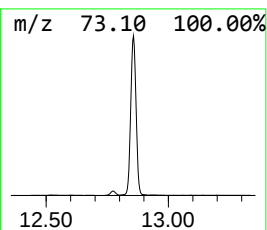
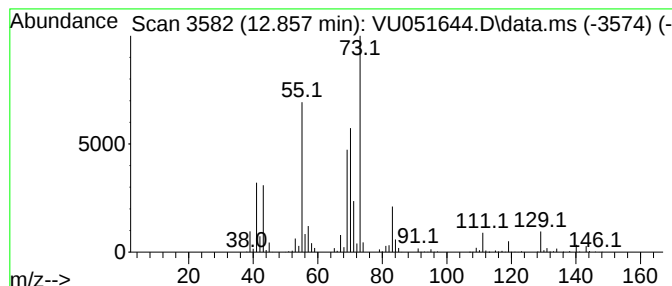
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 1-Octanol, 3,7-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.857	2.69 ug/L	1988500	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octanol, 3,7-dimethyl-	158	C10H22O	000106-21-8	50
2			3-Octanol, 3,7-dimethyl-	158	C10H22O	000078-69-3	43
3			3-Octanol, 3,7-dimethyl-	158	C10H22O	000078-69-3	40
4			5-Ethyl-1-nonene	154	C11H22	019780-74-6	40
5			1-Heptene, 5-methyl-	112	C8H16	013151-04-7	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU103122\
 Data File : VU051644.D
 Acq On : 01 Nov 2022 05:22
 Operator : JC/MD
 Sample : N5319-08
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHAA1

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

TIC Library : C:\Database\NIST0.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, propyl-	10.902	3.8	ug/L	2777940	3	11.809	3695110	5.0
Benzene, 1-ethy...	10.996	7.1	ug/L	5270720	3	11.809	3695110	5.0
Benzene, 1-ethy...	11.288	3.8	ug/L	2809850	3	11.809	3695110	5.0
Benzene, 1,2,3-...	11.893	5.0	ug/L	3695110	3	11.809	3695110	5.0
Benzene, 1-prop...	12.092	3.1	ug/L	2261020	3	11.809	3695110	5.0
Cyclohexanone, ...	12.478	4.8	ug/L	3556450	3	11.809	3695110	5.0
1-Octanol, 3,7-...	12.857	2.7	ug/L	1988500	3	11.809	3695110	5.0