

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121422\
 Data File : VU052396.D
 Acq On : 14 Dec 2022 13:36
 Operator : JC/MD
 Sample : N6031-02
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0B24

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: VU052396.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.491	37	47	67	rBV	28713	89533	8.51%	1.053%
2	1.601	72	81	94	rVB	110019	138397	13.16%	1.628%
3	1.916	170	179	193	rVB	96623	128540	12.22%	1.512%
4	2.568	367	382	397	rBV	173150	284484	27.05%	3.347%
5	4.639	1011	1026	1066	rBV	133287	442943	42.12%	5.211%
6	4.809	1068	1079	1105	rVB3	36088	93114	8.86%	1.096%
7	5.060	1141	1157	1177	rBV	169578	370559	35.24%	4.360%
8	5.723	1342	1363	1386	rBV2	333437	882888	83.96%	10.388%
9	6.247	1511	1526	1550	rBV	286256	546067	51.93%	6.425%
10	6.687	1646	1663	1685	rBV	214604	422557	40.18%	4.972%
11	7.163	1794	1811	1824	rBV2	21829	46449	4.42%	0.546%
12	7.562	1923	1935	1959	rBV	88015	159922	15.21%	1.882%
13	7.896	2024	2039	2059	rBV	358026	636236	60.51%	7.486%
14	8.176	2113	2126	2143	rBV	56213	97478	9.27%	1.147%
15	8.632	2252	2268	2308	rBV2	514496	1051540	100.00%	12.372%
16	9.414	2497	2511	2529	rBV	422290	708183	67.35%	8.332%
17	10.751	2910	2927	2946	rBV	191856	313604	29.82%	3.690%
18	11.809	3243	3256	3274	rBV	356280	572371	54.43%	6.734%
19	12.189	3359	3374	3394	rBV	354210	581185	55.27%	6.838%
20	16.677	4761	4770	4782	rBV4	39528	61620	5.86%	0.725%
21	16.883	4822	4834	4850	rBV	565562	871785	82.91%	10.257%

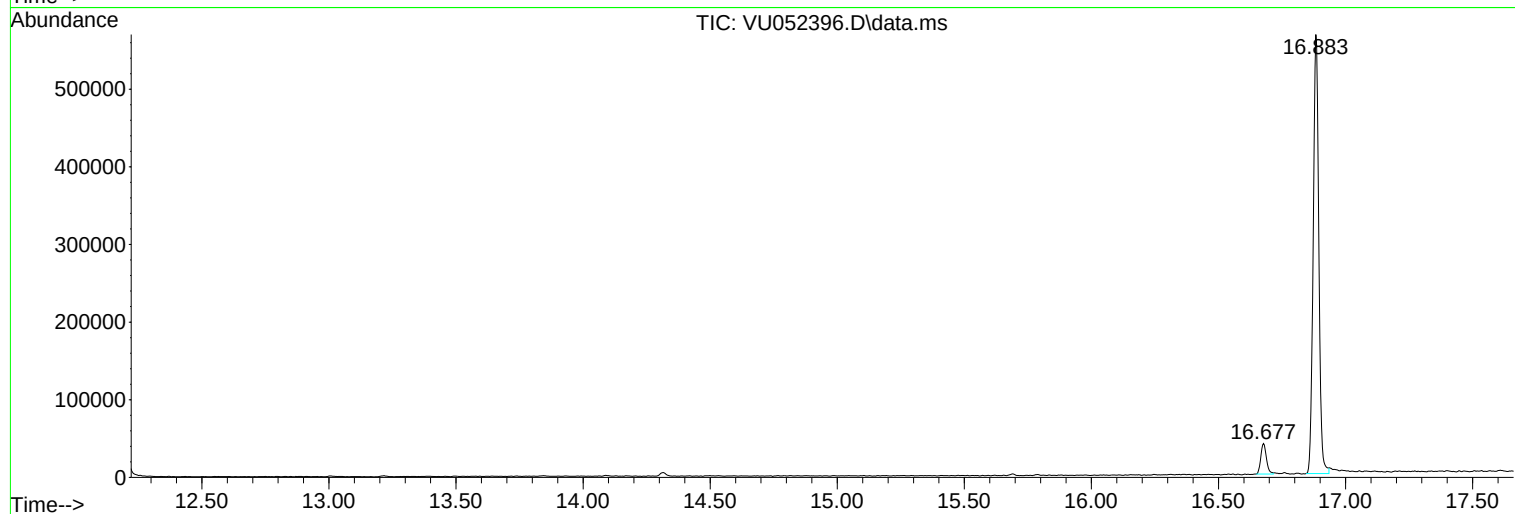
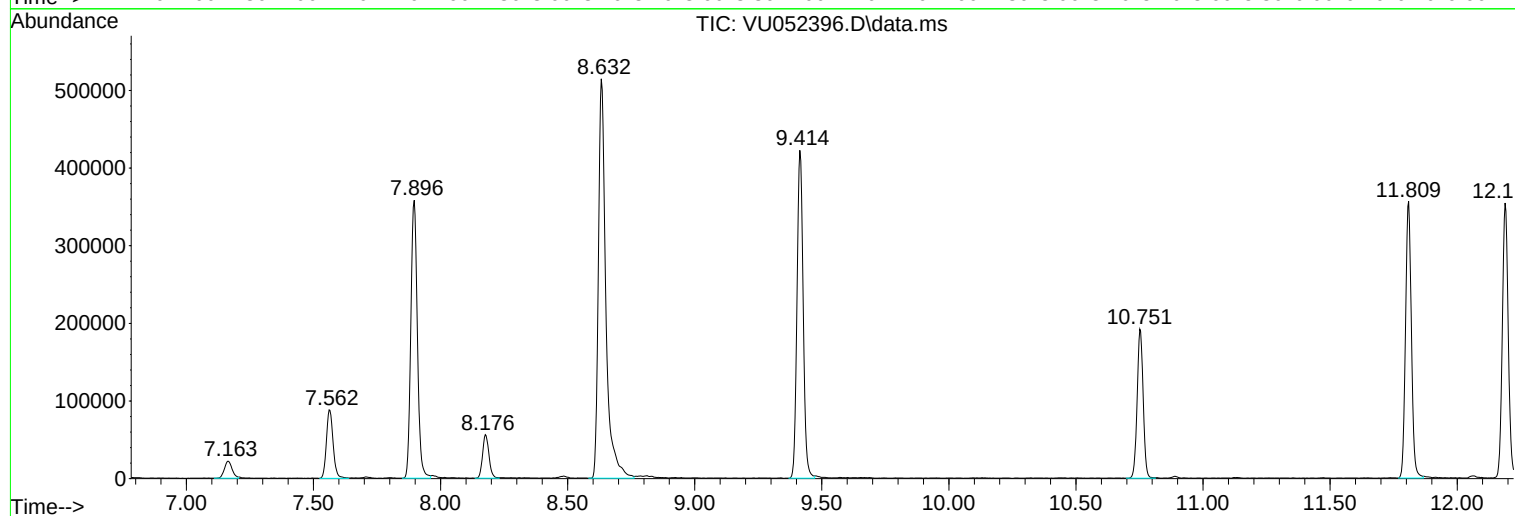
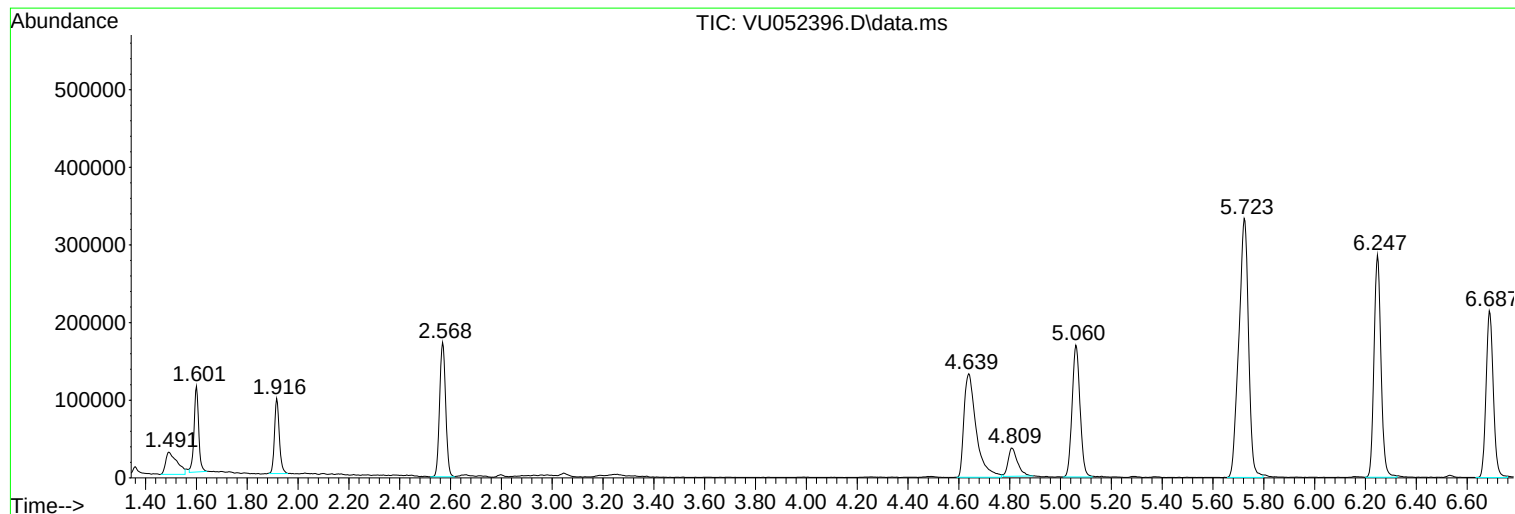
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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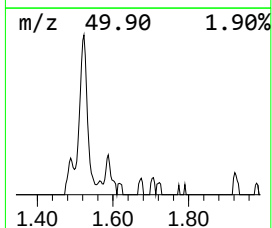
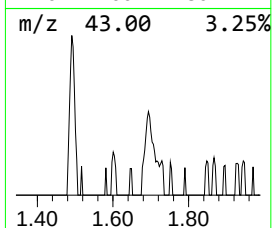
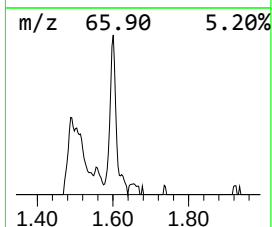
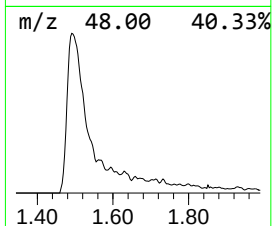
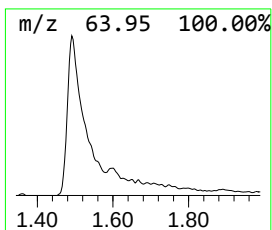
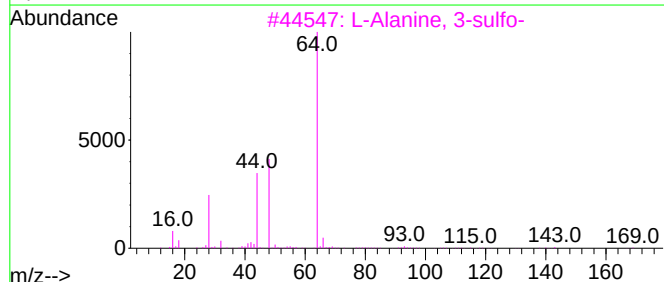
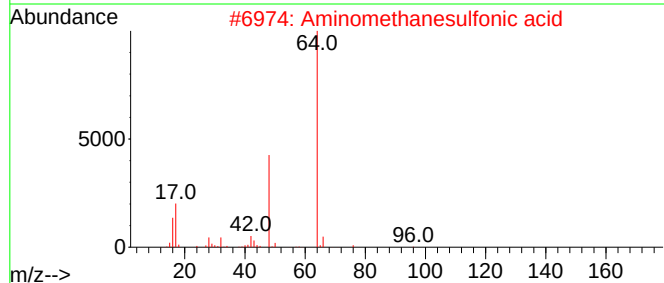
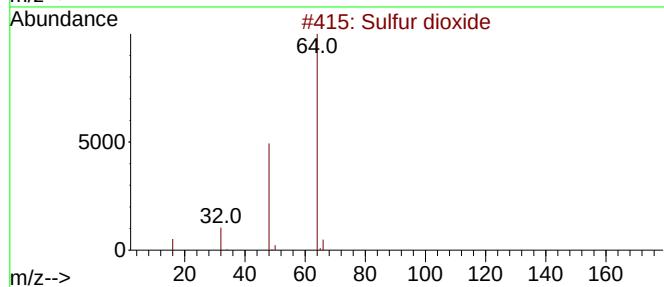
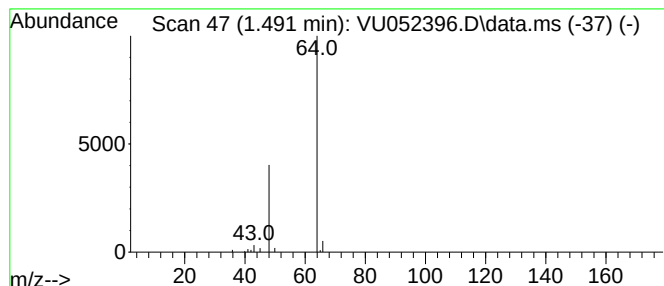
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.491	0.82 ug/L	89533	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Sulfur dioxide	64	O2S	007446-09-5	5
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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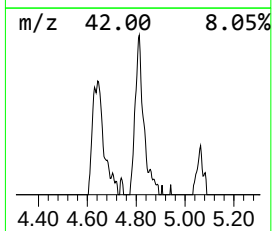
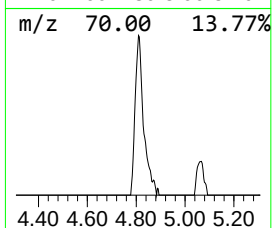
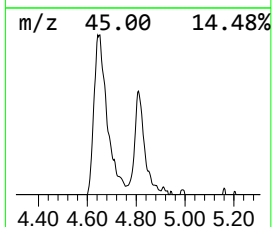
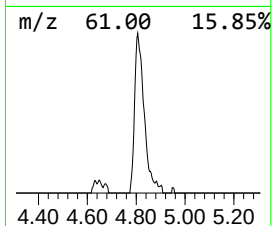
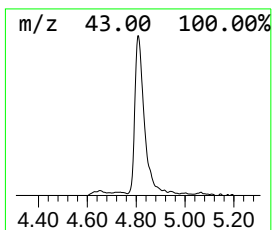
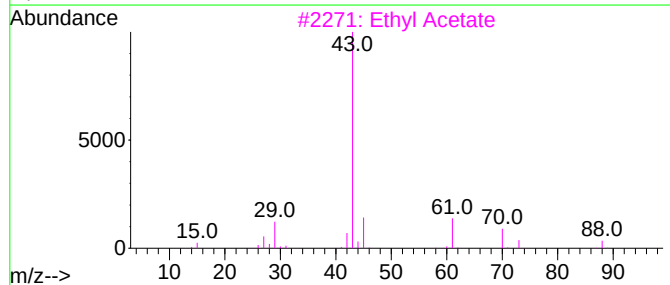
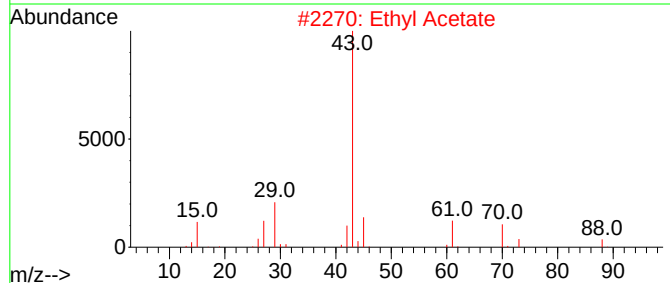
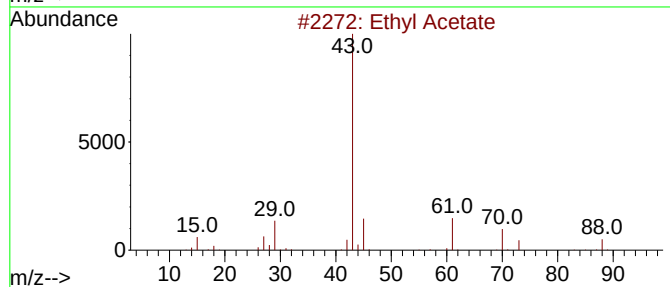
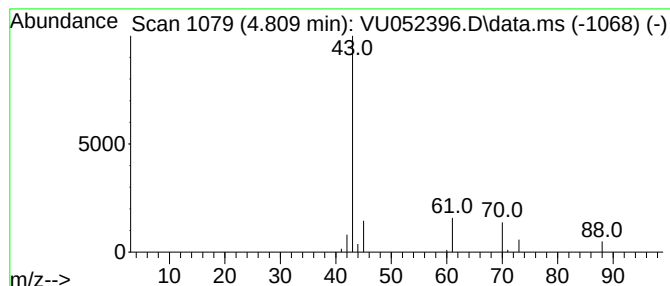
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Ethyl Acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.809	0.85 ug/L	93114	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	90
3			Ethyl Acetate	88	C4H8O2	000141-78-6	86
4			Ethyl Acetate	88	C4H8O2	000141-78-6	83
5			CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	78



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ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0B24

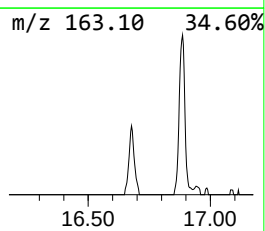
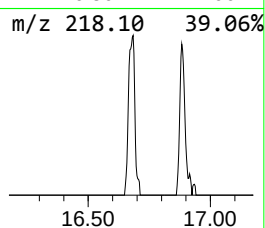
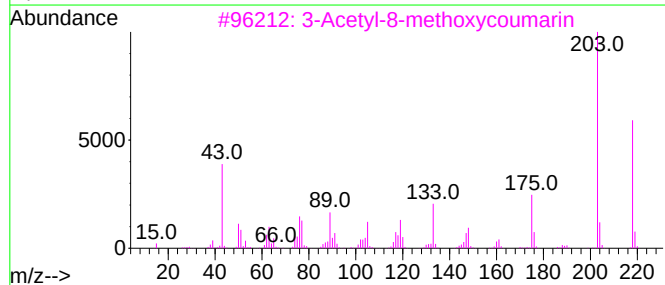
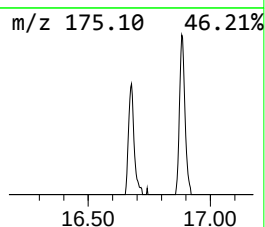
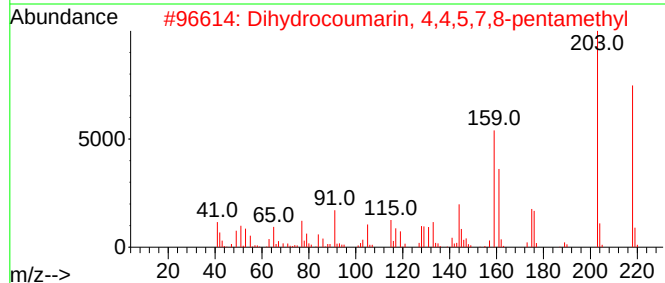
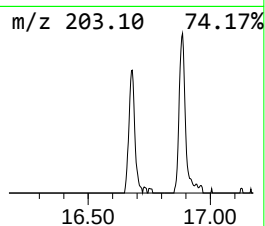
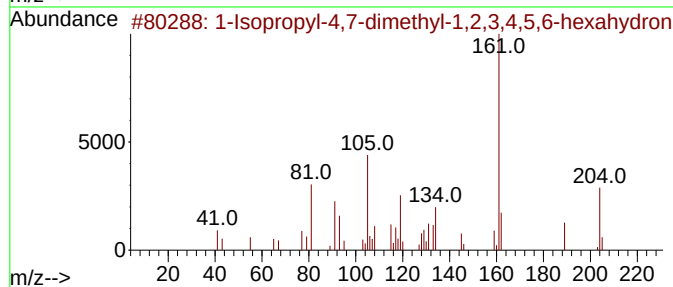
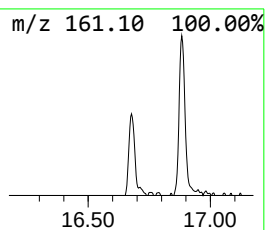
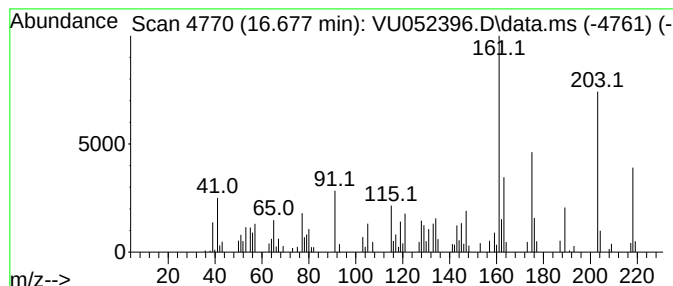
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 1-Isopropyl-4,7-dimethyl-1,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.677	0.54 ug/L	61620	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Isopropyl-4,7-dimethyl-1,2,3,4...	204	C15H24	016729-00-3	60
2			Dihydrocoumarin, 4,4,5,7,8-penta...	218	C14H18O2	039170-97-3	50
3			3-Acetyl-8-methoxycoumarin	218	C12H10O4	005452-39-1	46
4			(4aS)-3,5,5,9-Tetramethyl-1,2,5...	218	C15H22O	064825-84-9	46
5			1s,4R,7R,11R-1,3,4,7-Tetramethyl...	218	C15H22O	137235-42-8	42



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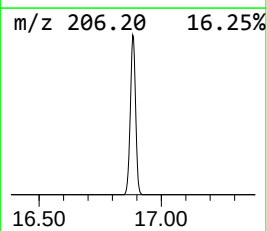
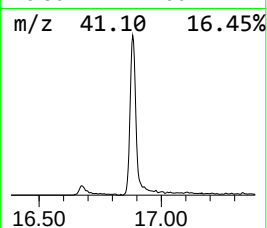
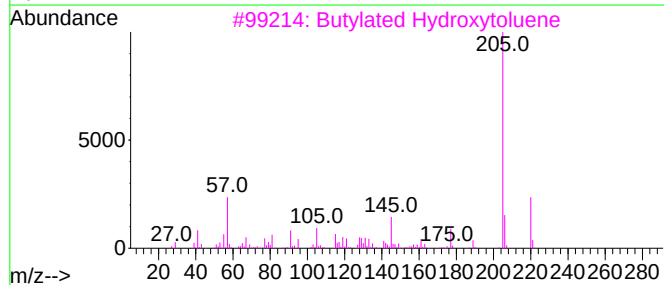
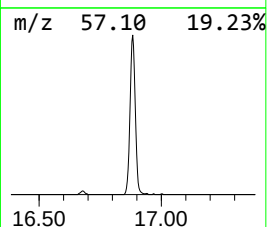
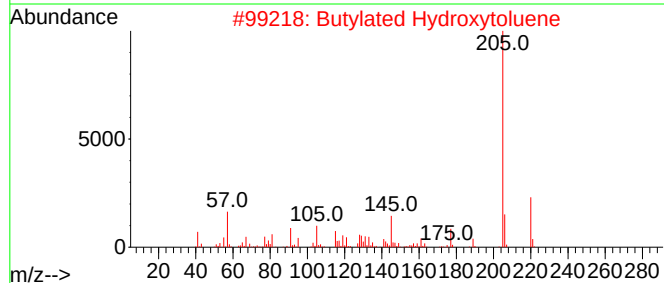
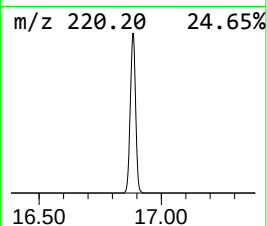
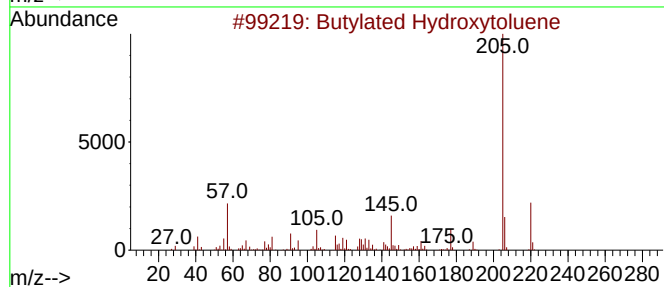
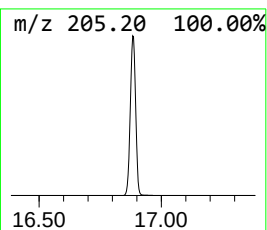
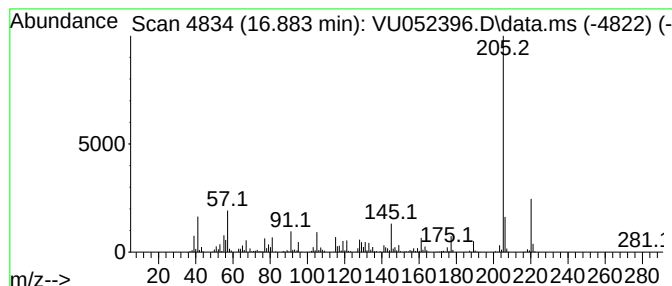
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.883	7.62 ug/L	871785	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	97
5			Ethyl 4-oxo-2-phenylpentanoate	220	C13H16O3	1000427-11-2	96



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.491	0.8	ug/L	89533	1	6.247	546067	5.0
Ethyl Acetate	4.809	0.8	ug/L	93114	1	6.247	546067	5.0
1-Isopropyl-4,7...	16.677	0.5	ug/L	61620	3	11.809	572371	5.0
Butylated Hydro...	16.883	7.6	ug/L	871785	3	11.809	572371	5.0