

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU103122\
 Data File : VU051609.D
 Acq On : 31 Oct 2022 14:12
 Operator : JC/MD
 Sample : N5319-02
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHA97

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: VU051609.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.469	30	40	52	rBV	166775	309163	25.31%	3.366%
2	1.597	74	80	120	rVB2	127842	327123	26.78%	3.561%
3	1.912	170	178	190	rVB	94931	127295	10.42%	1.386%
4	2.375	314	322	338	rVB2	67466	112474	9.21%	1.225%
5	2.565	369	381	394	rBV	125198	204784	16.76%	2.230%
6	3.044	519	530	541	rBV2	8298	15313	1.25%	0.167%
7	3.356	616	627	642	rVB6	6388	13036	1.07%	0.142%
8	3.928	775	805	816	rBV	9139	46809	3.83%	0.510%
9	3.996	820	826	843	rVB2	9922	20424	1.67%	0.222%
10	4.620	1004	1020	1066	rBV	192640	507332	41.53%	5.523%
11	5.060	1141	1157	1180	rBV	189835	425895	34.86%	4.637%
12	5.722	1343	1363	1392	rBV2	310014	876435	71.74%	9.542%
13	6.247	1510	1526	1551	rBV	217797	426640	34.92%	4.645%
14	6.690	1650	1664	1681	rBV	220979	433969	35.52%	4.725%
15	7.565	1921	1936	1957	rBV	65373	118600	9.71%	1.291%
16	7.713	1969	1982	1994	rVB4	9971	19353	1.58%	0.211%
17	7.896	2028	2039	2056	rBV	293392	508162	41.60%	5.533%
18	8.179	2114	2127	2144	rBV	41072	73488	6.02%	0.800%
19	8.481	2210	2221	2233	rVB4	6939	14098	1.15%	0.153%
20	8.632	2256	2268	2303	rBV2	590666	1136439	93.03%	12.373%
21	8.783	2308	2315	2327	rVB8	8145	16300	1.33%	0.177%
22	9.417	2499	2512	2517	rBV	350216	608424	49.81%	6.624%
23	9.754	2608	2617	2629	rBV3	9388	15989	1.31%	0.174%
24	10.481	2835	2843	2852	rBV3	10710	17012	1.39%	0.185%
25	10.754	2914	2928	2940	rBV2	203681	329839	27.00%	3.591%
26	11.812	3244	3257	3276	rBV2	289540	543206	44.47%	5.914%
27	12.092	3329	3344	3358	rBV	29953	50928	4.17%	0.554%
28	12.192	3362	3375	3395	rBV	297805	509562	41.71%	5.548%
29	13.844	3878	3889	3901	rBV3	8745	14797	1.21%	0.161%
30	16.677	4761	4770	4785	rBV2	73906	123747	10.13%	1.347%
31	16.886	4823	4835	4859	rBV	798952	1221607	100.00%	13.300%
32	17.098	4894	4901	4908	rBV3	11992	16790	1.37%	0.183%

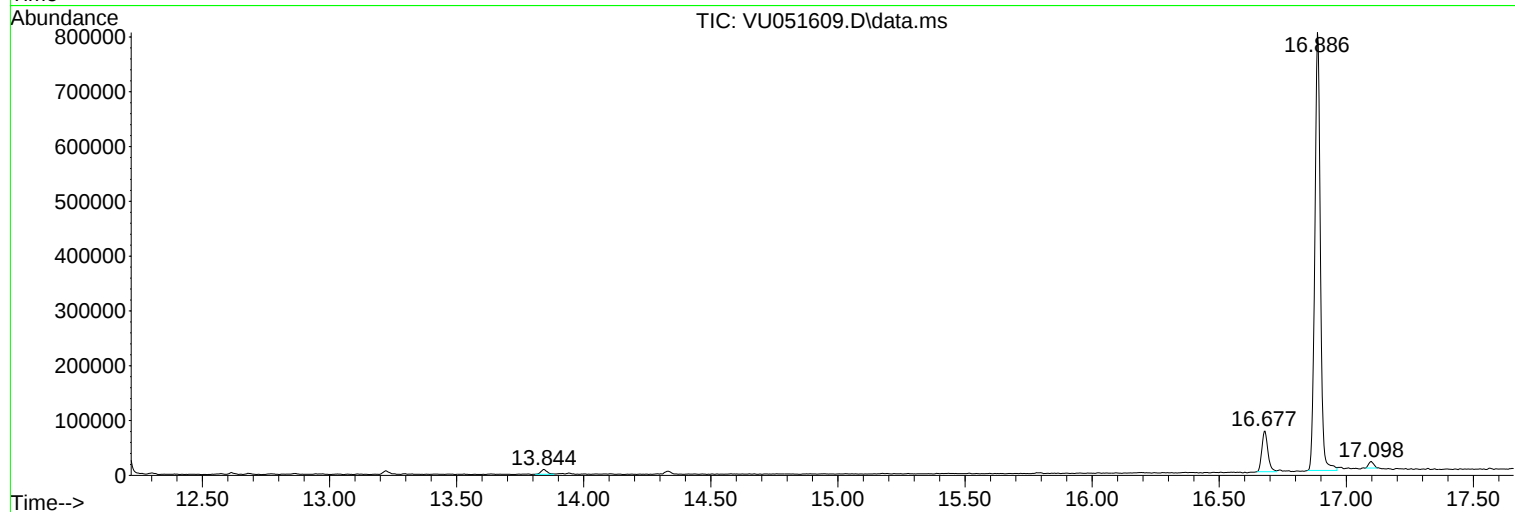
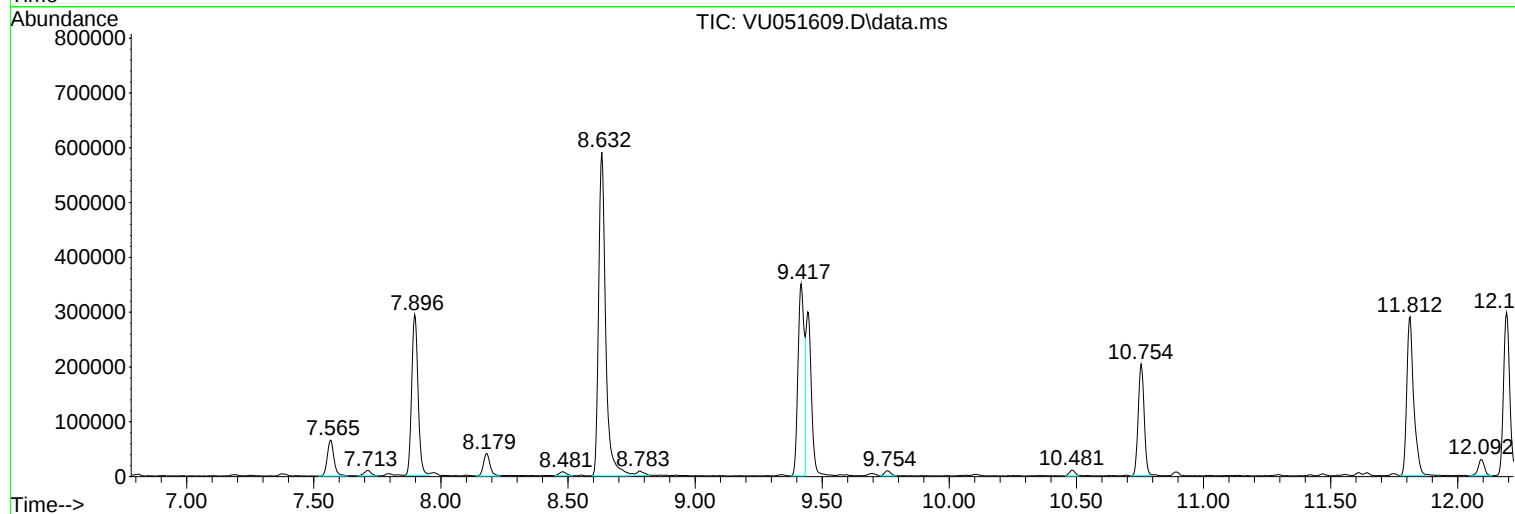
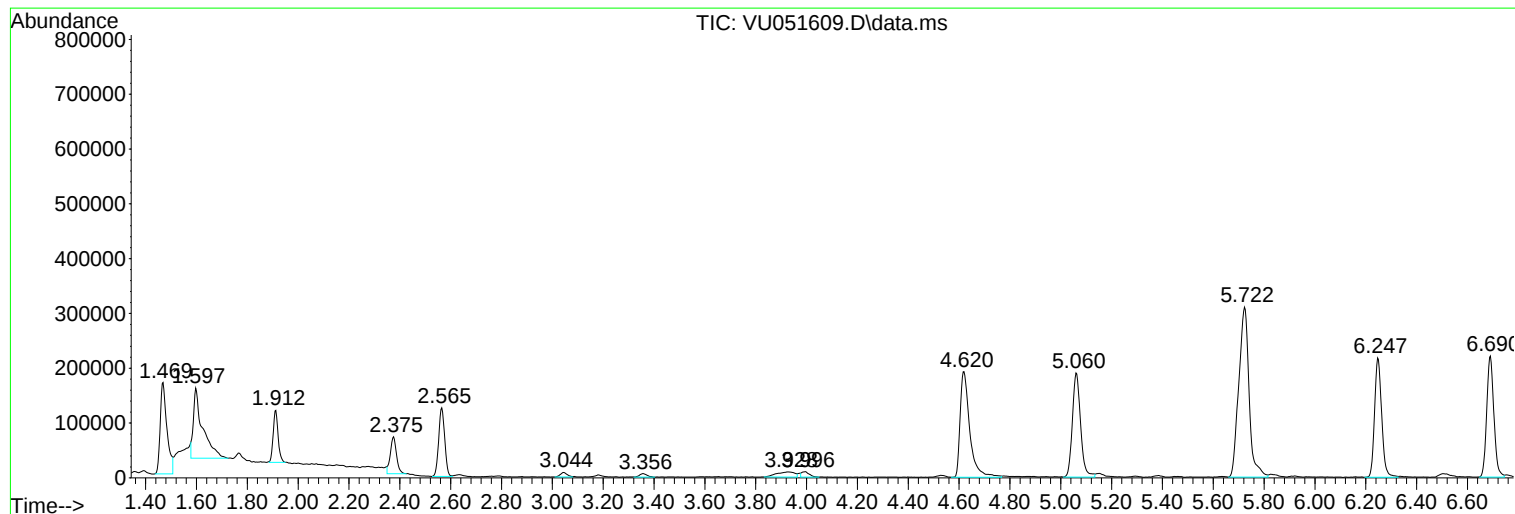
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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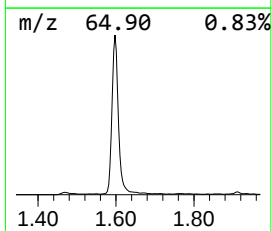
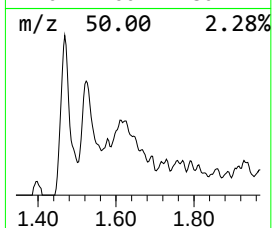
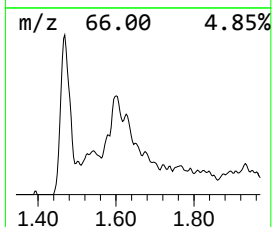
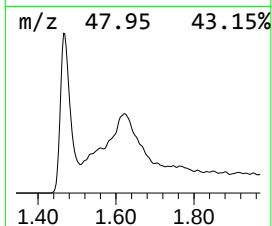
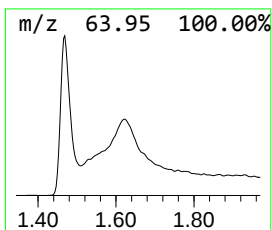
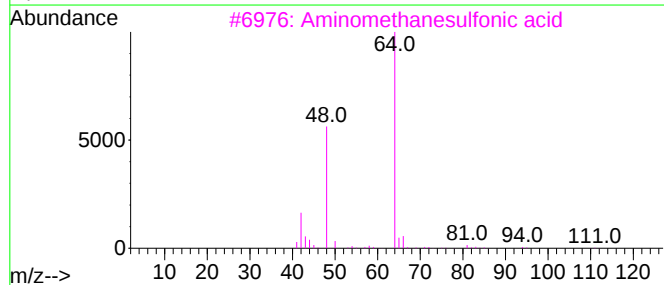
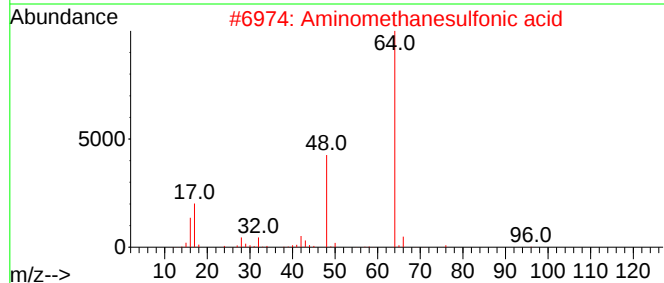
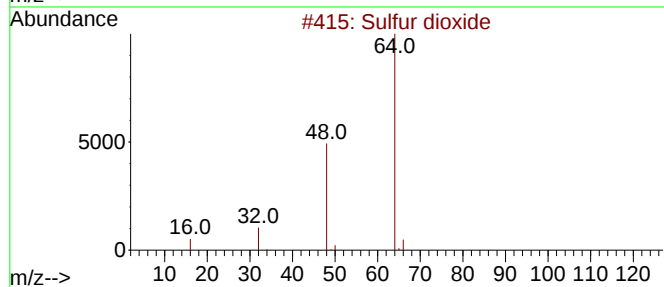
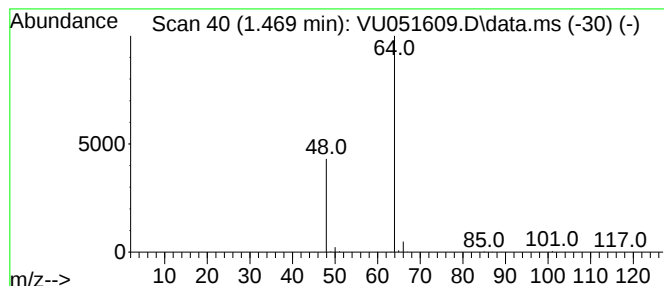
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.469	3.62 ug/L	309163	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	9
5			(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	9



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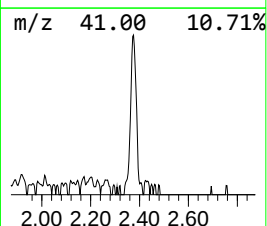
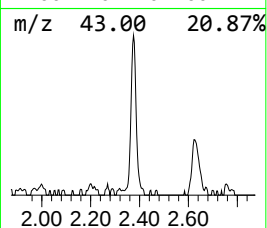
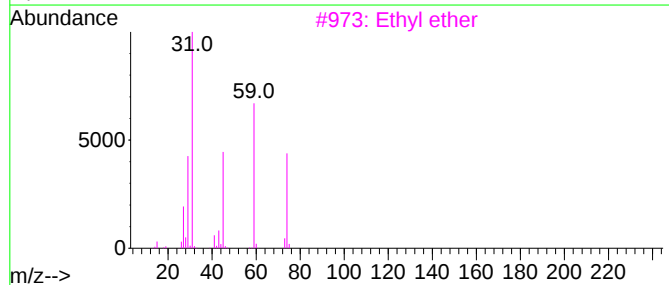
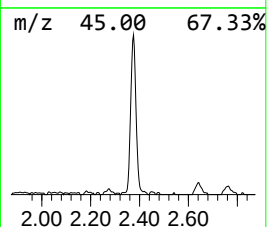
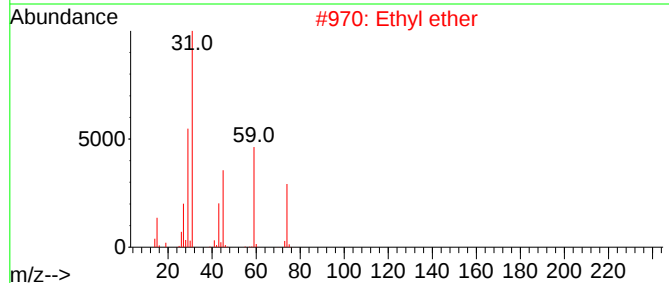
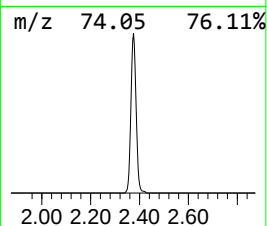
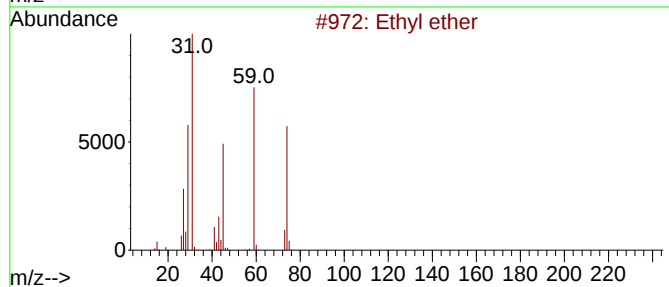
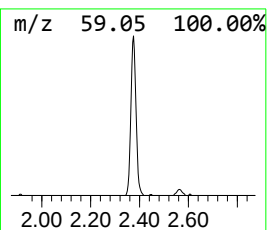
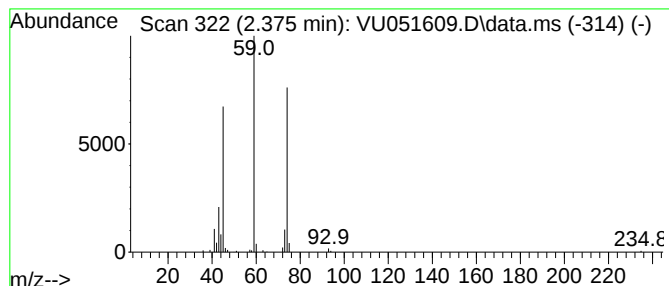
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Ethyl ether Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.375	1.32 ug/L	112474	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethyl ether			74	C4H10O	000060-29-7	91
2	Ethyl ether			74	C4H10O	000060-29-7	90
3	Ethyl ether			74	C4H10O	000060-29-7	90
4	Ethyl ether			74	C4H10O	000060-29-7	78
5	Ethane, 1,2-diethoxy-			118	C6H14O2	000629-14-1	74



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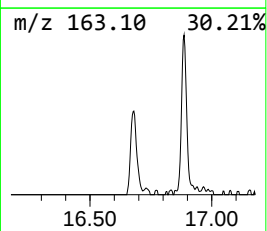
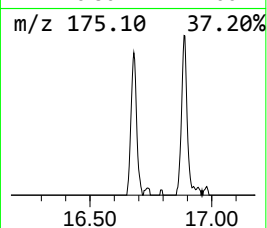
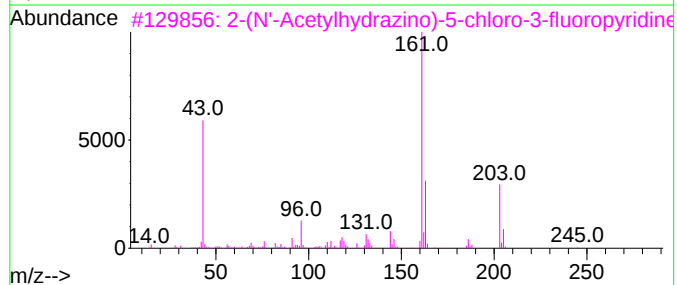
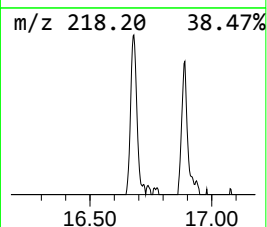
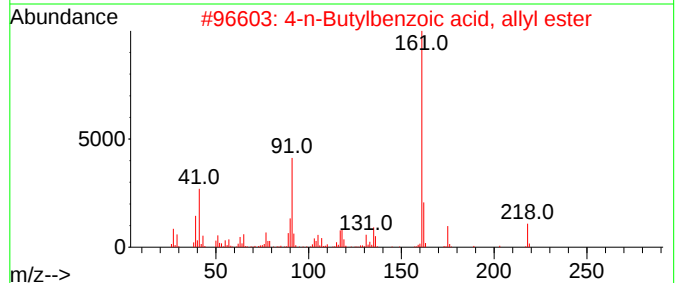
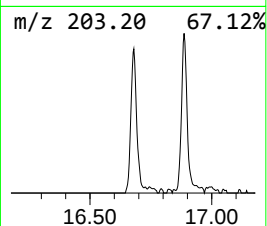
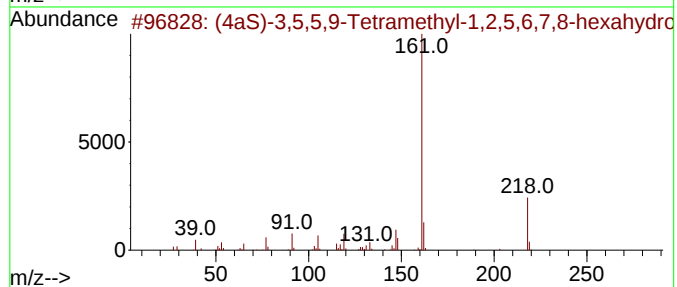
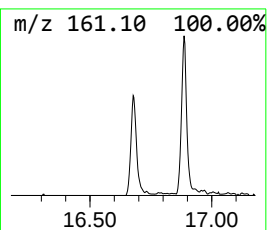
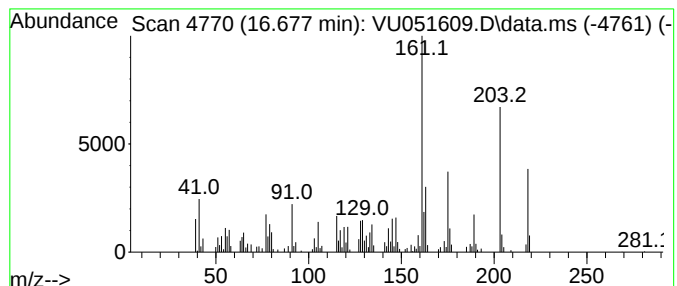
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 (4aS)-3,5,5,9-Tetramethyl-1... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.677	1.14 ug/L	123747	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(4aS)-3,5,5,9-Tetramethyl-1,2,5,...	218	C15H22O	064825-84-9	55
2			4-n-Butylbenzoic acid, allyl ester	218	C14H18O2	1000293-35-8	46
3			2-(N'-Acetylhydrazino)-5-chloro-...	245	C9H9ClFN3O2	1000512-28-8	43
4			1-Isopropyl-4,7-dimethyl-1,2,3,4...	204	C15H24	016729-00-3	42
5			1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	017334-55-3	42



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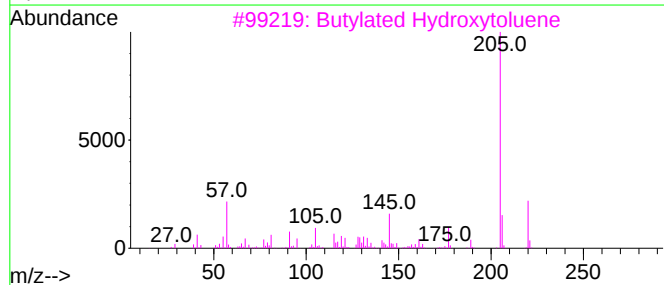
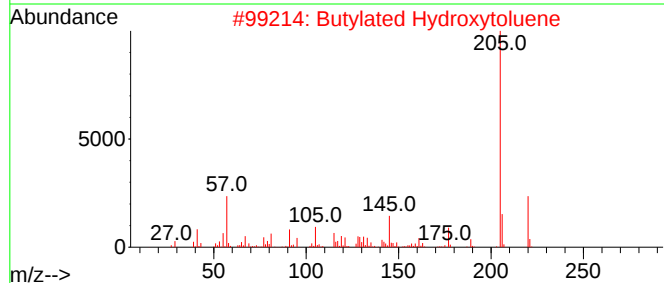
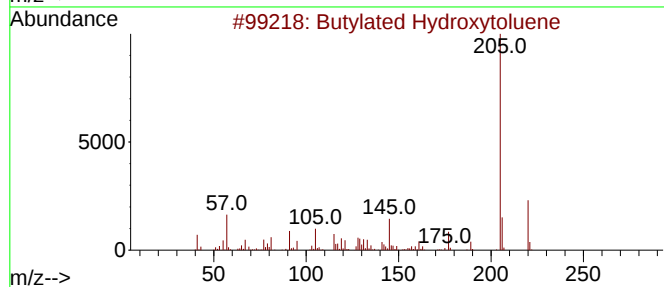
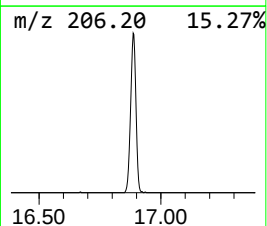
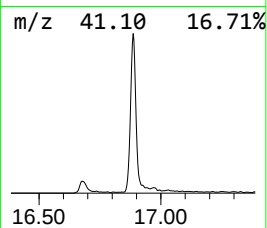
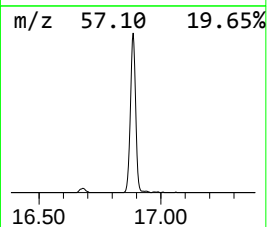
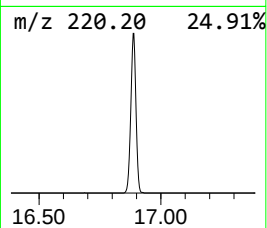
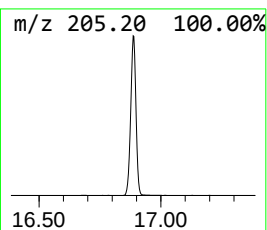
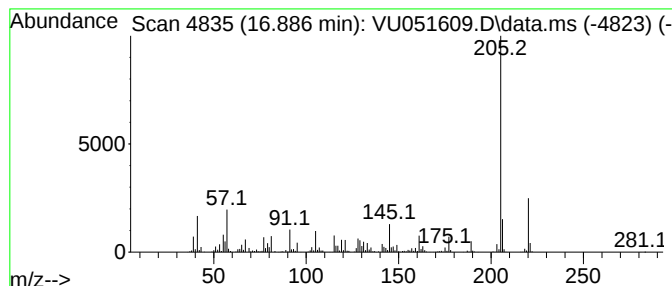
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.886	11.24 ug/L	1221610	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
2			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
3			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	96
4			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	95
5			Ethyl 4-oxo-2-phenylpentanoate	220	C13H16O3	1000427-11-2	94



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.469	3.6	ug/L	309163	1	6.250	426640	5.0
Ethyl ether	2.375	1.3	ug/L	112474	1	6.250	426640	5.0
(4aS)-3,5,5,9-T...	16.677	1.1	ug/L	123747	3	11.812	543206	5.0
Butylated Hydro...	16.886	11.2	ug/L	1221610	3	11.812	543206	5.0