

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120722\
 Data File : VU052233.D
 Acq On : 08 Dec 2022 06:34
 Operator : JC/MD
 Sample : N5916-14
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5N32

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: VU052233.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	70	81	101	rVB	108966	148875	15.42%	1.747%
2	1.916	171	179	198	rVB	84907	117378	12.16%	1.378%
3	2.568	370	382	399	rVB	171385	283165	29.34%	3.323%
4	3.858	756	783	785	rBV	7171	21668	2.24%	0.254%
5	4.649	1014	1029	1072	rBV	75256	333404	34.54%	3.913%
6	5.060	1140	1157	1175	rBV	149847	334102	34.61%	3.921%
7	5.723	1340	1363	1375	rBV2	290259	757799	78.51%	8.893%
8	5.793	1375	1385	1410	rVB	185388	393651	40.78%	4.620%
9	6.247	1511	1526	1554	rBV	250599	488571	50.62%	5.734%
10	6.687	1650	1663	1681	rBV	187358	373885	38.73%	4.388%
11	7.565	1923	1936	1958	rBV	75406	134154	13.90%	1.574%
12	7.896	2023	2039	2054	rBV	306943	536977	55.63%	6.302%
13	8.179	2115	2127	2145	rBV	47471	82536	8.55%	0.969%
14	8.636	2256	2269	2304	rBV2	423151	890851	92.29%	10.455%
15	9.414	2498	2511	2530	rBV	371171	624041	64.65%	7.324%
16	10.751	2911	2927	2941	rBV	174519	289552	30.00%	3.398%
17	11.118	3033	3041	3054	rVB2	10377	16905	1.75%	0.198%
18	11.809	3243	3256	3276	rBV	336854	551085	57.09%	6.467%
19	12.063	3326	3335	3346	rBV7	6323	10431	1.08%	0.122%
20	12.189	3363	3374	3395	rBV	319366	538333	55.77%	6.318%
21	15.690	4453	4463	4478	rBV4	43648	75099	7.78%	0.881%
22	15.783	4485	4492	4504	rBV4	9609	15426	1.60%	0.181%
23	16.690	4762	4774	4787	rBV2	135575	259578	26.89%	3.046%
24	16.764	4788	4797	4817	rVV2	161952	278302	28.83%	3.266%
25	16.883	4823	4834	4858	rBV	626502	965248	100.00%	11.328%

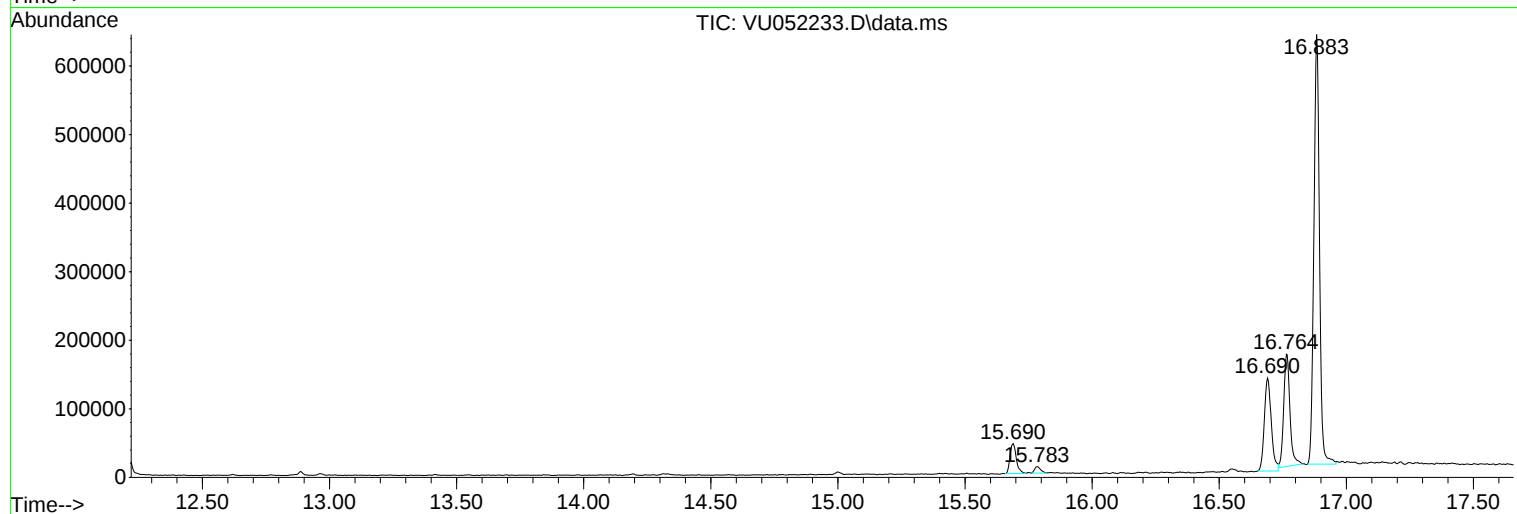
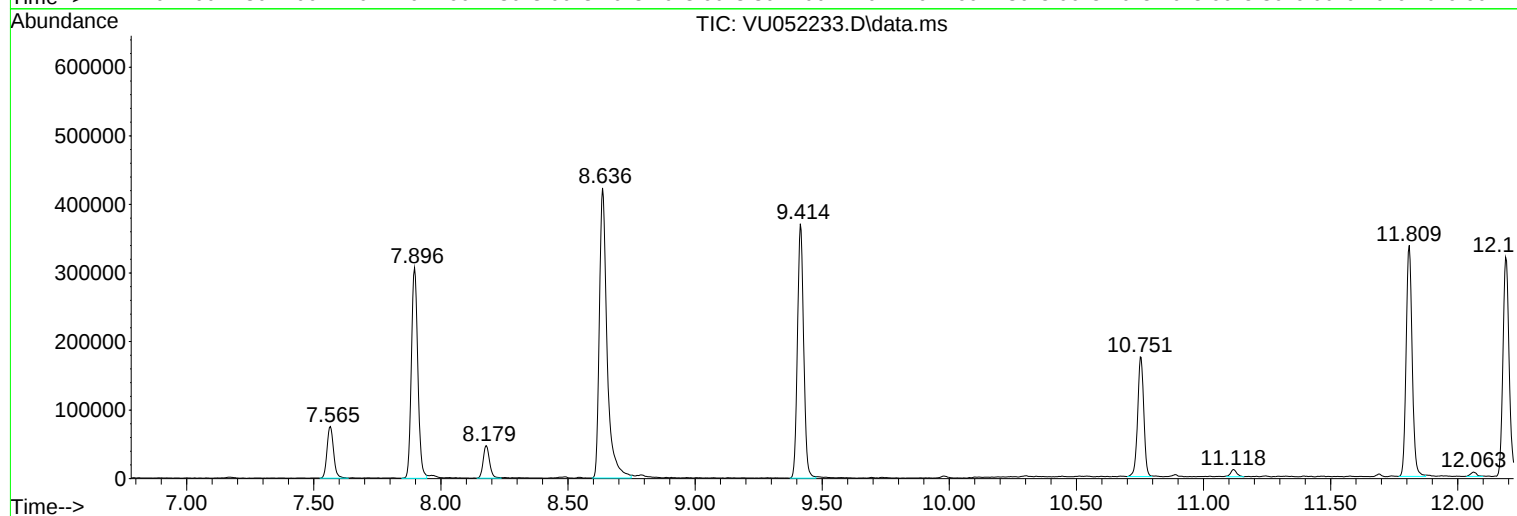
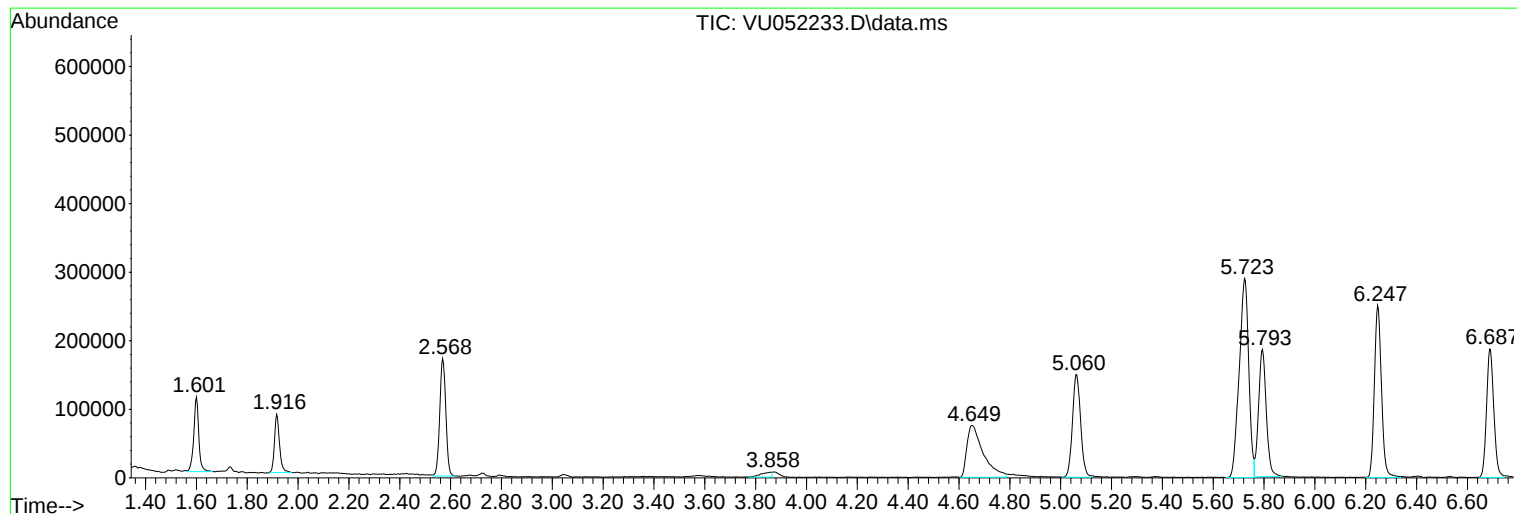
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F5N32

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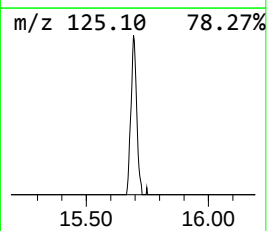
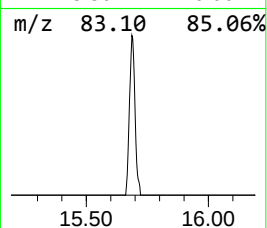
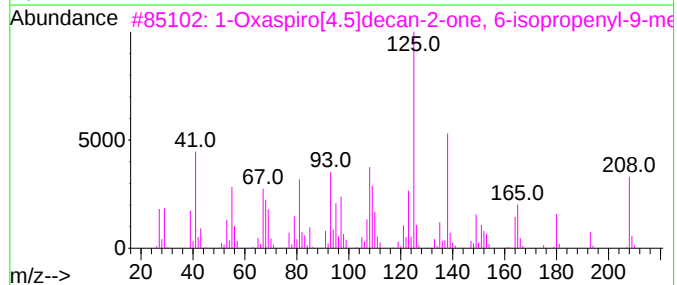
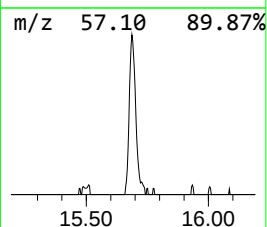
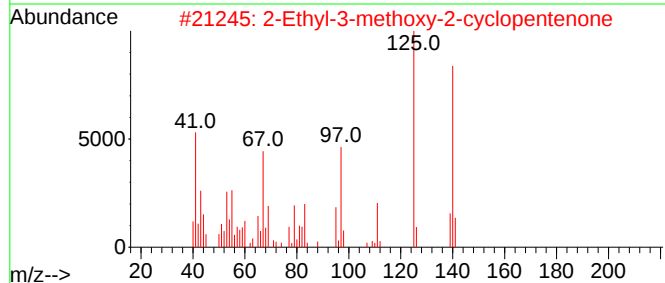
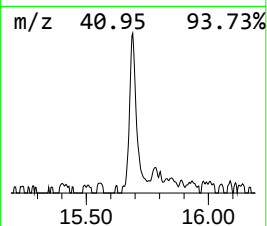
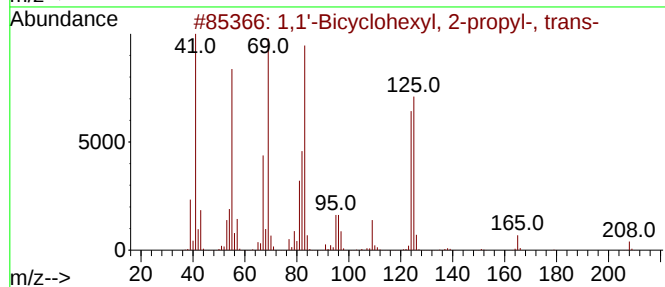
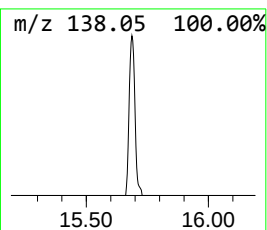
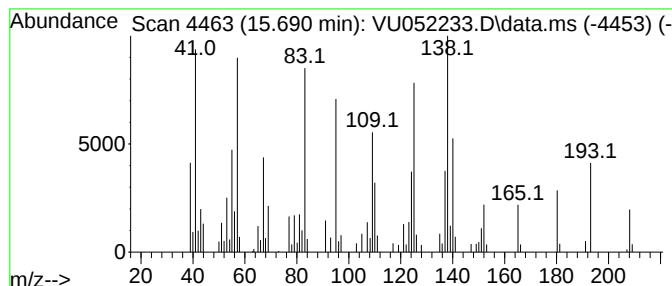
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.690	0.68 ug/L	75099	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Bicyclohexyl, 2-propyl-, tr...	208	C15H28	054934-89-3	38		
2	2-Ethyl-3-methoxy-2-cyclopentenone	140	C8H12O2	025112-86-1	20		
3	1-Oxaspiro[4.5]decan-2-one, 6-is...	208	C13H20O2	1010157-58-3	18		
4	9-Borabicyclo[3.3.1]nonane, 9-(3...	208	C13H25BO	1010160-84-8	15		
5	3,4-Dihydro-6-fluorocoumarin	166	C9H7FO2	075487-95-5	14		



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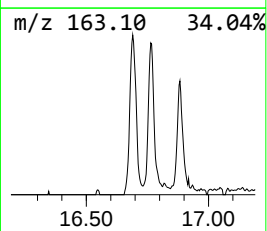
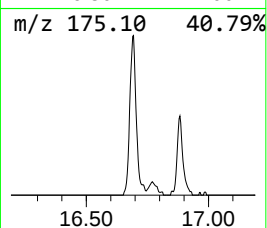
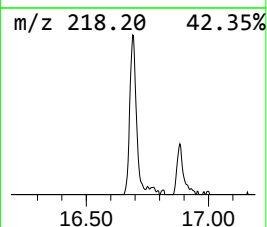
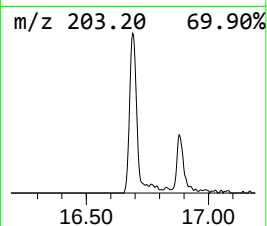
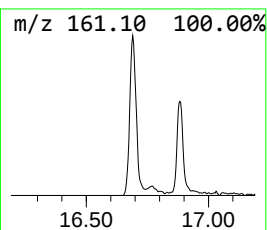
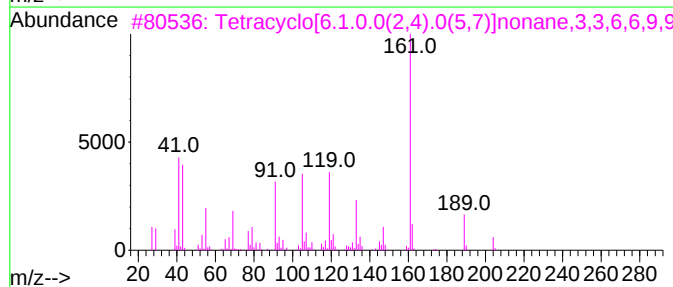
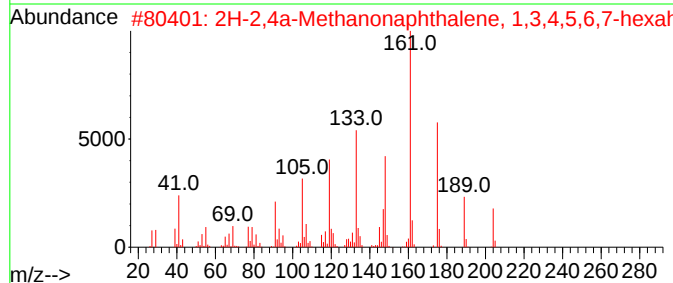
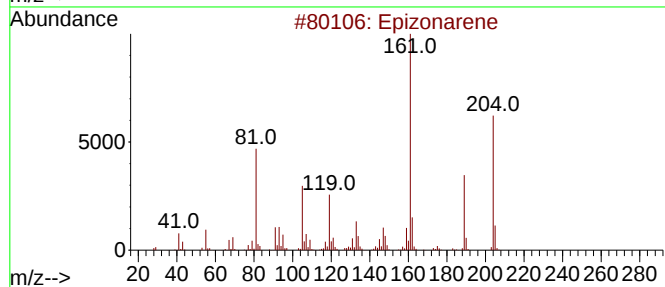
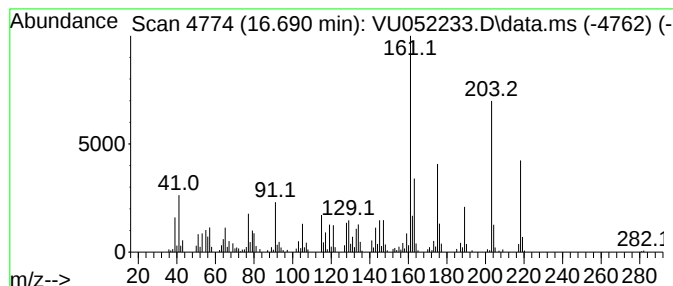
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Epizonarene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.690	2.36 ug/L	259578	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Epizonarene	204	C15H24	041702-63-0	53
2			2H-2,4a-Methanonaphthalene, 1,3,...	204	C15H24	001135-66-6	49
3			Tetracyclo[6.1.0.0(2,4).0(5,7)]n...	204	C15H24	051898-92-1	46
4			1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	017334-55-3	46
5			(4aS)-3,5,5,9-Tetramethyl-1,2,5,...	218	C15H22O	064825-84-9	45



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ALS Vial : 45 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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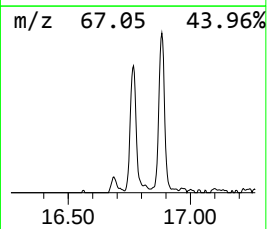
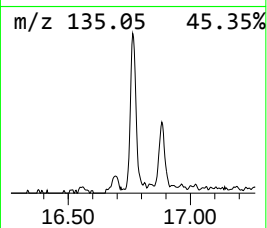
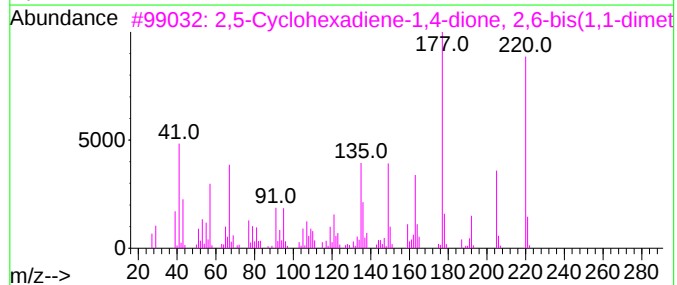
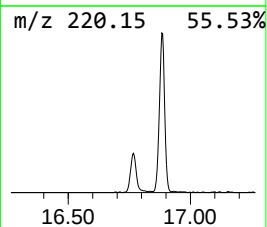
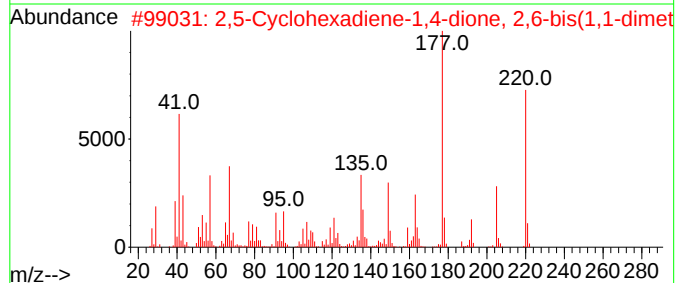
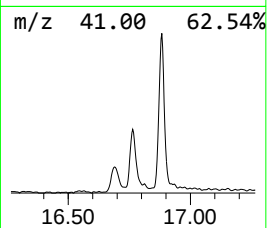
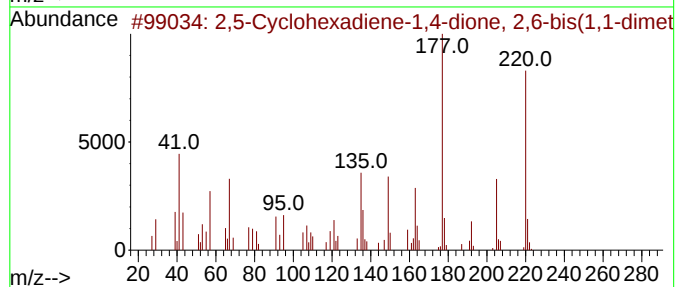
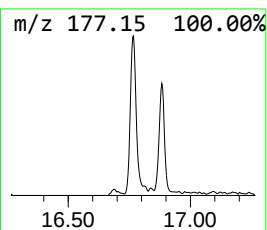
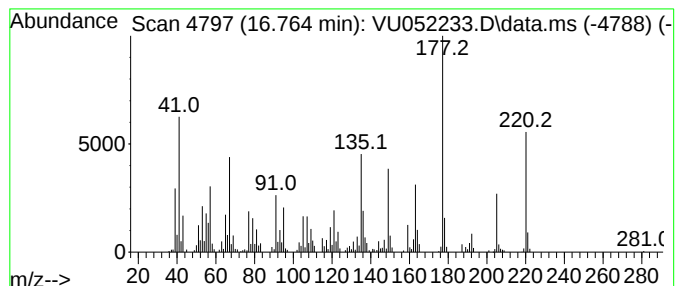
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.764	2.53 ug/L	278302	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	96		
2	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	96		
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	94		
4	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	94		
5	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	90		



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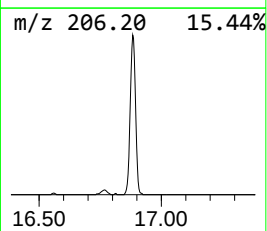
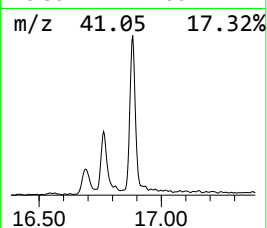
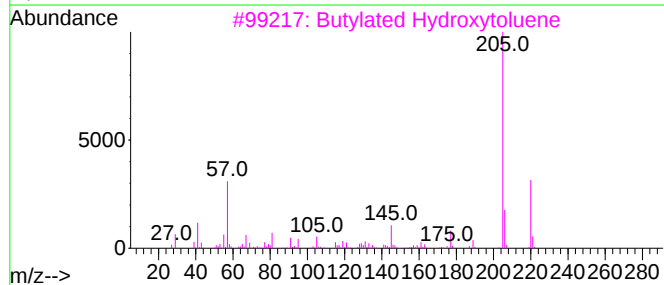
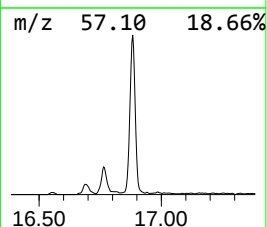
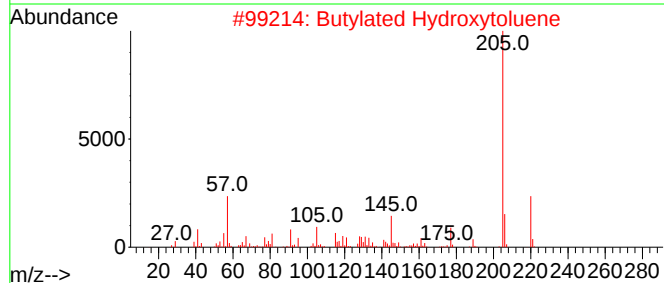
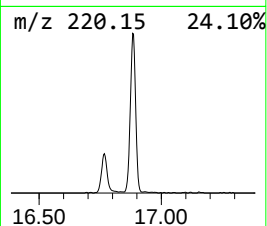
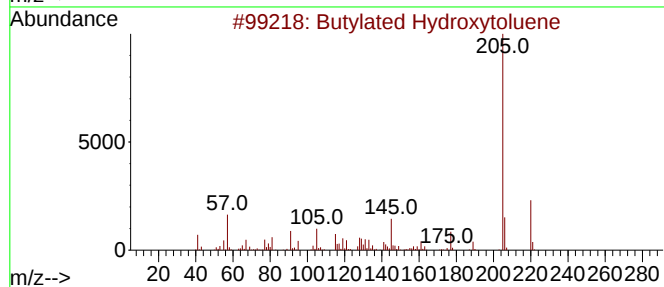
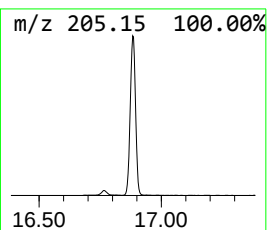
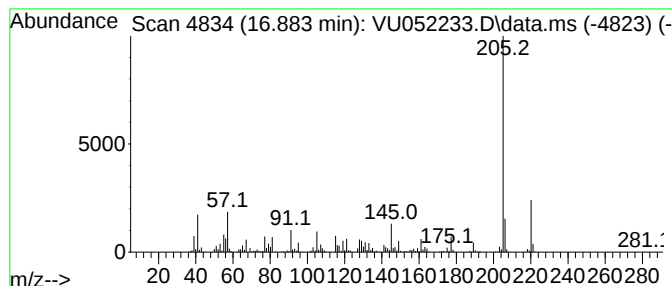
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Peak Number 5 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.883	8.76 ug/L	965248	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	98
3			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	97
4			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	97
5			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	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
unknown-01	15.690	0.7	ug/L	75099	3	11.809	551085	5.0
Epizonarene	16.690	2.4	ug/L	259578	3	11.809	551085	5.0
2,5-Cyclohexadi...	16.764	2.5	ug/L	278302	3	11.809	551085	5.0
Butylated Hydro...	16.883	8.8	ug/L	965248	3	11.809	551085	5.0