

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV111021\
 Data File : VV023353.D
 Acq On : 11 Nov 2021 00:13
 Operator : SY/MD
 Sample : M4558-12
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 GB874

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_V\Method\SFAMVTR110421WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VV023353.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.307	75	83	100	rVB	55369	58996	14.37%	1.392%
2	1.568	156	164	172	rBV	41096	47647	11.60%	1.125%
3	1.632	178	184	194	rVB	17761	22169	5.40%	0.523%
4	1.806	234	238	247	rVB7	4163	5319	1.30%	0.126%
5	2.024	300	306	316	rVB5	3302	5243	1.28%	0.124%
6	2.108	322	332	347	rVB	75928	112607	27.42%	2.658%
7	2.500	441	454	462	rBV10	4444	10357	2.52%	0.244%
8	3.770	833	849	858	rBV7	3829	9811	2.39%	0.232%
9	3.908	881	892	927	rBV	40972	156238	38.05%	3.687%
10	4.352	1014	1030	1053	rBV	70292	173740	42.31%	4.100%
11	4.683	1117	1133	1147	rVB7	3931	9917	2.42%	0.234%
12	5.050	1230	1247	1282	rBV3	149879	410631	100.00%	9.691%
13	5.619	1409	1424	1454	rBV	151594	307972	75.00%	7.269%
14	5.921	1507	1518	1535	rVB5	16232	34859	8.49%	0.823%
15	6.072	1552	1565	1592	rBV	91600	191230	46.57%	4.513%
16	6.989	1841	1850	1865	rBV2	36224	69515	16.93%	1.641%
17	7.320	1939	1953	1970	rBV	167757	295542	71.97%	6.975%
18	7.400	1972	1978	1986	rVB5	3983	6799	1.66%	0.160%
19	7.628	2039	2049	2063	rBV	22259	41112	10.01%	0.970%
20	8.091	2183	2193	2228	rBV	201496	392201	95.51%	9.256%
21	8.853	2419	2430	2448	rBV	234893	380060	92.56%	8.970%
22	9.146	2513	2521	2530	rBV6	2495	4207	1.02%	0.099%
23	10.217	2844	2854	2867	rBV	74807	115184	28.05%	2.718%
24	11.091	3119	3126	3135	rBV6	3177	5177	1.26%	0.122%
25	11.249	3164	3175	3196	rBV	238462	371784	90.54%	8.775%
26	11.529	3248	3262	3277	rBV5	21373	38321	9.33%	0.904%
27	11.625	3280	3292	3312	rVB	193861	304589	74.18%	7.189%
28	12.049	3416	3424	3436	rVB3	5768	8696	2.12%	0.205%
29	12.303	3491	3503	3511	rVB5	3021	4560	1.11%	0.108%
30	12.885	3674	3684	3692	rBV7	3195	4523	1.10%	0.107%
31	13.374	3829	3836	3844	rVB7	3338	5791	1.41%	0.137%
32	13.696	3927	3936	3947	rVB6	7353	11003	2.68%	0.260%
33	13.754	3947	3954	3966	rVB8	2602	4423	1.08%	0.104%
34	15.773	4572	4582	4595	rBV	45795	67820	16.52%	1.601%
35	16.181	4698	4709	4723	rBV2	170515	274249	66.79%	6.473%
36	16.310	4738	4749	4762	rBV2	182769	274782	66.92%	6.485%

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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_V\Method\SFAMVTR110421WMA.M
Title : TRACE VOA SFAM1.0

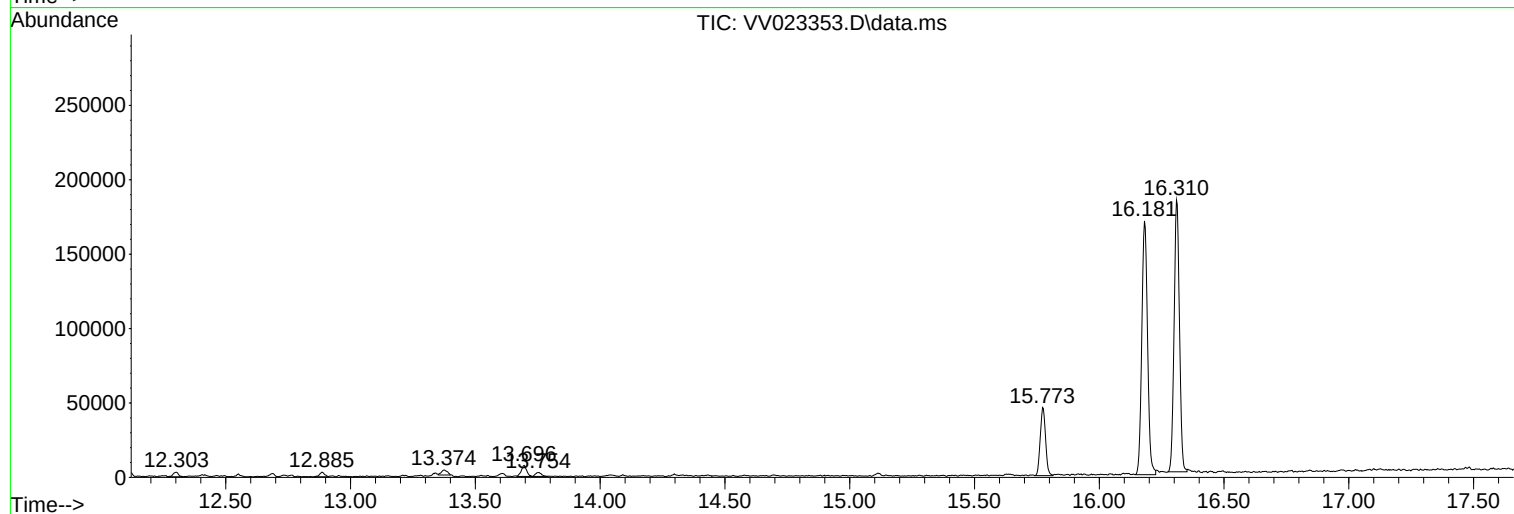
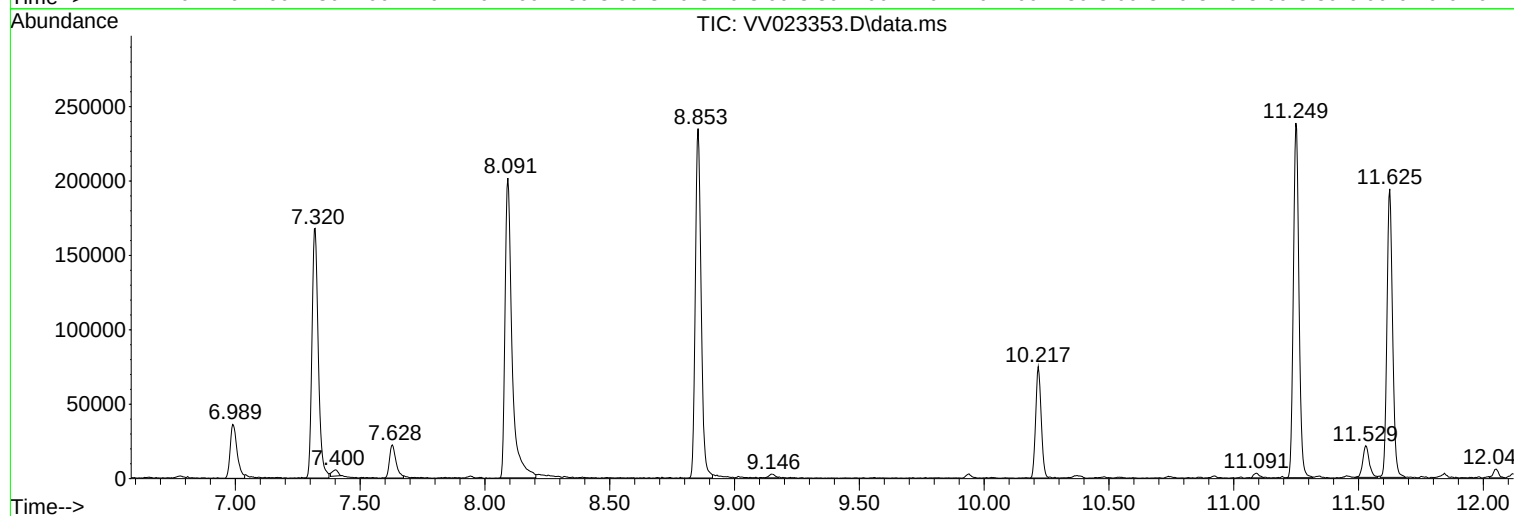
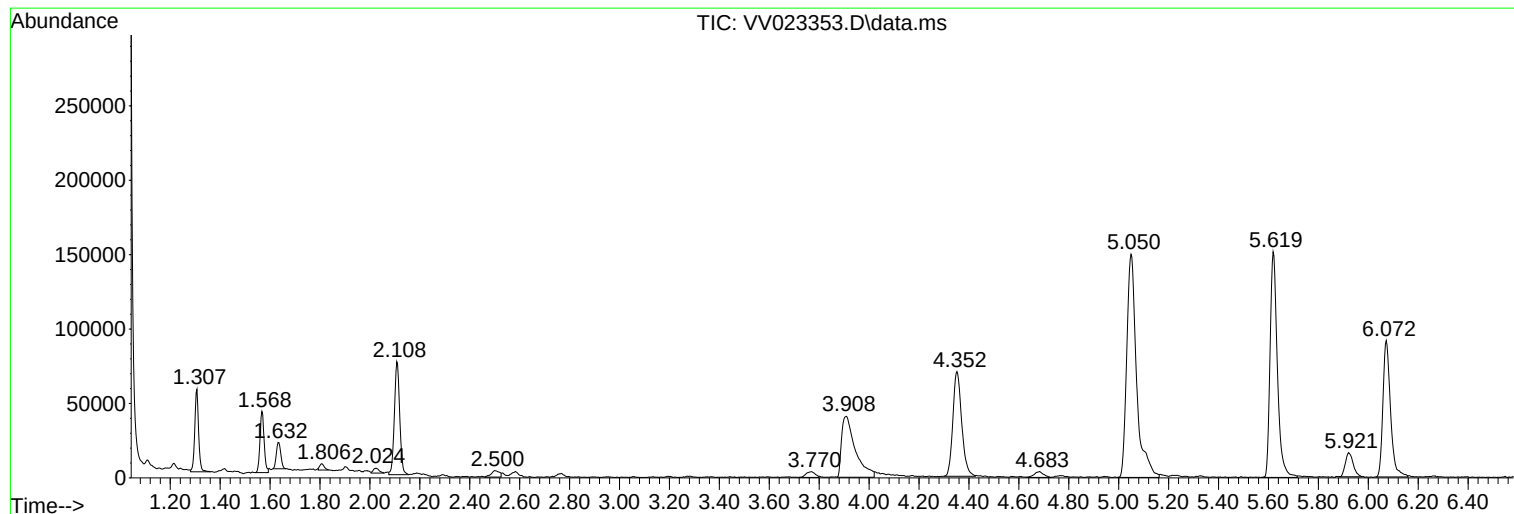
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Quant Title : TRACE VOA SFAM1.0

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



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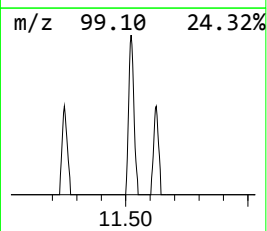
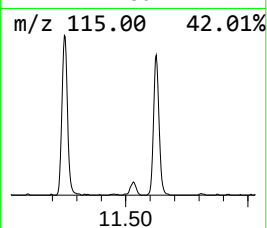
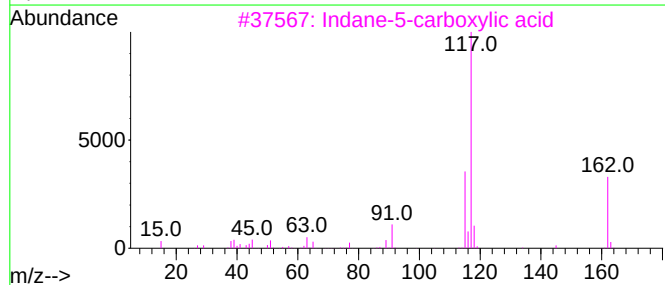
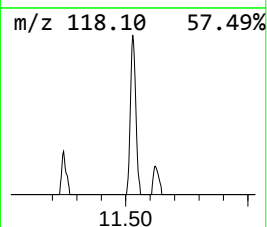
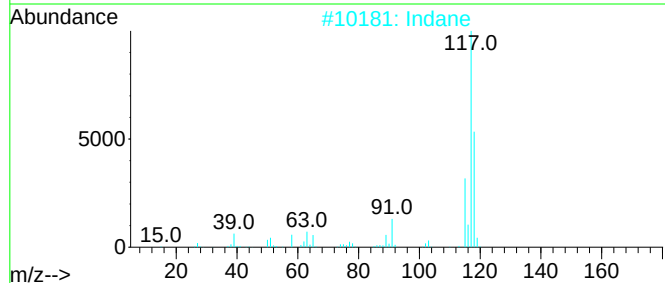
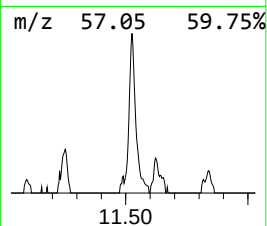
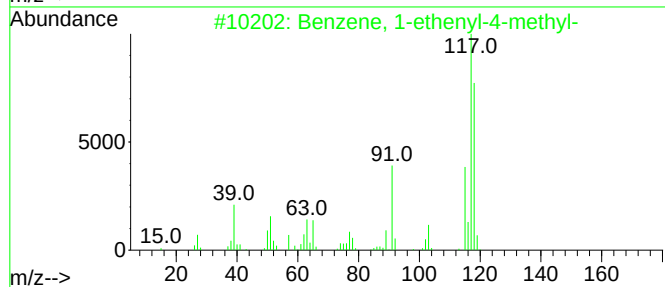
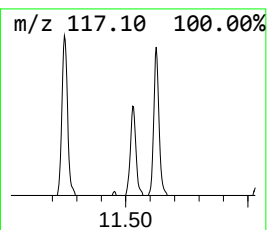
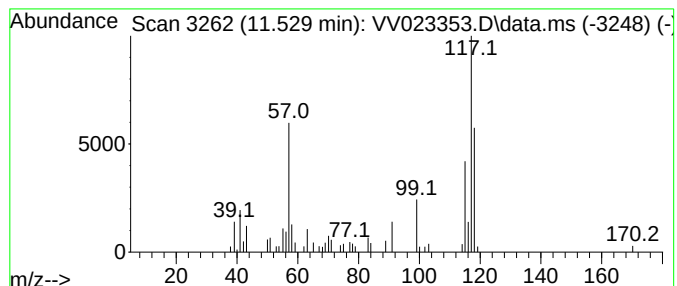
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Benzene, 1-ethenyl-4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.529	0.52 ug/L	38321	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	58
2			Indane	118	C9H10	000496-11-7	58
3			Indane-5-carboxylic acid	162	C10H10O2	065898-38-6	53
4			Benzene, (3-chloro-1-propenyl)-	152	C9H9Cl	002687-12-9	53
5			Indane	118	C9H10	000496-11-7	52



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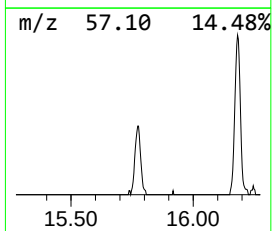
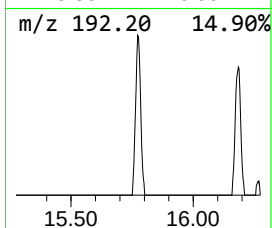
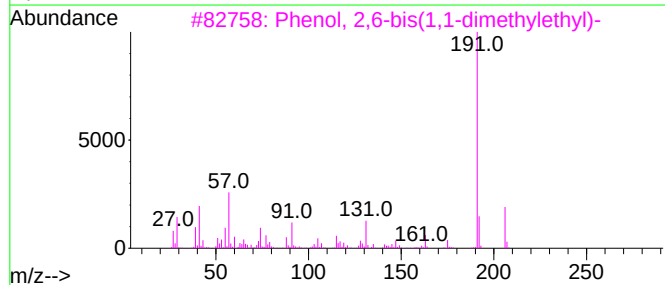
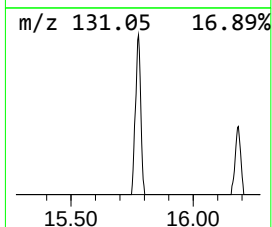
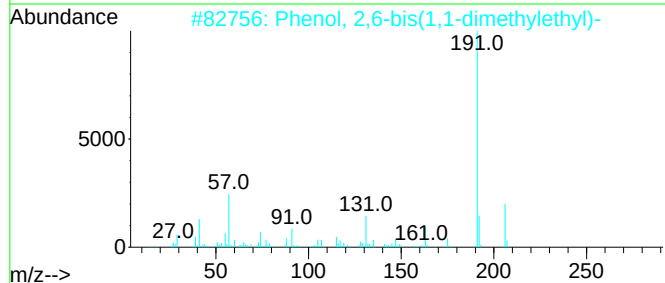
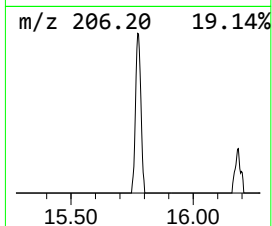
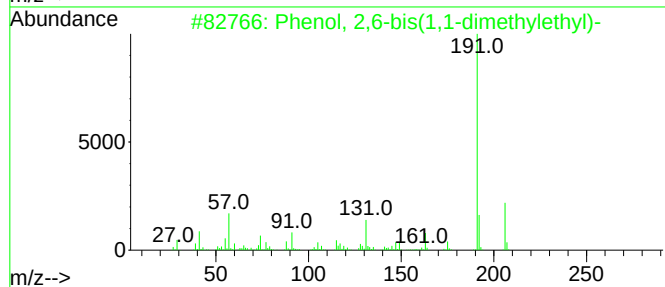
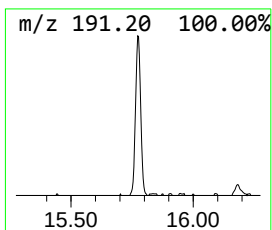
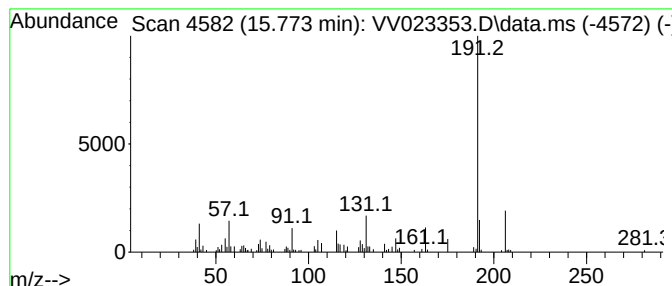
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR110421WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.773	0.91 ug/L	67820	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	94
2			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	94
3			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	93
4			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	93
5			Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	91



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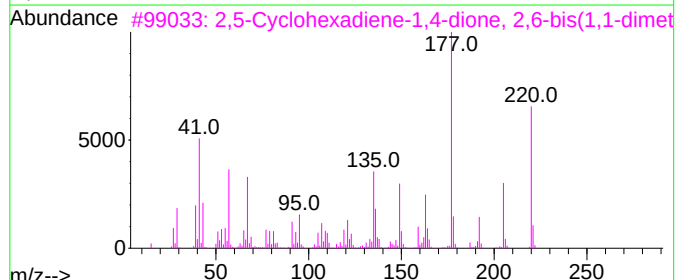
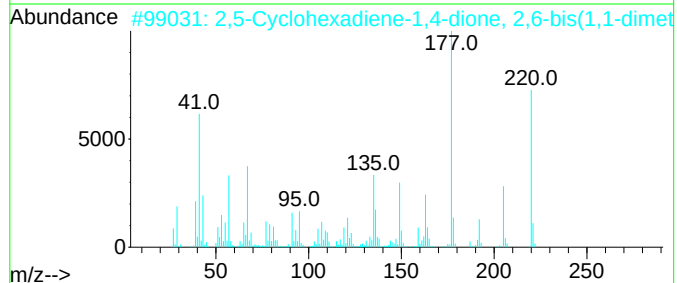
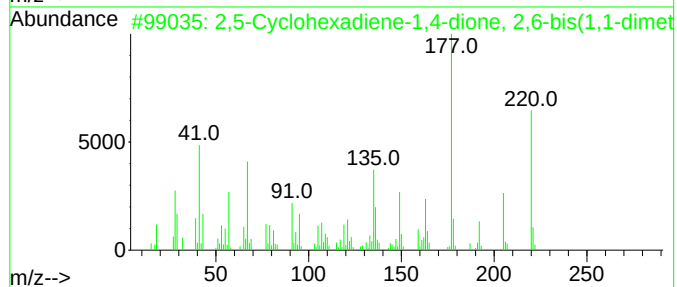
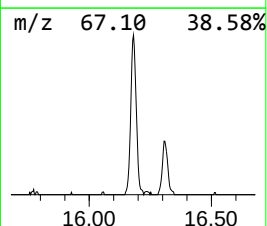
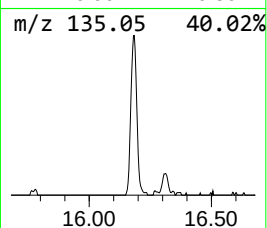
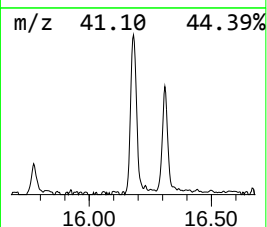
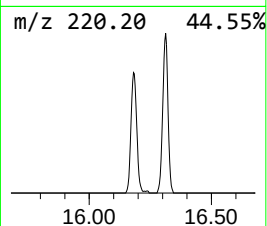
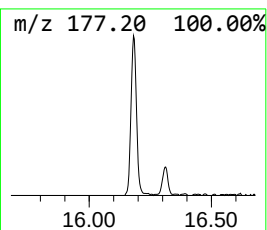
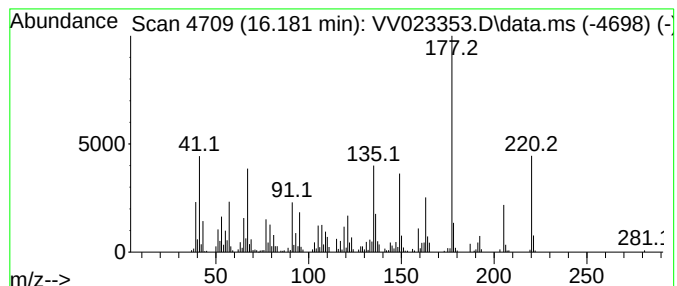
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Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.181	3.69 ug/L	274249	1,4-Dichlorobenzene-d4	11.249

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	95	
2	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	94	
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	87	
4	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	78	
5	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	64	



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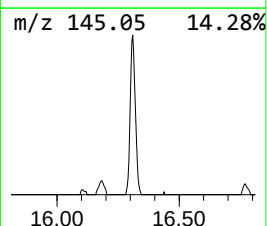
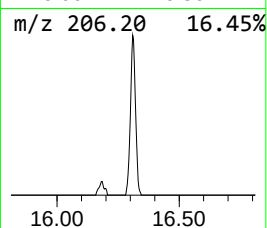
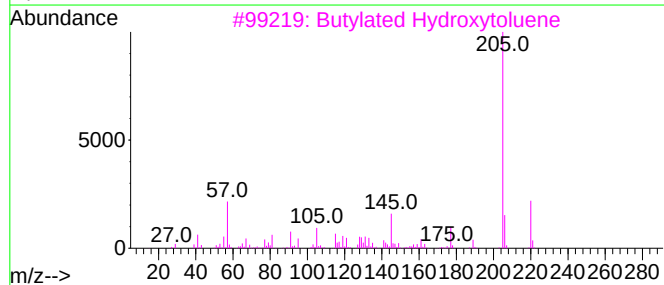
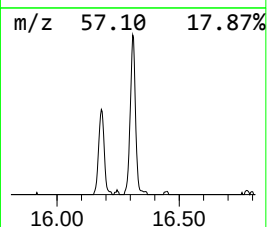
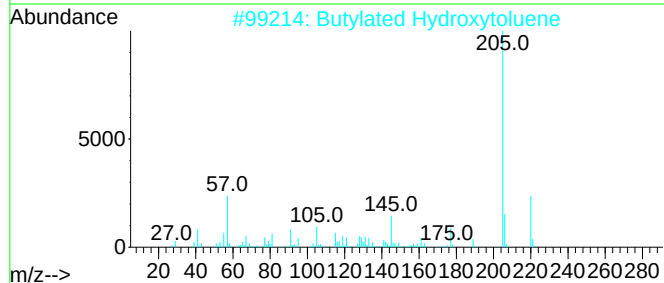
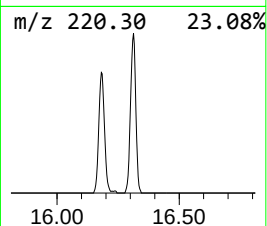
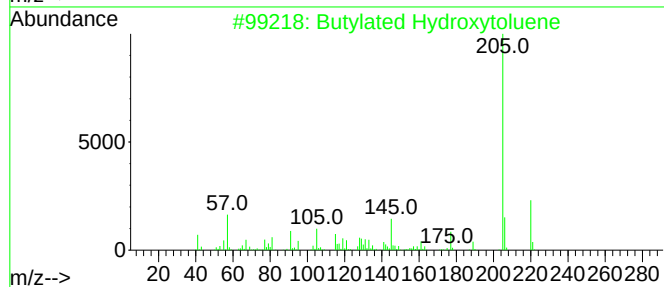
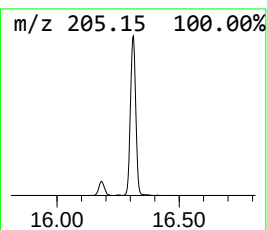
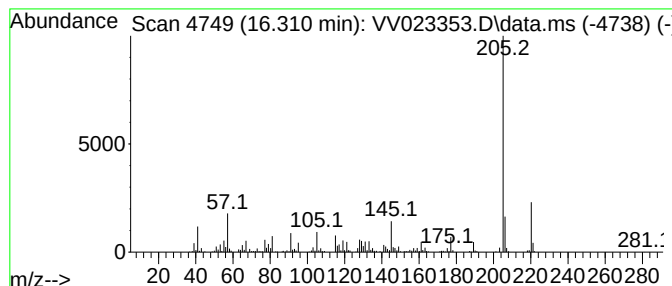
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Peak Number 5 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.310	3.70 ug/L	274782	1,4-Dichlorobenzene-d4	11.249

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	96
5			Ethyl 4-oxo-2-phenylpentanoate	220	C13H16O3	1000427-11-2	95



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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
Benzene, 1-ethe...	11.529	0.5	ug/L	38321	3	11.249	371784	5.0
Phenol, 2,6-bis...	15.773	0.9	ug/L	67820	3	11.249	371784	5.0
2,5-Cyclohexadi...	16.181	3.7	ug/L	274249	3	11.249	371784	5.0
Butylated Hydro...	16.310	3.7	ug/L	274782	3	11.249	371784	5.0