

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV111021\
 Data File : VV023396.D
 Acq On : 11 Nov 2021 18:35
 Operator : SY/MD
 Sample : M4558-12
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 4 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: VV023396.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	96	rVB	60197	63915	16.41%	1.671%
2	1.568	156	164	176	rBV	41082	48657	12.49%	1.272%
3	1.632	176	184	192	rBV2	16658	21157	5.43%	0.553%
4	1.812	231	240	253	rVB6	3797	7448	1.91%	0.195%
5	2.024	300	306	315	rVB2	4207	5839	1.50%	0.153%
6	2.105	320	331	343	rBV	87109	126914	32.58%	3.317%
7	2.503	447	455	461	rBV7	2916	5164	1.33%	0.135%
8	2.577	470	478	489	rVB7	3573	6822	1.75%	0.178%
9	2.764	524	536	547	rBV9	3605	7184	1.84%	0.188%
10	3.767	836	848	859	rBV6	3713	9367	2.40%	0.245%
11	3.902	881	890	917	rBV2	24215	86027	22.08%	2.249%
12	4.352	1013	1030	1056	rBV2	61934	158494	40.68%	4.143%
13	4.677	1119	1131	1145	rVB2	3908	9070	2.33%	0.237%
14	5.050	1232	1247	1279	rBV3	144080	389593	100.00%	10.184%
15	5.619	1413	1424	1448	rBV	137073	284253	72.96%	7.430%
16	5.918	1507	1517	1537	rVB8	8155	19031	4.88%	0.497%
17	6.072	1552	1565	1595	rBV	78767	172879	44.37%	4.519%
18	6.992	1840	1851	1873	rBV3	36654	72600	18.63%	1.898%
19	7.317	1941	1952	1970	rBV	169273	299197	76.80%	7.821%
20	7.397	1971	1977	1992	rVB3	7251	13417	3.44%	0.351%
21	7.628	2039	2049	2065	rBV2	21215	40257	10.33%	1.052%
22	7.944	2137	2147	2152	rBV3	2976	5228	1.34%	0.137%
23	7.982	2153	2159	2166	rVB7	2522	4061	1.04%	0.106%
24	8.091	2183	2193	2227	rBV	123831	264766	67.96%	6.921%
25	8.853	2419	2430	2449	rBV	209551	342946	88.03%	8.964%
26	9.149	2514	2522	2530	rBV3	3748	6558	1.68%	0.171%
27	9.934	2757	2766	2773	rBV4	4480	6687	1.72%	0.175%
28	10.217	2844	2854	2868	rBV	53641	84779	21.76%	2.216%
29	10.381	2891	2905	2914	rBB5	3367	6324	1.62%	0.165%
30	10.921	3062	3073	3084	rBV5	3839	6351	1.63%	0.166%
31	11.091	3118	3126	3136	rBV8	2828	4232	1.09%	0.111%
32	11.194	3150	3158	3164	rBV8	2852	4025	1.03%	0.105%
33	11.249	3164	3175	3197	rBV	198478	315638	81.02%	8.251%
34	11.529	3251	3262	3277	rBV3	18017	31494	8.08%	0.823%
35	11.625	3281	3292	3310	rVB	164309	259884	66.71%	6.793%
36	12.053	3416	3425	3435	rVB3	4945	7396	1.90%	0.193%

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37	12.300	3494	3502	3509	rBV5	2987	3912	1.00%	0.102%
38	12.648	3603	3610	3616	rBV3	3354	4026	1.03%	0.105%
39	13.268	3795	3803	3810	rBV6	3573	5207	1.34%	0.136%
40	13.374	3828	3836	3850	rVB6	3433	6755	1.73%	0.177%
41	13.692	3928	3935	3945	rBV7	5916	9730	2.50%	0.254%
42	13.747	3945	3952	3963	rVB8	5124	8089	2.08%	0.211%
43	14.043	4033	4044	4054	rVB2	4852	7975	2.05%	0.208%
44	15.773	4573	4582	4596	rBV	41993	61854	15.88%	1.617%
45	16.181	4697	4709	4724	rBV3	167019	268218	68.85%	7.011%
46	16.310	4738	4749	4761	rBV	166233	252220	64.74%	6.593%

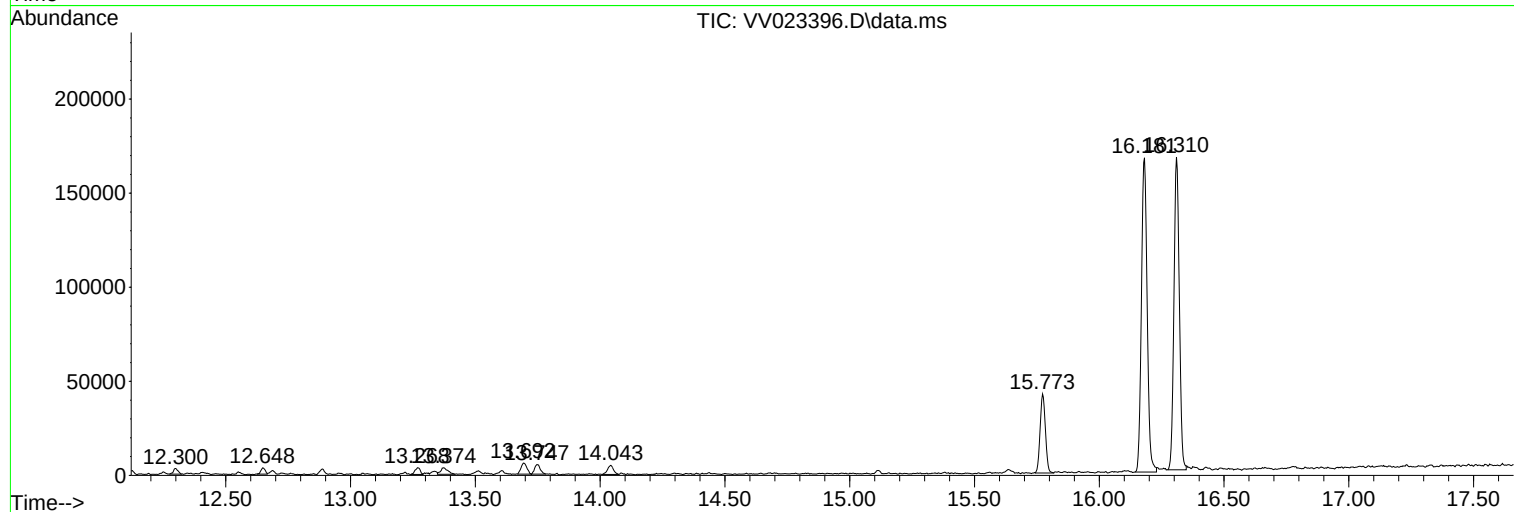
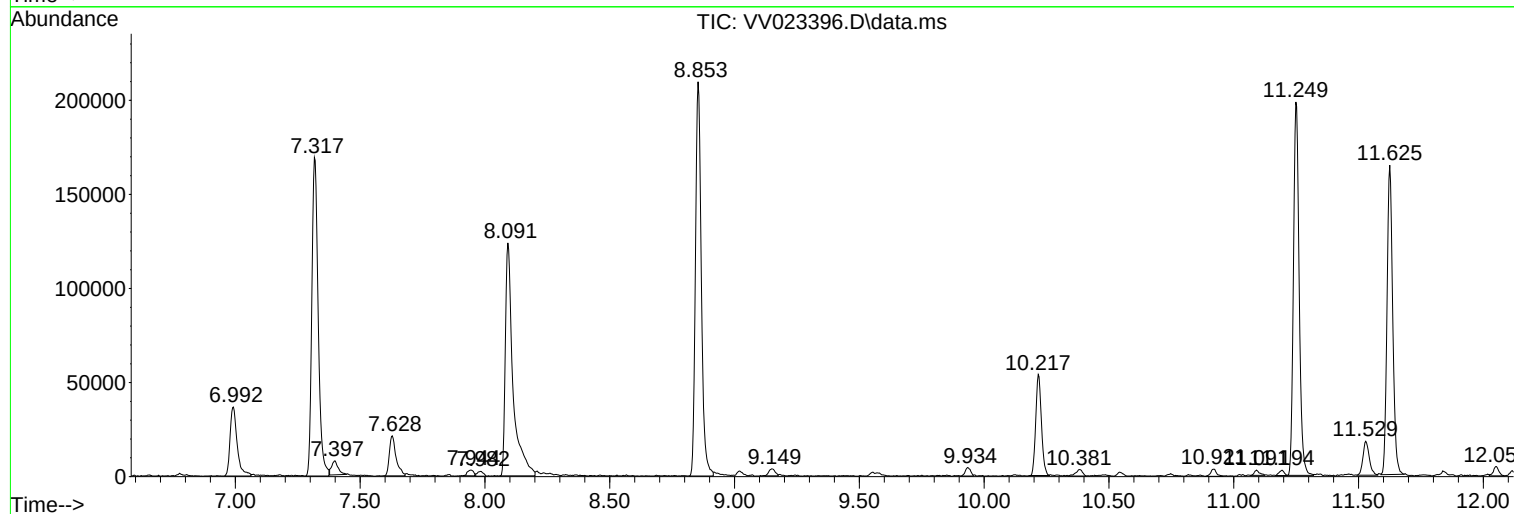
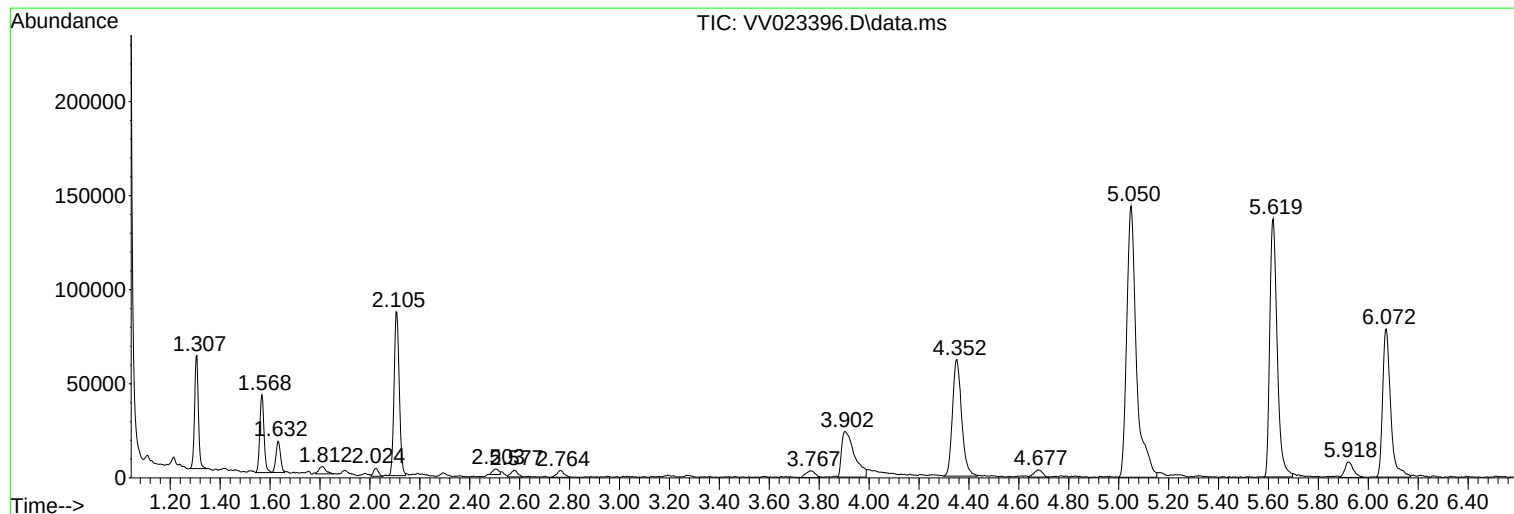
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Quant Title : TRACE VOA SFAM1.0

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



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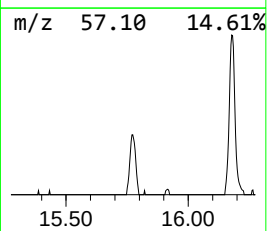
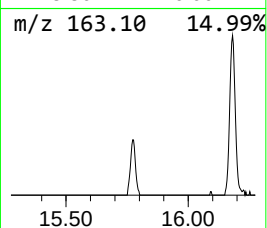
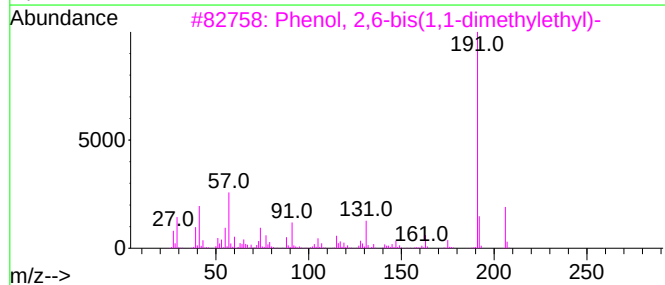
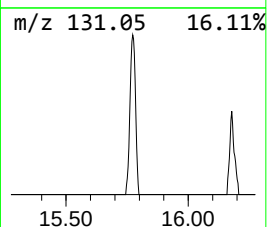
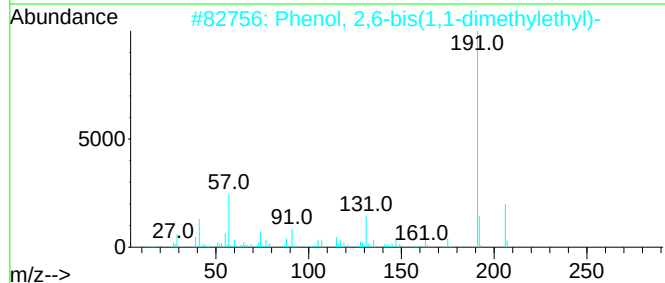
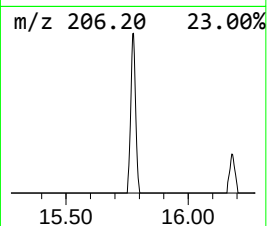
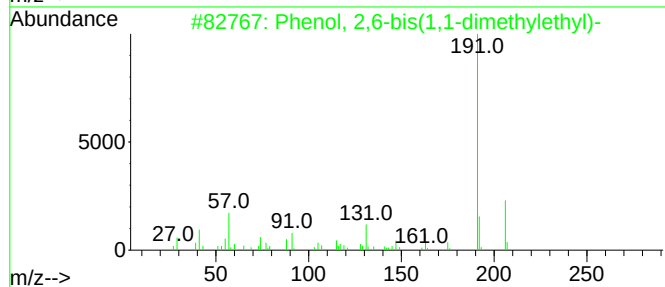
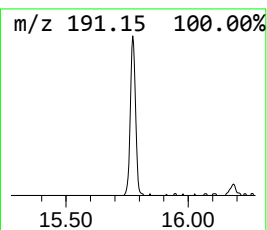
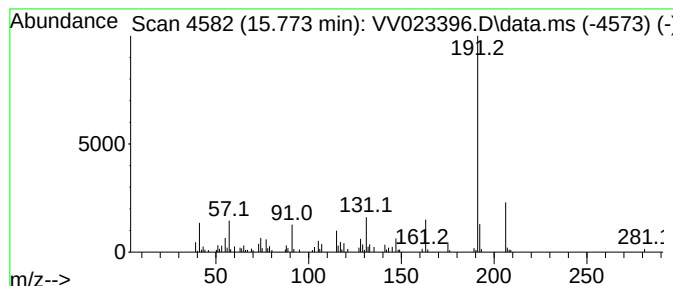
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Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.773	0.98 ug/L	61854	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	87



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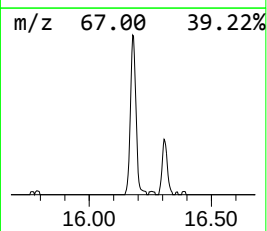
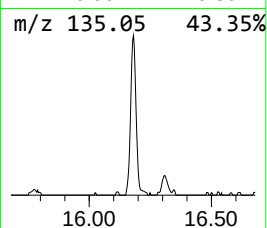
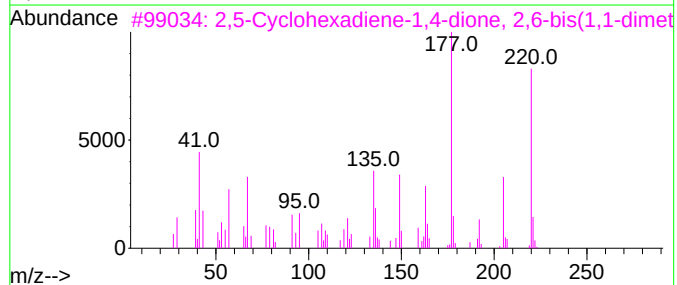
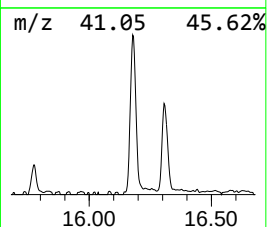
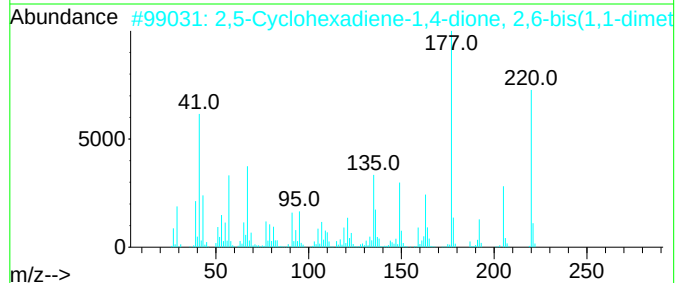
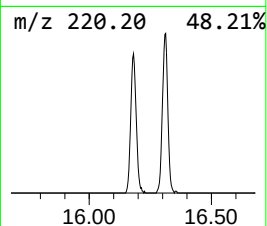
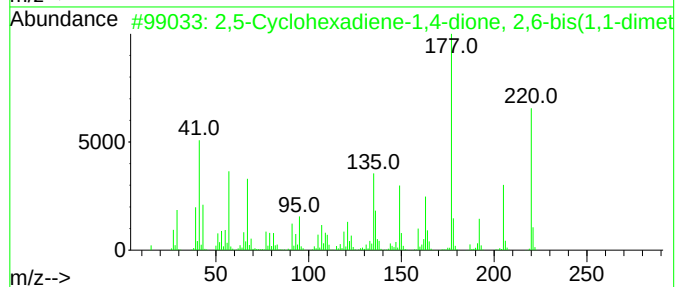
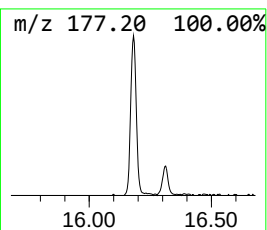
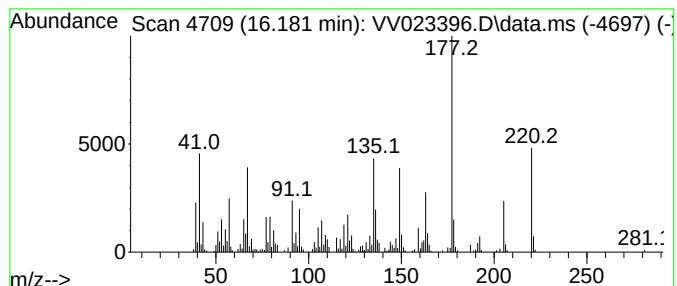
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR110421WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.181	4.25 ug/L	268218	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	96		
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	94		
4	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	93		
5	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	83		



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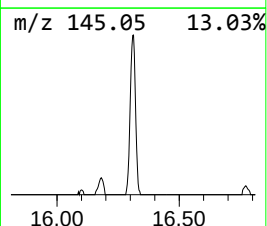
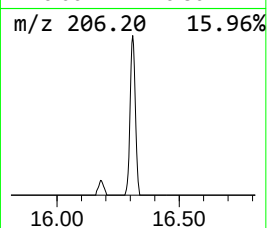
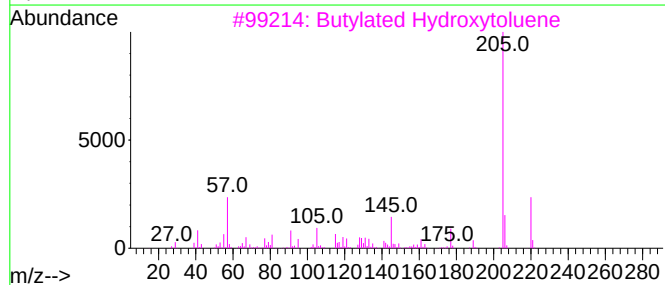
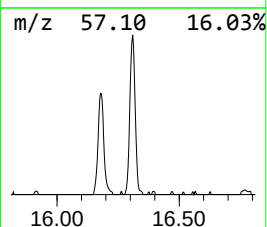
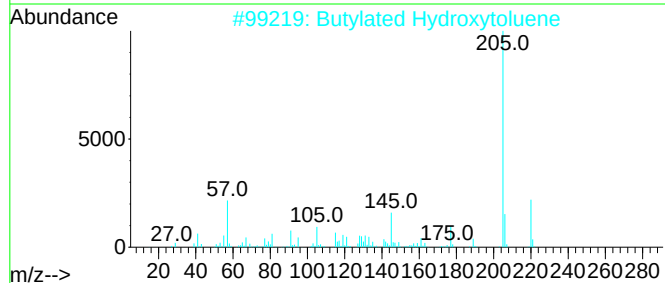
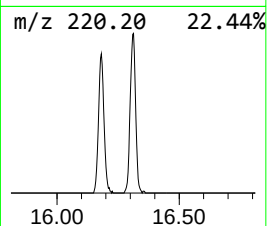
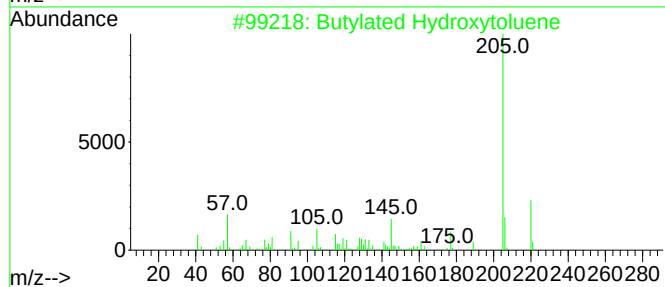
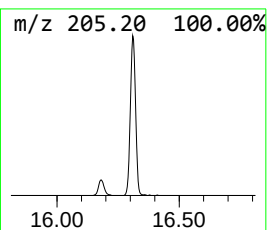
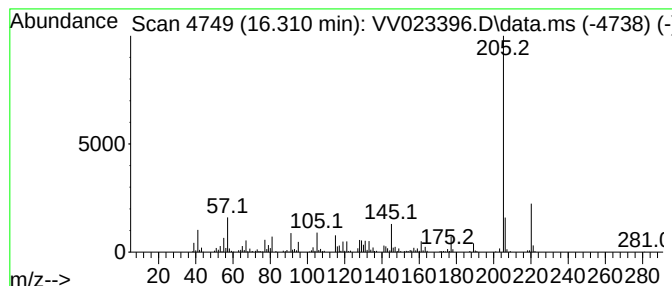
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
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Peak Number 4 Butylated Hydroxytoluene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.310	4.00 ug/L	252220	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	99
3			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
4			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	95
5			Ethyl 4-oxo-2-phenylpentanoate	220	C13H16O3	1000427-11-2	95



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Phenol, 2,6-bis...	15.773	1.0	ug/L	61854	3	11.249	315638	5.0
2,5-Cyclohexadi...	16.181	4.3	ug/L	268218	3	11.249	315638	5.0
Butylated Hydro...	16.310	4.0	ug/L	252220	3	11.249	315638	5.0