

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012425\
 Data File : VU062988.D
 Acq On : 24 Jan 2025 13:11
 Operator : MD/SY
 Sample : Q1174-02
 Misc : 25mL/MSVOA_U/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 E2932

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\SFAMUTR010225WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU062988.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.345	13	17	20	rBV	4447	3678	1.09%	0.102%
2	1.374	21	26	38	rVB3	23885	29616	8.80%	0.818%
3	1.618	92	102	117	rVB2	40271	69061	20.51%	1.906%
4	1.759	138	146	156	rVB2	6066	9558	2.84%	0.264%
5	1.824	158	166	175	rBV2	14084	18865	5.60%	0.521%
6	1.946	196	204	211	rBV	22414	28501	8.46%	0.787%
7	2.271	297	305	316	rVB3	4227	6957	2.07%	0.192%
8	2.586	393	403	418	rVB	42036	68834	20.44%	1.900%
9	2.711	429	442	458	rBV	93809	164136	48.75%	4.531%
10	2.811	458	473	488	rVB2	10990	24062	7.15%	0.664%
11	3.068	544	553	566	rVB4	4630	10243	3.04%	0.283%
12	3.898	796	811	826	rBV3	23161	54075	16.06%	1.493%
13	3.988	835	839	851	rVB7	2133	3867	1.15%	0.107%
14	4.753	1048	1077	1092	rBV	18183	76938	22.85%	2.124%
15	5.103	1168	1186	1207	rBV3	60610	138768	41.21%	3.831%
16	5.489	1300	1306	1318	rBV4	3980	7706	2.29%	0.213%
17	5.763	1375	1391	1428	rBV2	132220	318601	94.63%	8.795%
18	6.277	1539	1551	1576	rVB	147010	278797	82.80%	7.696%
19	6.563	1632	1640	1651	rVB8	6353	11623	3.45%	0.321%
20	6.647	1656	1666	1675	rBV8	1789	3572	1.06%	0.099%
21	6.714	1675	1687	1706	rBV2	72677	141280	41.96%	3.900%
22	6.846	1712	1728	1744	rBV5	6390	21365	6.35%	0.590%
23	7.579	1945	1956	1980	rVB2	38103	66943	19.88%	1.848%
24	7.692	1980	1991	2004	rBV3	3991	7701	2.29%	0.213%
25	7.824	2018	2032	2047	rBV5	35217	85106	25.28%	2.349%
26	7.907	2047	2058	2072	rVV	147494	261985	77.81%	7.232%
27	7.978	2074	2080	2093	rVV2	10648	18114	5.38%	0.500%
28	8.052	2096	2103	2112	rBV6	2318	4161	1.24%	0.115%
29	8.187	2135	2145	2160	rBV	23220	39924	11.86%	1.102%
30	8.647	2275	2288	2321	rBV2	100478	236173	70.14%	6.519%
31	8.795	2327	2334	2348	rVB6	6720	11979	3.56%	0.331%
32	9.415	2515	2527	2548	rBV	195477	336697	100.00%	9.294%
33	9.692	2604	2613	2625	rVB3	4256	7255	2.15%	0.200%
34	10.100	2732	2740	2749	rBV3	2156	3542	1.05%	0.098%
35	10.238	2773	2783	2795	rVB3	4155	7171	2.13%	0.198%
36	10.698	2916	2926	2931	rBV6	2298	3534	1.05%	0.098%

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37	10.746	2931	2941	2956	rVB	60060	99451	29.54%	2.745%
38	10.884	2975	2984	2994	rVB4	2452	4001	1.19%	0.110%
39	11.682	3218	3232	3239	rBV9	1720	3369	1.00%	0.093%
40	11.804	3256	3270	3285	rBV	193375	325579	96.70%	8.987%
41	12.065	3339	3351	3370	rBV4	13845	42076	12.50%	1.161%
42	12.183	3377	3388	3404	rVB	131867	219557	65.21%	6.061%
43	12.306	3419	3426	3429	rBV5	3646	4411	1.31%	0.122%
44	12.447	3462	3470	3477	rBV5	2942	4306	1.28%	0.119%
45	12.881	3597	3605	3611	rBV7	3647	4816	1.43%	0.133%
46	12.939	3614	3623	3635	rVV3	8058	13376	3.97%	0.369%
47	13.280	3718	3729	3741	rBV3	3836	8687	2.58%	0.240%
48	13.444	3768	3780	3786	rBV7	2347	3806	1.13%	0.105%
49	13.511	3795	3801	3808	rVB4	3252	4398	1.31%	0.121%
50	13.724	3859	3867	3877	rVB8	4751	6964	2.07%	0.192%
51	13.833	3892	3901	3908	rBV10	2932	5382	1.60%	0.149%
52	13.936	3922	3933	3941	rBV9	4522	8786	2.61%	0.243%
53	14.029	3951	3962	3969	rBV10	3907	6343	1.88%	0.175%
54	14.084	3970	3979	3992	rVB	4055	6913	2.05%	0.191%
55	14.412	4072	4081	4093	rVB2	11640	18021	5.35%	0.497%
56	14.817	4196	4207	4214	rBV8	3105	6661	1.98%	0.184%
57	15.212	4322	4330	4340	rBV	6808	10780	3.20%	0.298%
58	15.402	4379	4389	4400	rBV	12016	18746	5.57%	0.517%
59	15.473	4400	4411	4429	rBV	75994	136488	40.54%	3.768%
60	15.916	4541	4549	4557	rBV8	2664	4172	1.24%	0.115%
61	16.257	4648	4655	4663	rVB7	2428	3691	1.10%	0.102%
62	16.399	4691	4699	4706	rBV4	6787	9524	2.83%	0.263%
63	16.752	4799	4809	4825	rBV3	39188	61961	18.40%	1.710%

Sum of corrected areas: 3622653

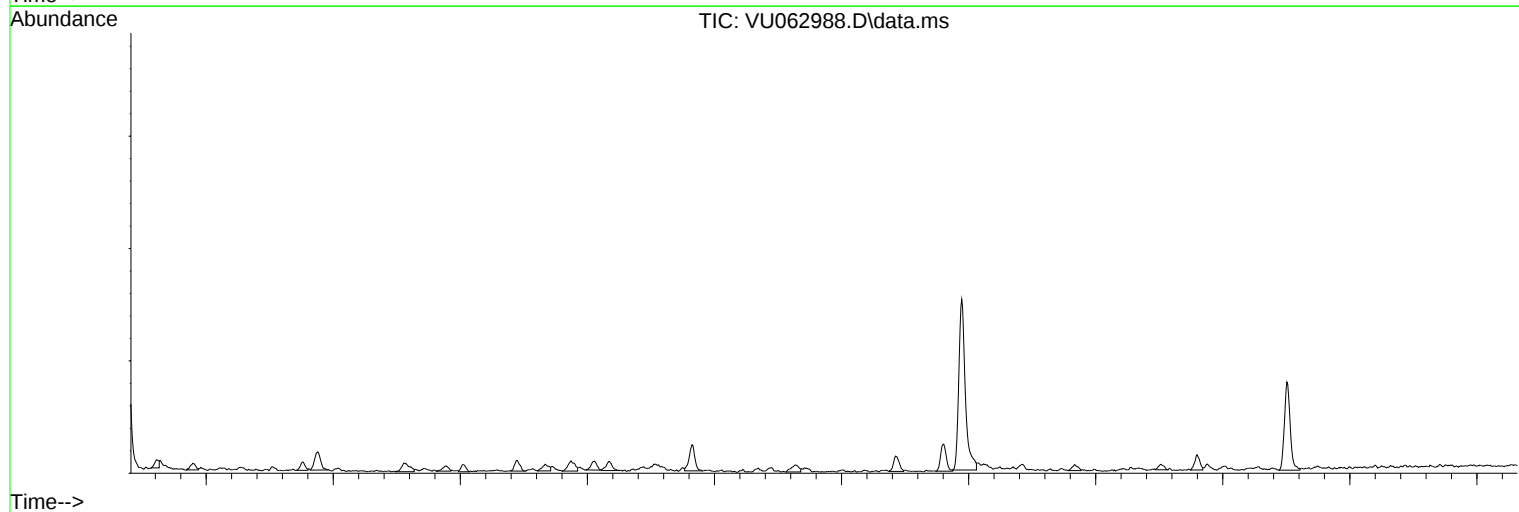
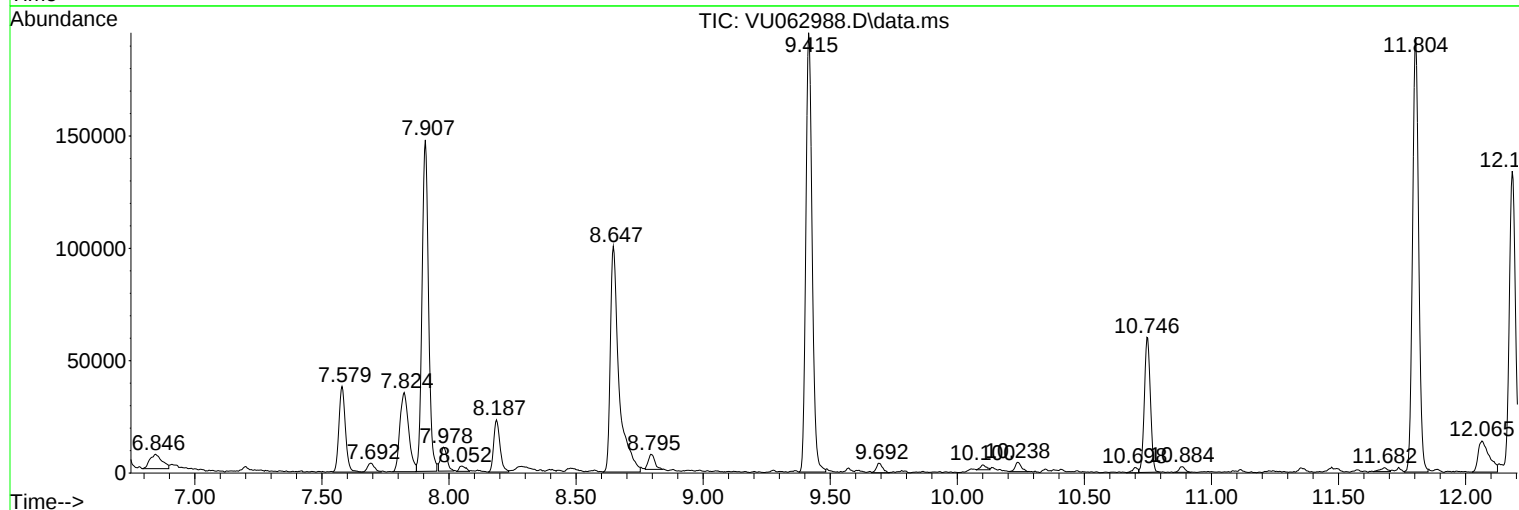
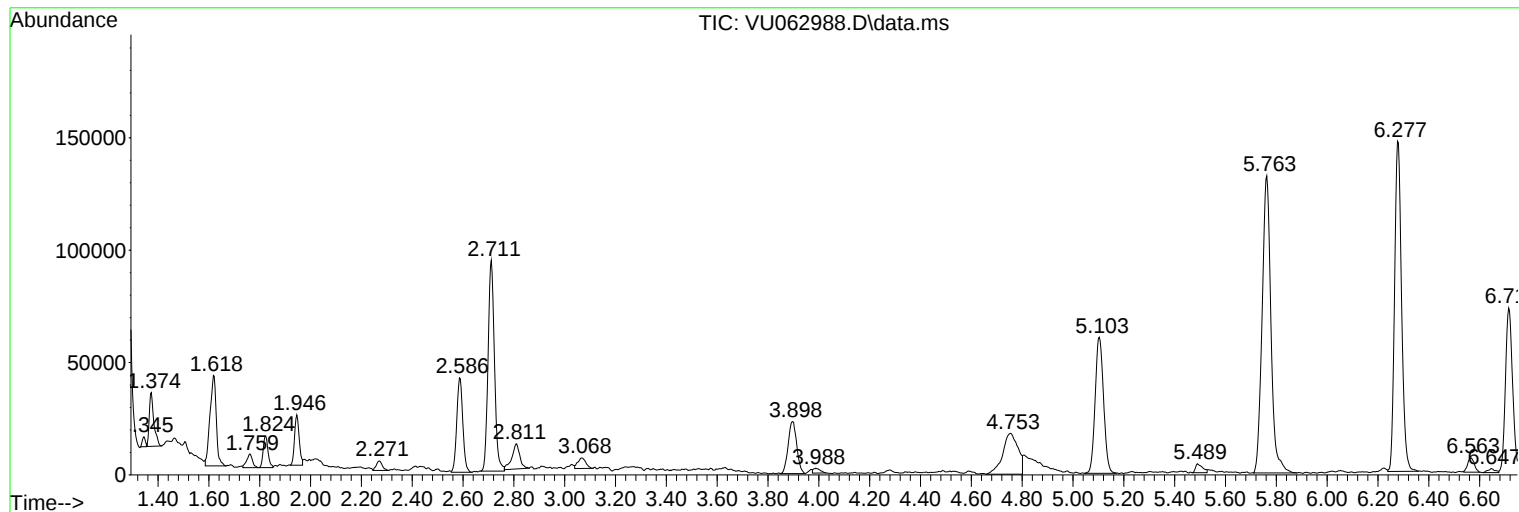
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR010225WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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ClientSampleId :
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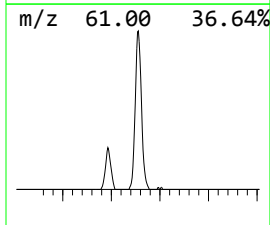
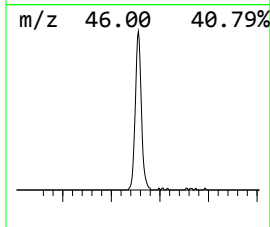
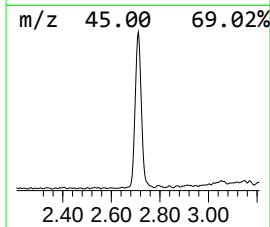
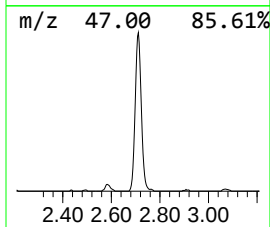
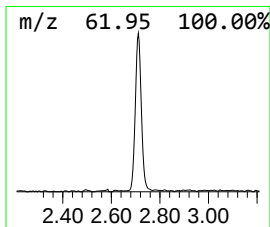
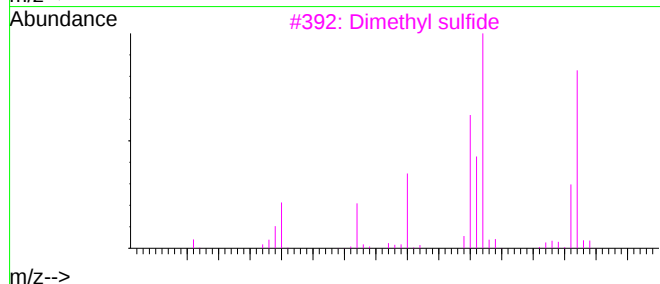
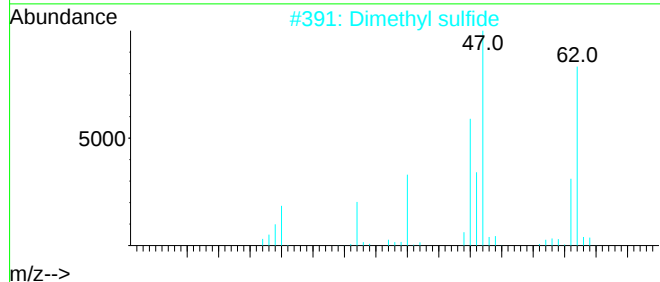
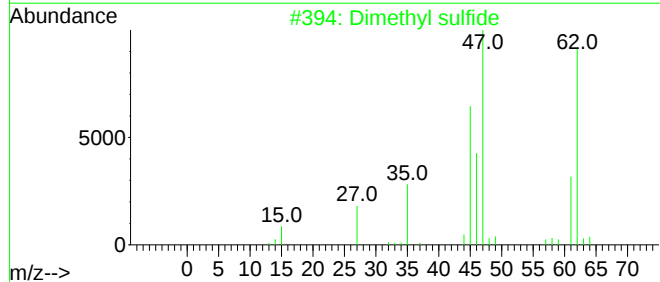
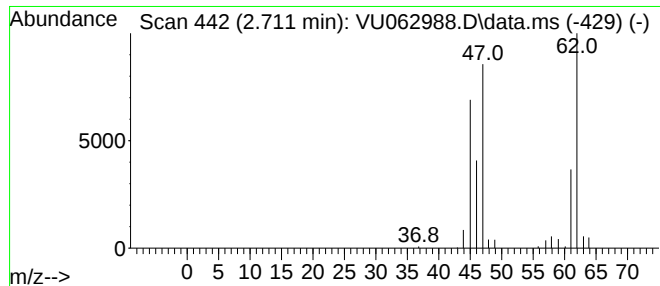
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR010225WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Dimethyl sulfide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.711	2.94 ug/L	164136	1,4-Difluorobenzene	6.277

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl sulfide	62	C2H6S	000075-18-3	94
2	Dimethyl sulfide	62	C2H6S	000075-18-3	94
3	Dimethyl sulfide	62	C2H6S	000075-18-3	94
4	Dimethyl sulfide	62	C2H6S	000075-18-3	91
5	Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	83



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Quant Title : TRACE VOA SFAM1.0

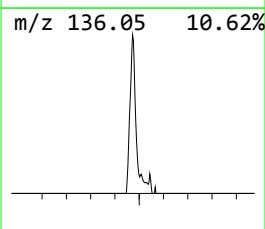
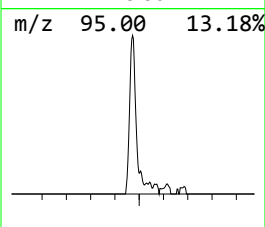
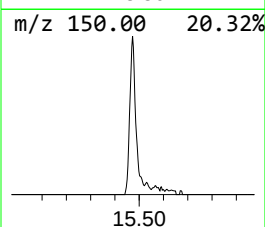
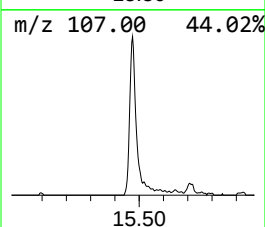
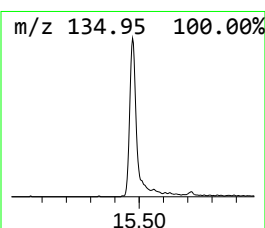
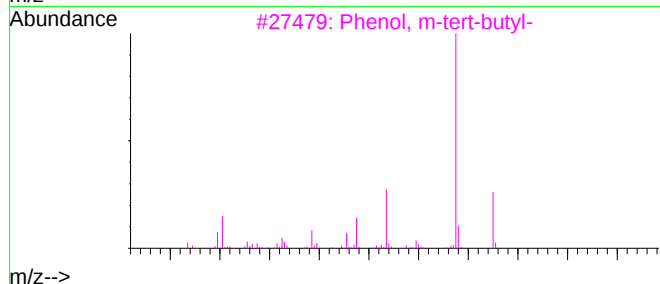
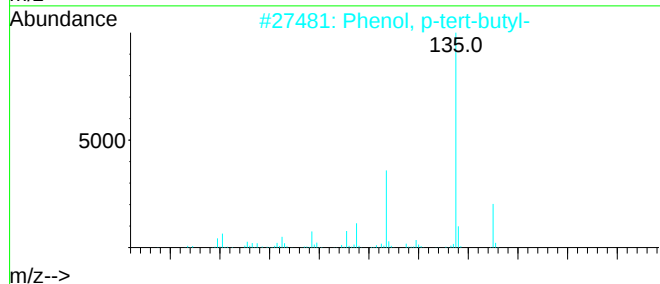
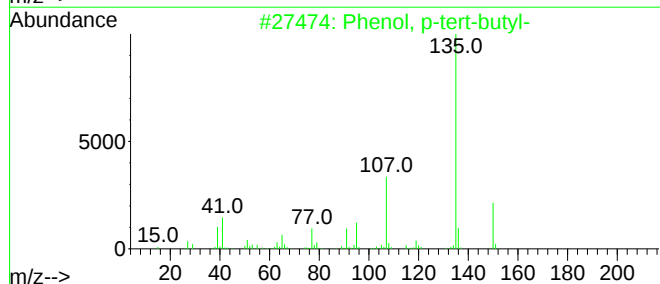
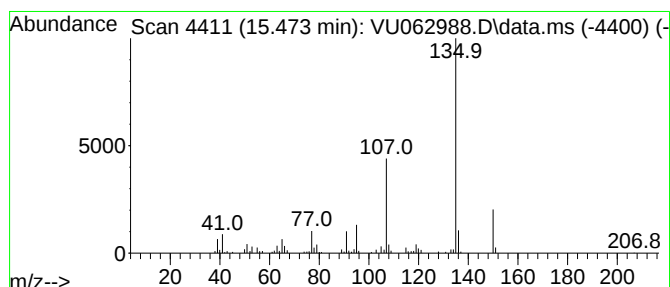
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 5 Phenol, p-tert-butyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.473	2.10 ug/L	136488	1,4-Dichlorobenzene-d4	11.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	96
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	96
3	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	93
4	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	93
5	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	91



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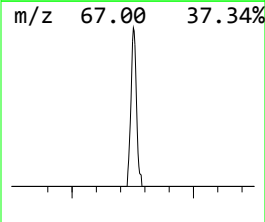
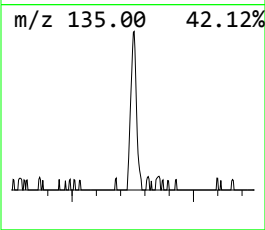
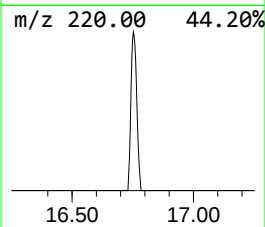
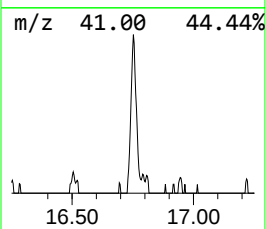
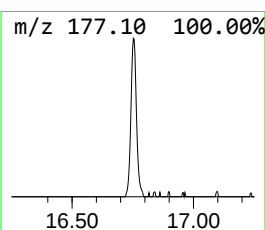
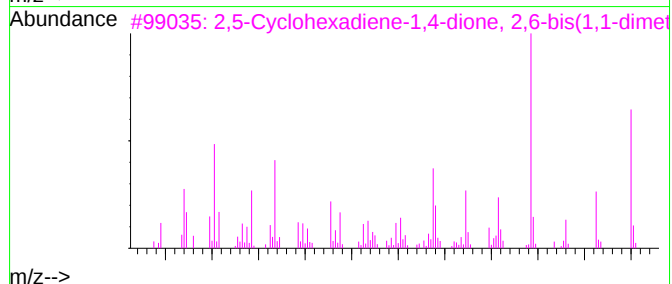
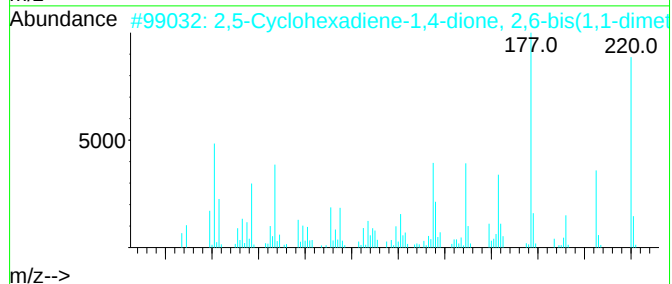
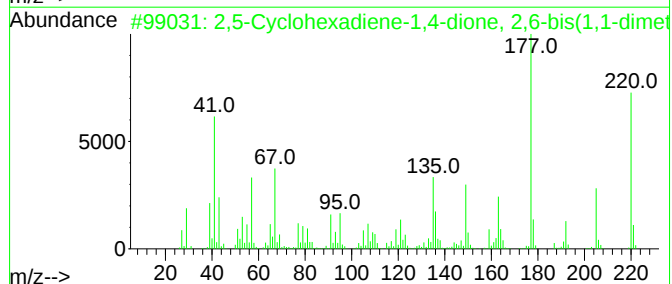
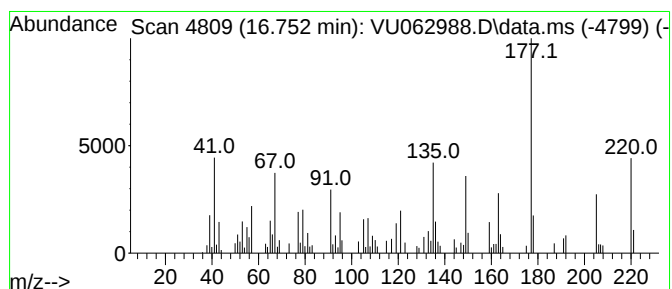
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 6 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.752	0.95 ug/L	61961	1,4-Dichlorobenzene-d4	11.804	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	95
2	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	94
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	94
4	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	60
5	1H-indene-4,7-diol, 2,3-dihydro-...	220	C14H20O2	1000396-25-5	53



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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
Dimethyl sulfide	2.711	2.9	ug/L	164136	1	6.277	278797	5.0
Phenol, p-tert-...	15.473	2.1	ug/L	136488	3	11.804	325579	5.0
2,5-Cyclohexadi...	16.752	0.9	ug/L	61961	3	11.804	325579	5.0