

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120922\
 Data File : VU052294.D
 Acq On : 09 Dec 2022 12:14
 Operator : JC/MD
 Sample : N5916-14
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 8 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: VU052294.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	71	81	97	rVB	103628	137462	14.12%	1.687%
2	1.916	171	179	196	rVB	87697	123973	12.74%	1.522%
3	2.568	370	382	396	rBV	167770	272415	27.99%	3.344%
4	4.649	1013	1029	1072	rBV	92073	385447	39.60%	4.731%
5	5.060	1141	1157	1178	rBV	158886	354852	36.46%	4.356%
6	5.723	1343	1363	1375	rBV2	306772	805952	82.80%	9.893%
7	5.793	1375	1385	1408	rVB	274027	563581	57.90%	6.918%
8	6.247	1512	1526	1553	rBV	288064	553414	56.85%	6.793%
9	6.543	1607	1618	1631	rVB3	14783	28751	2.95%	0.353%
10	6.687	1649	1663	1682	rBV	199470	397629	40.85%	4.881%
11	7.565	1924	1936	1956	rBV	86986	155439	15.97%	1.908%
12	7.896	2026	2039	2055	rBV	322566	566794	58.23%	6.957%
13	7.967	2056	2061	2073	rVB	6977	10779	1.11%	0.132%
14	8.176	2114	2126	2145	rBV	53403	93541	9.61%	1.148%
15	8.636	2253	2269	2307	rBV2	458328	973382	100.00%	11.948%
16	9.414	2499	2511	2537	rBV	413744	697386	71.65%	8.560%
17	10.751	2912	2927	2942	rBV	183973	304044	31.24%	3.732%
18	11.118	3023	3041	3051	rBV	11208	18439	1.89%	0.226%
19	11.809	3242	3256	3276	rBV	351530	569028	58.46%	6.985%
20	12.063	3324	3335	3345	rBV6	6757	12228	1.26%	0.150%
21	12.189	3362	3374	3394	rBV	315503	529358	54.38%	6.498%
22	15.690	4444	4463	4477	rBV3	39376	68011	6.99%	0.835%
23	16.677	4760	4770	4786	rBV2	116303	202117	20.76%	2.481%
24	16.764	4788	4797	4815	rVB3	54633	93516	9.61%	1.148%
25	16.883	4823	4834	4846	rBV	147949	229310	23.56%	2.815%

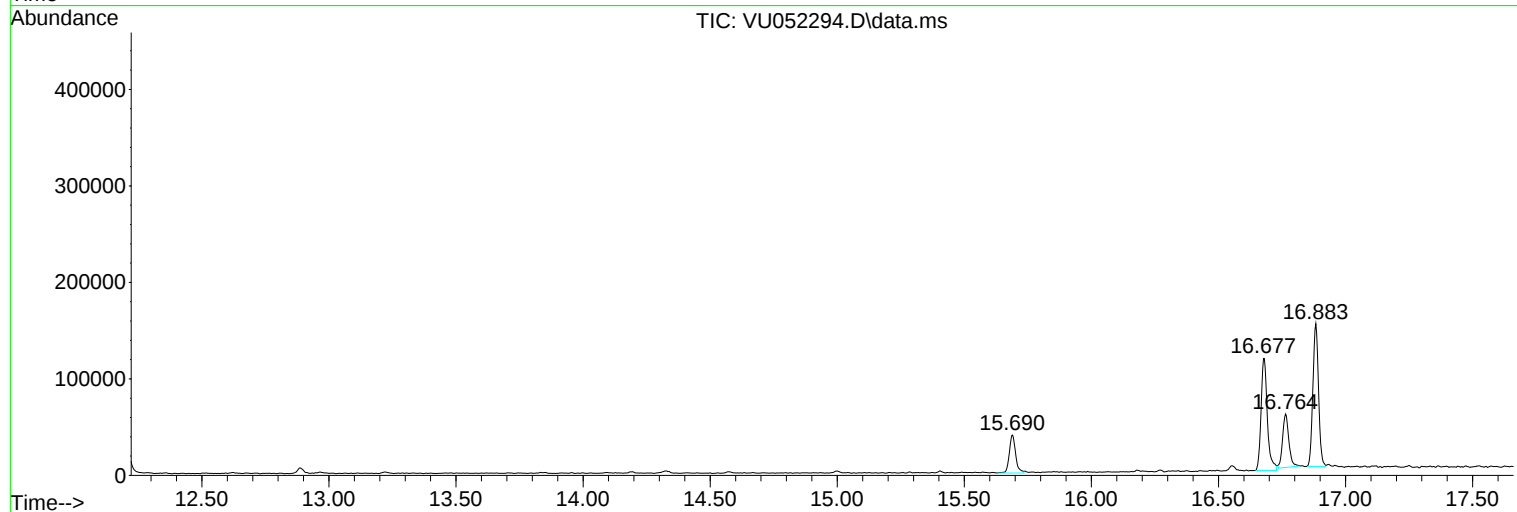
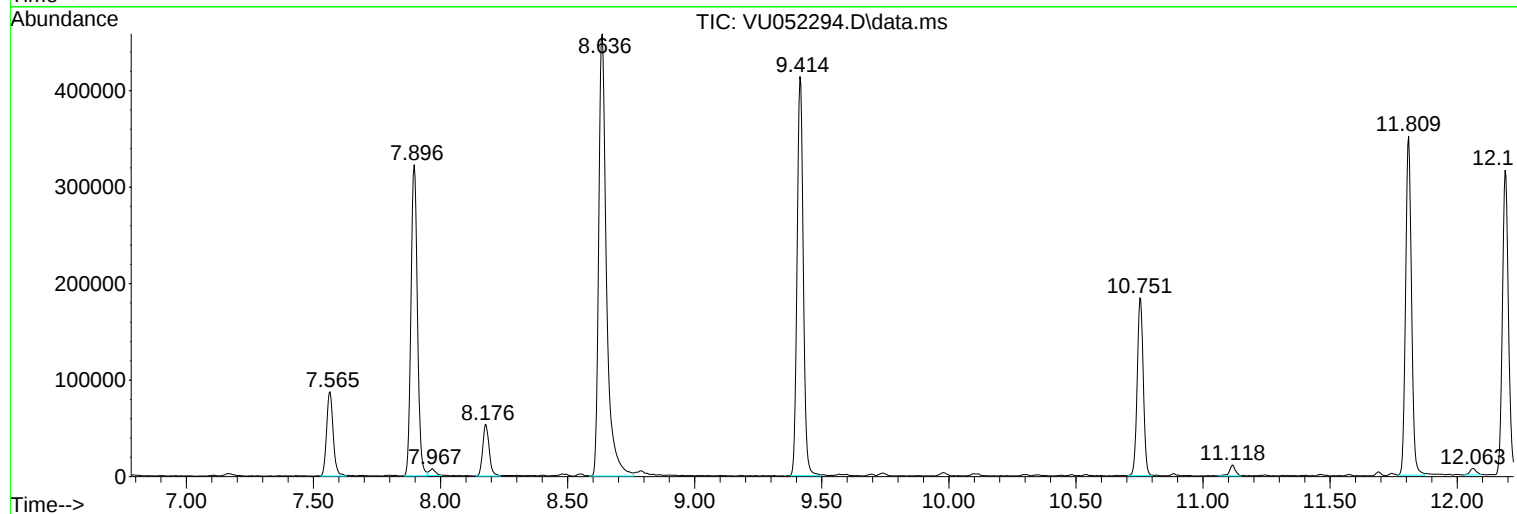
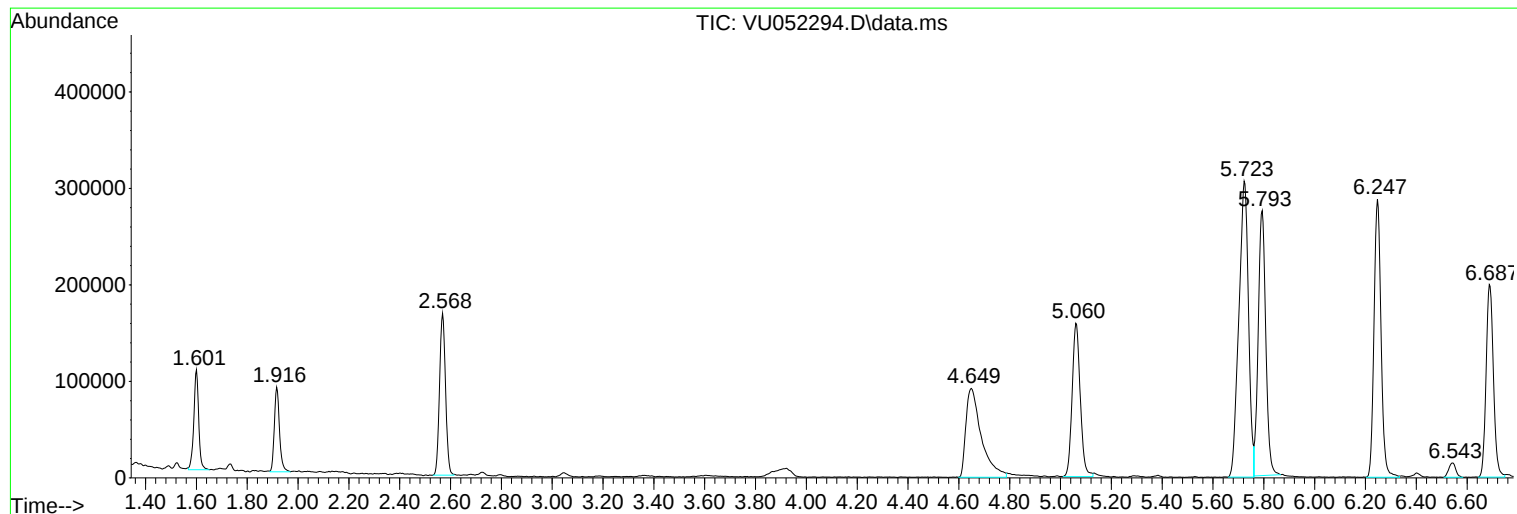
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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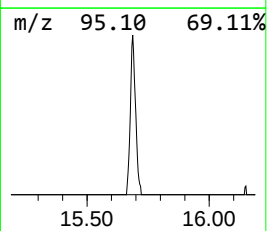
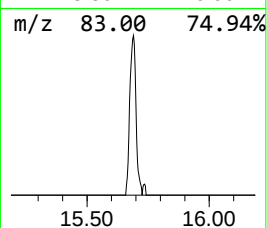
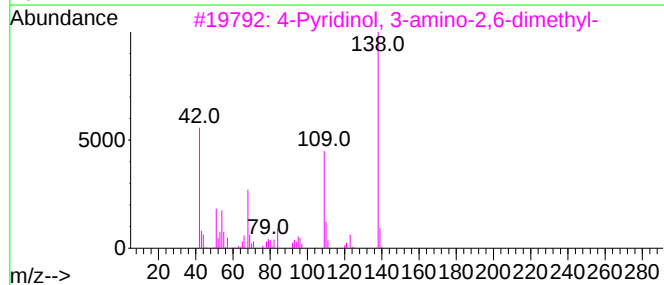
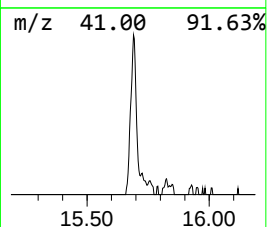
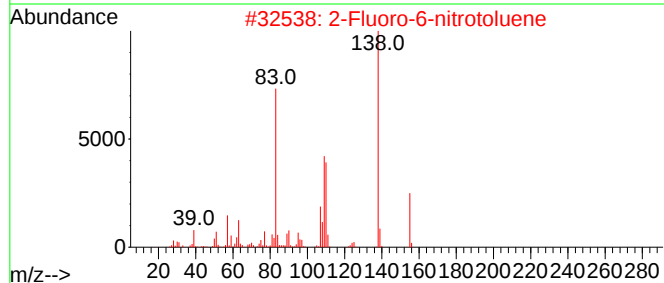
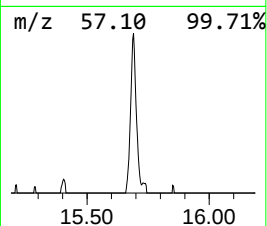
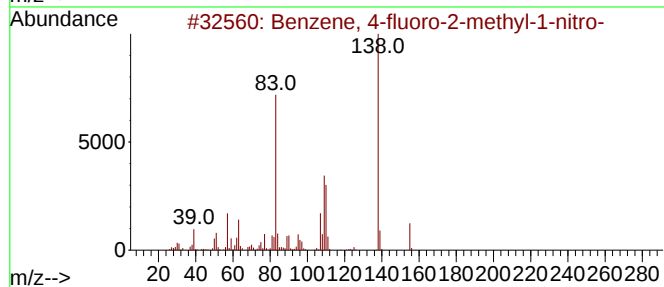
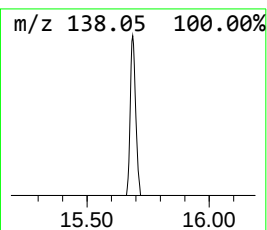
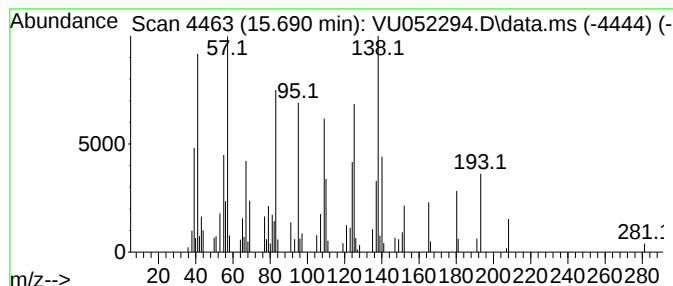
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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	0.60 ug/L	68011	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-fluoro-2-methyl-1-nitro-	155	C7H6FN02	000446-33-3	35
2			2-Fluoro-6-nitrotoluene	155	C7H6FN02	000769-10-8	35
3			4-Pyridinol, 3-amino-2,6-dimethyl-	138	C7H10N2O	1000252-94-0	18
4			3-Methoxybenzyl alcohol	138	C8H10O2	006971-51-3	18
5			2,3-Dimethylhydroquinone	138	C8H10O2	000608-43-5	15



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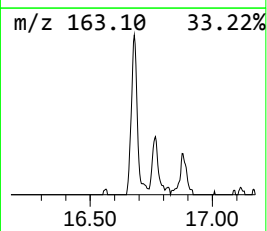
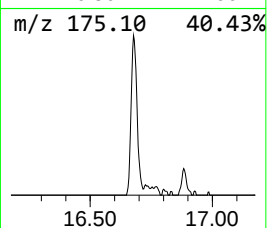
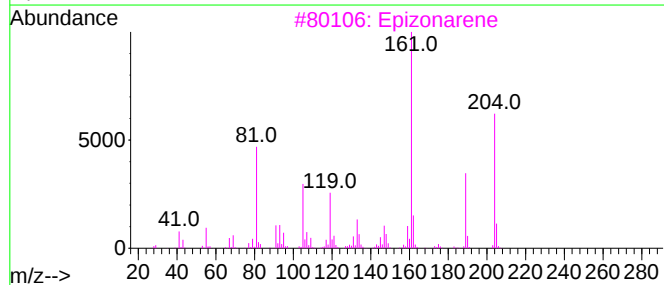
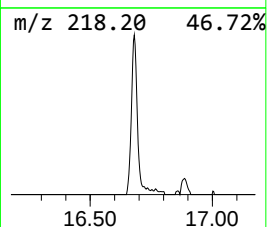
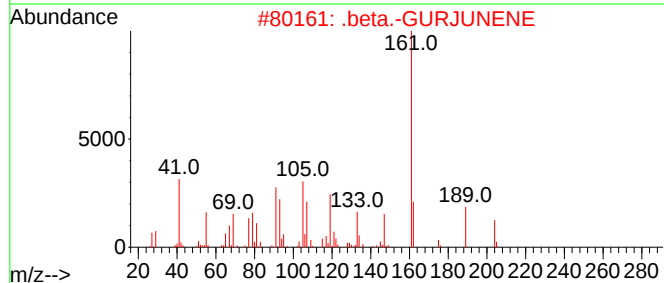
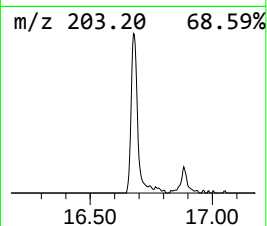
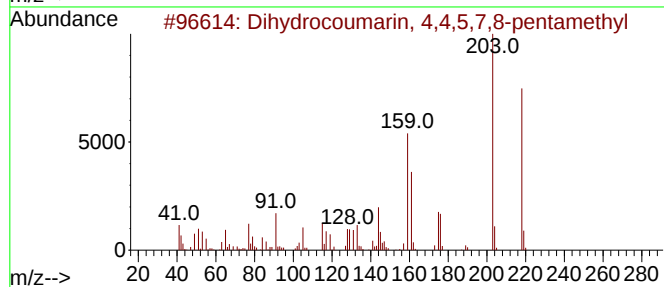
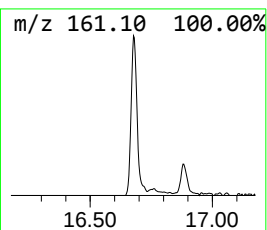
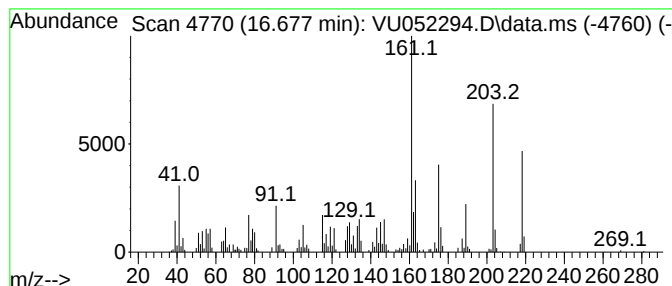
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 unknown-02 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.677	1.78 ug/L	202117	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dihydrocoumarin, 4,4,5,7,8-penta...	218	C14H18O2	039170-97-3	46
2			.beta.-GURJUNENE	204	C15H24	1000425-17-9	46
3			Epizonarene	204	C15H24	041702-63-0	46
4			4-n-Butylbenzoic acid, allyl ester	218	C14H18O2	1000293-35-8	43
5			1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	017334-55-3	42



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Sample : N5916-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5N32

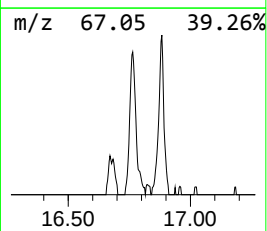
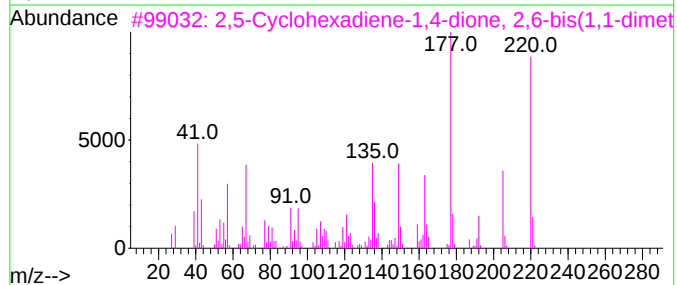
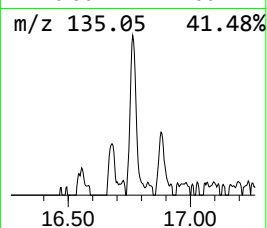
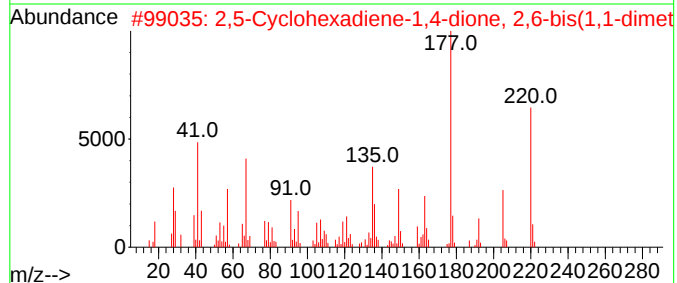
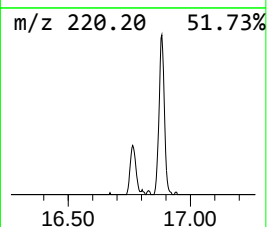
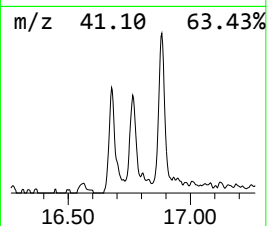
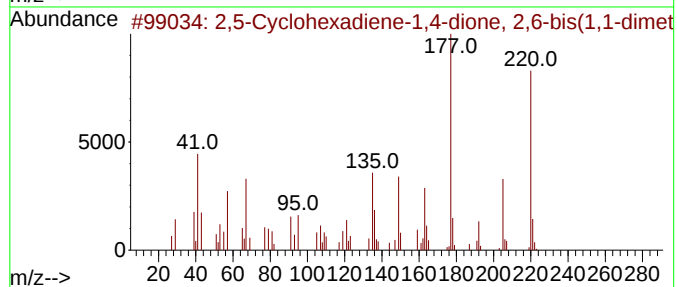
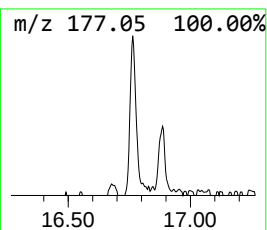
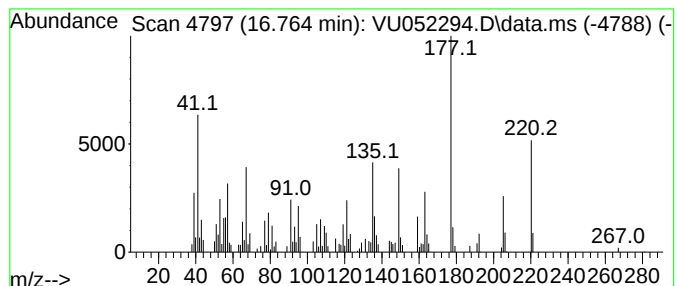
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.764	0.82 ug/L	93516	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	96
2			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	91
3			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	90
4			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	87
5			2,5-di-tert-Butyl-1,4-benzoquinone	220	C14H20O2	002460-77-7	51



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ClientSampleId :
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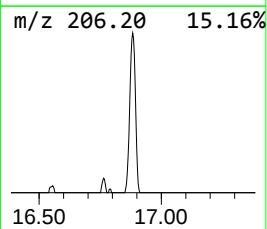
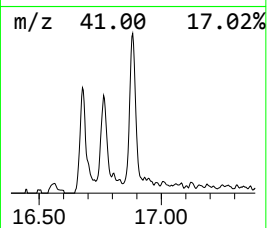
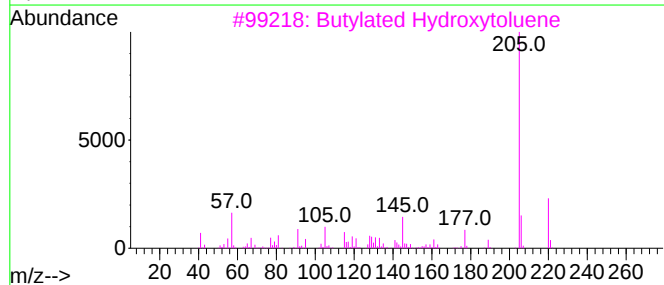
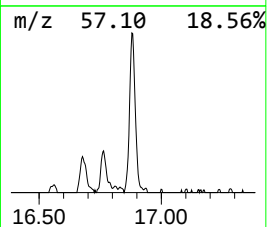
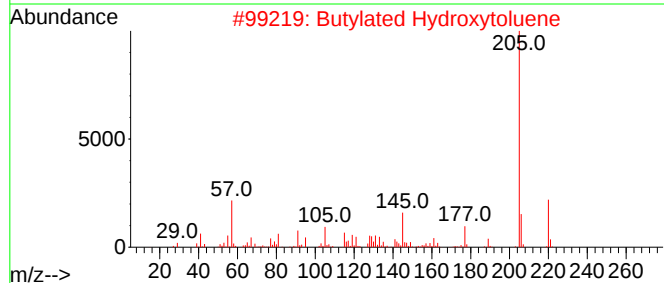
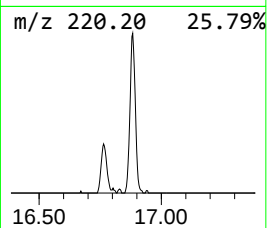
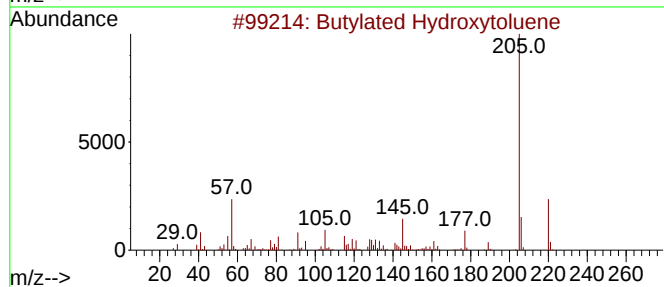
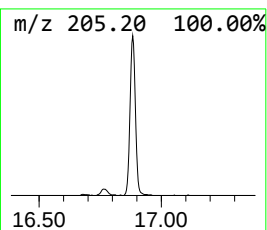
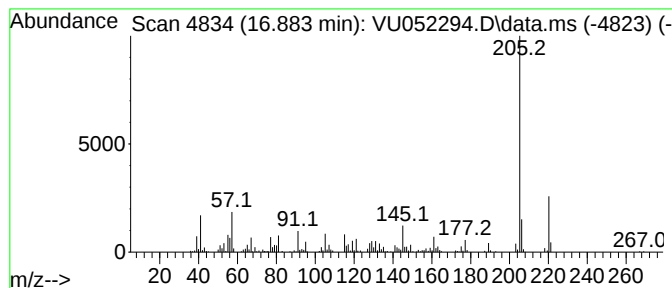
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.883	2.01 ug/L	229310	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	97
2			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	97
3			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	96
4			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	94
5			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	15.690	0.6	ug/L	68011	3	11.809	569028	5.0
unknown-02	16.677	1.8	ug/L	202117	3	11.809	569028	5.0
2,5-Cyclohexadi...	16.764	0.8	ug/L	93516	3	11.809	569028	5.0
Butylated Hydro...	16.883	2.0	ug/L	229310	3	11.809	569028	5.0