

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120822\
 Data File : VU052254.D
 Acq On : 08 Dec 2022 17:22
 Operator : JC/MD
 Sample : N5916-14
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 20 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: VU052254.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	96	rVB	107882	145060	15.10%	1.787%
2	1.732	117	122	132	rVB2	7819	10632	1.11%	0.131%
3	1.916	170	179	193	rBV	87515	119331	12.42%	1.470%
4	2.568	370	382	403	rVB	163529	269244	28.03%	3.317%
5	3.854	763	782	783	rBV4	5649	11684	1.22%	0.144%
6	4.649	1014	1029	1075	rBV2	91367	376715	39.21%	4.641%
7	5.060	1142	1157	1176	rBV	150683	334534	34.82%	4.122%
8	5.723	1337	1363	1375	rBV2	286200	756117	78.70%	9.316%
9	5.793	1375	1385	1412	rVB	165167	349316	36.36%	4.304%
10	6.247	1511	1526	1552	rBV	242520	469519	48.87%	5.785%
11	6.687	1646	1663	1691	rBV	186327	376175	39.16%	4.635%
12	7.565	1924	1936	1952	rBV	77079	138287	14.39%	1.704%
13	7.896	2025	2039	2058	rBV	304467	537935	55.99%	6.628%
14	8.179	2113	2127	2146	rBV	49479	87657	9.12%	1.080%
15	8.636	2255	2269	2305	rBV2	457676	960709	100.00%	11.836%
16	9.414	2499	2511	2533	rBV	362966	607788	63.26%	7.488%
17	10.754	2912	2928	2941	rVB	177712	297768	30.99%	3.669%
18	11.115	3033	3040	3053	rVB2	12917	21028	2.19%	0.259%
19	11.809	3244	3256	3277	rBV	332695	542867	56.51%	6.688%
20	12.060	3327	3334	3344	rBV3	6242	9663	1.01%	0.119%
21	12.189	3362	3374	3400	rBV	324129	533152	55.50%	6.569%
22	12.886	3585	3591	3604	rVB7	7114	10206	1.06%	0.126%
23	15.687	4452	4462	4477	rBV5	47452	82212	8.56%	1.013%
24	15.783	4486	4492	4504	rVB5	9827	15386	1.60%	0.190%
25	16.693	4766	4775	4787	rBV2	84764	149277	15.54%	1.839%
26	16.764	4789	4797	4817	rVB2	128171	212623	22.13%	2.620%
27	16.883	4824	4834	4855	rVB	448731	691664	72.00%	8.522%

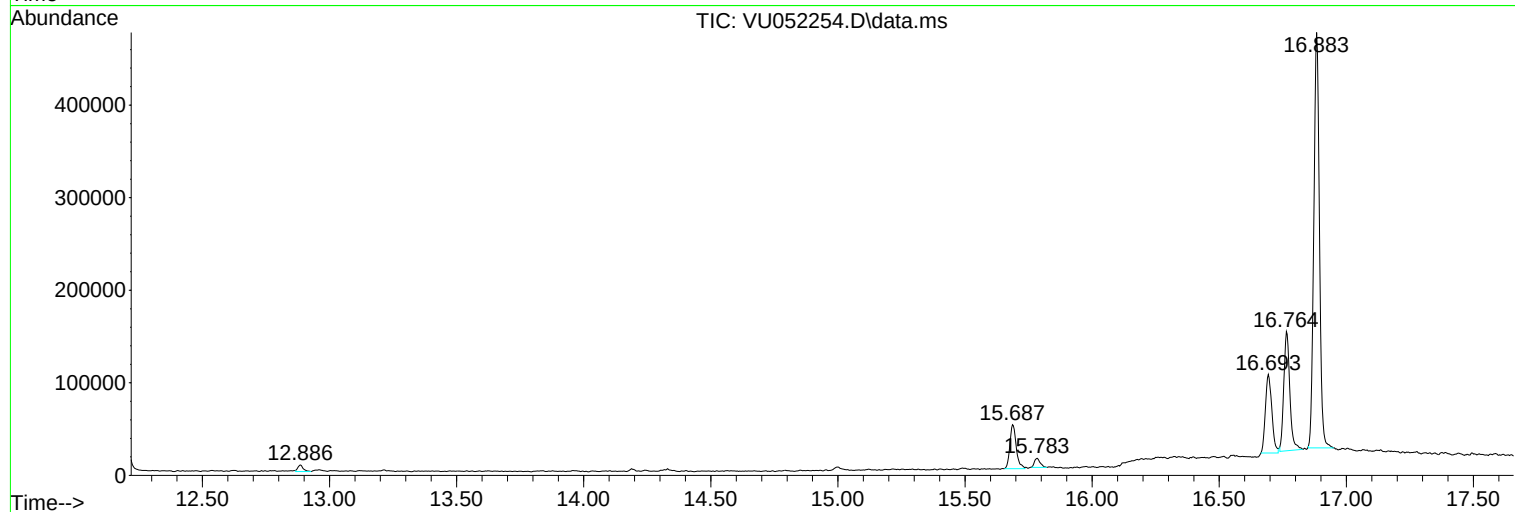
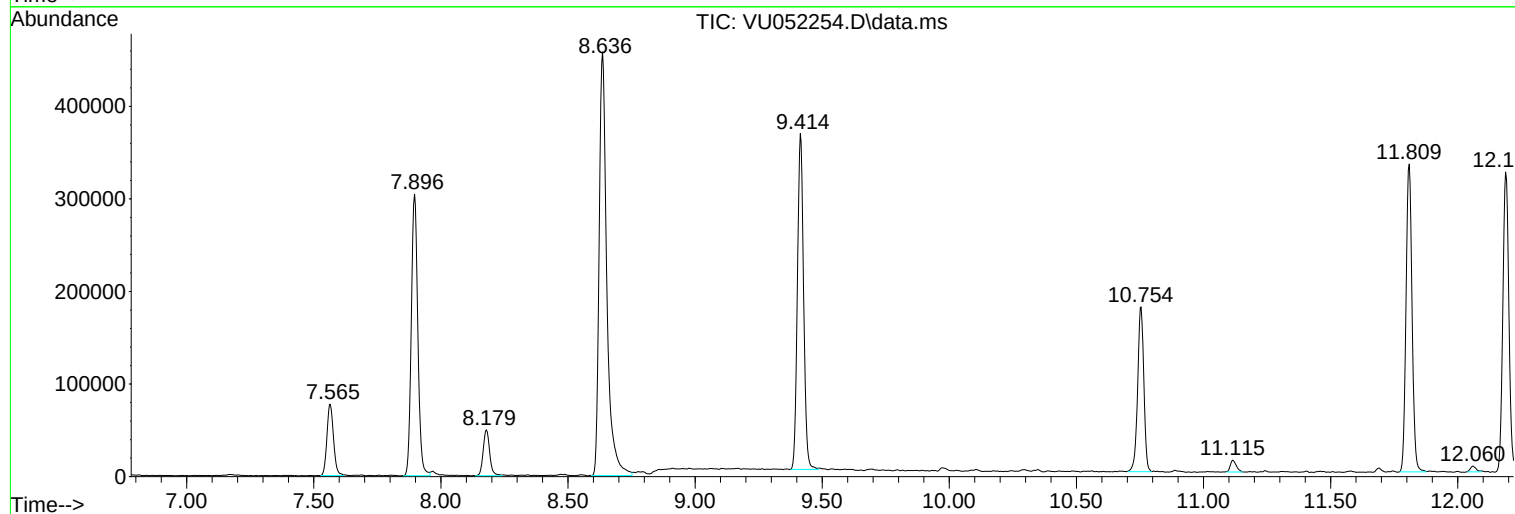
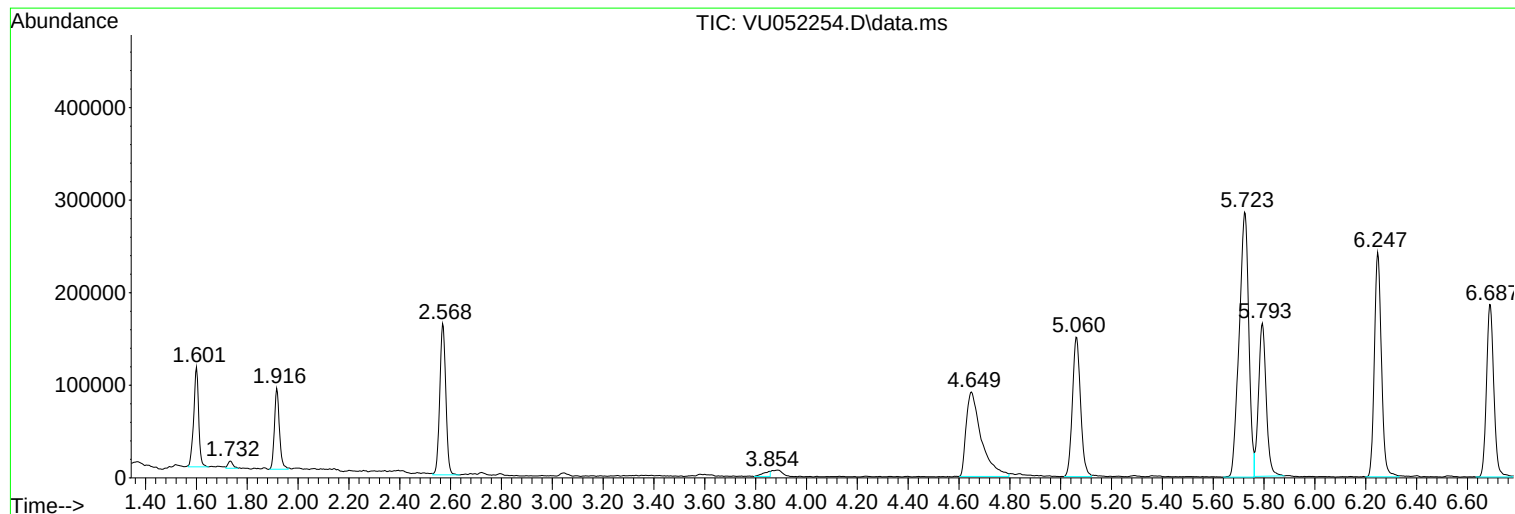
Sum of corrected areas: 8116549

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120822\
Data File : VU052254.D
Acq On : 08 Dec 2022 17:22
Operator : JC/MD
Sample : N5916-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 20 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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120822\
Data File : VU052254.D
Acq On : 08 Dec 2022 17:22
Operator : JC/MD
Sample : N5916-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5N32

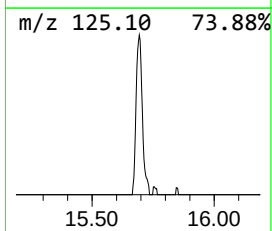
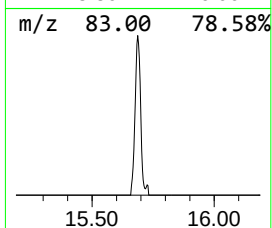
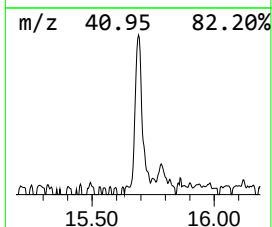
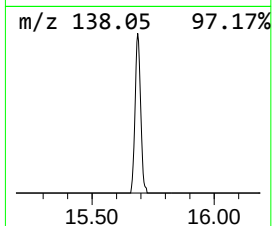
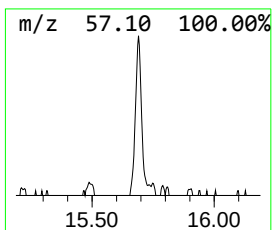
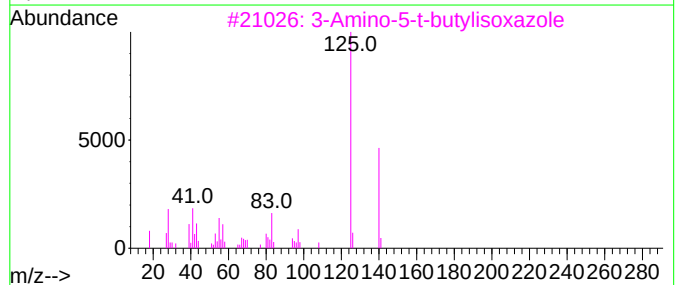
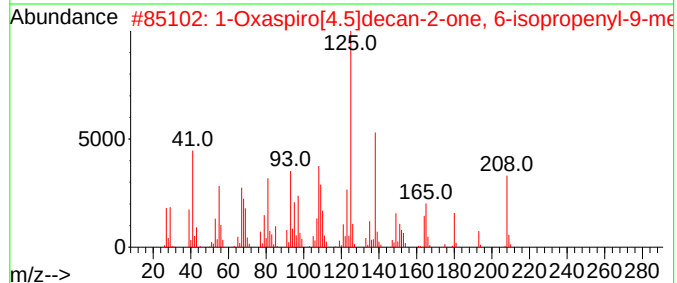
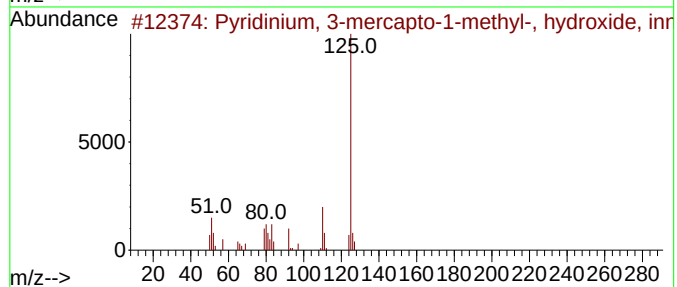
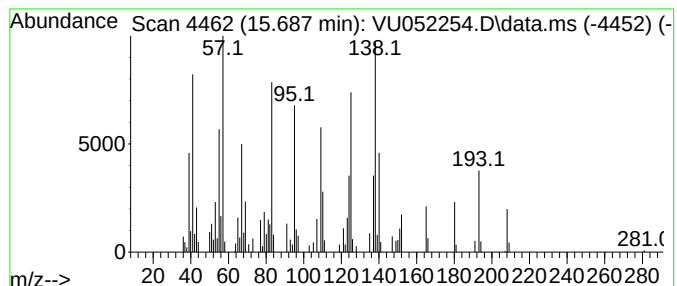
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.687	0.76 ug/L	82212	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pyridinium, 3-mercapto-1-methyl-...	125	C6H7NS	036880-58-7	25
2			1-Oxaspiro[4.5]decan-2-one, 6-is...	208	C13H20O2	1010157-58-3	25
3			3-Amino-5-t-butylisoxazole	140	C7H12N2O	055809-36-4	18
4			3-Amino-5-t-butylisoxazole	140	C7H12N2O	055809-36-4	18
5			Benzene, 1,3-dimethoxy-	138	C8H10O2	000151-10-0	14



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120822\
Data File : VU052254.D
Acq On : 08 Dec 2022 17:22
Operator : JC/MD
Sample : N5916-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5N32

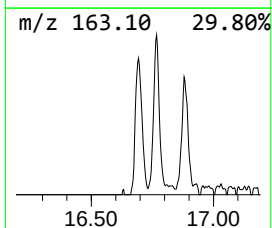
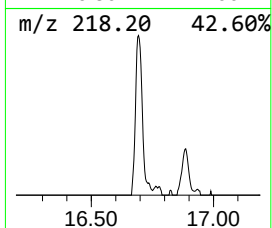
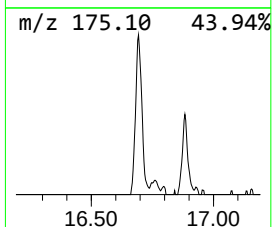
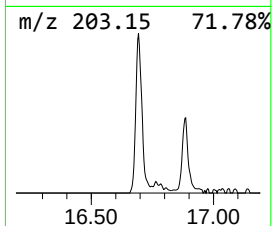
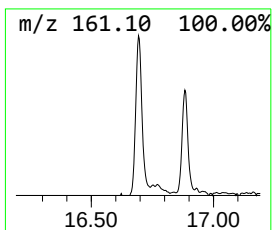
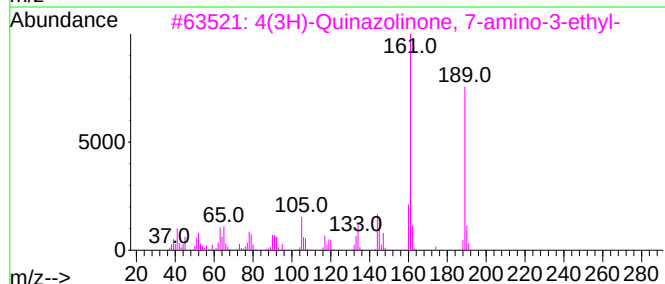
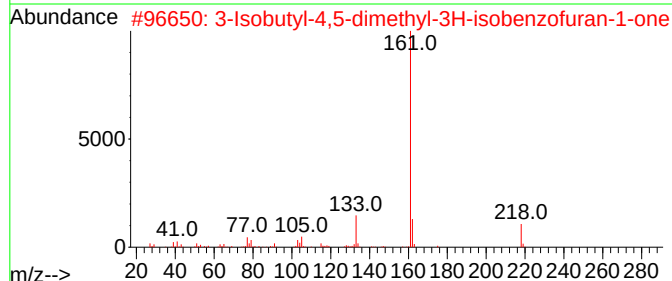
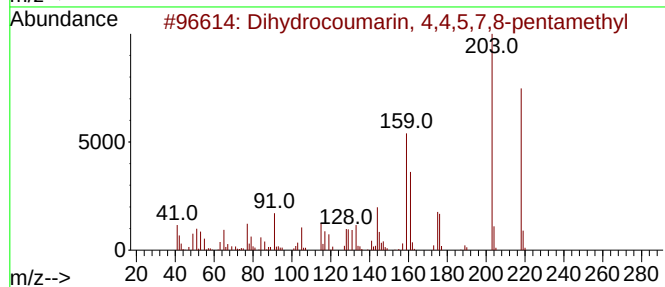
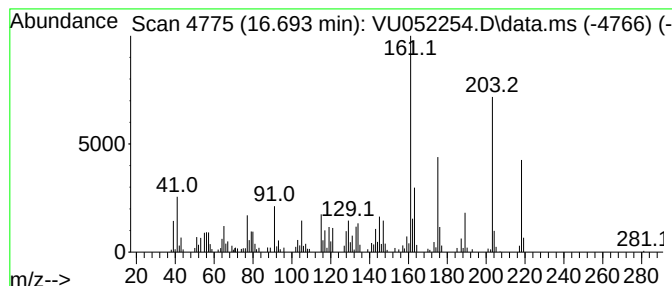
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Dihydrocoumarin, 4,4,5,7,8-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.693	1.37 ug/L	149277	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	50
2			3-Isobutyl-4,5-dimethyl-3H-isobe...	218	C14H18O2	1000187-23-3	50
3			4(3H)-Quinazolinone, 7-amino-3-e...	189	C10H11N3O	1000338-19-9	42
4			Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	000523-47-7	42
5			.beta.-GURJUNENE	204	C15H24	1000425-17-9	41



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120822\
Data File : VU052254.D
Acq On : 08 Dec 2022 17:22
Operator : JC/MD
Sample : N5916-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5N32

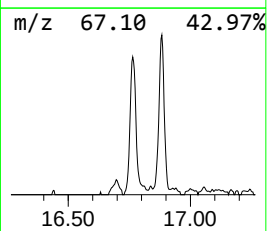
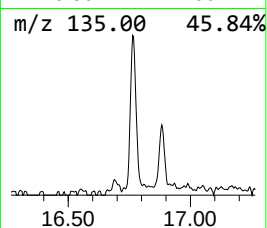
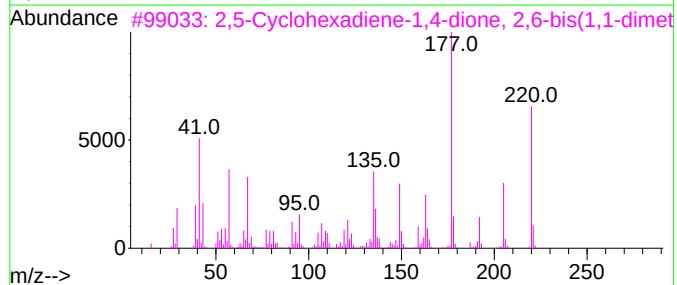
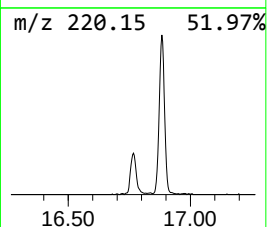
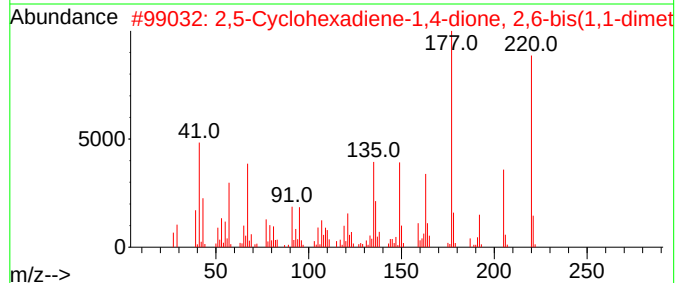
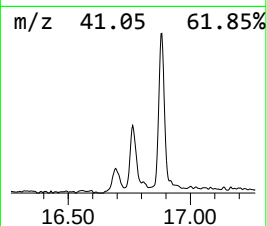
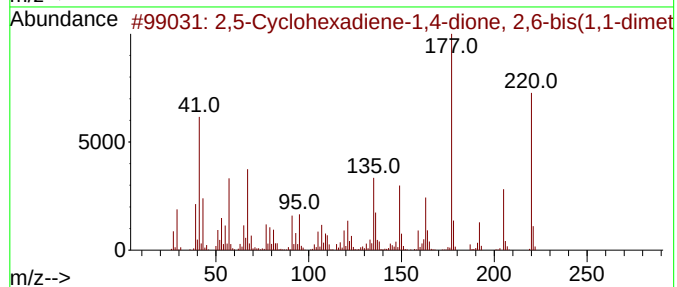
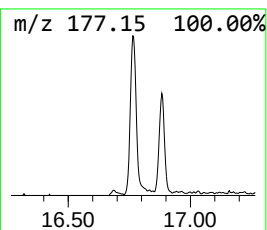
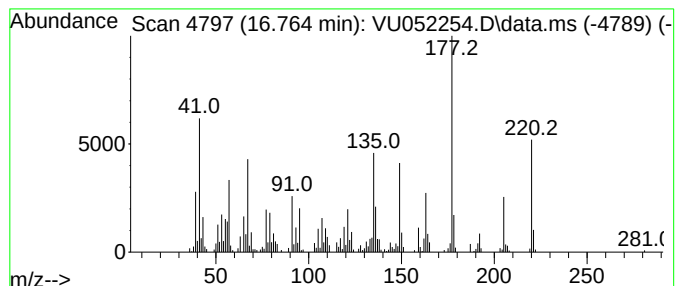
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.764	1.96 ug/L	212623	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	94		
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	94		
5	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	93		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120822\
Data File : VU052254.D
Acq On : 08 Dec 2022 17:22
Operator : JC/MD
Sample : N5916-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5N32

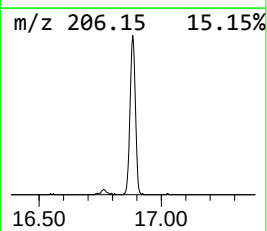
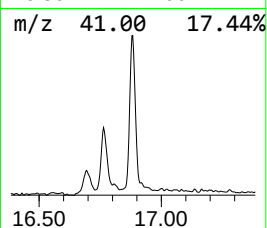
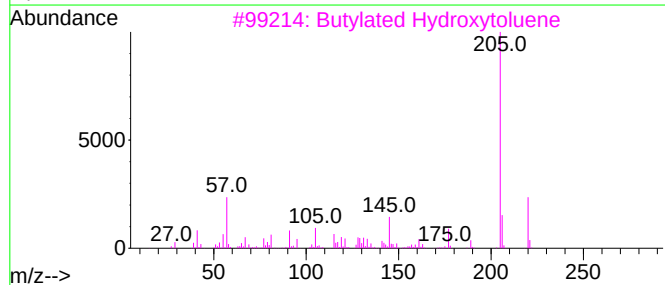
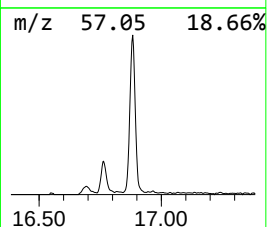
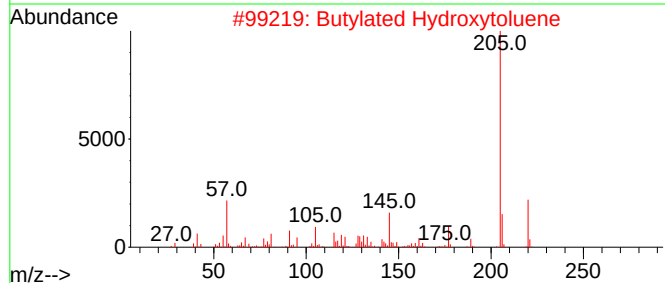
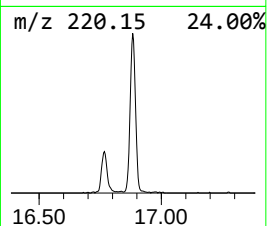
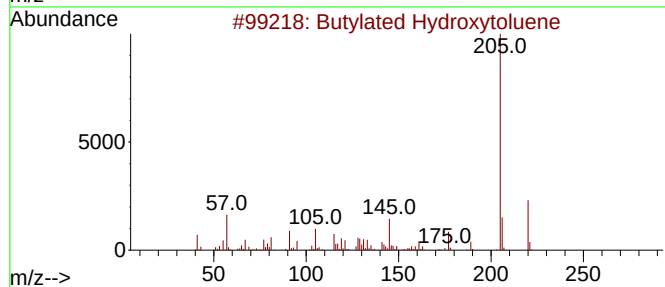
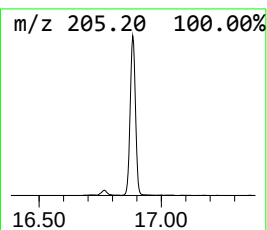
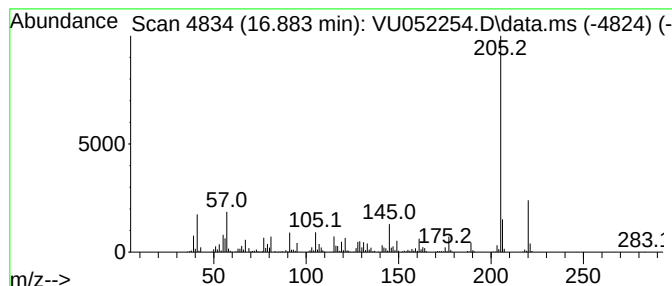
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.883	6.37 ug/L	691664	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	99
3			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
4			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	96
5			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120822\
Data File : VU052254.D
Acq On : 08 Dec 2022 17:22
Operator : JC/MD
Sample : N5916-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 20 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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	15.687	0.8	ug/L	82212	3	11.809	542867	5.0
Dihydrocoumarin...	16.693	1.4	ug/L	149277	3	11.809	542867	5.0
2,5-Cyclohexadi...	16.764	2.0	ug/L	212623	3	11.809	542867	5.0
Butylated Hydro...	16.883	6.4	ug/L	691664	3	11.809	542867	5.0