

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121222\
 Data File : VU052365.D
 Acq On : 12 Dec 2022 20:04
 Operator : JC/MD
 Sample : N5961-09
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 26 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5N36

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: VU052365.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.475	33	42	72	rBV	598230	1693541	100.00%	16.486%
2	1.600	76	81	93	rVB	137437	199625	11.79%	1.943%
3	1.916	174	179	195	rVB	98356	132668	7.83%	1.291%
4	2.578	370	385	401	rBV4	415054	801214	47.31%	7.799%
5	2.723	422	430	442	rVB2	11062	19681	1.16%	0.192%
6	3.870	770	787	806	rBV2	27332	65319	3.86%	0.636%
7	4.658	1013	1032	1085	rBV3	112421	462664	27.32%	4.504%
8	5.060	1141	1157	1182	rBV2	160197	359202	21.21%	3.497%
9	5.722	1342	1363	1379	rBV2	328390	862769	50.94%	8.399%
10	6.247	1508	1526	1549	rBV	272800	529781	31.28%	5.157%
11	6.542	1607	1618	1632	rVB3	19048	36933	2.18%	0.360%
12	6.687	1648	1663	1680	rBV	203285	408199	24.10%	3.974%
13	7.565	1921	1936	1953	rBV	87514	158922	9.38%	1.547%
14	7.896	2023	2039	2055	rBV	364590	639335	37.75%	6.224%
15	8.176	2112	2126	2140	rBV	55713	97722	5.77%	0.951%
16	8.549	2231	2242	2253	rVB2	12356	20961	1.24%	0.204%
17	8.636	2255	2269	2304	rBV	534904	1070425	63.21%	10.420%
18	9.414	2498	2511	2534	rBV	408410	682389	40.29%	6.643%
19	10.751	2911	2927	2940	rBV	199272	327911	19.36%	3.192%
20	11.690	3211	3219	3228	rBV8	11421	19627	1.16%	0.191%
21	11.738	3228	3234	3243	rVB6	12355	17751	1.05%	0.173%
22	11.809	3243	3256	3276	rBV	390593	632883	37.37%	6.161%
23	12.060	3324	3334	3354	rBV3	11754	26300	1.55%	0.256%
24	12.188	3362	3374	3393	rVB	393077	642964	37.97%	6.259%
25	12.886	3579	3591	3603	rBV6	13391	22733	1.34%	0.221%
26	12.973	3606	3618	3631	rVB10	16935	28156	1.66%	0.274%
27	14.188	3985	3996	4006	rBV2	24415	38299	2.26%	0.373%
28	15.687	4452	4462	4477	rBV6	23837	42647	2.52%	0.415%
29	16.764	4788	4797	4814	rBV3	43799	76680	4.53%	0.746%
30	16.883	4824	4834	4844	rBV	103615	155382	9.17%	1.513%

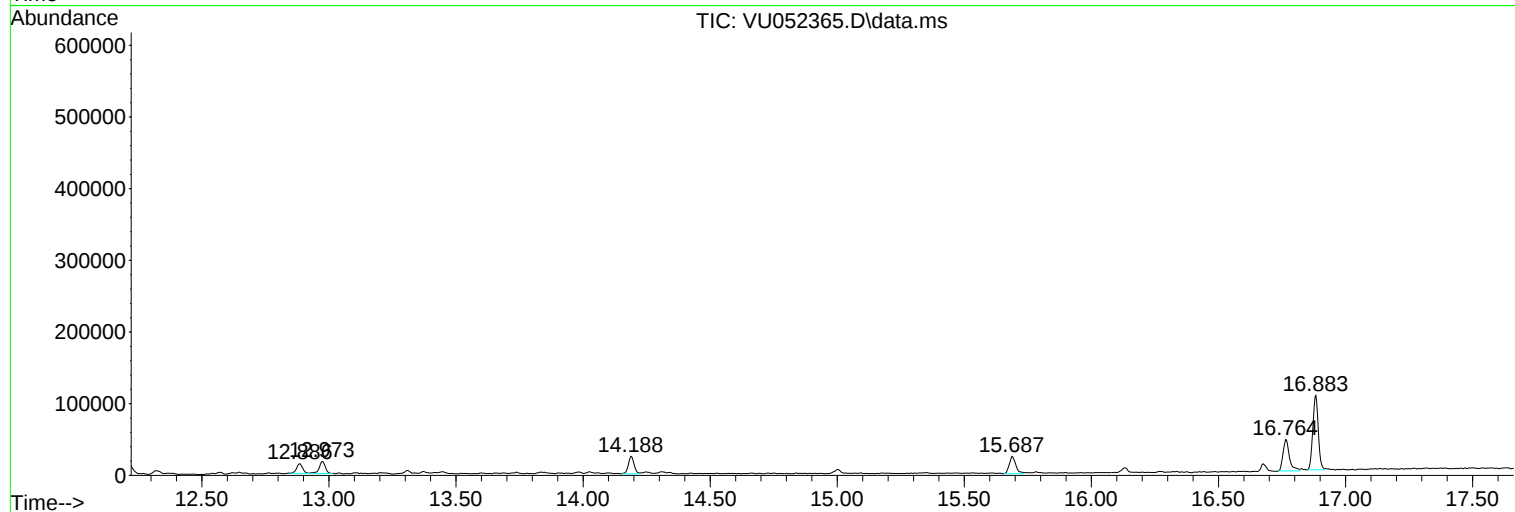
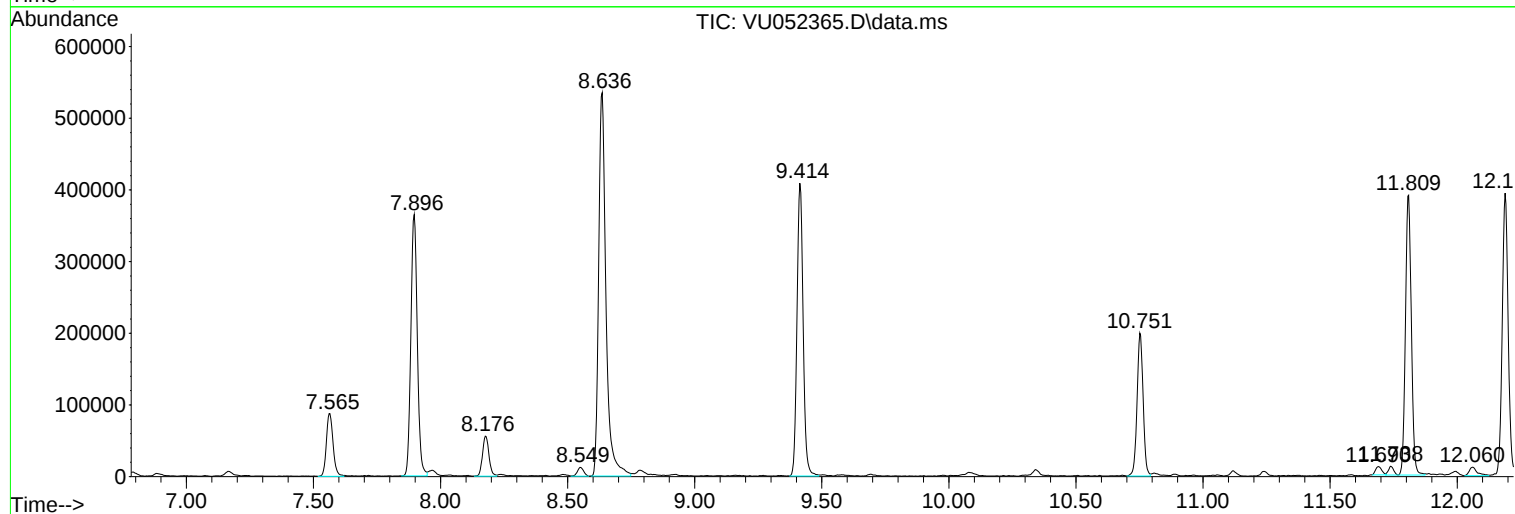
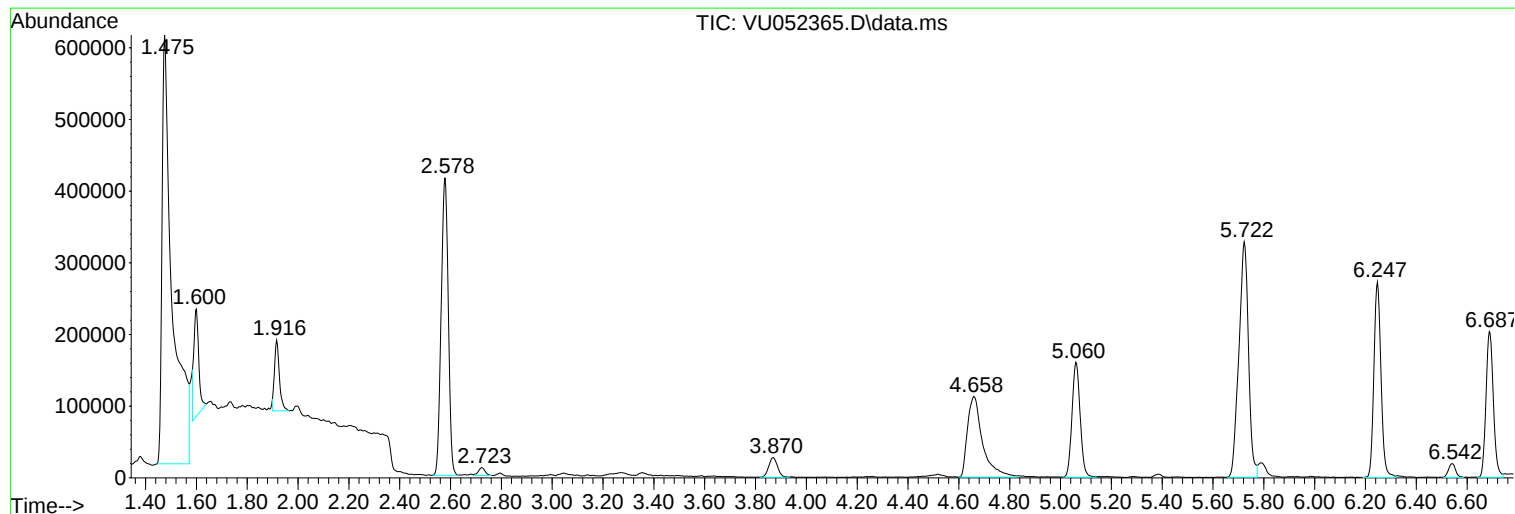
Sum of corrected areas: 10272683

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ClientSampleId :
F5N36

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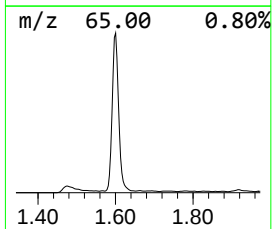
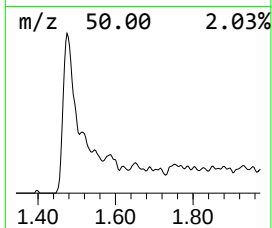
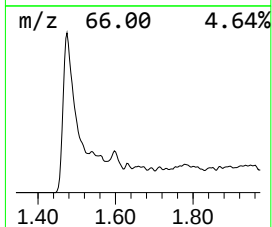
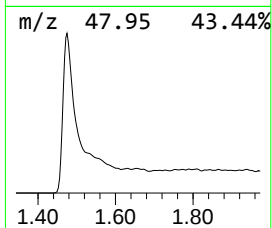
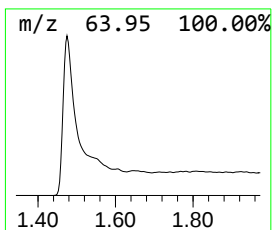
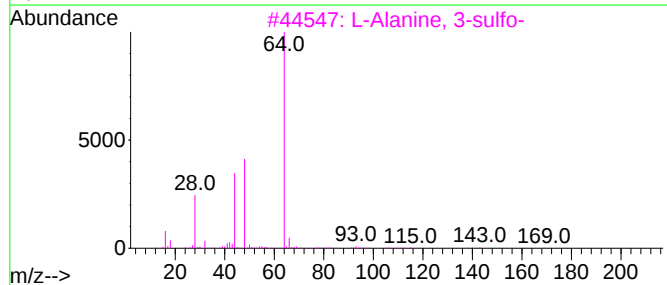
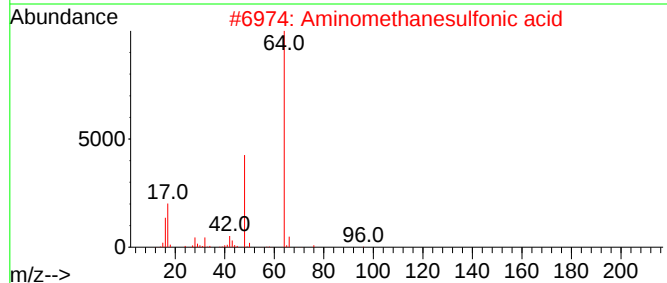
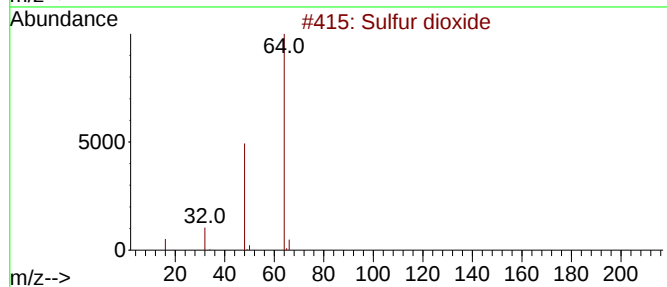
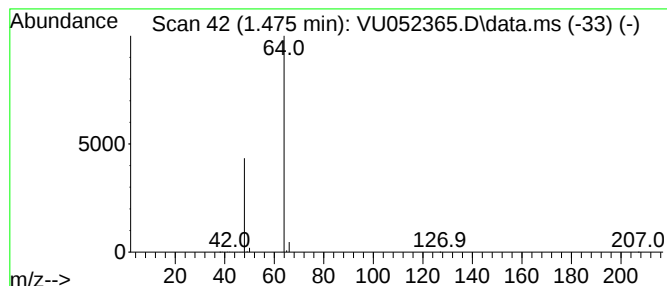
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.475	15.98 ug/L	1693540	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Sulfur dioxide	64	O2S	007446-09-5	5
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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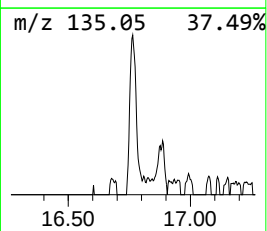
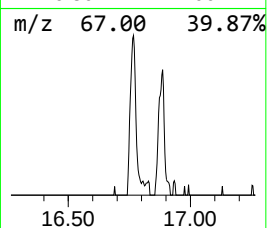
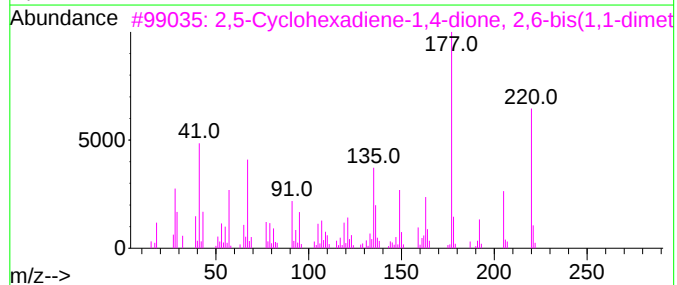
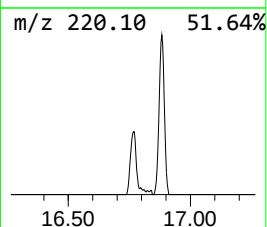
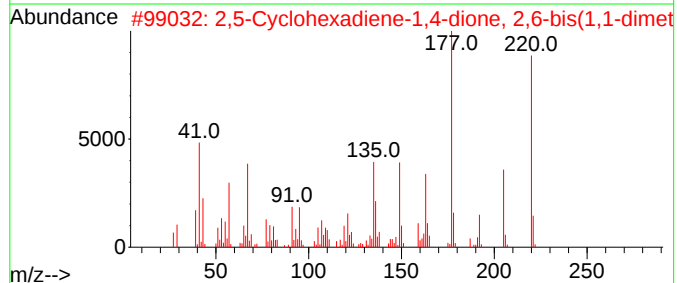
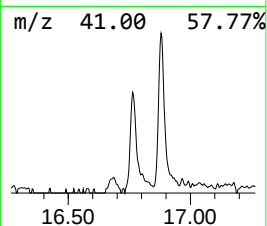
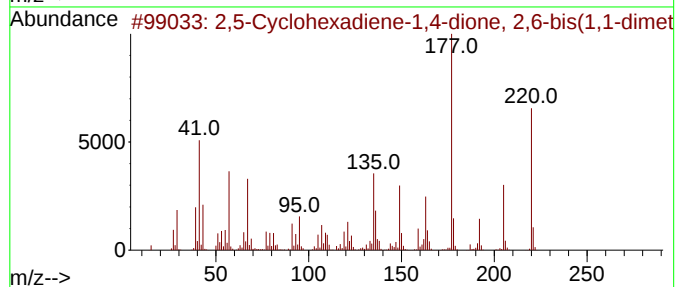
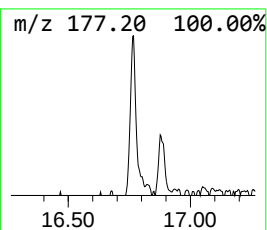
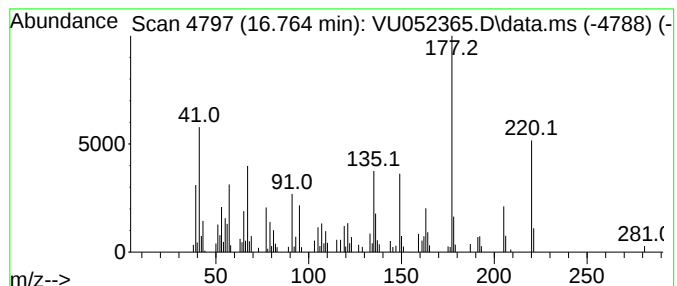
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Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.764	0.61 ug/L	76680	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	81		
2	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	70		
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	64		
4	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	64		
5	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	64		



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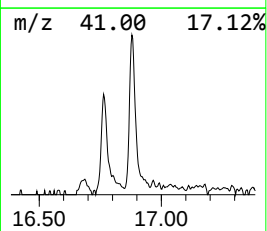
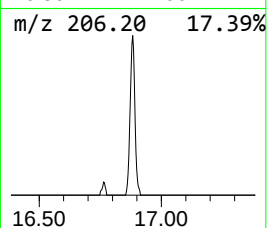
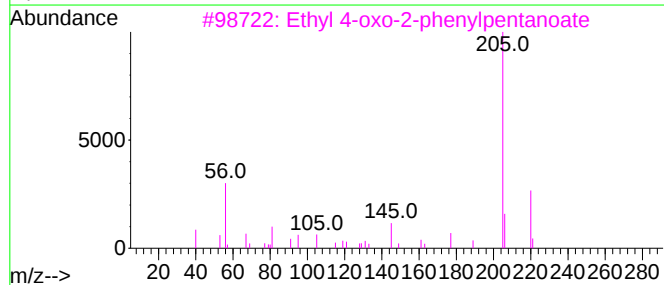
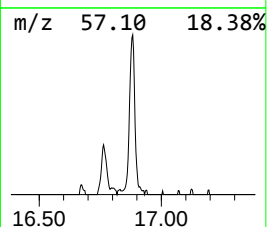
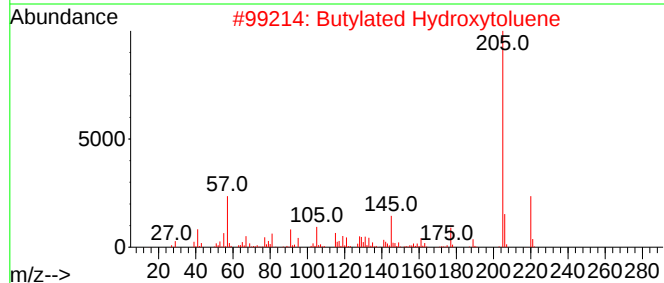
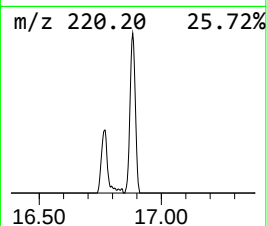
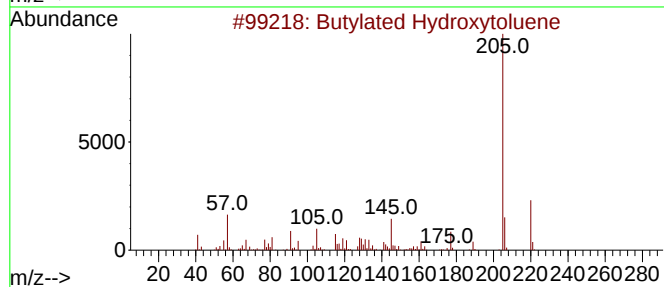
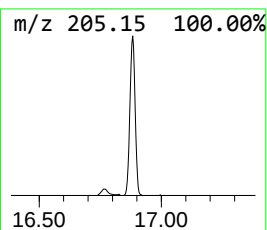
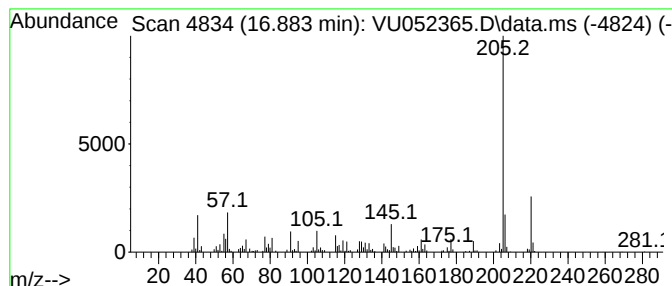
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Butylated Hydroxytoluene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.883	1.23 ug/L	155382	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	96
3			Ethyl 4-oxo-2-phenylpentanoate	220	C13H16O3	1000427-11-2	94
4			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	94
5			Phenol, 4,6-di(1,1-dimethylethyl...	220	C15H24O	000616-55-7	94



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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
Sulfur dioxide	1.475	16.0	ug/L	1693540	1	6.247	529781	5.0
2,5-Cyclohexadi...	16.764	0.6	ug/L	76680	3	11.809	632883	5.0
Butylated Hydro...	16.883	1.2	ug/L	155382	3	11.809	632883	5.0