

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120722\
 Data File : VU052234.D
 Acq On : 08 Dec 2022 06:58
 Operator : JC/MD
 Sample : N5916-15
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5N40

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: VU052234.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	70	81	93	rBV	111356	141473	14.07%	1.858%
2	1.916	170	179	201	rBV	92320	128893	12.82%	1.693%
3	2.568	370	382	396	rVB	175423	282820	28.12%	3.714%
4	2.658	396	410	411	rBV5	8044	12073	1.20%	0.159%
5	4.642	1013	1027	1070	rBV2	114993	435397	43.29%	5.718%
6	5.060	1140	1157	1183	rBV	169297	386809	38.46%	5.080%
7	5.726	1342	1364	1397	rBV2	317765	850645	84.58%	11.172%
8	6.247	1512	1526	1554	rBV	264149	508873	50.60%	6.683%
9	6.687	1649	1663	1685	rBV	204540	406928	40.46%	5.344%
10	7.565	1923	1936	1953	rBV	82590	149077	14.82%	1.958%
11	7.896	2021	2039	2059	rBV	338273	594817	59.14%	7.812%
12	8.176	2115	2126	2142	rBV2	53037	90058	8.95%	1.183%
13	8.636	2255	2269	2301	rBV2	491148	1005714	100.00%	13.208%
14	9.414	2498	2511	2537	rBV	393949	659941	65.62%	8.667%
15	10.751	2912	2927	2945	rBV	183048	307583	30.58%	4.040%
16	11.809	3243	3256	3285	rBV	351156	565823	56.26%	7.431%
17	12.189	3361	3374	3397	rBV	339970	569972	56.67%	7.486%
18	15.783	4485	4492	4508	rVB5	9803	16426	1.63%	0.216%
19	16.687	4763	4773	4784	rBV4	49960	87884	8.74%	1.154%
20	16.764	4788	4797	4810	rVB2	42467	66909	6.65%	0.879%
21	16.883	4822	4834	4847	rBV	221877	346098	34.41%	4.545%

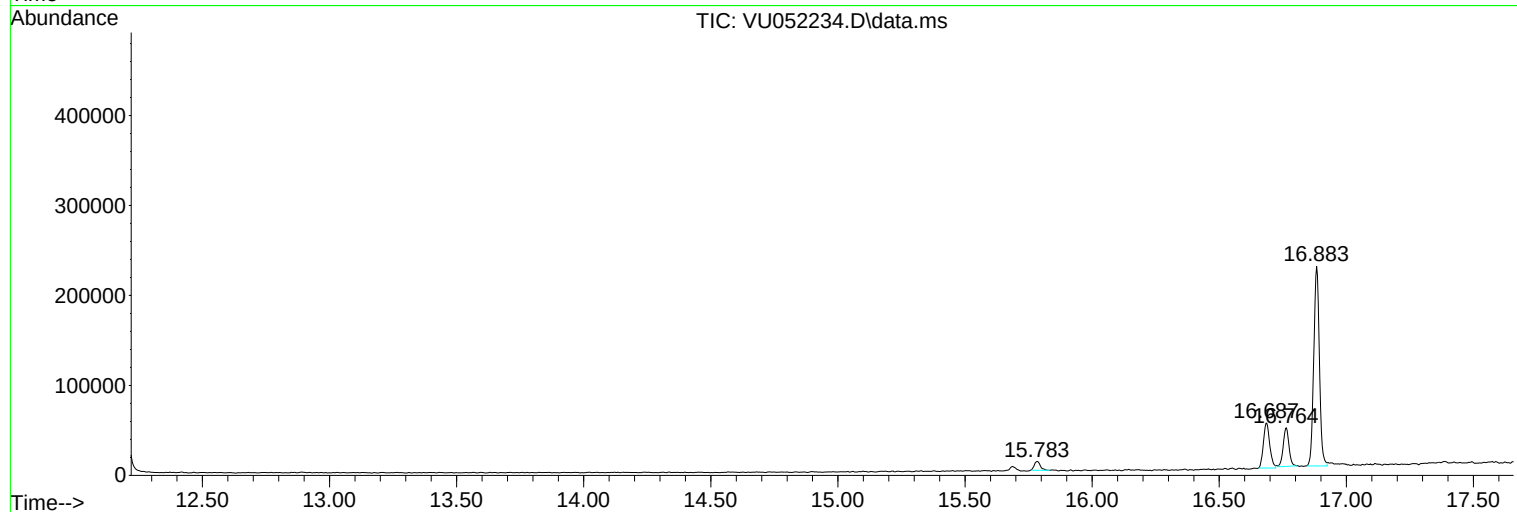
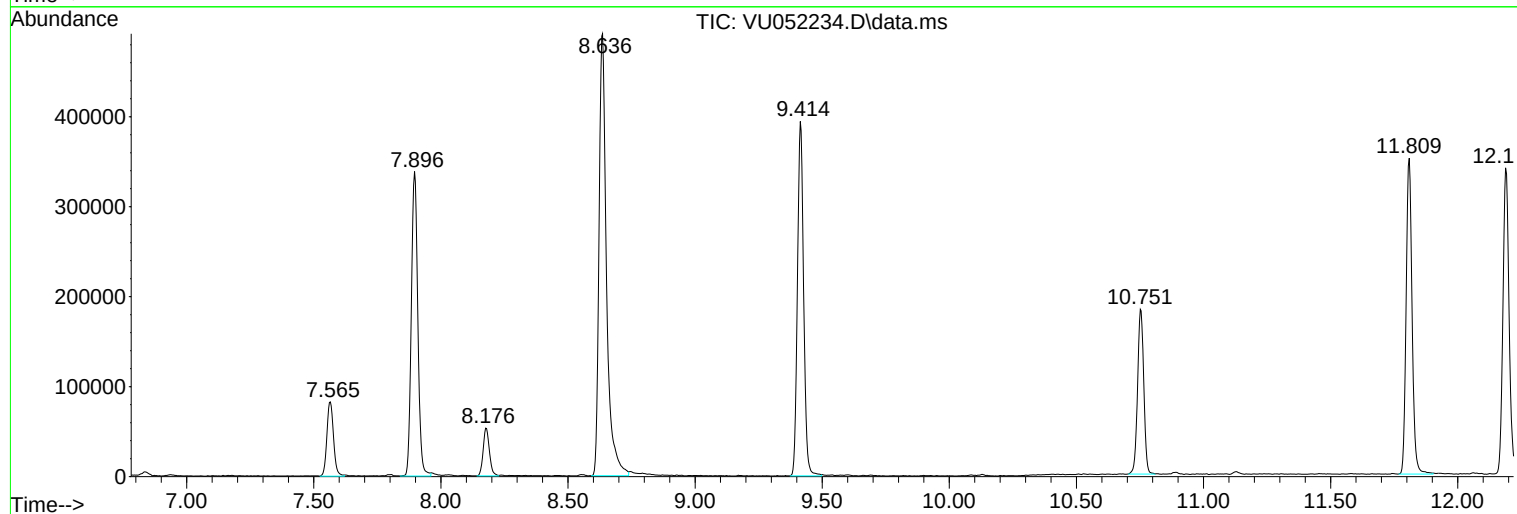
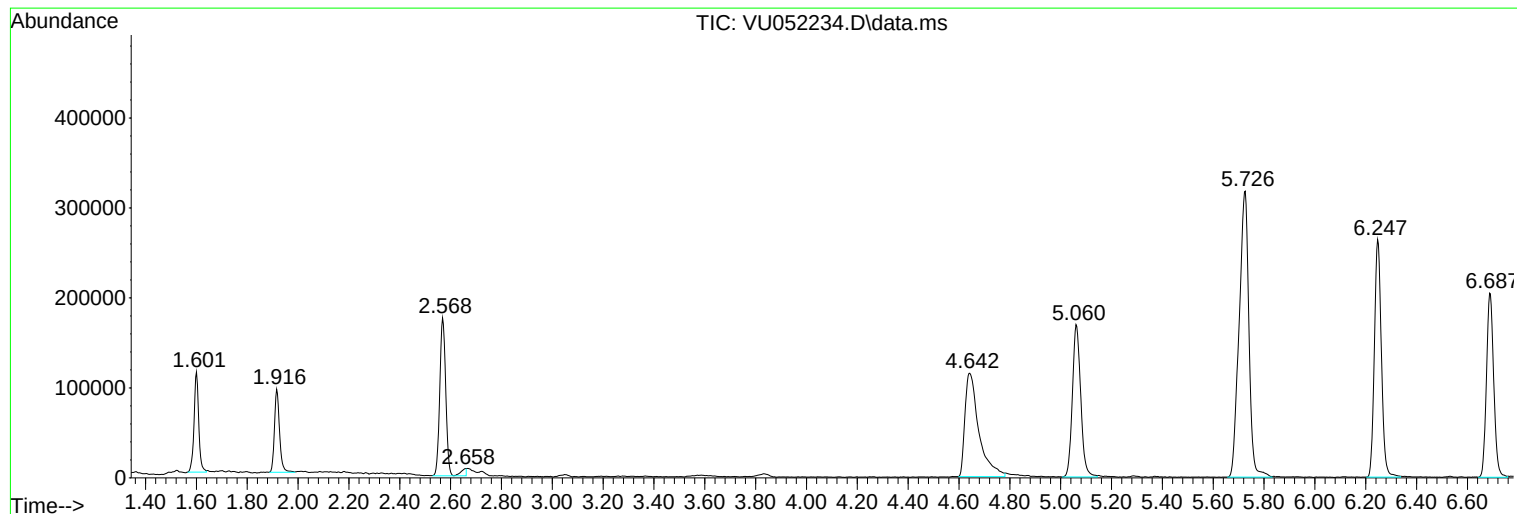
Sum of corrected areas: 7614213

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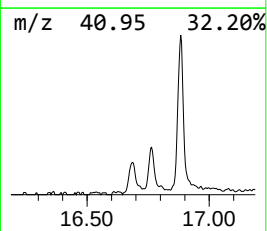
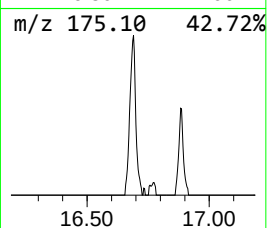
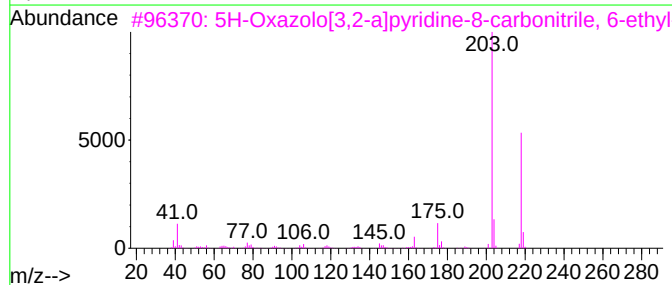
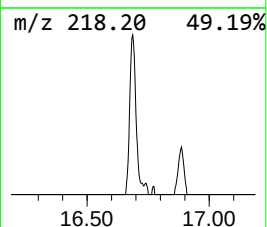
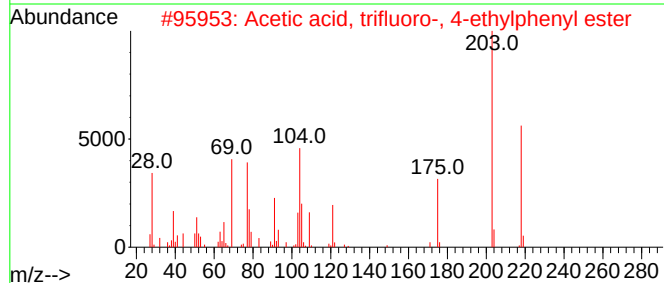
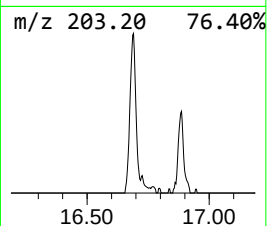
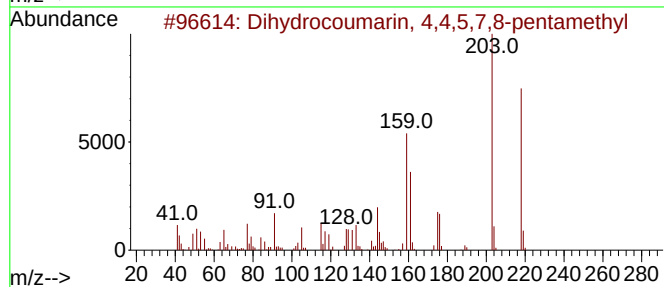
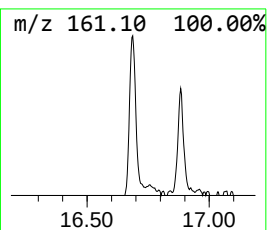
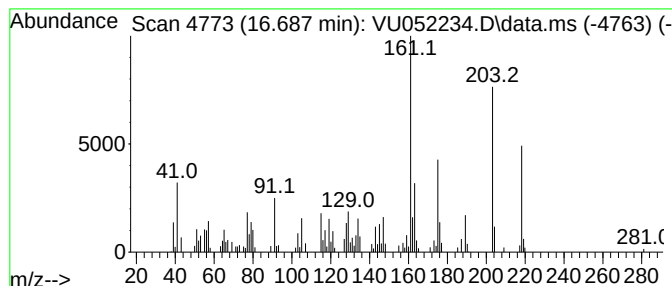
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.687	0.78 ug/L	87884	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	49
2			Acetic acid, trifluoro-, 4-ethyl...	218	C10H9F3O2	1000376-49-4	43
3			5H-Oxazolo[3,2-a]pyridine-8-carb...	218	C12H14N2O2	1000337-58-3	38
4			4-n-Butylbenzoic acid, allyl ester	218	C14H18O2	1000293-35-8	38
5			Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	000523-47-7	38



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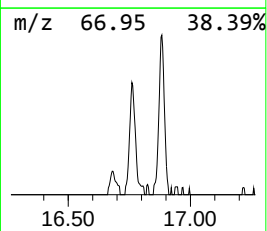
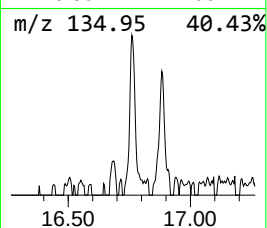
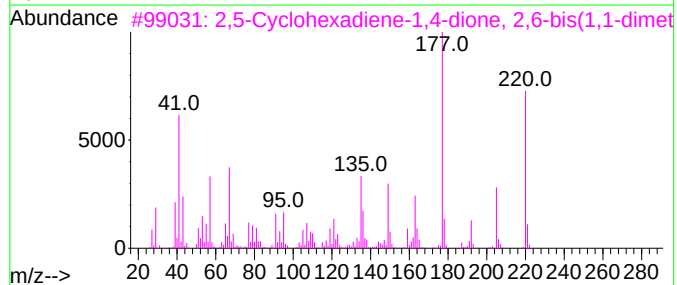
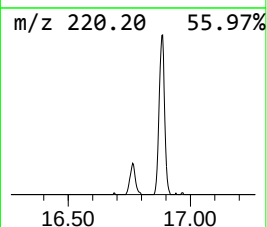
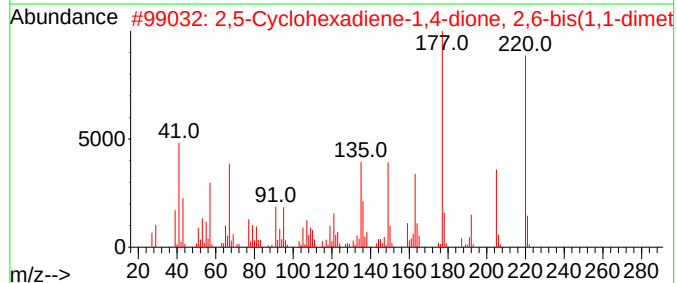
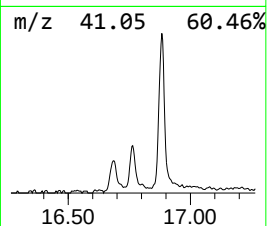
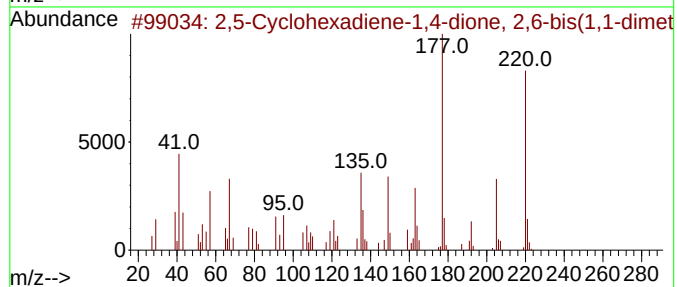
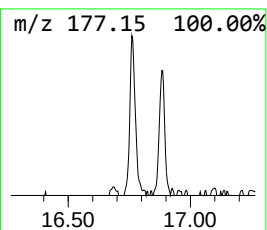
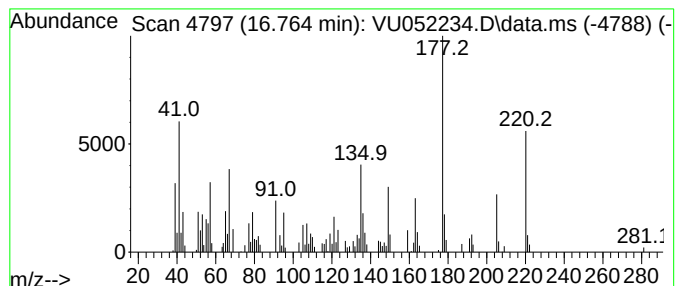
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
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Peak Number 3 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.764	0.59 ug/L	66909	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	98
2			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	98
3			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	95
4			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	94
5			Thiocoumarine, 4,4,6,7-tetramethyl-	220	C13H16OS	1000128-90-2	60



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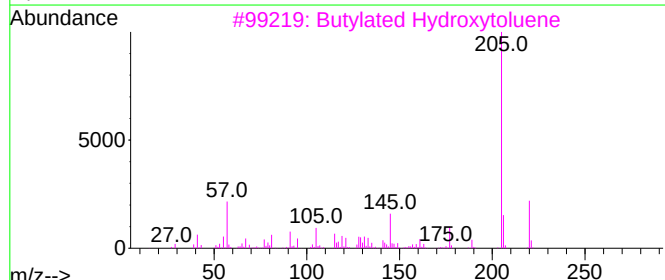
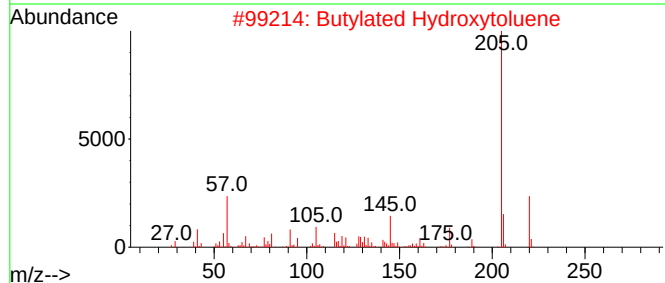
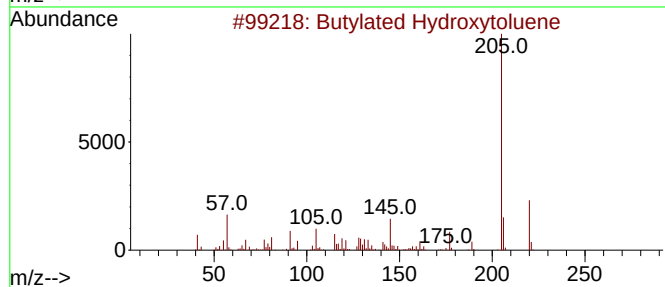
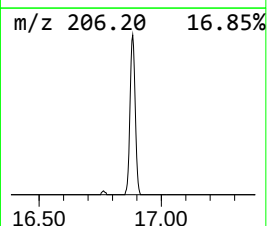
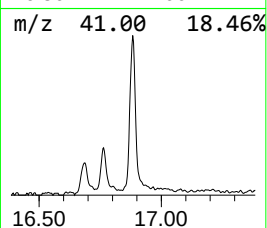
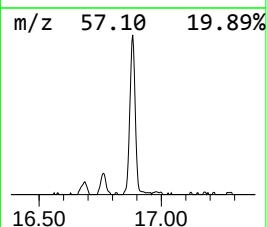
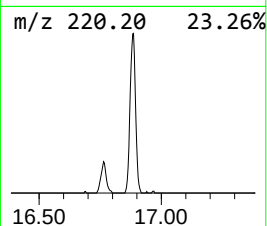
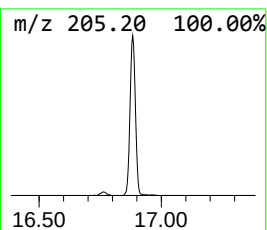
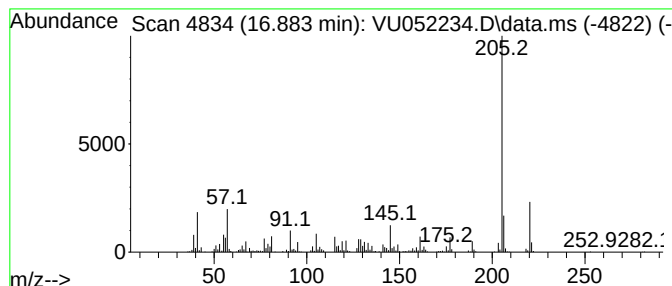
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.883	3.06 ug/L	346098	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	98
3			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
4			Ethyl 4-oxo-2-phenylpentanoate	220	C13H16O3	1000427-11-2	95
5			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	94



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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	16.687	0.8	ug/L	87884	3	11.809	565823	5.0
2,5-Cyclohexadi...	16.764	0.6	ug/L	66909	3	11.809	565823	5.0
Butylated Hydro...	16.883	3.1	ug/L	346098	3	11.809	565823	5.0