

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120822\
 Data File : VU052253.D
 Acq On : 08 Dec 2022 16:58
 Operator : JC/MD
 Sample : N5916-13
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5N31

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: VU052253.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	72	81	94	rVB	99886	120140	1.04%	0.631%
2	1.916	170	179	197	rVB	86378	118896	1.03%	0.624%
3	2.568	370	382	397	rBV	158919	256533	2.23%	1.347%
4	4.652	1014	1030	1089	rBV2	78358	398040	3.46%	2.090%
5	5.060	1142	1157	1182	rBV	147180	330929	2.88%	1.738%
6	5.723	1339	1363	1372	rBV2	283810	753508	6.55%	3.957%
7	5.793	1372	1385	1439	rVB	5615576	11502217	100.00%	60.407%
8	6.247	1512	1526	1546	rBV	261254	506363	4.40%	2.659%
9	6.690	1650	1664	1683	rBV	185832	374066	3.25%	1.965%
10	7.565	1923	1936	1957	rBV2	77694	143181	1.24%	0.752%
11	7.896	2025	2039	2055	rBV	302663	535791	4.66%	2.814%
12	8.636	2255	2269	2293	rBV2	445585	970653	8.44%	5.098%
13	9.414	2500	2511	2532	rVB	372977	616694	5.36%	3.239%
14	10.751	2912	2927	2947	rVB	179906	300337	2.61%	1.577%
15	11.809	3243	3256	3279	rBV	344863	562908	4.89%	2.956%
16	12.189	3363	3374	3391	rBV	325563	534604	4.65%	2.808%
17	16.693	4765	4775	4787	rBV4	77113	141556	1.23%	0.743%
18	16.764	4788	4797	4815	rVV	164735	268251	2.33%	1.409%
19	16.883	4824	4834	4854	rBV	391418	606609	5.27%	3.186%

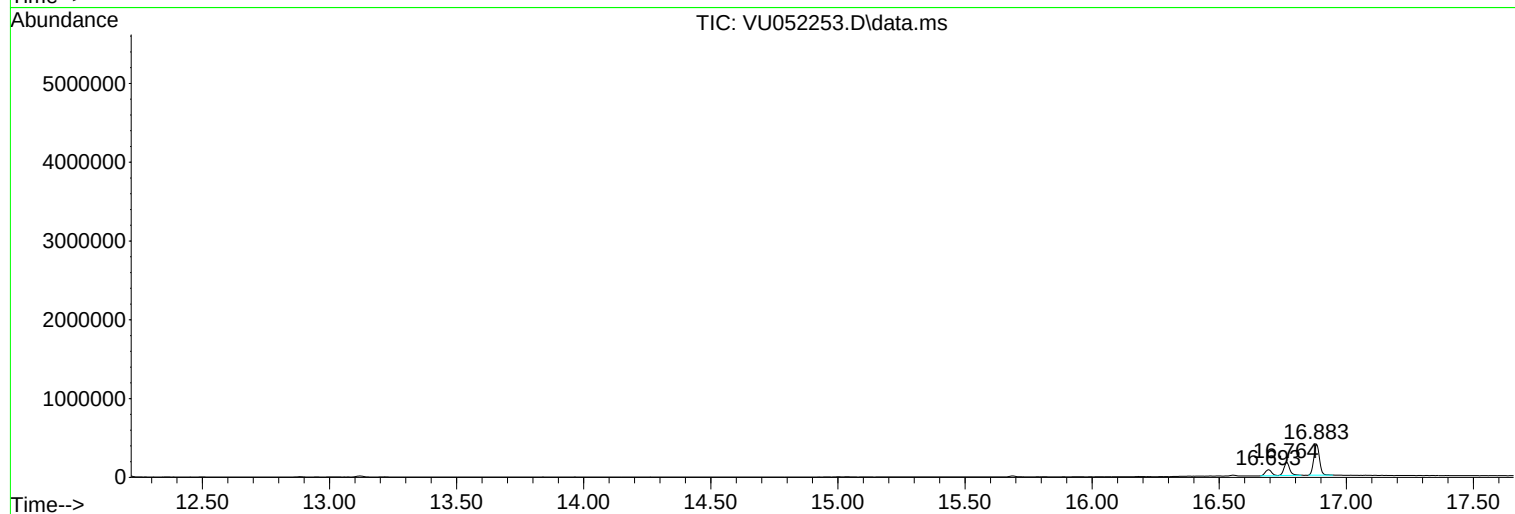
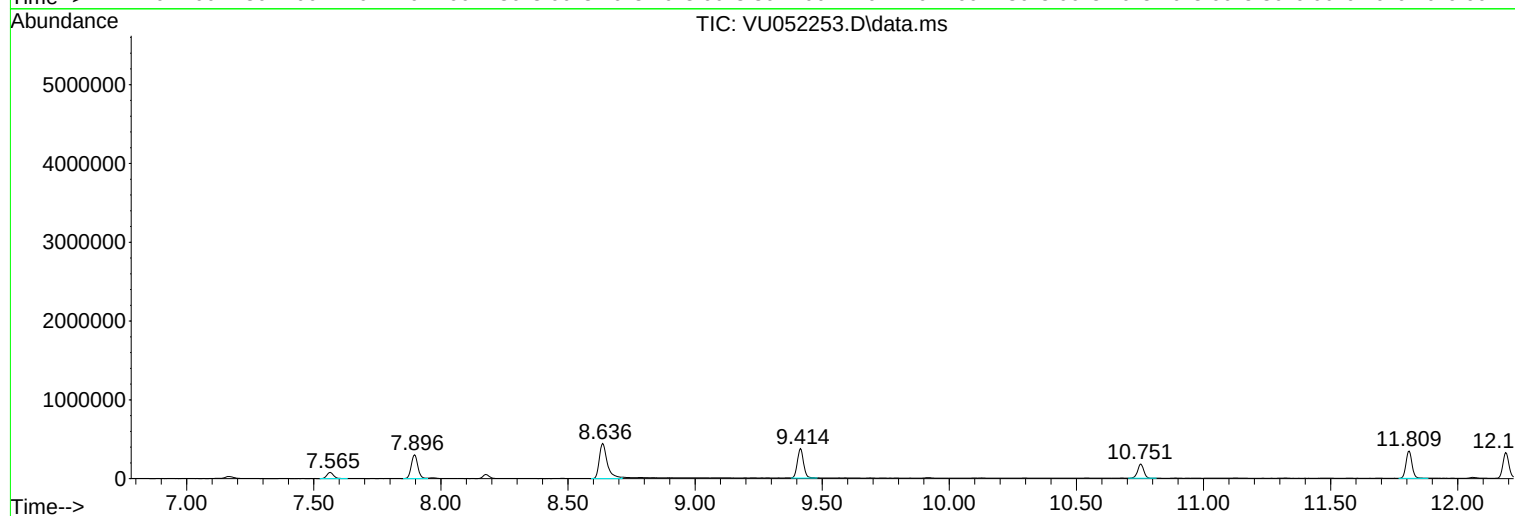
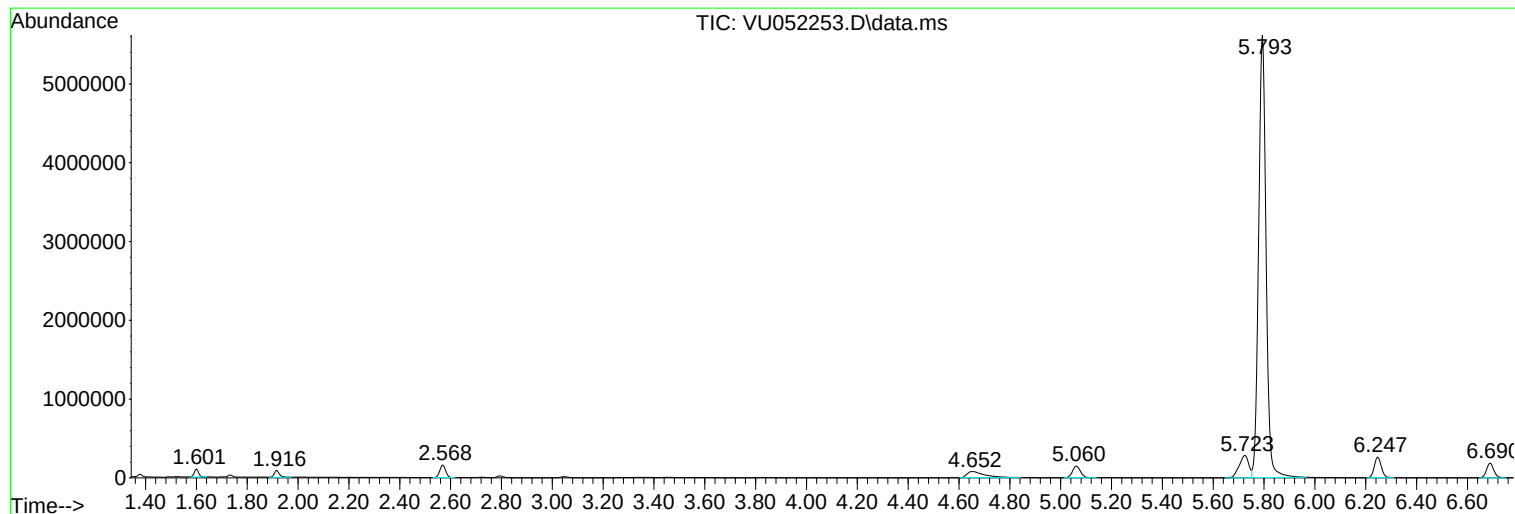
Sum of corrected areas: 19041276

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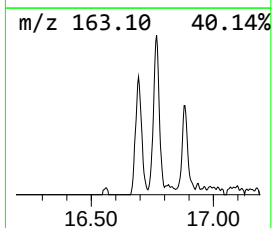
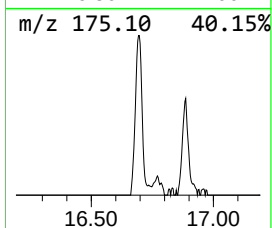
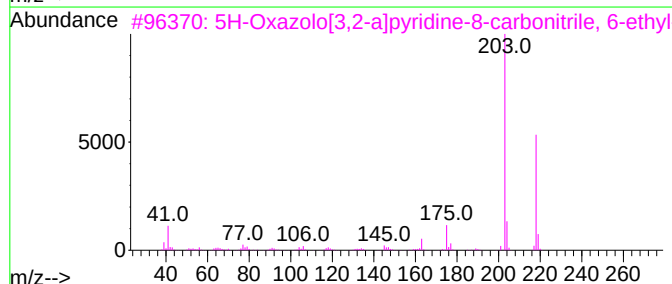
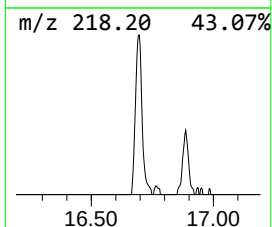
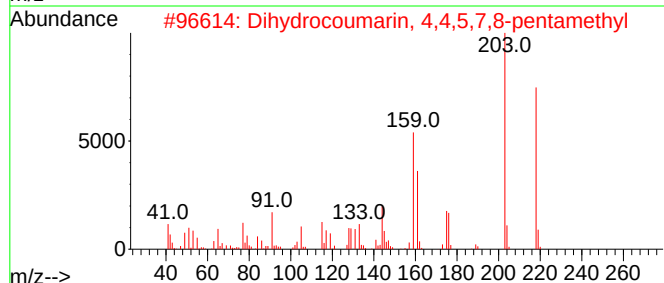
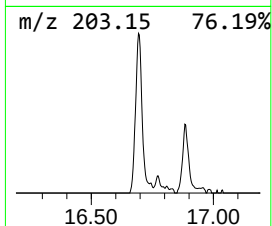
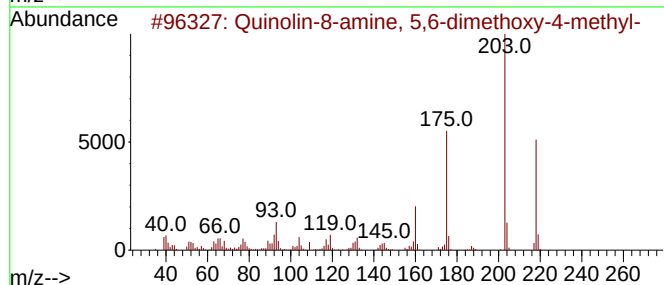
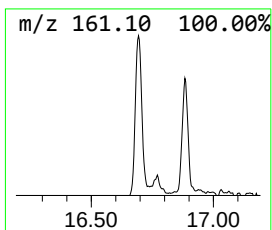
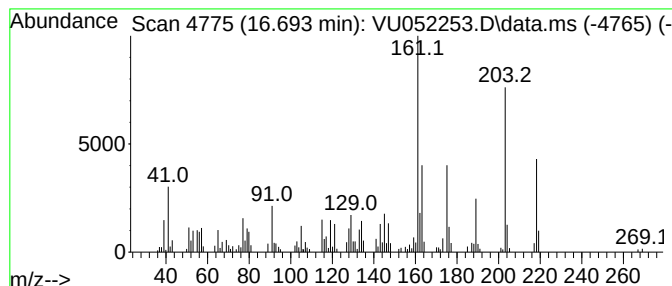
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.693	1.26 ug/L	141556	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Quinolin-8-amine, 5,6-dimethoxy-...	218	C12H14N2O2	064992-95-6	45
2			Dihydrocoumarin, 4,4,5,7,8-penta...	218	C14H18O2	039170-97-3	45
3			5H-Oxazolo[3,2-a]pyridine-8-carb...	218	C12H14N2O2	1000337-58-3	41
4			(4aS)-3,5,5,9-Tetramethyl-1,2,5,...	218	C15H22O	064825-84-9	38
5			1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	017334-55-3	35



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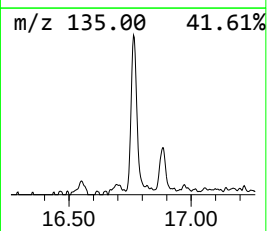
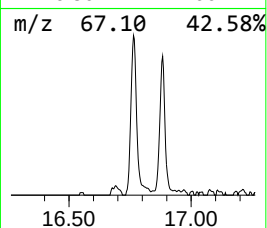
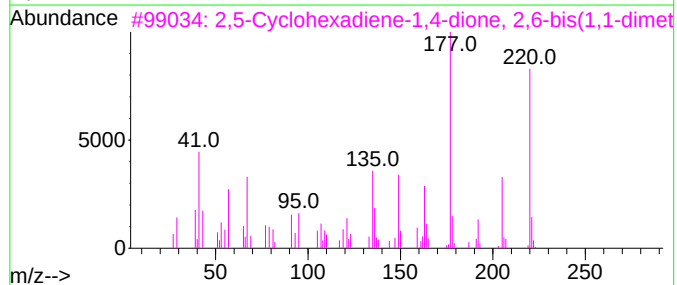
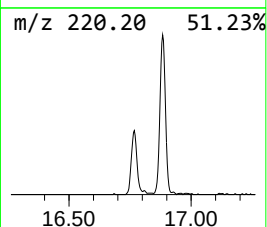
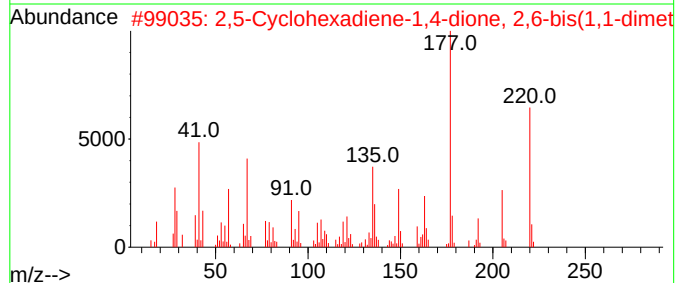
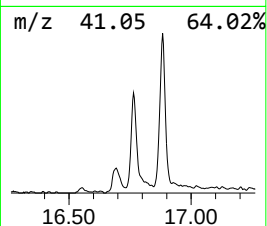
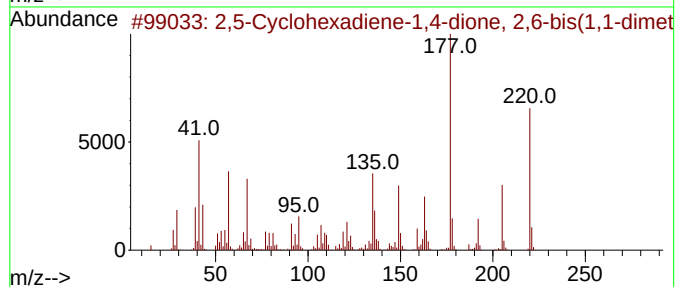
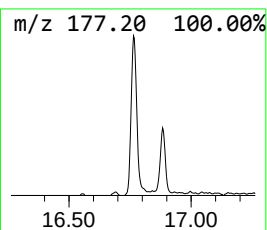
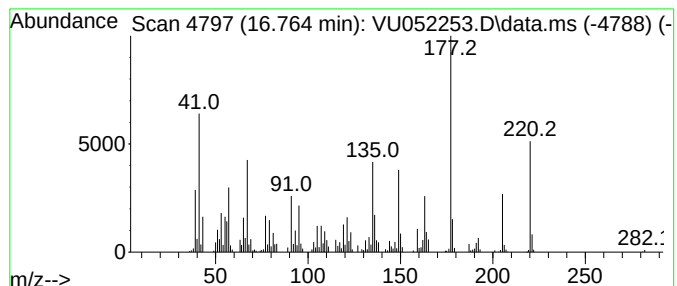
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Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.764	2.38 ug/L	268251	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	96		
2	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	96		
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	95		
4	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	95		
5	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	90		



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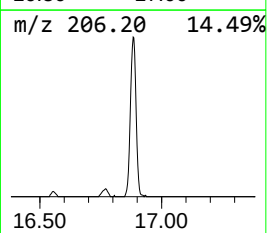
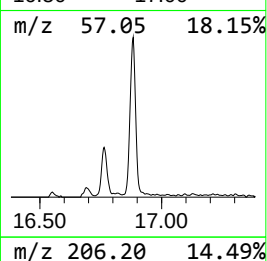
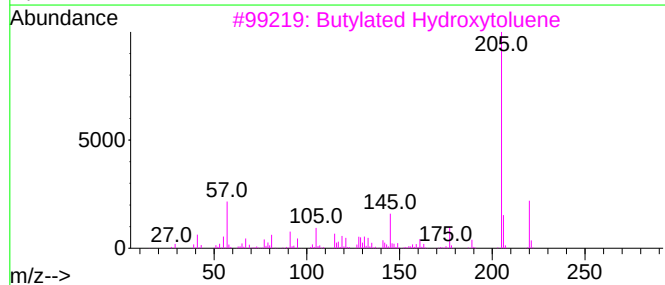
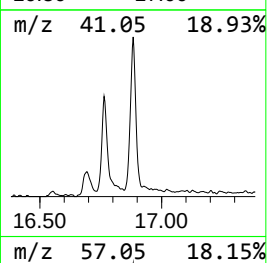
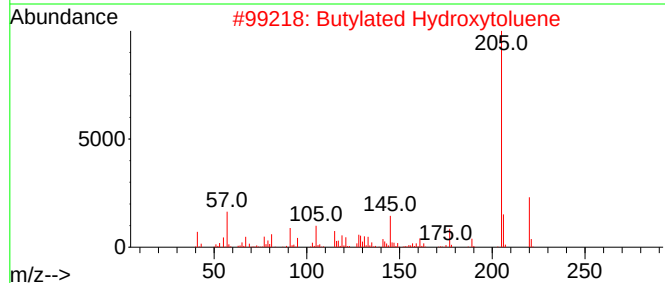
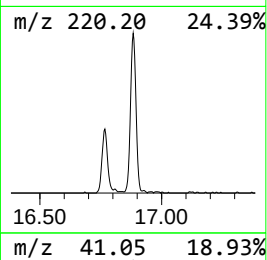
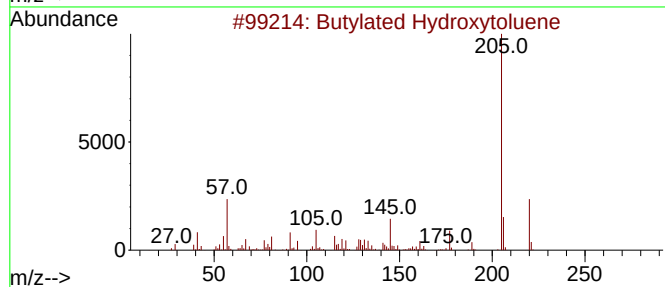
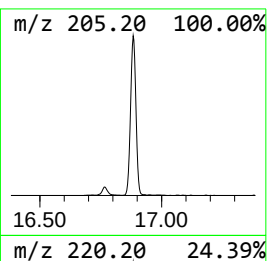
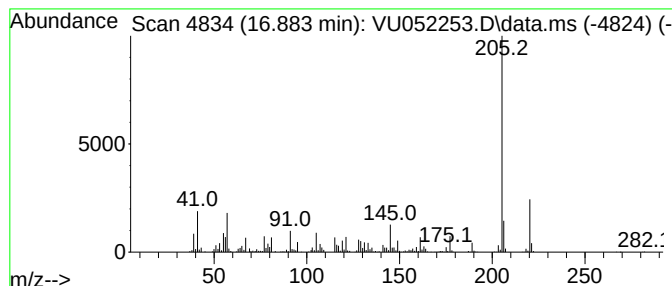
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Quant Title : TRACE VOA SFAM1.0

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	5.39 ug/L	606609	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
2			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
3			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	97
4			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	95
5			Ethyl 4-oxo-2-phenylpentanoate	220	C13H16O3	1000427-11-2	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
unknown-01	16.693	1.3	ug/L	141556	3	11.809	562908	5.0
2,5-Cyclohexadi...	16.764	2.4	ug/L	268251	3	11.809	562908	5.0
Butylated Hydro...	16.883	5.4	ug/L	606609	3	11.809	562908	5.0