

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012221\
 Data File : VU042174.D
 Acq On : 22 Jan 2021 16:58
 Operator : SY/MD
 Sample : M1222-09
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :

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\SOMUTR012021WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC: VU042174.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	93	rVB2	44151	58928	11.99%	1.514%
2	1.916	172	179	192	rVB	33882	43064	8.76%	1.107%
3	2.572	370	383	396	rBV	73691	119463	24.30%	3.070%
4	3.253	575	595	601	rBV7	4613	14419	2.93%	0.371%
5	4.652	1010	1030	1032	rBV	45172	86956	17.69%	2.235%
6	5.073	1146	1161	1182	rBV	69554	149420	30.40%	3.840%
7	5.735	1345	1367	1387	rBV2	133414	349463	71.09%	8.980%
8	6.256	1516	1529	1549	rBV	131982	243599	49.55%	6.260%
9	6.549	1611	1620	1631	rVB6	4894	9256	1.88%	0.238%
10	6.700	1654	1667	1684	rVB	86939	164624	33.49%	4.230%
11	7.179	1801	1816	1825	rBV4	4507	9042	1.84%	0.232%
12	7.575	1927	1939	1955	rBV	48765	86114	17.52%	2.213%
13	7.906	2028	2042	2056	rBV	169137	286849	58.35%	7.371%
14	8.185	2119	2129	2143	rBV	31130	53146	10.81%	1.366%
15	8.558	2237	2245	2255	rVB3	6510	10074	2.05%	0.259%
16	8.642	2255	2271	2316	rBV	217264	467271	95.06%	12.008%
17	9.423	2502	2514	2534	rBV	185908	307236	62.50%	7.895%
18	9.989	2680	2690	2702	rBV2	14958	25504	5.19%	0.655%
19	10.552	2855	2865	2875	rBV	8342	14140	2.88%	0.363%
20	10.693	2902	2909	2919	rVB3	3753	5929	1.21%	0.152%
21	10.764	2919	2931	2947	rBV	68130	112279	22.84%	2.885%
22	11.819	3247	3259	3273	rBV	209968	326874	66.50%	8.400%
23	12.070	3328	3337	3357	rBV3	6376	13337	2.71%	0.343%
24	12.201	3366	3378	3394	rVB	177223	284888	57.95%	7.321%
25	12.333	3402	3419	3429	rBV	6846	12638	2.57%	0.325%
26	12.896	3585	3594	3604	rVV3	12165	18022	3.67%	0.463%
27	14.201	3990	4000	4010	rBV2	26928	40206	8.18%	1.033%
28	14.323	4031	4038	4049	rBV6	4839	8210	1.67%	0.211%
29	15.703	4455	4467	4479	rBV7	6816	11145	2.27%	0.286%
30	16.143	4597	4604	4614	rVB5	6512	9257	1.88%	0.238%
31	16.783	4791	4803	4816	rBV2	33957	58452	11.89%	1.502%
32	16.899	4827	4839	4856	rBV	332260	491575	100.00%	12.632%

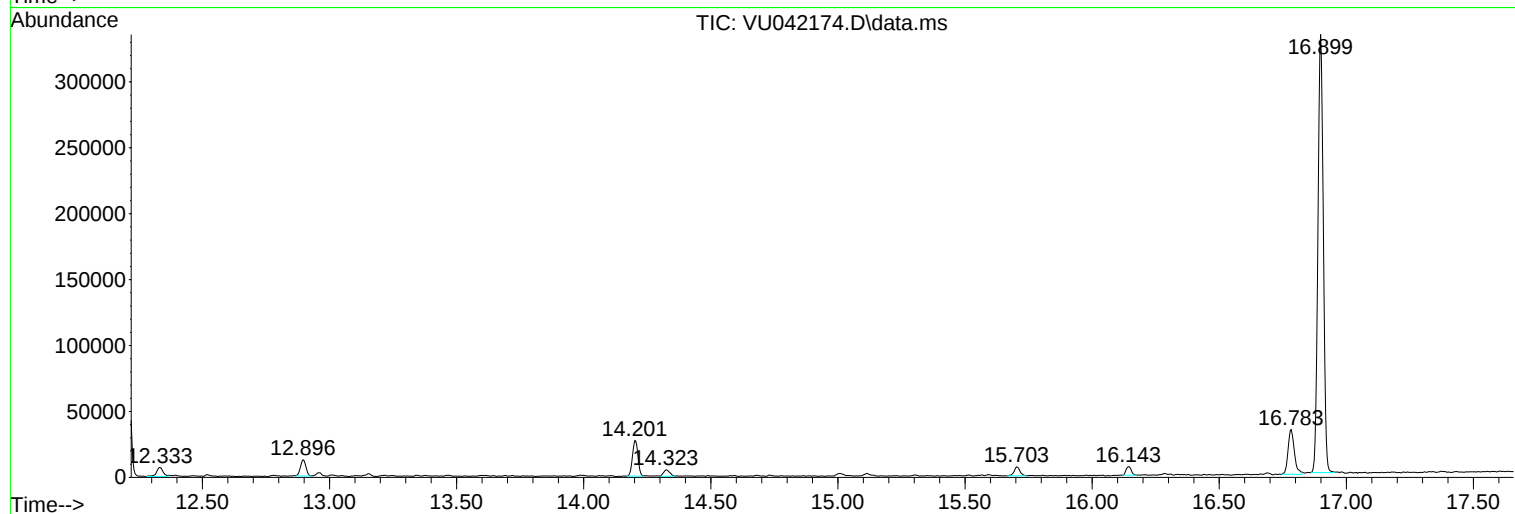
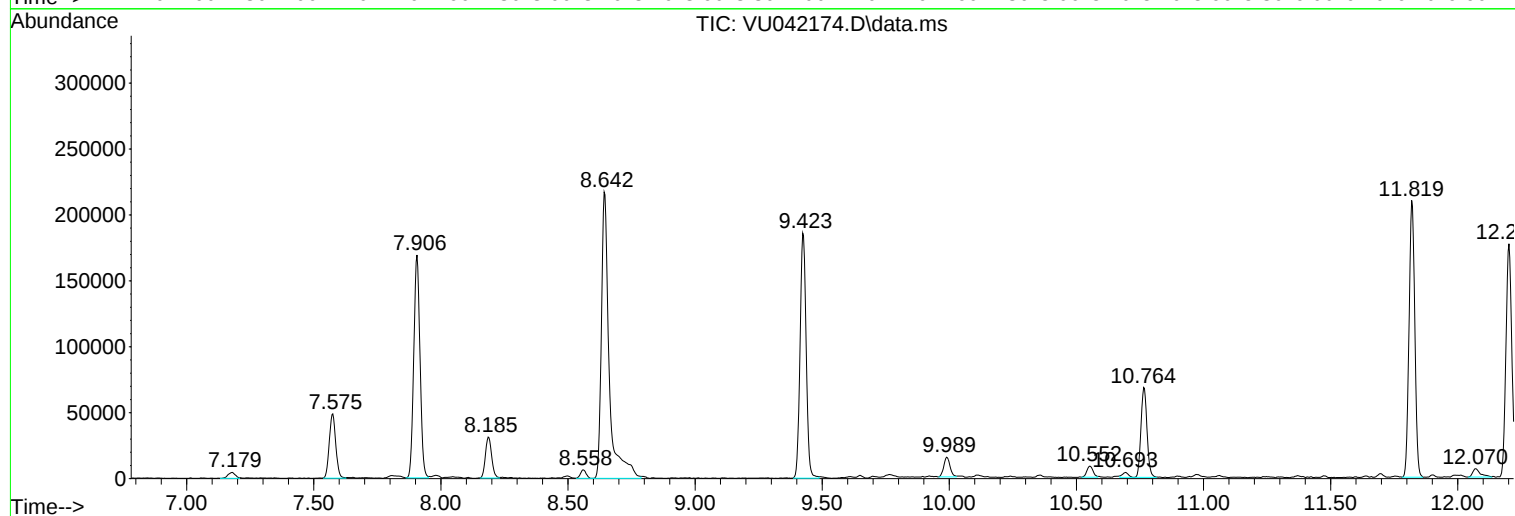
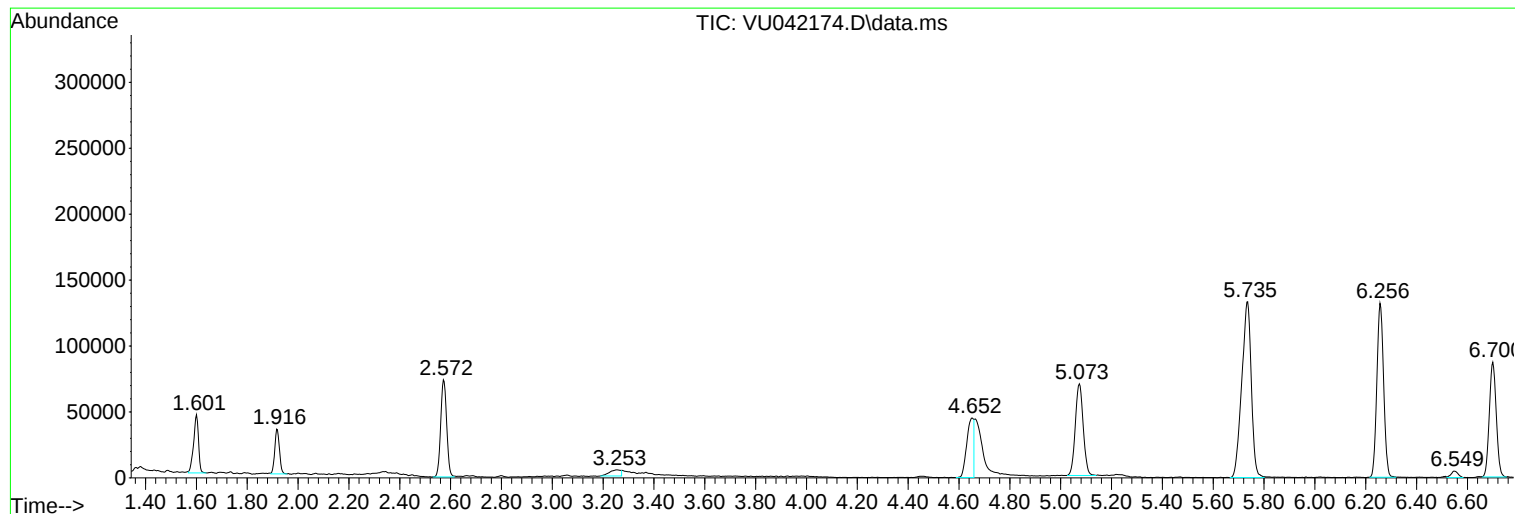
Sum of corrected areas: 3891380

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Instrument :
MSVOA_D
ClientSampled :

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Instrument :
MSVOA_D
ClientSampleId :

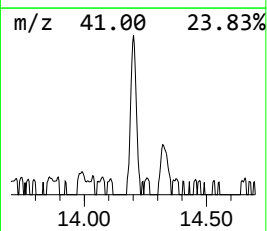
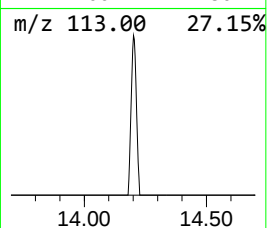
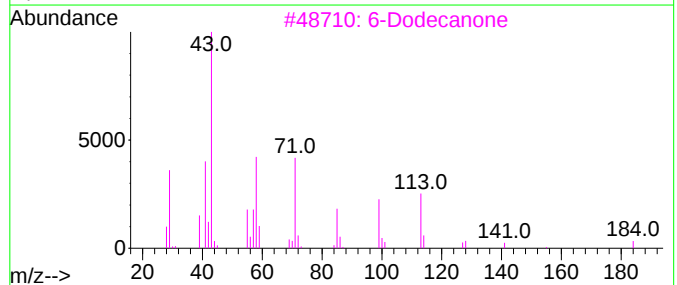
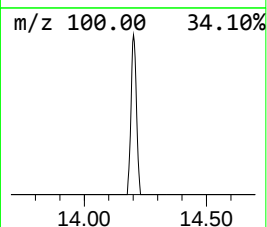
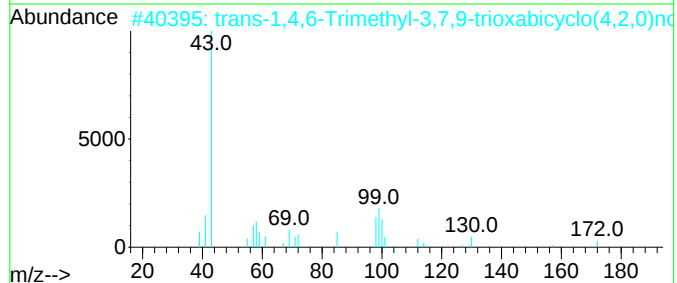
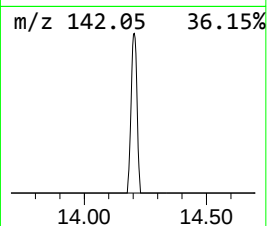
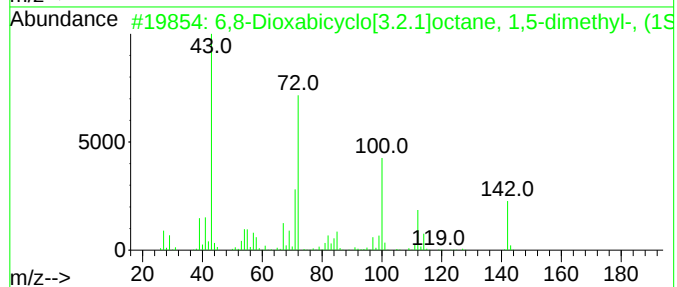
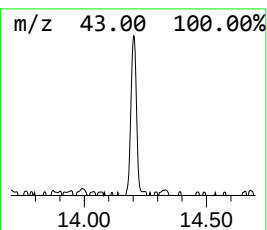
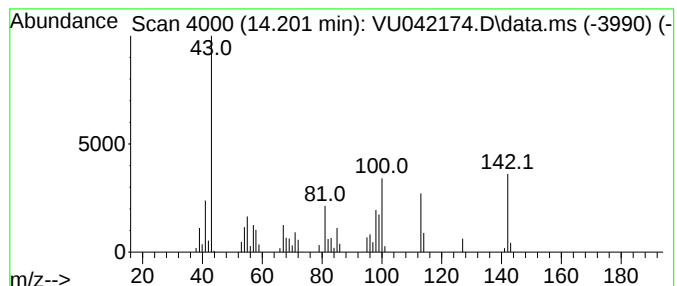
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.201	0.62 ug/L	40206	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	27		
2	trans-1,4,6-Trimethyl-3,7,9-trio...	172	C9H16O3	062759-59-5	16		
3	6-Dodecanone	184	C12H24O	006064-27-3	16		
4	3-t-Butylhexan-2-one	156	C10H20O	1000202-22-9	10		
5	1,4,6-Trimethyl-3,7,9-trioxabicy...	172	C9H16O3	062759-58-4	10		



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MSVOA_D
ClientSampleId :

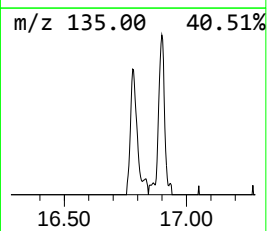
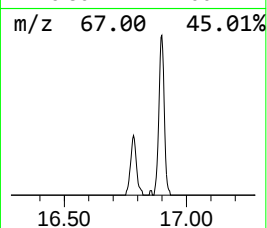
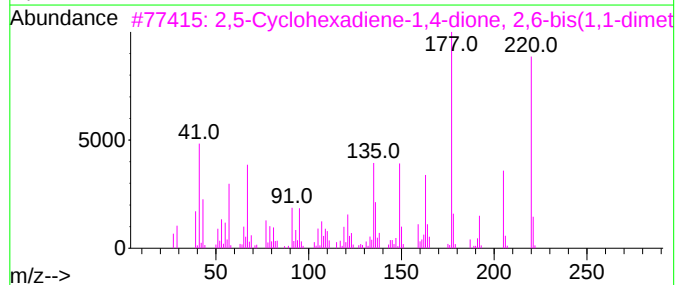
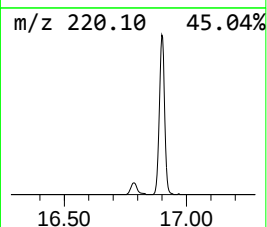
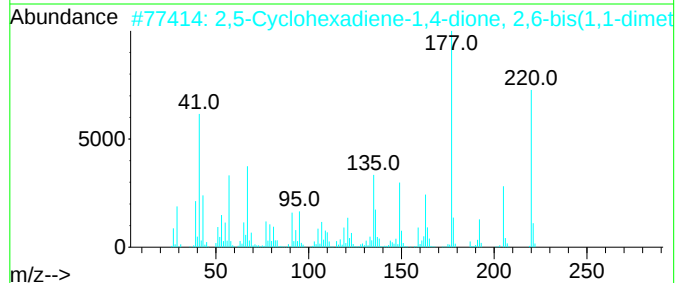
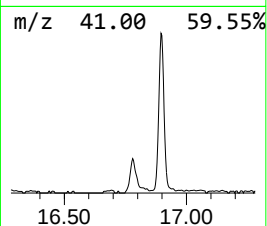
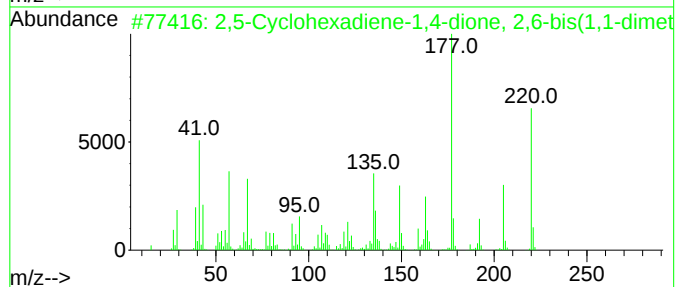
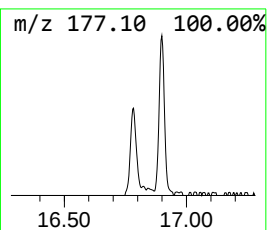
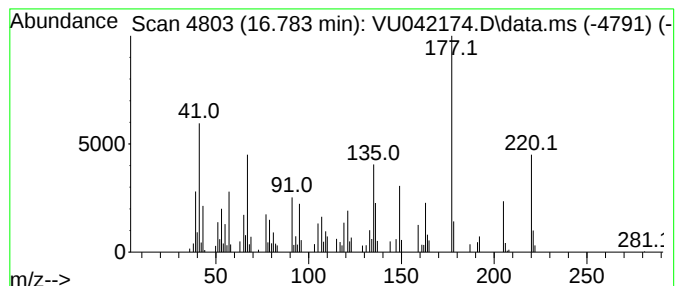
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Peak Number 3 2,5-Cyclohexadiene-1,4-dione... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.783	0.89 ug/L	58452	1,4-Dichlorobenzene-d4	11.819

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	87		
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H2002	000719-22-2	83		
4	trans-.beta.-Ionone	192	C13H200	000079-77-6	38		
5	Thiocoumarin, 4,4,6,8-tetramethyl-	220	C13H160S	1000128-90-3	38		



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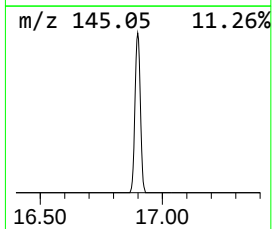
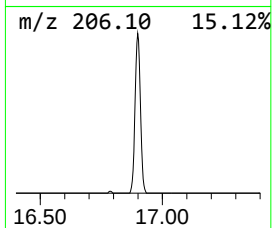
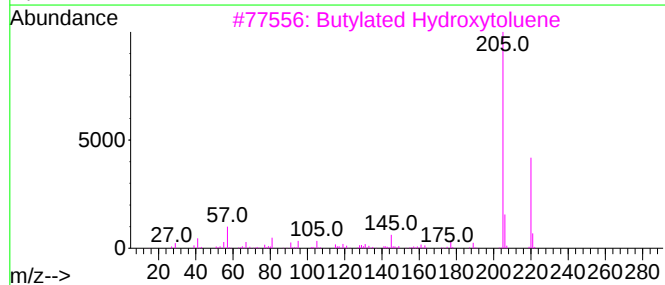
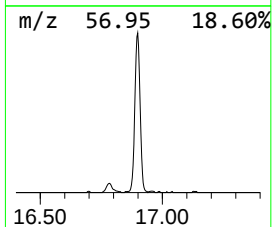
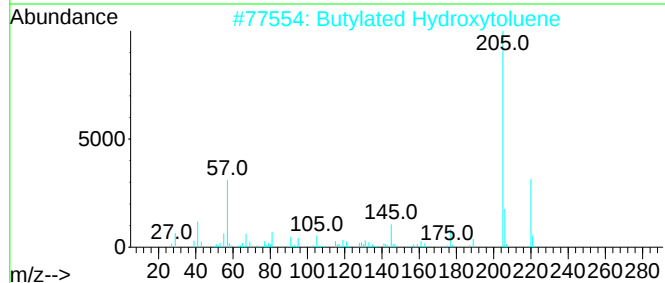
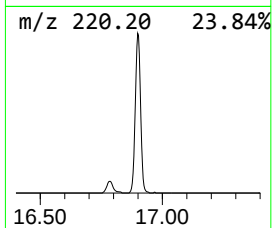
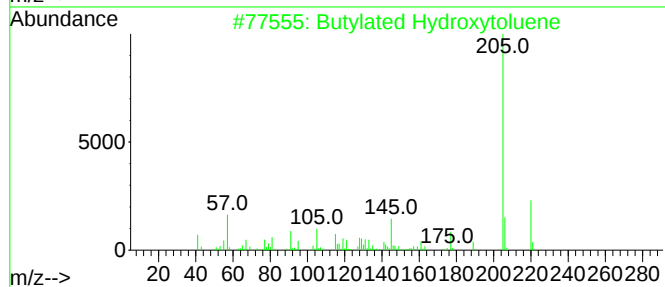
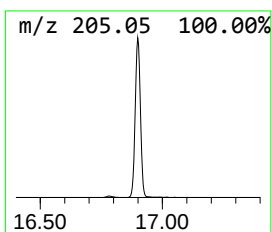
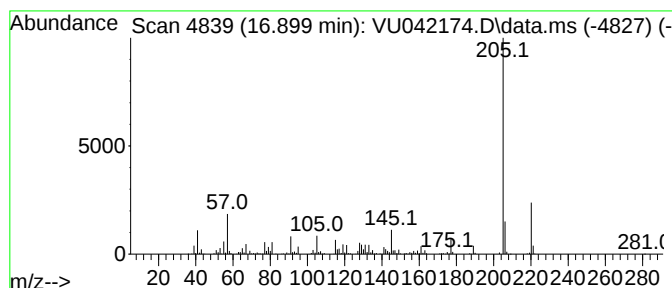
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Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.899	7.52 ug/L	491575	1,4-Dichlorobenzene-d4	11.819

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	96
3			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	94
4			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	94
5			Phenol, 4,6-di(1,1-dimethylethyl...	220	C15H24O	000616-55-7	81



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Quant Title : TRACE VOA SOM01.0

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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	14.201	0.6	ug/L	40206	3	11.819	326874	5.0
2,5-Cyclohexadi...	16.783	0.9	ug/L	58452	3	11.819	326874	5.0
Butylated Hydro...	16.899	7.5	ug/L	491575	3	11.819	326874	5.0