

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012221\
 Data File : VU042170.D
 Acq On : 22 Jan 2021 15:21
 Operator : SY/MD
 Sample : M1222-05
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F1E12

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: VU042170.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.362	3	7	19	rVB2	11144	11789	1.82%	0.286%
2	1.600	70	81	89	rVB2	46656	61941	9.58%	1.503%
3	1.919	170	180	191	rBV	34980	45245	7.00%	1.098%
4	2.571	371	383	399	rBV	76362	123556	19.12%	2.998%
5	3.260	572	597	598	rBV2	8934	22975	3.55%	0.558%
6	4.649	1013	1029	1056	rBV	41918	140152	21.68%	3.401%
7	5.073	1145	1161	1182	rVB	70399	157129	24.31%	3.813%
8	5.735	1345	1367	1389	rBV2	136225	358142	55.41%	8.691%
9	6.256	1512	1529	1549	rVB	128963	243464	37.67%	5.908%
10	6.700	1654	1667	1684	rVB	88246	168251	26.03%	4.083%
11	7.176	1797	1815	1827	rBV3	17162	35161	5.44%	0.853%
12	7.574	1924	1939	1953	rBV	51560	89712	13.88%	2.177%
13	7.832	2000	2019	2029	rBV8	2805	8502	1.32%	0.206%
14	7.906	2029	2042	2056	rVV	171545	291385	45.08%	7.071%
15	7.976	2056	2064	2076	rVB2	5994	10378	1.61%	0.252%
16	8.189	2119	2130	2144	rBV	32392	54642	8.45%	1.326%
17	8.497	2216	2226	2238	rVB3	4758	7599	1.18%	0.184%
18	8.562	2238	2246	2253	rBV3	6068	8892	1.38%	0.216%
19	8.642	2258	2271	2313	rBV	202161	449696	69.58%	10.912%
20	9.423	2502	2514	2537	rBV	179393	302710	46.84%	7.346%
21	9.648	2578	2584	2593	rVB2	6167	8540	1.32%	0.207%
22	10.693	2900	2909	2920	rVB2	10151	15575	2.41%	0.378%
23	10.764	2920	2931	2948	rVB2	69588	113283	17.53%	2.749%
24	10.973	2981	2996	3012	rBV2	13156	23435	3.63%	0.569%
25	11.819	3247	3259	3273	rBV	203127	320559	49.60%	7.779%
26	12.073	3326	3338	3355	rBV	10873	23024	3.56%	0.559%
27	12.201	3364	3378	3392	rVB	179896	286284	44.29%	6.947%
28	12.333	3409	3419	3428	rBV2	14979	22715	3.51%	0.551%
29	14.201	3988	4000	4015	rVB2	31260	47123	7.29%	1.144%
30	14.327	4030	4039	4048	rBV6	5204	8288	1.28%	0.201%
31	15.706	4459	4468	4476	rBV7	5126	7712	1.19%	0.187%
32	16.780	4794	4802	4811	rBV7	4422	6760	1.05%	0.164%
33	16.899	4827	4839	4859	rBV	443769	646324	100.00%	15.684%

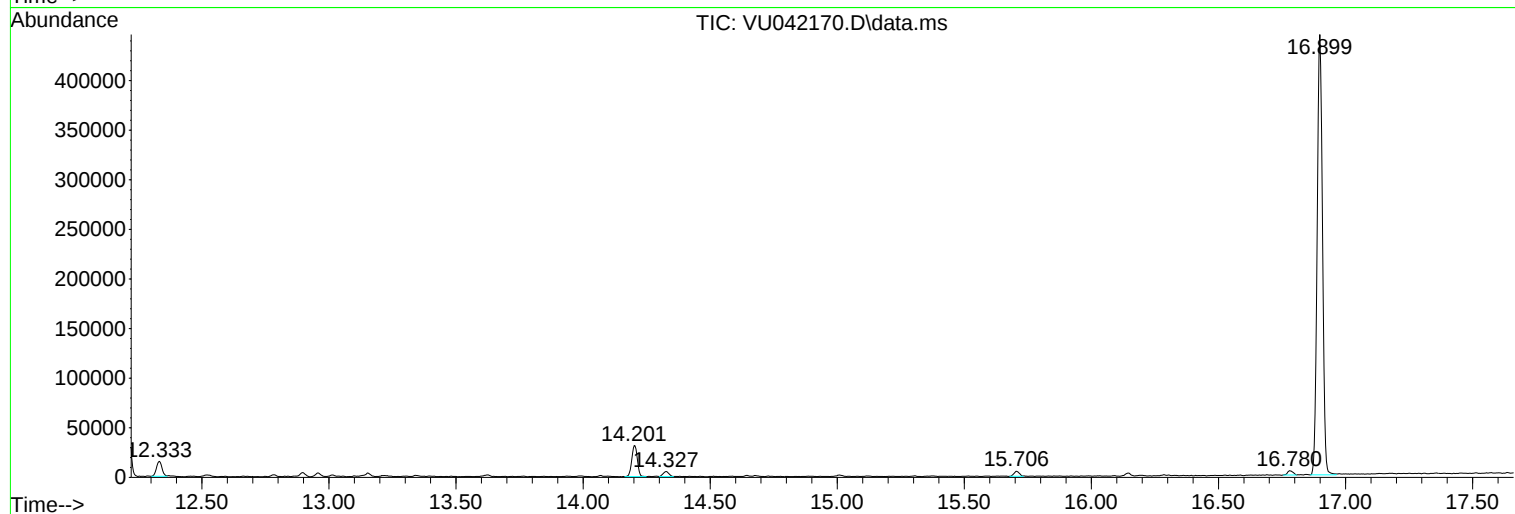
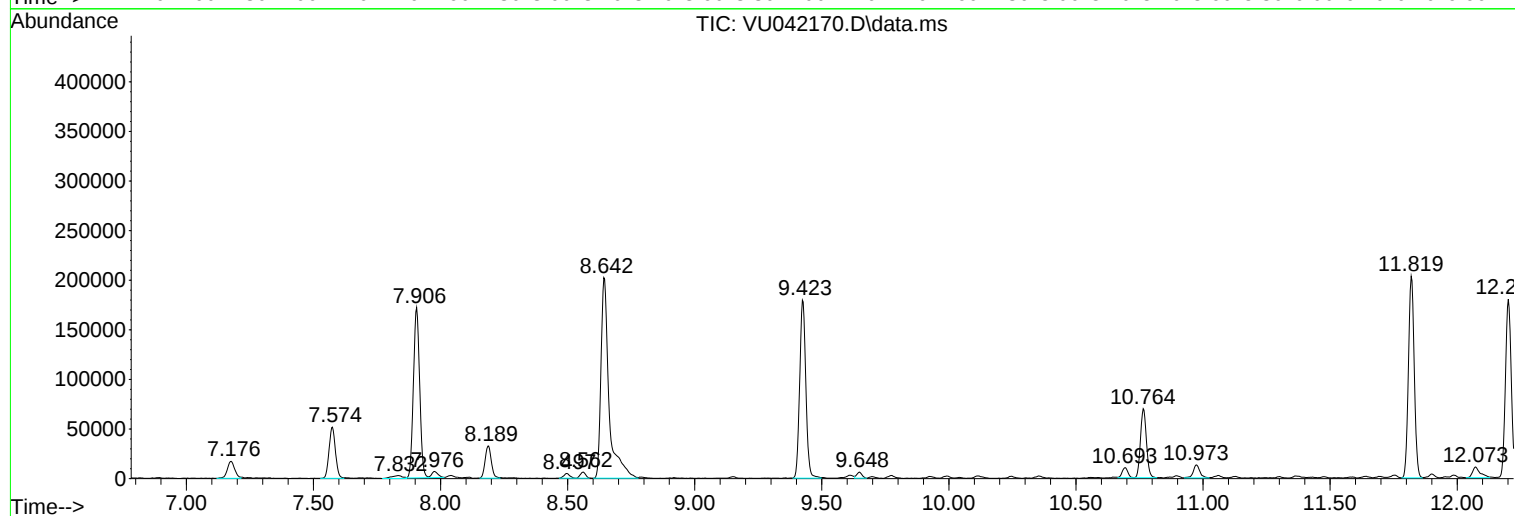
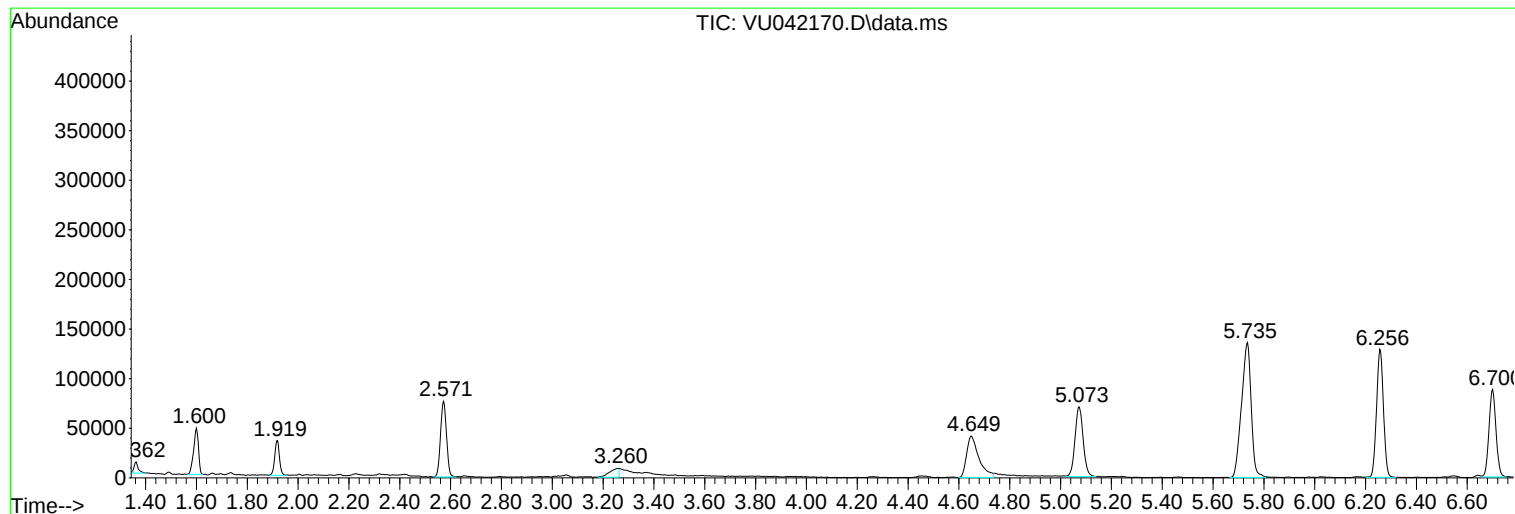
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Instrument :
MSVOA_U
ClientSampleId :
F1E12

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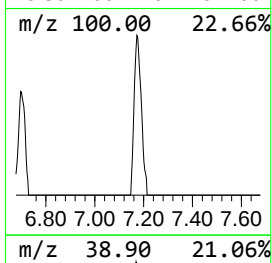
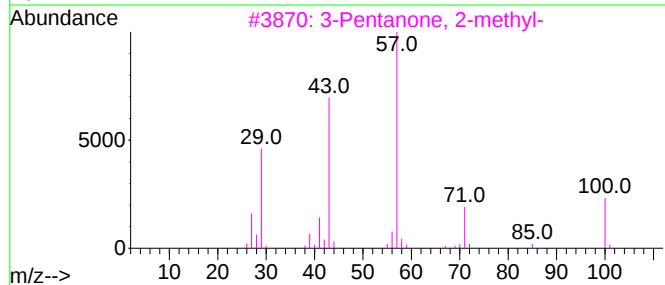
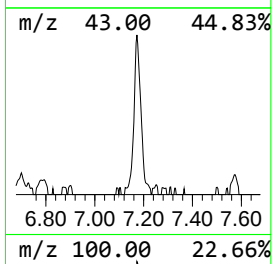
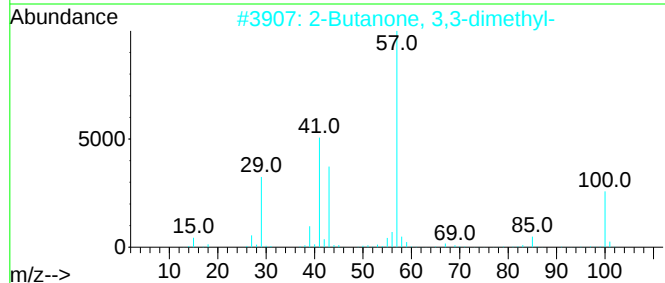
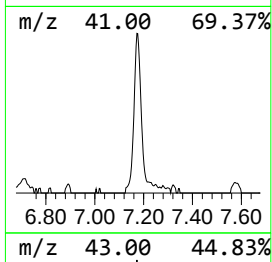
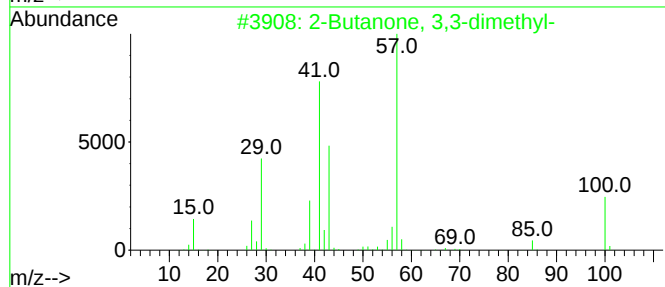
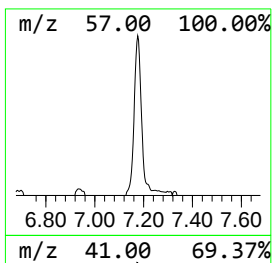
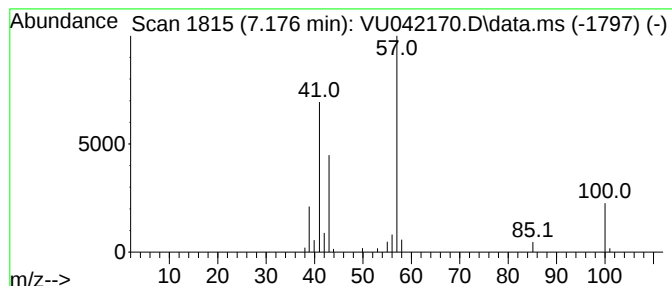
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Butanone, 3,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.176	0.72 ug/L	35161	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-		100	C6H12O	000075-97-8	91	
2	2-Butanone, 3,3-dimethyl-		100	C6H12O	000075-97-8	80	
3	3-Pentanone, 2-methyl-		100	C6H12O	000565-69-5	64	
4	3-Pentanone, 2-methyl-		100	C6H12O	000565-69-5	64	
5	2-Butanone, 3,3-dimethyl-		100	C6H12O	000075-97-8	56	



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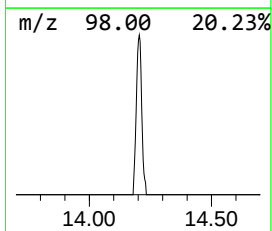
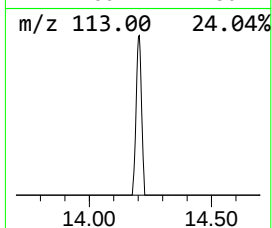
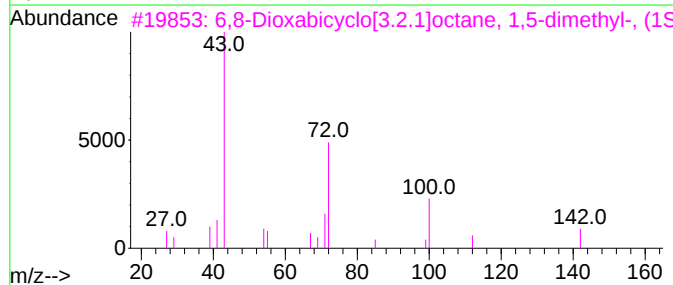
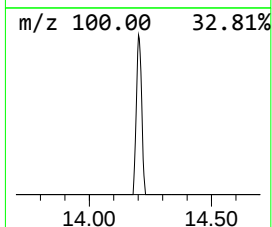
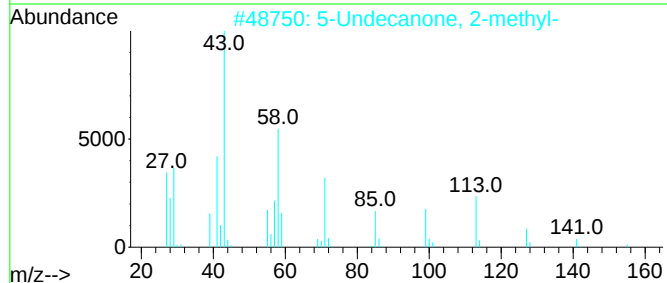
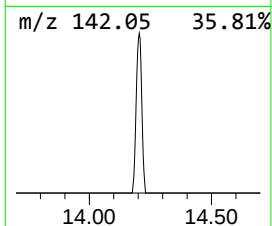
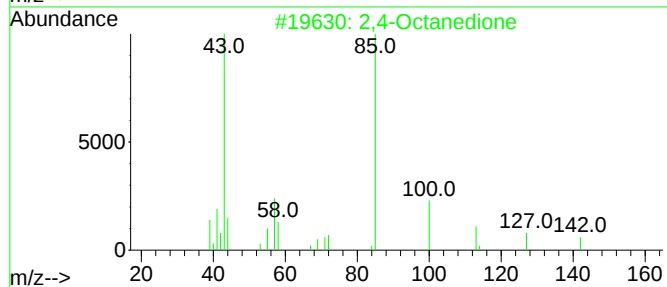
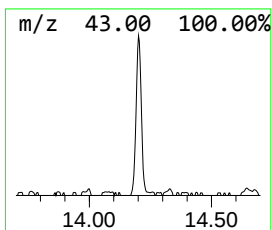
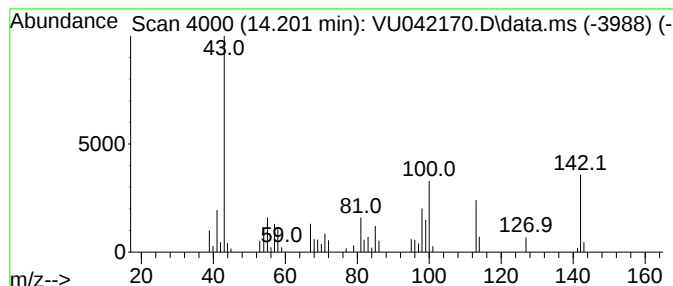
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 3 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.201	0.74 ug/L	47123	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Octanedione	142	C8H14O2	014090-87-0	25
2			5-Undecanone, 2-methyl-	184	C12H24O	050639-02-6	16
3			6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	16
4			6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	16
5			6-Dodecanone	184	C12H24O	006064-27-3	16



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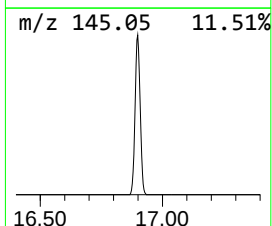
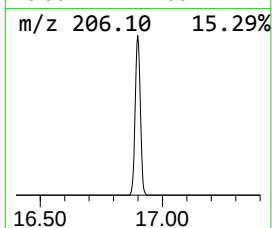
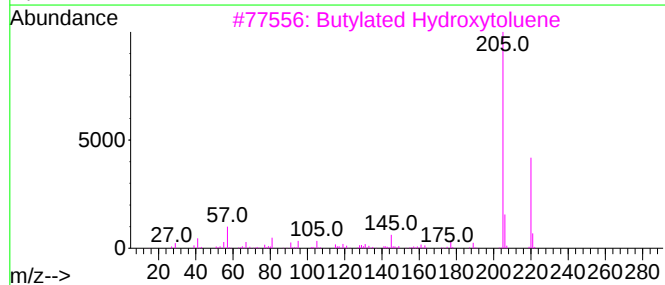
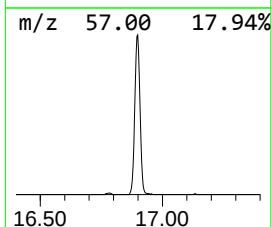
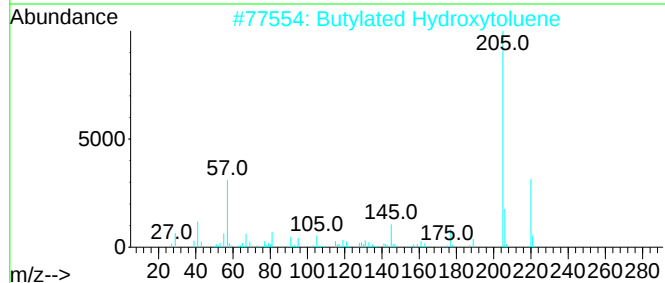
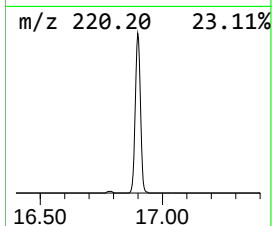
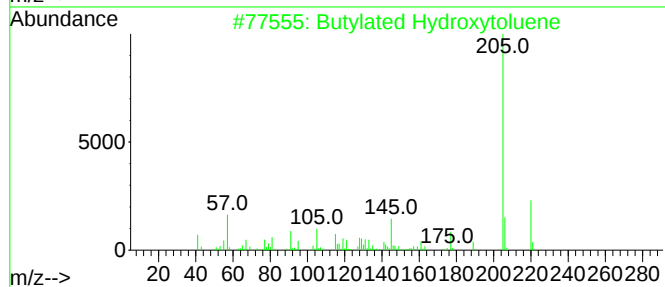
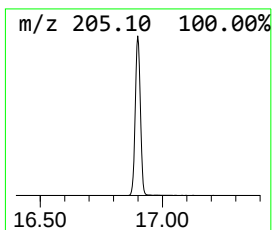
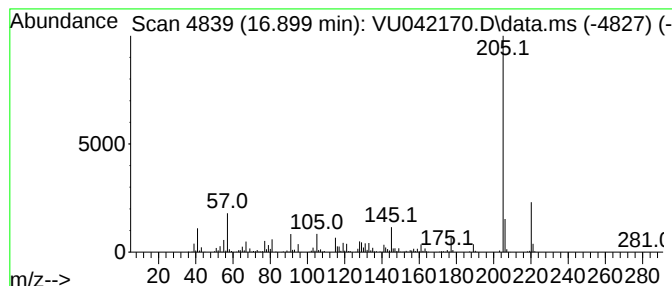
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Quant Title : TRACE VOA SOM01.0

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	10.08 ug/L	646324	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	93
5			Phenol, 4,6-di(1,1-dimethylethyl...	220	C15H24O	000616-55-7	93



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Quant Title : TRACE VOA SOM01.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Butanone, 3,3...	7.176	0.7	ug/L	35161	1	6.256	243464	5.0
unknown-01	14.201	0.7	ug/L	47123	3	11.819	320559	5.0
Butylated Hydro...	16.899	10.1	ug/L	646324	3	11.819	320559	5.0