

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012221\
 Data File : VU042176.D
 Acq On : 22 Jan 2021 17:46
 Operator : SY/MD
 Sample : M1222-11
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 16 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: VU042176.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	91	rVB	41641	48119	7.94%	1.165%
2	1.916	171	179	192	rVB	33773	42485	7.01%	1.028%
3	2.298	291	298	305	rBV	8614	13024	2.15%	0.315%
4	2.572	372	383	396	rBV	72865	117261	19.36%	2.838%
5	4.655	1014	1031	1084	rBV	48341	202196	33.38%	4.894%
6	5.073	1146	1161	1178	rBV	69074	152785	25.22%	3.698%
7	5.732	1345	1366	1393	rBV2	136183	354121	58.45%	8.572%
8	6.256	1515	1529	1547	rBV	131605	247142	40.79%	5.982%
9	6.700	1654	1667	1682	rVB	86046	166733	27.52%	4.036%
10	7.176	1800	1815	1832	rVB	18632	37819	6.24%	0.915%
11	7.575	1927	1939	1951	rBV	50758	88936	14.68%	2.153%
12	7.838	1998	2021	2030	rBV5	8508	24447	4.04%	0.592%
13	7.906	2030	2042	2057	rVB	167591	287074	47.39%	6.949%
14	8.041	2075	2084	2094	rVB3	3598	6718	1.11%	0.163%
15	8.186	2117	2129	2141	rBV	32866	54172	8.94%	1.311%
16	8.497	2216	2226	2235	rBV4	4077	6581	1.09%	0.159%
17	8.559	2235	2245	2255	rVB2	11704	19192	3.17%	0.465%
18	8.645	2255	2272	2292	rBV	241480	451420	74.51%	10.927%
19	9.423	2502	2514	2534	rBV	183975	308464	50.92%	7.466%
20	9.649	2578	2584	2593	rVB2	4974	7049	1.16%	0.171%
21	9.768	2612	2621	2634	rBV3	4159	8109	1.34%	0.196%
22	10.694	2901	2909	2919	rVB3	5716	9268	1.53%	0.224%
23	10.764	2919	2931	2946	rBV	70381	112988	18.65%	2.735%
24	10.976	2982	2997	3010	rBV3	5674	11676	1.93%	0.283%
25	11.819	3247	3259	3274	rVB	211067	328961	54.30%	7.963%
26	12.073	3328	3338	3346	rBV2	8789	16265	2.68%	0.394%
27	12.202	3362	3378	3393	rVB	178387	286963	47.37%	6.946%
28	12.330	3409	3418	3431	rBV2	7133	10363	1.71%	0.251%
29	14.201	3988	4000	4014	rBV	38764	59163	9.77%	1.432%
30	15.706	4459	4468	4478	rBV8	7134	12610	2.08%	0.305%
31	16.143	4595	4604	4614	rBV3	14053	22429	3.70%	0.543%
32	16.780	4795	4802	4813	rBV5	7615	10969	1.81%	0.266%
33	16.899	4827	4839	4854	rBV	412290	605827	100.00%	14.664%

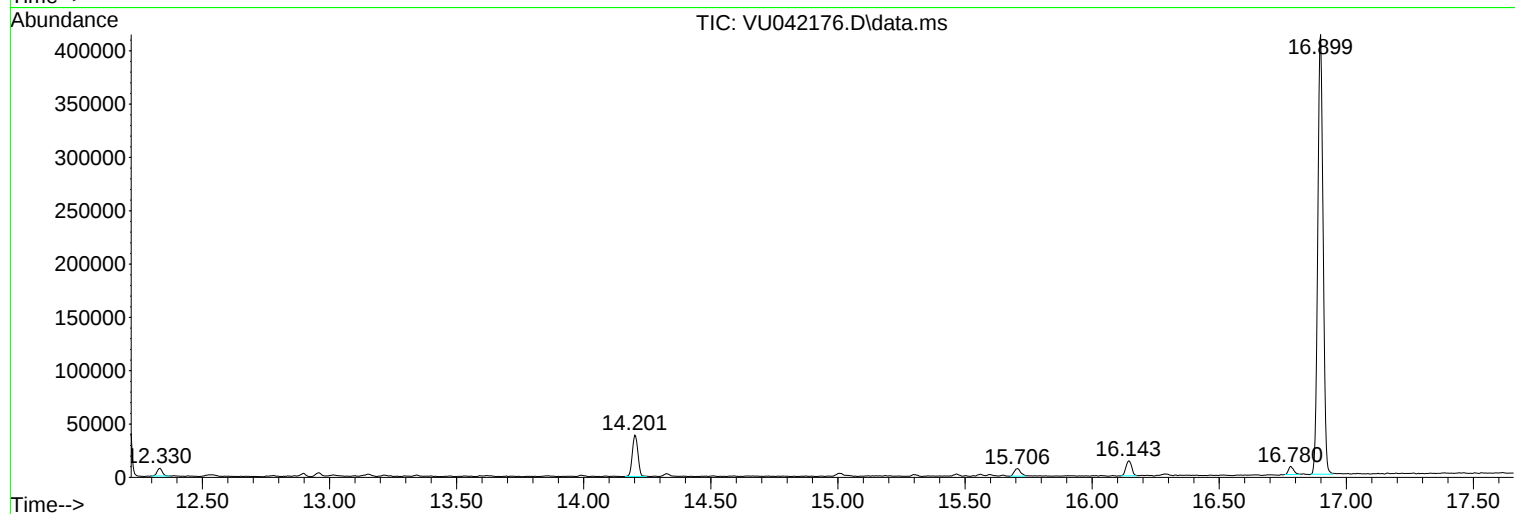
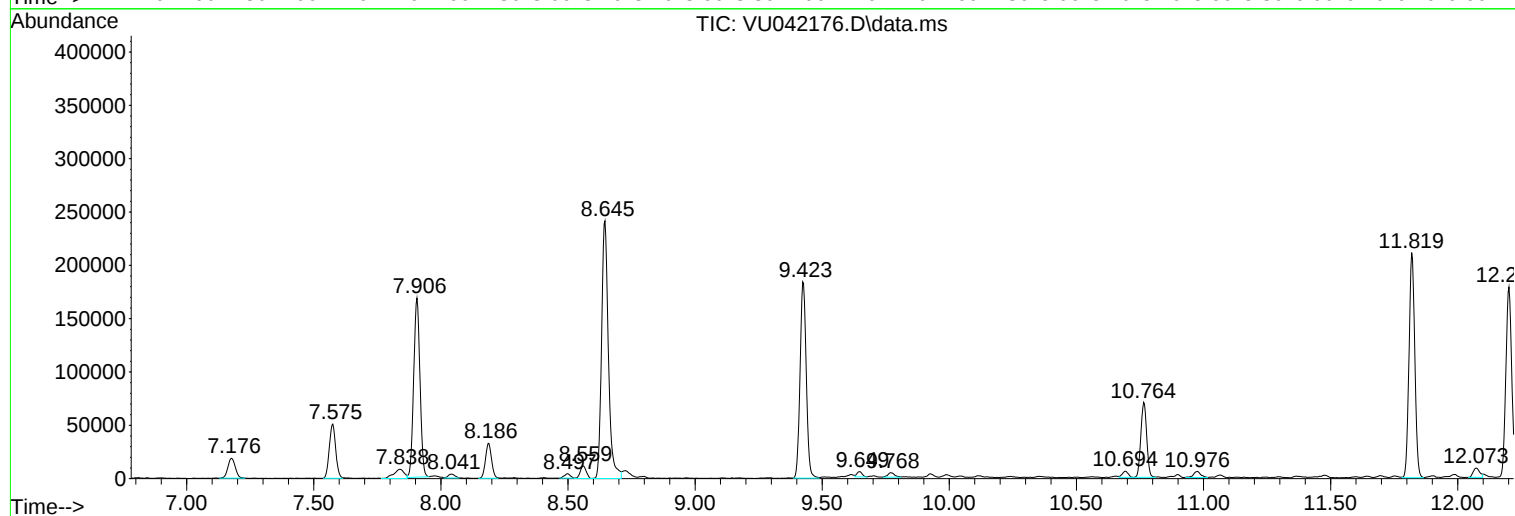
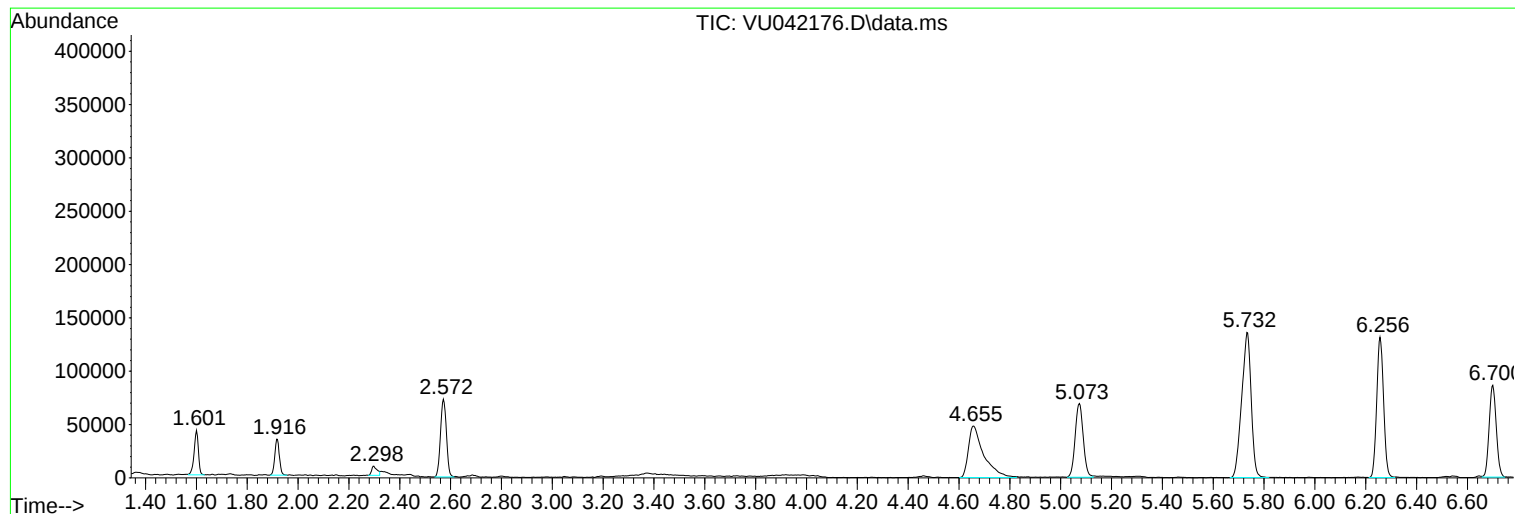
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ClientSampleId :

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



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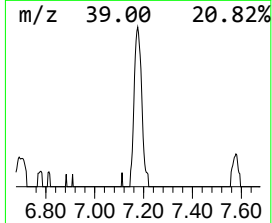
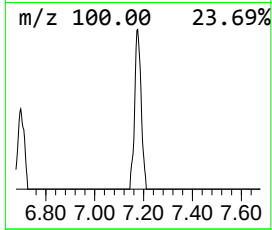
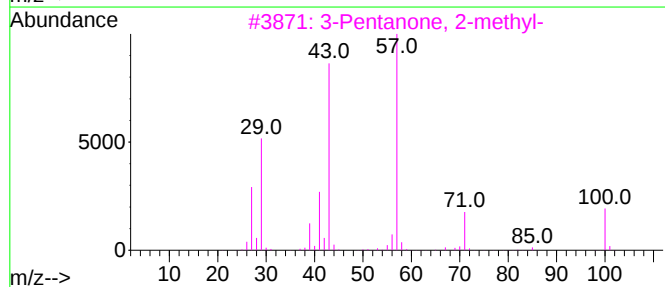
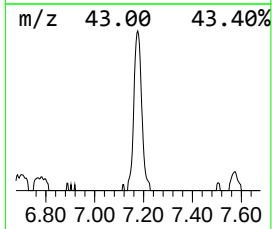
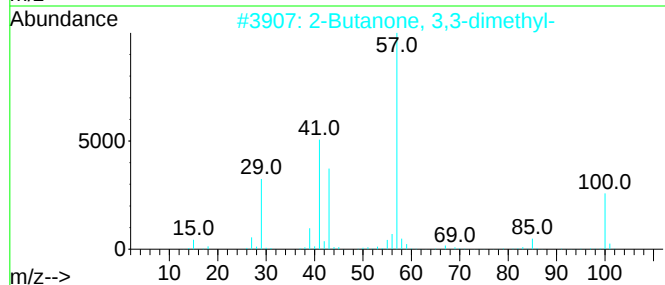
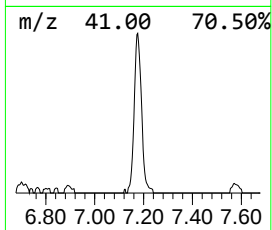
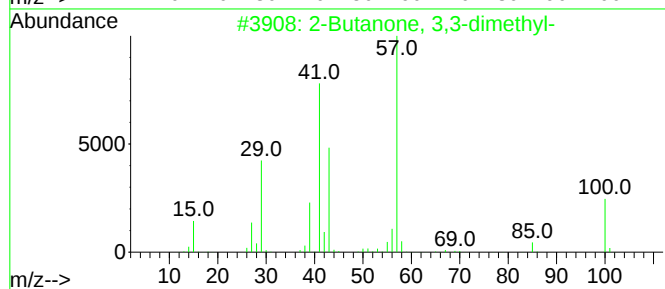
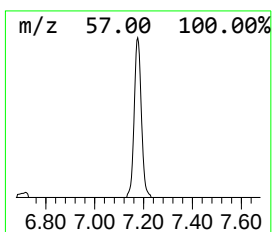
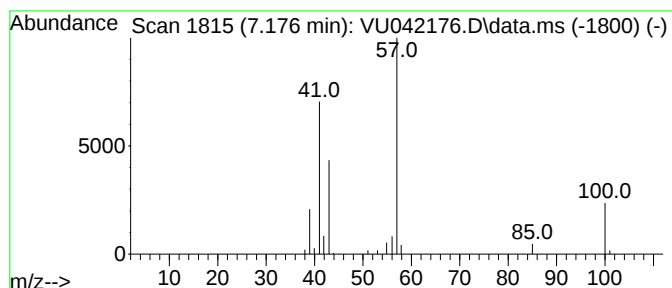
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR012021WMA.M
Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.176	0.77 ug/L	37819	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	90
3		3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	64
4		2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	64
5		3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	64



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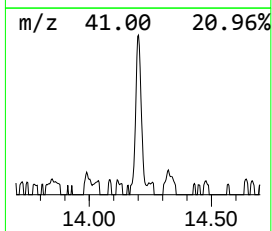
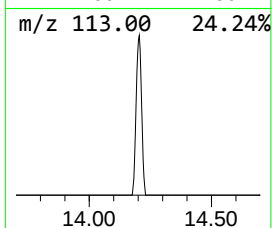
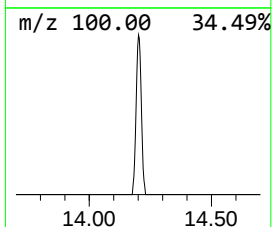
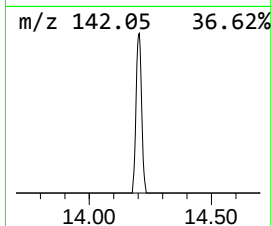
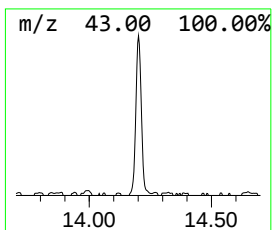
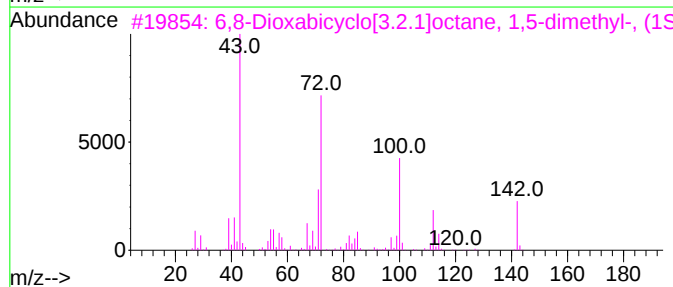
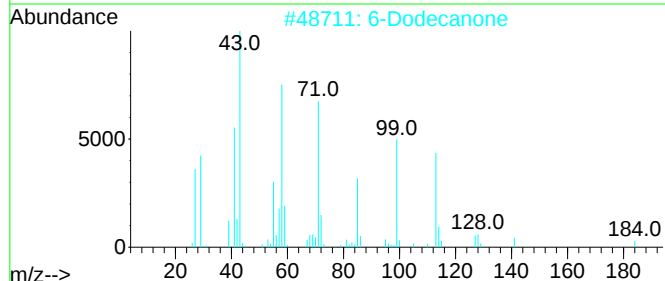
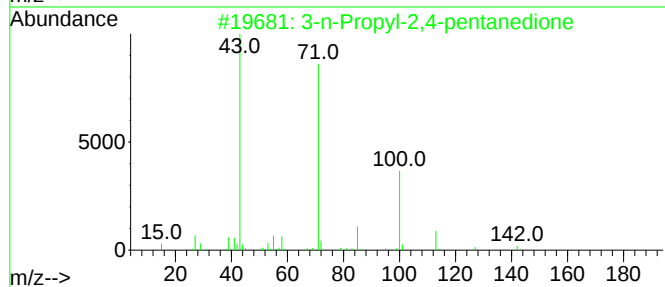
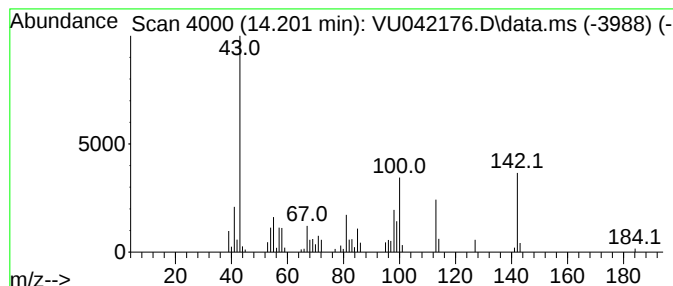
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Peak Number 3 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.201	0.90 ug/L	59163	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-n-Propyl-2,4-pentanedione	142	C8H14O2	001540-35-8	25
2			6-Dodecanone	184	C12H24O	006064-27-3	22
3			6,8-Dioxabicyclo[3.2.1]octane, 1...	142	C8H14O2	028401-39-0	22
4			Heptane, 4-ethyl-	128	C9H20	002216-32-2	12
5			Cyclohexanemethylamine	113	C7H15N	003218-02-8	11



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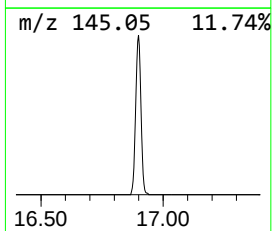
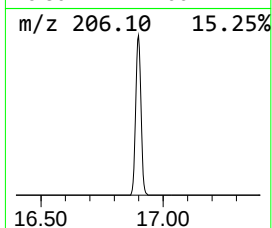
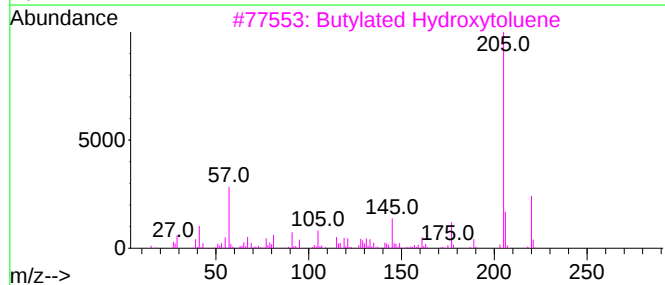
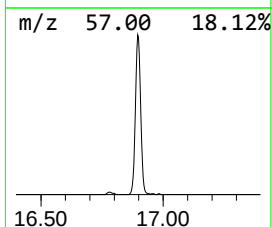
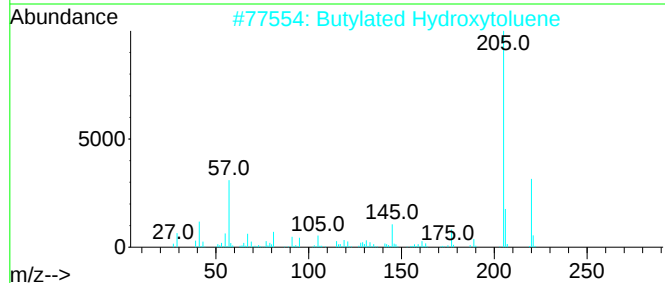
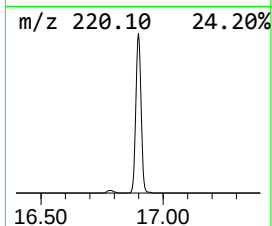
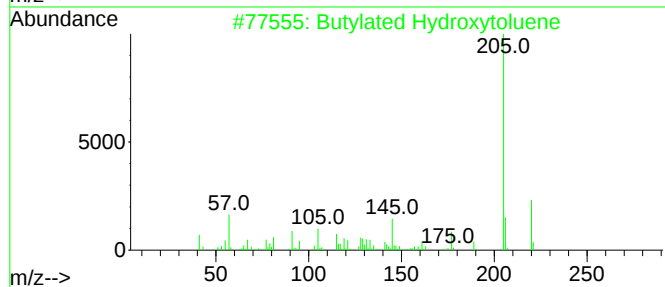
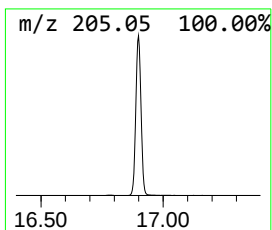
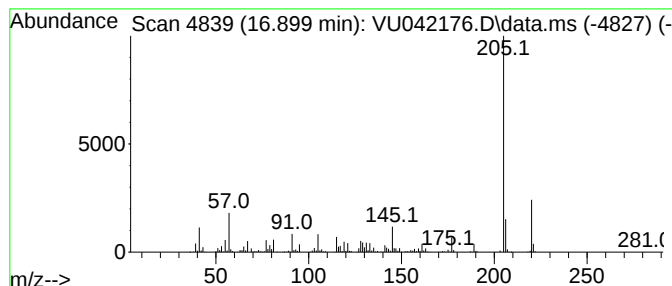
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Quant Title : TRACE VOA SOM01.0

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	9.21 ug/L	605827	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	97
3			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	96
4			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	94
5			Phenol, 4,6-di(1,1-dimethylethyl...	220	C15H24O	000616-55-7	93



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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	0.8	ug/L	37819	1	6.256	247142	5.0
unknown-01	14.201	0.9	ug/L	59163	3	11.819	328961	5.0
Butylated Hydro...	16.899	9.2	ug/L	605827	3	11.819	328961	5.0