

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU110920\
 Data File : VU041151.D
 Acq On : 09 Nov 2020 19:14
 Operator : SY/MD
 Sample : L4646-18
 Misc : 25.0mL/MSVOA U/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 GB0W2

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.1

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR102620WMA.M

Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.485	40	45	52	rVB2	4200	4143	1.24%	0.145%
2	1.594	69	79	89	rVB	42508	48076	14.39%	1.685%
3	1.912	170	178	192	rVV	24874	31317	9.37%	1.097%
4	1.993	194	203	215	rVB	25433	35192	10.53%	1.233%
5	2.202	260	268	279	rBV2	7014	11833	3.54%	0.415%
6	2.314	298	303	311	rVB2	4157	6038	1.81%	0.212%
7	2.414	330	334	343	rVB5	2785	3379	1.01%	0.118%
8	2.465	343	350	359	rVB4	5394	8842	2.65%	0.310%
9	2.568	371	382	398	rBV	47661	76463	22.89%	2.679%
10	3.038	514	528	535	rBV	3274	7779	2.33%	0.273%
11	3.076	535	540	548	rVB7	2457	3645	1.09%	0.128%
12	3.137	548	559	566	rBV7	2378	4825	1.44%	0.169%
13	3.359	615	628	638	rBV6	2705	6299	1.89%	0.221%
14	4.530	978	992	1003	rVB3	4981	11554	3.46%	0.405%
15	4.681	1026	1039	1044	rBV4	7596	14522	4.35%	0.509%
16	4.755	1045	1062	1089	rVB2	26018	103715	31.04%	3.634%
17	5.009	1127	1141	1143	rBV2	3436	5427	1.62%	0.190%
18	5.079	1150	1163	1183	rVB	53615	116161	34.77%	4.070%
19	5.391	1256	1260	1270	rVB5	3539	5391	1.61%	0.189%
20	5.732	1349	1366	1378	rBV2	110942	258679	77.42%	9.065%
21	6.259	1517	1530	1544	rBV	89991	165280	49.47%	5.792%
22	6.549	1603	1620	1636	rBV2	58856	111478	33.37%	3.906%
23	6.703	1650	1668	1681	rBV	65794	127084	38.04%	4.453%
24	7.574	1928	1939	1951	rBV	31113	53150	15.91%	1.862%
25	7.902	2029	2041	2057	rBV	107919	184296	55.16%	6.458%
26	8.185	2118	2129	2141	rBV	20049	32241	9.65%	1.130%
27	8.652	2261	2274	2285	rBV	190734	334108	100.00%	11.708%
28	9.417	2501	2512	2533	rBV	126574	207114	61.99%	7.258%
29	9.693	2588	2598	2610	rBV	15060	23884	7.15%	0.837%
30	10.758	2917	2929	2943	rVB	52077	84330	25.24%	2.955%
31	10.902	2959	2974	2984	rVB2	2716	4422	1.32%	0.155%
32	11.288	3086	3094	3105	rVB2	3320	4543	1.36%	0.159%
33	11.806	3244	3255	3268	rBV	124334	194334	58.17%	6.810%
34	12.063	3324	3335	3336	rBV	7276	8525	2.55%	0.299%

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ClientSampleId :
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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\SOMUTR102620WMA.M
Title : TRACE VOA SOM01.0

35	12.086	3338	3342	3351	rVB2	11246	16756	5.02%	0.587%
36	12.188	3362	3374	3388	rVB	128545	203862	61.02%	7.144%
37	12.876	3575	3588	3594	rBV5	2338	3648	1.09%	0.128%
38	14.272	4015	4022	4028	rBV5	3624	5344	1.60%	0.187%
39	16.339	4656	4665	4680	rBV3	22240	33333	9.98%	1.168%
40	16.754	4785	4794	4813	rBV2	85920	126682	37.92%	4.439%
41	16.870	4820	4830	4845	rBV	108920	166056	49.70%	5.819%

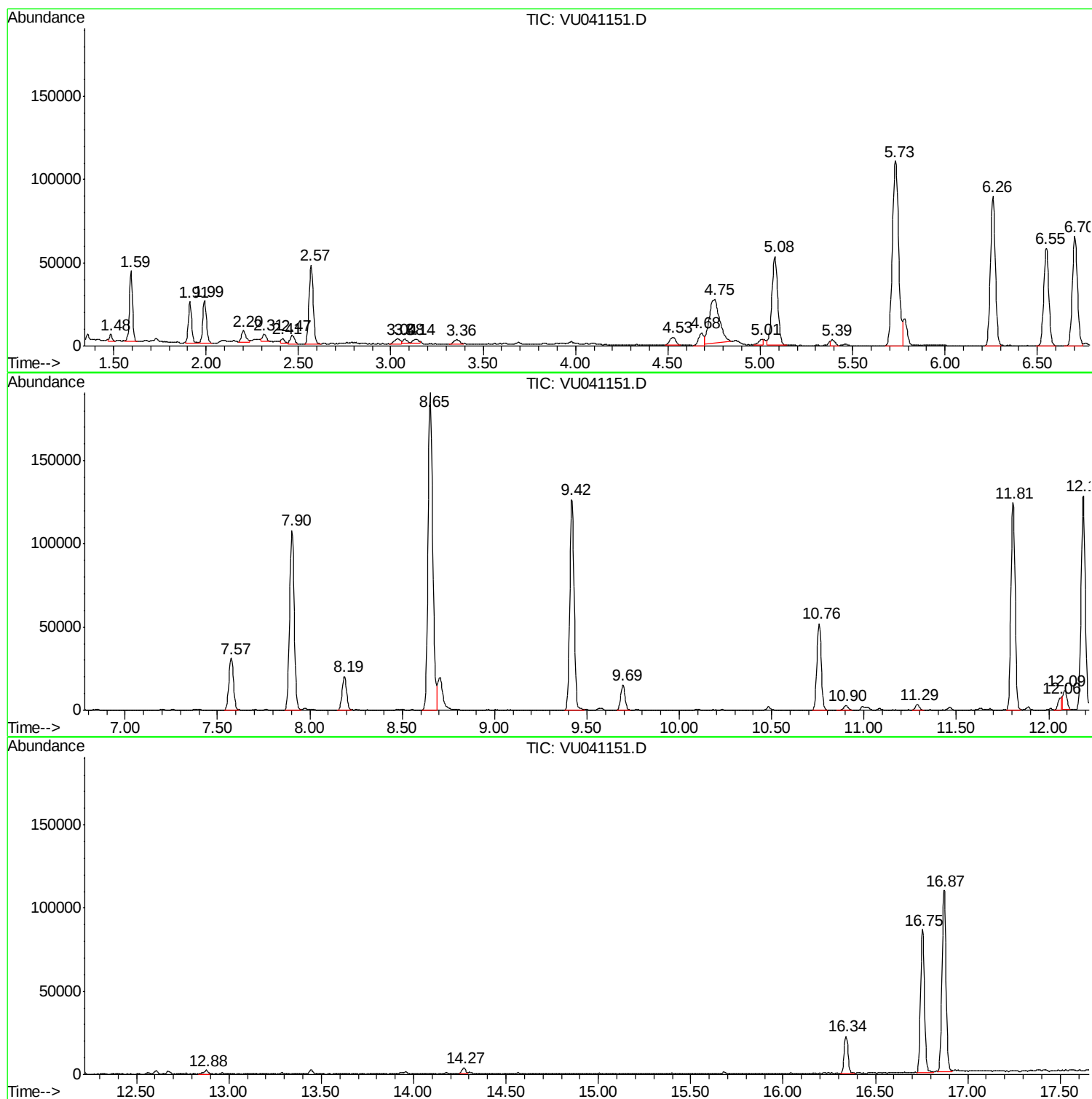
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ClientSampled :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR102620WMA.M
Quant Title : TRACE VOA SOM01.0

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



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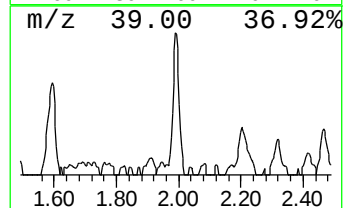
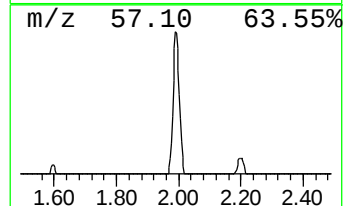
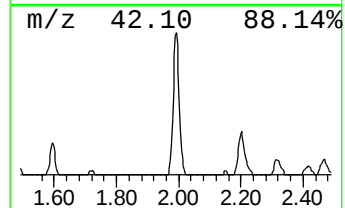
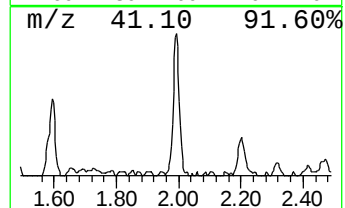
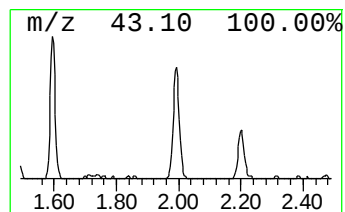
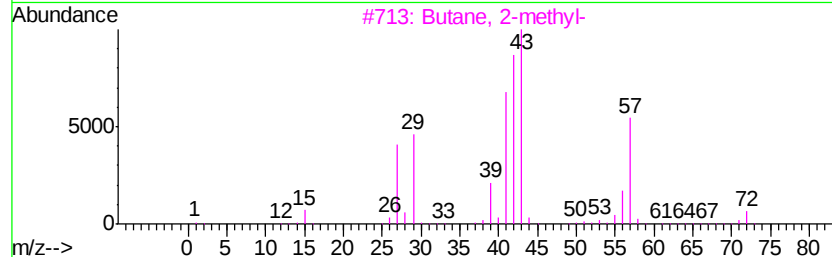
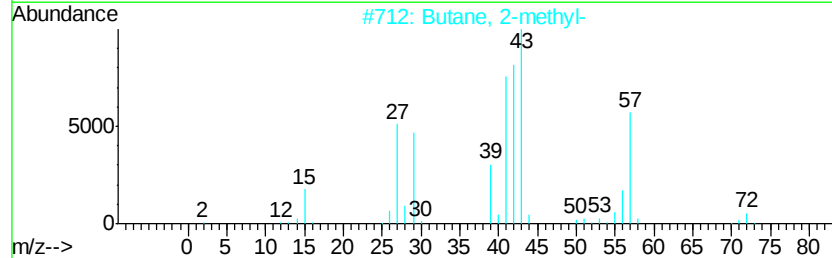
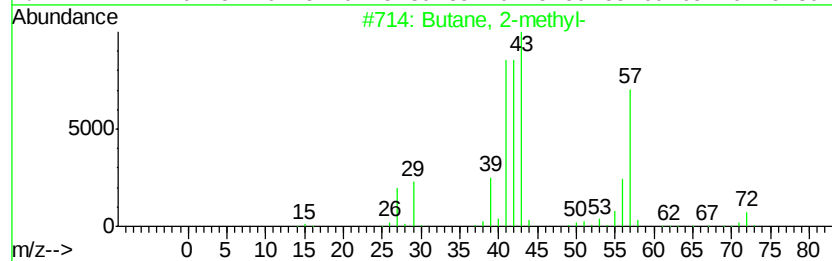
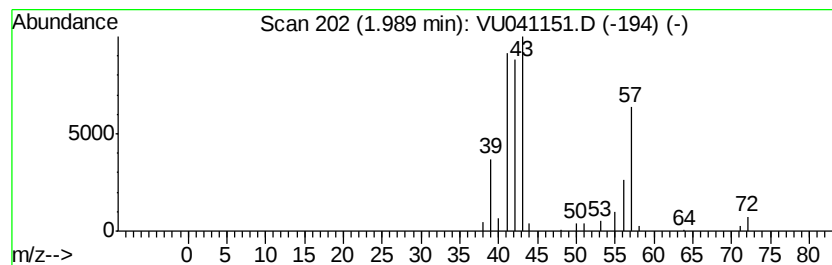
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR102620WMA.M
Quant Title : TRACE VOA SOM01.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.99	1.06 ug/L	35192	1,4-Difluorobenzene	6.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2		Butane, 2-methyl-	72	C5H12	000078-78-4	80
3		Butane, 2-methyl-	72	C5H12	000078-78-4	80
4		3-Buten-1-ol	72	C4H8O	000627-27-0	43
5		Oxirane, trimethyl-	86	C5H10O	005076-19-7	42



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ALS Vial : 20 Sample Multiplier: 1

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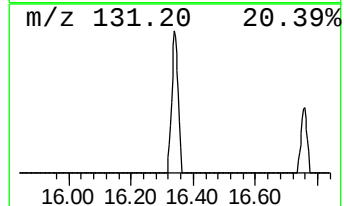
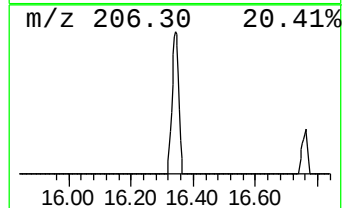
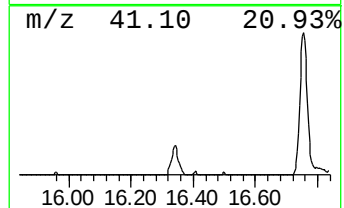
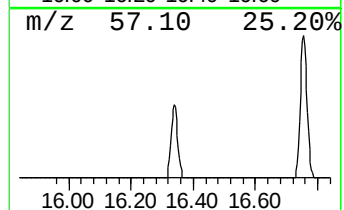
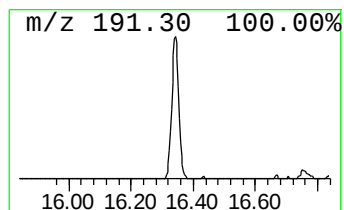
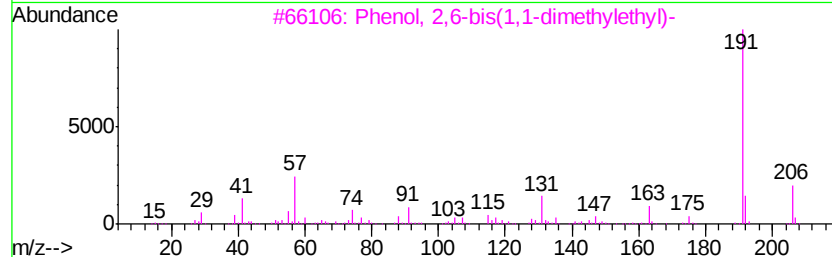
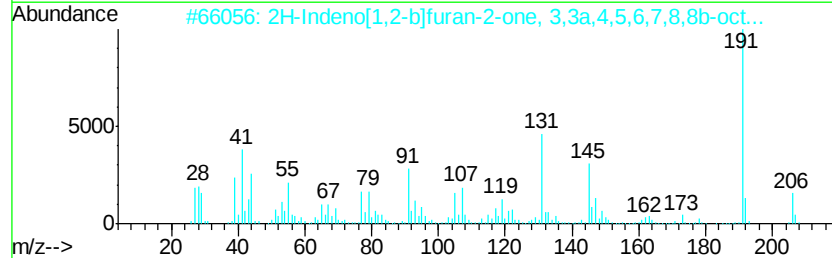
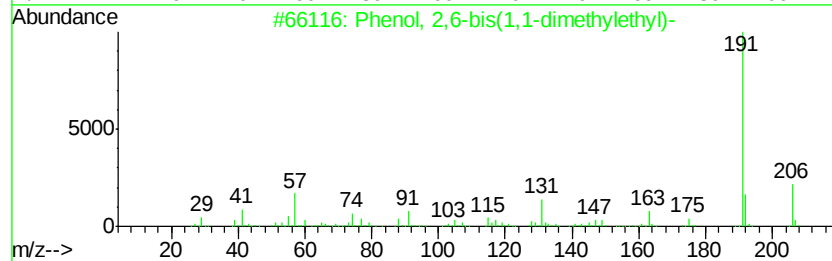
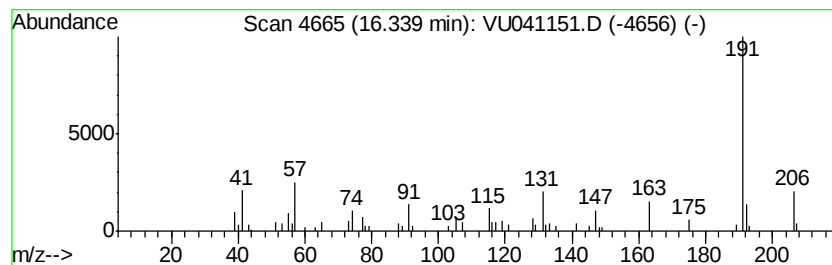
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.34	0.86 ug/L	33333	1,4-Dichlorobenzene-d4	11.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	91		
2	2H-Indeno[1,2-b]furan-2-one, 3,3...	206	C13H18O2	1000196-74-3	87		
3	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	87		
4	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	81		
5	Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	76		



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ALS Vial : 20 Sample Multiplier: 1

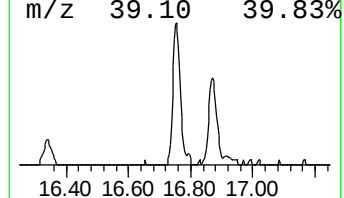
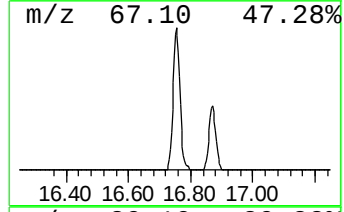
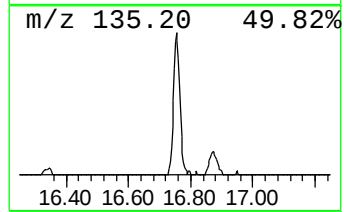
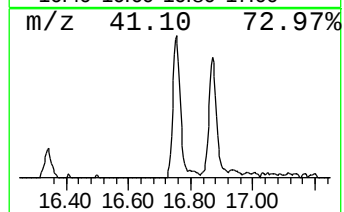
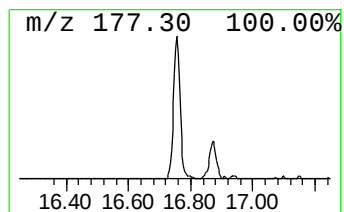
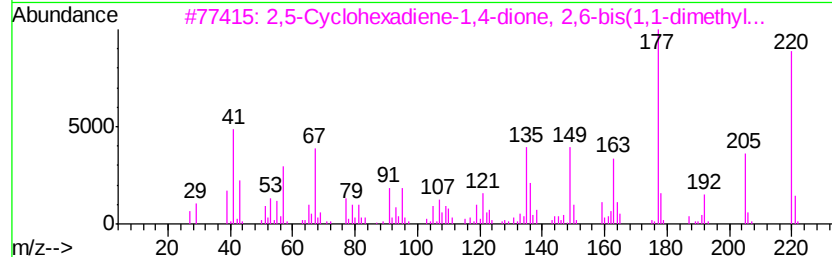
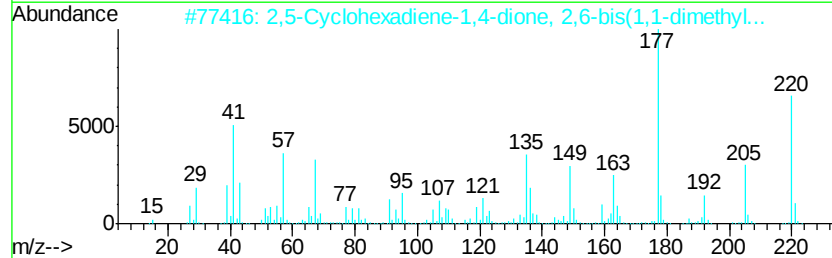
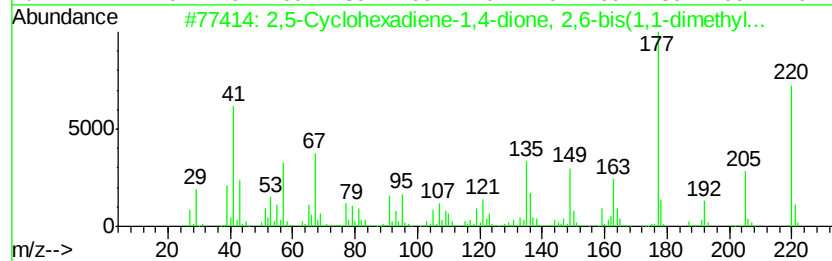
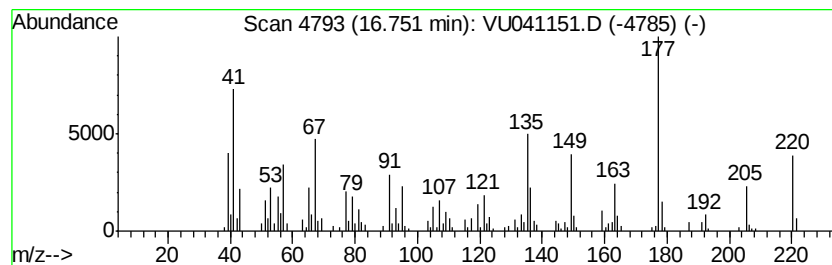
Instrument :
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR102620WMA.M
Quant Title : TRACE VOA SOM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD		R.T.		
16.75	3.26 ug/L	126682	1,4-Dichlorobenzene-d4		11.81		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	95		
2	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	90		
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	70		
4	3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	014901-07-6	47		
5	trans-.beta.-Ionone	192	C13H20O	000079-77-6	47		



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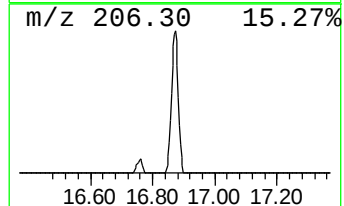
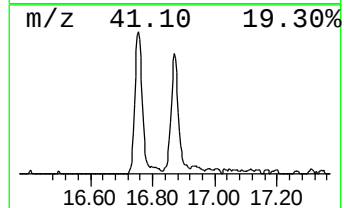
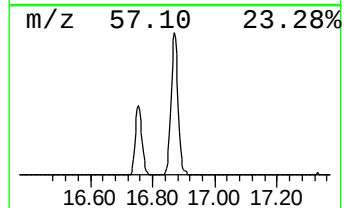
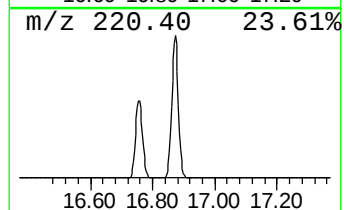
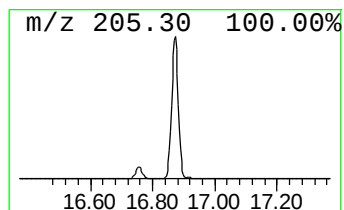
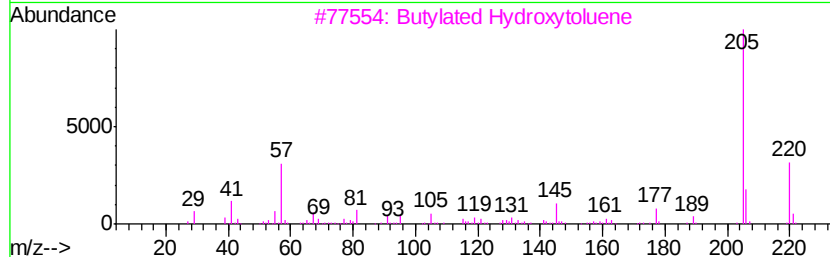
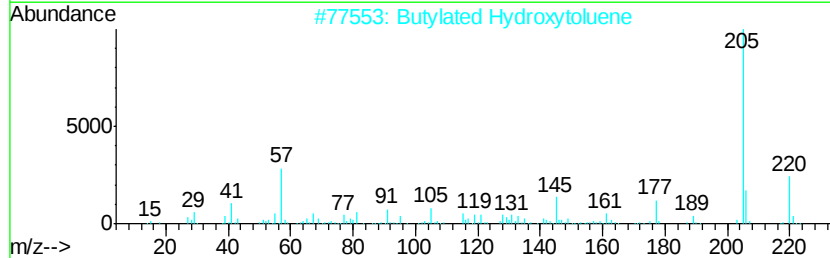
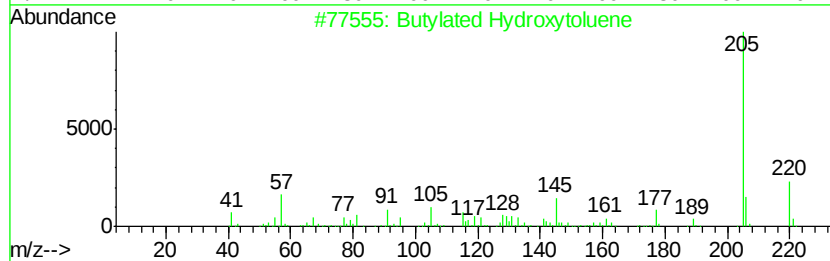
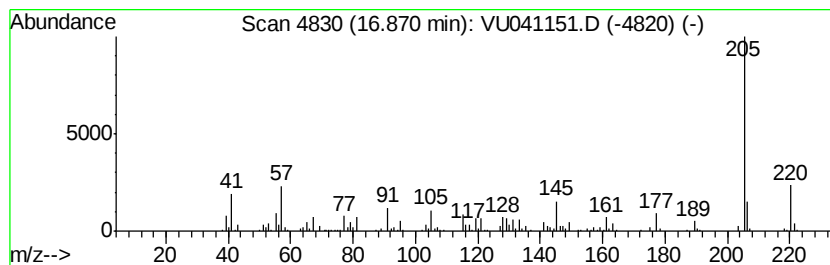
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Quant Title : TRACE VOA SOM01.0

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

Peak Number 5 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.87	4.27 ug/L	166056	1,4-Dichlorobenzene-d4	11.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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	95
4		Butylated Hydroxytoluene	220	C15H24O	000128-37-0	94
5		Phenol, 2,4,6-tris(1-methylethyl)-	220	C15H24O	002934-07-8	87



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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
(DEL) Alkane: Str...	1.99	1.1	ug/L	35192	1	6.26	165280	5.0
Phenol, 2,6-bis(1...	16.34	0.9	ug/L	33333	3	11.81	194334	5.0
2,5-Cyclohexadien...	16.75	3.3	ug/L	126682	3	11.81	194334	5.0
Butylated Hydroxy...	16.87	4.3	ug/L	166056	3	11.81	194334	5.0