

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032019\
 Data File : VN054472.D
 Acq On : 20 Mar 2019 19:12
 Operator : JC/SP
 Sample : K2004-05
 Misc : 4.48g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 SB-24(7-8)

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 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_N\METHODS\82N032019W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.558	240	244	255	rVB3	53821	90142	2.87%	0.542%
2	7.587	1789	1808	1819	rBV	387631	957625	30.46%	5.762%
3	7.664	1820	1832	1872	rVB	718665	1768084	56.24%	10.638%
4	8.027	1928	1945	1966	rBV	446471	1022290	32.52%	6.151%
5	8.583	2102	2118	2163	rVB	1040259	2296867	73.06%	13.820%
6	10.088	2571	2586	2630	rBV	1556027	3143595	100.00%	18.914%
7	11.406	2982	2996	3036	rBV	1364838	2537581	80.72%	15.268%
8	12.310	3269	3277	3286	rVB3	22124	36131	1.15%	0.217%
9	12.403	3293	3306	3326	rBV	1052767	1846315	58.73%	11.109%
10	13.342	3585	3598	3617	rBV	1204268	2059154	65.50%	12.389%
11	14.593	3977	3987	3993	rBV9	15030	32261	1.03%	0.194%
12	14.699	4013	4020	4031	rBV4	32444	46620	1.48%	0.280%
13	16.413	4543	4553	4575	rVB7	140131	317472	10.10%	1.910%
14	16.599	4599	4611	4624	rVB4	223987	466191	14.83%	2.805%

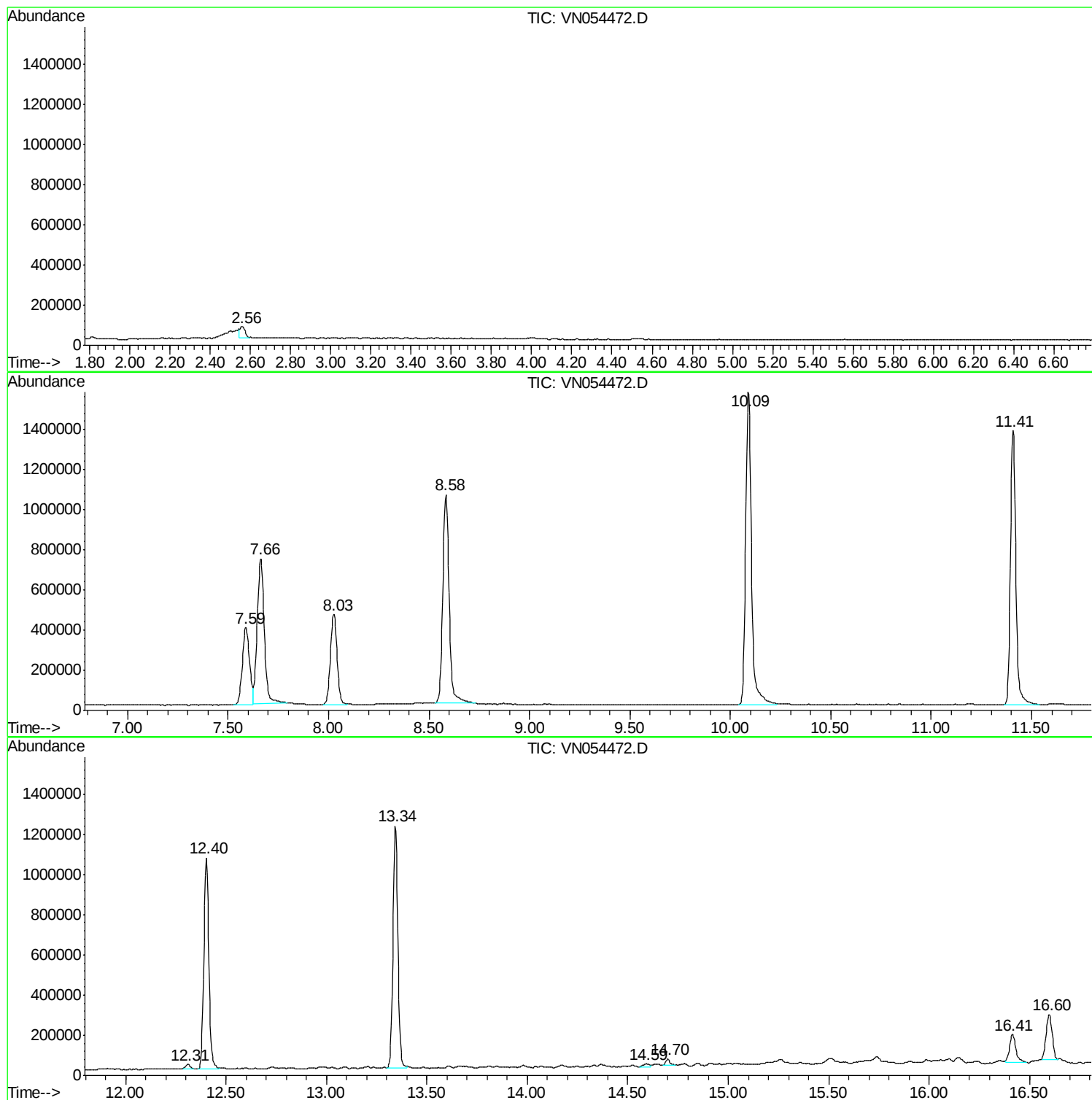
Sum of corrected areas: 16620328

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



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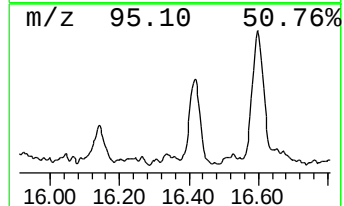
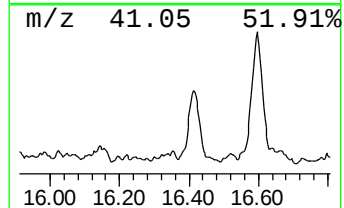
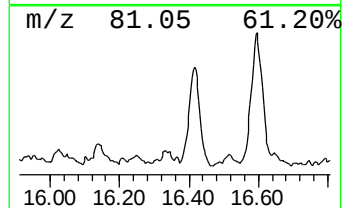
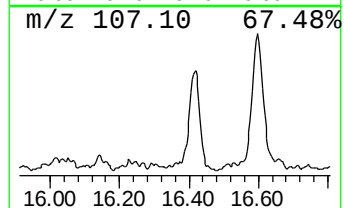
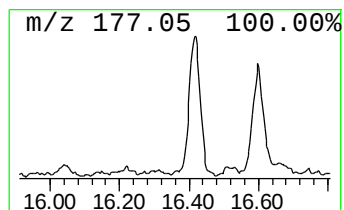
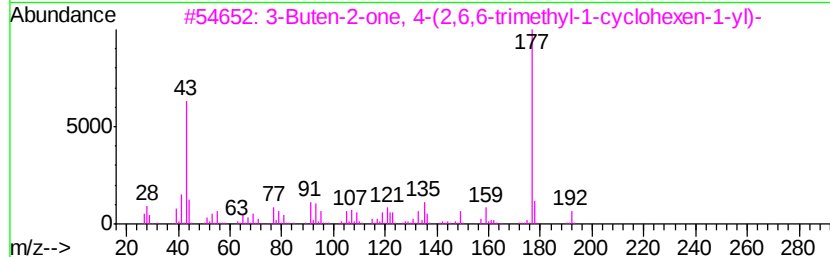
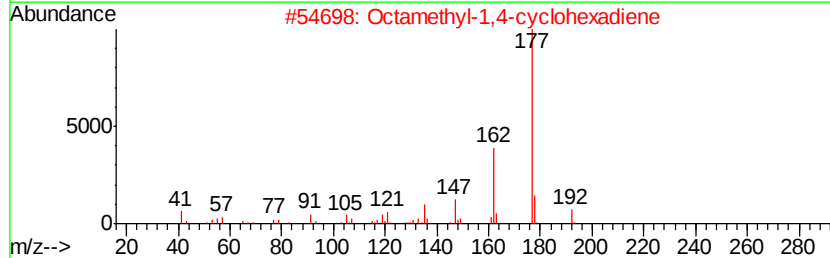
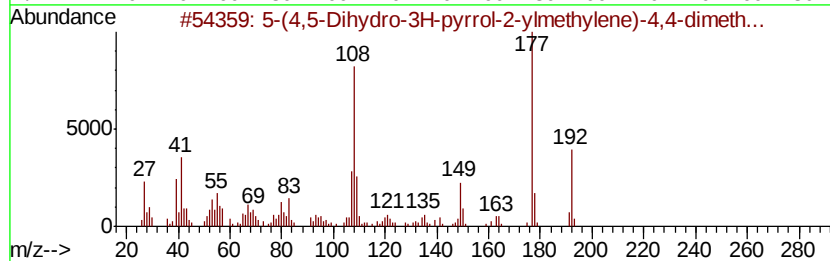
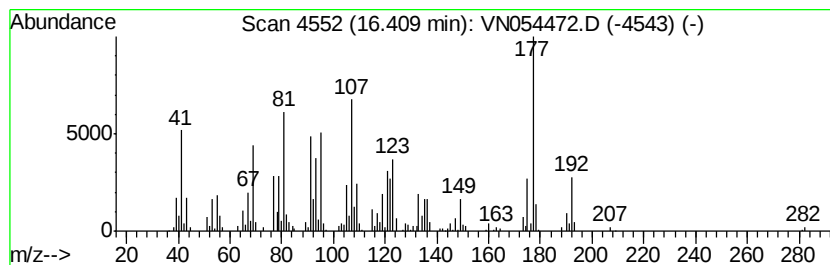
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Peak Number 1 unknown16.41 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.41	7.71 ug/l	317472	1,4-Dichlorobenzene-d4	13.34

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-(4,5-Dihydro-3H-pyrrol-2-yl)met...	192	C11H16N2O	051430-87-6	38		
2	Octamethyl-1,4-cyclohexadiene	192	C14H24	172684-93-4	38		
3	3-Buten-2-one, 4-(2,6,6-trimethyl...	192	C13H20O	014901-07-6	30		
4	5-Methyl-2,4-diisopropylphenol	192	C13H20O	040625-96-5	30		
5	N-(1,1-Dimethylpropynyl)-2-furan...	177	C10H11NO2	039108-97-9	30		



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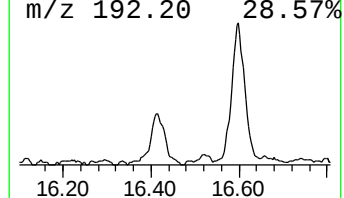
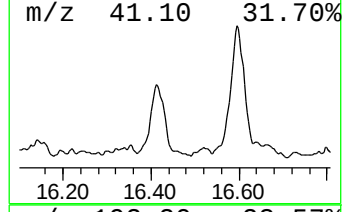
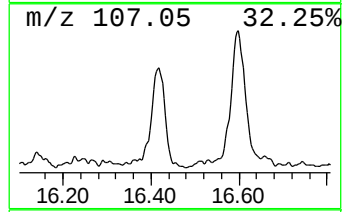
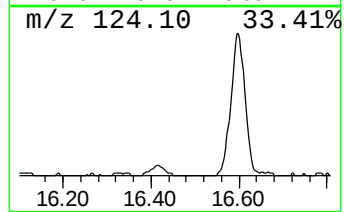
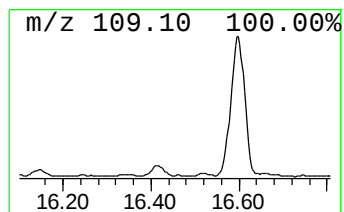
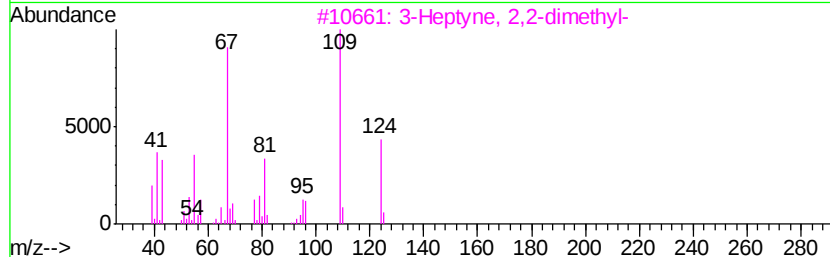
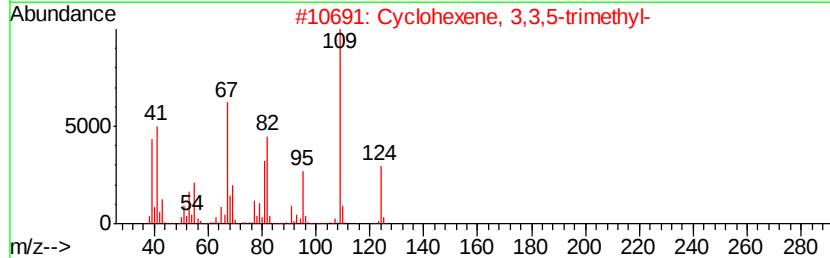
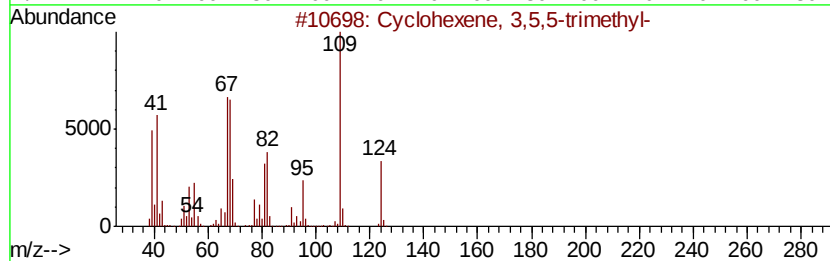
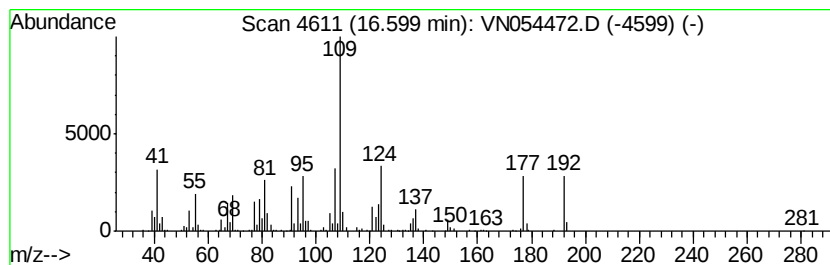
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Peak Number 2 Cyclohexene, 3,5,5-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.60	11.32 ug/l	466191	1,4-Dichlorobenzene-d4	13.34

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexene, 3,5,5-trimethyl-	124	C9H16	000933-12-0	53
2		Cyclohexene, 3,3,5-trimethyl-	124	C9H16	000503-45-7	49
3		3-Heptyne, 2,2-dimethyl-	124	C9H16	029022-29-5	46
4		1,3-Hexadiene, 2,3,5-trimethyl-	124	C9H16	061142-34-5	43
5		2-Cyclopenten-1-one, 3,4,5-trime...	124	C8H12O	055683-21-1	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown16.41	16.41	7.7	ug/l	317472	4	13.34	2059150	50.0
Cyclohexene, 3,5,...	16.60	11.3	ug/l	466191	4	13.34	2059150	50.0