

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN062221\
 Data File : VN067442.D
 Acq On : 22 Jun 2021 17:14
 Operator : JC/MD
 Sample : M2787-02
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 41828

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\82N061421W.M
 Title : SW846 8260

Signal : TIC: VN067442.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.030	7	15	33	rVB5	24276	39411	1.80%	0.340%
2	2.239	83	93	109	rVB5	11337	25775	1.18%	0.222%
3	4.293	839	859	884	rBV	78444	231025	10.55%	1.993%
4	4.594	954	971	1001	rBV2	17120	54513	2.49%	0.470%
5	7.069	1872	1894	1927	rBV5	34906	105461	4.81%	0.910%
6	7.340	1972	1995	1996	rBV2	17991	24477	1.12%	0.211%
7	8.027	2228	2251	2261	rBV2	247272	588322	26.86%	5.075%
8	8.088	2262	2274	2298	rVB3	440811	1009050	46.07%	8.705%
9	8.440	2385	2405	2429	rBV	315836	733605	33.49%	6.328%
10	8.971	2584	2603	2631	rBV	708886	1493385	68.18%	12.883%
11	9.507	2788	2803	2814	rBV6	9854	22791	1.04%	0.197%
12	10.446	3134	3153	3191	rBV	1141535	2190400	100.00%	18.895%
13	11.747	3617	3638	3667	rBV	968198	1811008	82.68%	15.623%
14	12.103	3757	3771	3788	rVB3	50805	88482	4.04%	0.763%
15	12.275	3822	3835	3844	rBV4	24972	50300	2.30%	0.434%
16	12.734	3989	4006	4036	rVB	737357	1314183	60.00%	11.337%
17	13.157	4148	4164	4174	rBV6	17985	51024	2.33%	0.440%
18	13.431	4257	4266	4279	rVB3	42866	71434	3.26%	0.616%
19	13.527	4289	4302	4324	rVB4	29791	66473	3.03%	0.573%
20	13.678	4342	4358	4381	rBV	788445	1376971	62.86%	11.878%
21	13.774	4381	4394	4414	rBV2	142140	244169	11.15%	2.106%

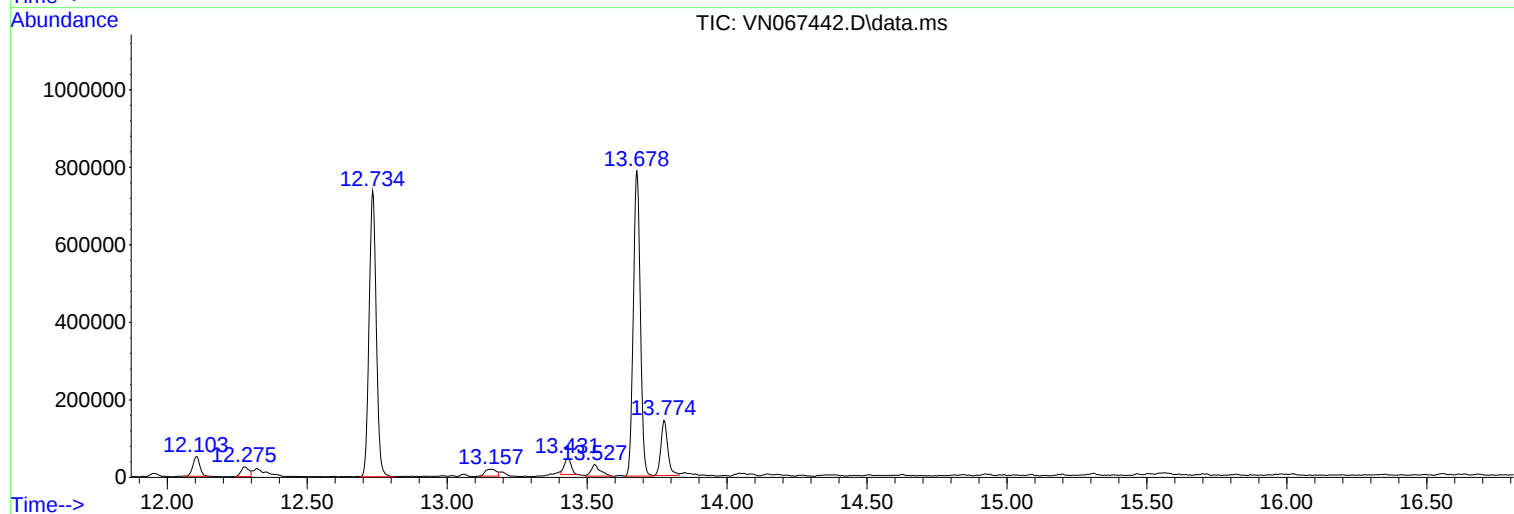
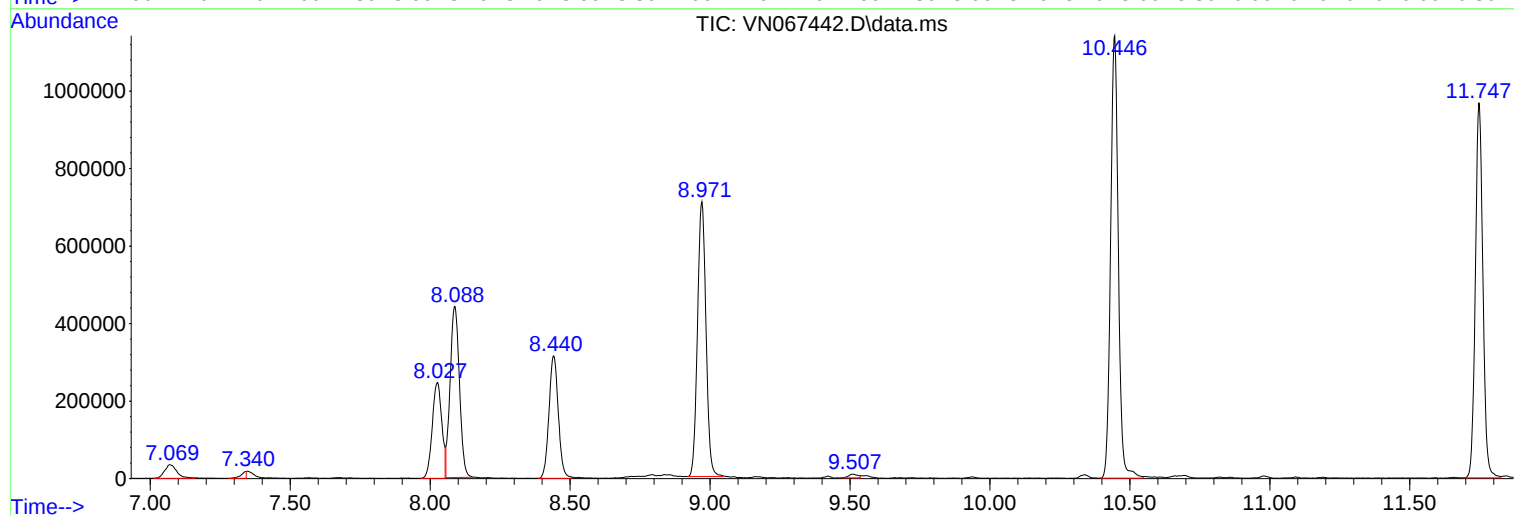
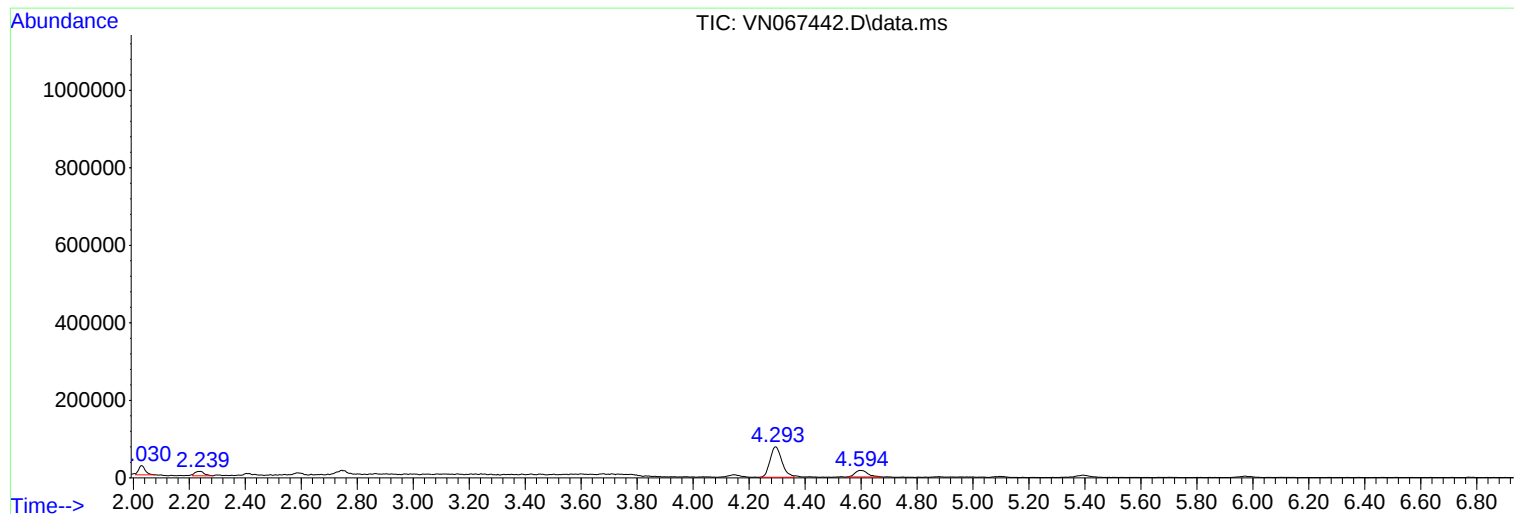
Sum of corrected areas: 11592259

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061421W.M
Quant Title : SW846 8260

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



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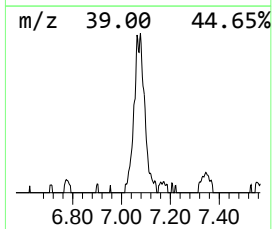
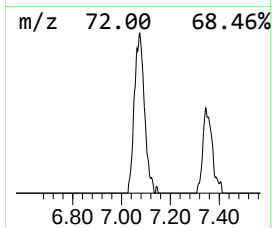
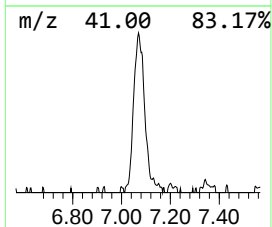
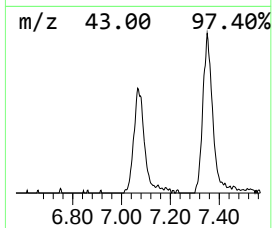
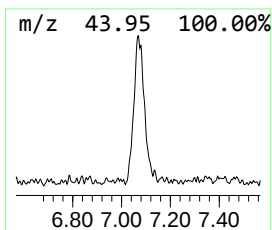
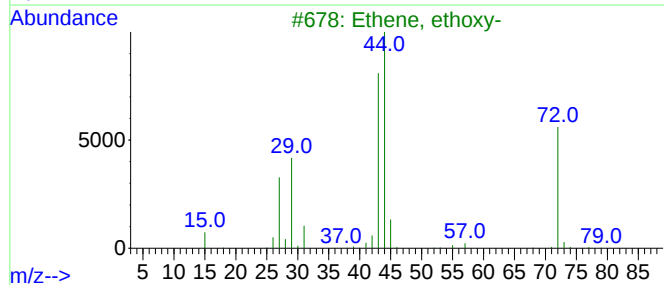
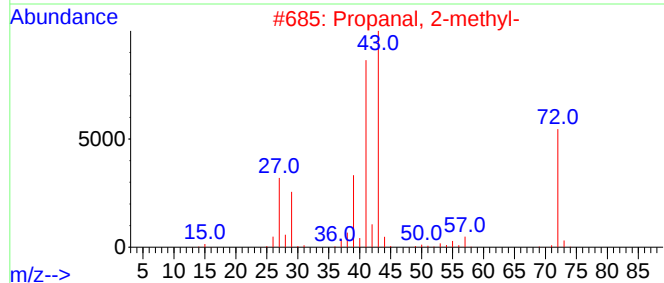
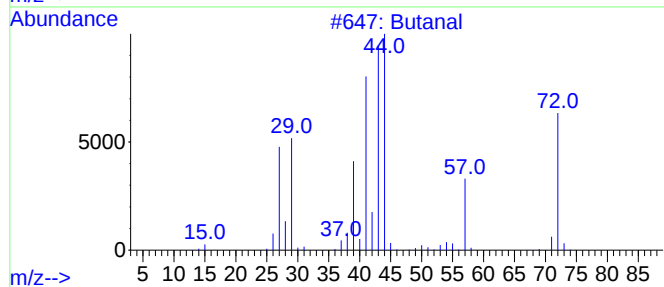
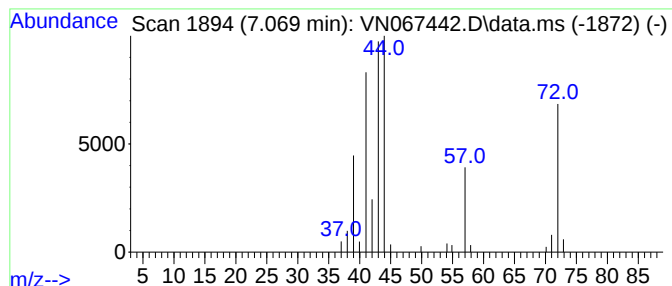
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N061421W.M
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 1 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.069	5.23 ug/l	105461	Pentafluorobenzene	8.088

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanal	72	C4H8O	000123-72-8	94
2		Propanal, 2-methyl-	72	C4H8O	000078-84-2	49
3		Ethene, ethoxy-	72	C4H8O	000109-92-2	47
4		1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	46
5		Isobutylene epoxide	72	C4H8O	000558-30-5	17



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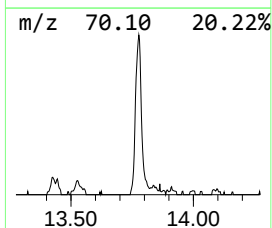
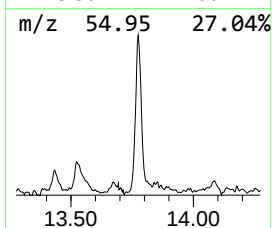
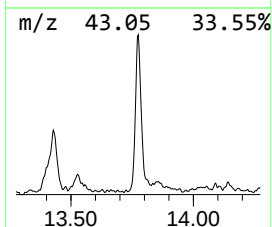
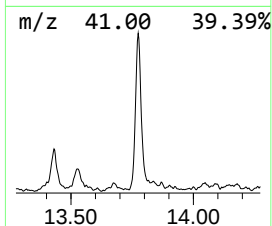
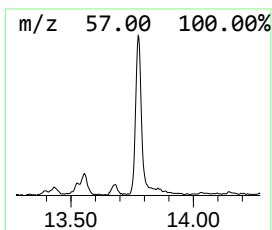
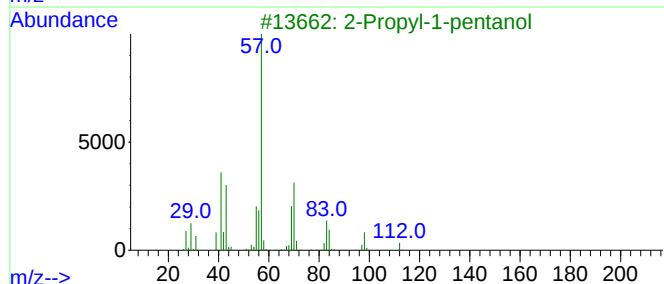
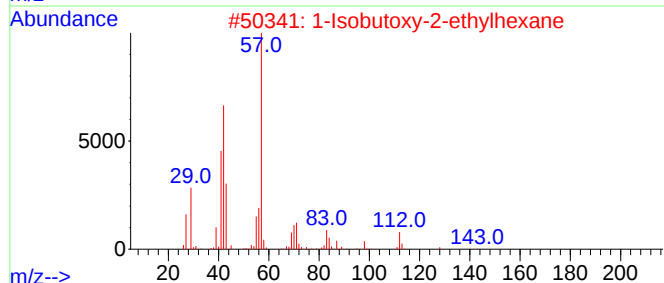
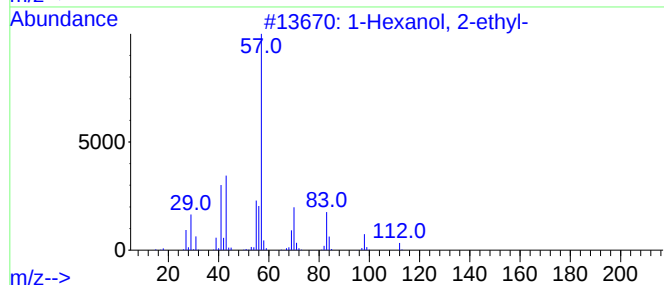
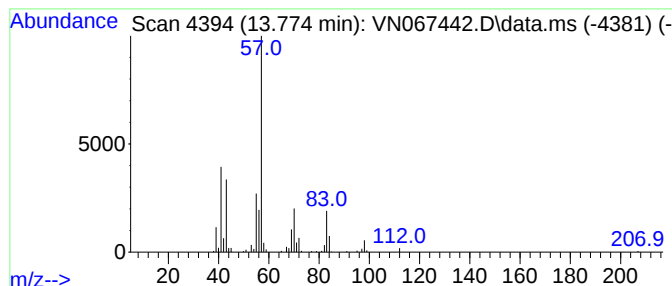
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Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	8.87 ug/l	244169	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	72
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
4			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47
5			Oxalic acid, 2-ethylhexyl octyl ...	314	C18H34O4	1000309-39-1	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanal	7.069	5.2	ug/l	105461	1	8.088	1009050	50.0
1-Hexanol, 2-et...	13.774	8.9	ug/l	244169	4	13.678	1376970	50.0