

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU090219\
 Data File : VU034176.D
 Acq On : 01 Sep 2019 18:02
 Operator : JC/SP
 Sample : K4527-07
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 T9-12-13-N2-(0)

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_U\METHOD\82U082919W.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	2.688	484	497	512	rVB	26565	48954	1.99%	0.271%
2	4.862	1157	1173	1190	rBV	333220	767187	31.20%	4.254%
3	4.961	1190	1204	1233	rVB	555615	1240452	50.45%	6.878%
4	5.289	1290	1306	1332	rBV	360222	796604	32.40%	4.417%
5	5.534	1367	1382	1408	rBV2	54854	127620	5.19%	0.708%
6	5.865	1471	1485	1513	rBV	812370	1677739	68.24%	9.303%
7	6.685	1728	1740	1780	rBV	1025531	1920510	78.11%	10.649%
8	7.402	1951	1963	1975	rBV	183499	316256	12.86%	1.754%
9	7.546	1994	2008	2042	rBV	1356502	2458575	100.00%	13.633%
10	7.829	2086	2096	2113	rVB3	24807	46775	1.90%	0.259%
11	8.138	2172	2192	2208	rBV	339331	578301	23.52%	3.207%
12	8.292	2232	2240	2259	rVB	107091	186914	7.60%	1.036%
13	8.398	2262	2273	2301	rBV	480646	788685	32.08%	4.373%
14	8.887	2412	2425	2457	rBV	682971	1114115	45.32%	6.178%
15	9.070	2462	2482	2522	rVV	1257987	2174619	88.45%	12.058%
16	9.752	2683	2694	2709	rBV2	58400	101176	4.12%	0.561%
17	10.289	2849	2861	2888	rBV	965970	1593982	64.83%	8.839%
18	11.463	3213	3226	3252	rBV	1281445	2095618	85.24%	11.620%

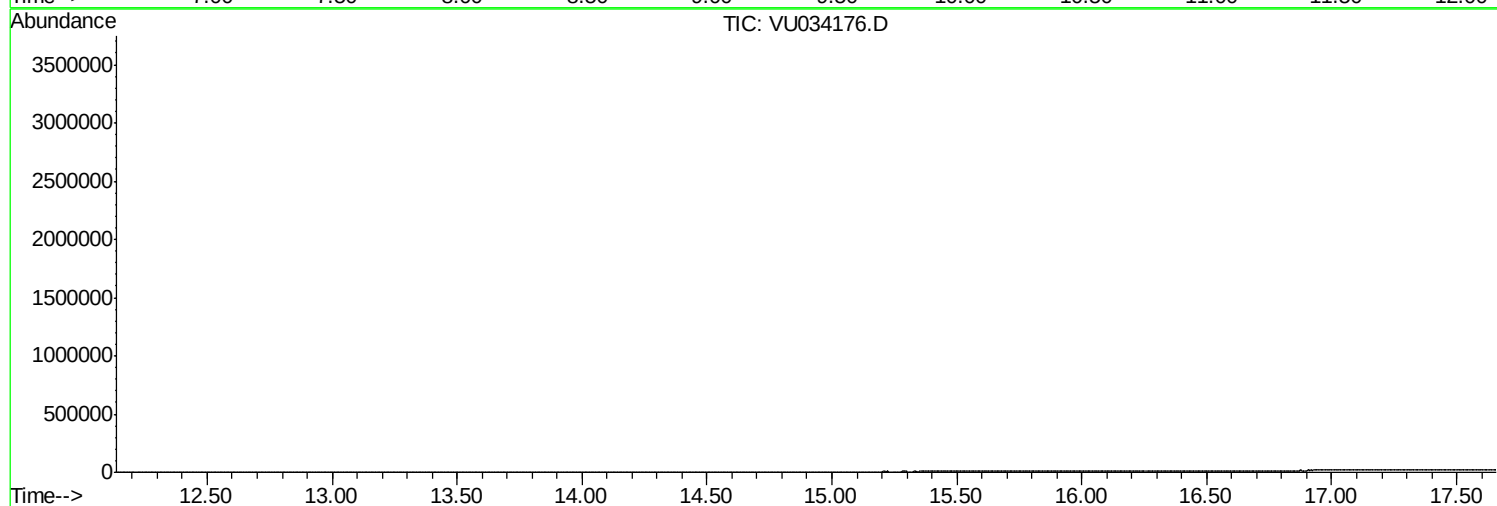
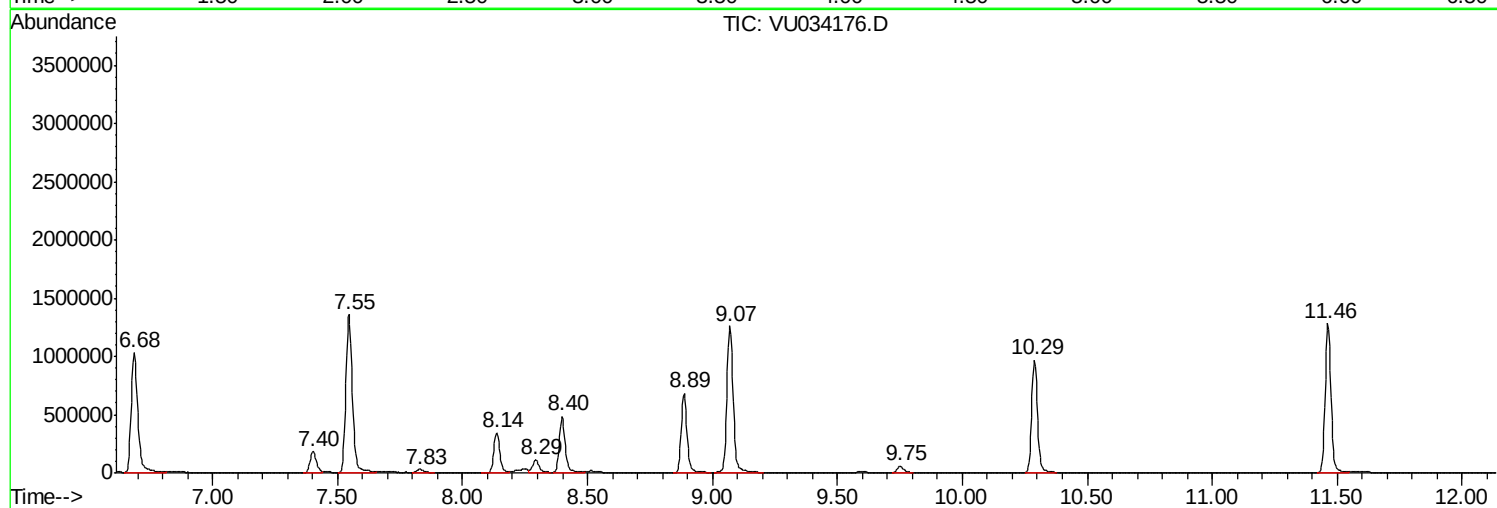
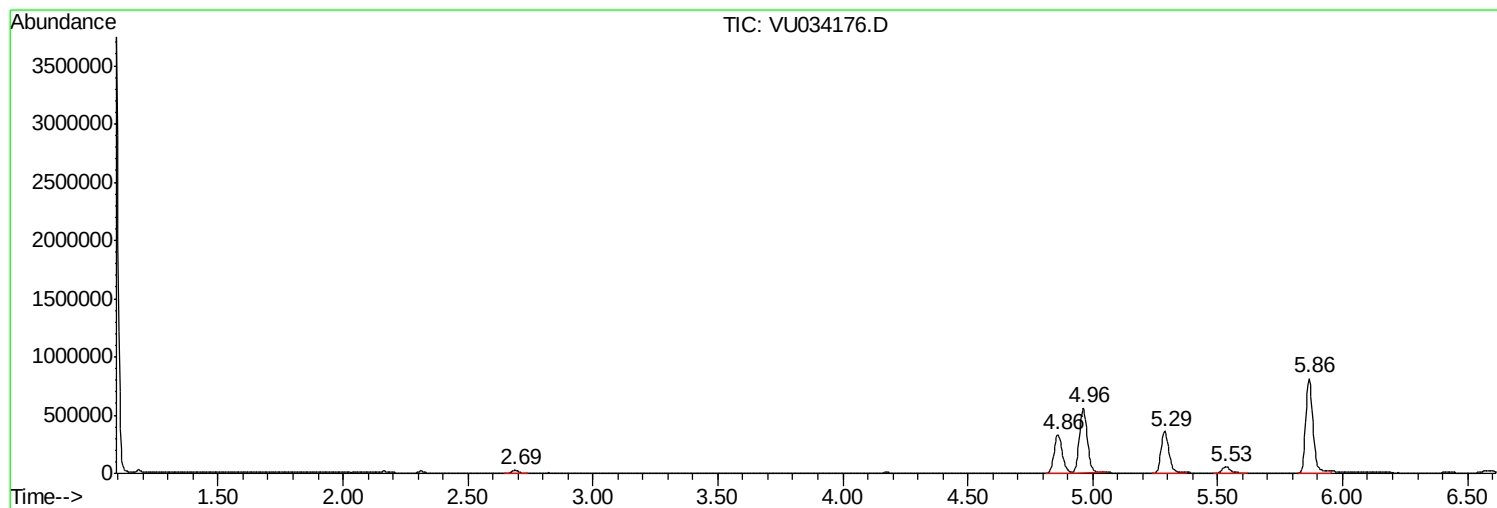
Sum of corrected areas: 18034082

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



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 Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.68	57.24 ug/l	1920510	1,4-Difluorobenzene	5.86
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		n-Propyl acetate	102 C5H10O2	000109-60-4 83
2		Isopropyl acetate	102 C5H10O2	000108-21-4 36
3		1-Butanamine	73 C4H11N	000109-73-9 9
4		Isobutylamine	73 C4H11N	000078-81-9 5
5		Butane, 2-methyl-	72 C5H12	000078-78-4 4

 Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.40	9.43 ug/l	316256	1,4-Difluorobenzene	5.86
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Propanoic acid, 1-methylethyl ester	116 C6H12O2	000637-78-5 90
2		Propanoic acid, propyl ester	116 C6H12O2	000106-36-5 50
3		Diethyl 2-(N-(tert-butoxycarbonyl)-2-oxoethyl)malonate	275 C12H21NO6	102831-44-7 25
4		Propane, 1-(1-methylethoxy)-	102 C6H14O	000627-08-7 23
5		o-Isopropylhydroxylamine	75 C3H9NO	1000322-42-6 9

 Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.14	13.30 ug/l	578301	Chlorobenzene-d5	9.07
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Propanoic acid, 2-methyl-, 1-methylethyl ester	130 C7H14O2	000617-50-5 83
2		Butanoic acid, 1-methylethyl ester	130 C7H14O2	000638-11-9 43
3		2,3-Hexanedione	114 C6H10O2	003848-24-6 42
4		Butanoic acid, pentyl ester	158 C9H18O2	000540-18-1 42
5		Propanoic acid, 2-methyl-, propyl ester	130 C7H14O2	000644-49-5 39

 Peak Number 4 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
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8.40	18.13 ug/l	788685	Chlorobenzene-d5	9.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
3	S-(-)-2-Methylbutylamine	87	C5H13N	020626-52-2	9
4	Isobutyl ether	130	C8H18O	000628-55-7	9
5	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7

Peak Number 5 Butanoic acid, 1-methylethy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.89	25.62 ug/l	1114120	Chlorobenzene-d5	9.07	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	94
2	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	64
3	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	64
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	56
5	Ethane-1,1-diol dibutanoate	202	C10H18O4	025572-25-2	50

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	6.68	57.2	ug/l	1920510	2	5.86	1677740	50.0
Propanoic acid, 1...	7.40	9.4	ug/l	316256	2	5.86	1677740	50.0
Propanoic acid, 2...	8.14	13.3	ug/l	578301	3	9.07	2174620	50.0
Propanoic acid, p...	8.40	18.1	ug/l	788685	3	9.07	2174620	50.0
Butanoic acid, 1-...	8.89	25.6	ug/l	1114120	3	9.07	2174620	50.0