

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110821\
 Data File : VU045645.D
 Acq On : 09 Nov 2021 03:26
 Operator : SY/MD
 Sample : M4541-01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 48 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 WC-3-AS

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\82U110521W.M
 Title : SW846 8260

Signal : TIC: VU045645.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.051	521	532	545	rVB2	16221	30417	1.06%	0.235%
2	5.292	1211	1229	1243	rBV	143118	299575	10.45%	2.318%
3	5.379	1243	1256	1275	rVB	216973	444132	15.49%	3.436%
4	5.703	1341	1357	1373	rBV	158206	317670	11.08%	2.458%
5	5.912	1409	1422	1440	rBV2	17642	35103	1.22%	0.272%
6	6.044	1448	1463	1465	rBV3	33276	73970	2.58%	0.572%
7	6.250	1515	1527	1575	rVB	358143	765588	26.71%	5.924%
8	6.925	1717	1737	1756	rBV3	15014	46852	1.63%	0.363%
9	7.041	1758	1773	1804	rBV	1133851	1971340	68.77%	15.253%
10	7.739	1973	1990	2001	rBV	182843	304231	10.61%	2.354%
11	7.899	2023	2040	2071	rBV	551775	966535	33.72%	7.478%
12	8.465	2204	2216	2231	rBV	46150	76316	2.66%	0.590%
13	8.575	2232	2250	2261	rVV	120162	199124	6.95%	1.541%
14	8.729	2282	2298	2320	rVV	1870968	2866744	100.00%	22.181%
15	8.835	2321	2331	2349	rVB	183201	288885	10.08%	2.235%
16	9.211	2434	2448	2483	rBV	1164568	1786343	62.31%	13.821%
17	9.420	2501	2513	2543	rVB	519319	860951	30.03%	6.661%
18	10.073	2705	2716	2732	rVB2	34577	52635	1.84%	0.407%
19	10.636	2878	2891	2911	rVB	417057	653009	22.78%	5.053%
20	11.812	3244	3257	3272	rBV	569030	885050	30.87%	6.848%

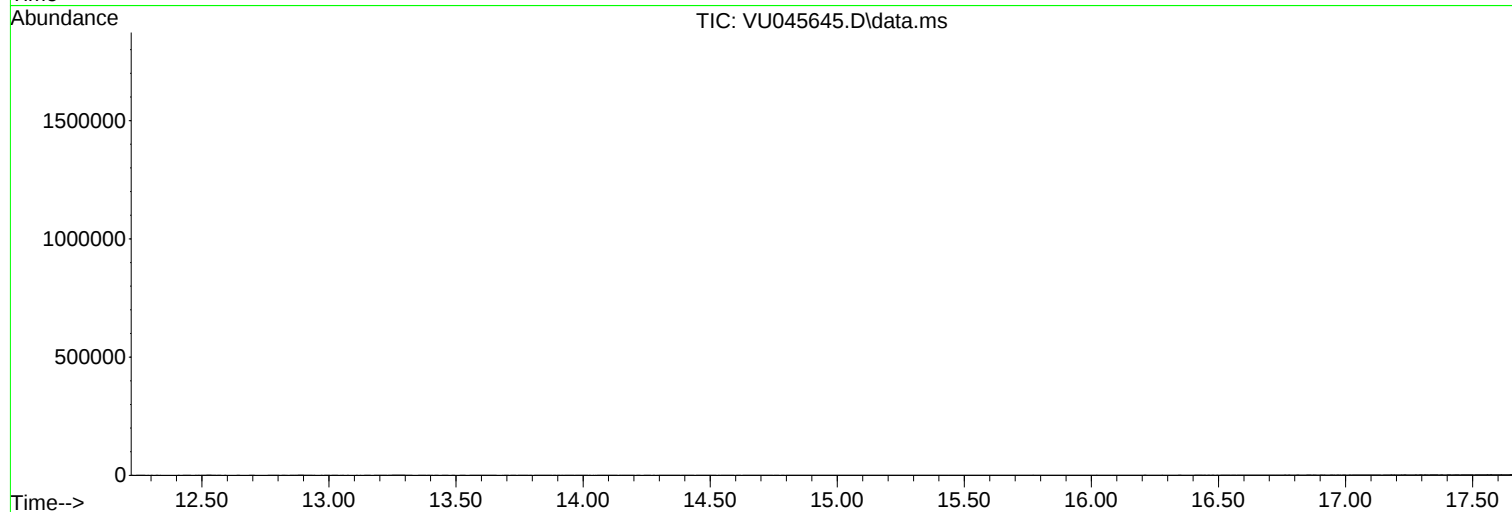
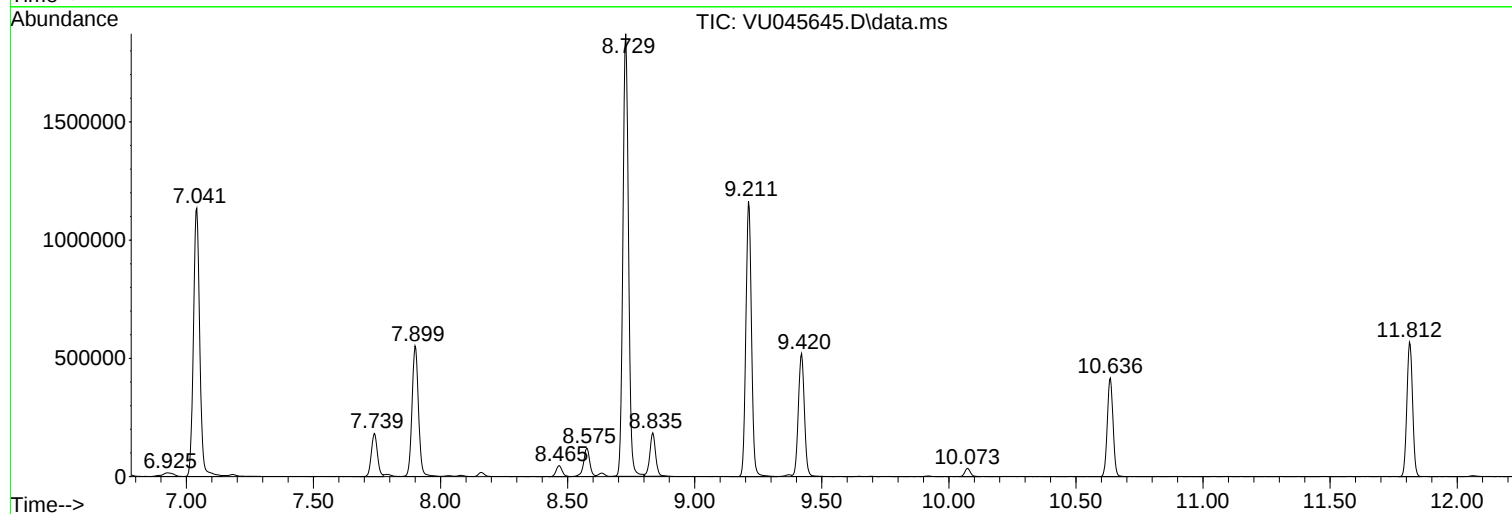
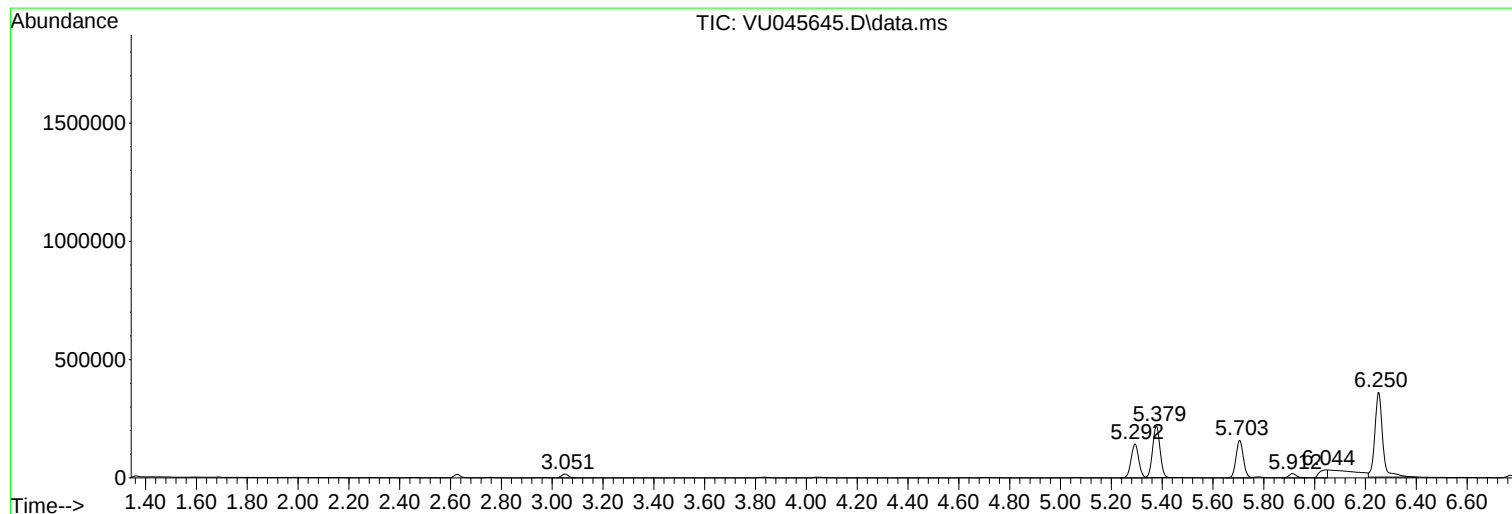
Sum of corrected areas: 12924470

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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U110521W.M
 Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
 TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Propyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.041	128.75 ug/l	1971340	1,4-Difluorobenzene	6.253

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	7
4			Isobutylamine	73	C4H11N	000078-81-9	4
5			5-Methyloxazolidine	87	C4H9NO	058328-22-6	4

Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.739	19.87 ug/l	304231	1,4-Difluorobenzene	6.253

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			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	25
4			Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	25
5			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	10

Peak Number 3 Butanoic acid, ethyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.575	11.56 ug/l	199124	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	94
2			3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	45
3			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	43
4			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	42
5			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	38

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.729	166.49 ug/l	2866740	Chlorobenzene-d5	9.420

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Hit#	of	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		2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
4		di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
5		1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7

Peak Number 5 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.835	16.78 ug/l	288885	Chlorobenzene-d5	9.420

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1		Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2		Isobutylamine	73	C4H11N	000078-81-9	9
3		Isobutyl acetate	116	C6H12O2	000110-19-0	9
4		Isopropyl acetate	102	C5H10O2	000108-21-4	9
5		Ethanol, 2-chloro-, acetate	122	C4H7ClO2	000542-58-5	9

Peak Number 6 Isopropyl butyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.211	103.74 ug/l	1786340	Chlorobenzene-d5	9.420

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1		Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
3		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
4		Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64
5		Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	50

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Propyl acetate	7.041	128.8	ug/l	1971340	2	6.253	765588	50.0
Propanoic acid,...	7.739	19.9	ug/l	304231	2	6.253	765588	50.0
Butanoic acid, ...	8.575	11.6	ug/l	199124	3	9.420	860951	50.0
Propanoic acid,...	8.729	166.5	ug/l	2866740	3	9.420	860951	50.0
Acetic acid, bu...	8.835	16.8	ug/l	288885	3	9.420	860951	50.0
Isopropyl butyrate	9.211	103.7	ug/l	1786340	3	9.420	860951	50.0