

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081522\
 Data File : VN073903.D
 Acq On : 15 Aug 2022 18:20
 Operator : JC\MD
 Sample : N4107-09
 Misc : 5.09g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 SOIL-STOCKPILE

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\82N081522W.M
 Title : SW846 8260

Signal : TIC: VN073903.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.693	129	137	138	rBV7	19608	38138	1.35%	0.226%
2	4.787	480	493	510	rBV2	25827	96208	3.40%	0.570%
3	5.216	553	566	578	rBV2	12426	51578	1.82%	0.306%
4	7.304	908	921	935	rBV	50253	150357	5.31%	0.891%
5	7.945	1018	1030	1035	rBV	369235	907715	32.05%	5.380%
6	8.004	1035	1040	1056	rVB	702684	1592164	56.22%	9.437%
7	8.363	1092	1101	1113	rBV	330394	756649	26.72%	4.485%
8	8.581	1131	1138	1146	rBV3	59585	203928	7.20%	1.209%
9	8.692	1147	1157	1183	rVV	170003	545991	19.28%	3.236%
10	8.898	1183	1192	1209	rVB	933323	1923981	67.93%	11.404%
11	9.186	1236	1241	1251	rVB	15611	35424	1.25%	0.210%
12	10.375	1435	1443	1452	rBV	1272638	2376659	83.92%	14.087%
13	10.445	1452	1455	1461	rVB3	25468	45613	1.61%	0.270%
14	11.128	1560	1571	1581	rBV5	14802	41105	1.45%	0.244%
15	11.686	1658	1666	1674	rBV	1392793	2449967	86.51%	14.522%
16	12.674	1827	1834	1843	rVB	1302083	2161718	76.33%	12.813%
17	13.616	1986	1994	2005	rBV	1717445	2832125	100.00%	16.787%
18	13.798	2016	2025	2027	rBV7	59535	137058	4.84%	0.812%
19	15.086	2236	2244	2255	rVB6	28445	94249	3.33%	0.559%
20	15.221	2258	2267	2277	rBV6	20785	77873	2.75%	0.462%
21	15.410	2288	2299	2315	rVB6	62643	310706	10.97%	1.842%
22	16.110	2413	2418	2432	rVB6	11469	42078	1.49%	0.249%

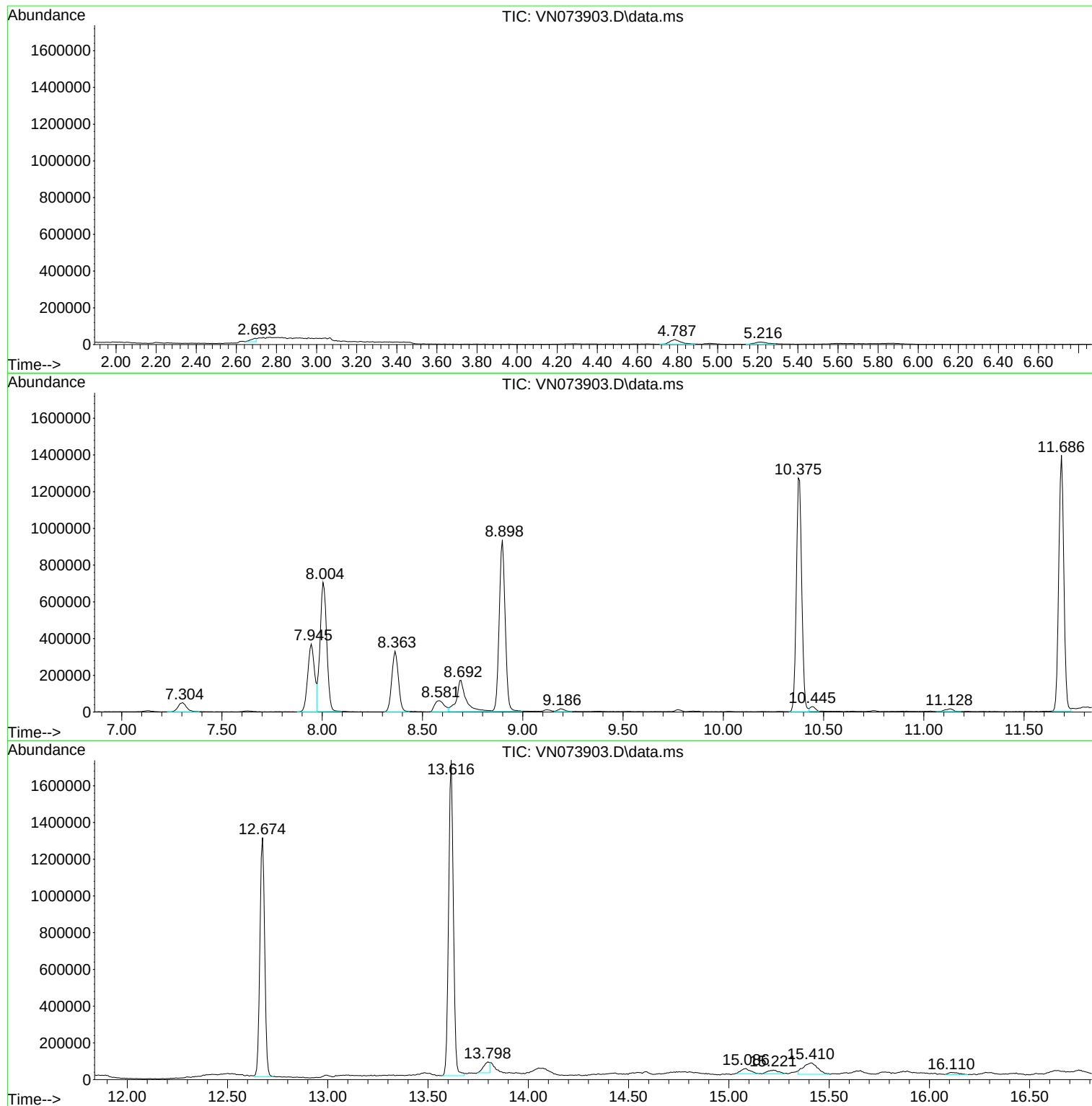
Sum of corrected areas: 16871284

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

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



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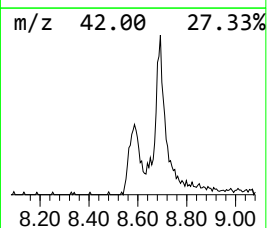
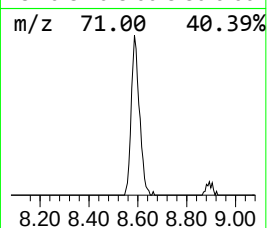
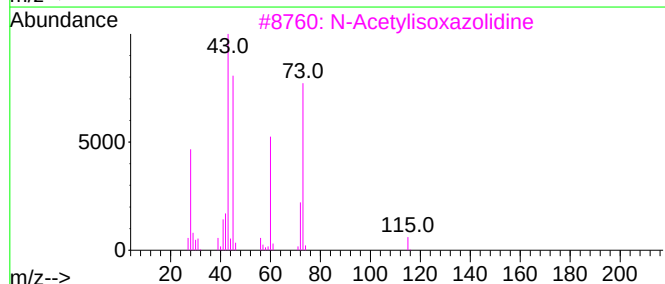
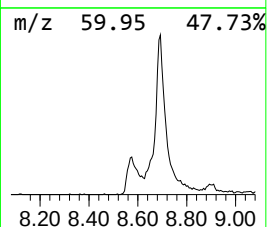
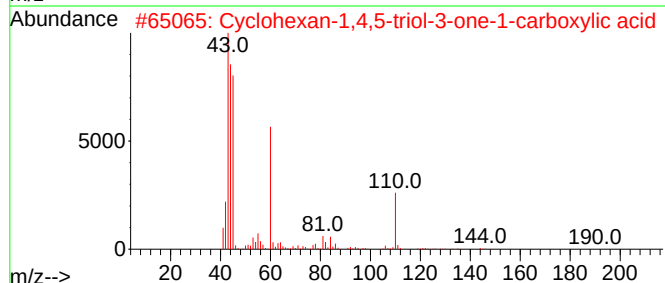
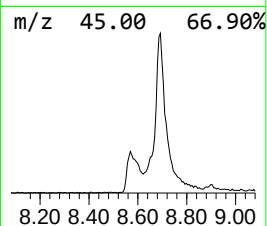
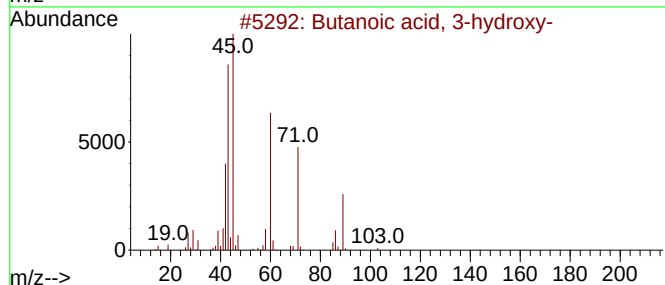
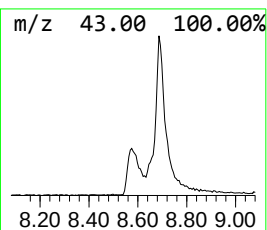
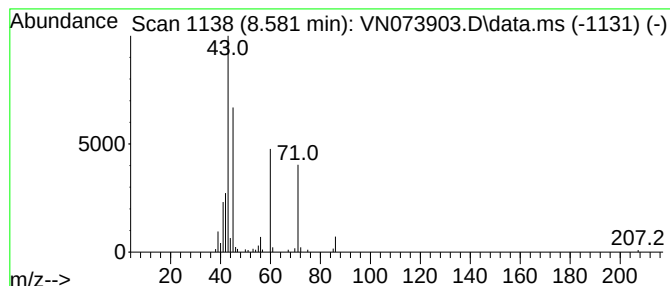
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N081522W.M
Quant Title : SW846 8260

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

Peak Number 1 Butanoic acid, 3-hydroxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.581	5.30 ug/l	203928	1,4-Difluorobenzene	8.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 3-hydroxy-	104	C4H8O3	000300-85-6	64
2			Cyclohexan-1,4,5-triol-3-one-1-c...	190	C7H10O6	1000128-45-5	53
3			N-Acetylisoaxazolidine	115	C5H9N02	115615-36-6	50
4			2,4-Pentanediol	104	C5H12O2	000625-69-4	50
5			Acetic acid	60	C2H4O2	000064-19-7	47



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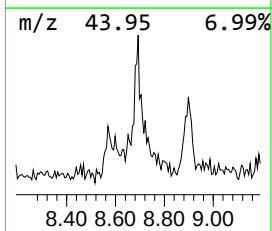
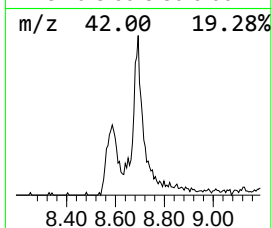
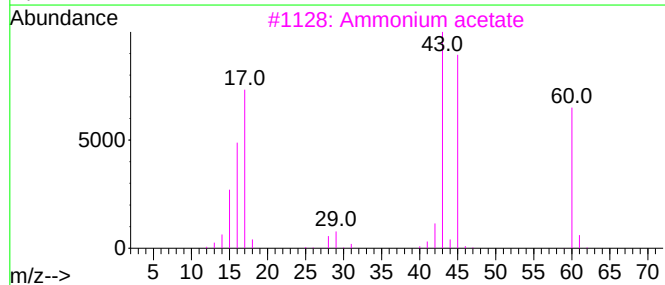
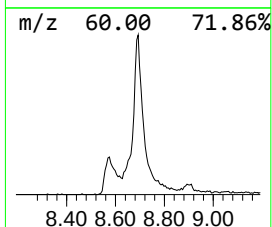
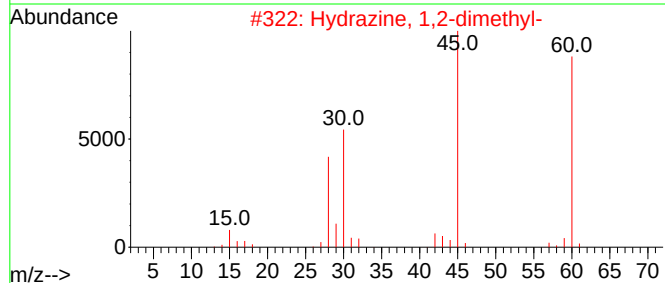
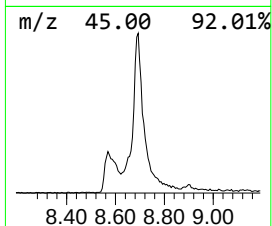
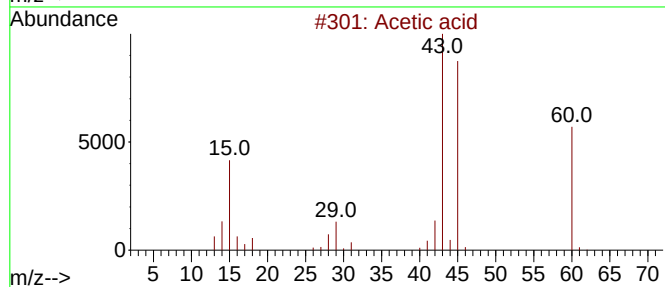
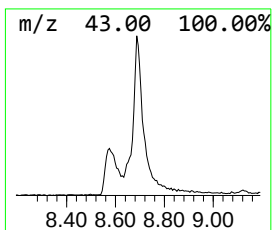
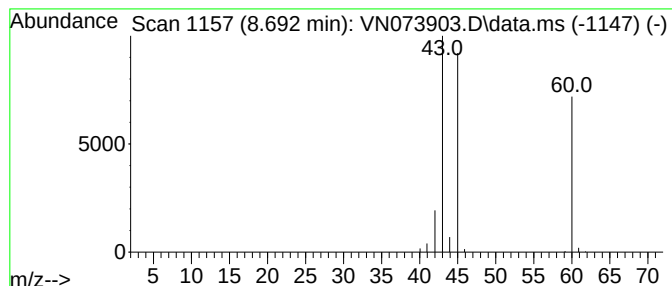
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Peak Number 2 Acetic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.692	14.19 ug/l	545991	1,4-Difluorobenzene	8.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid	60	C2H4O2	000064-19-7	90
2			Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	50
3			Ammonium acetate	77	C2H7NO2	000631-61-8	43
4			Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
5			Propanal, 3-methoxy-	88	C4H8O2	002806-84-0	9



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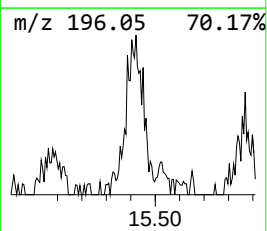
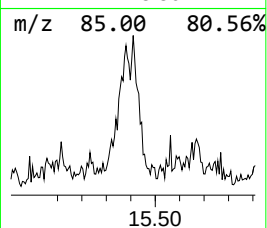
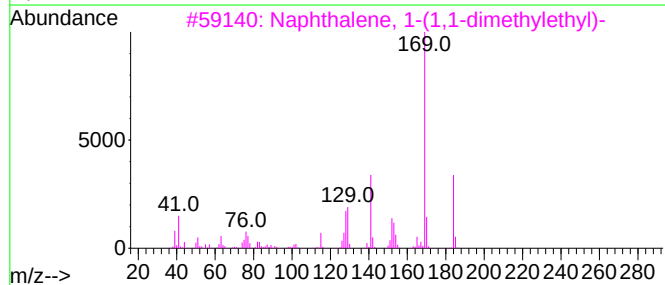
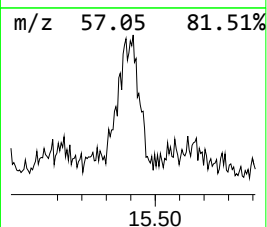
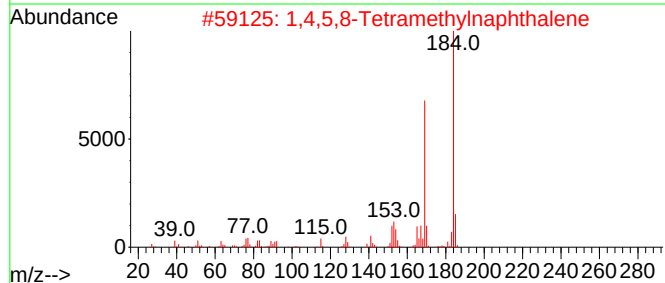
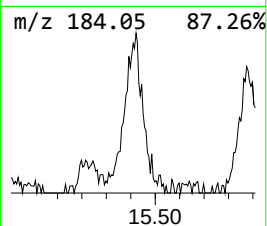
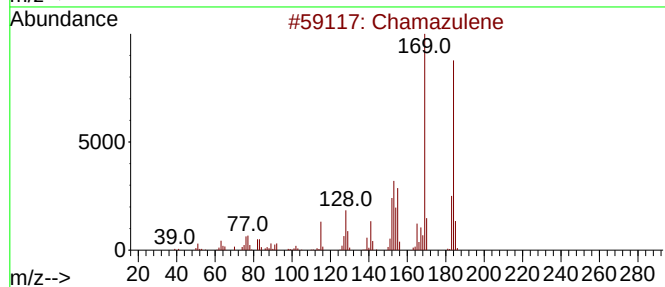
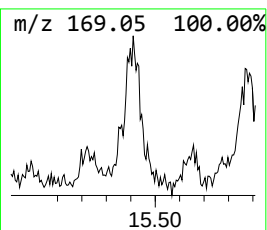
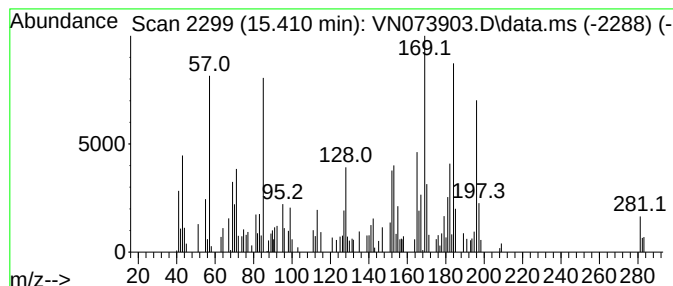
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Peak Number 3 unknown15.410 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.410	5.49 ug/l	310706	1,4-Dichlorobenzene-d4	13.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Chamazulene	184	C14H16	000529-05-5	35
2			1,4,5,8-Tetramethylnaphthalene	184	C14H16	002717-39-7	35
3			Naphthalene, 1-(1,1-dimethylethyl)-	184	C14H16	017085-91-5	30
4			2-Isopropyl-3-methylnaphthalene	184	C14H16	1000383-71-2	30
5			6'-Methyl-2'-acetophenone	184	C13H12O	024875-94-3	22



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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butanoic acid, ...	8.581	5.3	ug/l	203928	2	8.898	1923980	50.0
Acetic acid	8.692	14.2	ug/l	545991	2	8.898	1923980	50.0
unknown15.410	15.410	5.5	ug/l	310706	4	13.616	2832130	50.0