LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080723\
Data File : VX036843.D
Acq On : 07 Aug 2023 17:41
Operator : JC/MD
Sample : 03891-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-2

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_X\Method\82X072123W.M
Title : SW846 8260

Signal : TIC: VX036843.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.379	206	212	223	rBV	33532	57106	3.20%	0.537%
2	2.788	273	279	293	rBV	26344	53977	3.02%	0.508%
3	4.568	560	571	587	rBV2	11220	36063	2.02%	0.339%
4	5.385	695	705	720	rBV	89315	261987	14.68%	2.466%
5	5.550	722	732	749	rVB	142069	407627	22.84%	3.837%
6	5.958	789	799	816	rBV	96228	255363	14.31%	2.403%
7	6.342	853	862	878	rBV	91690	234709	13.15%	2.209%
8	6.763	922	931	943	rBV	240116	567240	31.78%	5.339%
9	7.641	1064	1075	1080	rBV	57354	104522	5.86%	0.984%
10	7.696	1080	1084	1093	rVB	17305	31585	1.77%	0.297%
11	7.799	1093	1101	1115	rBV	1044553	1784908	100.00%	16.799%
12	8.549	1218	1224	1234	rBV2	285947	559259	31.33%	5.264%
13	8.647	1234	1240	1249	rBV	476482	770571	43.17%	7.253%
14	8.951	1285	1290	1301	rBV	239211	350139	19.62%	3.295%
15	9.244	1332	1338	1344	rBV	375391	516093	28.91%	4.857%
16	9.311	1344	1349	1351	rVV	35022	49841	2.79%	0.469%
17	9.348	1351	1355	1356	rVV	43807	57504	3.22%	0.541%
18	9.378	1356	1360	1367	rVB	155285	223412	12.52%	2.103%
19	9.482	1372	1377	1383	rBV	519125	659637	36.96%	6.208%
20	9.579	1388	1393	1409	rVB	273373	346649	19.42%	3.263%
21	9.915	1442	1448	1460	rBV	1020047	1296230	72.62%	12.200%
22	10.055	1462	1471	1477	rBV	514466	714656	40.04%	6.726%
23	10.506	1540	1545	1551	rVB	18187	23202	1.30%	0.218%
24	10.640	1562	1567	1572	rBV	55857	65658	3.68%	0.618%
25	11.079	1634	1639	1652	rBV	405614	527715	29.57%	4.967%
26	11.555	1712	1717	1722	rBV	14170	18233	1.02%	0.172%
27	12.024	1788	1794	1804	rBV	490239	627943	35.18%	5.910%
28	12.219	1821	1826	1836	rBV	13931	22954	1.29%	0.216%

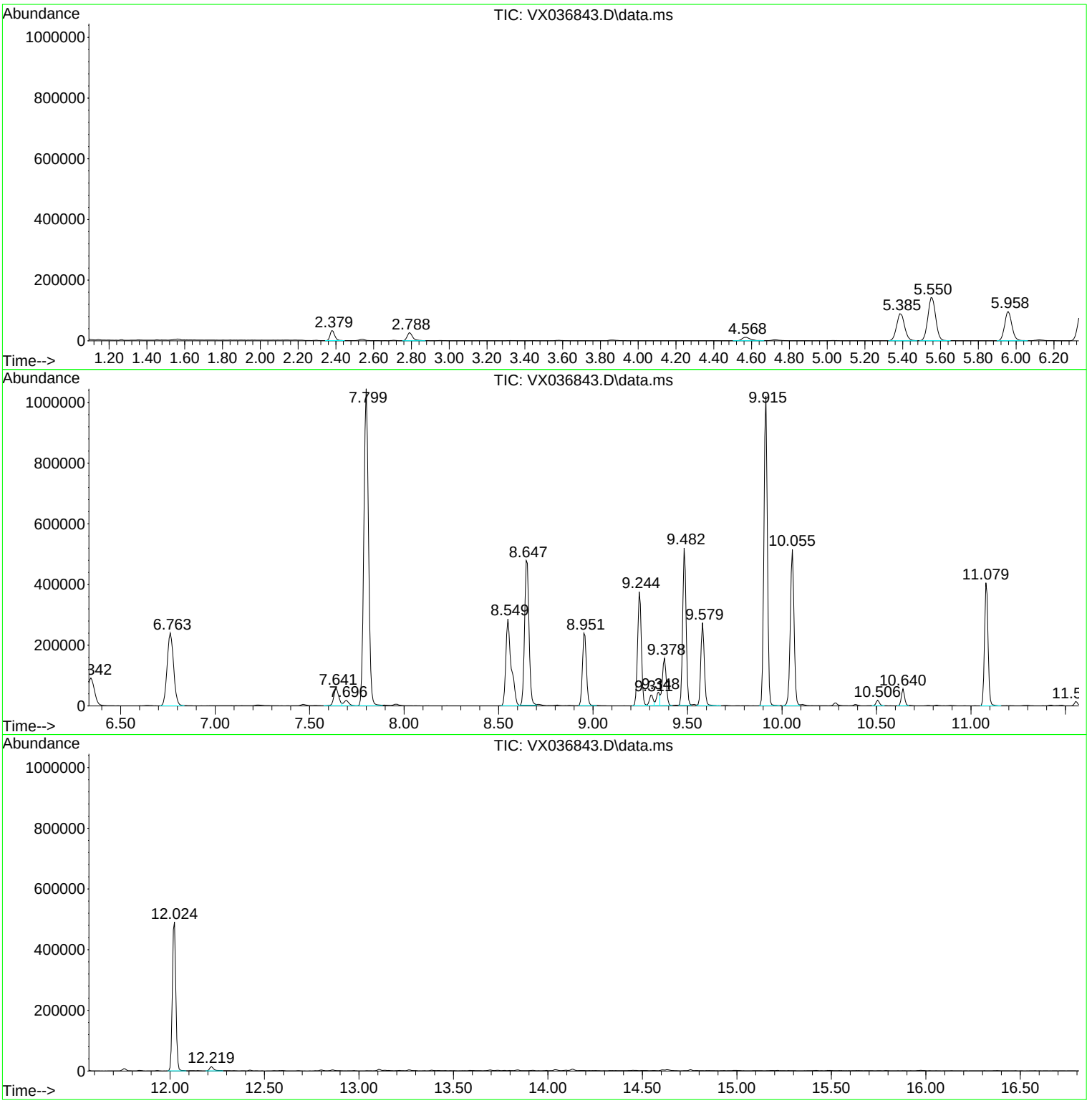
Sum of corrected areas: 10624783

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080723\
Data File : VX036843.D
Acq On : 07 Aug 2023 17:41
Operator : JC/MD
Sample : 03891-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080723\
Data File : VX036843.D
Acq On : 07 Aug 2023 17:41
Operator : JC/MD
Sample : 03891-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-2

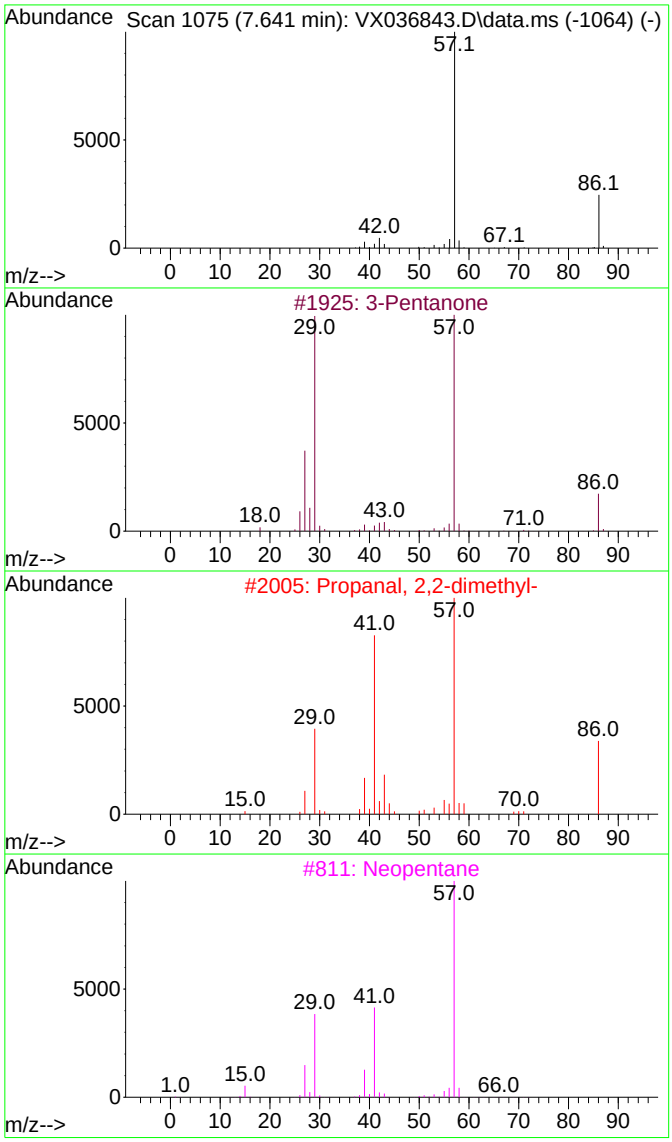
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

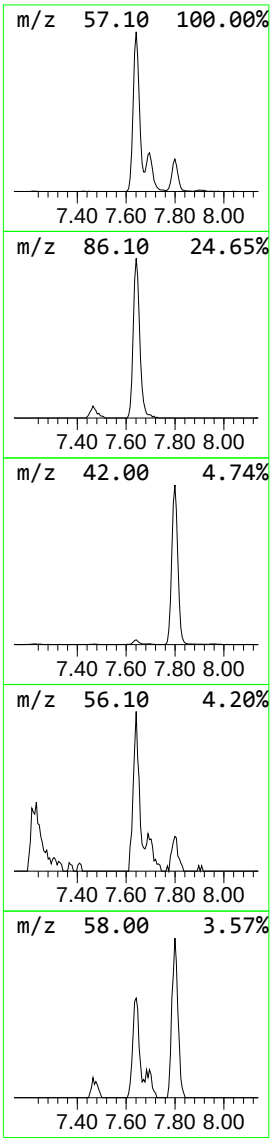
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 3-Pentanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.641	9.21 ug/l	104522	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	90
2	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	39
3	Neopentane	72	C5H12	000463-82-1	9
4	Azetidine, 1-nitroso-	86	C3H6N2O	015216-10-1	7
5	Ethyl-1-propenyl ether	86	C5H10O	000928-55-2	7





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080723\
Data File : VX036843.D
Acq On : 07 Aug 2023 17:41
Operator : JC/MD
Sample : 03891-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-2

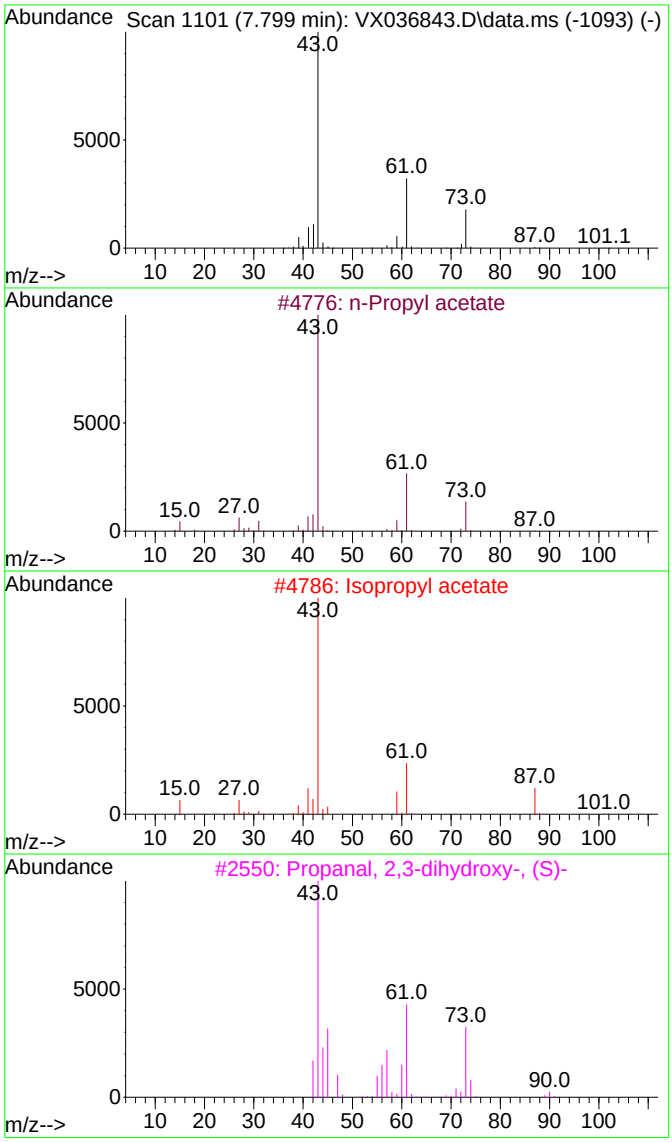
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

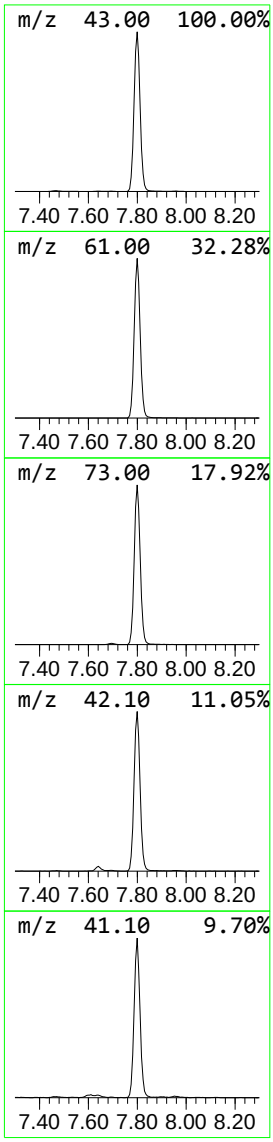
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.799	157.33 ug/l	1784910	1,4-Difluorobenzene	6.763

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	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	36
4	Isobutyl acetate	116	C6H12O2	000110-19-0	9
5	1-Butanamine	73	C4H11N	000109-73-9	7





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080723\
Data File : VX036843.D
Acq On : 07 Aug 2023 17:41
Operator : JC/MD
Sample : 03891-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-2

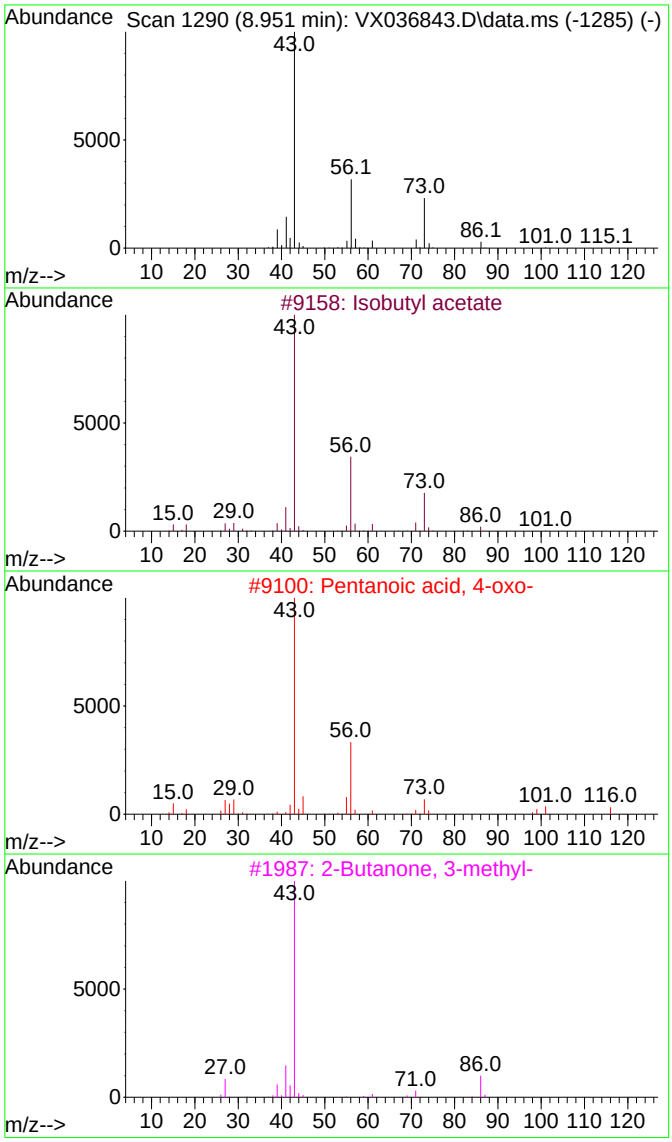
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

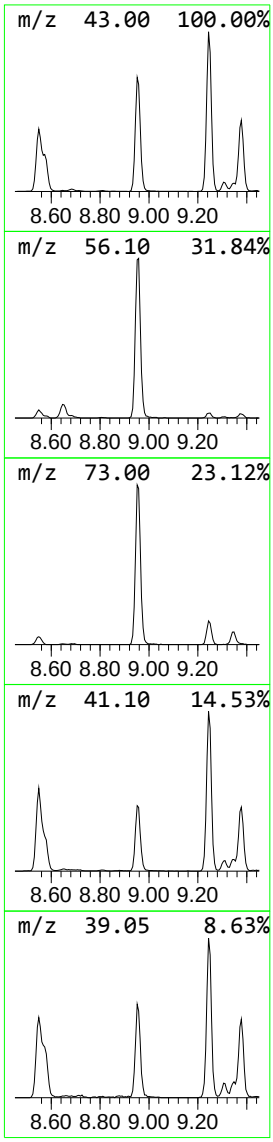
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Isobutyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.951	24.50 ug/l	350139	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl acetate	116	C6H12O2	000110-19-0	78
2	Pentanoic acid, 4-oxo-	116	C5H8O3	000123-76-2	38
3	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	9
5	Propane, 1-isocyanato-2-methyl-	99	C5H9NO	001873-29-6	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080723\
Data File : VX036843.D
Acq On : 07 Aug 2023 17:41
Operator : JC/MD
Sample : 03891-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-2

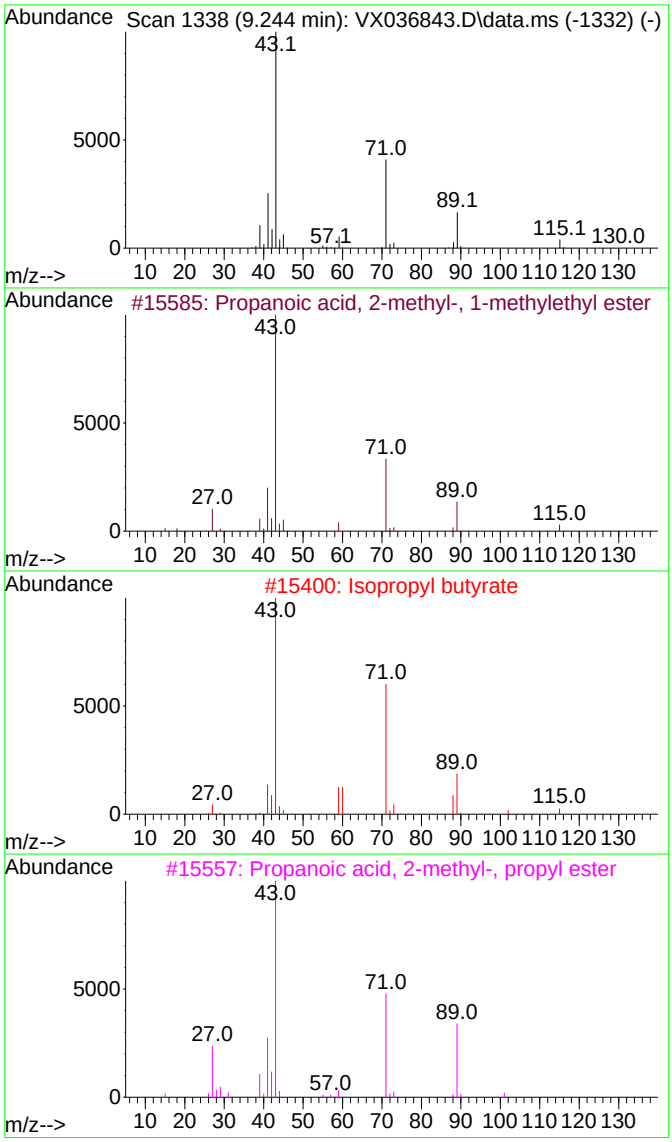
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

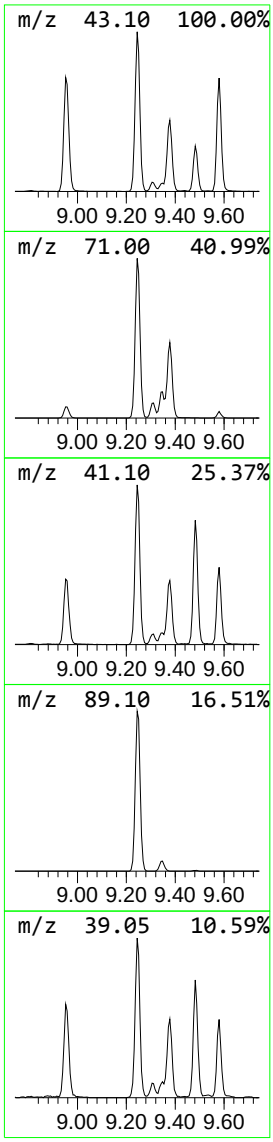
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.244	36.11 ug/l	516093	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2	Isopropyl butyrate	130	C7H14O2	000638-11-9	72
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4	2,3-Hexanedione	114	C6H10O2	003848-24-6	53
5	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	42





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080723\
Data File : VX036843.D
Acq On : 07 Aug 2023 17:41
Operator : JC/MD
Sample : 03891-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-2

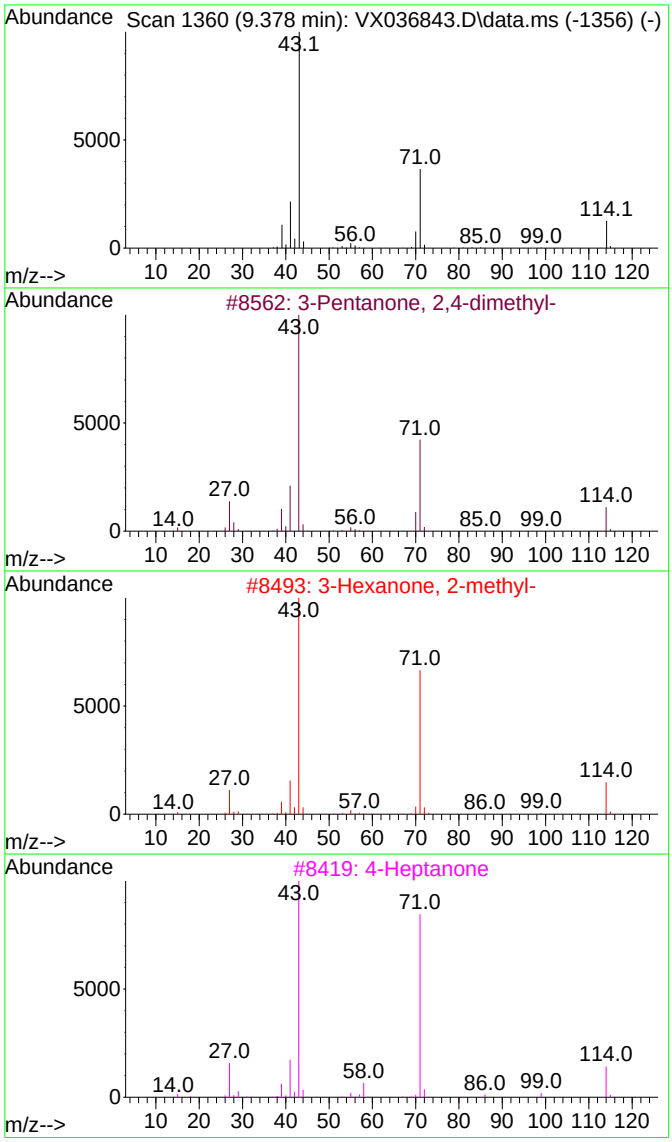
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

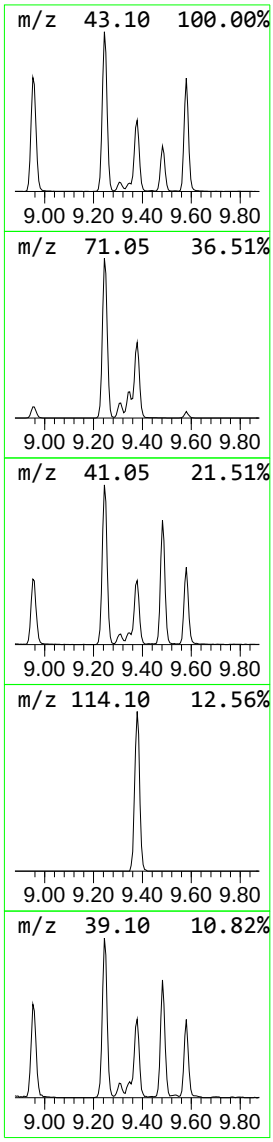
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 3-Pentanone, 2,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.378	15.63 ug/l	223412	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	80
2	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	78
3	4-Heptanone	114	C7H14O	000123-19-3	72
4	3,4-Dimethyl-2-pentanone	114	C7H14O	1000202-23-1	50
5	2,3-Hexanedione	114	C6H10O2	003848-24-6	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080723\
Data File : VX036843.D
Acq On : 07 Aug 2023 17:41
Operator : JC/MD
Sample : 03891-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-2

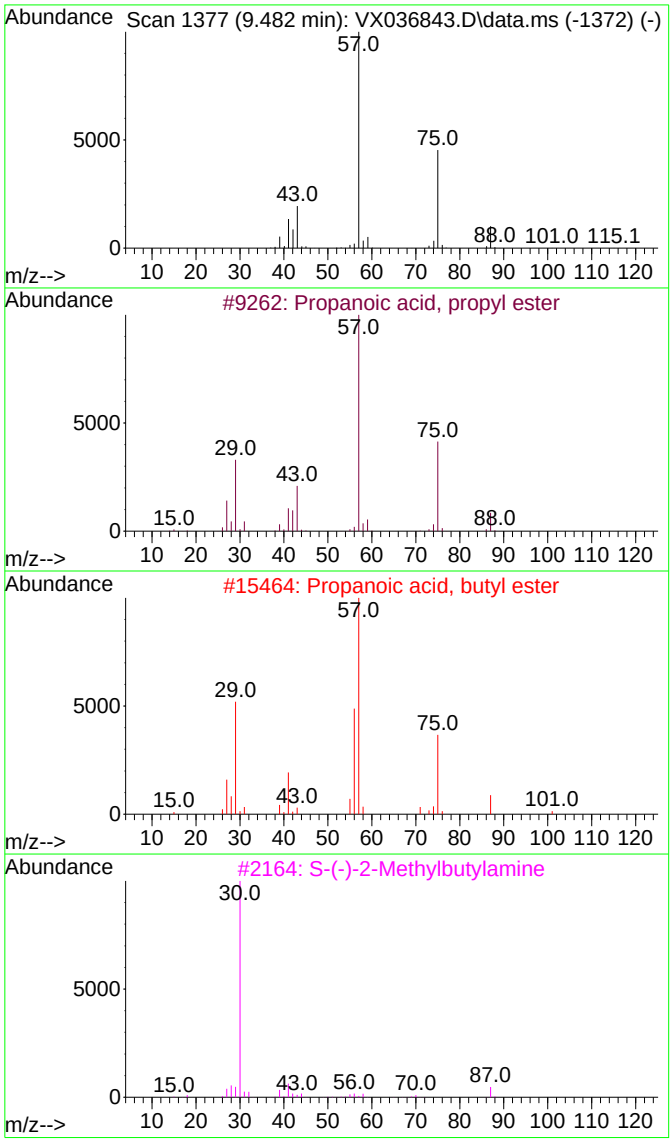
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

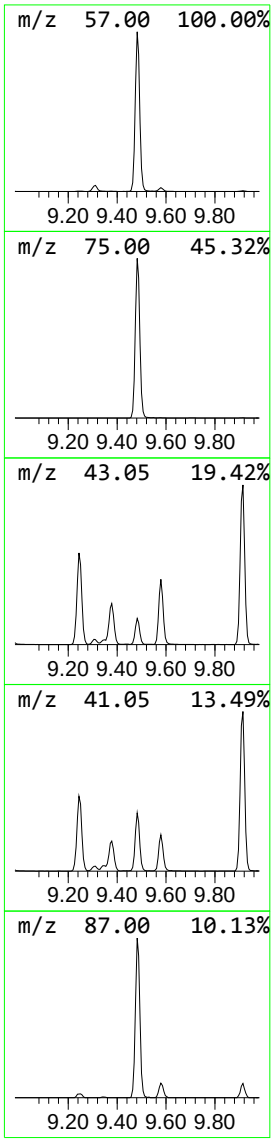
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.482	46.15 ug/l	659637	Chlorobenzene-d5	10.055

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	40
3	S-(-)-2-Methylbutylamine	87	C5H13N	020626-52-2	9
4	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
5	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080723\
Data File : VX036843.D
Acq On : 07 Aug 2023 17:41
Operator : JC/MD
Sample : 03891-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-2

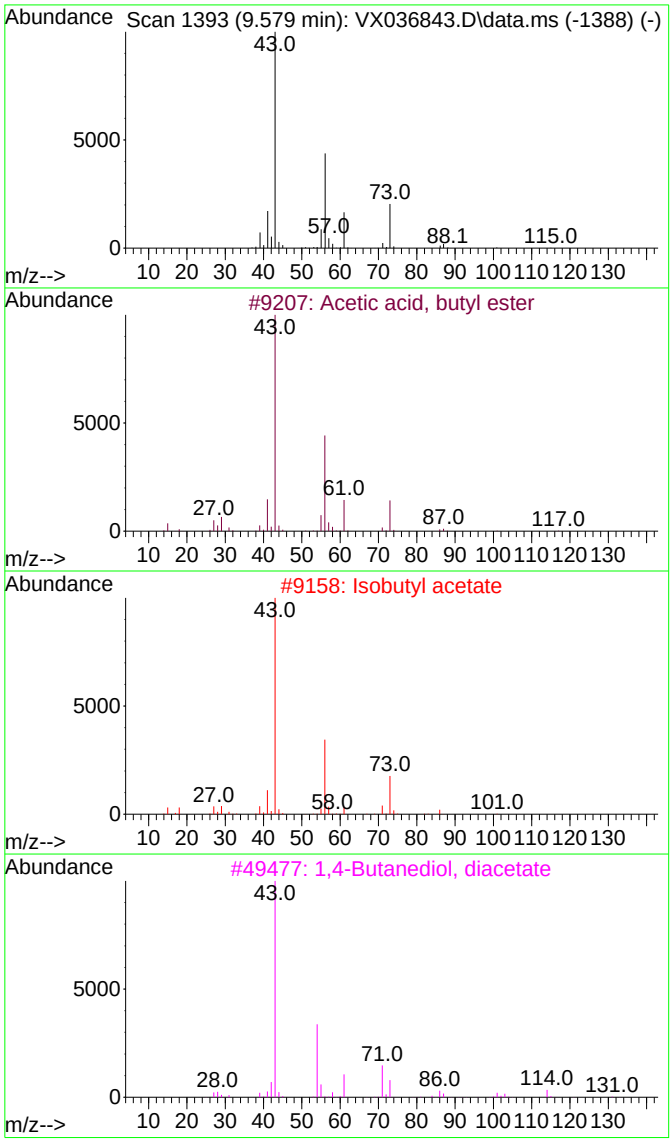
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

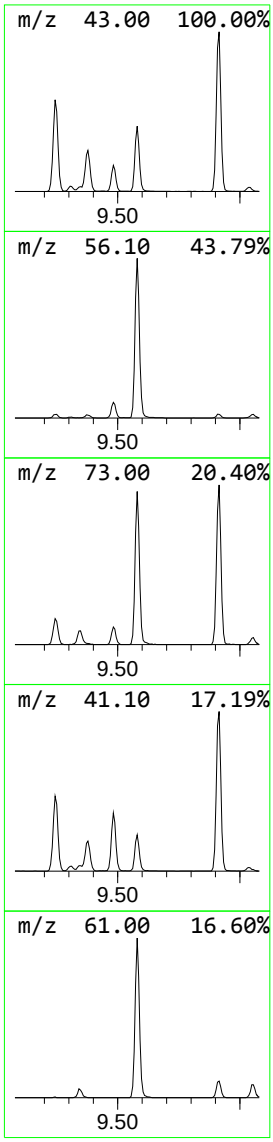
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.579	24.25 ug/l	346649	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2	Isobutyl acetate	116	C6H12O2	000110-19-0	40
3	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	12
4	Isobutylamine	73	C4H11N	000078-81-9	9
5	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080723\
Data File : VX036843.D
Acq On : 07 Aug 2023 17:41
Operator : JC/MD
Sample : 03891-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-2

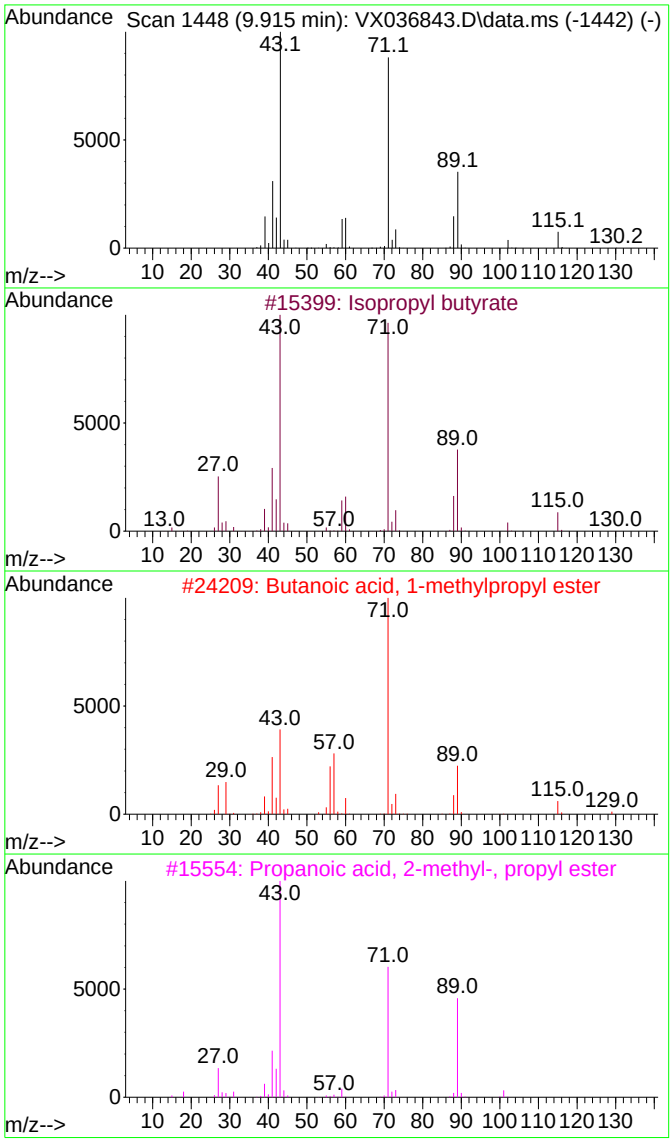
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

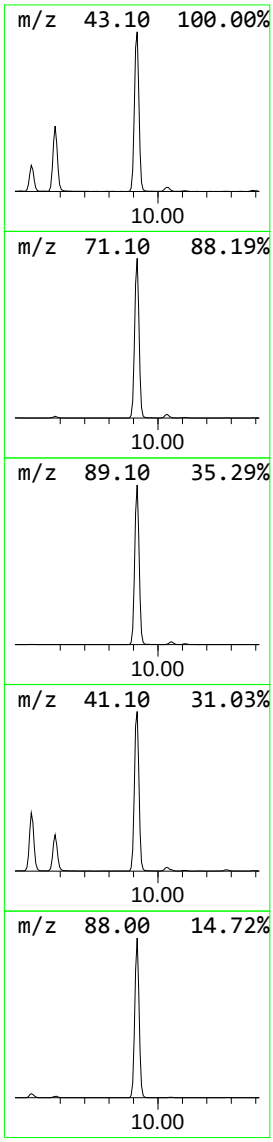
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	90.69 ug/l	1296230	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2	Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	72
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
5	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080723\
Data File : VX036843.D
Acq On : 07 Aug 2023 17:41
Operator : JC/MD
Sample : 03891-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Pentanone	7.641	9.2	ug/l	104522	2	6.763	567240	50.0
n-Propyl acetate	7.799	157.3	ug/l	1784910	2	6.763	567240	50.0
Isobutyl acetate	8.951	24.5	ug/l	350139	3	10.055	714656	50.0
Propanoic acid,...	9.244	36.1	ug/l	516093	3	10.055	714656	50.0
3-Pentanone, 2,...	9.378	15.6	ug/l	223412	3	10.055	714656	50.0
Propanoic acid,...	9.482	46.1	ug/l	659637	3	10.055	714656	50.0
Acetic acid, bu...	9.579	24.3	ug/l	346649	3	10.055	714656	50.0
Isopropyl butyrate	9.915	90.7	ug/l	1296230	3	10.055	714656	50.0