LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011323\
Data File : VN076241.D
Acq On : 13 Jan 2023 12:14
Operator : JC\MD
Sample : PB150223TB
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PB150223TB

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\82N121422W.M
Title : SW846 8260

Signal : TIC: VN076241.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.442	398	406	421	rBV2	24870	81804	2.40%	0.339%
2	6.477	742	752	762	rBV4	13258	43391	1.27%	0.180%
3	7.577	931	939	950	rVB2	24733	62851	1.84%	0.260%
4	8.177	1031	1041	1045	rBV	284604	674319	19.76%	2.793%
5	8.235	1045	1051	1067	rVB	534933	1198623	35.12%	4.965%
6	8.588	1097	1111	1121	rBV	279204	636500	18.65%	2.637%
7	8.694	1121	1129	1143	rBV	182062	412921	12.10%	1.711%
8	9.106	1189	1199	1210	rBV	732014	1492579	43.73%	6.183%
9	9.677	1288	1296	1301	rBV2	93816	196375	5.75%	0.813%
10	9.747	1301	1308	1327	rVV	1886422	3413242	100.00%	14.139%
11	10.359	1405	1412	1421	rBV	429121	760967	22.29%	3.152%
12	10.447	1421	1427	1438	rVB3	19318	49583	1.45%	0.205%
13	10.571	1440	1448	1458	rBV	1116085	2034874	59.62%	8.429%
14	10.729	1468	1475	1486	rVB	541258	918052	26.90%	3.803%
15	10.988	1511	1519	1529	rBV	657488	1099703	32.22%	4.556%
16	11.082	1529	1535	1543	rVV2	120419	225930	6.62%	0.936%
17	11.206	1543	1556	1564	rVV2	974886	1958515	57.38%	8.113%
18	11.294	1564	1571	1584	rVB	601292	1003325	29.40%	4.156%
19	11.606	1616	1624	1638	rBV	2014089	3215253	94.20%	13.319%
20	11.770	1647	1652	1660	rVB3	29424	52693	1.54%	0.218%
21	11.870	1660	1669	1680	rVV	952386	1712756	50.18%	7.095%
22	11.965	1680	1685	1693	rVB2	25299	44077	1.29%	0.183%
23	12.212	1720	1727	1735	rBV3	22644	38910	1.14%	0.161%
24	12.306	1735	1743	1753	rBV	161841	267917	7.85%	1.110%
25	12.853	1827	1836	1846	rBV	707215	1207417	35.37%	5.002%
26	13.794	1989	1996	2005	rVB	796208	1337403	39.18%	5.540%

Sum of corrected areas: 24139980

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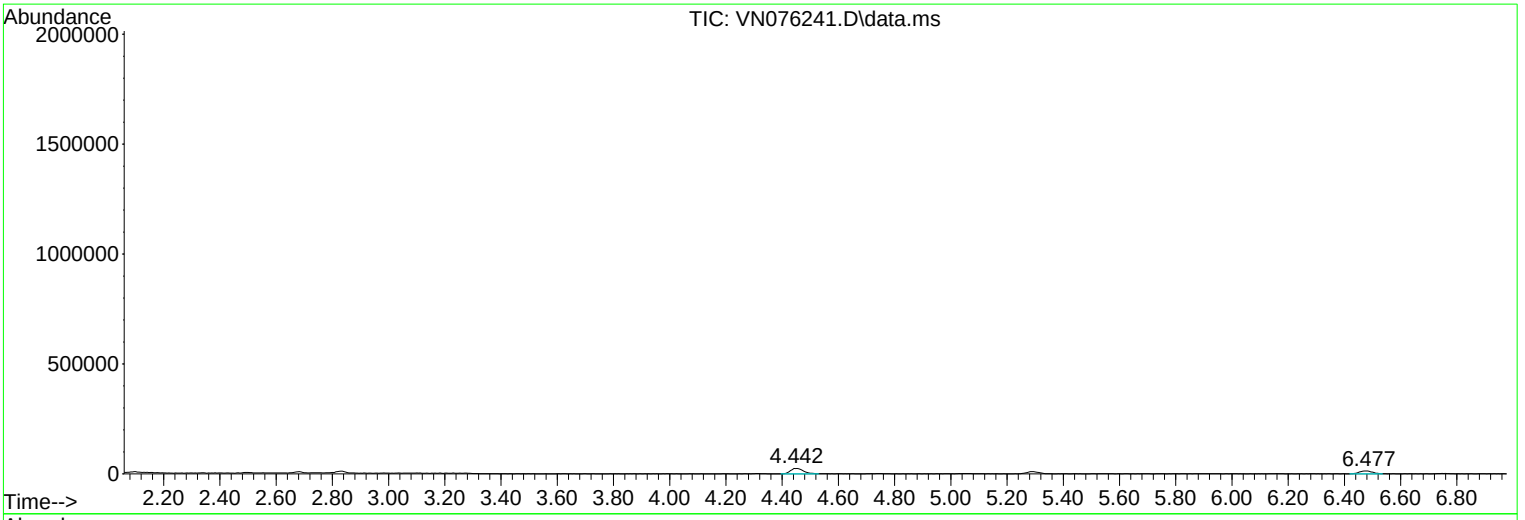
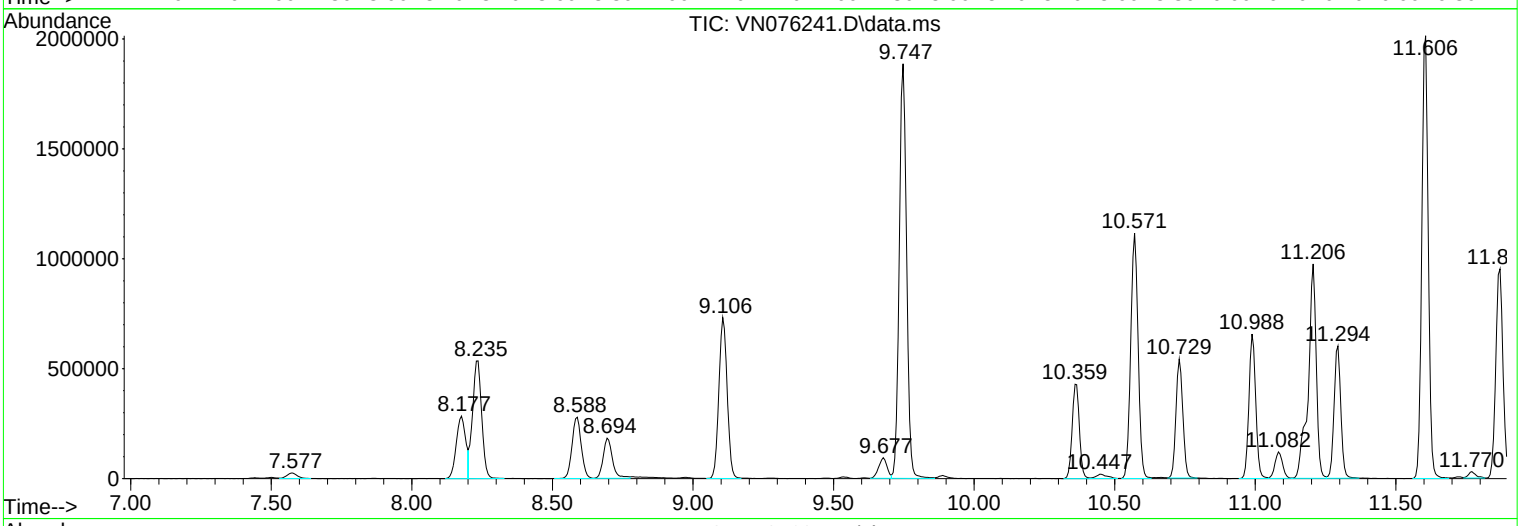
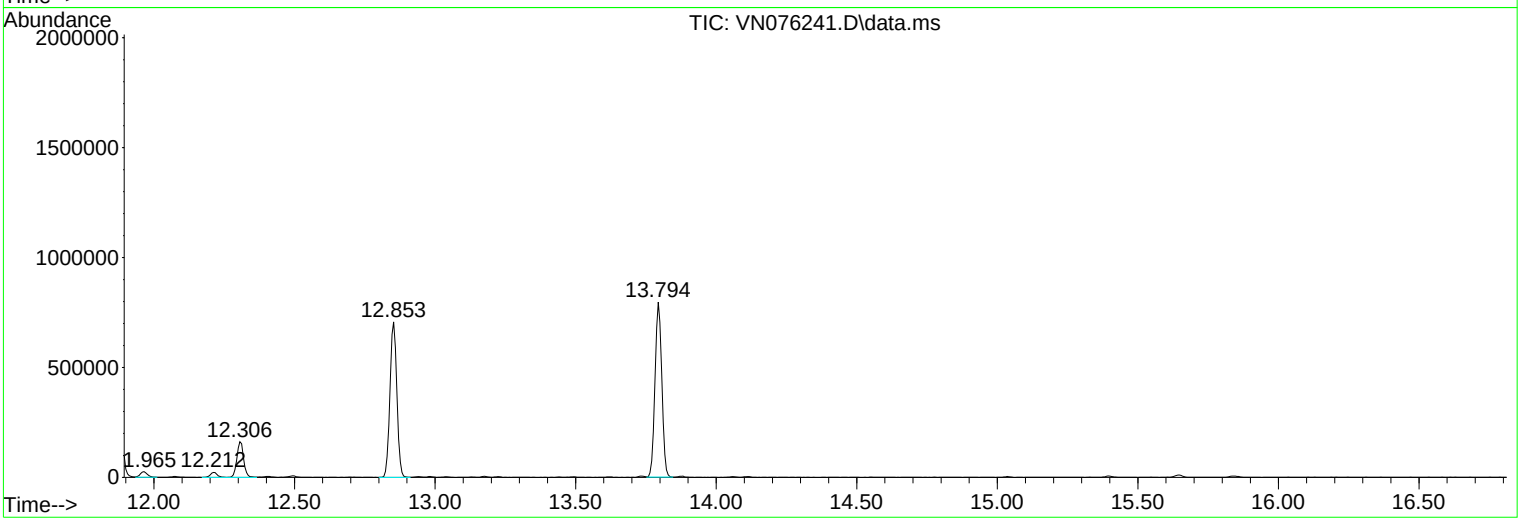
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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







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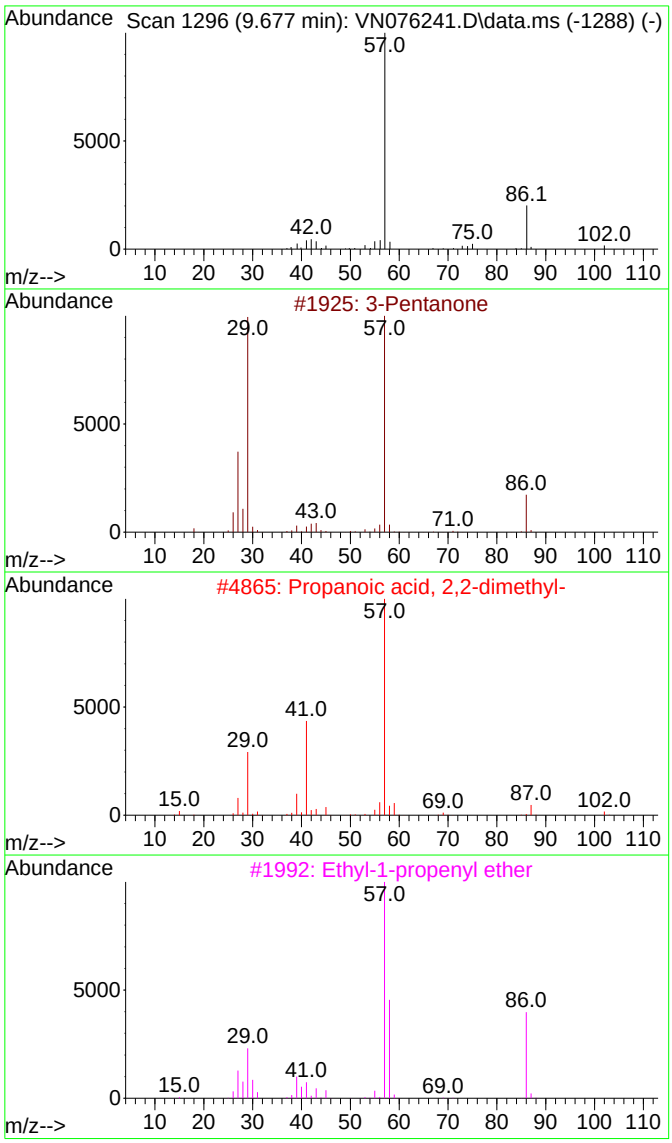
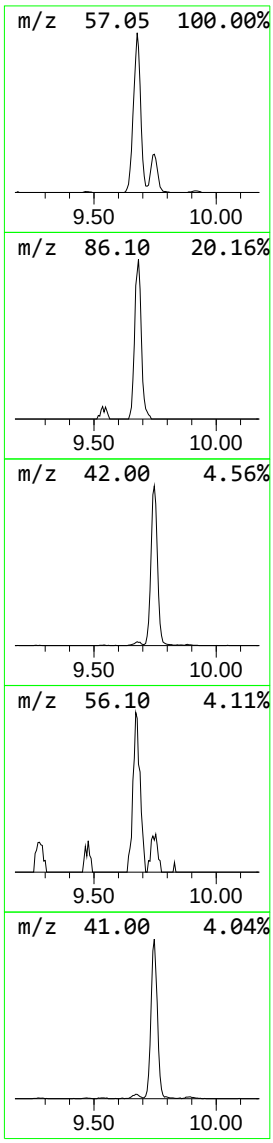
****
Peak Number 1 3-Pentanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.677	6.58 ug/l	196375	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	80
2	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	23
3	Ethyl-1-propenyl ether	86	C5H10O	000928-55-2	9
4	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	9
5	Butanoic acid, 2-oxo-	102	C4H6O3	000600-18-0	9





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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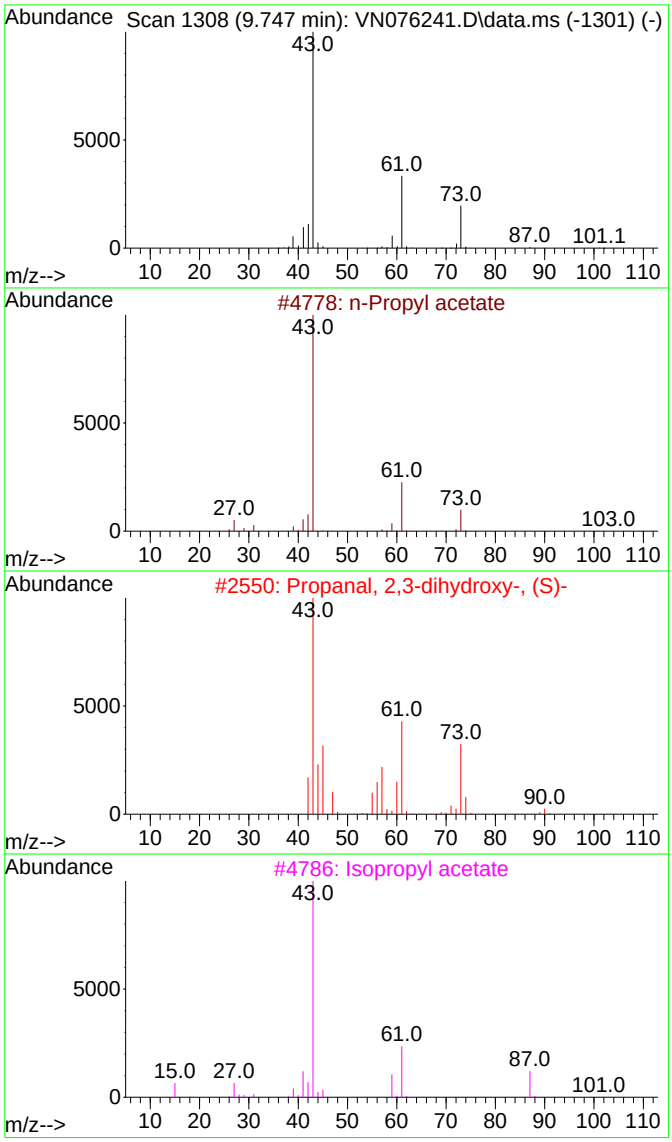
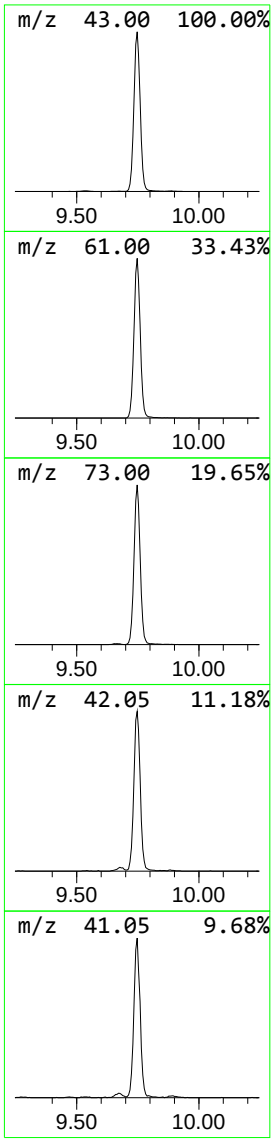
****

Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.747	114.34 ug/l	3413240	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	38
3	Isopropyl acetate	102	C5H10O2	000108-21-4	33
4	Isobutyl acetate	116	C6H12O2	000110-19-0	9
5	Acetamide, N-acetyl-N-methyl-	115	C5H9NO2	001113-68-4	9





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MSVOA_N
ClientSampleId :
PB150223TB

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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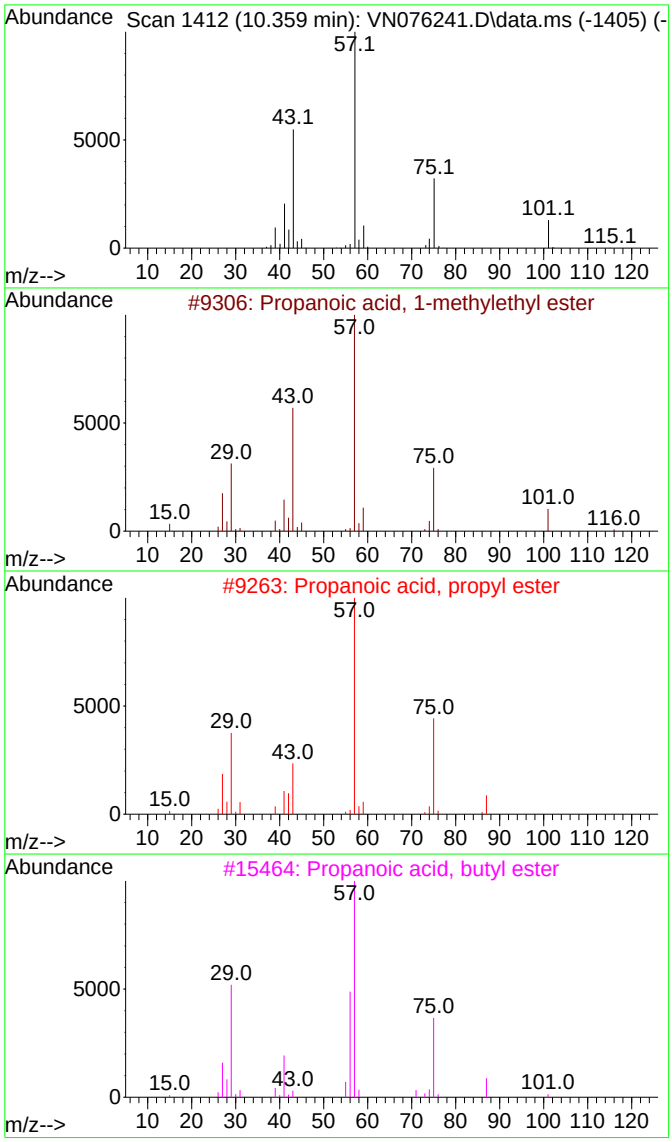
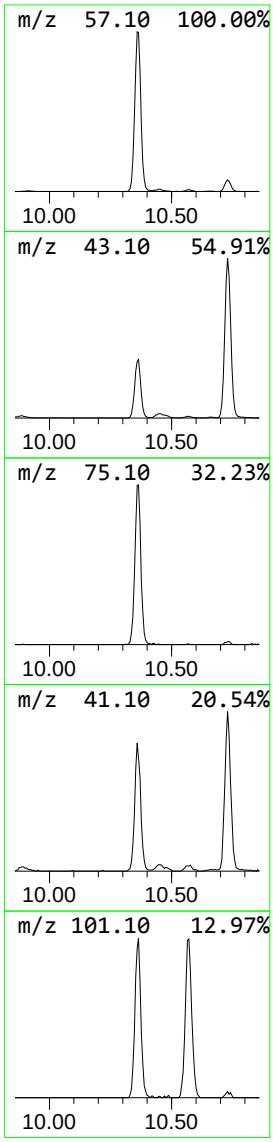
****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.359	25.49 ug/l	760967	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
2	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	53
3	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	9





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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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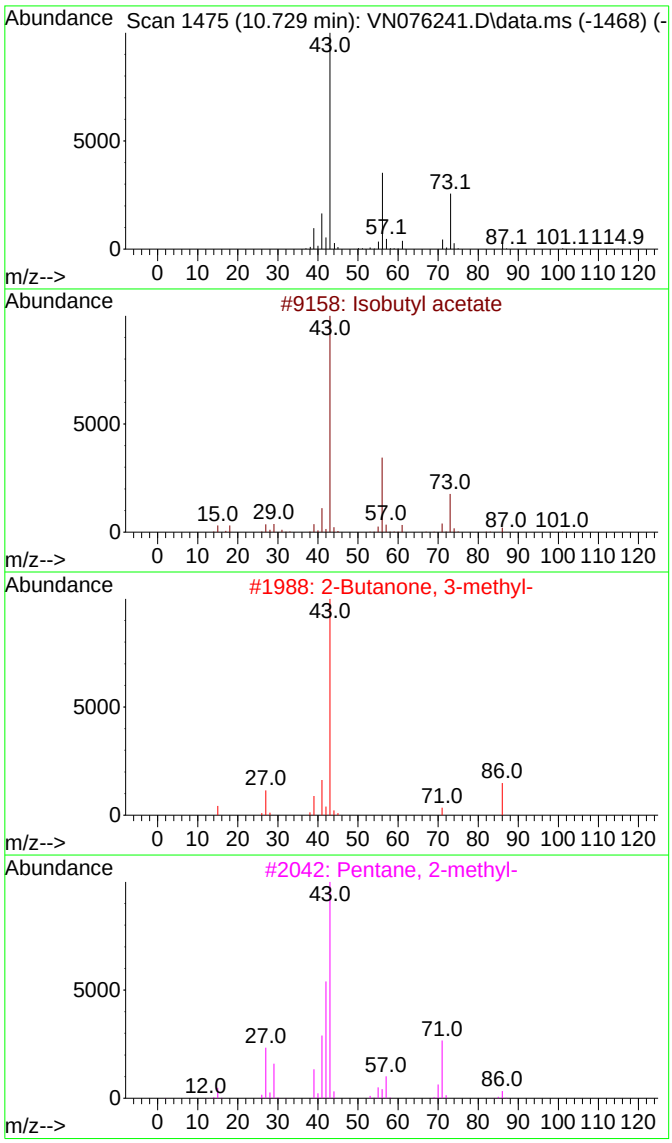
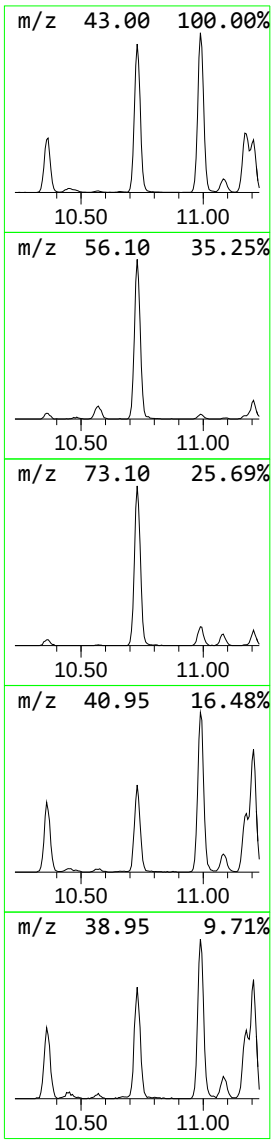
****

Peak Number 4 Isobutyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.729	26.80 ug/l	918052	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl acetate	116	C6H12O2	000110-19-0	83
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	22
3	Pentane, 2-methyl-	86	C6H14	000107-83-5	9
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	9
5	3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	9





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ALS Vial : 7 Sample Multiplier: 1

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MSVOA_N
ClientSampleId :
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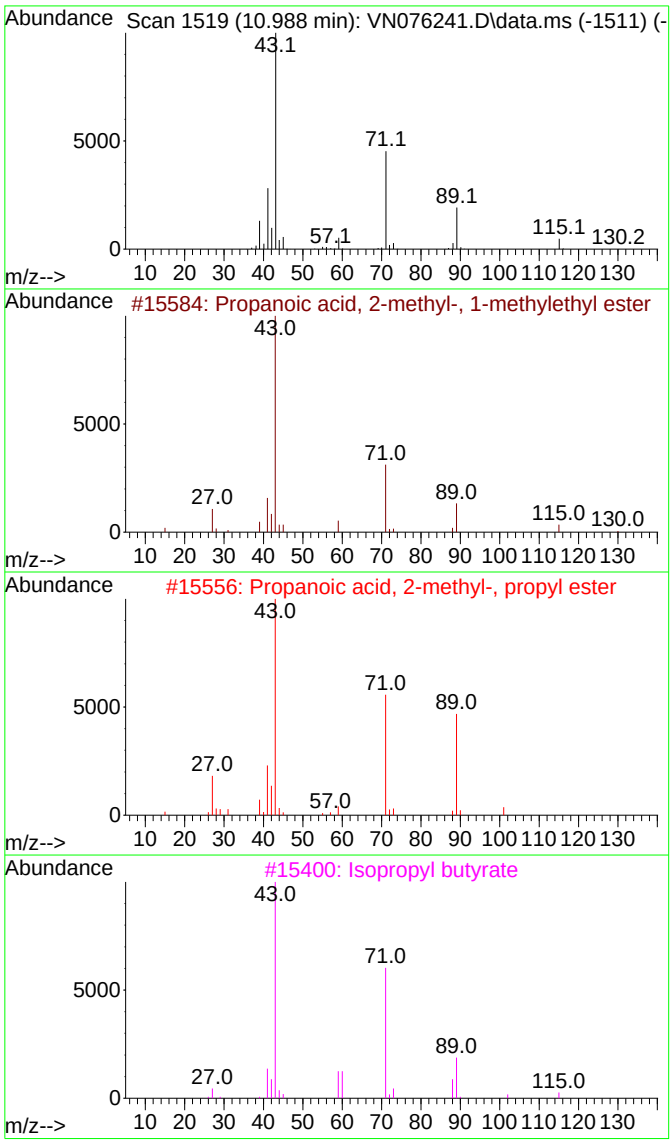
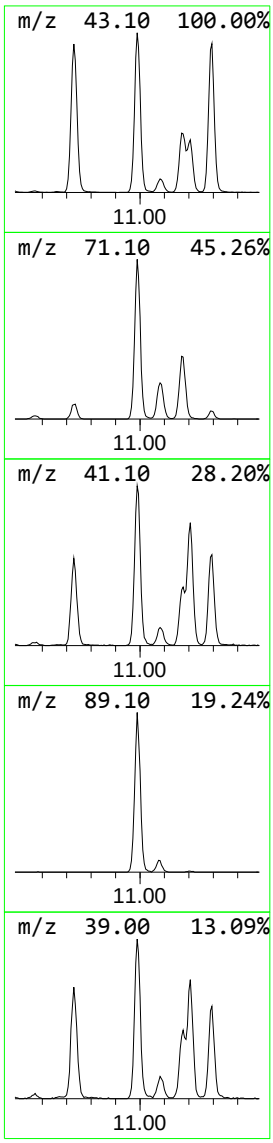
****
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.988	32.10 ug/l	1099700	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	90
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	64
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	45
5	Propanoic acid, 2-methyl-, 2-met...	172	C10H20O2	084254-82-0	40





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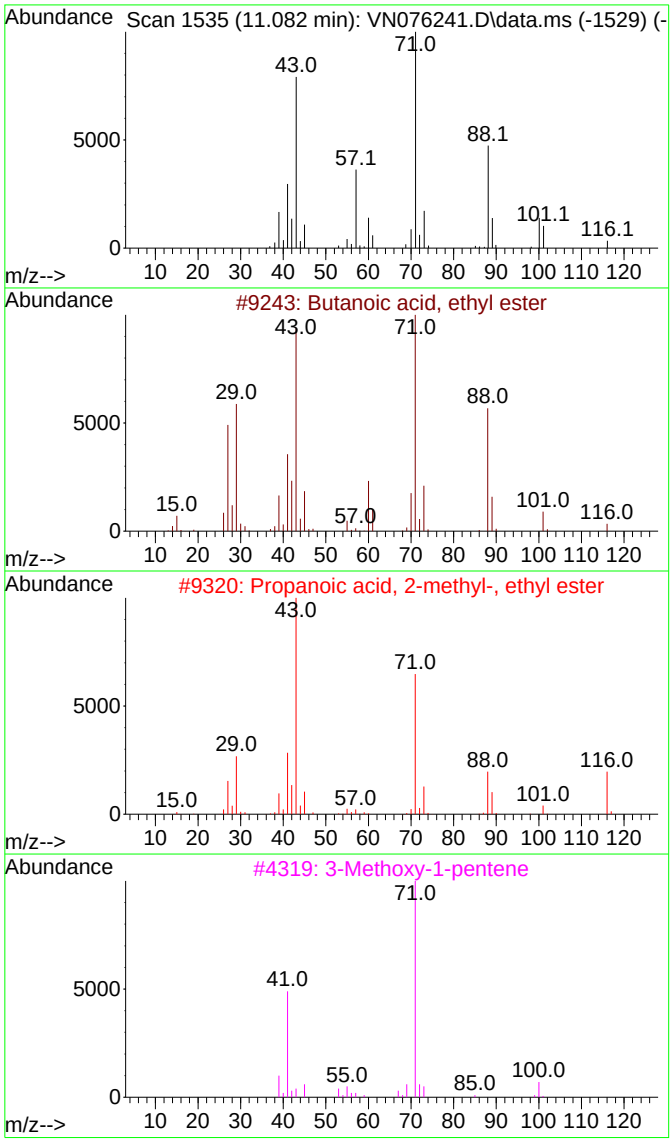
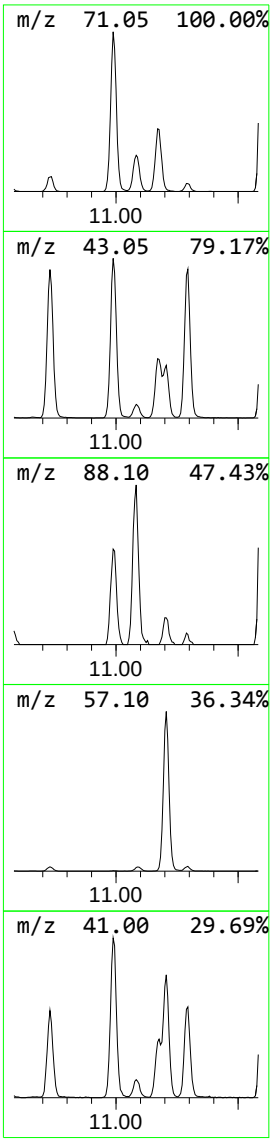
****

Peak Number 6 Butanoic acid, ethyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.082	6.60 ug/l	225930	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	64
2	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	58
3	3-Methoxy-1-pentene	100	C6H12O	014092-18-3	43
4	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	43
5	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	40





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Quant Title : SW846 8260

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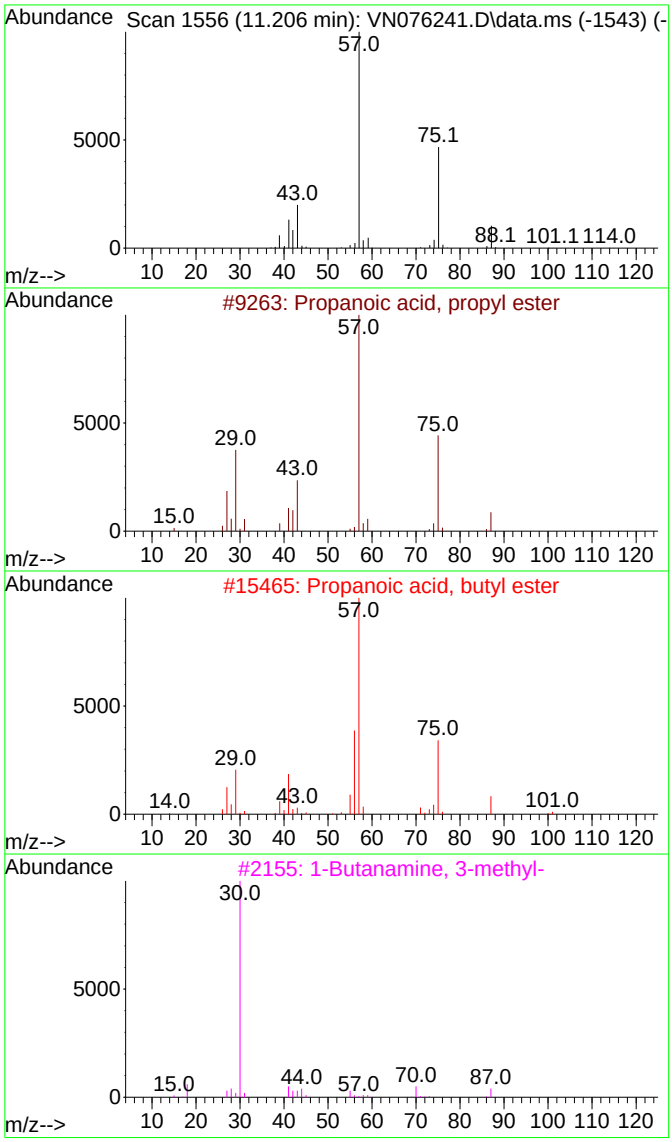
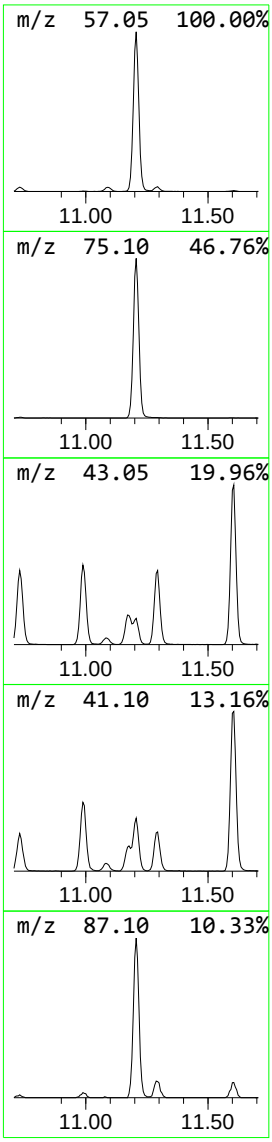
****
Peak Number 7 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.206	57.17 ug/l	1958520	Chlorobenzene-d5	11.871

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	39
3	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	9
4	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
5	1-Penten-3-ol	86	C5H10O	000616-25-1	7





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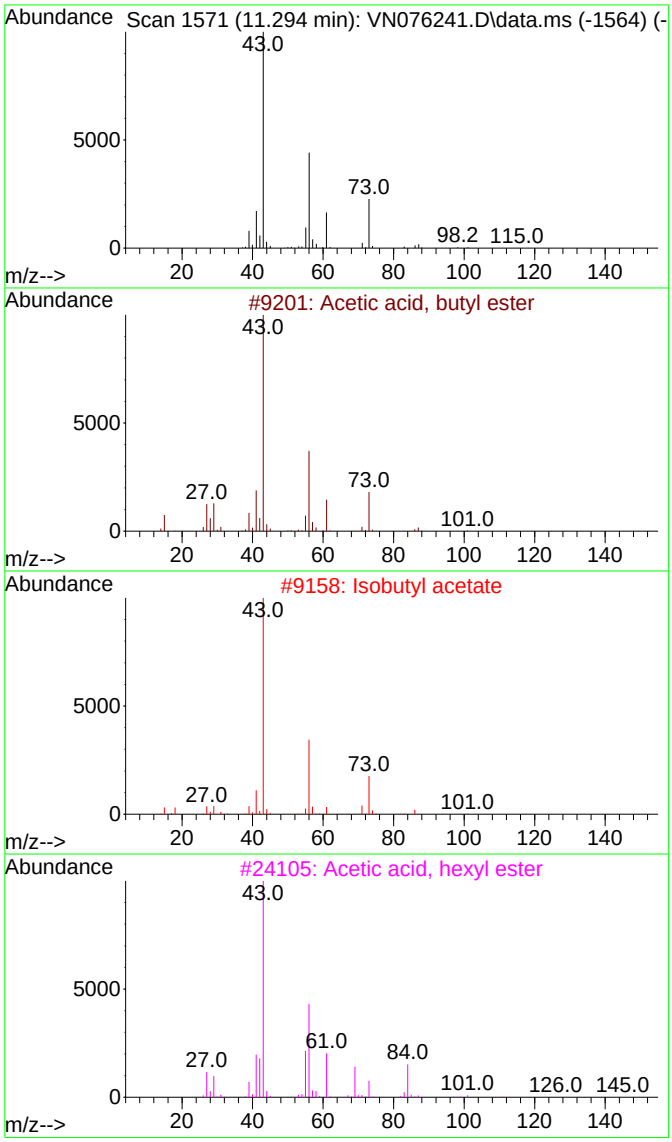
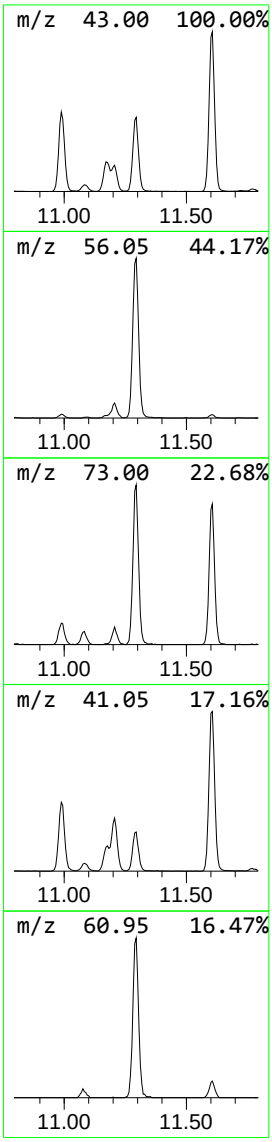
****
Peak Number 8 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.294	29.29 ug/l	1003330	Chlorobenzene-d5	11.871

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	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	36
4	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	10
5	Isobutylamine	73	C4H11N	000078-81-9	9





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MSVOA_N
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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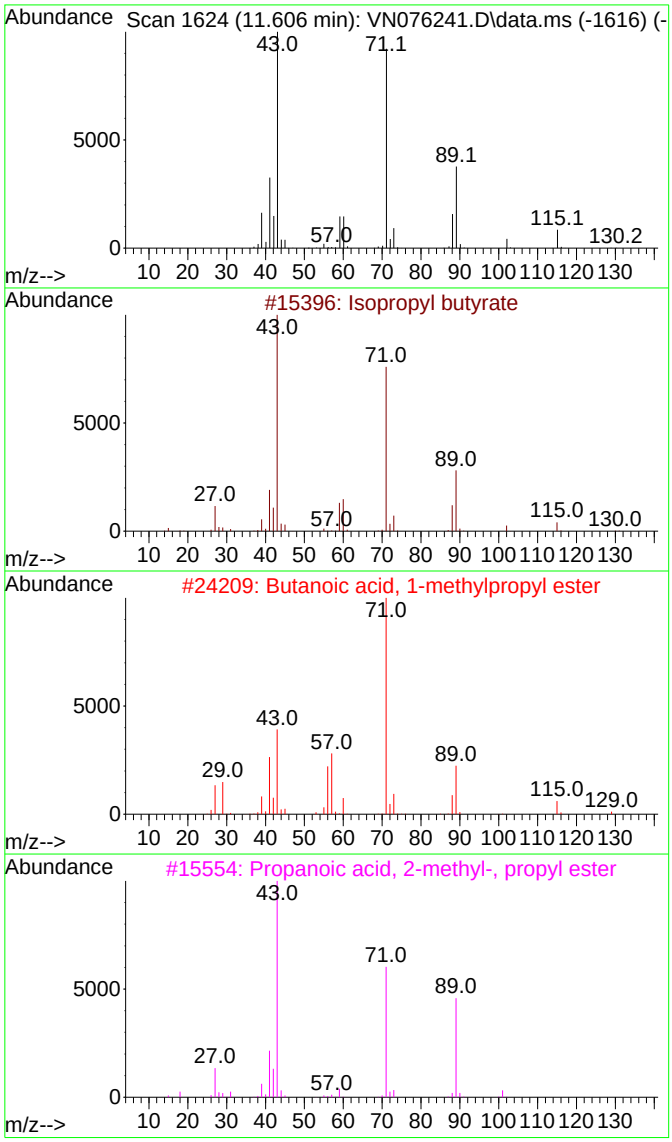
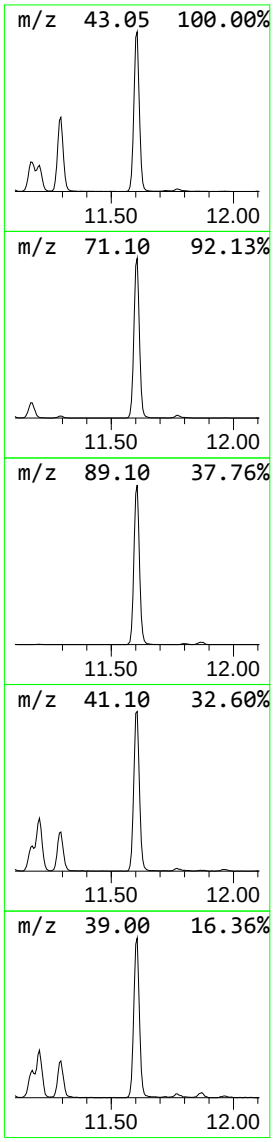
Peak Number 9 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.606	93.86 ug/l	3215250	Chlorobenzene-d5	11.871

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, propyl ester	130	C7H14O2	000105-66-8	72
5	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011323\
Data File : VN076241.D
Acq On : 13 Jan 2023 12:14
Operator : JC\MD
Sample : PB150223TB
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PB150223TB

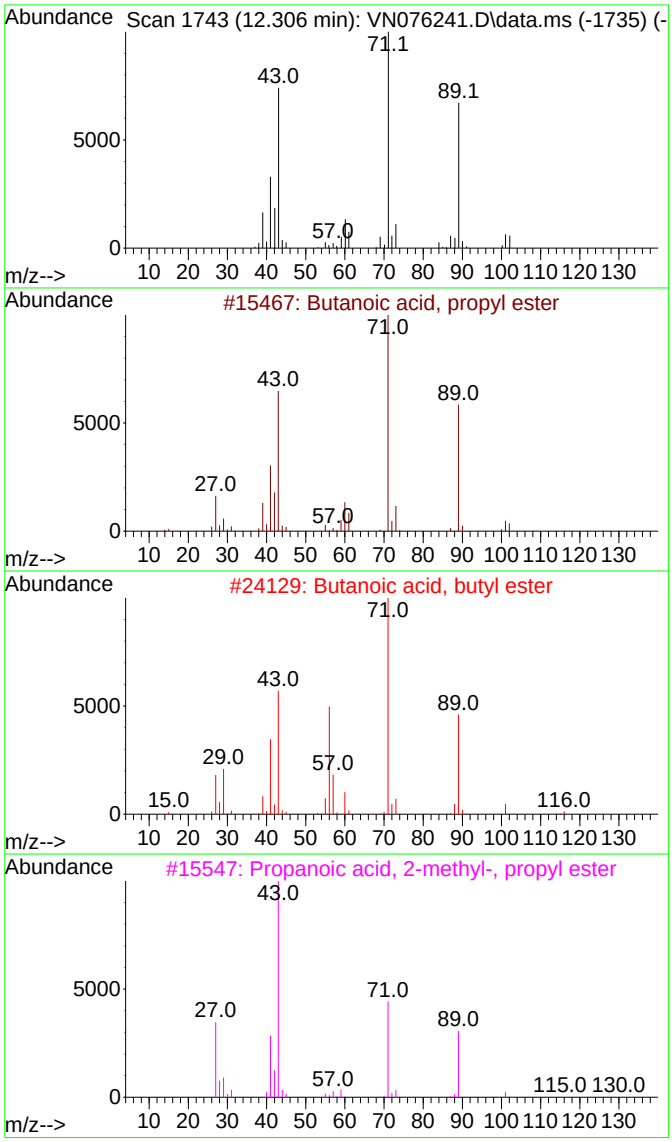
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

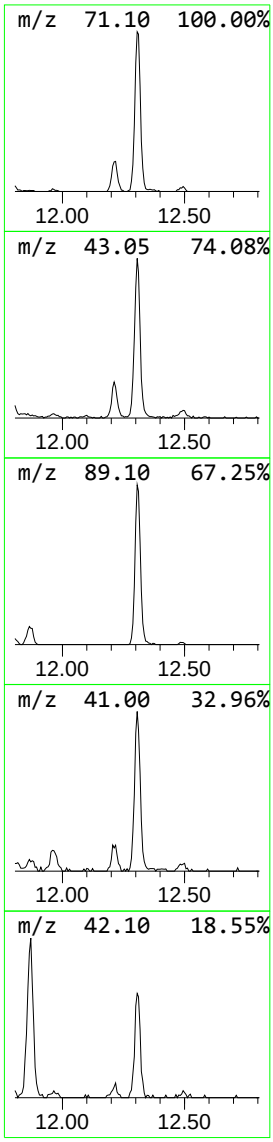
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Butanoic acid, propyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.306	7.82 ug/l	267917	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
2	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	78
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	72
5	Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011323\
Data File : VN076241.D
Acq On : 13 Jan 2023 12:14
Operator : JC\MD
Sample : PB150223TB
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
PB150223TB

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.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	9.677	6.6	ug/l	196375	2	9.106	1492580	50.0
n-Propyl acetate	9.747	114.3	ug/l	3413240	2	9.106	1492580	50.0
Propanoic acid,...	10.359	25.5	ug/l	760967	2	9.106	1492580	50.0
Isobutyl acetate	10.729	26.8	ug/l	918052	3	11.871	1712760	50.0
Propanoic acid,...	10.988	32.1	ug/l	1099700	3	11.871	1712760	50.0
Butanoic acid, ...	11.082	6.6	ug/l	225930	3	11.871	1712760	50.0
Propanoic acid,...	11.206	57.2	ug/l	1958520	3	11.871	1712760	50.0
Acetic acid, bu...	11.294	29.3	ug/l	1003330	3	11.871	1712760	50.0
Isopropyl butyrate	11.606	93.9	ug/l	3215250	3	11.871	1712760	50.0
Butanoic acid, ...	12.306	7.8	ug/l	267917	3	11.871	1712760	50.0