LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091522\
Data File : VN074468.D
Acq On : 15 Sep 2022 17:58
Operator : JC\MD
Sample : N4578-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CHERRY-HILL-COMP-1

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\82N091522W.M
Title : SW846 8260

Signal : TIC: VN074468.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	47	52	60	rBV	949648	1656964	18.93%	3.489%
2	4.228	388	398	406	rBV	72455	199590	2.28%	0.420%
3	5.010	522	531	542	rBV4	39791	119974	1.37%	0.253%
4	7.340	920	927	935	rVB3	75118	178072	2.03%	0.375%
5	7.951	1021	1031	1036	rBV	384644	930875	10.63%	1.960%
6	8.016	1036	1042	1055	rVB	634650	1456201	16.63%	3.066%
7	8.369	1093	1102	1115	rBV	430896	999405	11.42%	2.104%
8	8.492	1115	1123	1130	rBV	425910	939709	10.73%	1.978%
9	8.904	1184	1193	1210	rVB	1025510	2156670	24.63%	4.541%
10	9.492	1283	1293	1298	rBV	241263	518947	5.93%	1.093%
11	9.563	1298	1305	1317	rVB	4974024	8754796	100.00%	18.433%
12	10.181	1403	1410	1420	rBV	902952	1570764	17.94%	3.307%
13	10.381	1436	1444	1453	rBV	1575133	2843428	32.48%	5.987%
14	10.557	1467	1474	1483	rVB	1218385	2012302	22.99%	4.237%
15	10.816	1510	1518	1527	rBV	1311696	2099505	23.98%	4.420%
16	10.910	1527	1534	1543	rVV3	273651	489942	5.60%	1.032%
17	10.998	1543	1549	1551	rVV	482023	813009	9.29%	1.712%
18	11.033	1551	1555	1563	rVV	2015611	3197493	36.52%	6.732%
19	11.122	1563	1570	1581	rVB	1445484	2283195	26.08%	4.807%
20	11.433	1615	1623	1638	rBV	3759917	5809770	66.36%	12.232%
21	11.598	1646	1651	1658	rBV2	61431	96078	1.10%	0.202%
22	11.686	1658	1666	1677	rVV	1714676	2944612	33.63%	6.200%
23	12.039	1720	1726	1733	rBV3	59614	98019	1.12%	0.206%
24	12.139	1736	1743	1749	rBV	306525	467247	5.34%	0.984%
25	12.674	1826	1834	1844	rBV	1285174	2197999	25.11%	4.628%
26	13.616	1987	1994	2003	rBV	1650743	2661510	30.40%	5.604%

Sum of corrected areas: 47496076

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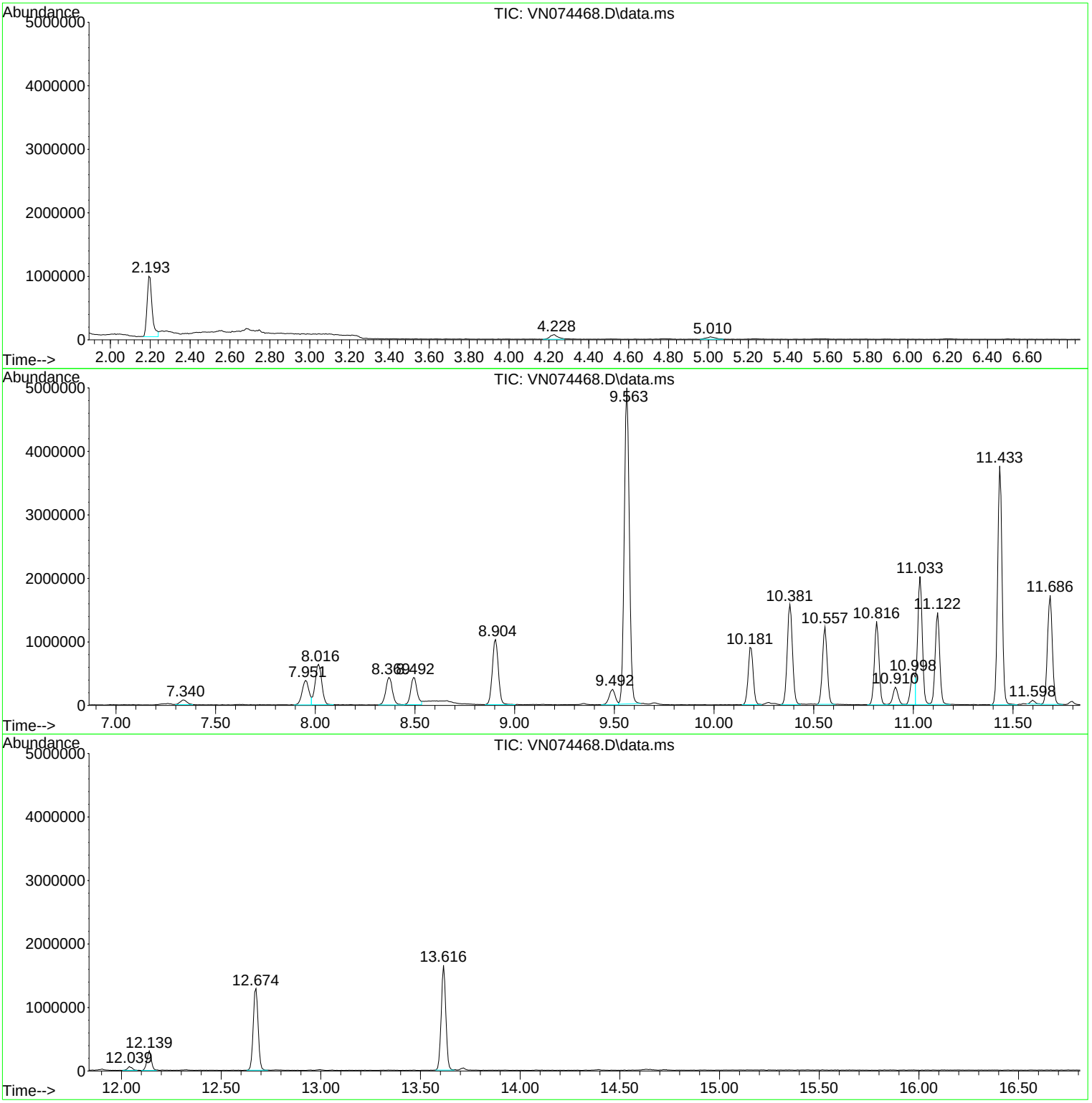
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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



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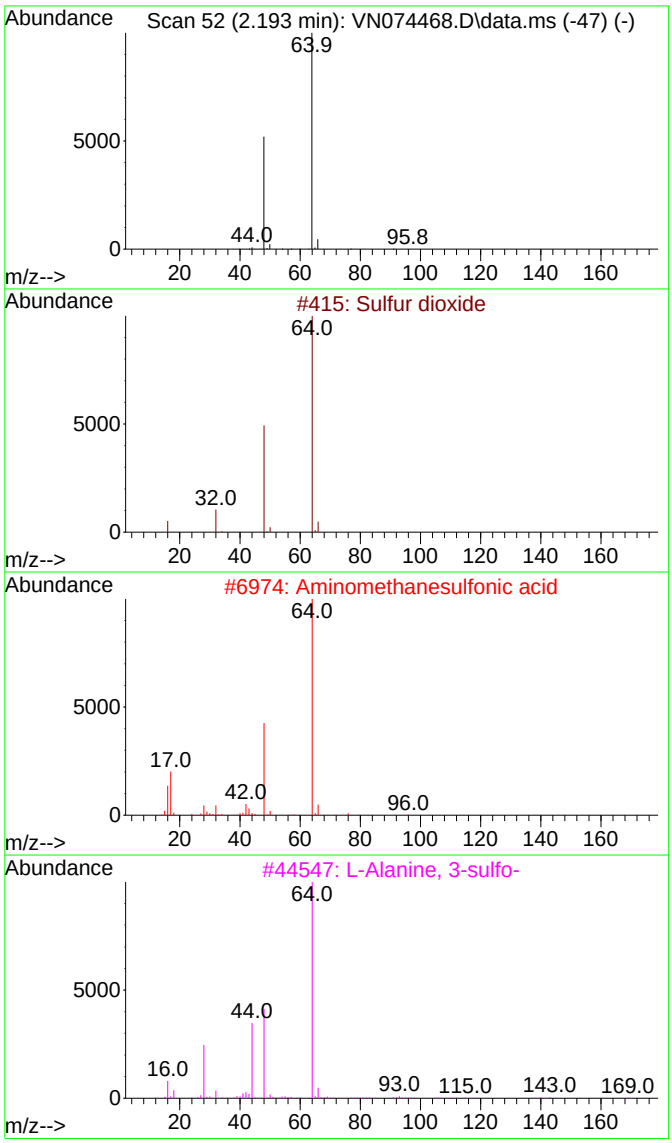
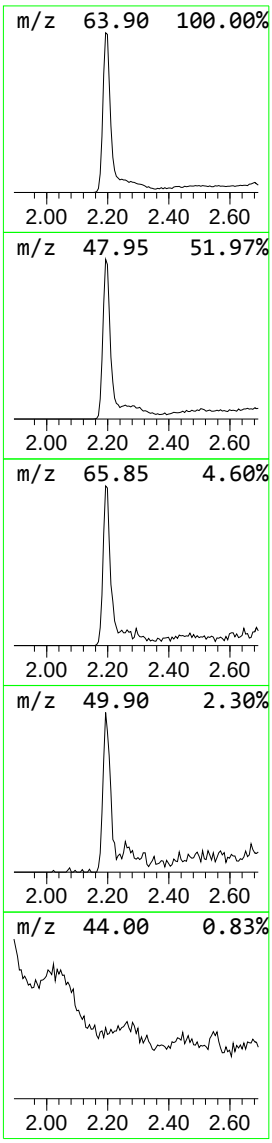
****

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	56.89 ug/l	1656960	Pentafluorobenzene	8.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





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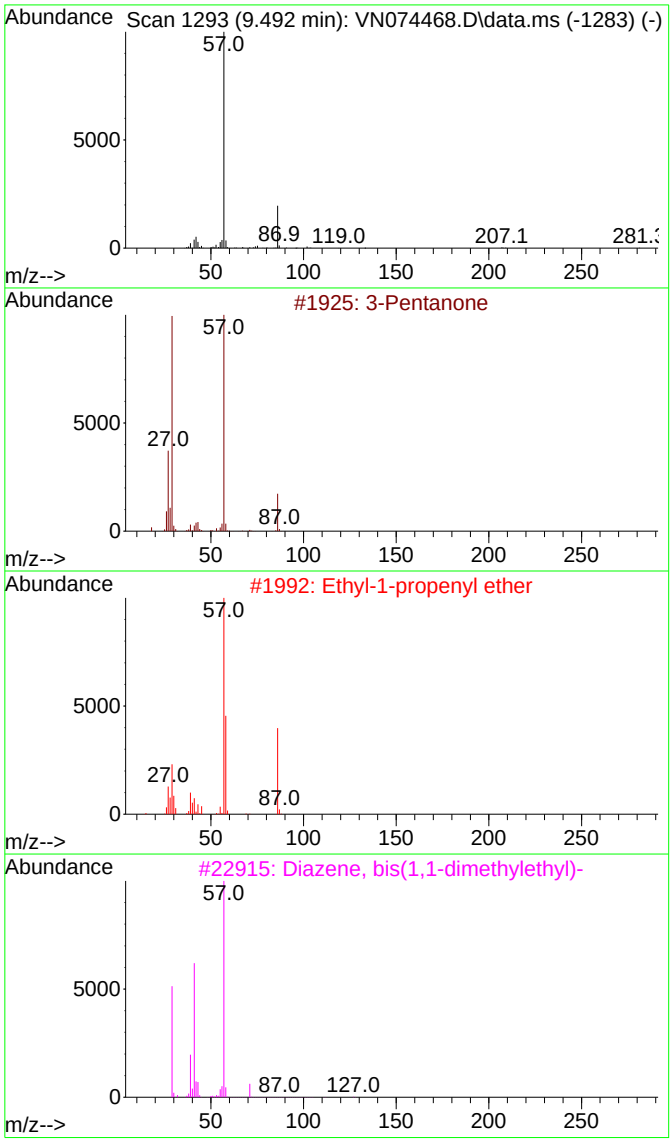
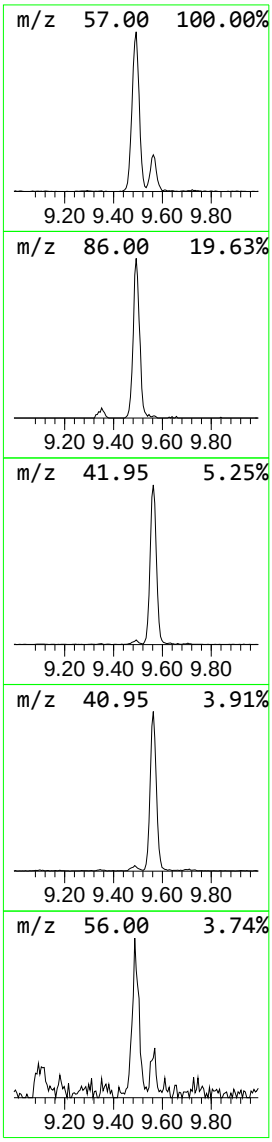
****
Peak Number 2 3-Pentanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.492	12.03 ug/l	518947	1,4-Difluorobenzene	8.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	80
2	Ethyl-1-propenyl ether	86	C5H10O	000928-55-2	9
3	Diazene, bis(1,1-dimethylethyl)-	142	C8H18N2	000927-83-3	9
4	Neopentane	72	C5H12	000463-82-1	9
5	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	7





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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
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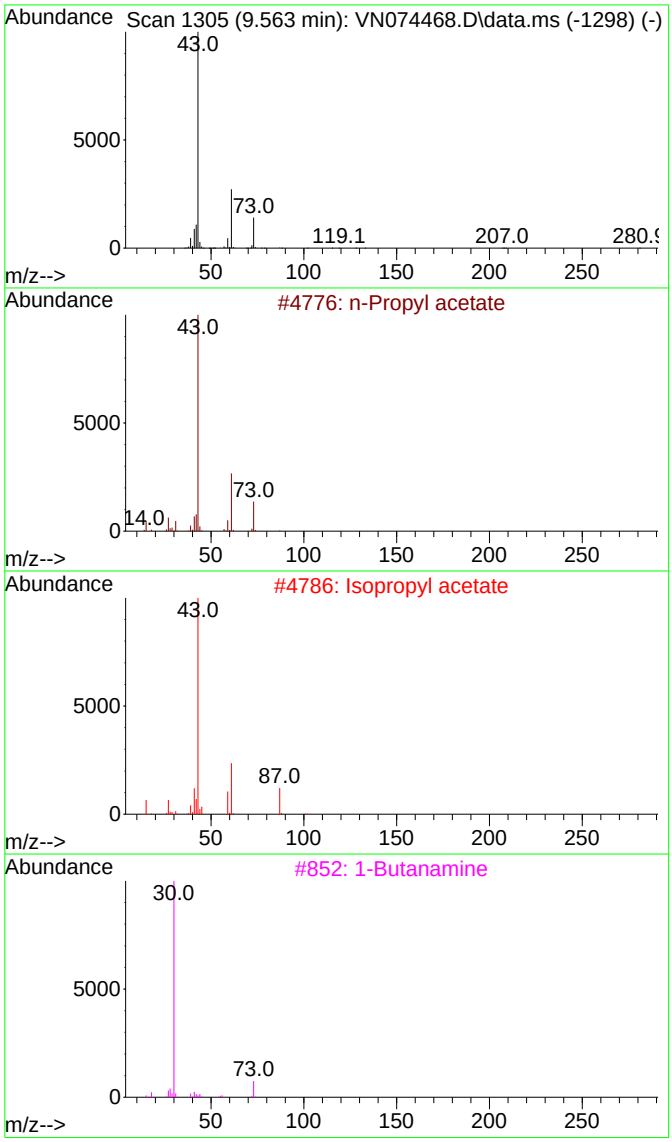
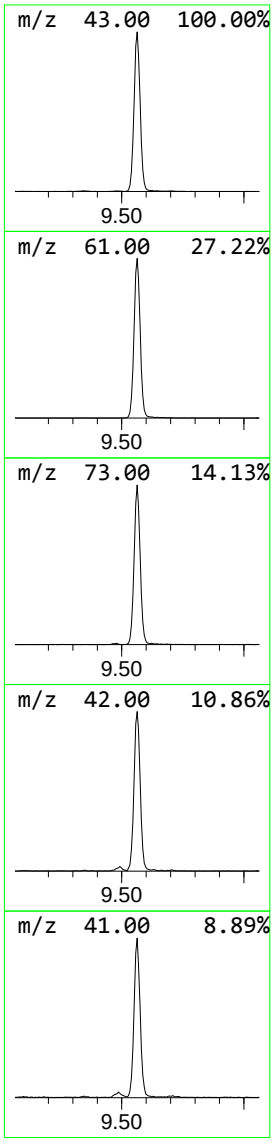
****
Peak Number 3 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.563	202.97 ug/l	8754800	1,4-Difluorobenzene	8.904

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	9
3	1-Butanamine	73	C4H11N	000109-73-9	7
4	Isobutylamine	73	C4H11N	000078-81-9	4
5	Hydrogen azide	43	HN3	007782-79-8	4





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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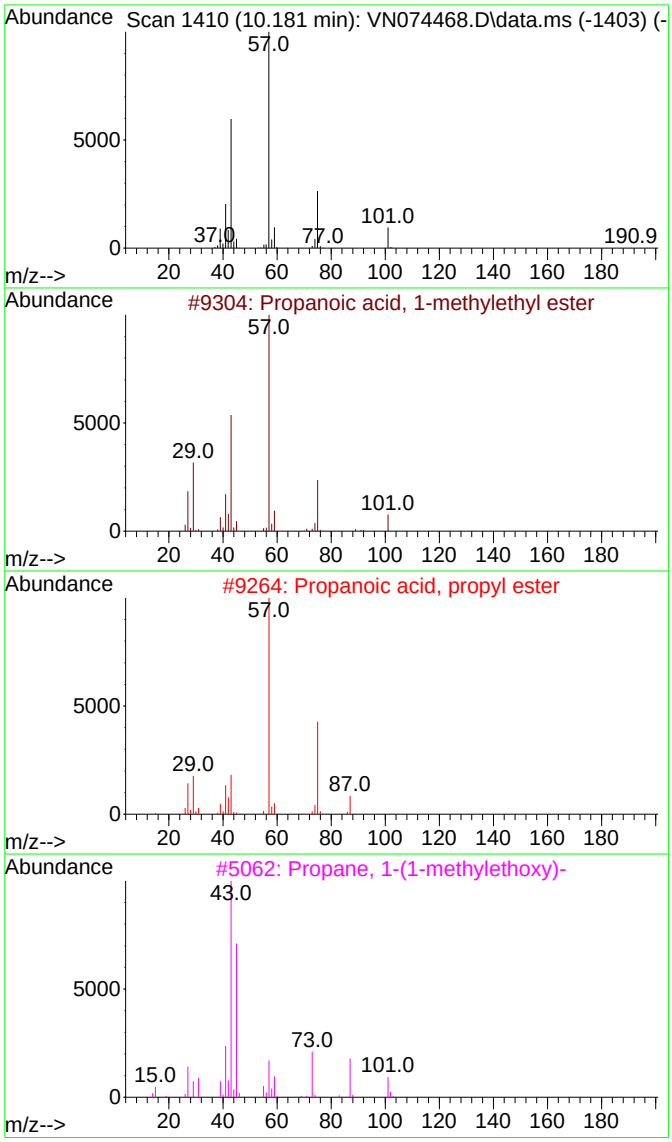
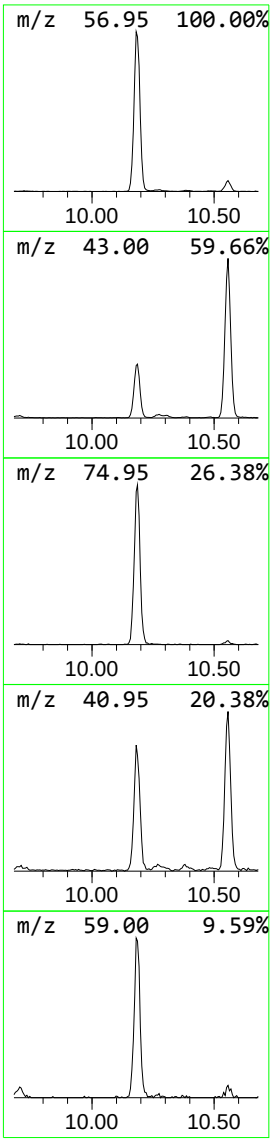
****
Peak Number 4 Propanoic acid, 1-methyleth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.181	36.42 ug/l	1570760	1,4-Difluorobenzene	8.904

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	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	o-Isopropylhydroxylamine	75	C3H9NO	1000322-42-6	9





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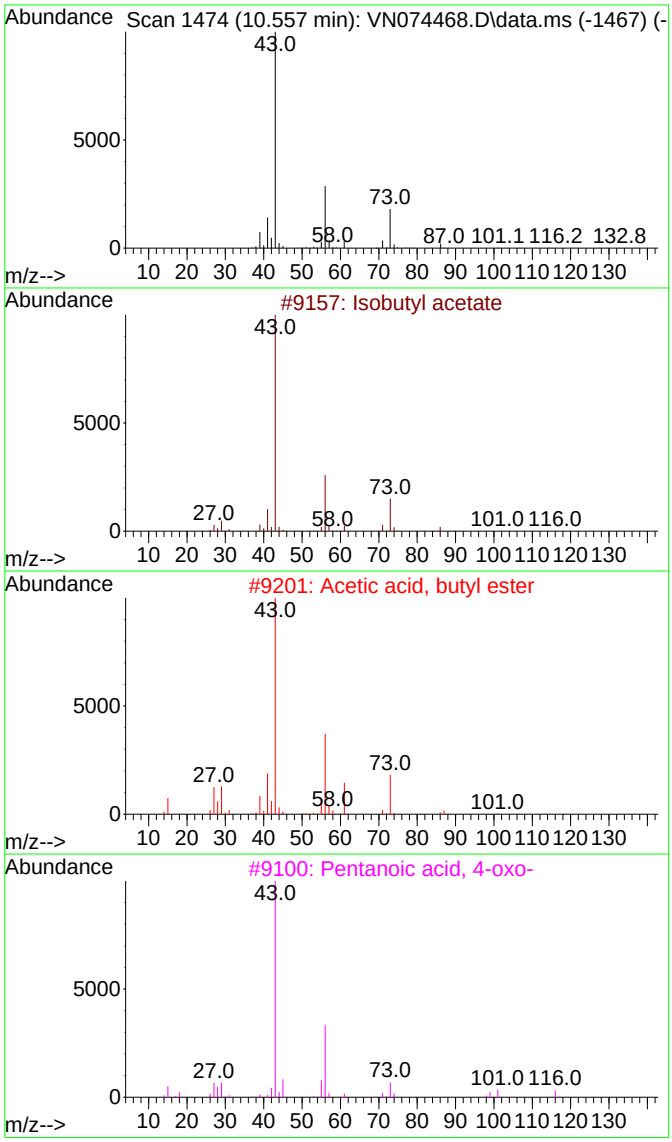
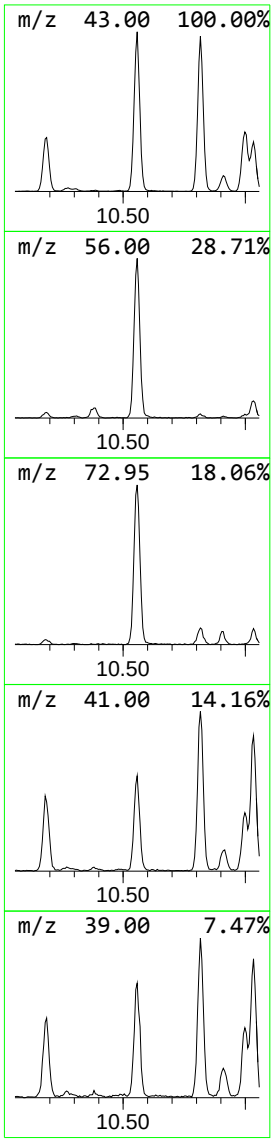
****
Peak Number 5 Isobutyl acetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.557	34.17 ug/l	2012300	Chlorobenzene-d5	11.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl acetate	116	C6H12O2	000110-19-0	78
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	50
3	Pentanoic acid, 4-oxo-	116	C5H8O3	000123-76-2	40
4	Pentane, 2-methyl-	86	C6H14	000107-83-5	9
5	Isobutylamine	73	C4H11N	000078-81-9	9





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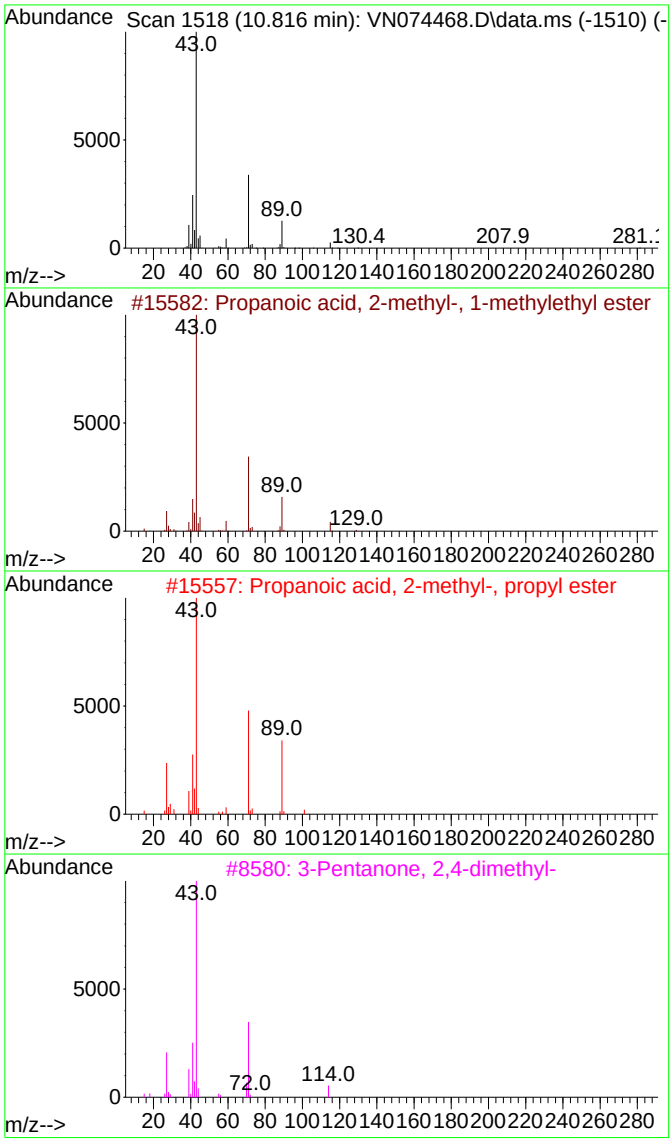
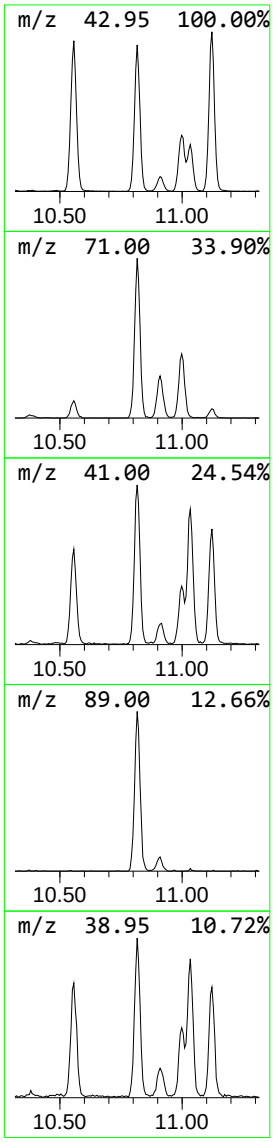
****
Peak Number 6 Propanoic acid, 2-methyl-, ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.816	35.65 ug/l	2099510	Chlorobenzene-d5	11.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	45
3	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	40
4	2,3-Hexanedione	114	C6H10O2	003848-24-6	40
5	Isopropyl butyrate	130	C7H14O2	000638-11-9	38





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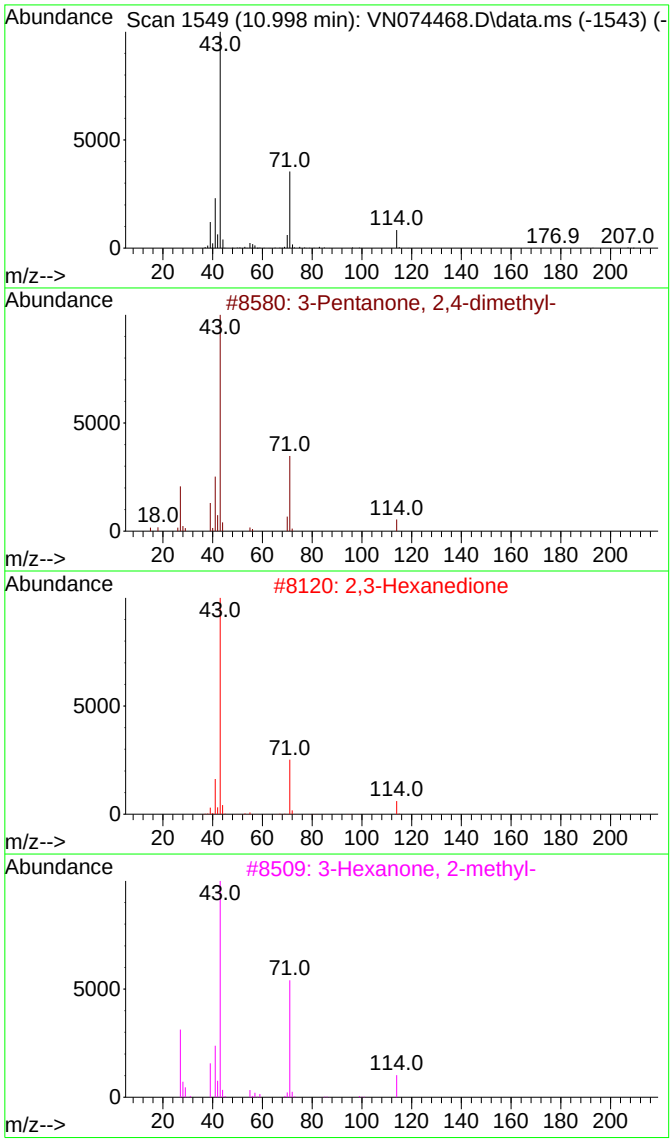
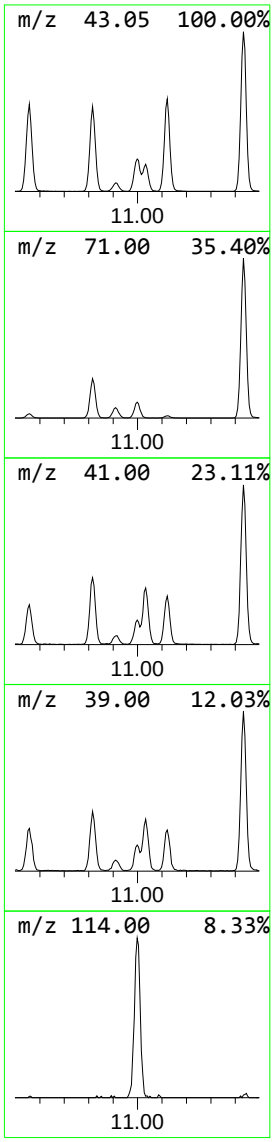
****
Peak Number 7 3-Pentanone, 2,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.998	13.81 ug/l	813009	Chlorobenzene-d5	11.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	86
2	2,3-Hexanedione	114	C6H10O2	003848-24-6	72
3	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	53
4	Piperazine, 1,4-dimethyl-	114	C6H14N2	000106-58-1	16
5	Cyanic acid, ethyl ester	71	C3H5NO	000627-48-5	9





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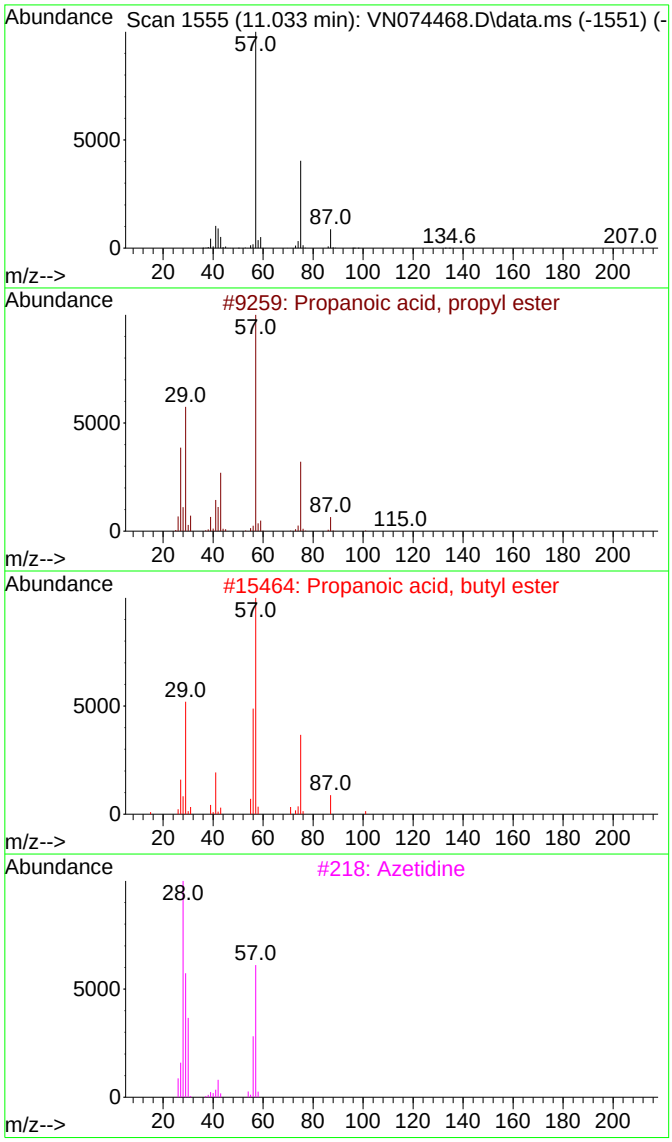
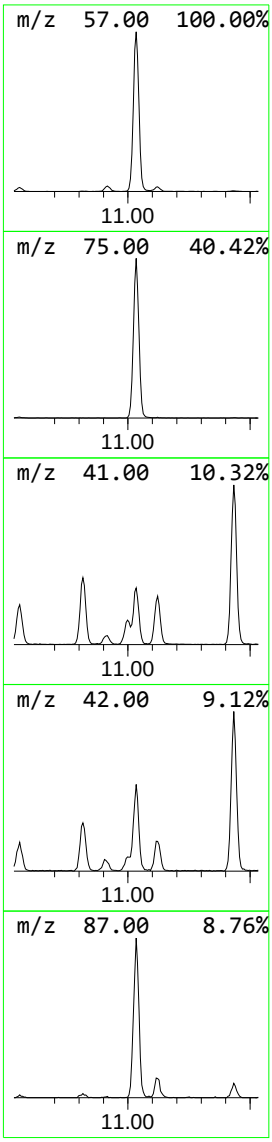
****
Peak Number 8 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.033	54.29 ug/l	3197490	Chlorobenzene-d5	11.686

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	38
3	Azetidine	57	C3H7N	000503-29-7	9
4	Isobutyl ether	130	C8H18O	000628-55-7	9
5	Trimethylaluminum	72	C3H9Al	000075-24-1	9





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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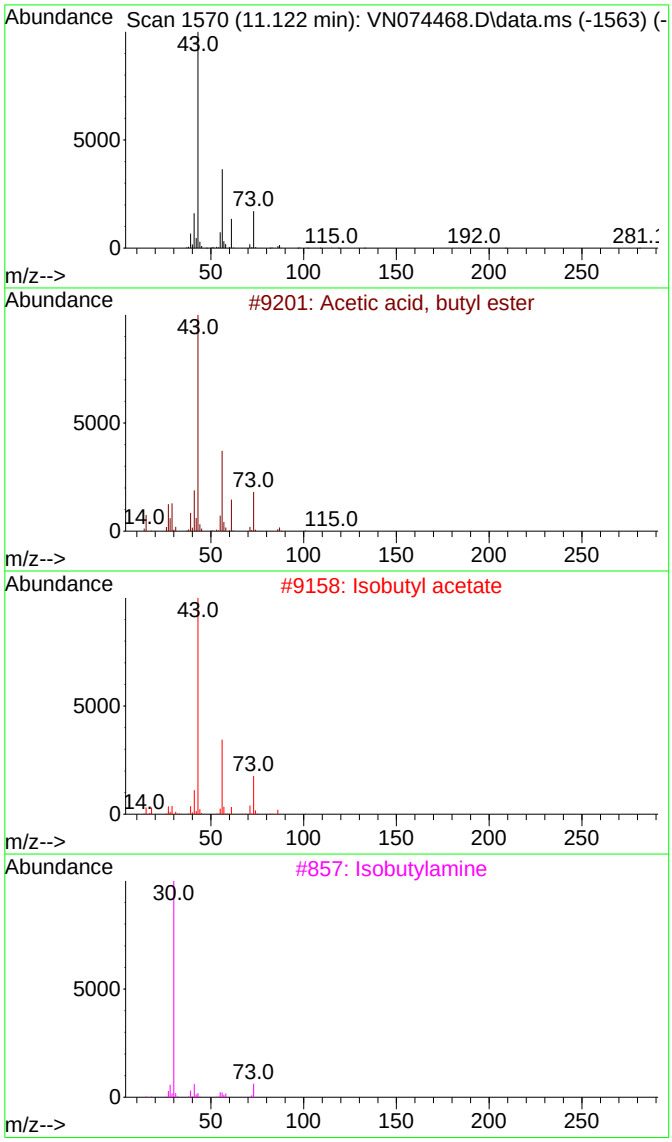
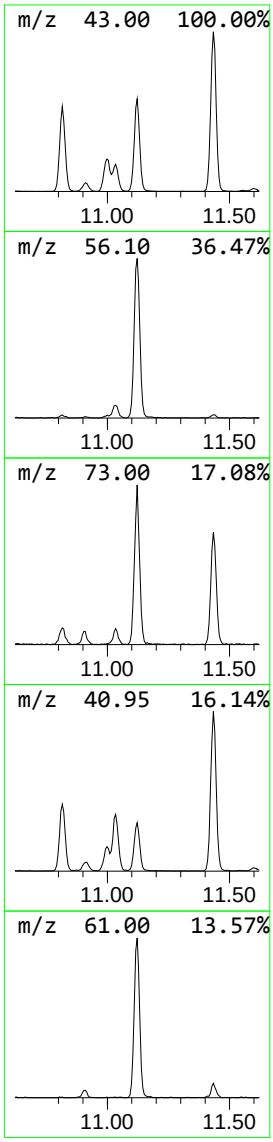
****
Peak Number 9 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.122	38.77 ug/l	2283200	Chlorobenzene-d5	11.686

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	38
3	Isobutylamine	73	C4H11N	000078-81-9	9
4	Isopropyl pyruvate	130	C6H10O3	1000431-41-9	9
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





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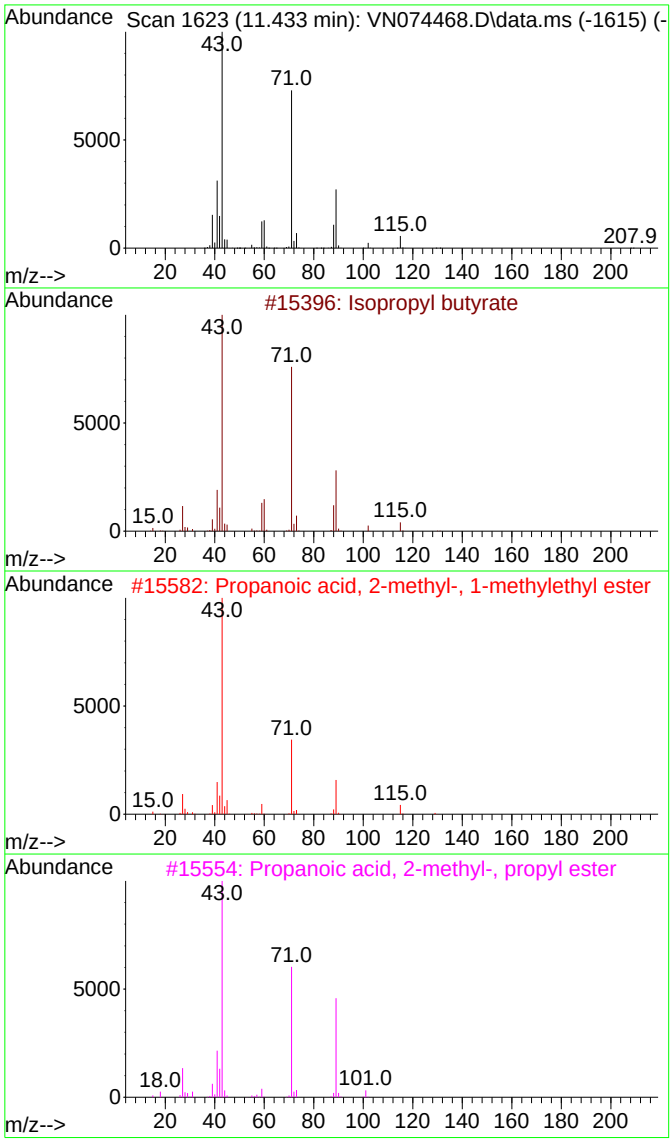
Quant Title : SW846 8260

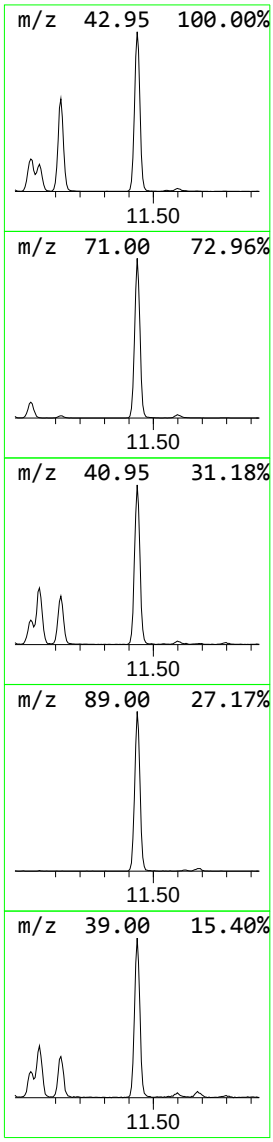
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.433	98.65 ug/l	5809770	Chlorobenzene-d5	11.686

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	72
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	59
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59
5	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091522\
Data File : VN074468.D
Acq On : 15 Sep 2022 17:58
Operator : JC\MD
Sample : N4578-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CHERRY-HILL-COMP-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.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
Sulfur dioxide	2.193	56.9	ug/l	1656960	1	8.016	1456200	50.0
3-Pentanone	9.492	12.0	ug/l	518947	2	8.904	2156670	50.0
n-Propyl acetate	9.563	203.0	ug/l	8754800	2	8.904	2156670	50.0
Propanoic acid,...	10.181	36.4	ug/l	1570760	2	8.904	2156670	50.0
Isobutyl acetate	10.557	34.2	ug/l	2012300	3	11.686	2944610	50.0
Propanoic acid,...	10.816	35.6	ug/l	2099510	3	11.686	2944610	50.0
3-Pentanone, 2,...	10.998	13.8	ug/l	813009	3	11.686	2944610	50.0
Propanoic acid,...	11.033	54.3	ug/l	3197490	3	11.686	2944610	50.0
Acetic acid, bu...	11.122	38.8	ug/l	2283200	3	11.686	2944610	50.0
Isopropyl butyrate	11.433	98.7	ug/l	5809770	3	11.686	2944610	50.0