LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078058.D
Acq On : 05 Jun 2023 20:44
Operator : JC\MD
Sample : 03029-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-6

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\82N051523W.M
Title : SW846 8260

Signal : TIC: VN078058.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.824	140	148	153	rBV2	34274	77174	1.63%	0.268%
2	5.289	555	567	576	rBV4	19940	64758	1.37%	0.225%
3	7.577	948	956	968	rVB2	42786	110609	2.34%	0.384%
4	8.177	1047	1058	1062	rBV	306944	731646	15.50%	2.538%
5	8.235	1062	1068	1078	rVB	513801	1164933	24.68%	4.041%
6	8.588	1119	1128	1136	rBV	314580	697033	14.77%	2.418%
7	8.694	1136	1146	1155	rBV	305939	793053	16.80%	2.751%
8	9.106	1207	1216	1230	rVB	783090	1619794	34.32%	5.619%
9	9.677	1304	1313	1318	rBV2	122306	272949	5.78%	0.947%
10	9.747	1318	1325	1344	rVV	2577410	4720196	100.00%	16.375%
11	10.365	1422	1430	1438	rBV	598017	1024331	21.70%	3.554%
12	10.576	1456	1466	1475	rBV	1174742	2269610	48.08%	7.874%
13	10.735	1485	1493	1501	rVB	672868	1170839	24.80%	4.062%
14	10.988	1527	1536	1546	rBV	793949	1366180	28.94%	4.739%
15	11.088	1546	1553	1561	rVV2	149899	283512	6.01%	0.984%
16	11.206	1561	1573	1582	rVV2	1185766	2476015	52.46%	8.590%
17	11.294	1582	1588	1602	rVB	692064	1174182	24.88%	4.073%
18	11.606	1633	1641	1656	rBV	2368071	3740955	79.25%	12.978%
19	11.771	1665	1669	1678	rVB4	32136	59661	1.26%	0.207%
20	11.871	1678	1686	1697	rVV	1085301	1948865	41.29%	6.761%
21	11.965	1697	1702	1709	rVB2	26761	47384	1.00%	0.164%
22	12.312	1753	1761	1769	rBV	158367	268865	5.70%	0.933%
23	12.853	1845	1853	1864	rBV	792579	1422538	30.14%	4.935%
24	13.800	2005	2014	2024	rBV	769646	1320373	27.97%	4.581%

Sum of corrected areas: 28825455

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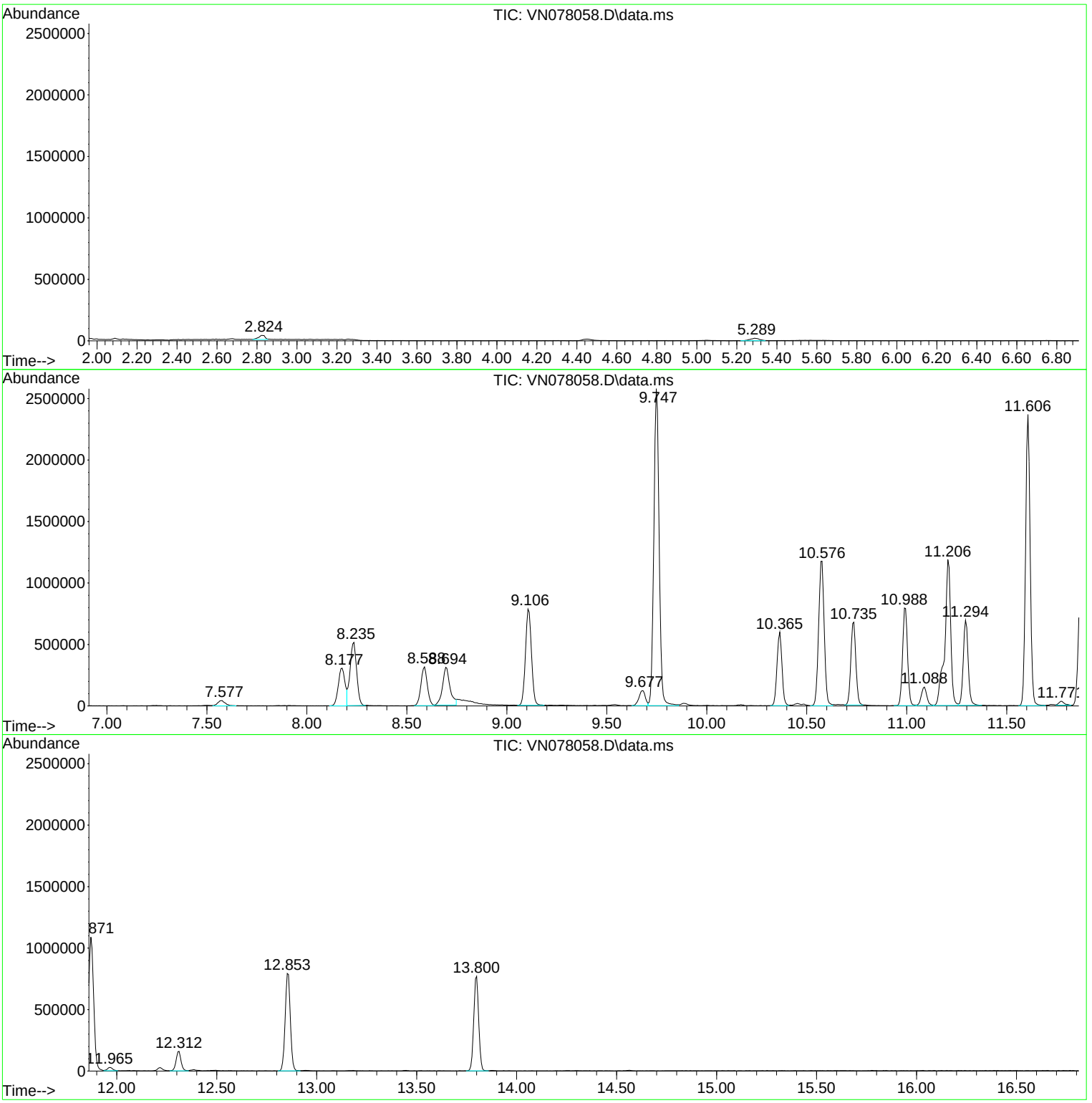
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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



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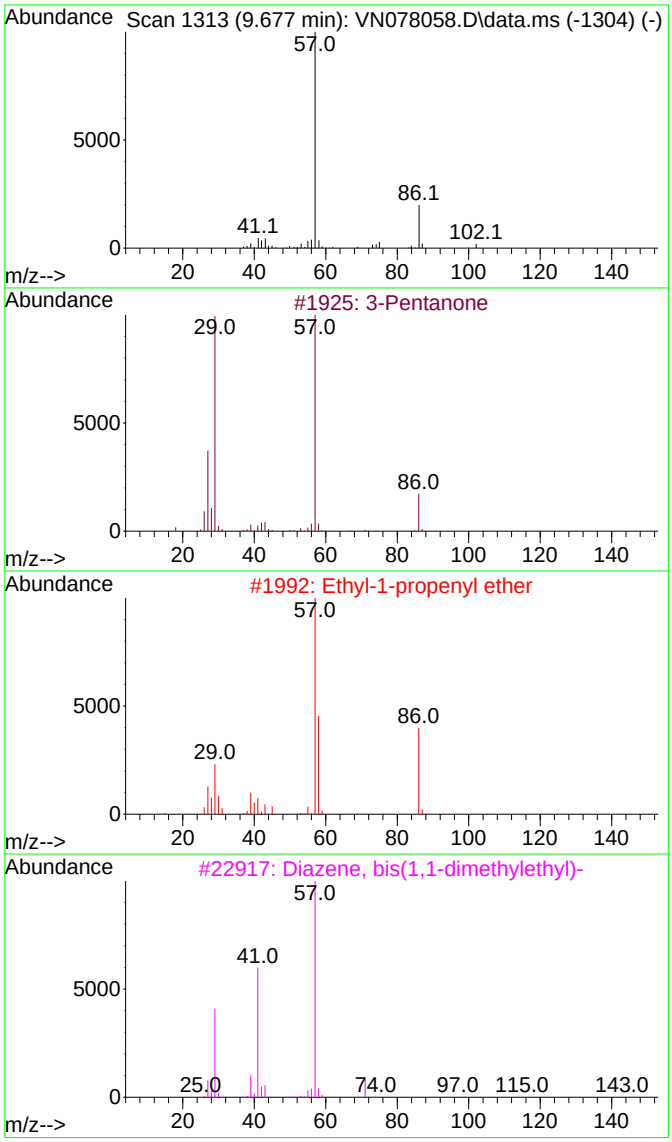
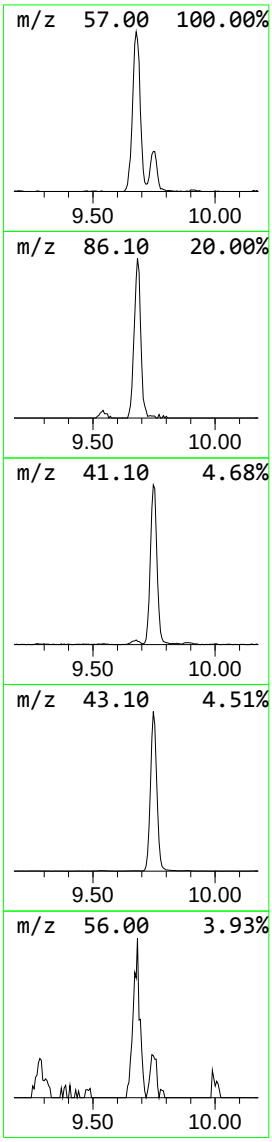
****
Peak Number 1 3-Pentanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.677	8.43 ug/l	272949	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	64
2	Ethyl-1-propenyl ether	86	C5H10O	000928-55-2	40
3	Diazene, bis(1,1-dimethylethyl)-	142	C8H18N2	000927-83-3	17
4	Butanoic acid, 2-oxo-	102	C4H6O3	000600-18-0	12
5	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	9





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Quant Title : SW846 8260

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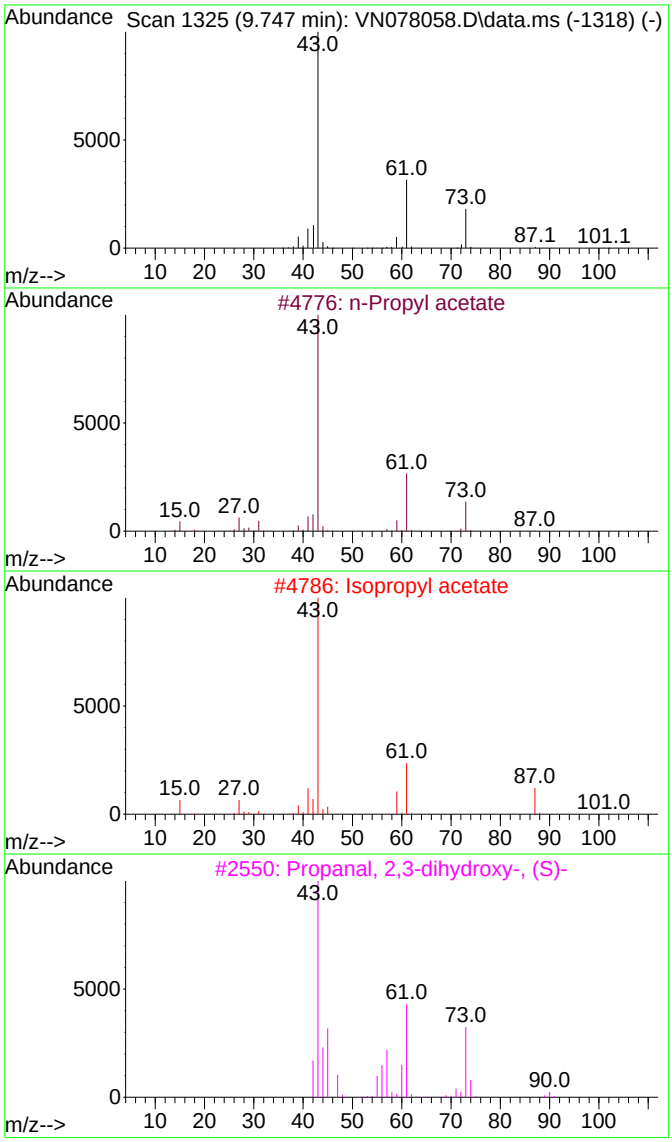
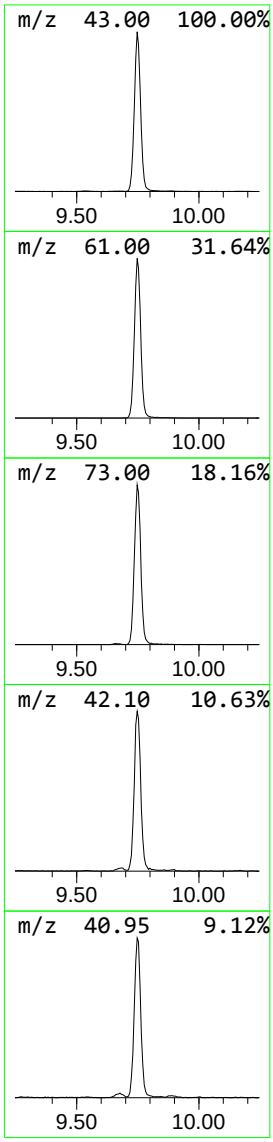
****
Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.747	145.70 ug/l	4720200	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	Isopropyl acetate	102	C5H10O2	000108-21-4	38
3	Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	36
4	1-Butanamine	73	C4H11N	000109-73-9	7
5	Isobutylamine	73	C4H11N	000078-81-9	4





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
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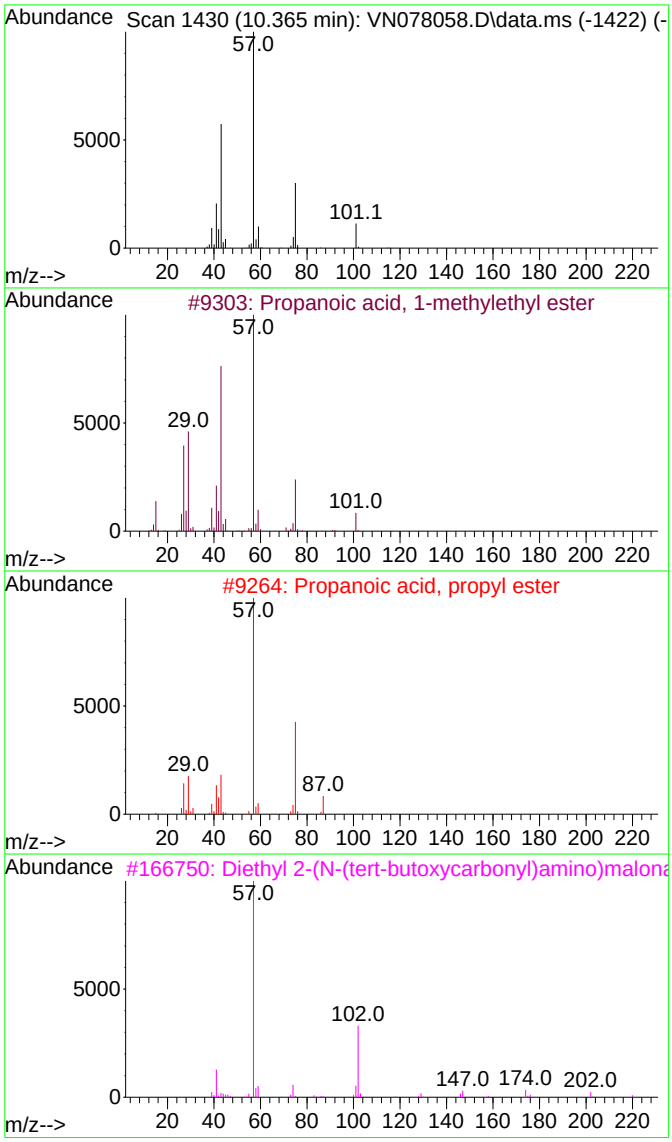
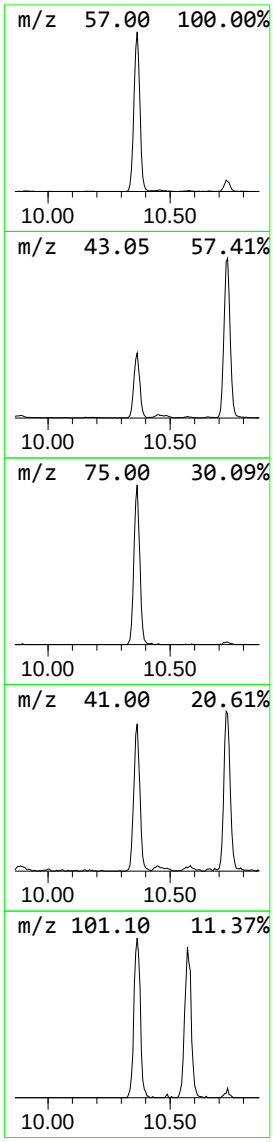
****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.365	31.62 ug/l	1024330	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	Diethyl 2-(N-(tert-butoxycarbony...	275	C12H21NO6	102831-44-7	25
4	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	23
5	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	10





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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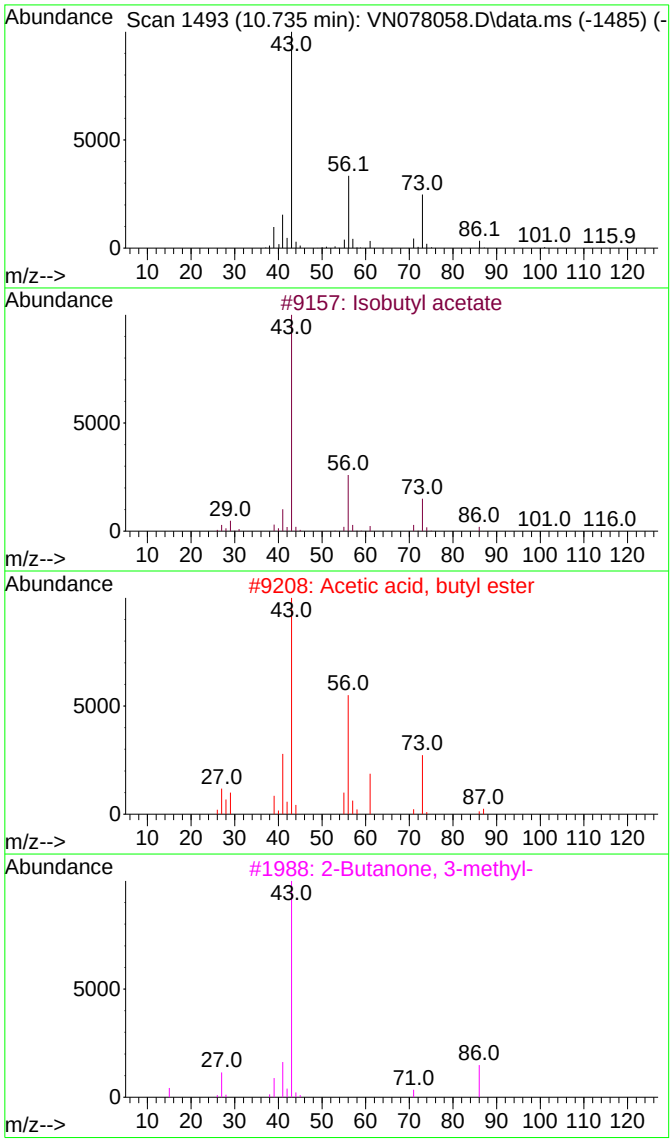
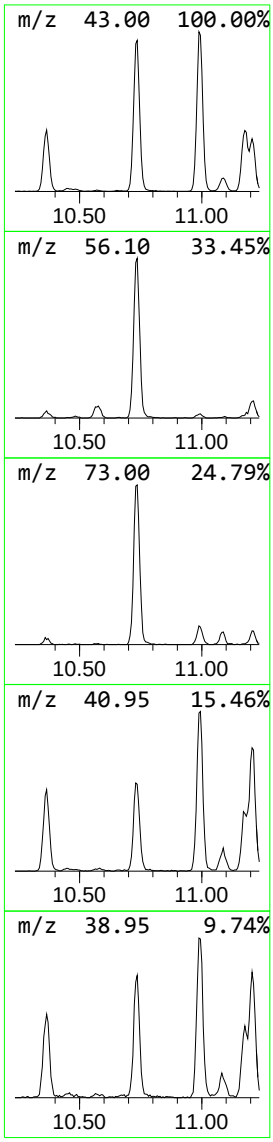
****
Peak Number 4 Isobutyl acetate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.735	30.04 ug/l	1170840	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutyl acetate	116	C6H12O2	000110-19-0	83
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	36
3	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	22
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5	Pentanoic acid, 4-oxo-	116	C5H8O3	000123-76-2	9





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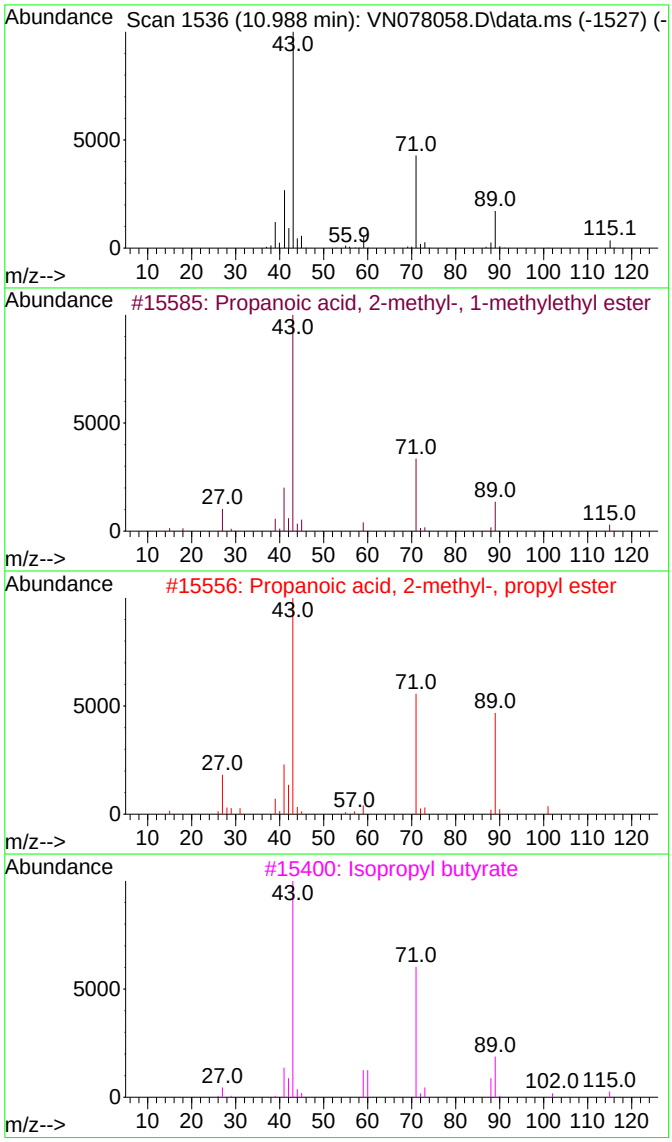
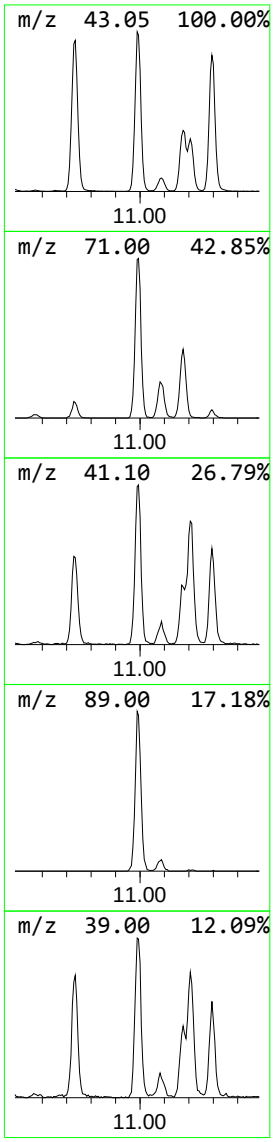
****
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.988	35.05 ug/l	1366180	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	83
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	56
4	Propanoic acid, 2-methyl-, 2-met...	172	C10H20O2	084254-82-0	56
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	53





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Instrument :
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TIC Library : C:\Database\NIST20.L
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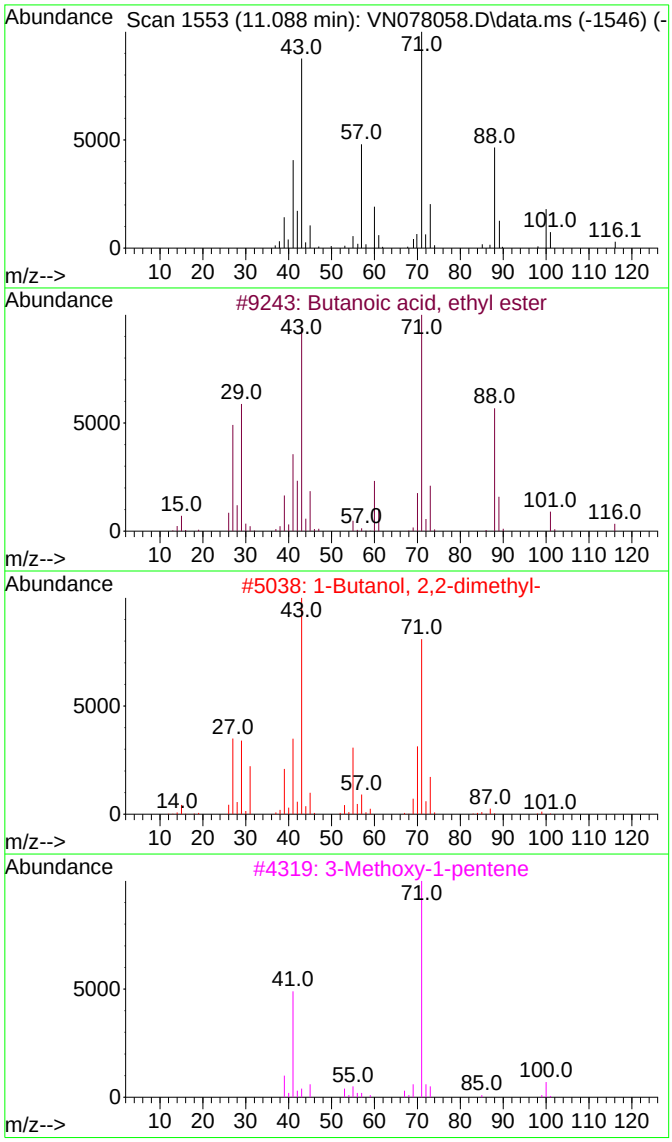
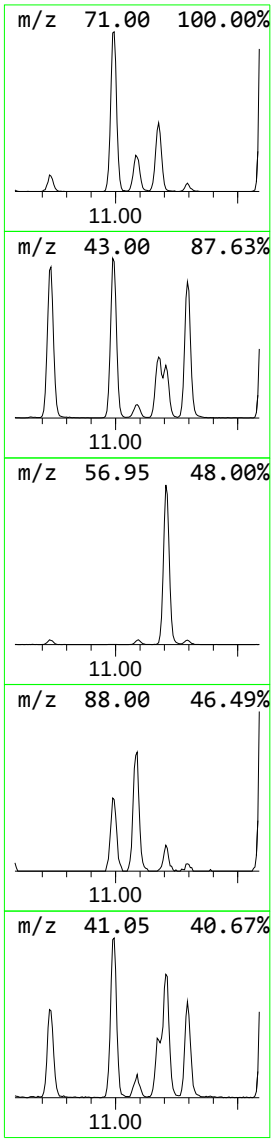
****
Peak Number 6 Butanoic acid, ethyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.088	7.27 ug/l	283512	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	1-Butanol, 2,2-dimethyl-	102	C6H14O	001185-33-7	43
3	3-Methoxy-1-pentene	100	C6H12O	014092-18-3	43
4	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	40
5	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	38





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TIC Library : C:\Database\NIST20.L
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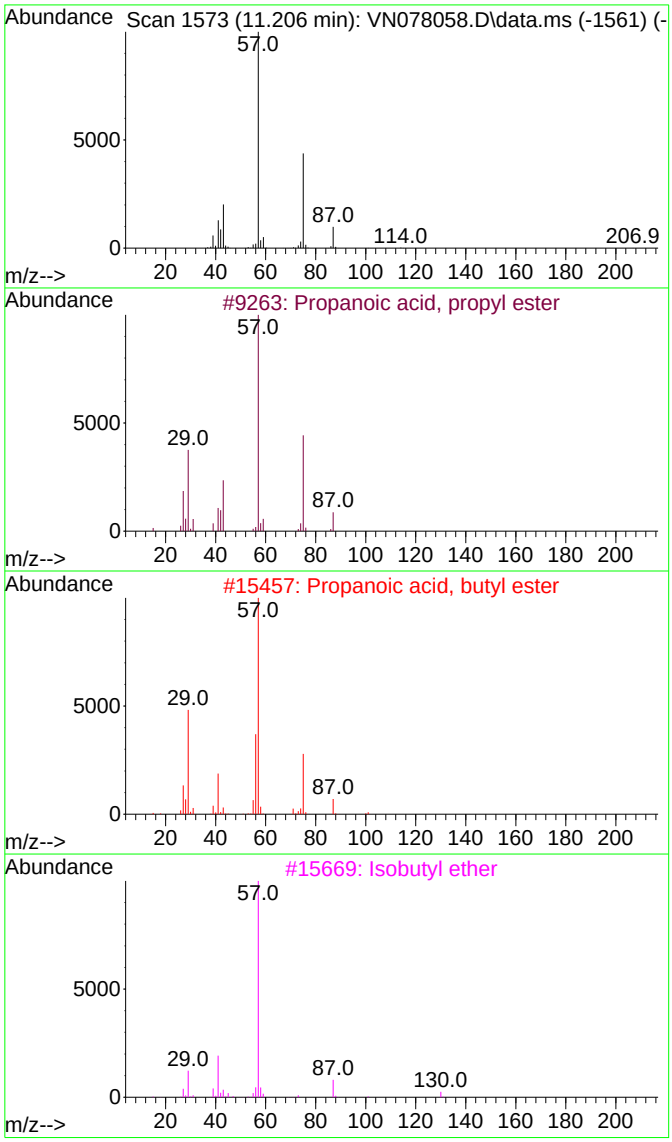
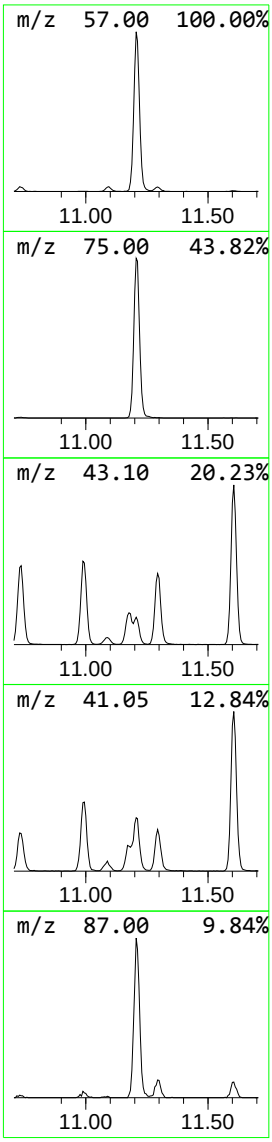
****
Peak Number 7 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.206	63.52 ug/l	2476020	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	28
3	Isobutyl ether	130	C8H18O	000628-55-7	17
4	S-(-)-2-Methylbutylamine	87	C5H13N	020626-52-2	9
5	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9





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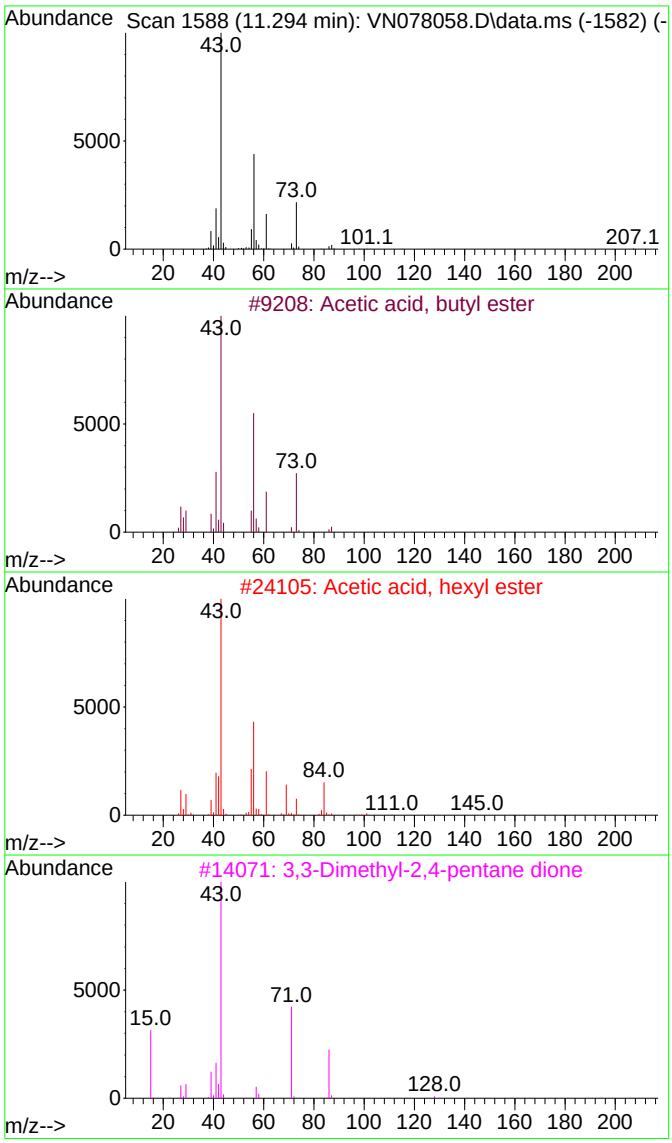
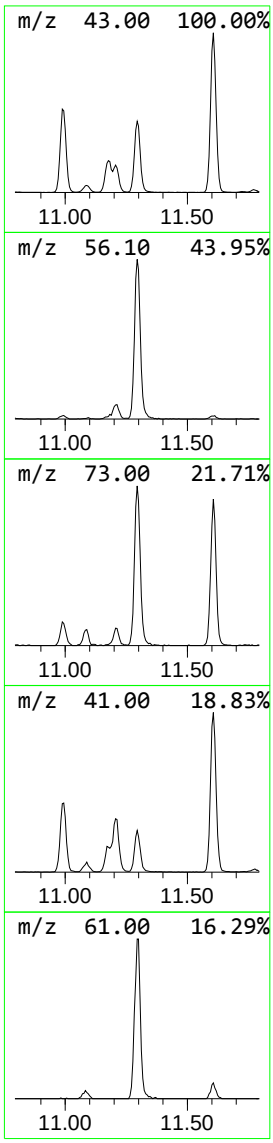
****
Peak Number 8 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.294	30.12 ug/l	1174180	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	90
2	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	36
3	3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	10
4	1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	10
5	Isobutylamine	73	C4H11N	000078-81-9	9





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Quant Title : SW846 8260

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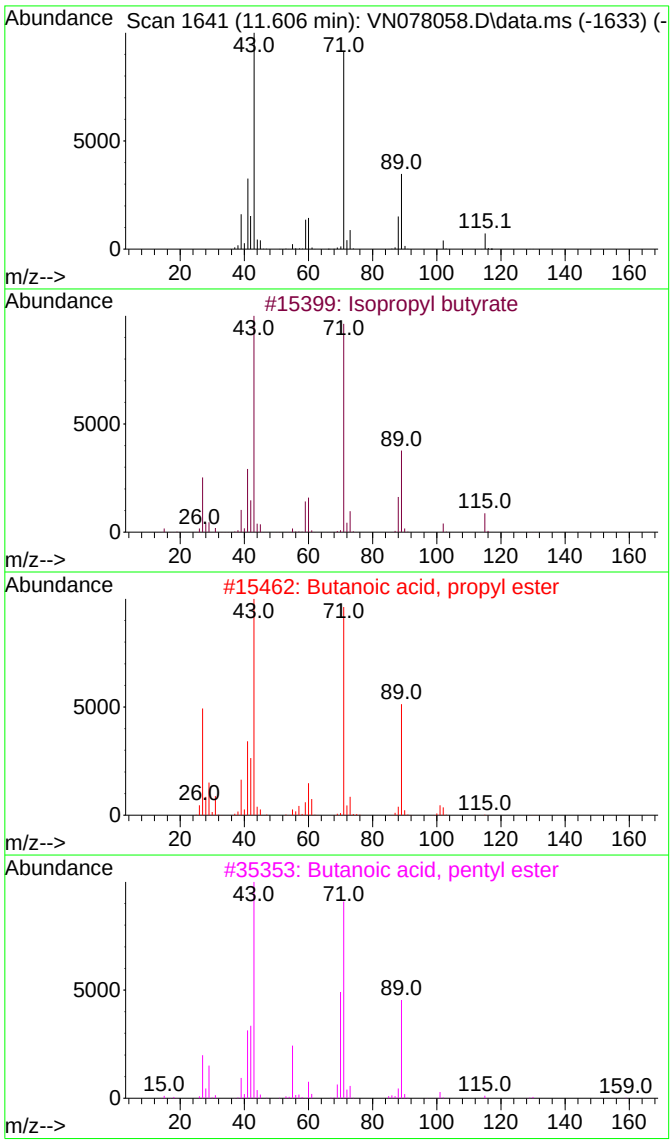
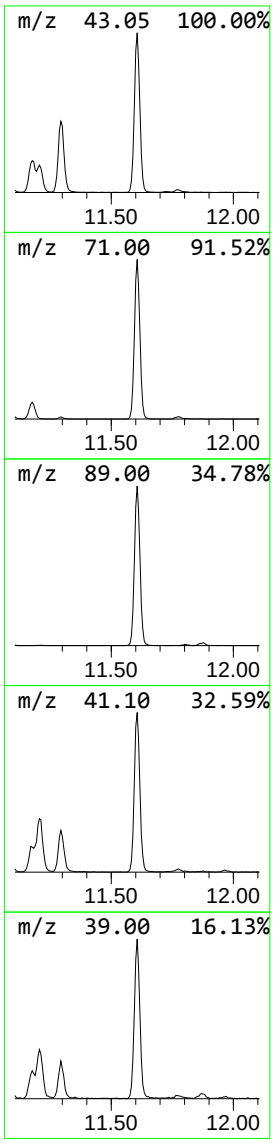
****
Peak Number 9 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.606	95.98 ug/l	3740960	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, propyl ester	130	C7H14O2	000105-66-8	72
3	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
4	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64
5	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	64





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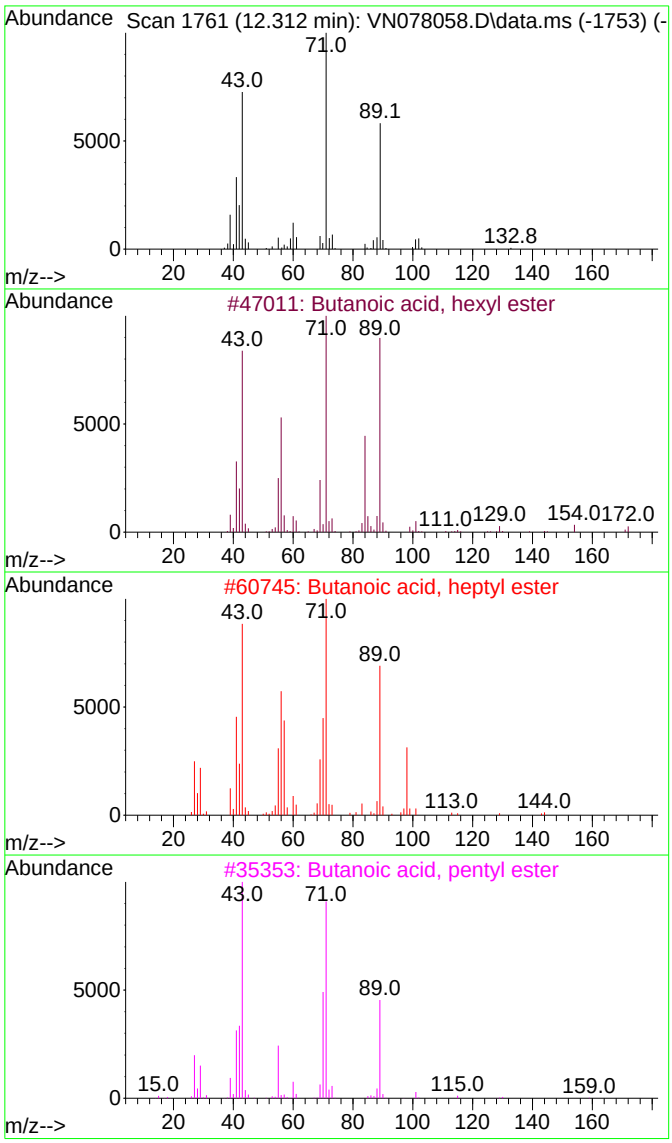
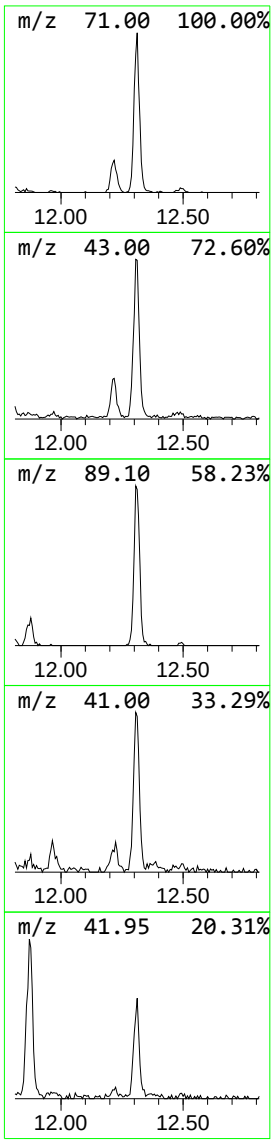
****
Peak Number 10 Butanoic acid, hexyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.312	6.90 ug/l	268865	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	83
2	Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	78
3	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	78
4	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078058.D
Acq On : 05 Jun 2023 20:44
Operator : JC\MD
Sample : 03029-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.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	8.4	ug/l	272949	2	9.106	1619790	50.0
n-Propyl acetate	9.747	145.7	ug/l	4720200	2	9.106	1619790	50.0
Propanoic acid,...	10.365	31.6	ug/l	1024330	2	9.106	1619790	50.0
Isobutyl acetate	10.735	30.0	ug/l	1170840	3	11.871	1948870	50.0
Propanoic acid,...	10.988	35.0	ug/l	1366180	3	11.871	1948870	50.0
Butanoic acid, ...	11.088	7.3	ug/l	283512	3	11.871	1948870	50.0
Propanoic acid,...	11.206	63.5	ug/l	2476020	3	11.871	1948870	50.0
Acetic acid, bu...	11.294	30.1	ug/l	1174180	3	11.871	1948870	50.0
Isopropyl butyrate	11.606	96.0	ug/l	3740960	3	11.871	1948870	50.0
Butanoic acid, ...	12.312	6.9	ug/l	268865	3	11.871	1948870	50.0