LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013124\
Data File : VN080851.D
Acq On : 31 Jan 2024 19:31
Operator : JC\MD
Sample : P1284-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1251

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\82N012924W.M
Title : SW846 8260

Signal : TIC: VN080851.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.500	419	433	442	rBV	34161	141663	2.96%	1.234%
2	8.165	1045	1056	1060	rBV	95687	218826	4.57%	1.906%
3	8.218	1060	1065	1074	rVB	151370	328017	6.85%	2.857%
4	8.577	1117	1126	1137	rBV	109779	255988	5.35%	2.230%
5	9.100	1204	1215	1221	rBV2	302650	677913	14.16%	5.904%
6	9.218	1221	1235	1249	rVB	1757470	4788349	100.00%	41.704%
7	9.888	1344	1349	1356	rVB2	50439	90888	1.90%	0.792%
8	10.565	1455	1464	1473	rBV	400214	760938	15.89%	6.627%
9	11.865	1674	1685	1694	rBV	463124	857293	17.90%	7.467%
10	12.423	1769	1780	1785	rBV2	48349	88506	1.85%	0.771%
11	12.853	1841	1853	1859	rBV	294835	551219	11.51%	4.801%
12	13.259	1912	1922	1929	rBV3	89738	198966	4.16%	1.733%
13	13.341	1929	1936	1946	rVB	638618	955279	19.95%	8.320%
14	13.688	1990	1995	2001	rVV3	56286	92511	1.93%	0.806%
15	13.794	2005	2013	2020	rBV	423836	689629	14.40%	6.006%
16	13.876	2020	2027	2037	rVV	242960	398163	8.32%	3.468%
17	15.082	2228	2232	2240	rVB4	38233	66142	1.38%	0.576%
18	15.394	2280	2285	2294	rVV3	39578	70698	1.48%	0.616%
19	15.594	2314	2319	2326	rVB4	45402	91532	1.91%	0.797%
20	16.641	2488	2497	2511	rBV3	36145	159188	3.32%	1.386%

Sum of corrected areas: 11481708

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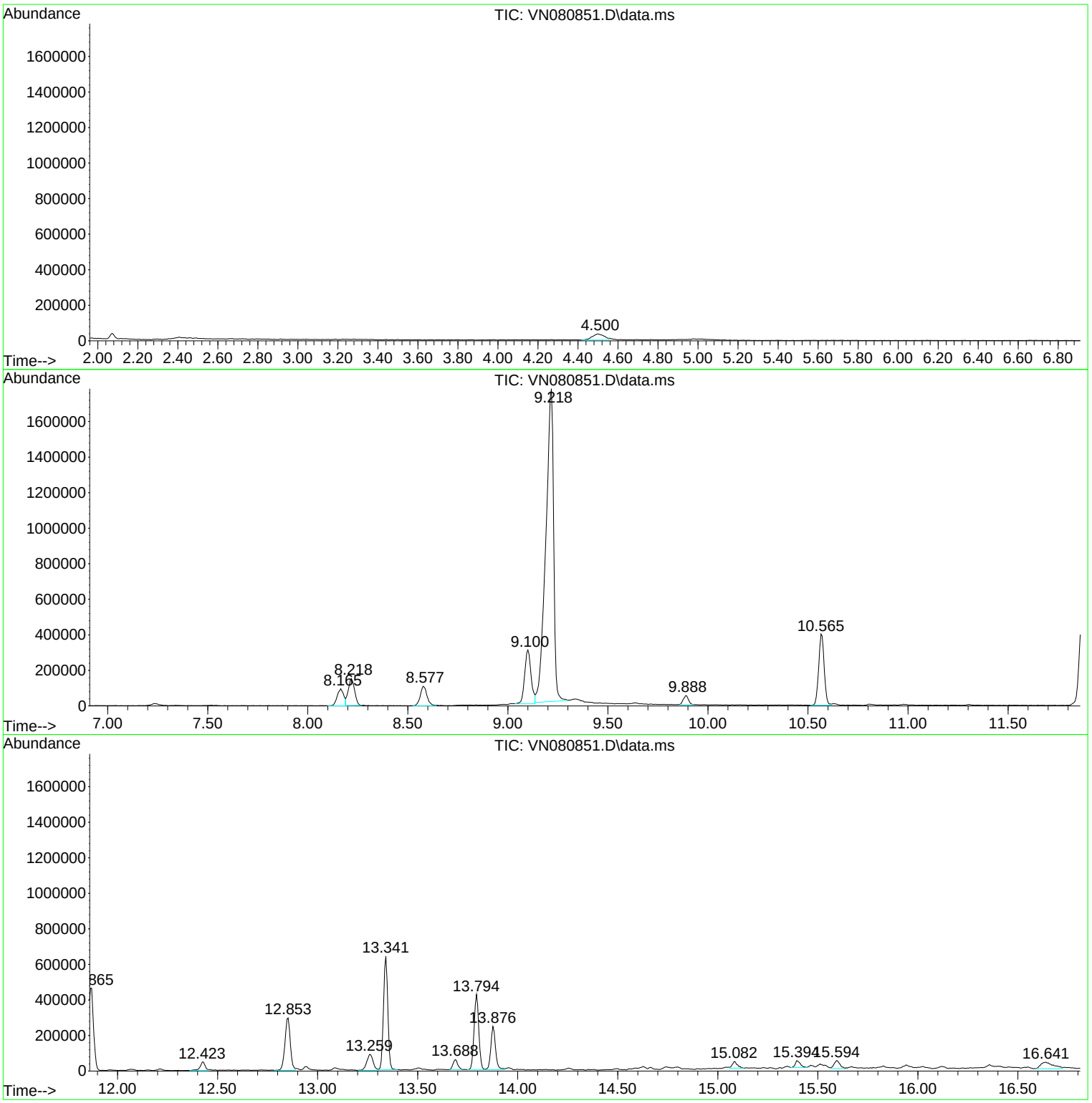
Instrument :
MSVOA_N
ClientSampleId :
1251

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

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



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Quant Title : SW846 8260

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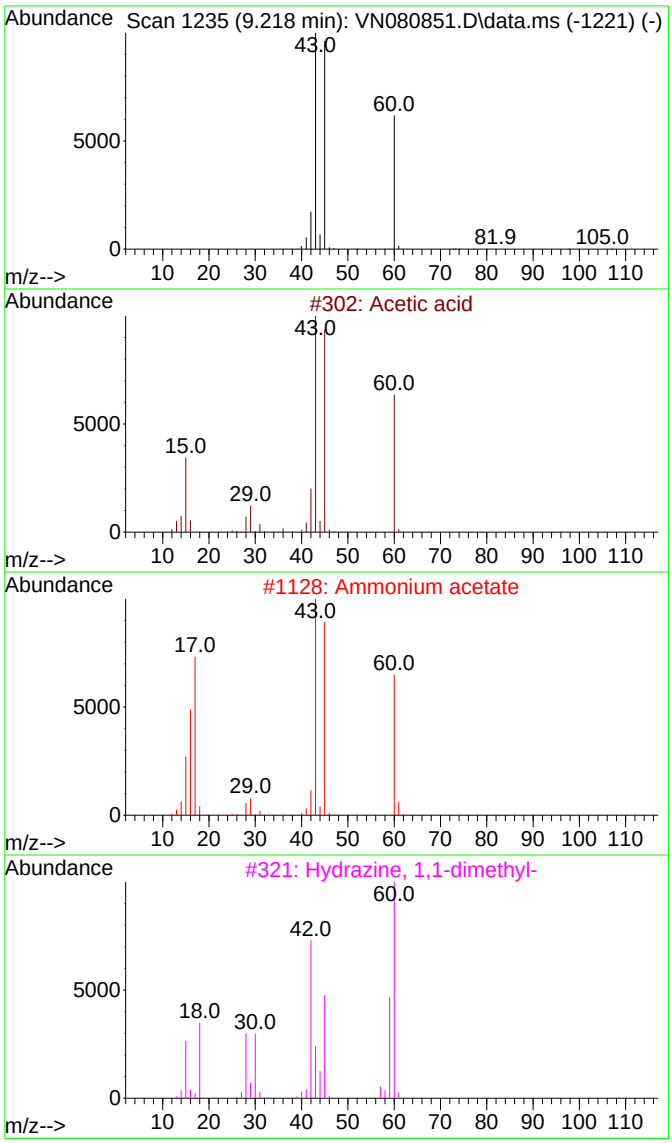
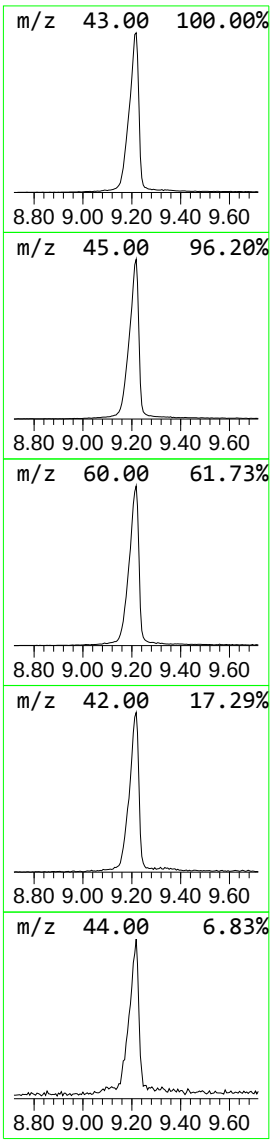
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Acetic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.218	353.17 ug/l	4788350	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	90
2	Ammonium acetate	77	C2H7NO2	000631-61-8	74
3	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
4	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
5	Thiirane	60	C2H4S	000420-12-2	5





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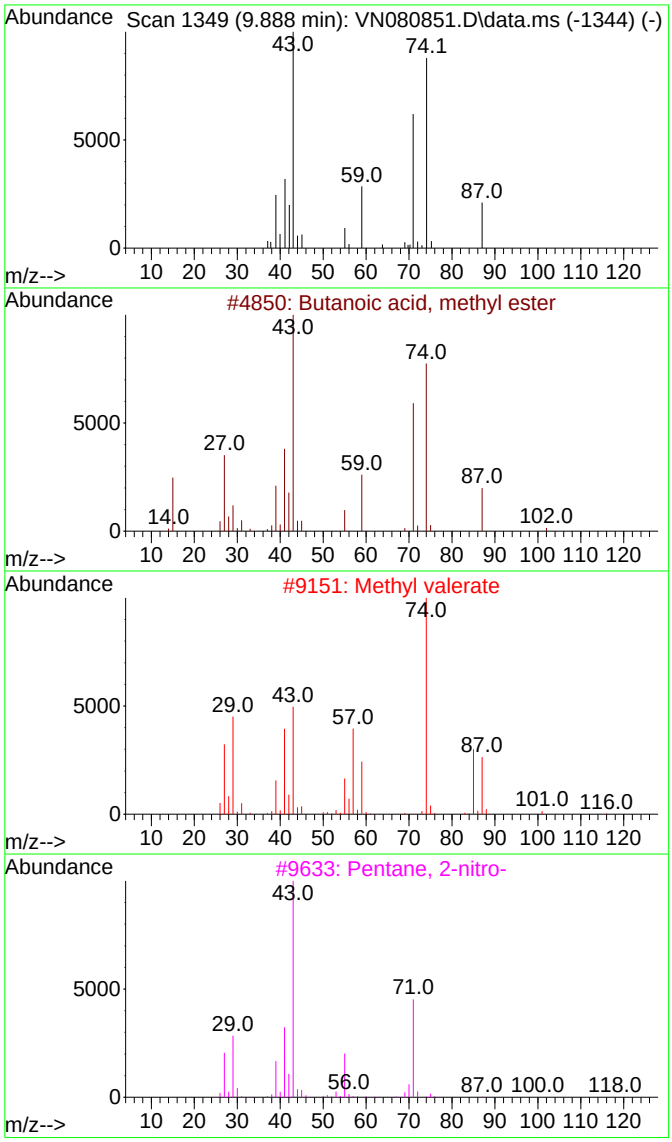
Quant Title : SW846 8260

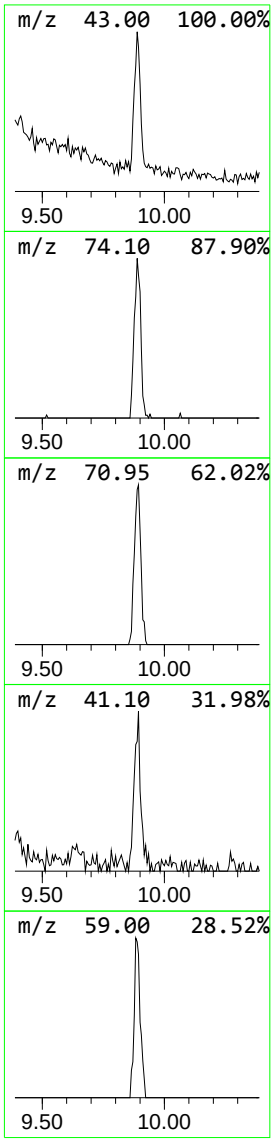
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butanoic acid, methyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.888	6.70 ug/l	90888	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	83
2	Methyl valerate	116	C6H12O2	000624-24-8	25
3	Pentane, 2-nitro-	117	C5H11NO2	004609-89-6	10
4	Sulfurous acid, pentyl 2-propyl ...	194	C8H18O3S	1000309-11-5	10
5	(3S)-3-Pyrrolidinol	87	C4H9NO	100243-39-8	10





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Instrument :
MSVOA_N
ClientSampleId :
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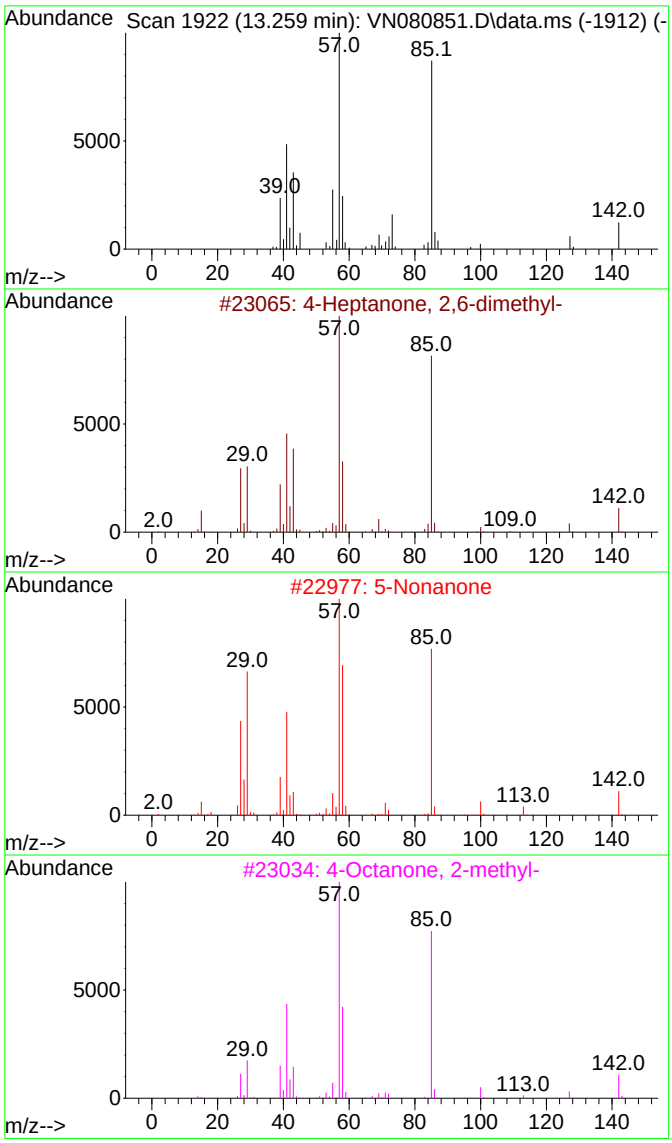
Quant Title : SW846 8260

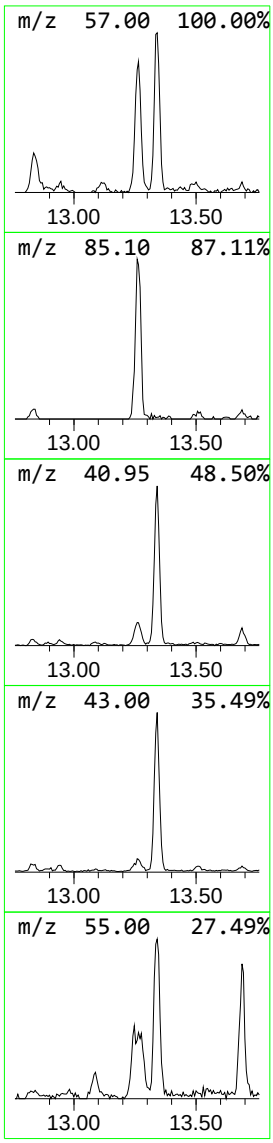
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 4-Heptanone, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.259	14.43 ug/l	198966	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanone, 2,6-dimethyl-	142	C9H18O	000108-83-8	87
2	5-Nonanone	142	C9H18O	000502-56-7	64
3	4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	64
4	Allyl isovalerate	142	C8H14O2	002835-39-4	53
5	Sulfurous acid, butyl hexyl ester	222	C10H22O3S	1000309-17-3	53





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Instrument :
MSVOA_N
ClientSampleId :
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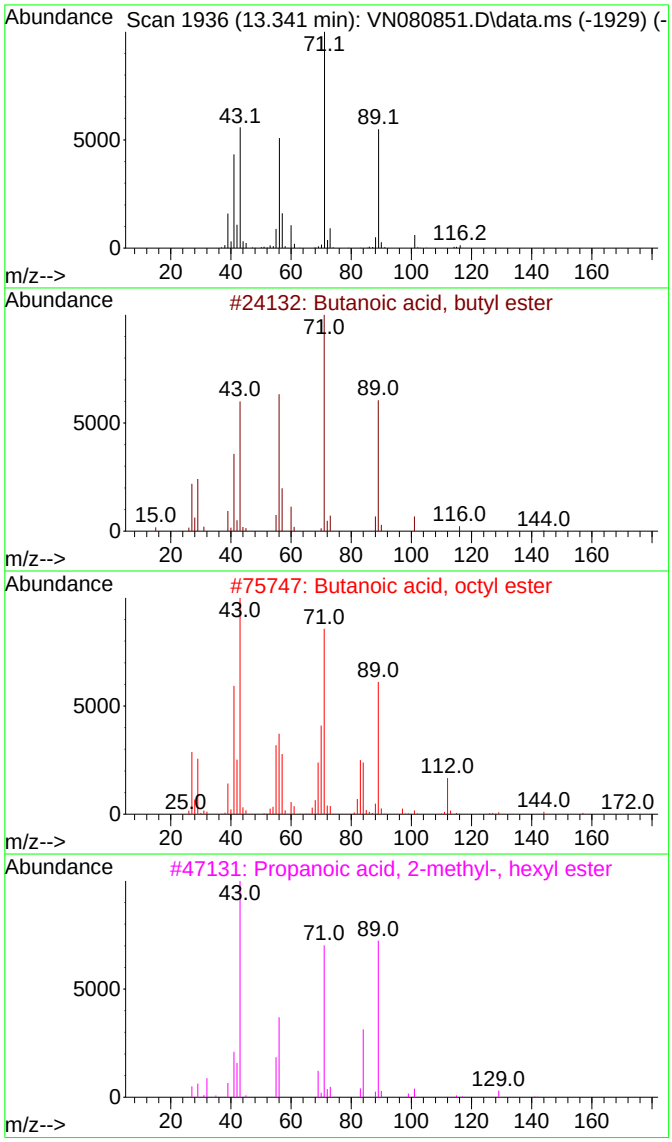
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

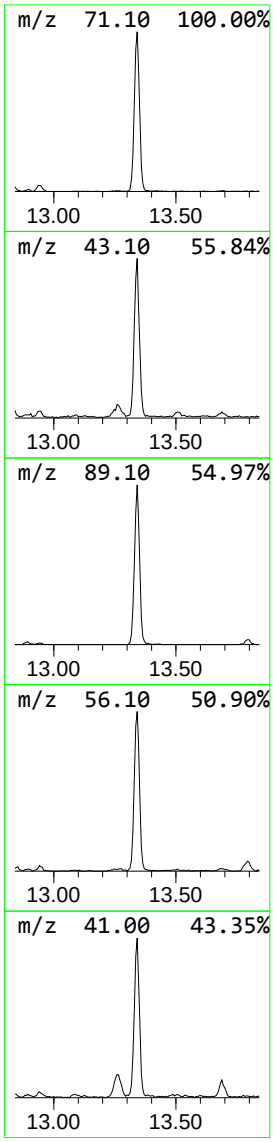
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butanoic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	69.26 ug/l	955279	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	83
2	Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	72
3	Propanoic acid, 2-methyl-, hexyl...	172	C10H20O2	002349-07-7	72
4	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	64
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59





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Sample : P1284-05
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ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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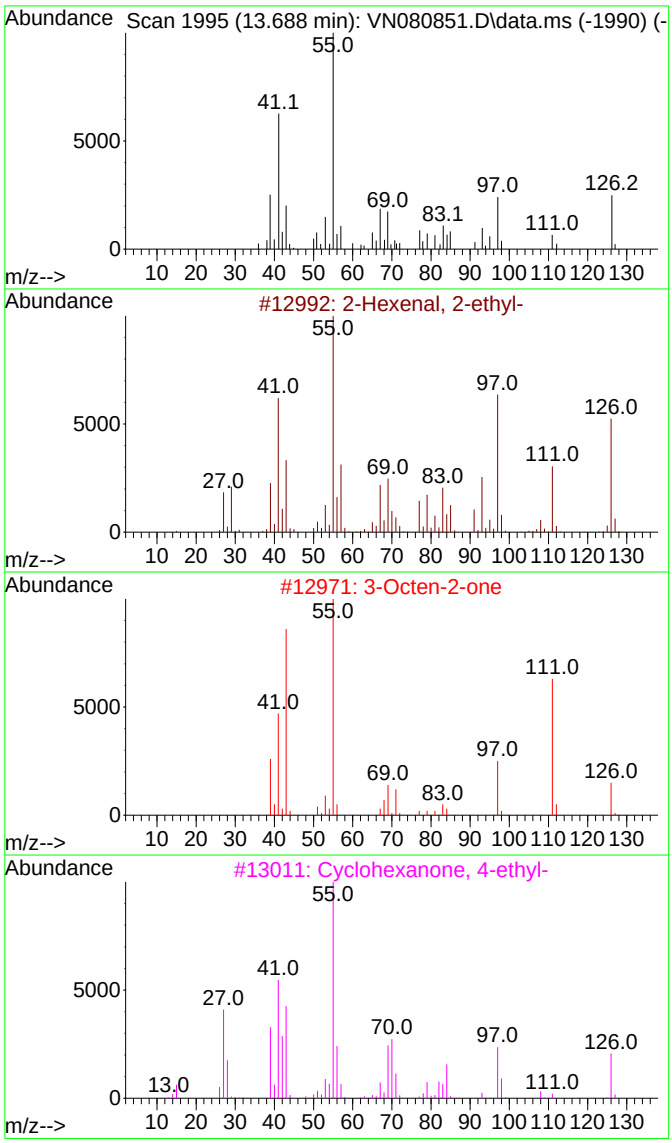
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

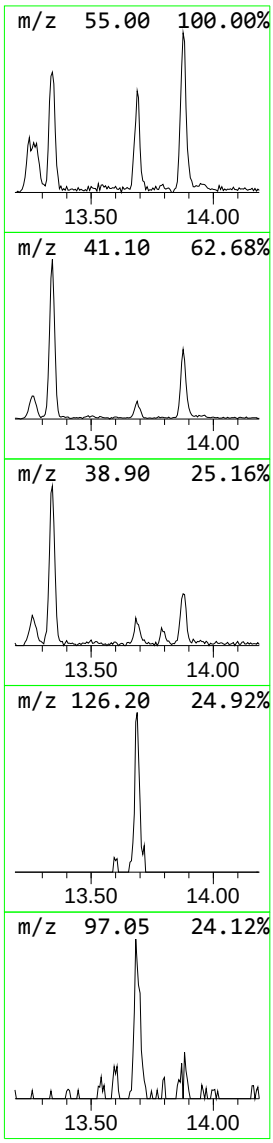
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Hexenal, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.688	6.71 ug/l	92511	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexenal, 2-ethyl-	126	C8H14O	000645-62-5	68
2	3-Octen-2-one	126	C8H14O	001669-44-9	43
3	Cyclohexanone, 4-ethyl-	126	C8H14O	005441-51-0	42
4	3,5-Octadien-2-ol	126	C8H14O	069668-82-2	42
5	2,4-Pentadien-1-ol, 3-propyl-, (...	126	C8H14O	1000142-17-9	38





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MSVOA_N
ClientSampleId :
1251

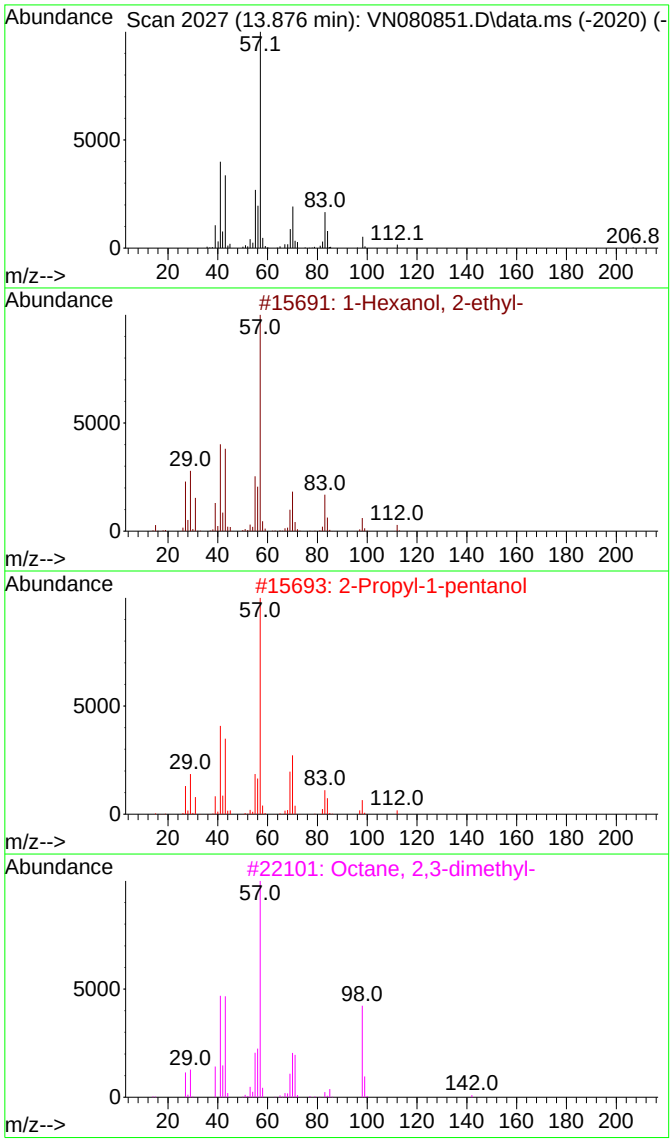
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

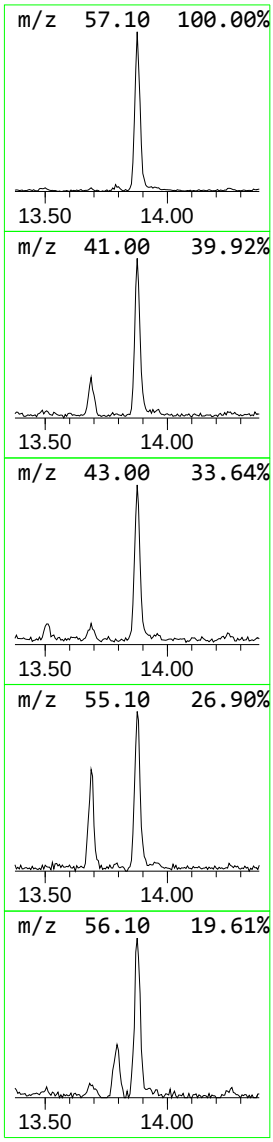
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	28.87 ug/l	398163	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	59
4	1-Decene, 3,4-dimethyl-	168	C12H24	050871-03-9	50
5	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	45





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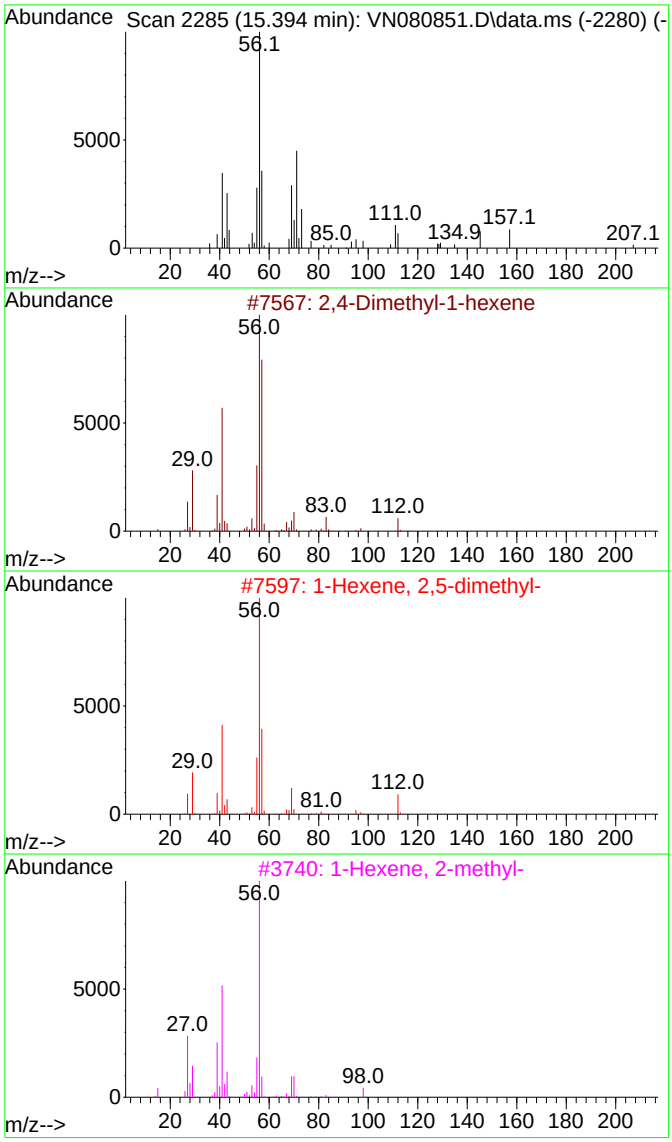
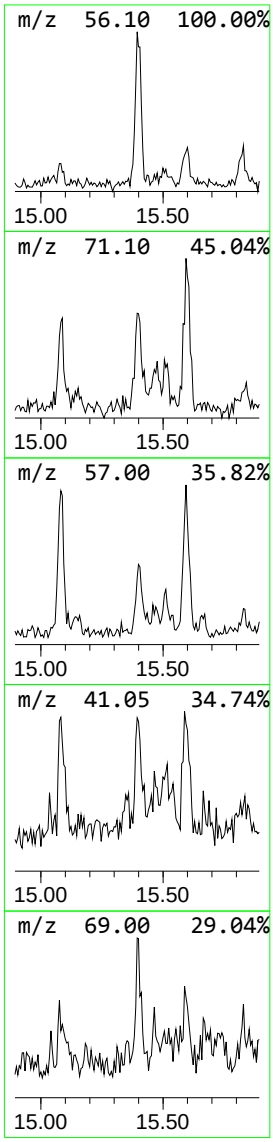
****

Peak Number 7 unknown15.394 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.394	5.13 ug/l	70698	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Dimethyl-1-hexene	112	C8H16	016746-87-5	38
2	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	38
3	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	35
4	1-Octene, 2-methyl-	126	C9H18	004588-18-5	32
5	1-Undecene, 2-methyl-	168	C12H24	018516-37-5	32





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ClientSampleId :
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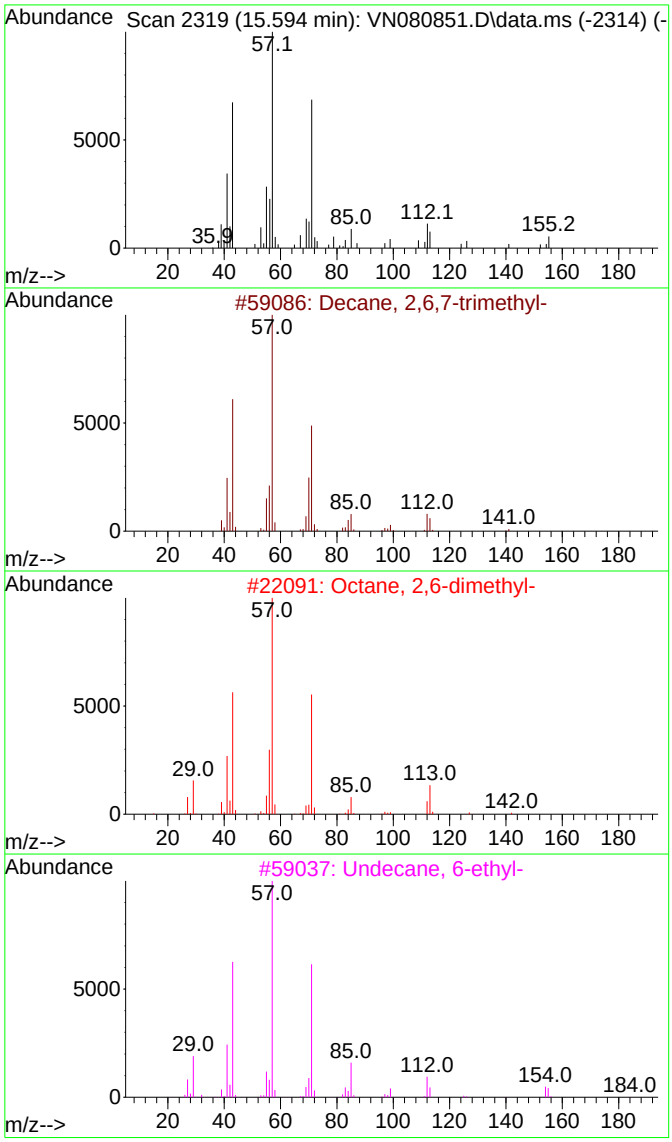
Quant Title : SW846 8260

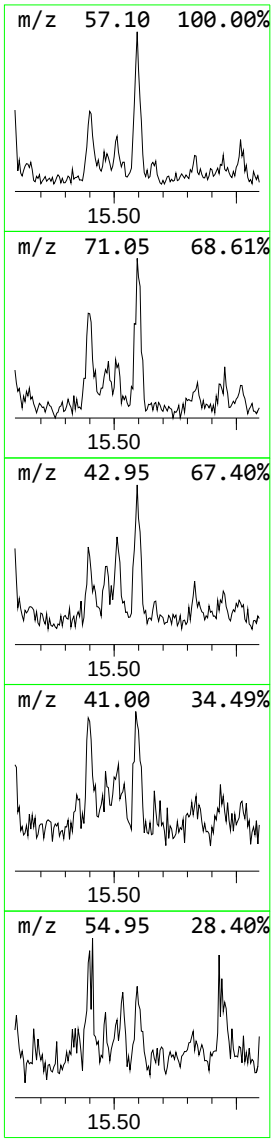
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Decane, 2,6,7-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.594	6.64 ug/l	91532	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	78
2	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	64
3	Undecane, 6-ethyl-	184	C13H28	017312-60-6	64
4	Undecane, 4,5-dimethyl-	184	C13H28	017312-79-7	64
5	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	64





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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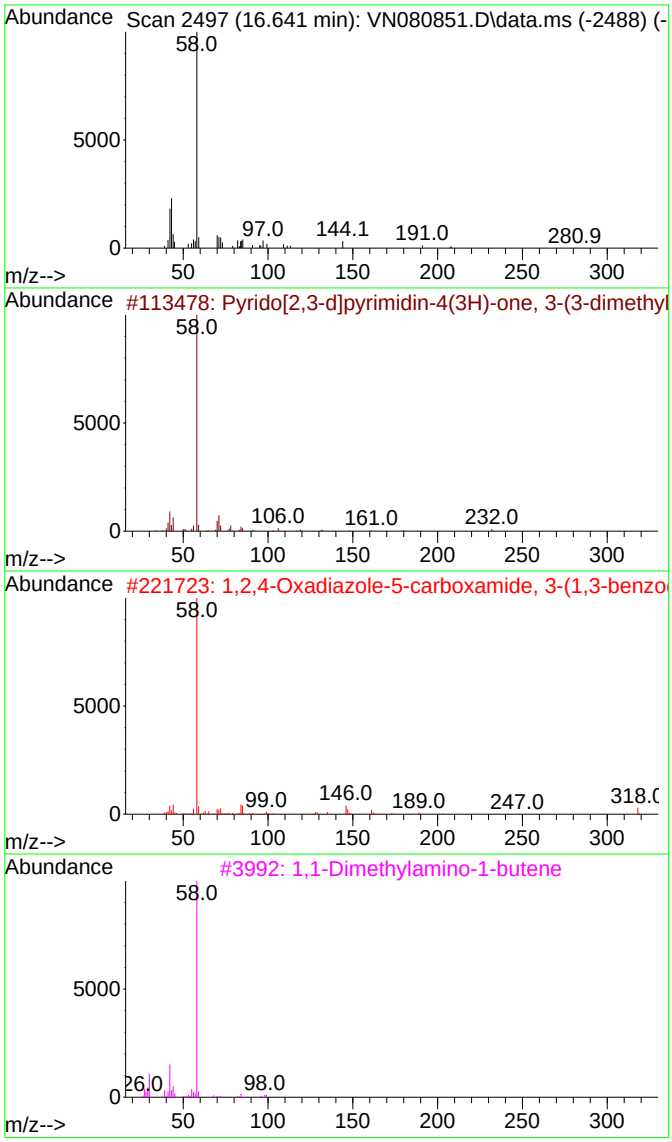
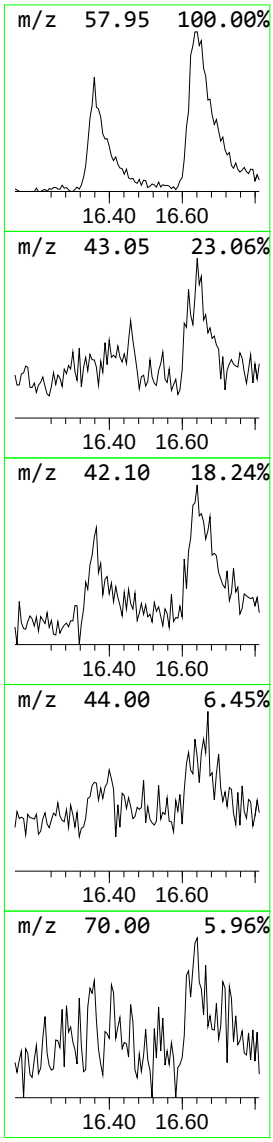
****
Peak Number 9 Pyrido[2,3-d]pyrimidin-4(3H... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.641	11.54 ug/l	159188	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrido[2,3-d]pyrimidin-4(3H)-one...	232	C12H16N4O	1000264-17-8	72
2	1,2,4-Oxadiazole-5-carboxamide, ...	318	C15H18N4O4	1000350-15-5	72
3	1,1-Dimethylamino-1-butene	99	C6H13N	014548-12-0	72
4	3-(Dimethylamino)propyl isothioc...	144	C6H12N2S	027421-70-1	64
5	4-Pentenylamine, N,N-dimethyl-	113	C7H15N	001001-91-8	64





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Acetic acid	9.218	353.2	ug/l	4788350	2	9.100	677913	50.0
Butanoic acid, ...	9.888	6.7	ug/l	90888	2	9.100	677913	50.0
4-Heptanone, 2,...	13.259	14.4	ug/l	198966	4	13.794	689629	50.0
Butanoic acid, ...	13.341	69.3	ug/l	955279	4	13.794	689629	50.0
2-Hexenal, 2-et...	13.688	6.7	ug/l	92511	4	13.794	689629	50.0
1-Hexanol, 2-et...	13.876	28.9	ug/l	398163	4	13.794	689629	50.0
unknown15.394	15.394	5.1	ug/l	70698	4	13.794	689629	50.0
Decane, 2,6,7-t...	15.594	6.6	ug/l	91532	4	13.794	689629	50.0
Pyrido[2,3-d]py...	16.641	11.5	ug/l	159188	4	13.794	689629	50.0