LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN013124\
Data File : VN080854.D
Acq On : 31 Jan 2024 20:42
Operator : JC\MD
Sample : P1284-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
1142

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: VN080854.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.659	112	120	131	rBV	521806	918860	8.04%	3.612%
2	3.789	304	312	322	rBV	70304	190752	1.67%	0.750%
3	4.177	368	378	385	rBV2	77187	230330	2.02%	0.905%
4	4.283	385	396	411	rVV	3744560	11423764	100.00%	44.904%
5	4.424	412	420	437	rVB	219028	703438	6.16%	2.765%
6	6.135	698	711	723	rBV2	41527	141558	1.24%	0.556%
7	6.730	799	812	830	rBV	1157364	3526100	30.87%	13.860%
8	7.224	883	896	907	rBV2	378485	1036671	9.07%	4.075%
9	7.482	932	940	950	rBV	95815	236936	2.07%	0.931%
10	8.165	1045	1056	1061	rBV2	86018	211642	1.85%	0.832%
11	8.224	1061	1066	1075	rVB2	141173	319564	2.80%	1.256%
12	8.582	1121	1127	1137	rVB2	104378	239985	2.10%	0.943%
13	9.100	1208	1215	1225	rVB	267864	551219	4.83%	2.167%
14	9.265	1235	1243	1250	rBV2	88562	173518	1.52%	0.682%
15	9.653	1299	1309	1320	rBV2	53405	126847	1.11%	0.499%
16	10.570	1456	1465	1472	rBV	388049	728872	6.38%	2.865%
17	11.865	1680	1685	1698	rVB	437929	811834	7.11%	3.191%
18	12.212	1738	1744	1752	rVB	69003	119421	1.05%	0.469%
19	12.382	1764	1773	1777	rBV	140002	233665	2.05%	0.918%
20	12.459	1782	1786	1798	rVB2	68100	118945	1.04%	0.468%
21	12.800	1835	1844	1848	rBV	152923	271342	2.38%	1.067%
22	12.853	1848	1853	1862	rVB	293718	511105	4.47%	2.009%
23	13.259	1915	1922	1927	rBV	100124	183685	1.61%	0.722%
24	13.635	1976	1986	1990	rBV	82189	150779	1.32%	0.593%
25	13.688	1990	1995	2005	rVB	324524	525914	4.60%	2.067%
26	13.794	2005	2013	2020	rBV	434055	728091	6.37%	2.862%
27	13.876	2020	2027	2037	rBV	561692	894727	7.83%	3.517%
28	14.635	2149	2156	2163	rVB	81054	130997	1.15%	0.515%

Sum of corrected areas: 25440561

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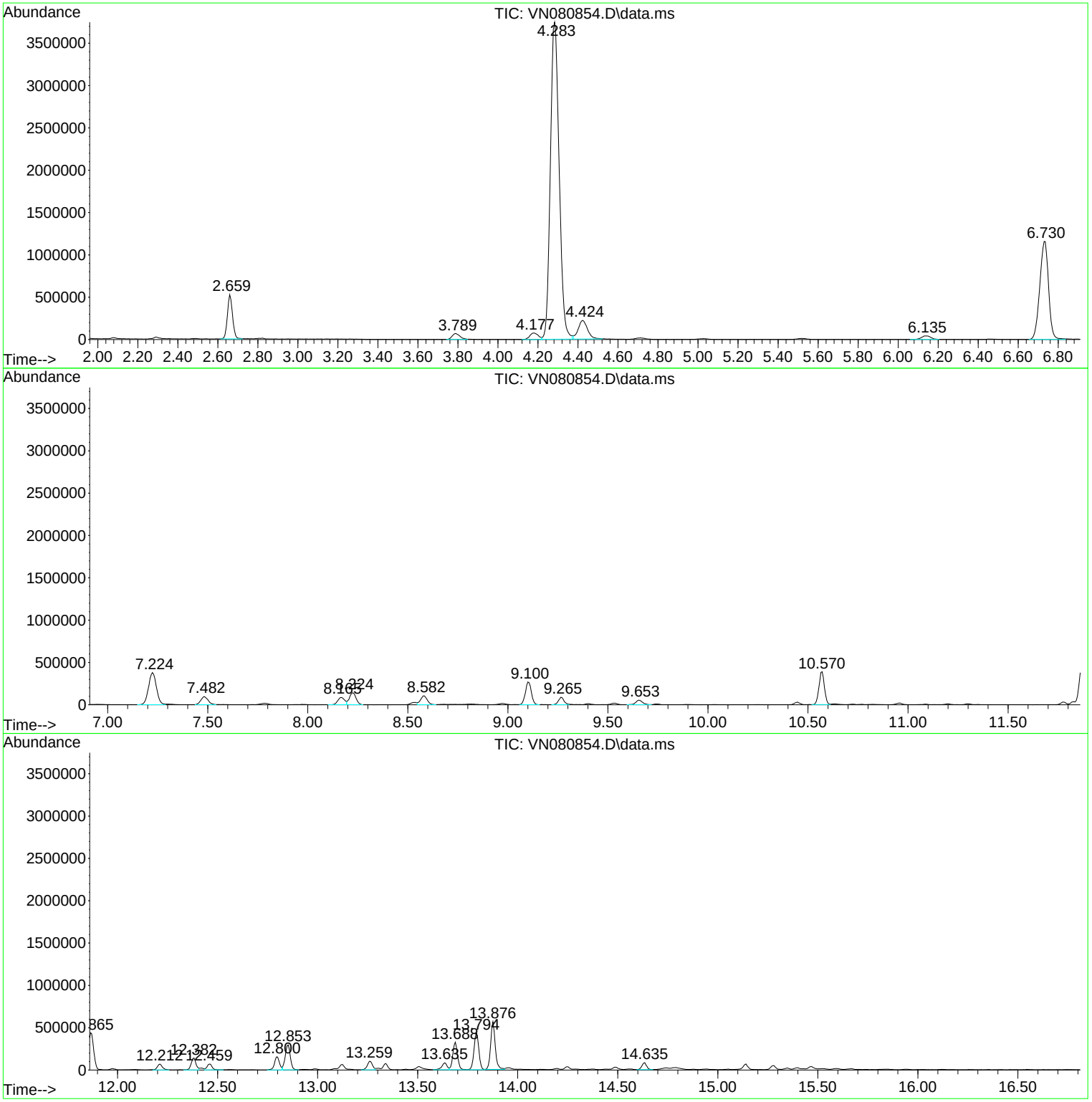
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

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



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Quant Title : SW846 8260

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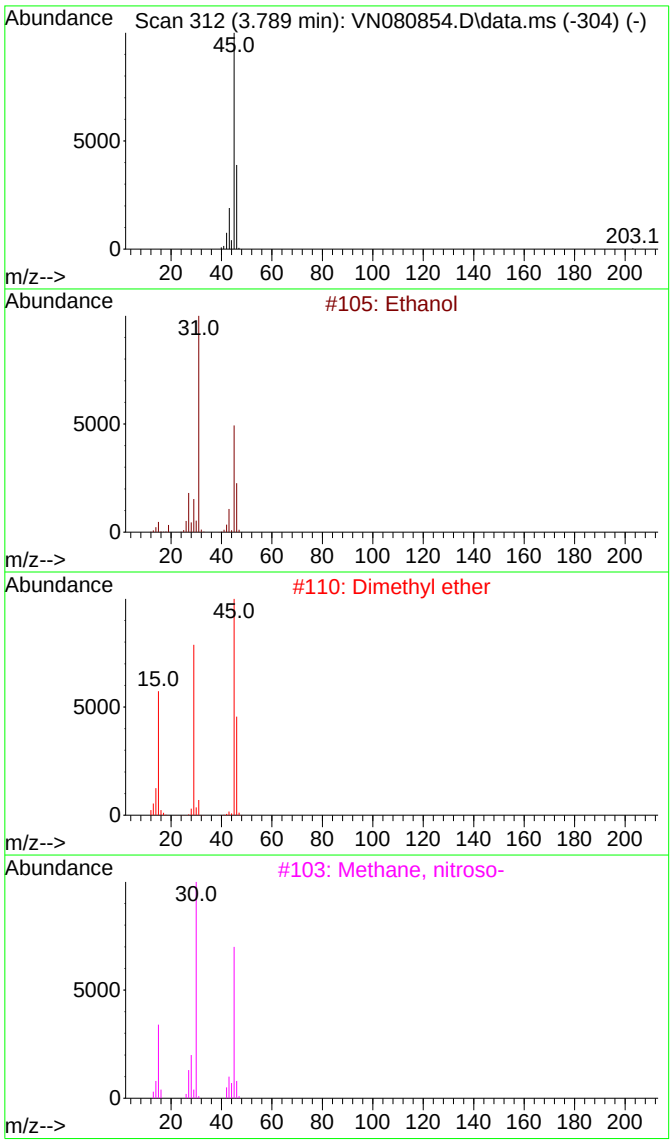
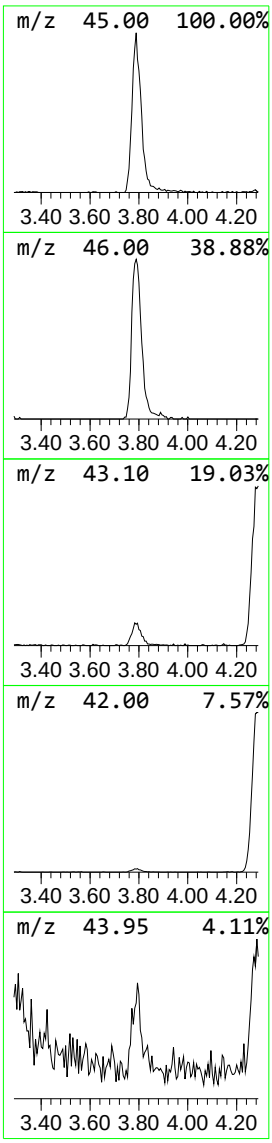
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.789	29.85 ug/l	190752	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	74
2	Dimethyl ether	46	C2H6O	000115-10-6	5
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Nitric acid, pentyl ester	133	C5H11NO3	001002-16-0	4
5	Formamide	45	CH3NO	000075-12-7	3





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Instrument :
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Quant Title : SW846 8260

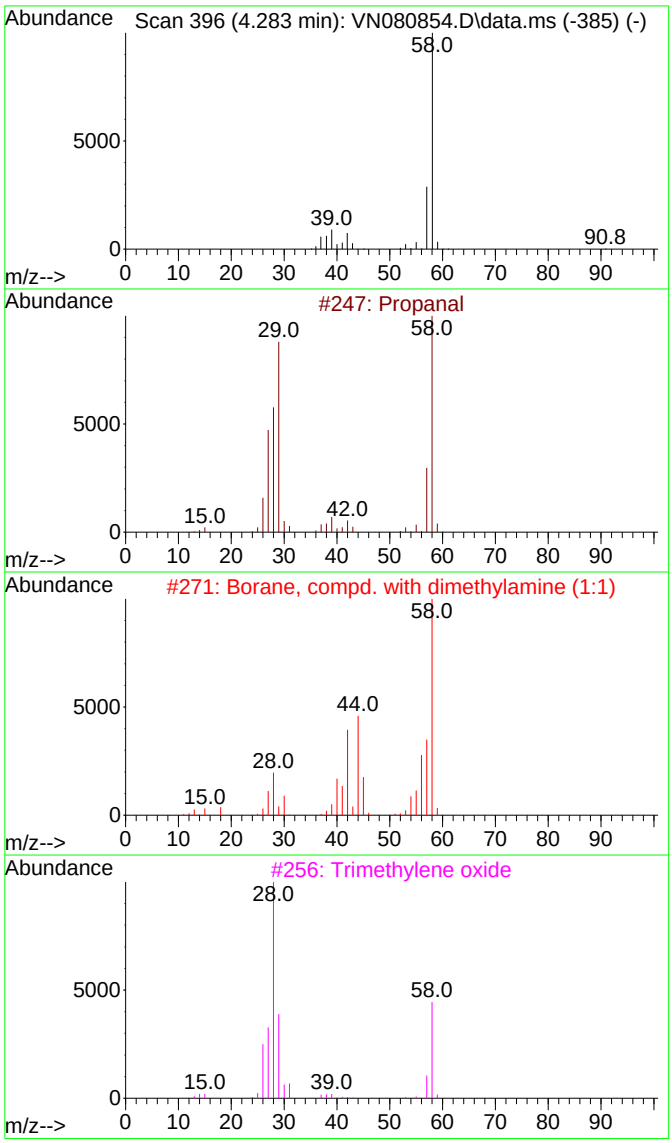
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

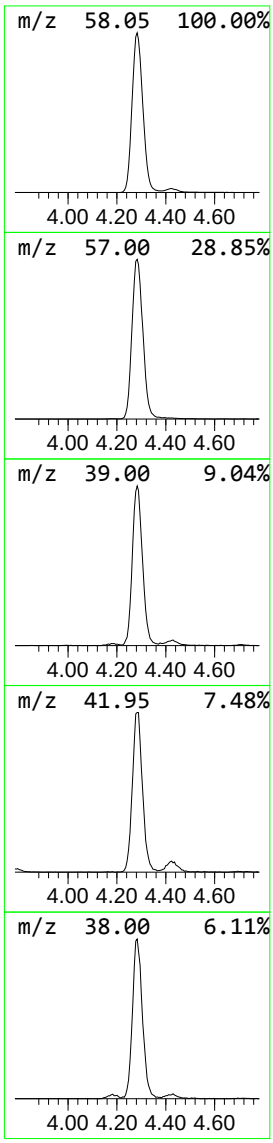
****

Peak Number 3 Propanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.283	1787.40 ug/l	11423800	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal	58	C3H6O	000123-38-6	72
2	Borane, compd. with dimethylamin...	59	C2H10BN	000074-94-2	9
3	Trimethylene oxide	58	C3H6O	000503-30-0	9
4	2-(Aminomethyl)-4-methylpentanoi...	187	C10H21NO2	1891211-54-3	9
5	Propylene oxide	58	C3H6O	000075-56-9	7





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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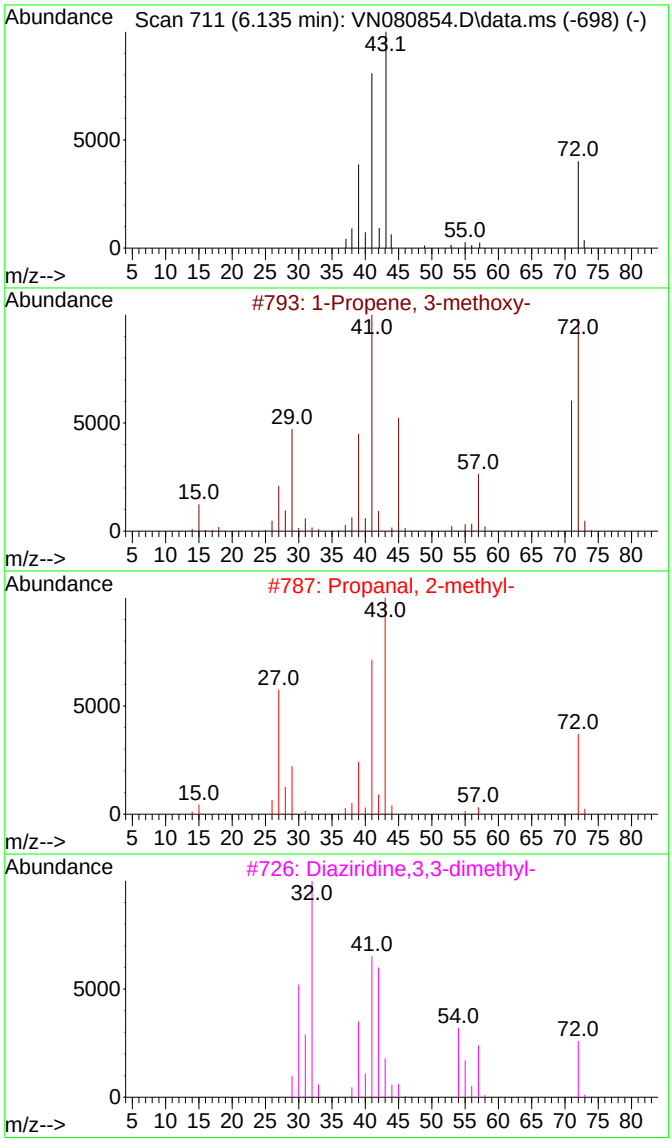
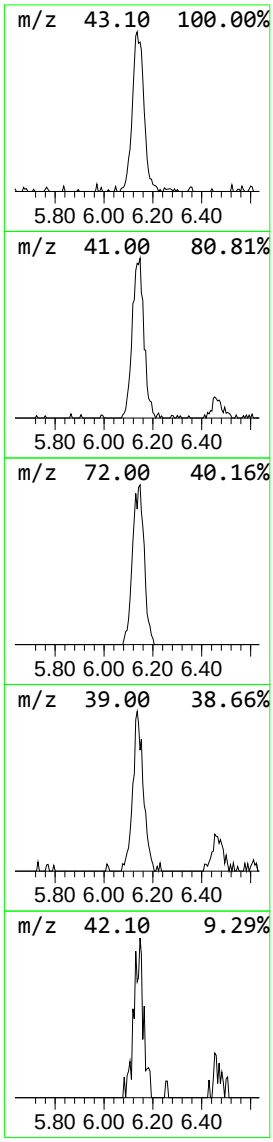
****
Peak Number 4 1-Propene, 3-methoxy- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.135	22.15 ug/l	141558	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	64
2	Propanal, 2-methyl-	72	C4H8O	000078-84-2	58
3	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	45
4	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	36
5	Ethene, ethoxy-	72	C4H8O	000109-92-2	32





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

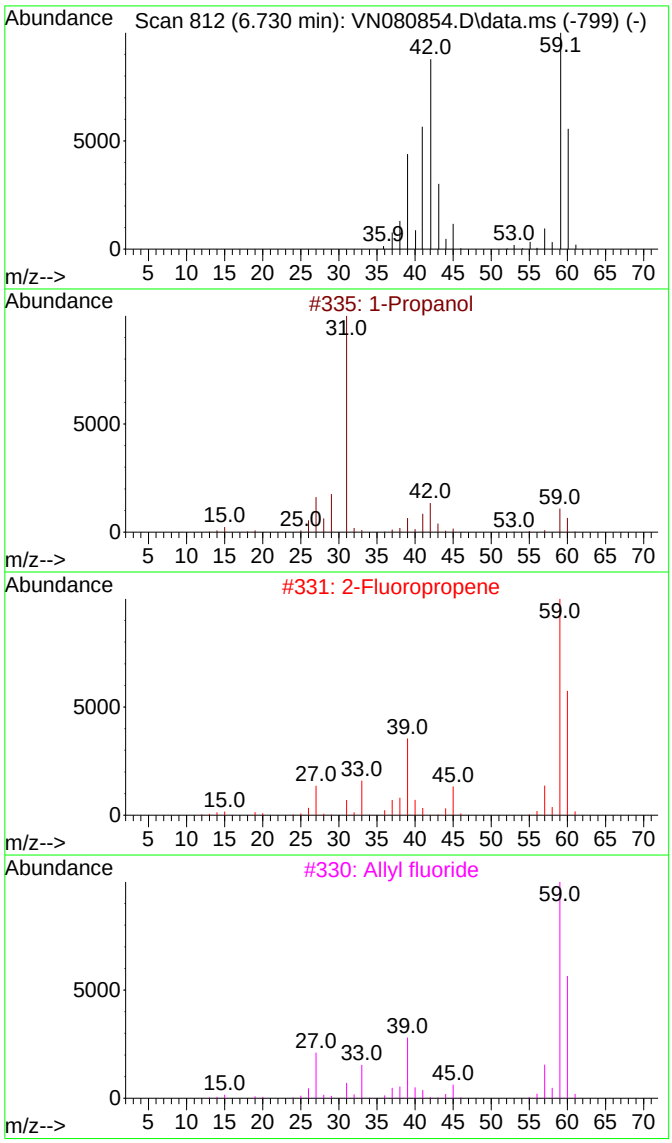
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

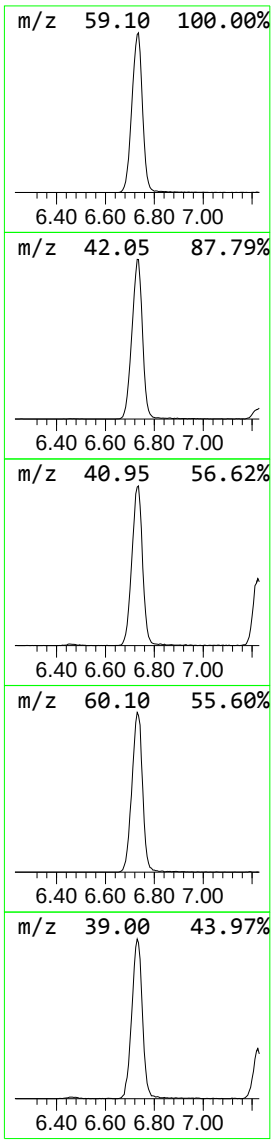
****

Peak Number 5 1-Propanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.730	551.71 ug/l	3526100	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	64
2	2-Fluoropropene	60	C3H5F	001184-60-7	52
3	Allyl fluoride	60	C3H5F	000818-92-8	32
4	Cyclopropane	42	C3H6	000075-19-4	25
5	Propene	42	C3H6	000115-07-1	17





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Instrument :
MSVOA_N
ClientSampleId :
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Quant Title : SW846 8260

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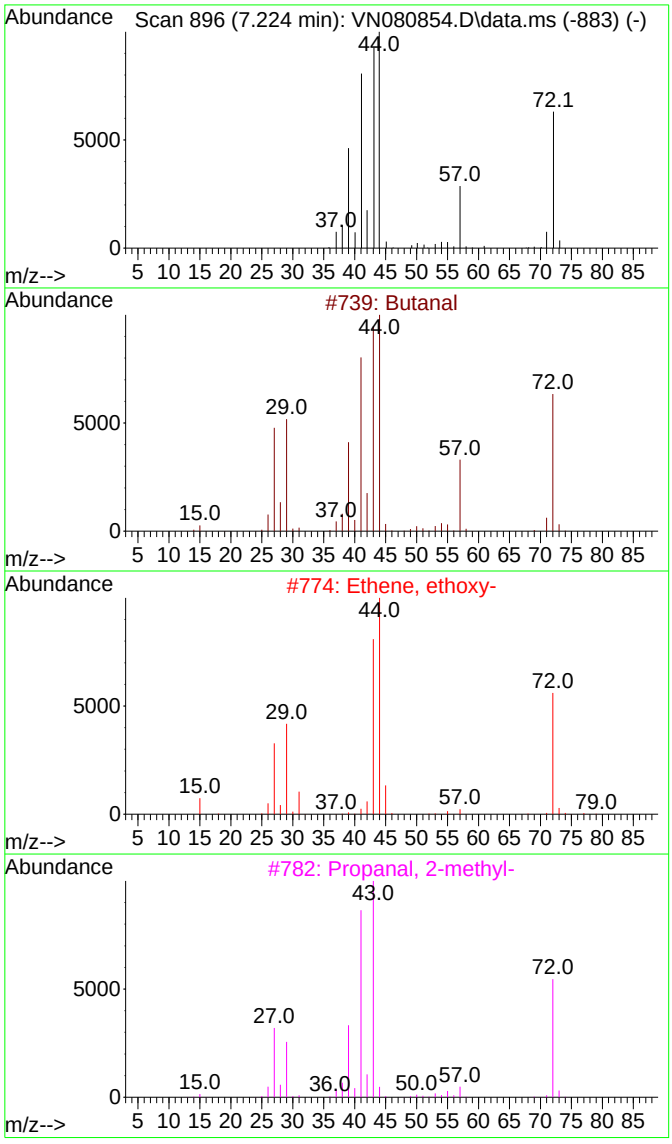
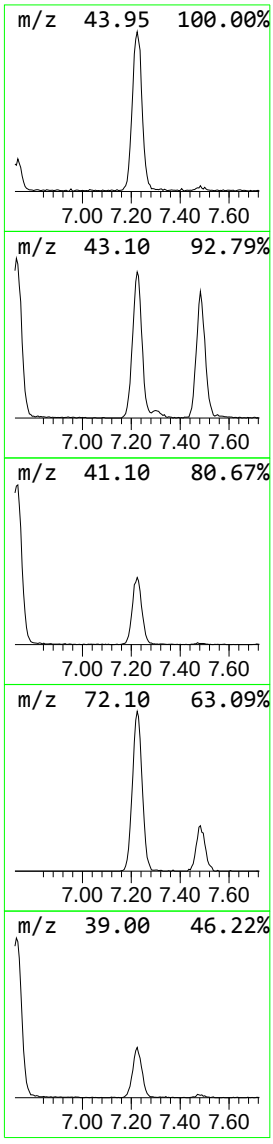
****

Peak Number 6 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	162.20 ug/l	1036670	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	52
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	52
4	2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	23
5	2-Butenal, (Z)-	70	C4H6O	015798-64-8	14





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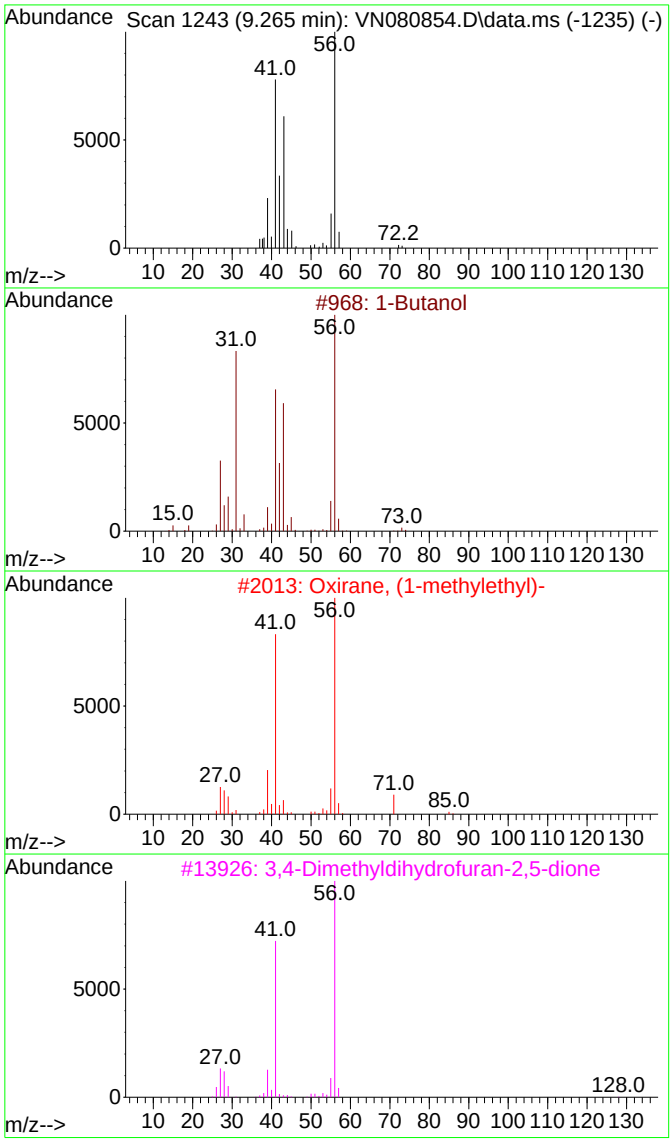
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N012924W.M
Quant Title : SW846 8260

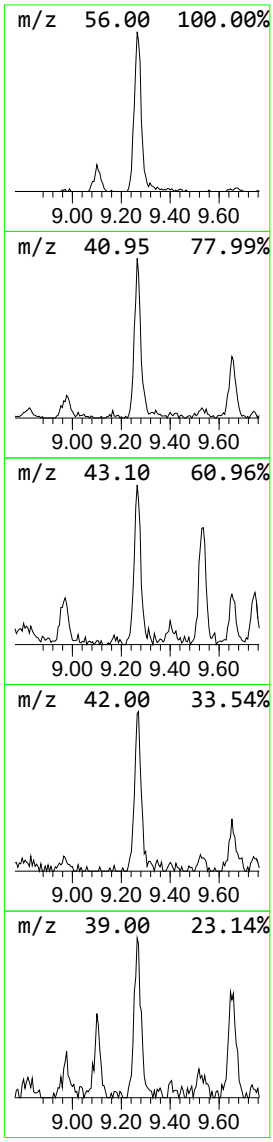
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1-Butanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.265	15.74 ug/l	173518	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	72
2	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	42
3	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	42
4	o-Allylhydroxylamine	73	C3H7NO	006542-54-7	9
5	Aziridine, 1-(2-buten-2-yl)-	97	C6H11N	1000158-95-2	9





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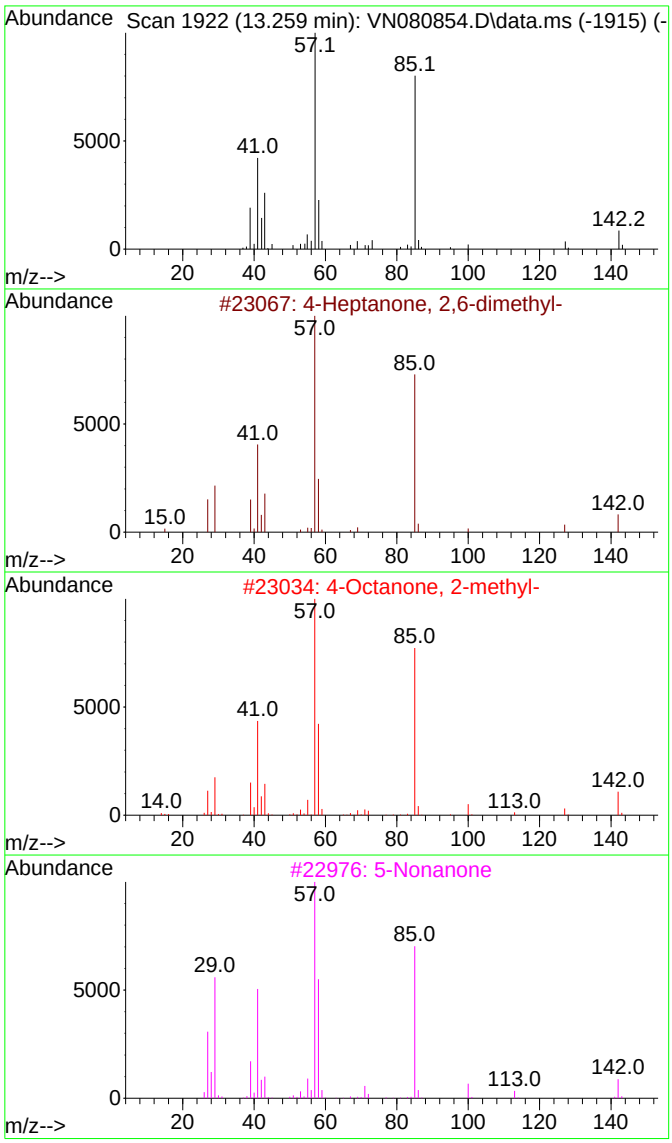
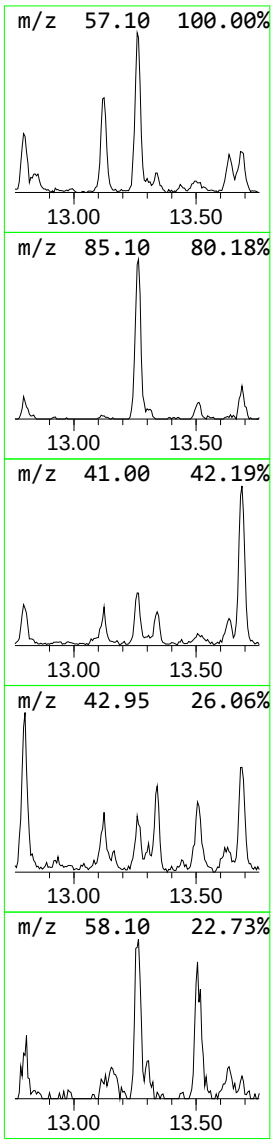
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 4-Heptanone, 2,6-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.259	12.61 ug/l	183685	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	90
2	4-Octanone, 2-methyl-	142	C9H18O	007492-38-8	74
3	5-Nonanone	142	C9H18O	000502-56-7	64
4	1-Propoxypropan-2-yl 2-methylbut...	202	C11H22O3	1000367-10-7	56
5	2,4-Hexanedione, 5,5-dimethyl-	142	C8H14O2	007307-04-2	53





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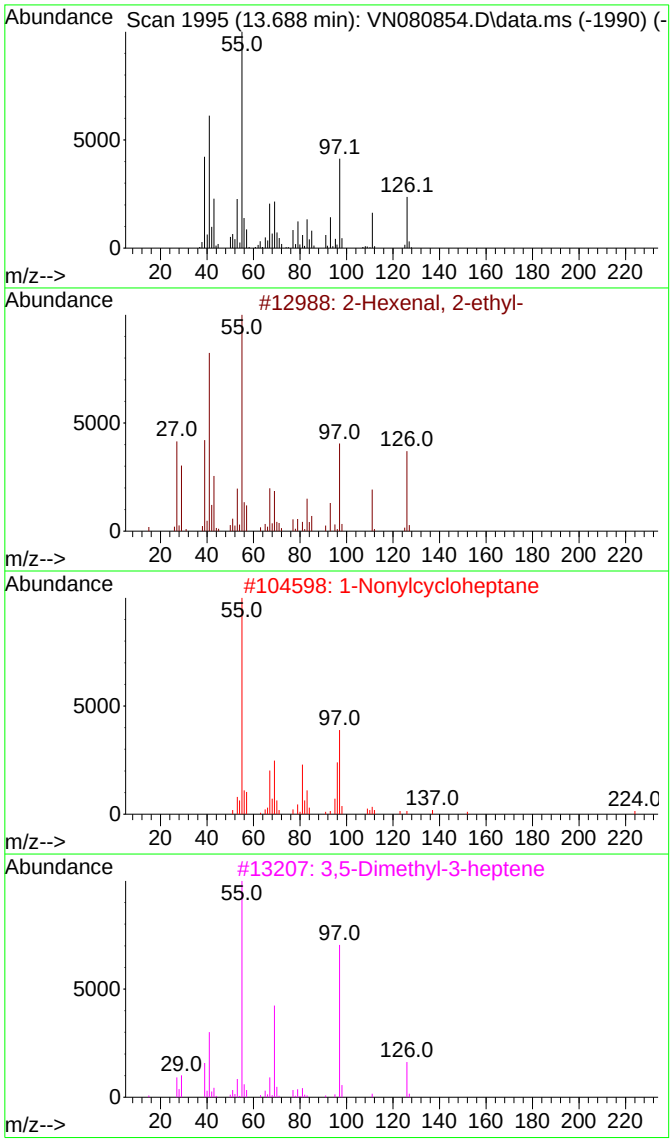
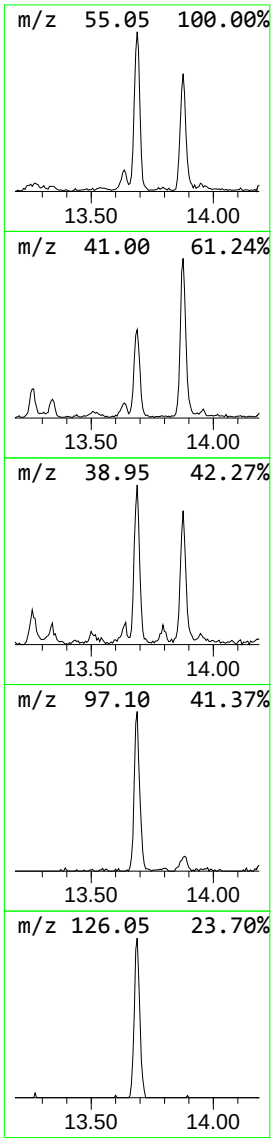
****
Peak Number 9 2-Hexenal, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.688	36.12 ug/l	525914	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	64
2	1-Nonylcycloheptane	224	C16H32	1000371-47-7	38
3	3,5-Dimethyl-3-heptene	126	C9H18	059643-68-4	38
4	2,4-Pentadien-1-ol, 3-propyl-, (...	126	C8H14O	1000142-17-9	35
5	3,5-Octadien-2-ol	126	C8H14O	069668-82-2	35





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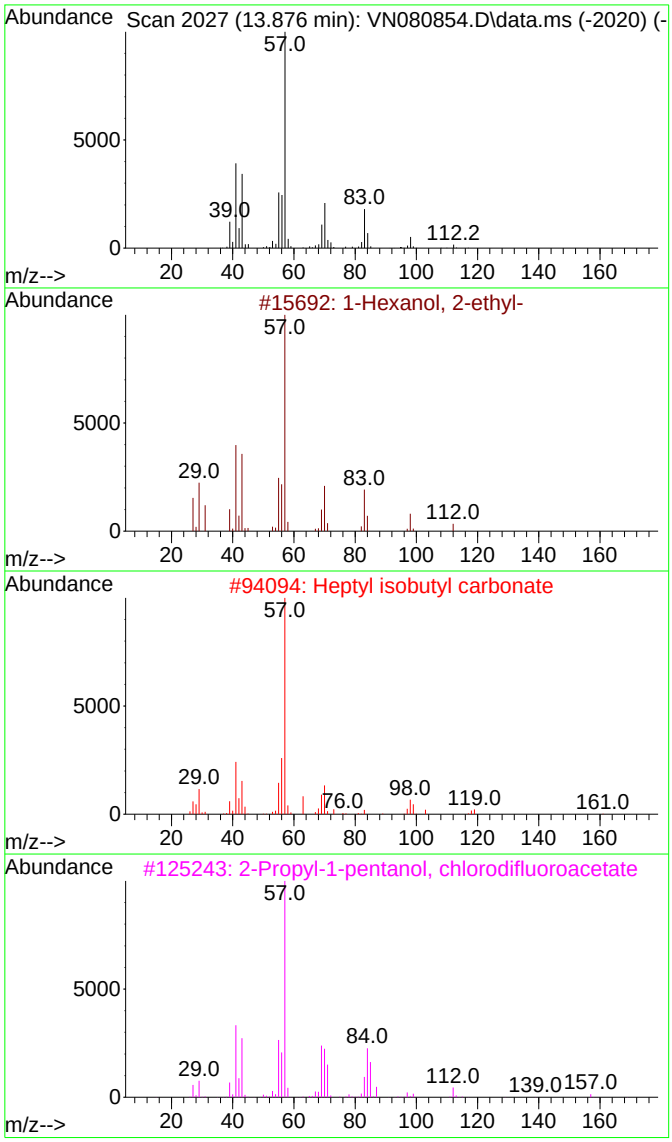
Quant Title : SW846 8260

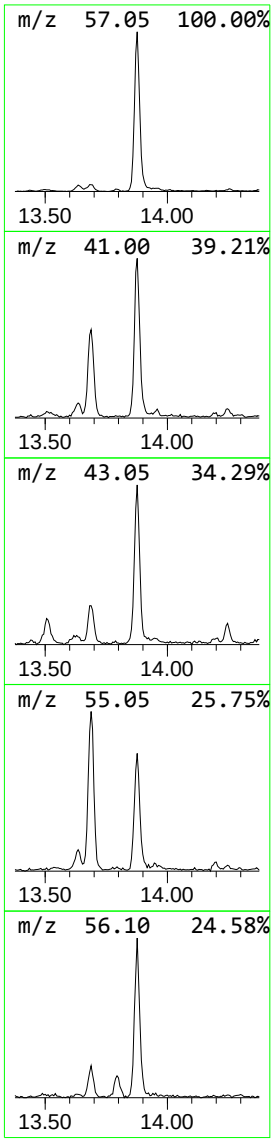
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	61.44 ug/l	894727	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	72
2	Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	64
3	2-Propyl-1-pentanol, chlorodiflu...	242	C10H17ClF2O2	1000447-27-3	59
4	Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	53
5	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	53





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethanol	3.789	29.9	ug/l	190752	1	8.224	319564	50.0
Propanal	4.283	1787.4	ug/l	11423800	1	8.224	319564	50.0
1-Propene, 3-me...	6.135	22.1	ug/l	141558	1	8.224	319564	50.0
1-Propanol	6.730	551.7	ug/l	3526100	1	8.224	319564	50.0
Butanal	7.224	162.2	ug/l	1036670	1	8.224	319564	50.0
1-Butanol	9.265	15.7	ug/l	173518	2	9.100	551219	50.0
4-Heptanone, 2,...	13.259	12.6	ug/l	183685	4	13.794	728091	50.0
2-Hexenal, 2-et...	13.688	36.1	ug/l	525914	4	13.794	728091	50.0
1-Hexanol, 2-et...	13.876	61.4	ug/l	894727	4	13.794	728091	50.0