LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091124\
Data File : VN083801.D
Acq On : 11 Sep 2024 17:33
Operator : JC\MD
Sample : P3839-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
830

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\82N091024W.M
Title : SW846 8260

Signal : TIC: VN083801.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.077	16	21	29	rVB	64465	100454	1.17%	0.547%
2	2.295	52	58	72	rVB2	35952	101283	1.18%	0.551%
3	3.824	308	318	334	rBV	92500	262264	3.06%	1.428%
4	4.289	386	397	407	rBV2	26816	86494	1.01%	0.471%
5	4.747	460	475	492	rBV	77809	299004	3.49%	1.628%
6	5.577	601	616	629	rBV5	28066	93169	1.09%	0.507%
7	6.765	785	818	839	rBV	2321507	8567745	100.00%	46.647%
8	7.218	883	895	907	rBV4	36101	107213	1.25%	0.584%
9	7.977	1015	1024	1043	rVB	67026	154733	1.81%	0.842%
10	8.165	1046	1056	1060	rBV	101770	236313	2.76%	1.287%
11	8.218	1060	1065	1075	rVB	173832	384408	4.49%	2.093%
12	8.577	1109	1126	1134	rBV2	110683	298691	3.49%	1.626%
13	9.100	1206	1215	1226	rBV	293486	596288	6.96%	3.246%
14	9.276	1237	1245	1256	rBV	86387	191189	2.23%	1.041%
15	10.565	1456	1464	1471	rBV	403506	747310	8.72%	4.069%
16	10.959	1520	1531	1547	rBV	652541	1144381	13.36%	6.231%
17	11.200	1563	1572	1580	rVB	99057	163566	1.91%	0.891%
18	11.865	1671	1685	1694	rBV	507839	907488	10.59%	4.941%
19	12.847	1845	1852	1860	rBV	359922	606769	7.08%	3.304%
20	13.335	1930	1935	1943	rVB	97261	154193	1.80%	0.840%
21	13.541	1964	1970	1978	rBV3	72796	140893	1.64%	0.767%
22	13.788	2006	2012	2020	rBV	531311	928534	10.84%	5.055%
23	13.870	2020	2026	2033	rVV	1060132	1692599	19.76%	9.215%
24	13.941	2033	2038	2048	rVV3	151447	402224	4.69%	2.190%

Sum of corrected areas: 18367205

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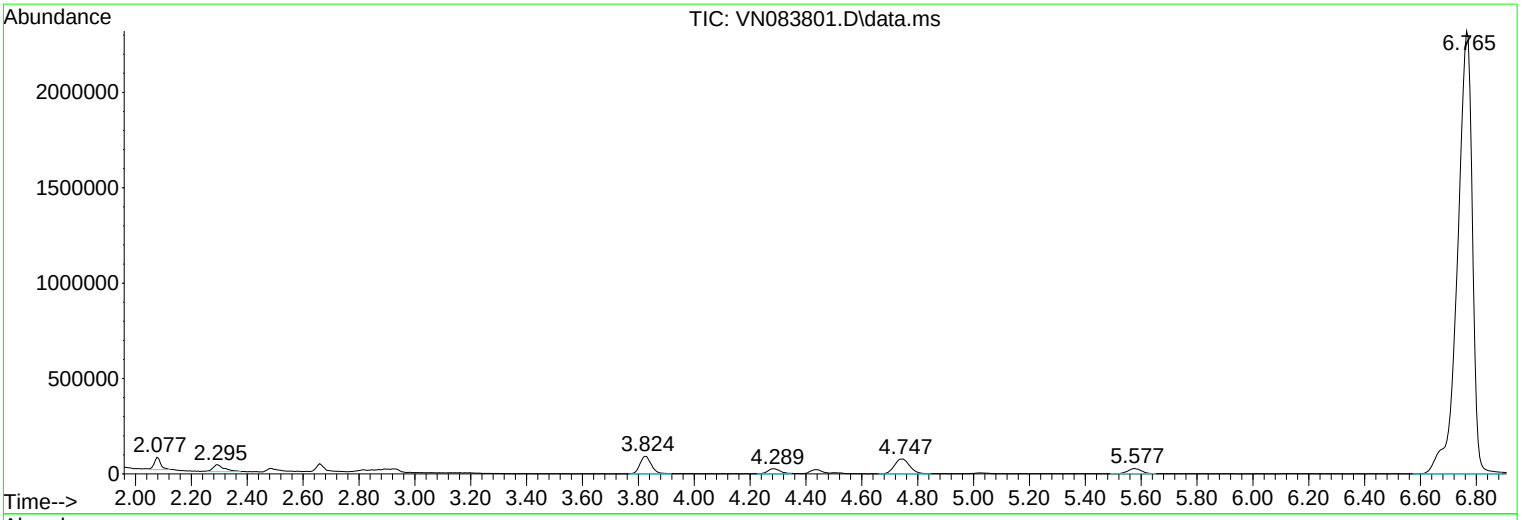
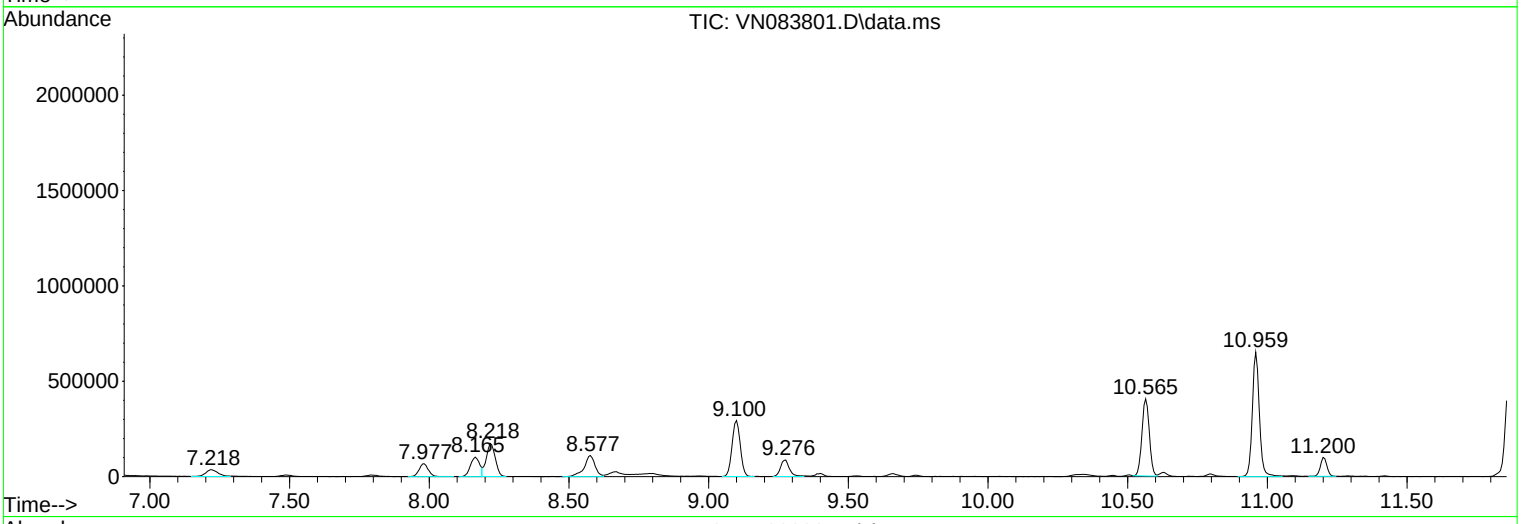
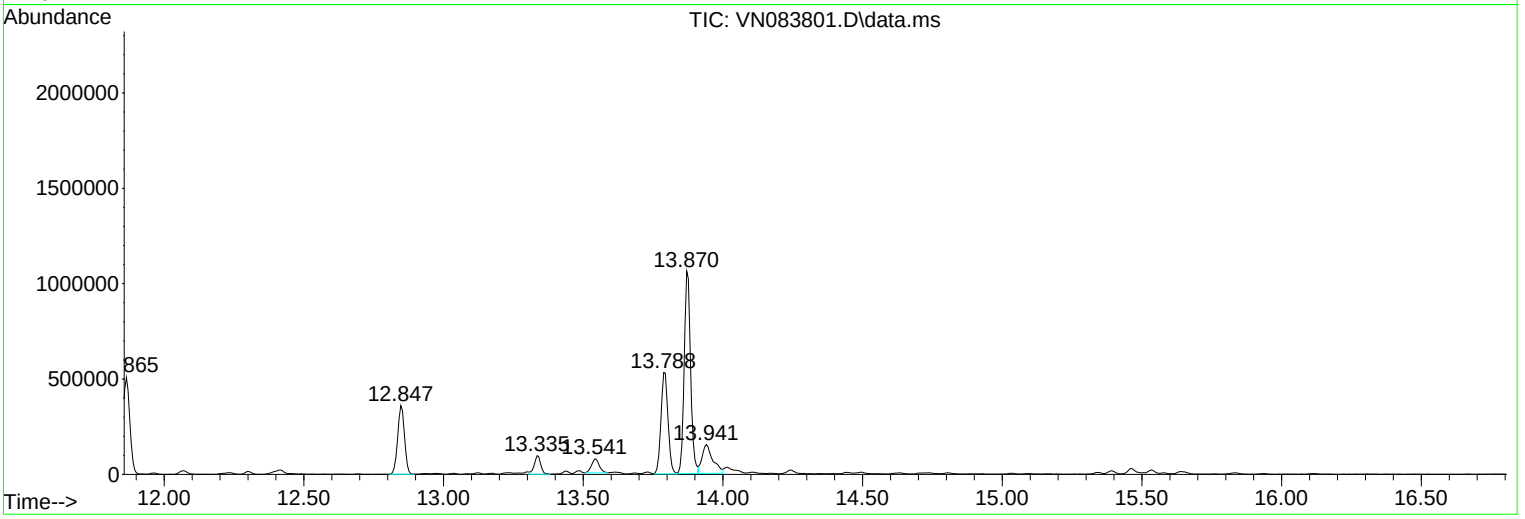
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

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







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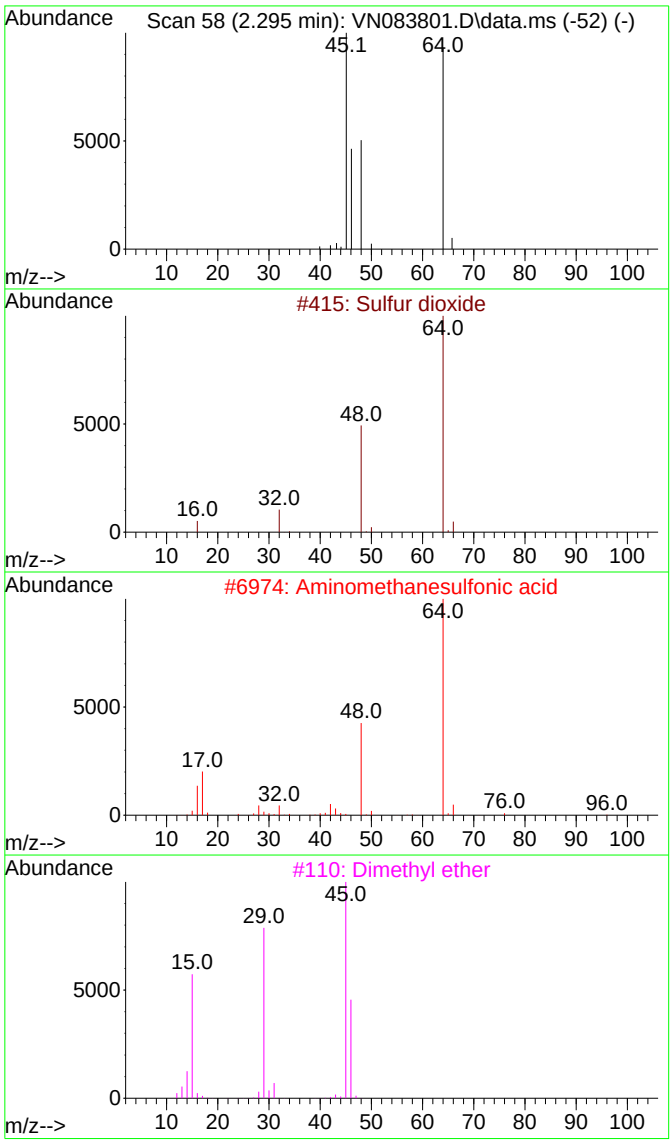
Quant Title : SW846 8260

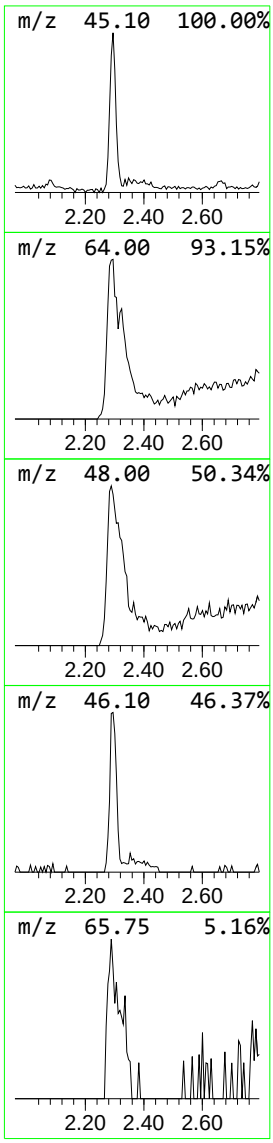
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 unknown2.295 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.295	13.17 ug/l	101283	Pentafluorobenzene	8.218

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	45
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	38
3	Dimethyl ether	46	C2H6O	000115-10-6	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	7
5	Ethanol	46	C2H6O	000064-17-5	4





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Data File : VN083801.D
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Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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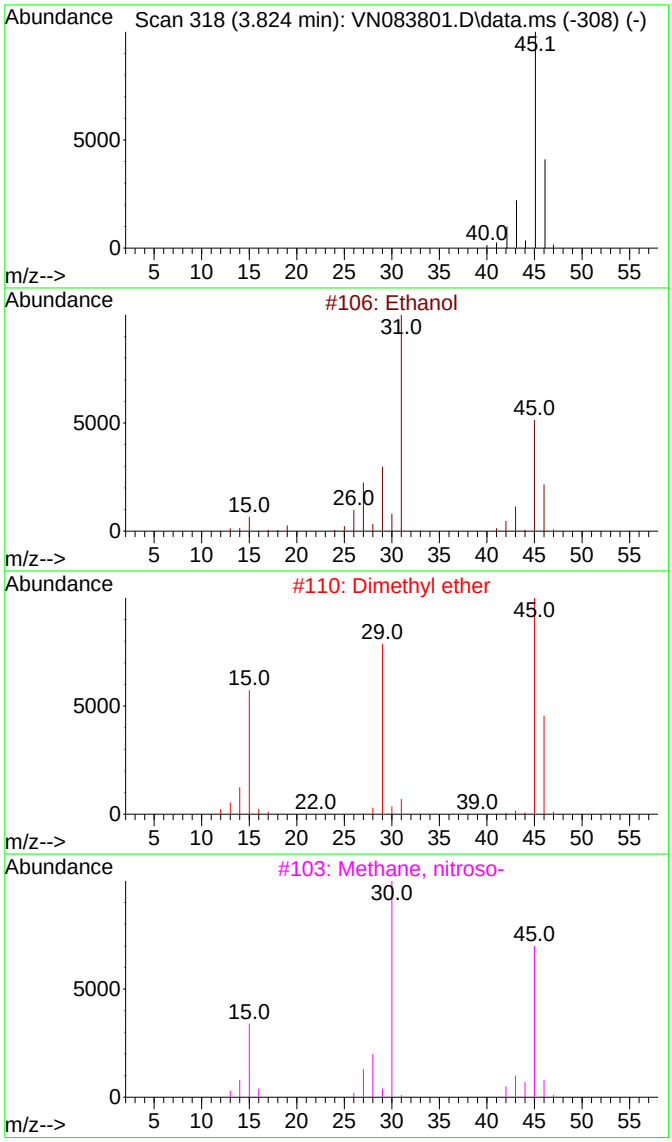
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

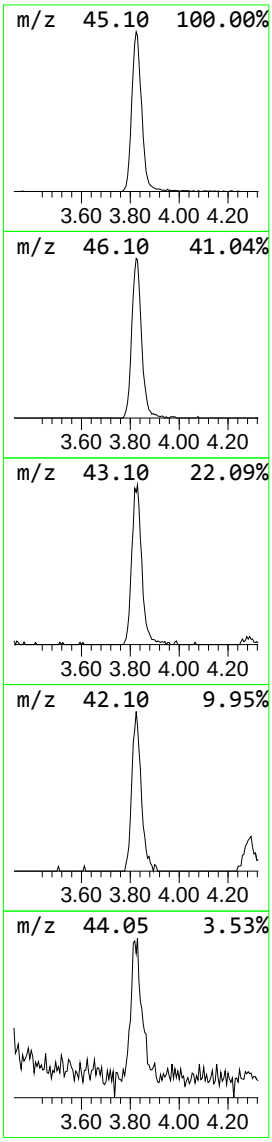
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.824	34.11 ug/l	262264	Pentafluorobenzene	8.218

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	90
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Formic acid	46	CH2O2	000064-18-6	4
5	Nitrogen dioxide	46	NO2	010102-44-0	2





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Operator : JC\MD
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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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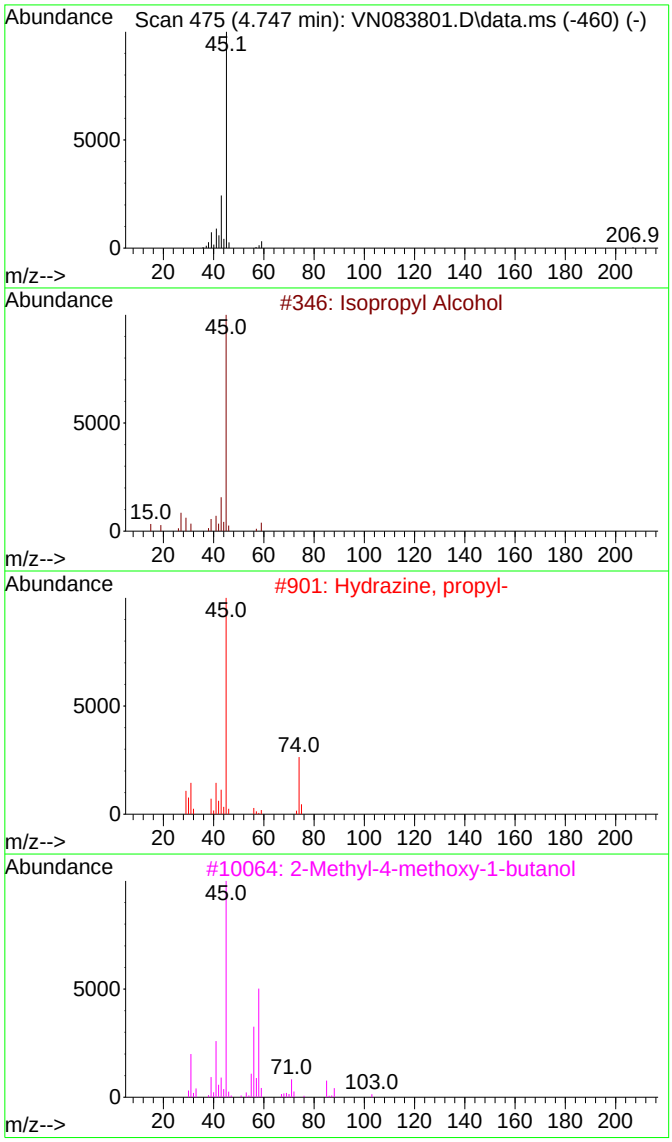
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

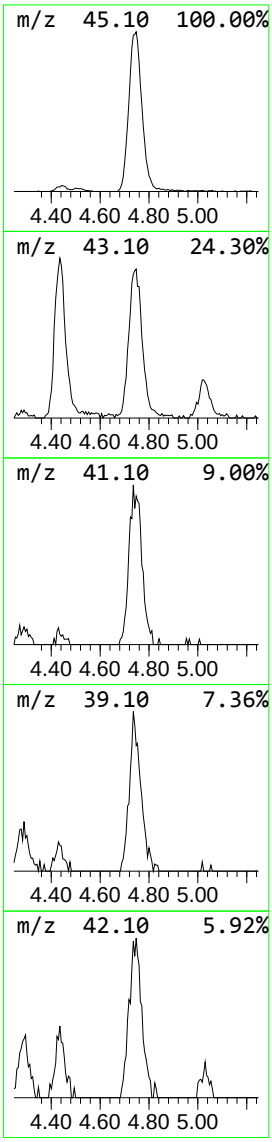
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Isopropyl Alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.747	38.89 ug/l	299004	Pentafluorobenzene	8.218

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	64
2	Hydrazine, propyl-	74	C3H10N2	005039-61-2	9
3	2-Methyl-4-methoxy-1-butanol	118	C6H14O2	071052-94-3	9
4	2-Pentanol	88	C5H12O	006032-29-7	9
5	2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	9





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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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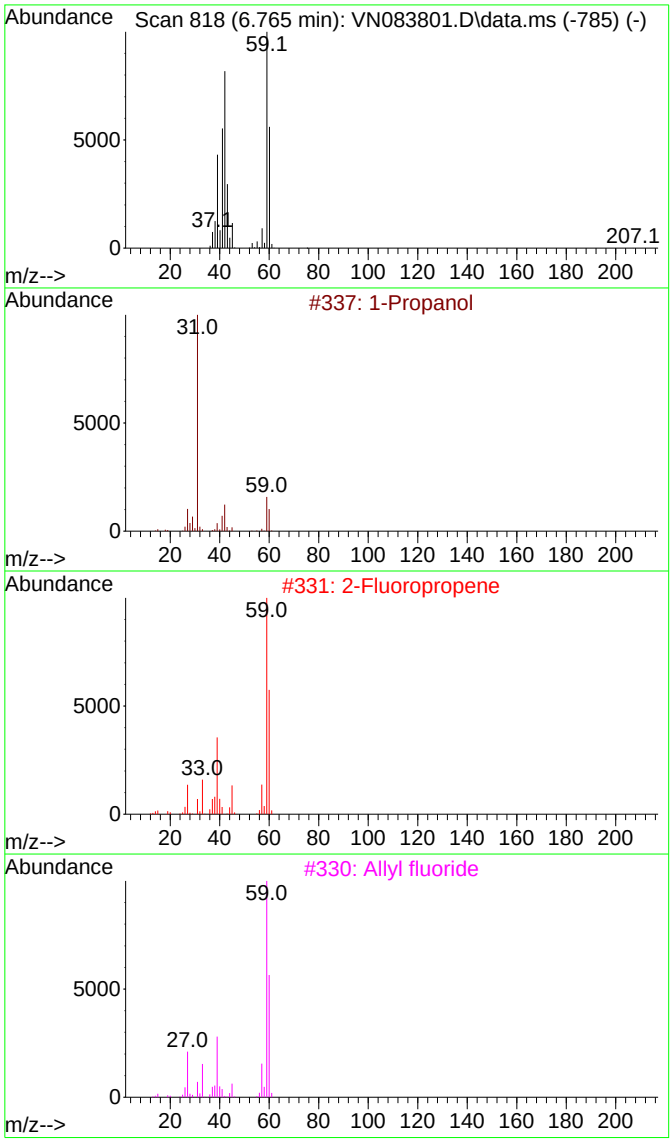
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

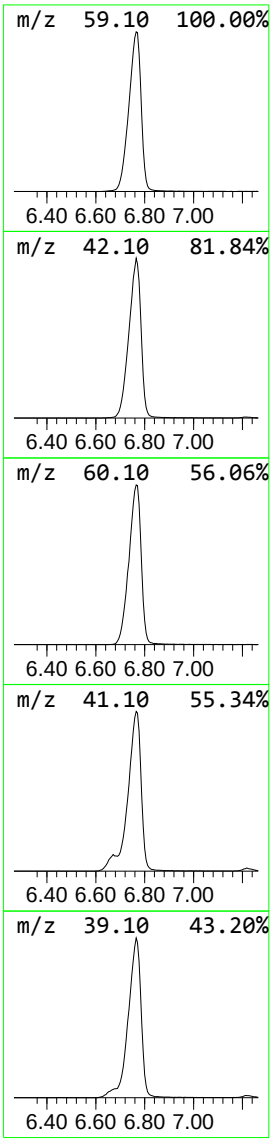
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.765	1114.41 ug/l	8567750	Pentafluorobenzene	8.218

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	50
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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ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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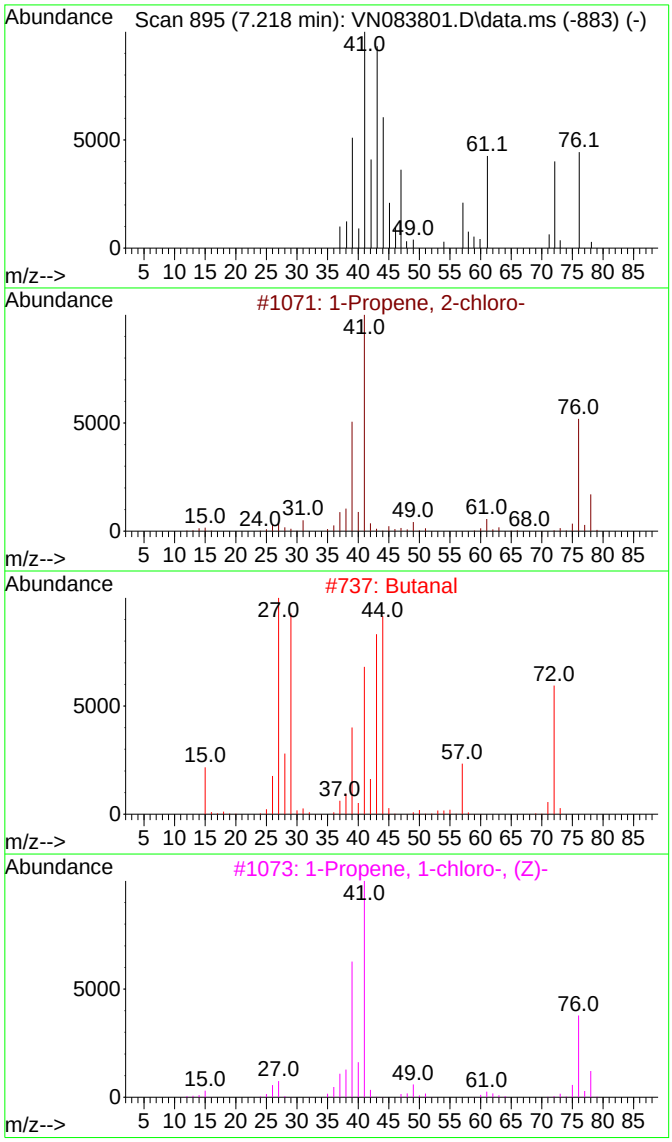
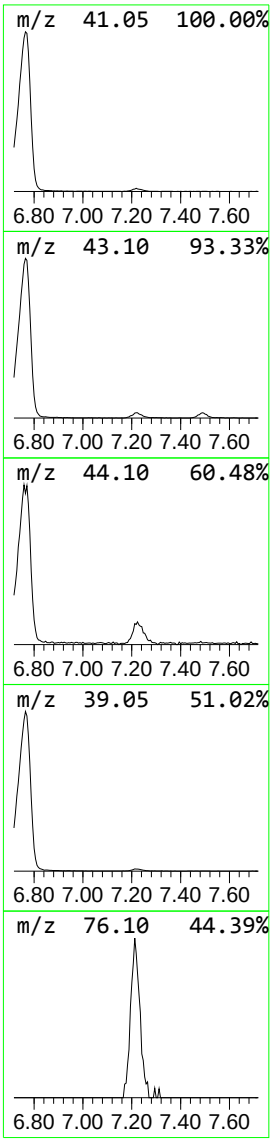
****
Peak Number 5 unknown7.218 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.218	13.95 ug/l	107213	Pentafluorobenzene	8.218

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-chloro-	76	C3H5Cl	000557-98-2	22
2	Butanal	72	C4H8O	000123-72-8	22
3	1-Propene, 1-chloro-, (Z)-	76	C3H5Cl	016136-84-8	14
4	1-Propene, 1-chloro-	76	C3H5Cl	000590-21-6	14
5	trans-1-Chloropropene	76	C3H5Cl	016136-85-9	14





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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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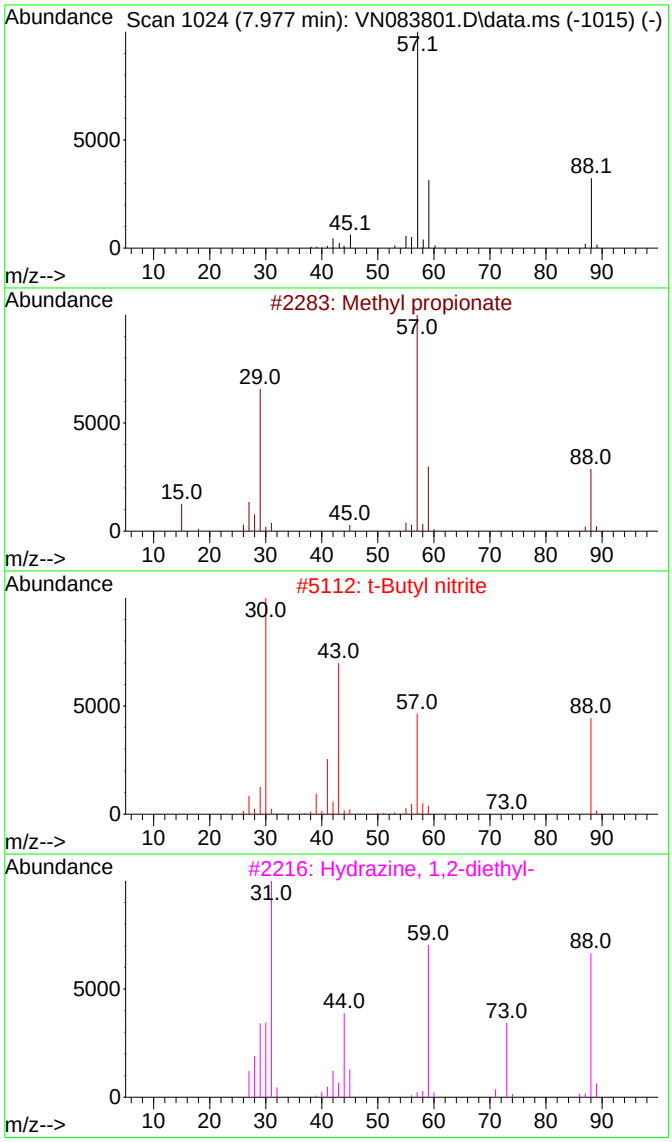
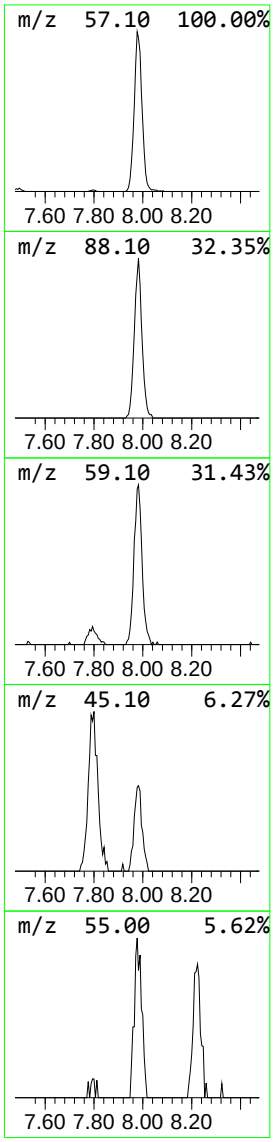
****

Peak Number 6 Methyl propionate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.977	20.13 ug/l	154733	Pentafluorobenzene	8.218

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl propionate	88	C4H8O2	000554-12-1	90
2	t-Butyl nitrite	103	C4H9NO2	000540-80-7	23
3	Hydrazine, 1,2-diethyl-	88	C4H12N2	001615-80-1	9
4	Sulfurous acid, dibutyl ester	194	C8H18O3S	000626-85-7	9
5	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	9





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

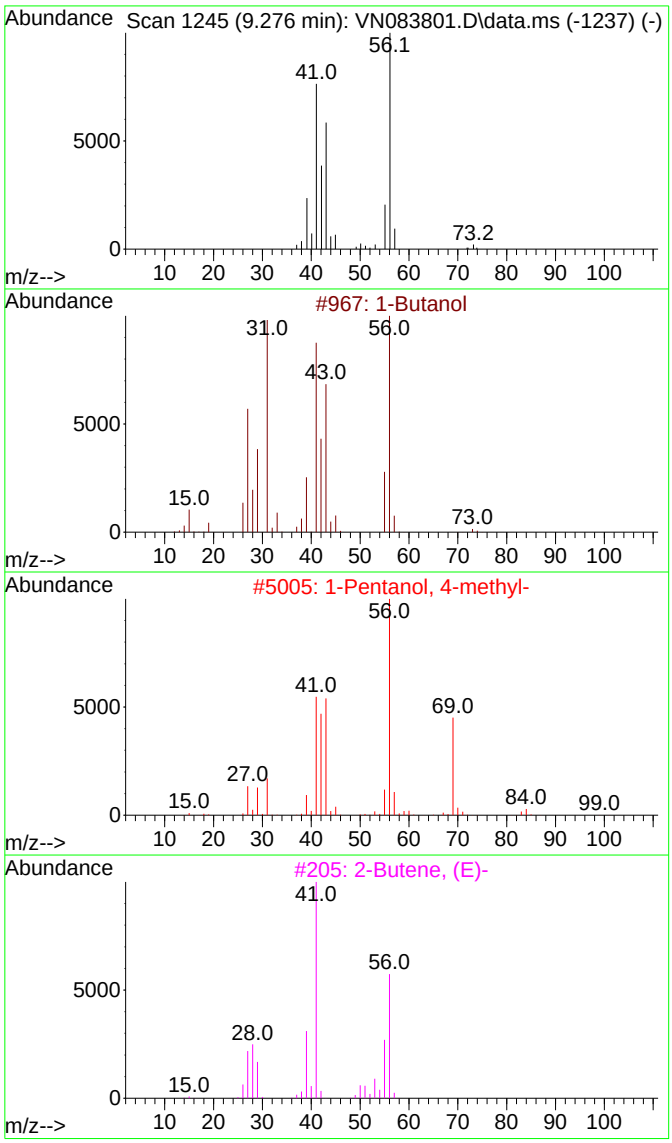
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

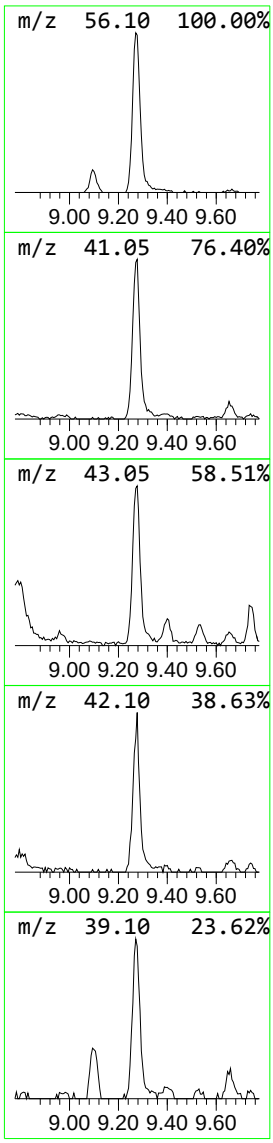
****

Peak Number 7 1-Butanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.276	16.03 ug/l	191189	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	91
2	1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	40
3	2-Butene, (E)-	56	C4H8	000624-64-6	38
4	2-Butene, (Z)-	56	C4H8	000590-18-1	28
5	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	9





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ClientSampleId :
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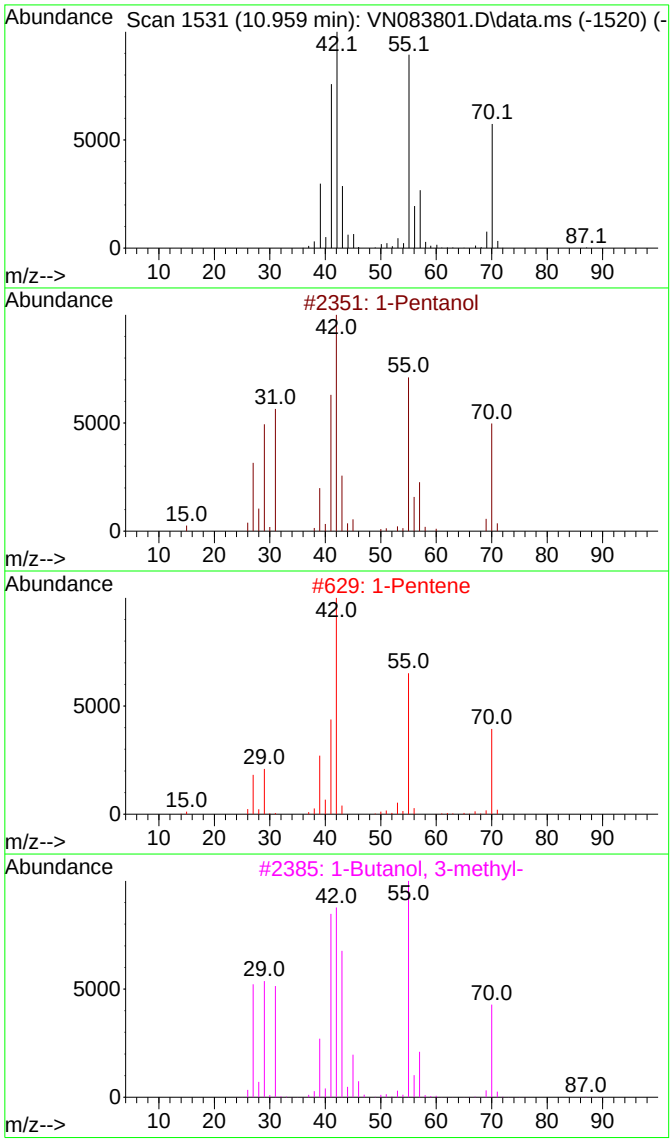
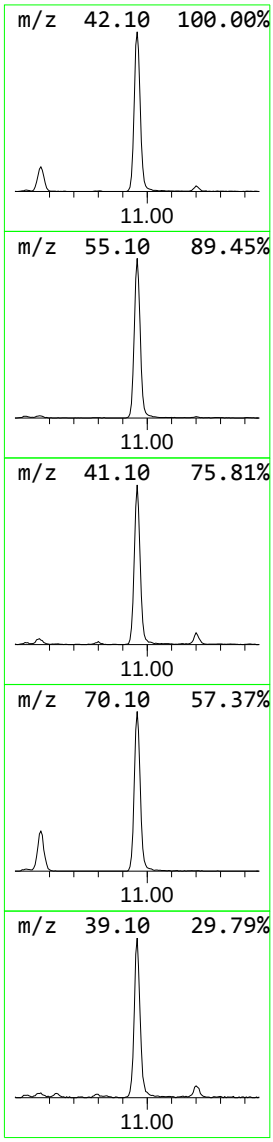
****
Peak Number 8 1-Pentanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.959	63.05 ug/l	1144380	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol	88	C5H12O	000071-41-0	90
2	1-Pentene	70	C5H10	000109-67-1	59
3	1-Butanol, 3-methyl-	88	C5H12O	000123-51-3	56
4	Formic acid, pentyl ester	116	C6H12O2	000638-49-3	56
5	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	50





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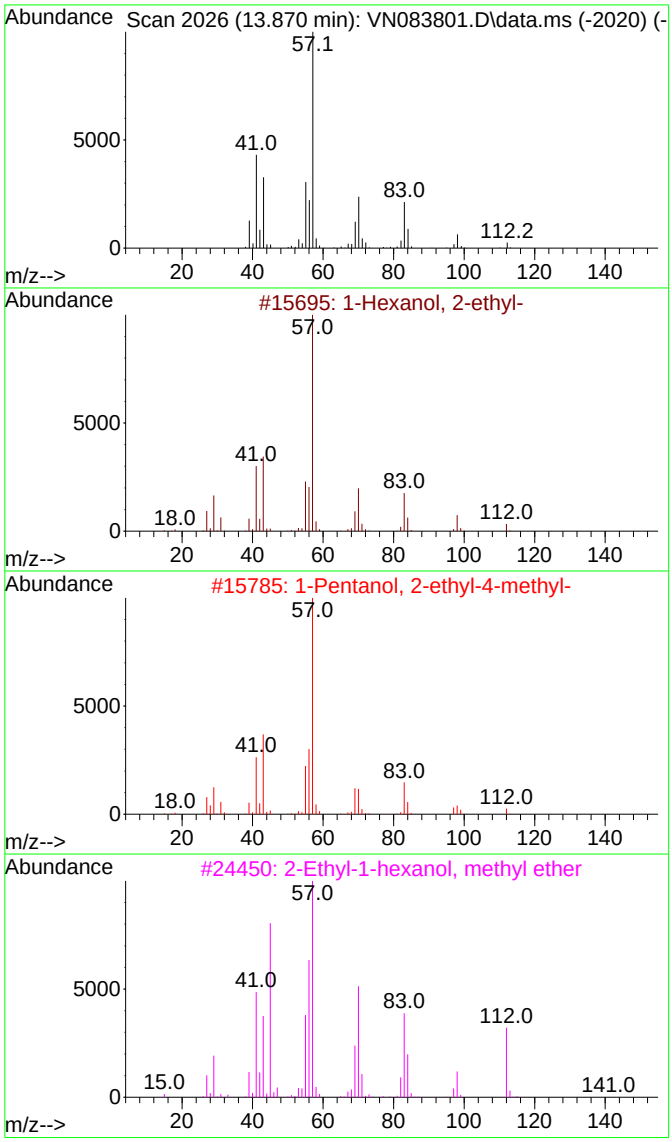
Quant Title : SW846 8260

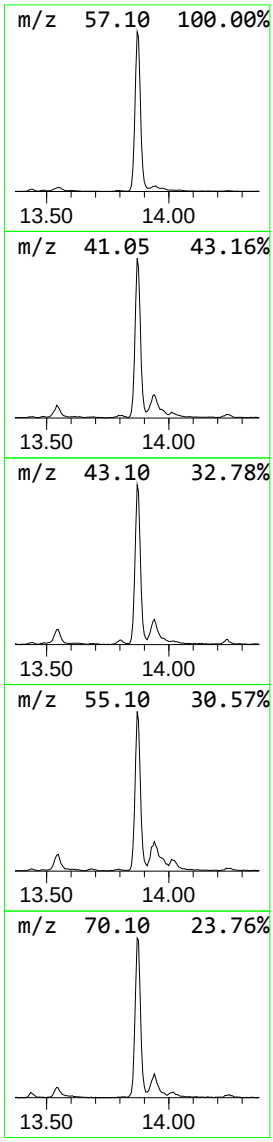
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.870	91.14 ug/l	1692600	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
4	Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	50
5	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47





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Instrument :
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ClientSampleId :
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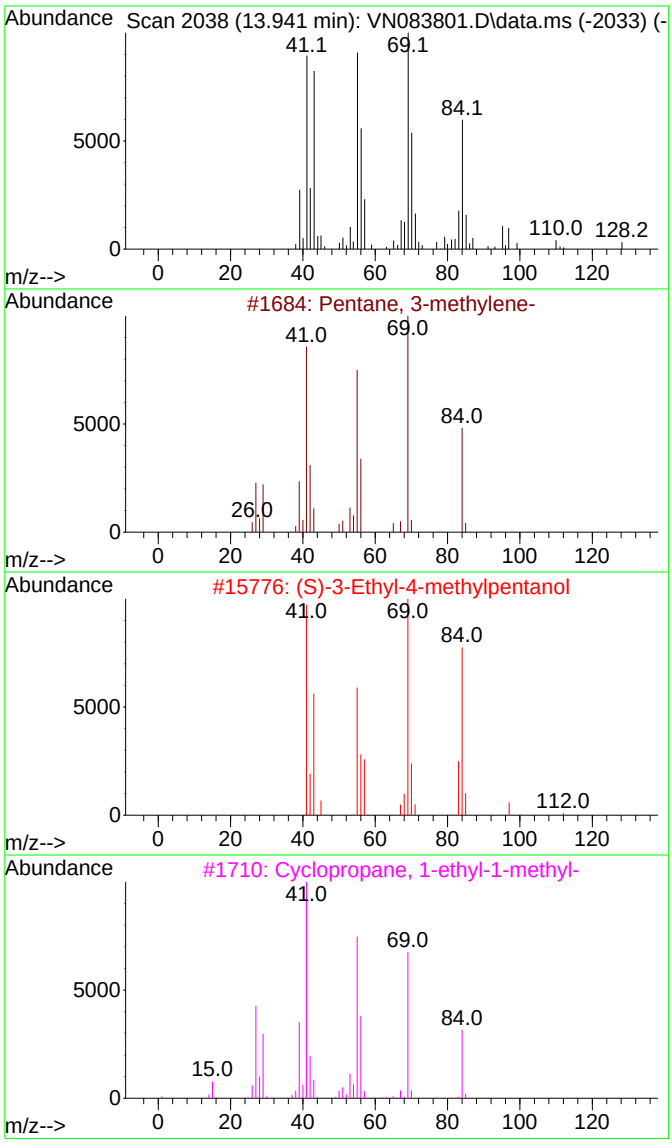
Quant Title : SW846 8260

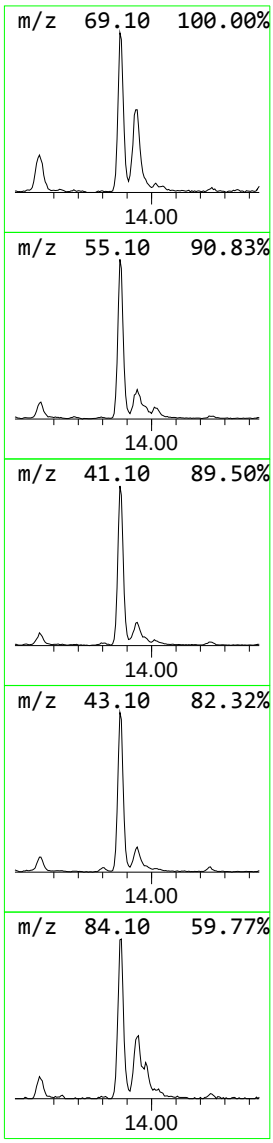
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Pentane, 3-methylene- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.941	21.66 ug/l	402224	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methylene-	84	C6H12	000760-21-4	58
2	(S)-3-Ethyl-4-methylpentanol	130	C8H18O	1000144-07-1	53
3	Cyclopropane, 1-ethyl-1-methyl-	84	C6H12	053778-43-1	53
4	2-Propenoic acid, 2-methyl-, hex...	170	C10H18O2	000142-09-6	50
5	Cyclobutane, butyl-	112	C8H16	013152-44-8	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091124\
Data File : VN083801.D
Acq On : 11 Sep 2024 17:33
Operator : JC\MD
Sample : P3839-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
830

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.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
unknown2.295	2.295	13.2	ug/l	101283	1	8.218	384408	50.0
Ethanol	3.824	34.1	ug/l	262264	1	8.218	384408	50.0
Isopropyl Alcohol	4.747	38.9	ug/l	299004	1	8.218	384408	50.0
1-Propanol	6.765	1114.4	ug/l	8567750	1	8.218	384408	50.0
unknown7.218	7.218	13.9	ug/l	107213	1	8.218	384408	50.0
Methyl propionate	7.977	20.1	ug/l	154733	1	8.218	384408	50.0
1-Butanol	9.276	16.0	ug/l	191189	2	9.100	596288	50.0
1-Pentanol	10.959	63.0	ug/l	1144380	3	11.865	907488	50.0
1-Hexanol, 2-et...	13.870	91.1	ug/l	1692600	4	13.788	928534	50.0
Pentane, 3-meth...	13.941	21.7	ug/l	402224	4	13.788	928534	50.0