LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083826.D
Acq On : 12 Sep 2024 12:31
Operator : JC\MD
Sample : P3913-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
82924-A-C

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: VN083826.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	42	rVB	80433	177949	9.59%	1.177%
2	2.289	51	57	76	rVB3	34872	116446	6.28%	0.770%
3	2.660	115	120	127	rBV	32193	52874	2.85%	0.350%
4	2.807	140	145	149	rBV5	11055	22883	1.23%	0.151%
5	3.513	256	265	275	rVB2	8782	21816	1.18%	0.144%
6	4.283	386	396	408	rBV	27022	83251	4.49%	0.551%
7	4.430	411	421	443	rVB	197410	592854	31.96%	3.921%
8	4.736	457	473	485	rBV2	26974	105458	5.69%	0.697%
9	7.230	884	897	907	rBV3	18546	57906	3.12%	0.383%
10	7.483	930	940	957	rBV	126653	327023	17.63%	2.163%
11	7.789	982	992	1003	rBV	130303	357122	19.25%	2.362%
12	8.165	1045	1056	1060	rBV	122931	282488	15.23%	1.868%
13	8.218	1060	1065	1077	rVB	198917	455052	24.53%	3.009%
14	8.536	1108	1119	1132	rBV2	654370	1854879	100.00%	12.267%
15	8.653	1132	1139	1147	rVV2	28326	118779	6.40%	0.786%
16	9.100	1206	1215	1225	rBV	349069	706317	38.08%	4.671%
17	9.271	1233	1244	1258	rBV2	54073	120757	6.51%	0.799%
18	9.530	1280	1288	1296	rBV	45842	92660	5.00%	0.613%
19	9.653	1302	1309	1322	rVB	71823	155010	8.36%	1.025%
20	10.565	1456	1464	1470	rBV	497189	916492	49.41%	6.061%
21	10.630	1470	1475	1487	rVB	161409	292166	15.75%	1.932%
22	10.959	1524	1531	1539	rBV3	9644	19439	1.05%	0.129%
23	11.124	1546	1559	1569	rBV3	41309	132036	7.12%	0.873%
24	11.259	1576	1582	1586	rBV2	17512	29039	1.57%	0.192%
25	11.406	1603	1607	1614	rVB2	14216	24975	1.35%	0.165%
26	11.512	1616	1625	1639	rBV	250949	609484	32.86%	4.031%
27	11.865	1674	1685	1697	rVB	608680	1107973	59.73%	7.328%
28	11.965	1697	1702	1707	rVV2	24763	46534	2.51%	0.308%
29	12.024	1707	1712	1714	rVV5	18701	31983	1.72%	0.212%
30	12.065	1714	1719	1728	rVB	97412	193068	10.41%	1.277%
31	12.165	1730	1736	1741	rBV2	34665	66823	3.60%	0.442%
32	12.236	1743	1748	1759	rVB	38623	73386	3.96%	0.485%
33	12.412	1769	1778	1783	rBV6	60638	164478	8.87%	1.088%
34	12.459	1783	1786	1796	rVB3	37141	68949	3.72%	0.456%
35	12.565	1798	1804	1813	rBV5	39453	97521	5.26%	0.645%
36	12.688	1820	1825	1832	rVB4	33674	59922	3.23%	0.396%

LSC Area Percent Report

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Sample : P3913-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
82924-A-C

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

37	12.847	1845	1852	1859	rBV	471147	797453	42.99%	5.274%
38	13.035	1879	1884	1888	rBV2	19192	35129	1.89%	0.232%
39	13.124	1888	1899	1905	rVV5	44577	100173	5.40%	0.662%
40	13.241	1912	1919	1922	rBV5	19011	38118	2.06%	0.252%
41	13.271	1922	1924	1927	rVV3	16473	21075	1.14%	0.139%
42	13.335	1930	1935	1944	rVB	221752	371592	20.03%	2.458%
43	13.435	1944	1952	1953	rBV5	11145	22251	1.20%	0.147%
44	13.494	1953	1962	1966	rVV8	69275	204637	11.03%	1.353%
45	13.541	1966	1970	1980	rVV	102288	204940	11.05%	1.355%
46	13.630	1981	1985	1989	rVV6	10469	18828	1.02%	0.125%
47	13.788	2005	2012	2021	rBV	707758	1314387	70.86%	8.693%
48	13.871	2021	2026	2036	rVB	485424	810142	43.68%	5.358%
49	14.106	2061	2066	2072	rBV5	24541	46721	2.52%	0.309%
50	14.177	2072	2078	2083	rBV	58281	106962	5.77%	0.707%
51	14.241	2084	2089	2094	rBV	122849	194059	10.46%	1.283%
52	14.547	2133	2141	2149	rBV3	63723	141914	7.65%	0.939%
53	14.712	2163	2169	2174	rBV3	17713	39295	2.12%	0.260%
54	14.953	2207	2210	2216	rVB	32504	47145	2.54%	0.312%
55	15.100	2228	2235	2244	rVB10	31922	99991	5.39%	0.661%
56	15.200	2248	2252	2260	rVB9	13568	30588	1.65%	0.202%
57	15.394	2281	2285	2290	rBV8	10026	18897	1.02%	0.125%
58	15.465	2294	2297	2300	rVV5	12099	22129	1.19%	0.146%
59	15.500	2301	2303	2312	rVB8	20196	41586	2.24%	0.275%
60	15.594	2312	2319	2322	rBV4	41599	87168	4.70%	0.576%
61	15.641	2322	2327	2336	rVB	90066	191830	10.34%	1.269%
62	15.824	2347	2358	2370	rVB2	103543	332376	17.92%	2.198%
63	16.465	2461	2467	2474	rVB8	12689	26654	1.44%	0.176%
64	16.541	2476	2480	2486	rVB7	11532	23233	1.25%	0.154%
65	16.612	2488	2492	2502	rVB9	15751	36334	1.96%	0.240%
66	16.782	2513	2521	2522	rBV2	33969	59202	3.19%	0.392%

Sum of corrected areas: 15120601

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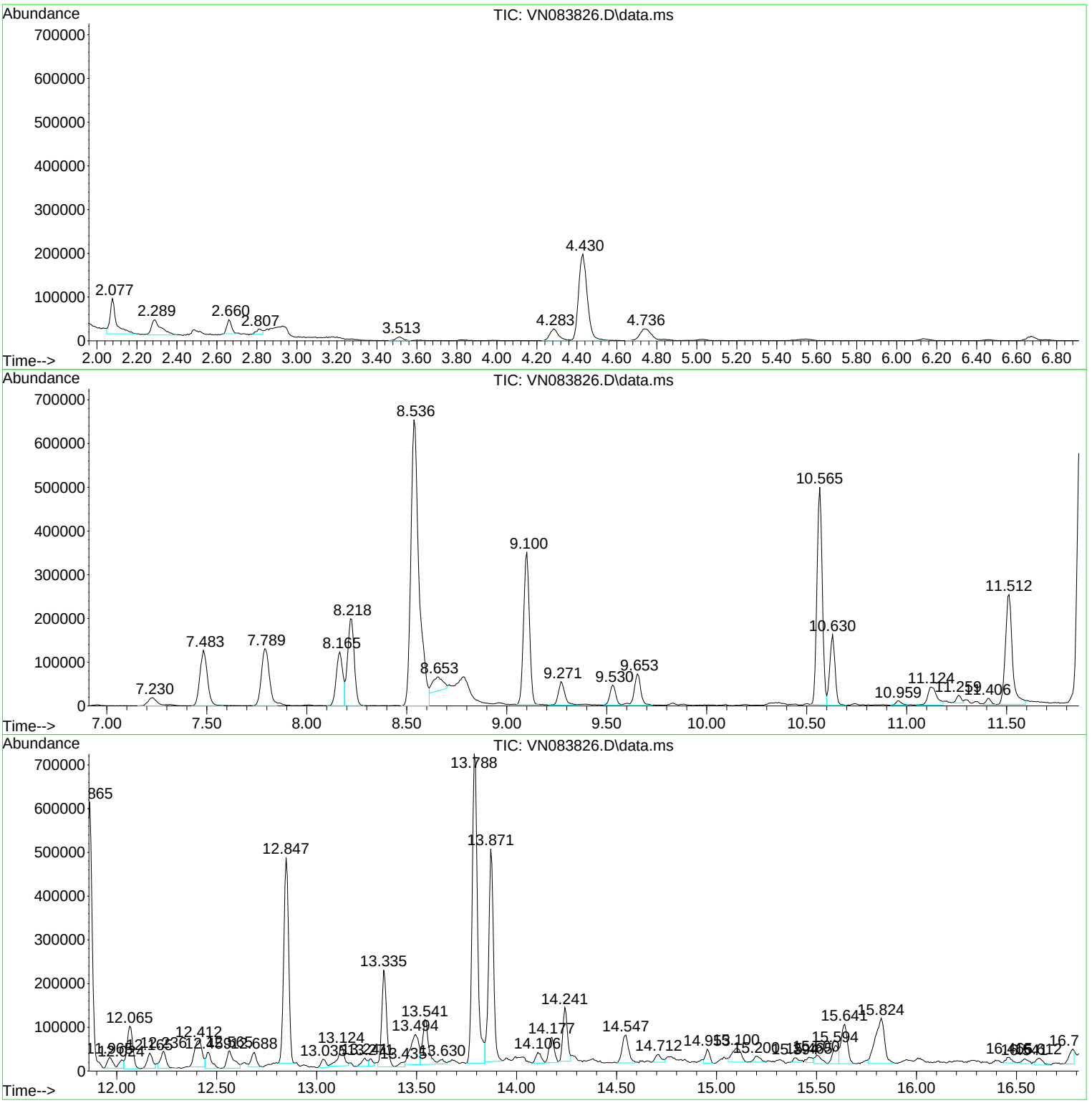
Instrument :
MSVOA_N
ClientSampleId :
82924-A-C

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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Data File : VN083826.D
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Quant Title : SW846 8260

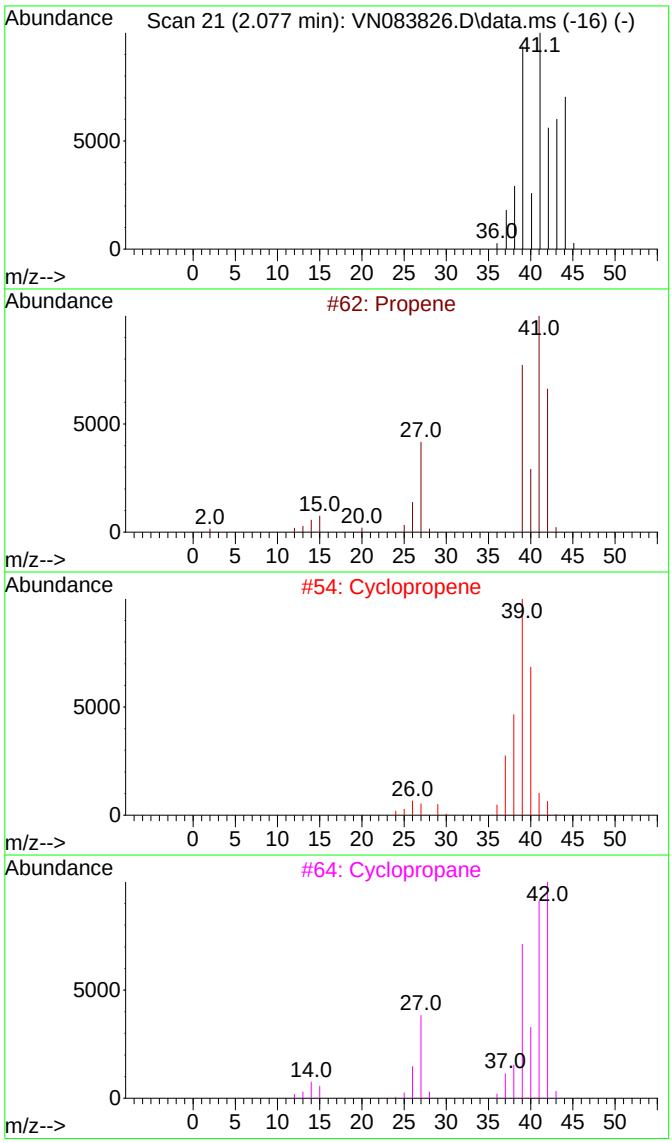
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

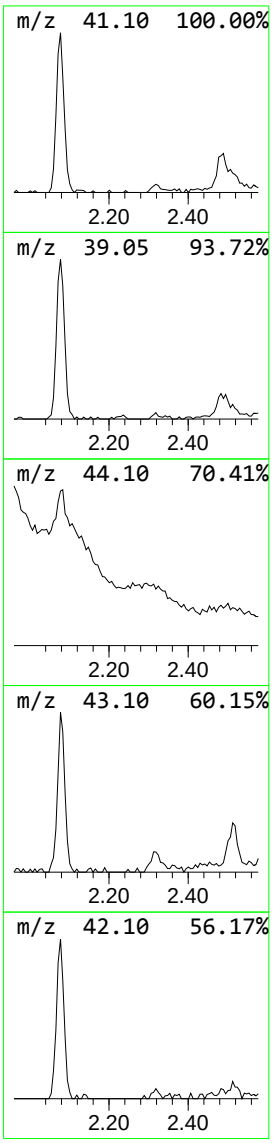
****

Peak Number 1 unknown2.077 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.077	19.55 ug/l	177949	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	42
2	Cyclopropene	40	C3H4	002781-85-3	9
3	Cyclopropane	42	C3H6	000075-19-4	4
4	Propane	44	C3H8	000074-98-6	4
5	Cyclobutylamine	71	C4H9N	002516-34-9	2





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083826.D
Acq On : 12 Sep 2024 12:31
Operator : JC\MD
Sample : P3913-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
82924-A-C

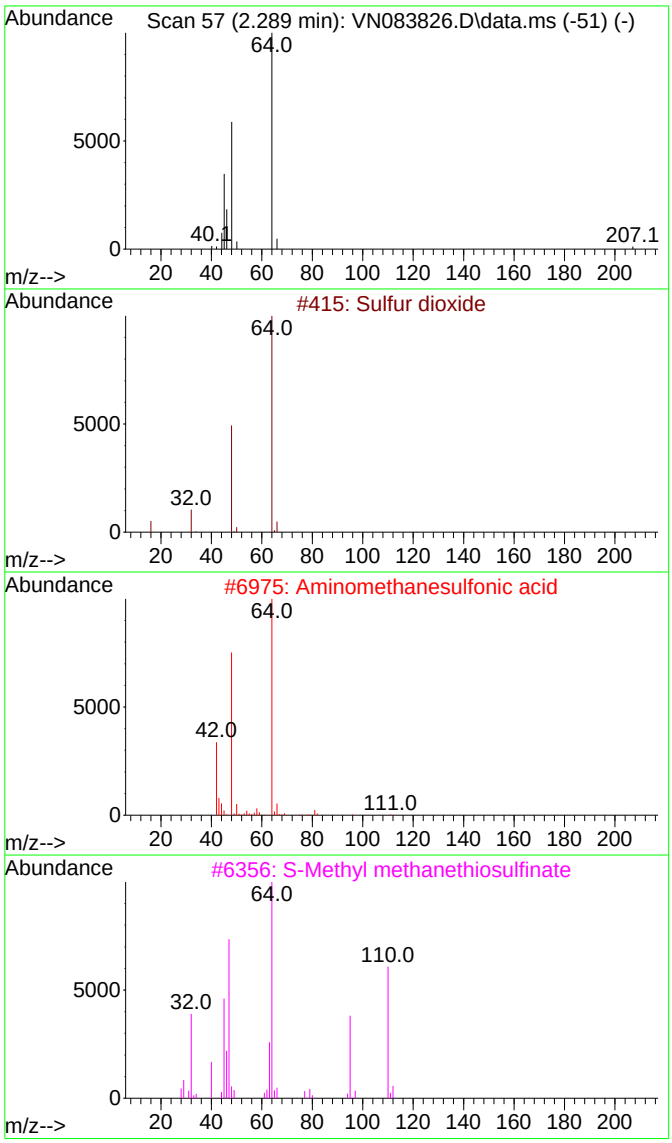
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

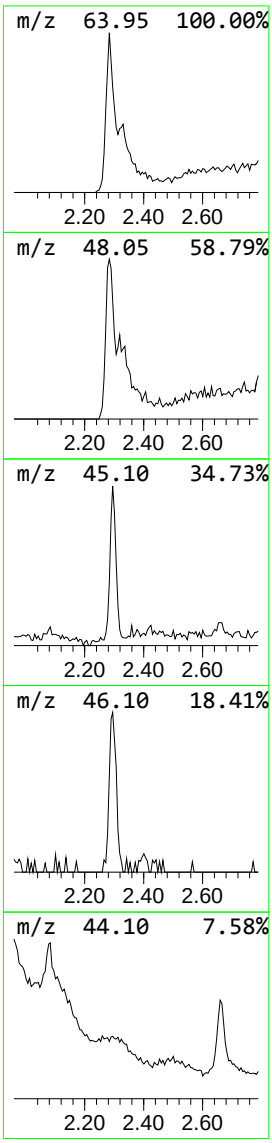
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Sulfur dioxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.289	12.79 ug/l	116446	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	64
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3	S-Methyl methanethiosulfinate	110	C2H6OS2	013882-12-7	43
4	Benzenesulfonic acid, 2,5-diamino-	188	C6H8N2O3S	000088-45-9	9
5	1,1,1,2,2,3,3,4,4,5,5-Undecafluo...	602	C10F22O2S	1000486-78-5	9





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Operator : JC\MD
Sample : P3913-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
82924-A-C

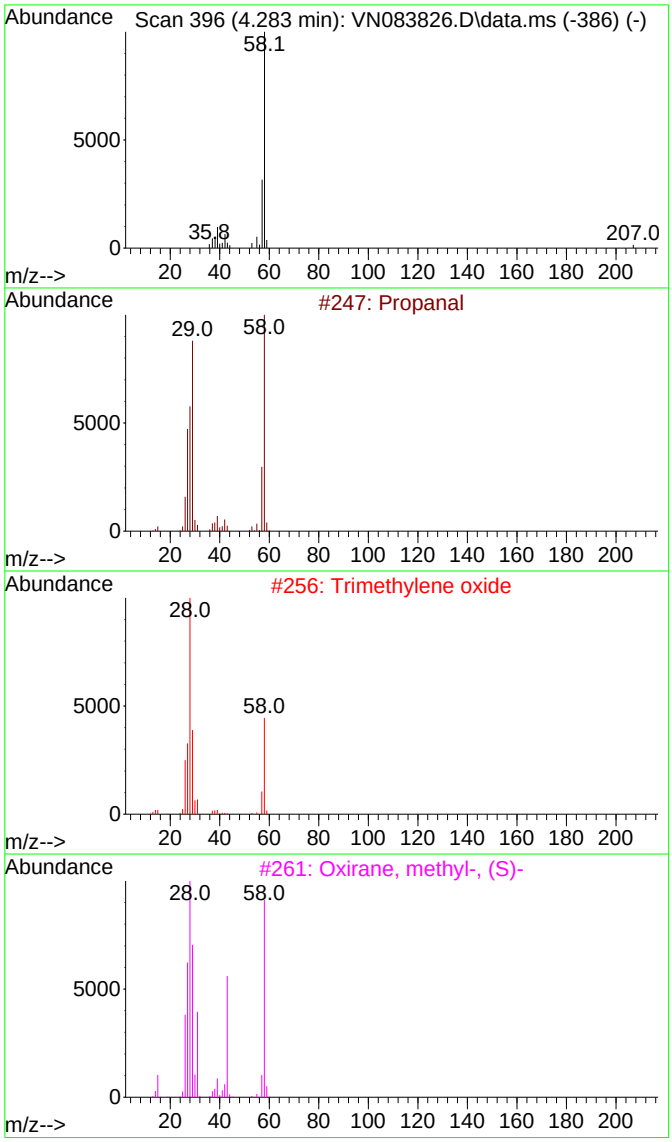
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

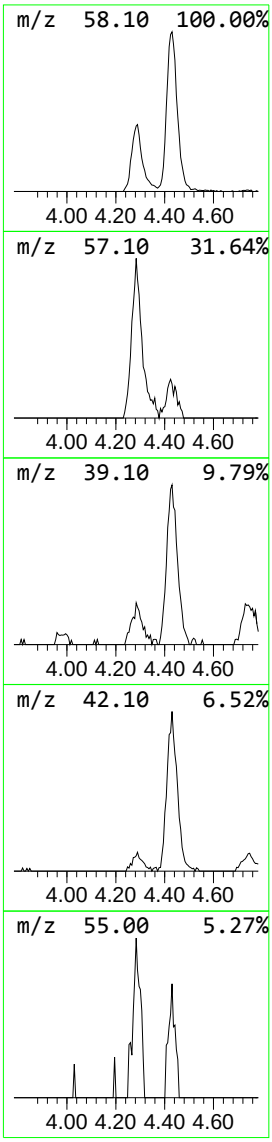
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Propanal Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.283	9.15 ug/l	83251	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal	58	C3H6O	000123-38-6	72
2	Trimethylene oxide	58	C3H6O	000503-30-0	9
3	Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	9
4	4-(3-Dimethylaminopropoxy)benzal...	207	C12H17NO2	026934-35-0	9
5	Propylene oxide	58	C3H6O	000075-56-9	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
82924-A-C

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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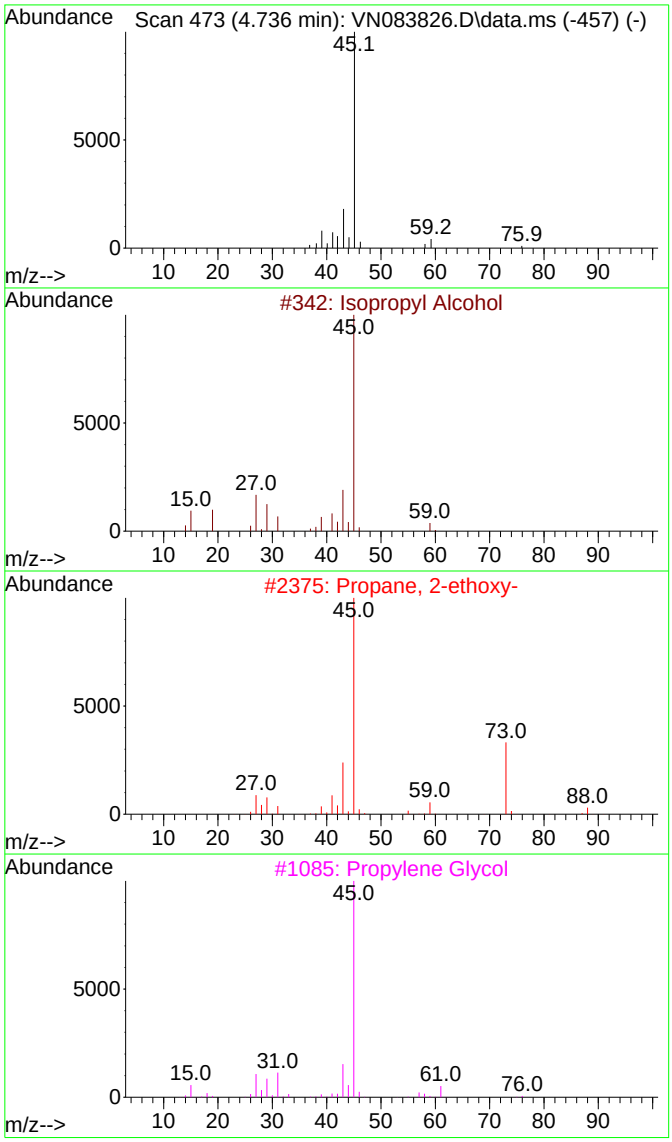
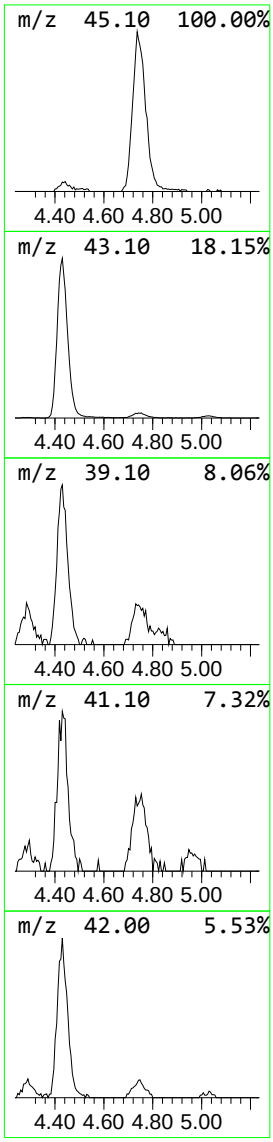
Peak Number 4 Isopropyl Alcohol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.736	11.59 ug/l	105458	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	64
2	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	40
3	Propylene Glycol	76	C3H8O2	000057-55-6	9
4	4-Penten-2-ol	86	C5H10O	000625-31-0	9
5	2-Pentanol	88	C5H12O	006032-29-7	9





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ALS Vial : 9 Sample Multiplier: 1

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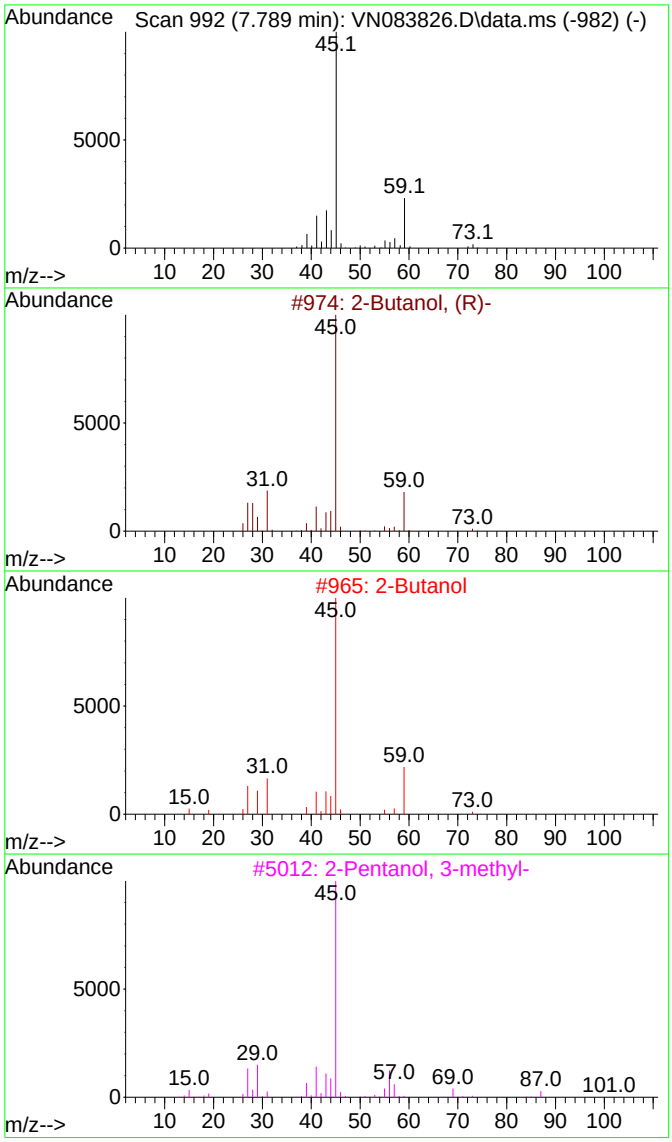
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

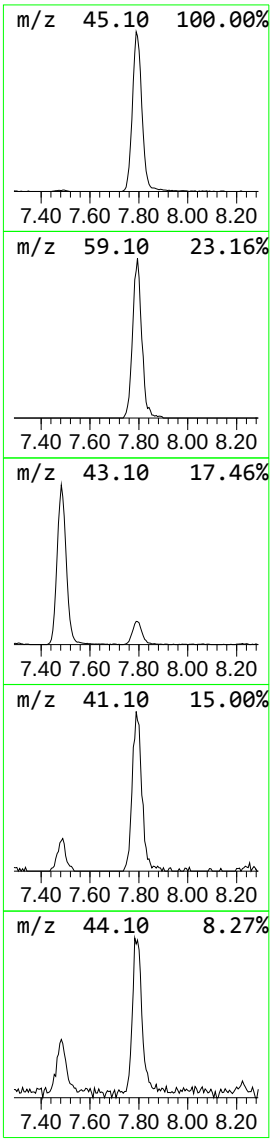
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Butanol, (R)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.789	39.24 ug/l	357122	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol, (R)-	74	C4H10O	014898-79-4	83
2	2-Butanol	74	C4H10O	000078-92-2	83
3	2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	59
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	45
5	2-Hexanol	102	C6H14O	000626-93-7	38





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Quant Title : SW846 8260

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

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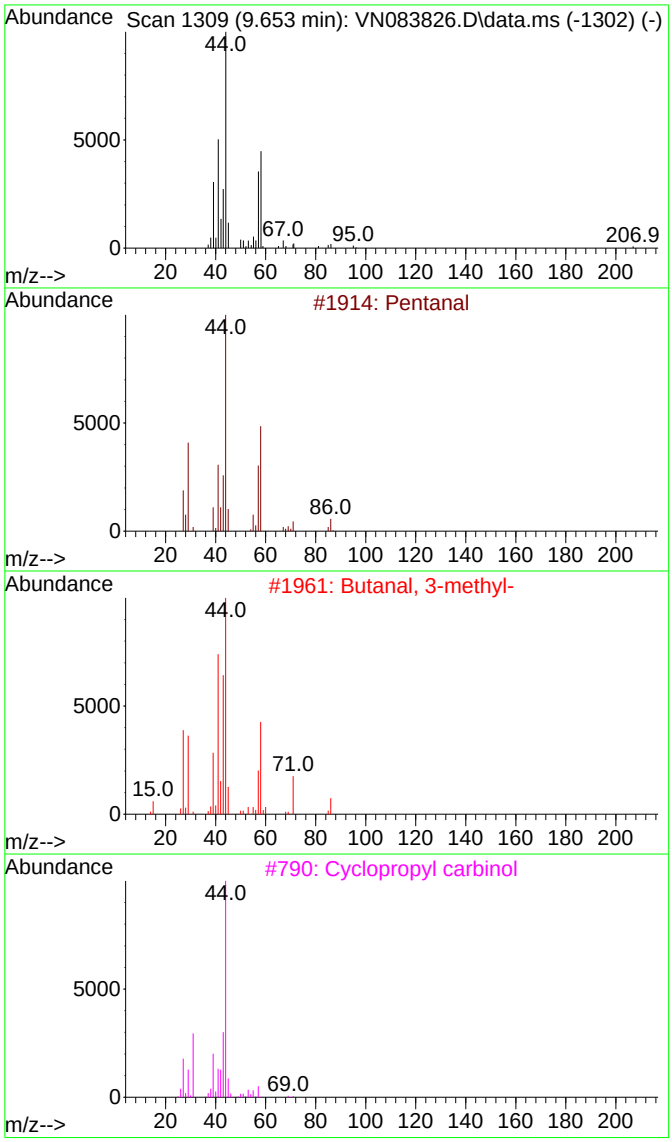
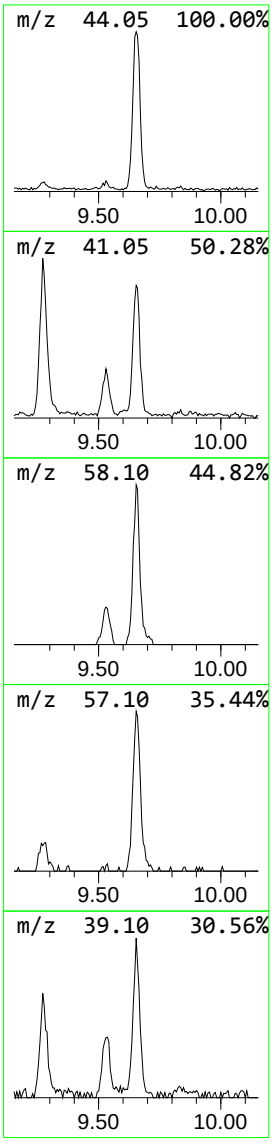
Peak Number 6 Pentanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.653	10.97 ug/l	155010	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal	86	C5H10O	000110-62-3	74
2	Butanal, 3-methyl-	86	C5H10O	000590-86-3	64
3	Cyclopropyl carbinol	72	C4H8O	002516-33-8	50
4	Hexanal	100	C6H12O	000066-25-1	33
5	Ethanol, 2-(2-propenyloxy)-	102	C5H10O2	000111-45-5	12





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083826.D
Acq On : 12 Sep 2024 12:31
Operator : JC\MD
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
82924-A-C

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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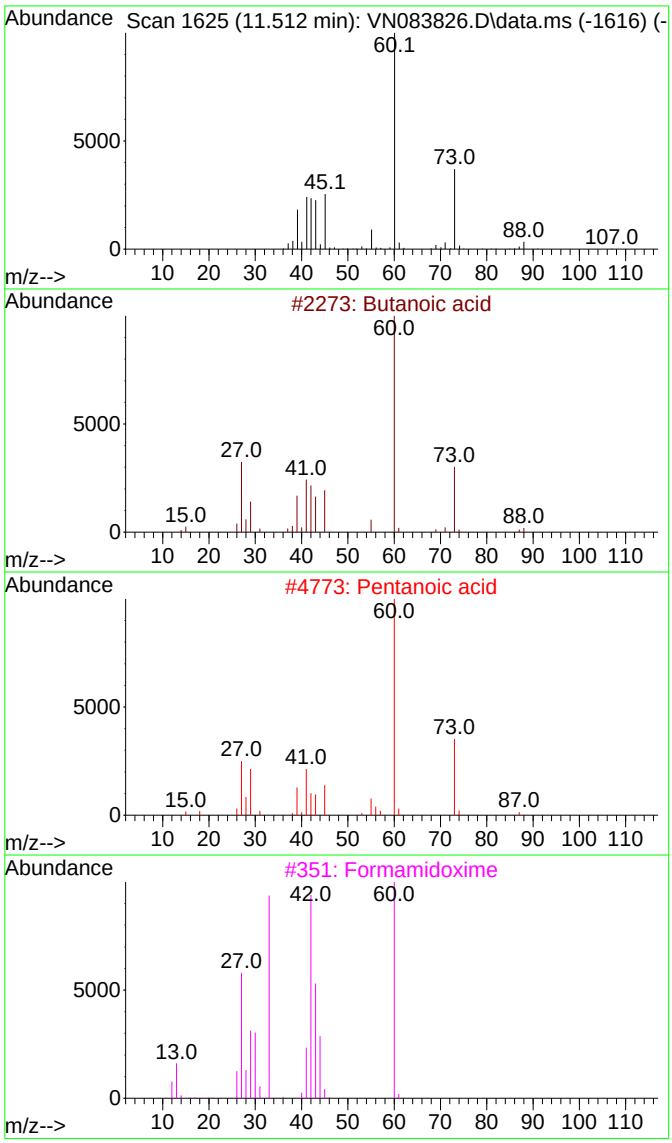
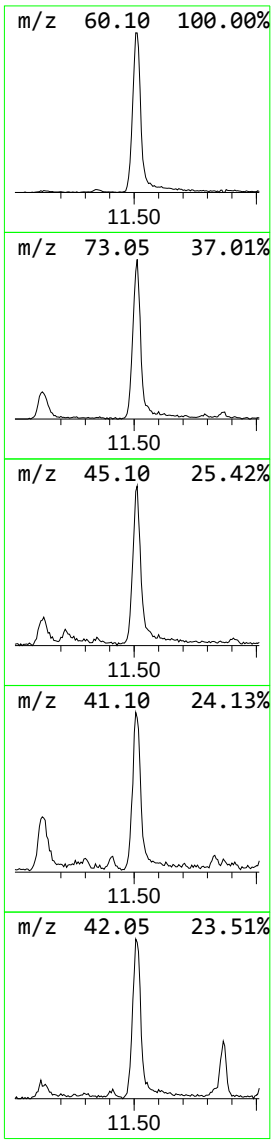
Peak Number 7 Butanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.512	27.50 ug/l	609484	Chlorobenzene-d5	11.865

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid	88	C4H8O2	000107-92-6	90
2	Pentanoic acid	102	C5H10O2	000109-52-4	38
3	Formamidoxime	60	CH4N2O	000624-82-8	9
4	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
5	Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083826.D
Acq On : 12 Sep 2024 12:31
Operator : JC\MD
Sample : P3913-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
82924-A-C

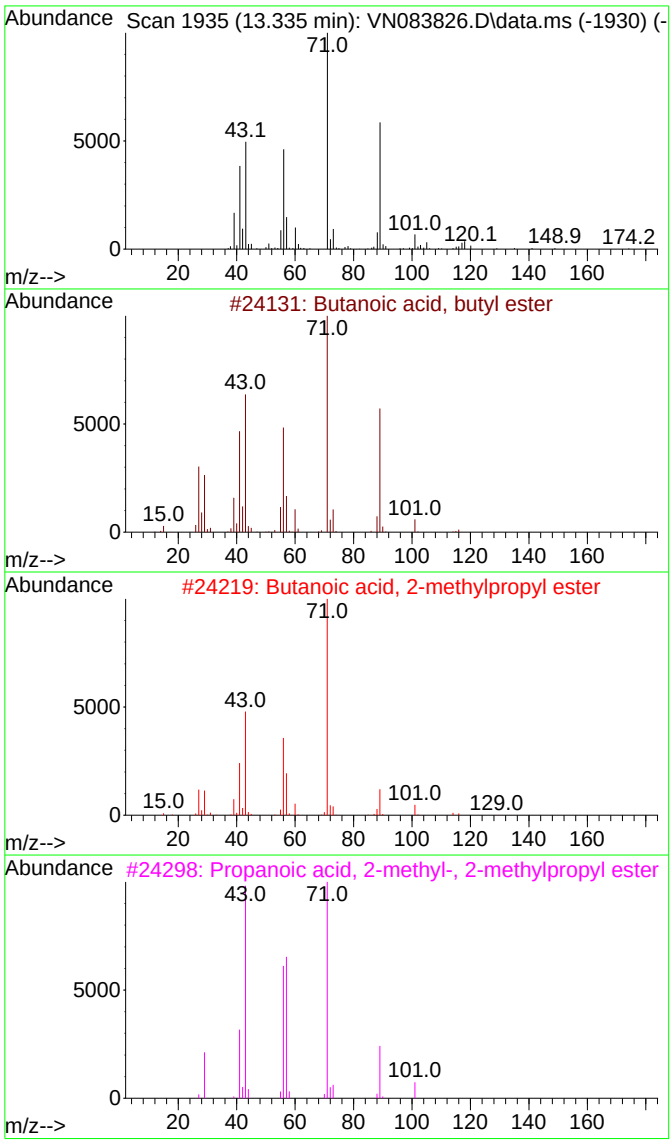
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

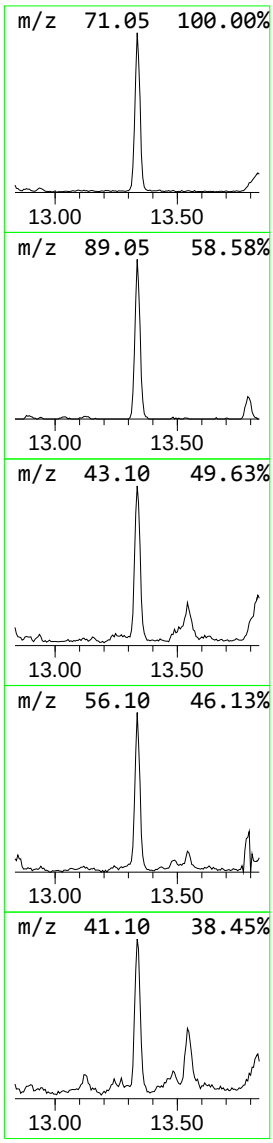
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Butanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.336	14.14 ug/l	371592	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	91
2	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	59
3	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	59
4	Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	56
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083826.D
Acq On : 12 Sep 2024 12:31
Operator : JC\MD
Sample : P3913-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
82924-A-C

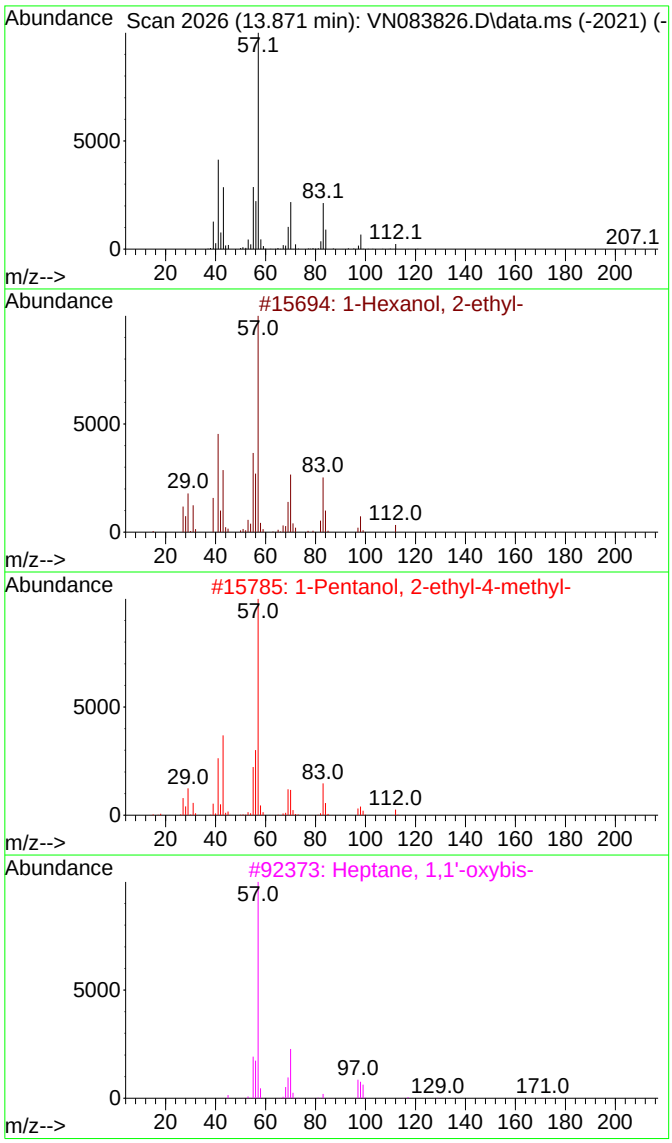
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

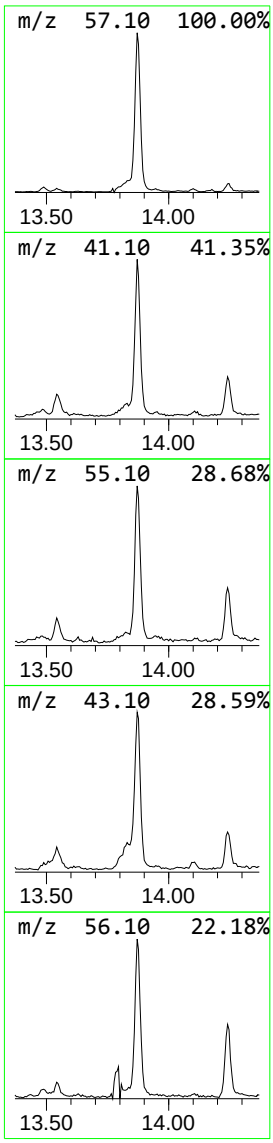
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.871	30.82 ug/l	810142	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	90
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
4	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	50
5	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083826.D
Acq On : 12 Sep 2024 12:31
Operator : JC\MD
Sample : P3913-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
82924-A-C

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

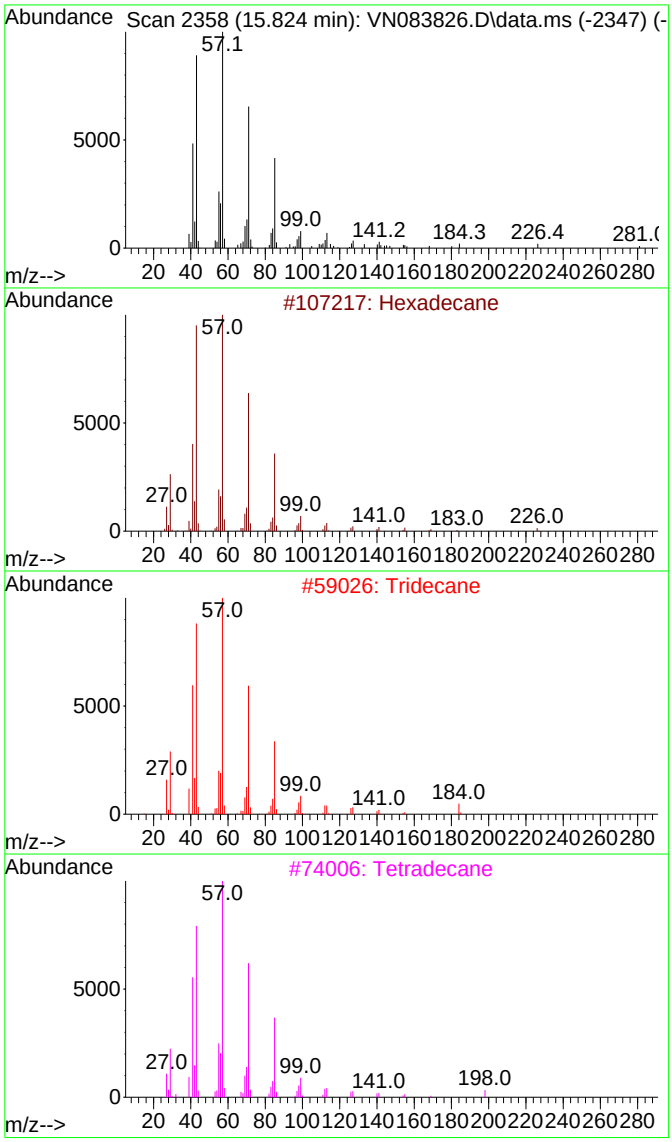
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

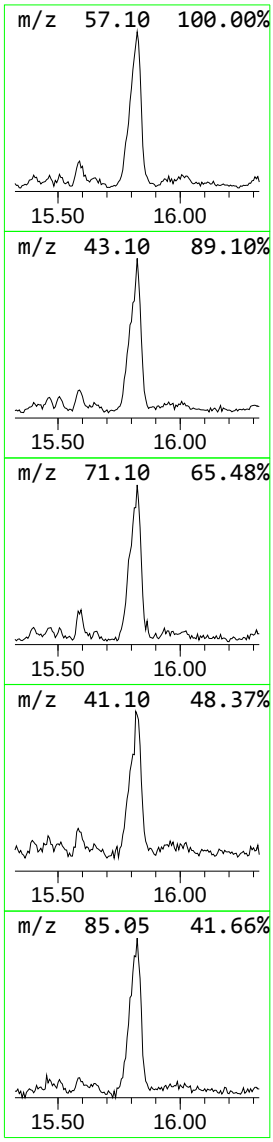
****

Peak Number 10 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.823	12.64 ug/l	332376	1,4-Dichlorobenzene-d4	13.788

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	96
2	Tridecane	184	C13H28	000629-50-5	95
3	Tetradecane	198	C14H30	000629-59-4	91
4	Dodecane	170	C12H26	000112-40-3	90
5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083826.D
Acq On : 12 Sep 2024 12:31
Operator : JC\MD
Sample : P3913-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
82924-A-C

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
unknown2.077	2.077	19.6	ug/l	177949	1	8.224	455052	50.0
Sulfur dioxide	2.289	12.8	ug/l	116446	1	8.224	455052	50.0
Propanal	4.283	9.2	ug/l	83251	1	8.224	455052	50.0
Isopropyl Alcohol	4.736	11.6	ug/l	105458	1	8.224	455052	50.0
2-Butanol, (R)-	7.789	39.2	ug/l	357122	1	8.224	455052	50.0
Pentanal	9.653	11.0	ug/l	155010	2	9.100	706317	50.0
Butanoic acid	11.512	27.5	ug/l	609484	3	11.865	1107970	50.0
Butanoic acid, ...	13.336	14.1	ug/l	371592	4	13.788	1314390	50.0
1-Hexanol, 2-et...	13.871	30.8	ug/l	810142	4	13.788	1314390	50.0
Hexadecane	15.823	12.6	ug/l	332376	4	13.788	1314390	50.0