LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083823.D
Acq On : 12 Sep 2024 11:20
Operator : JC\MD
Sample : P3913-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
9424-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: VN083823.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	17	21	28	rVB3	42652	68272	4.20%	0.589%
2	2.295	50	58	75	rBV3	50710	135447	8.33%	1.169%
3	2.659	114	120	130	rBV	83884	159828	9.82%	1.379%
4	3.518	257	266	278	rVB4	7394	18030	1.11%	0.156%
5	4.283	385	396	411	rBV	69233	216289	13.29%	1.867%
6	4.430	411	421	438	rVB	113711	341559	20.99%	2.948%
7	4.730	459	472	485	rBV	28572	106692	6.56%	0.921%
8	6.142	700	712	724	rBV3	12079	40898	2.51%	0.353%
9	6.671	792	802	813	rBV4	7492	22985	1.41%	0.198%
10	7.224	886	896	907	rBV3	44473	130284	8.01%	1.124%
11	7.483	924	940	952	rBV	95153	248601	15.28%	2.146%
12	7.789	980	992	1003	rBV2	116691	310901	19.11%	2.683%
13	8.165	1044	1056	1060	rBV	112951	260867	16.03%	2.251%
14	8.218	1060	1065	1078	rVB	187482	414997	25.51%	3.582%
15	8.536	1107	1119	1134	rBV2	580483	1626949	100.00%	14.041%
16	9.100	1206	1215	1225	rBV	317696	646396	39.73%	5.579%
17	9.271	1237	1244	1255	rBV2	47821	107763	6.62%	0.930%
18	9.530	1280	1288	1296	rBV	63690	125817	7.73%	1.086%
19	9.653	1299	1309	1321	rVB	175488	349942	21.51%	3.020%
20	10.565	1456	1464	1471	rBV	442616	828130	50.90%	7.147%
21	10.624	1471	1474	1483	rVB3	18784	33344	2.05%	0.288%
22	11.124	1548	1559	1565	rBV2	14036	38701	2.38%	0.334%
23	11.259	1576	1582	1585	rBV2	15657	29150	1.79%	0.252%
24	11.300	1585	1589	1595	rVB	31838	53122	3.27%	0.458%
25	11.406	1601	1607	1613	rVB4	9599	18752	1.15%	0.162%
26	11.506	1615	1624	1637	rBV2	42278	108418	6.66%	0.936%
27	11.865	1674	1685	1696	rVB	554373	994331	61.12%	8.581%
28	11.971	1696	1703	1708	rVV3	14298	27603	1.70%	0.238%
29	12.024	1708	1712	1715	rVV5	14226	28716	1.77%	0.248%
30	12.065	1715	1719	1728	rVV2	36839	67130	4.13%	0.579%
31	12.165	1728	1736	1741	rVV2	25417	46329	2.85%	0.400%
32	12.235	1741	1748	1760	rVB3	17748	38836	2.39%	0.335%
33	12.418	1766	1779	1783	rBV5	38650	103981	6.39%	0.897%
34	12.559	1797	1803	1811	rBV	89975	155114	9.53%	1.339%
35	12.688	1818	1825	1832	rVB5	18445	38612	2.37%	0.333%
36	12.847	1845	1852	1860	rBV	418506	712087	43.77%	6.146%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083823.D
Acq On : 12 Sep 2024 11:20
Operator : JC\MD
Sample : P3913-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
9424-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	13.035	1878	1884	1888	rBV	21545	32102	1.97%	0.277%
38	13.118	1895	1898	1903	rVV4	12098	20108	1.24%	0.174%
39	13.235	1911	1918	1921	rVV6	10452	25561	1.57%	0.221%
40	13.335	1928	1935	1943	rVB	137929	224341	13.79%	1.936%
41	13.494	1955	1962	1975	rVB3	66656	167410	10.29%	1.445%
42	13.623	1979	1984	1989	rVB5	13916	21002	1.29%	0.181%
43	13.682	1989	1994	1999	rBV2	40181	72202	4.44%	0.623%
44	13.788	2005	2012	2020	rBV	616045	1057274	64.99%	9.125%
45	13.871	2020	2026	2037	rBV	360671	591711	36.37%	5.107%
46	14.106	2062	2066	2071	rVB3	11566	19091	1.17%	0.165%
47	14.171	2071	2077	2084	rBV	38388	66233	4.07%	0.572%
48	14.241	2084	2089	2094	rBV2	31621	54895	3.37%	0.474%
49	14.547	2133	2141	2149	rBV3	57271	120617	7.41%	1.041%
50	14.706	2163	2168	2179	rBV	16335	35633	2.19%	0.308%
51	14.959	2203	2211	2215	rVB3	13284	22573	1.39%	0.195%
52	15.041	2218	2225	2227	rBV2	10571	20498	1.26%	0.177%
53	15.118	2233	2238	2245	rVB4	12347	24661	1.52%	0.213%
54	15.200	2245	2252	2259	rVB4	9918	20648	1.27%	0.178%
55	15.394	2279	2285	2292	rBV5	19785	38298	2.35%	0.331%
56	15.506	2294	2304	2311	rVV5	15169	42546	2.62%	0.367%
57	15.588	2311	2318	2319	rVV3	12283	16737	1.03%	0.144%
58	15.641	2321	2327	2334	rVB	74626	143644	8.83%	1.240%
59	15.829	2351	2359	2367	rBV5	28986	57462	3.53%	0.496%
60	16.776	2513	2520	2522	rBV2	20633	36822	2.26%	0.318%

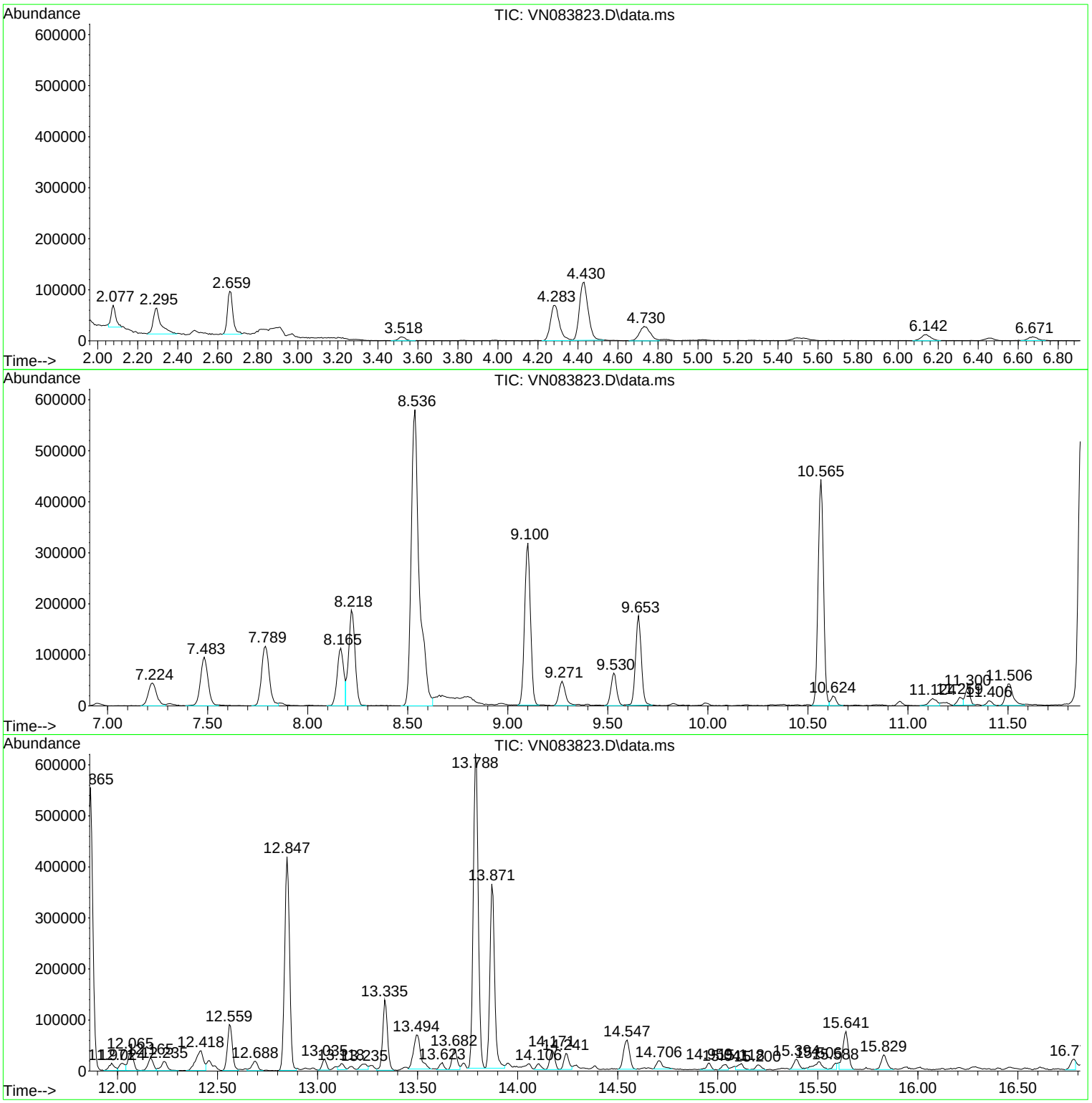
Sum of corrected areas: 11586942

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083823.D
Acq On : 12 Sep 2024 11:20
Operator : JC\MD
Sample : P3913-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
9424-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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083823.D
Acq On : 12 Sep 2024 11:20
Operator : JC\MD
Sample : P3913-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
9424-A-C

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

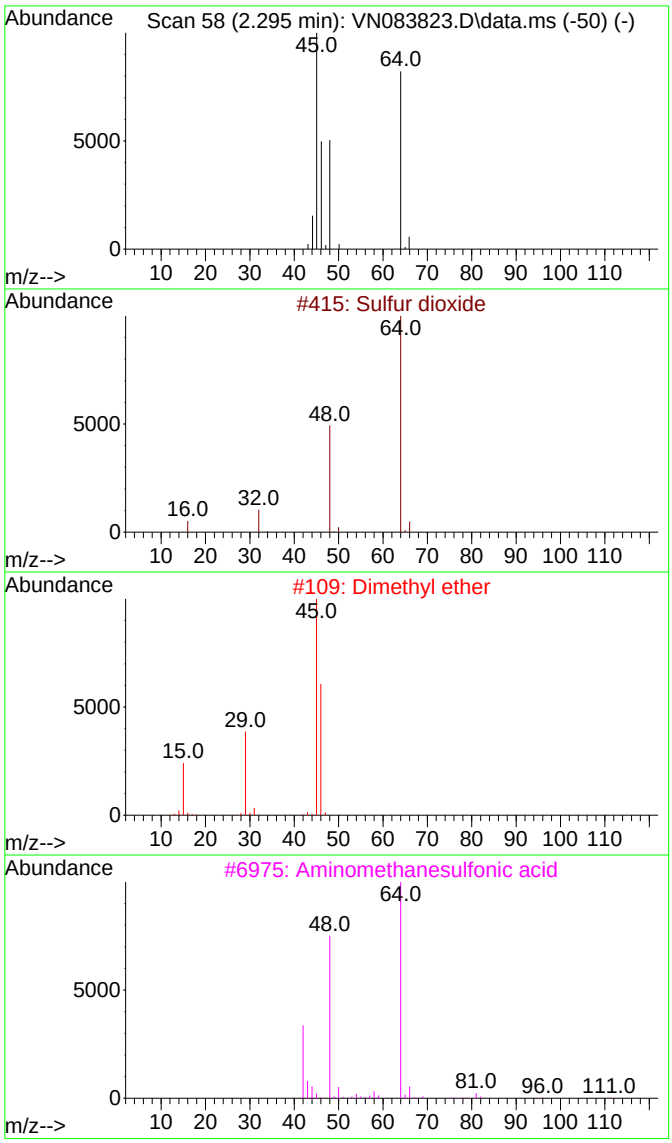
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

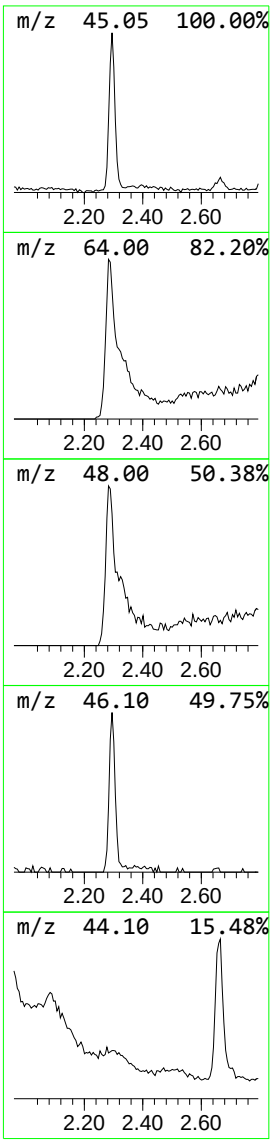
****

Peak Number 1 Sulfur dioxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.295	16.32 ug/l	135447	Pentafluorobenzene	8.218

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	58
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5	Oxalic acid	90	C2H2O4	000144-62-7	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083823.D
Acq On : 12 Sep 2024 11:20
Operator : JC\MD
Sample : P3913-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
9424-A-C

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

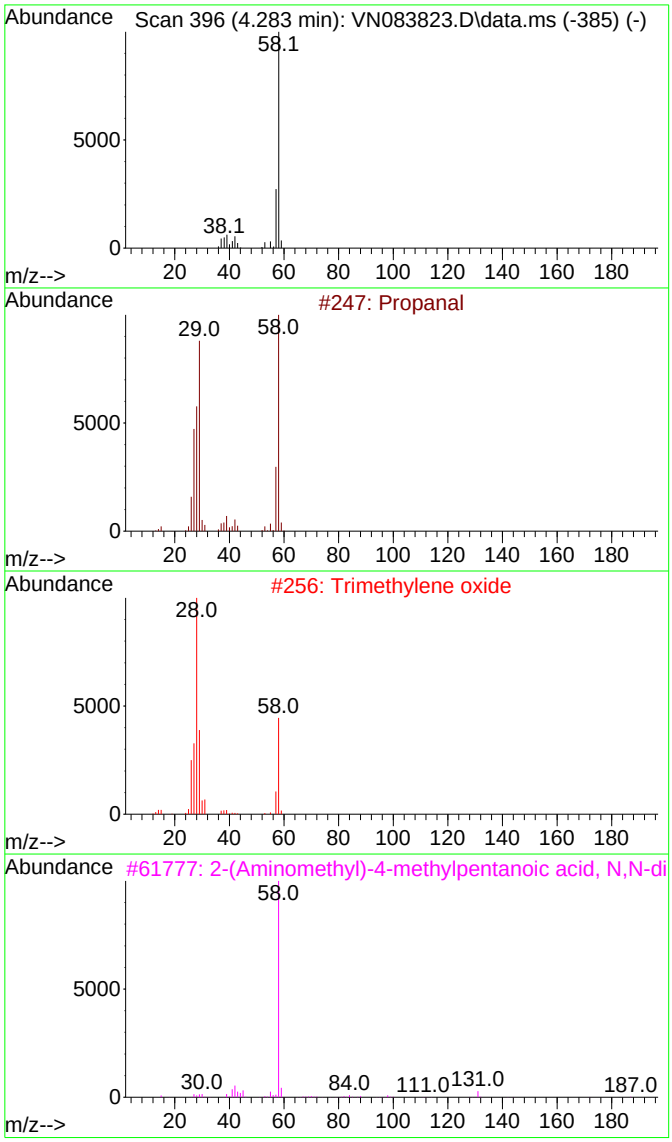
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

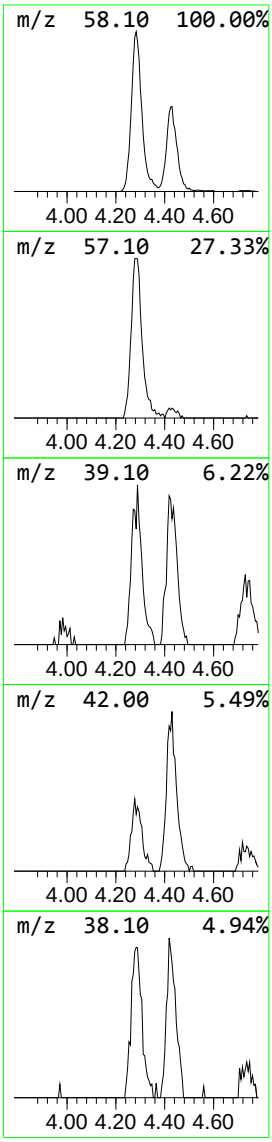
****

Peak Number 3 Propanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.283	26.06 ug/l	216289	Pentafluorobenzene	8.218

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal	58	C3H6O	000123-38-6	78
2	Trimethylene oxide	58	C3H6O	000503-30-0	9
3	2-(Aminomethyl)-4-methylpentanoi...	187	C10H21NO2	1891211-54-3	9
4	Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7
5	Propylene oxide	58	C3H6O	000075-56-9	7





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083823.D
Acq On : 12 Sep 2024 11:20
Operator : JC\MD
Sample : P3913-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
9424-A-C

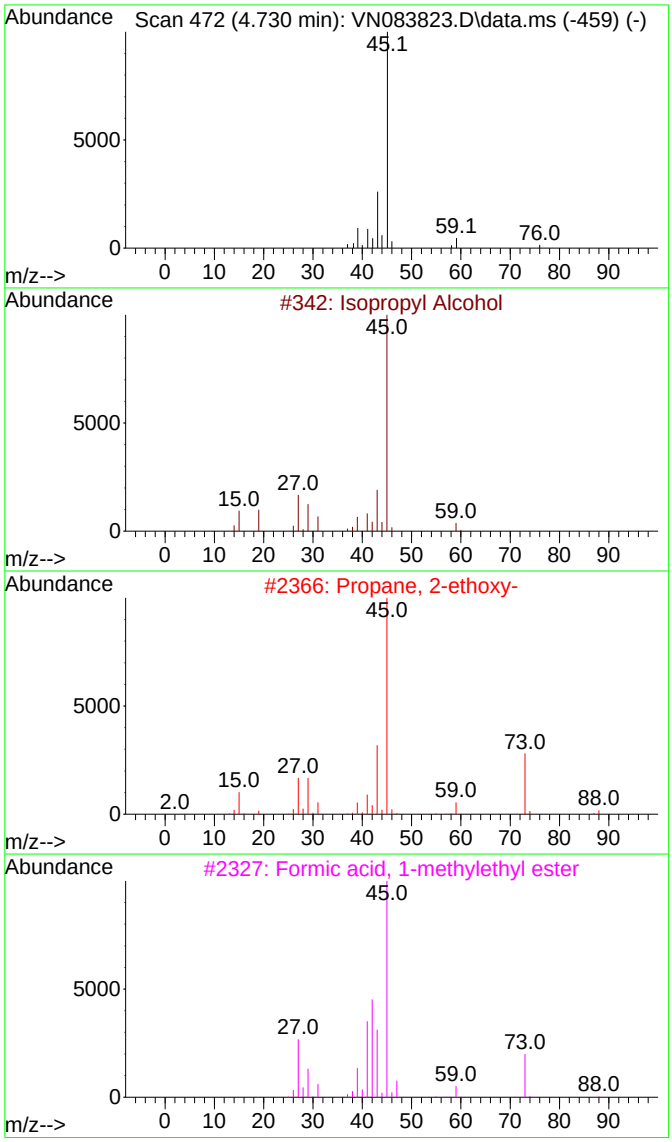
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

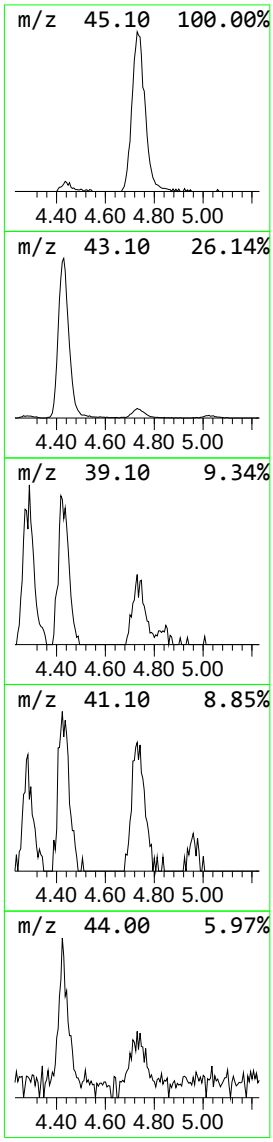
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Isopropyl Alcohol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.730	12.85 ug/l	106692	Pentafluorobenzene	8.218

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	43
3	Formic acid, 1-methylethyl ester	88	C4H8O2	000625-55-8	40
4	2-Pentanol	88	C5H12O	006032-29-7	9
5	(S)-(+)-2-Pentanol	88	C5H12O	026184-62-3	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083823.D
Acq On : 12 Sep 2024 11:20
Operator : JC\MD
Sample : P3913-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
9424-A-C

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

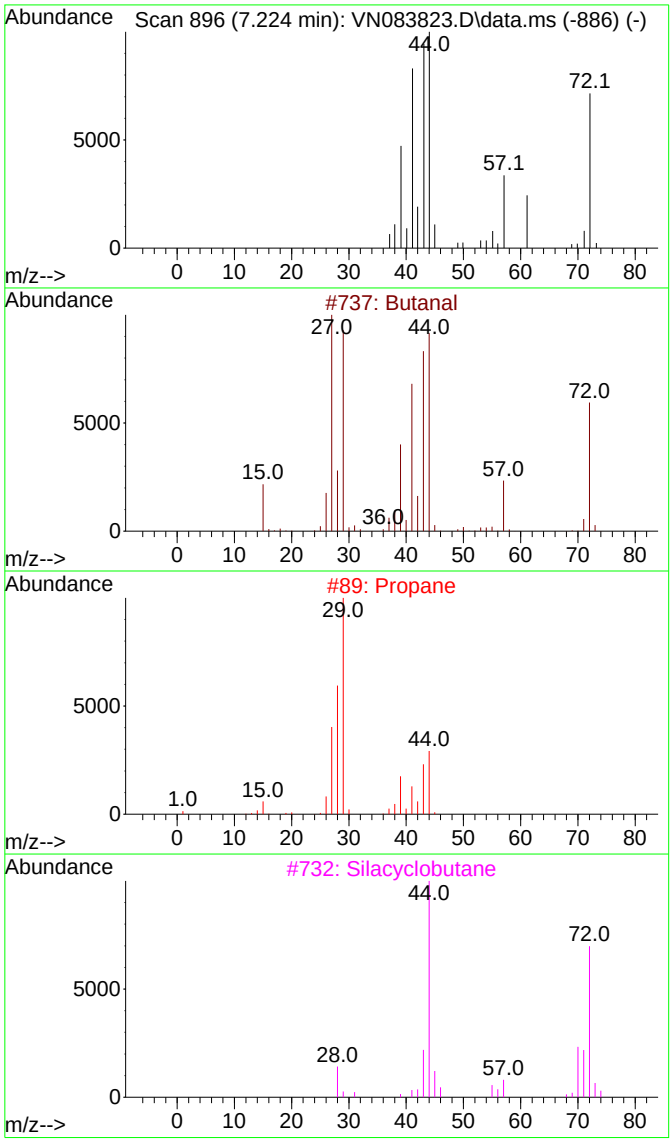
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

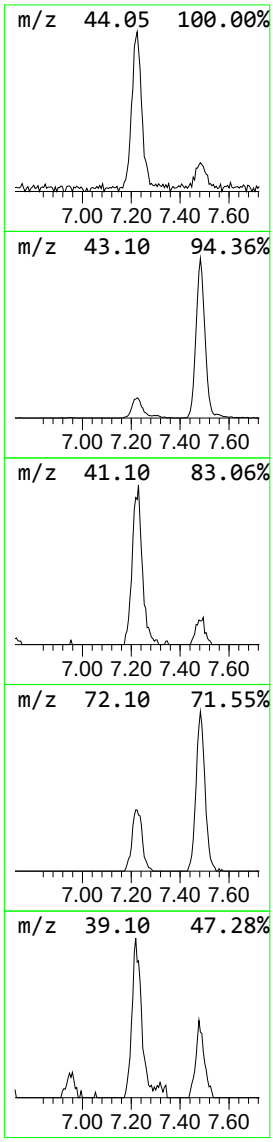
****

Peak Number 5 Butanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.224	15.70 ug/l	130284	Pentafluorobenzene	8.218

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	87
2	Propane	44	C3H8	000074-98-6	50
3	Silacyclobutane	72	C3H8Si	1000434-34-1	38
4	Propanal, 2-methyl-	72	C4H8O	000078-84-2	27
5	N-Formyl-dl-alanine	117	C4H7NO3	005893-10-7	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083823.D
Acq On : 12 Sep 2024 11:20
Operator : JC\MD
Sample : P3913-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
9424-A-C

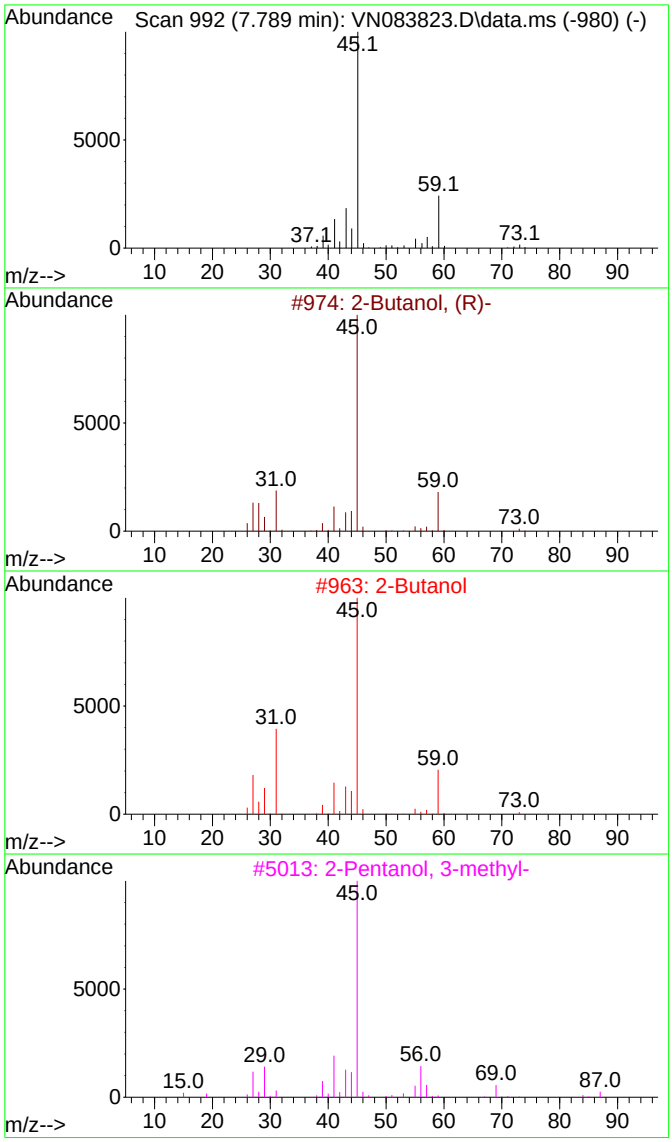
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

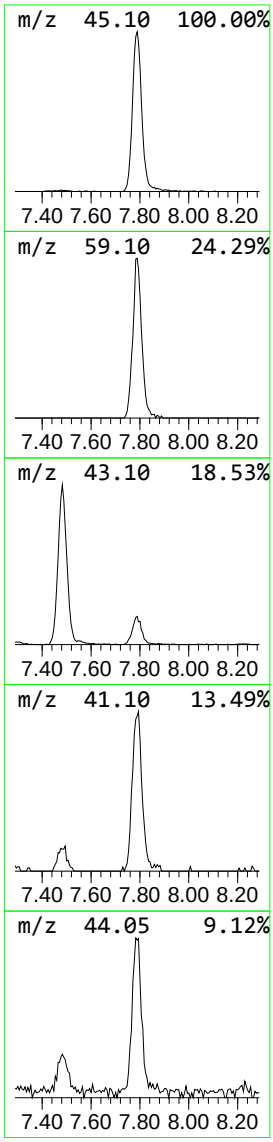
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Butanol, (R)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.789	37.46 ug/l	310901	Pentafluorobenzene	8.218

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	2-Hexanol, (R)-	102	C6H14O	026549-24-6	38
5	2-Hexanol	102	C6H14O	000626-93-7	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083823.D
Acq On : 12 Sep 2024 11:20
Operator : JC\MD
Sample : P3913-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
9424-A-C

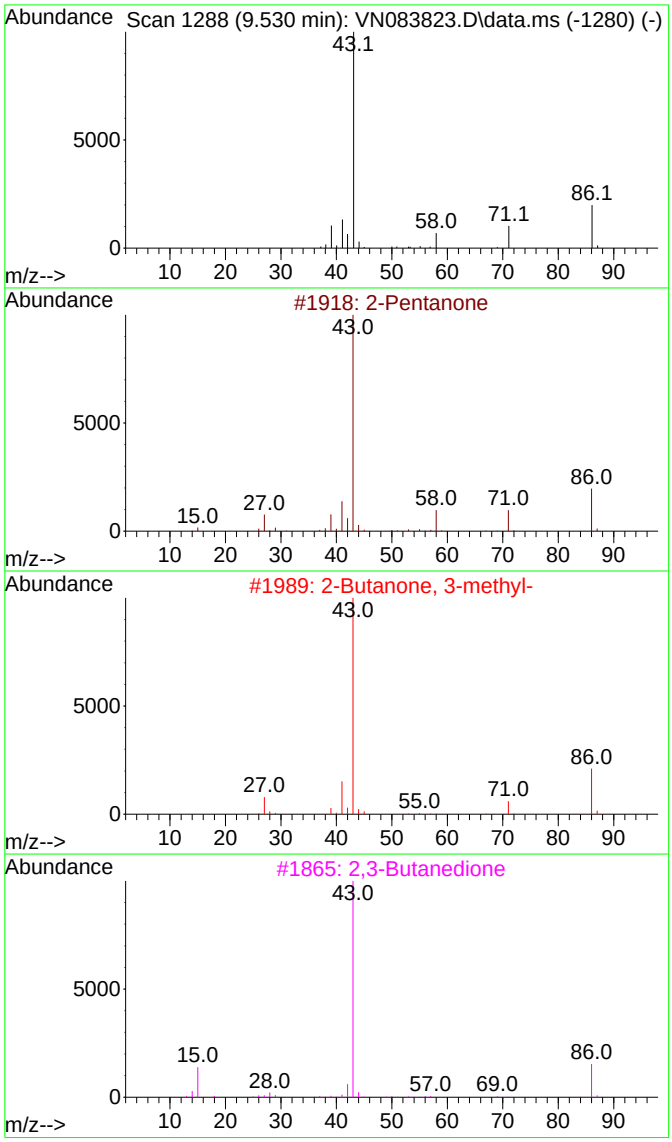
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

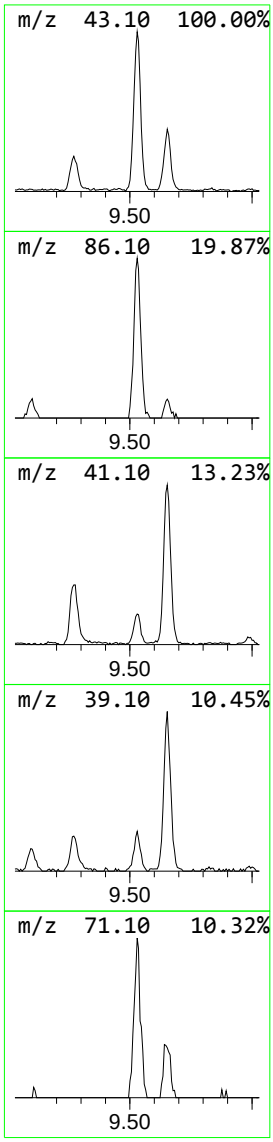
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2-Pentanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.530	9.73 ug/l	125817	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	90
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	64
3	2,3-Butanedione	86	C4H6O2	000431-03-8	58
4	3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	36
5	Acetic acid ethenyl ester	86	C4H6O2	000108-05-4	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083823.D
Acq On : 12 Sep 2024 11:20
Operator : JC\MD
Sample : P3913-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
9424-A-C

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

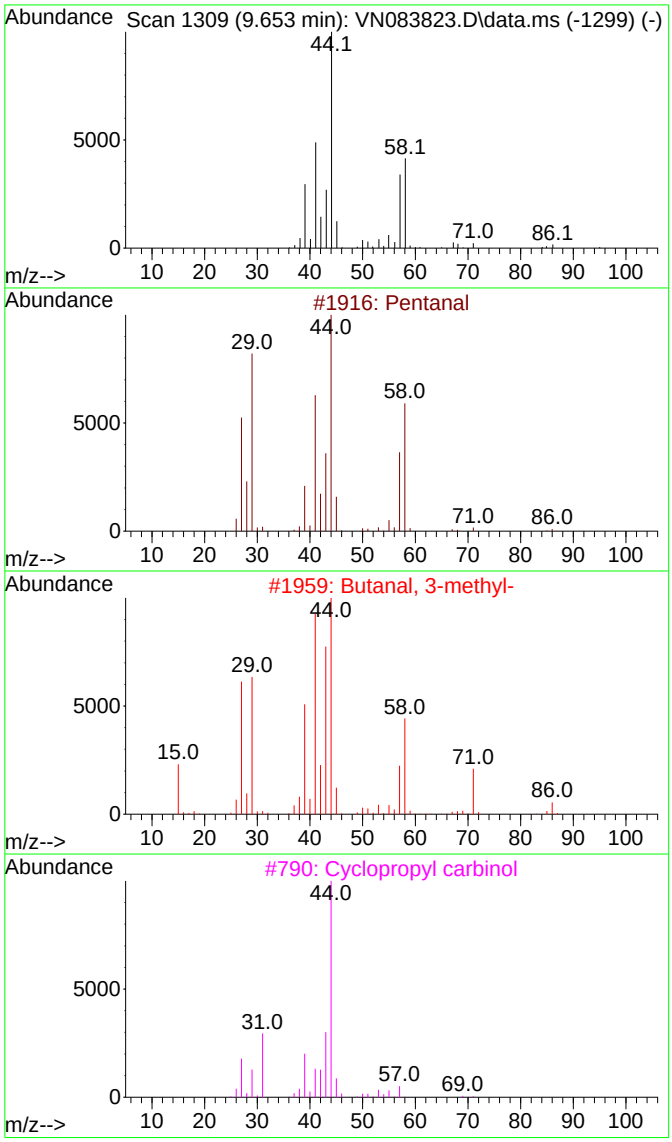
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

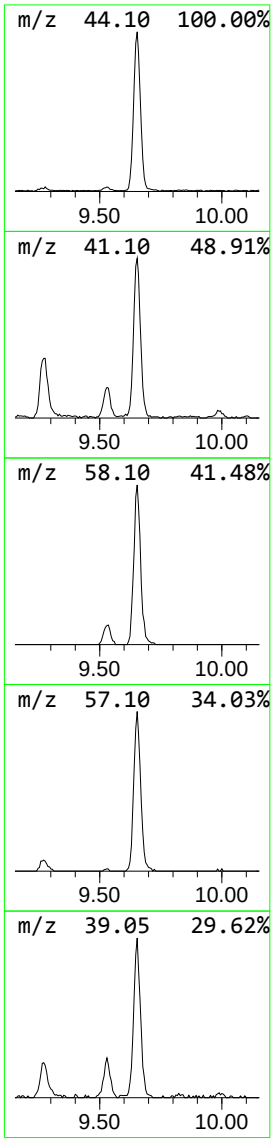
****

Peak Number 8 Pentanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.653	27.07 ug/l	349942	1,4-Difluorobenzene	9.100

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal	86	C5H10O	000110-62-3	78
2	Butanal, 3-methyl-	86	C5H10O	000590-86-3	53
3	Cyclopropyl carbinol	72	C4H8O	002516-33-8	42
4	2-Formylhistamine	139	C6H9N3O	1000132-95-8	28
5	2-Pentanamine	87	C5H13N	063493-28-7	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083823.D
Acq On : 12 Sep 2024 11:20
Operator : JC\MD
Sample : P3913-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
9424-A-C

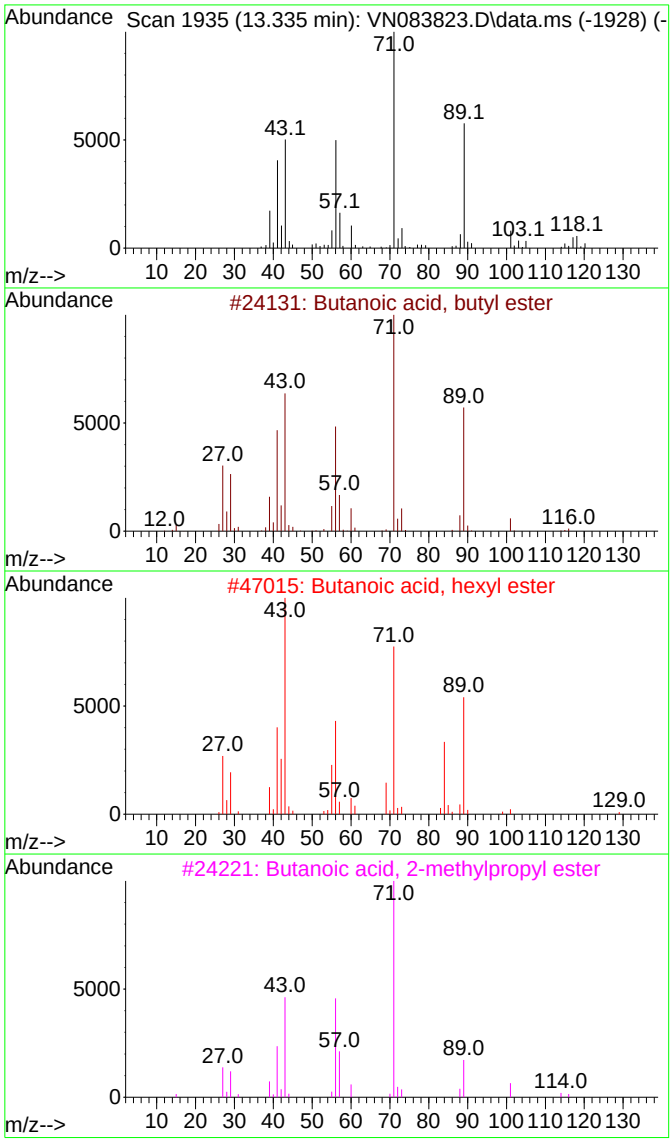
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091024W.M
Quant Title : SW846 8260

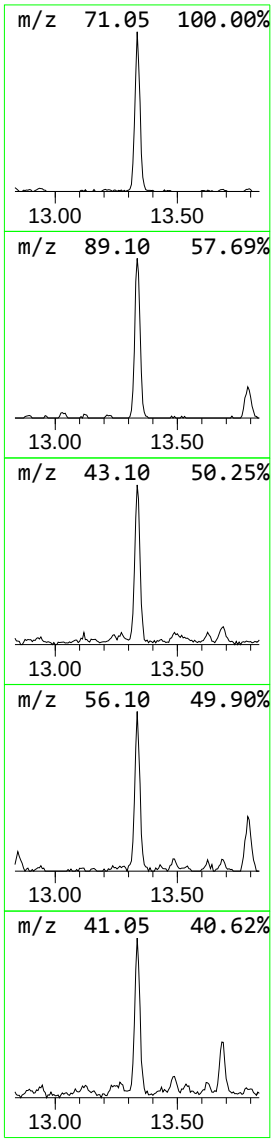
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Butanoic acid, butyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.335	10.61 ug/l	224341	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	87
2	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	72
3	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	59
4	Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	59
5	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083823.D
Acq On : 12 Sep 2024 11:20
Operator : JC\MD
Sample : P3913-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
9424-A-C

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

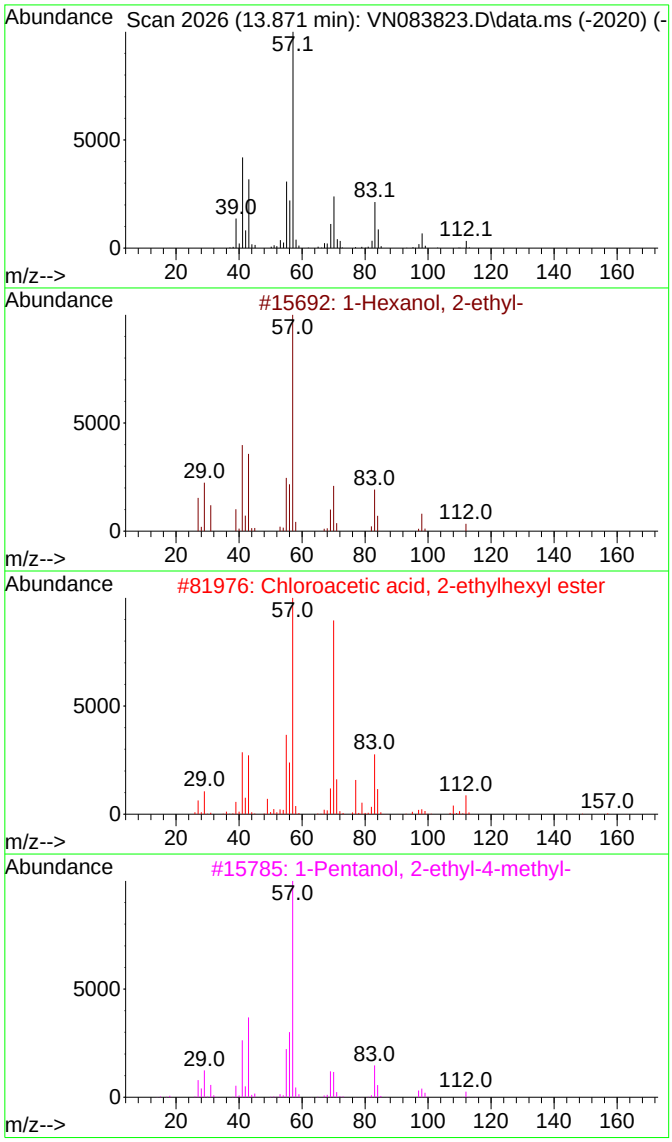
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

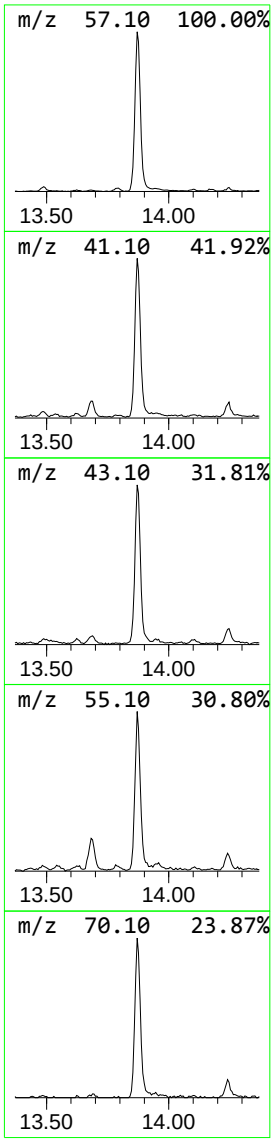
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.871	27.98 ug/l	591711	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	Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	59
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
5	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091224\
Data File : VN083823.D
Acq On : 12 Sep 2024 11:20
Operator : JC\MD
Sample : P3913-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
9424-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
Sulfur dioxide	2.295	16.3	ug/l	135447	1	8.218	414997	50.0
Propanal	4.283	26.1	ug/l	216289	1	8.218	414997	50.0
Isopropyl Alcohol	4.730	12.9	ug/l	106692	1	8.218	414997	50.0
Butanal	7.224	15.7	ug/l	130284	1	8.218	414997	50.0
2-Butanol, (R)-	7.789	37.5	ug/l	310901	1	8.218	414997	50.0
2-Pentanone	9.530	9.7	ug/l	125817	2	9.100	646396	50.0
Pentanal	9.653	27.1	ug/l	349942	2	9.100	646396	50.0
Butanoic acid, ...	13.335	10.6	ug/l	224341	4	13.788	1057270	50.0
1-Hexanol, 2-et...	13.871	28.0	ug/l	591711	4	13.788	1057270	50.0