LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121522\
Data File : VN075830.D
Acq On : 15 Dec 2022 20:11
Operator : JC\MD
Sample : N6066-09
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ORA-583

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\82N121422W.M
Title : SW846 8260

Signal : TIC: VN075830.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.095	3	7	16	rVB	209375	310524	18.29%	2.155%
2	2.336	40	48	55	rVB	40648	63273	3.73%	0.439%
3	2.524	70	80	90	rBV2	56306	135787	8.00%	0.942%
4	2.677	101	106	115	rVB	11587	20665	1.22%	0.143%
5	2.824	125	131	137	rVB4	10274	23384	1.38%	0.162%
6	3.253	198	204	213	rVB2	14288	33127	1.95%	0.230%
7	3.806	291	298	311	rBV2	19171	51710	3.05%	0.359%
8	4.447	394	407	418	rBV	44561	134733	7.93%	0.935%
9	4.730	444	455	467	rBV2	15843	52563	3.10%	0.365%
10	5.530	580	591	603	rBV	8345	29352	1.73%	0.204%
11	6.159	687	698	709	rBV5	5357	17604	1.04%	0.122%
12	6.694	775	789	807	rBV4	73537	291322	17.16%	2.022%
13	7.235	869	881	894	rBV	247538	684891	40.33%	4.753%
14	7.494	916	925	937	rBV2	93063	237938	14.01%	1.651%
15	8.177	1030	1041	1045	rBV	234763	563226	33.17%	3.908%
16	8.229	1045	1050	1065	rVB	481003	1059961	62.42%	7.356%
17	8.606	1095	1114	1134	rBV3	366273	1241577	73.12%	8.616%
18	9.106	1190	1199	1212	rVB	611633	1249559	73.59%	8.671%
19	9.271	1219	1227	1236	rBV2	31597	65631	3.87%	0.455%
20	9.659	1287	1293	1304	rVB4	23685	53415	3.15%	0.371%
21	10.571	1439	1448	1454	rBV	918401	1698071	100.00%	11.784%
22	10.635	1454	1459	1470	rVB	334528	611445	36.01%	4.243%
23	10.959	1507	1514	1523	rVB4	12931	26489	1.56%	0.184%
24	11.353	1576	1581	1587	rVB3	16203	26513	1.56%	0.184%
25	11.870	1656	1669	1679	rBV	778594	1434929	84.50%	9.958%
26	11.965	1680	1685	1692	rVV	28848	51352	3.02%	0.356%
27	12.070	1696	1703	1715	rVV2	116978	225679	13.29%	1.566%
28	12.206	1719	1726	1738	rVB3	78234	135432	7.98%	0.940%
29	12.406	1751	1760	1767	rBV5	59024	141592	8.34%	0.983%
30	12.853	1827	1836	1847	rBV	615820	1059230	62.38%	7.350%
31	13.100	1873	1878	1882	rBV2	20016	35975	2.12%	0.250%
32	13.176	1887	1891	1896	rVB	17841	25521	1.50%	0.177%
33	13.247	1896	1903	1906	rBV4	9053	17360	1.02%	0.120%
34	13.341	1911	1919	1926	rVB2	40555	72712	4.28%	0.505%
35	13.488	1937	1944	1949	rBV	46893	82010	4.83%	0.569%
36	13.535	1949	1952	1961	rVB6	17188	27089	1.60%	0.188%

LSC Area Percent Report

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ALS Vial : 24 Sample Multiplier: 1

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ClientSampleId :
ORA-583

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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Title : SW846 8260

37	13.688	1972	1978	1984	rBV4	11109	20337	1.20%	0.141%
38	13.794	1988	1996	2004	rBV	744108	1289517	75.94%	8.949%
39	13.876	2004	2010	2019	rBV	498912	795931	46.87%	5.523%
40	13.953	2019	2023	2027	rVV5	17973	26133	1.54%	0.181%
41	14.176	2054	2061	2068	rVB3	30262	54867	3.23%	0.381%
42	14.247	2068	2073	2078	rBV7	13559	25389	1.50%	0.176%
43	14.459	2101	2109	2116	rBV5	7323	18609	1.10%	0.129%
44	14.611	2129	2135	2140	rBV5	9235	18689	1.10%	0.130%
45	15.047	2202	2209	2214	rBV5	7190	17727	1.04%	0.123%
46	15.470	2275	2281	2287	rVB8	13370	26566	1.56%	0.184%
47	15.647	2305	2311	2321	rVB	54932	124972	7.36%	0.867%

Sum of corrected areas: 14410378

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Instrument :
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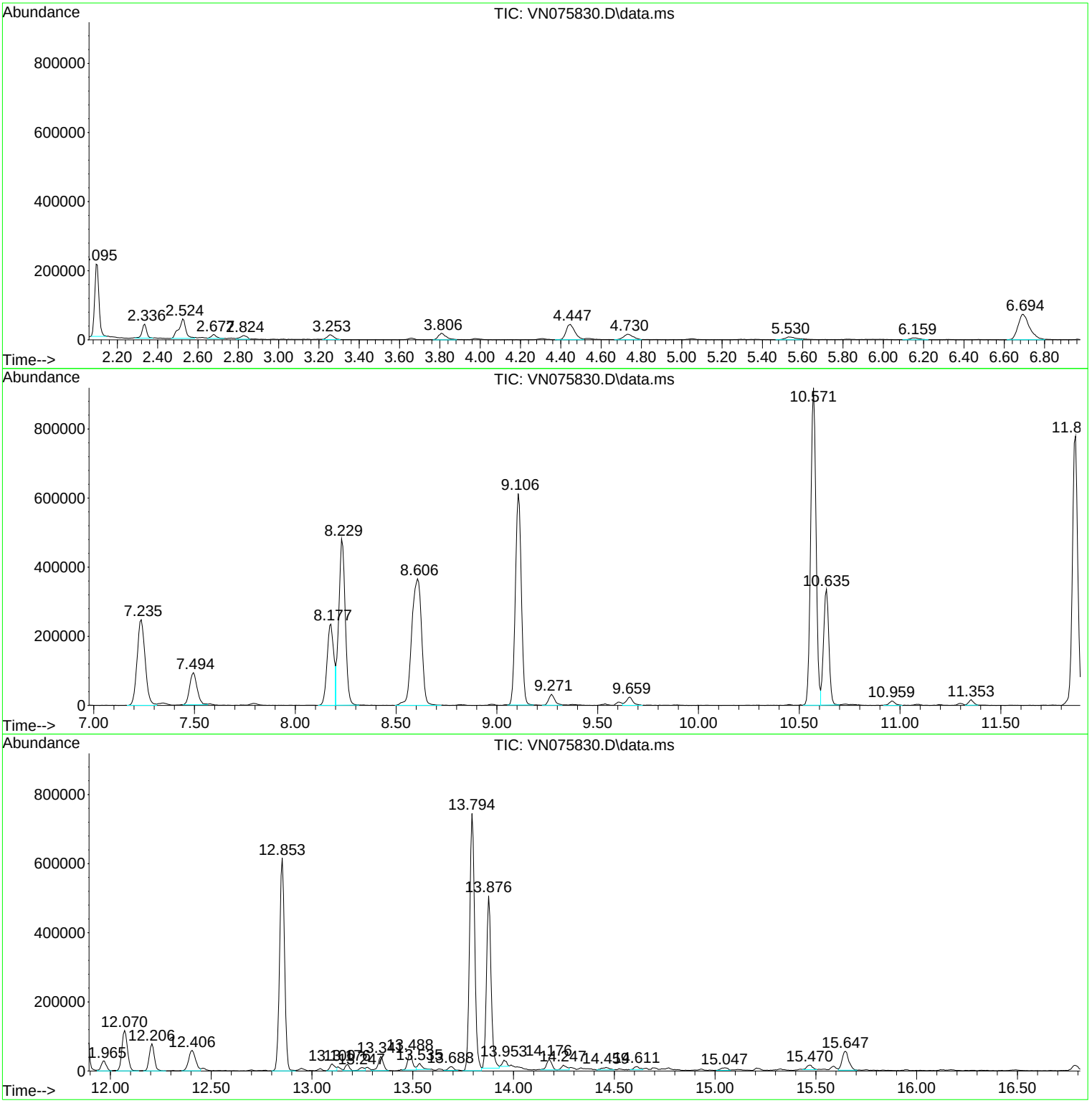
ClientSampleId :
ORA-583

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

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



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Acq On : 15 Dec 2022 20:11
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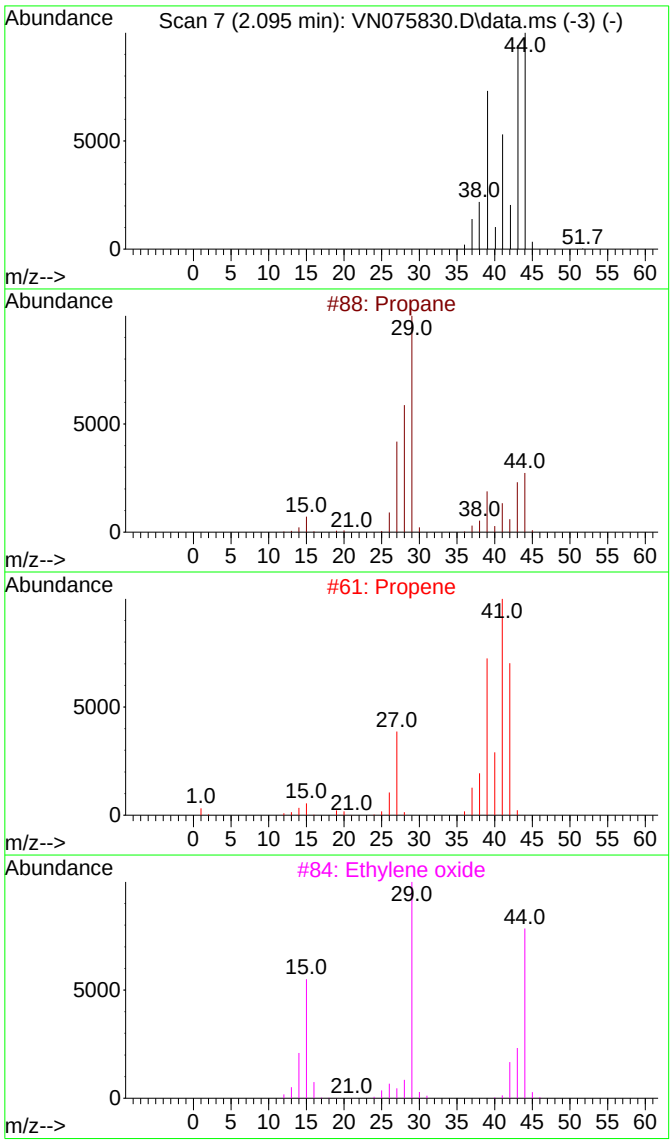
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

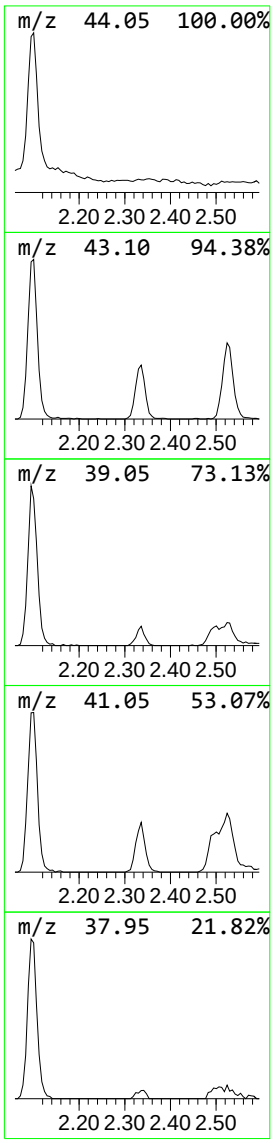
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Propane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.095	14.65 ug/l	310524	Pentafluorobenzene	8.229

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane	44	C3H8	000074-98-6	90
2	Propene	42	C3H6	000115-07-1	9
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Acetaldehyde	44	C2H4O	000075-07-0	5
5	Cyclopropene	40	C3H4	002781-85-3	2





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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
ORA-583

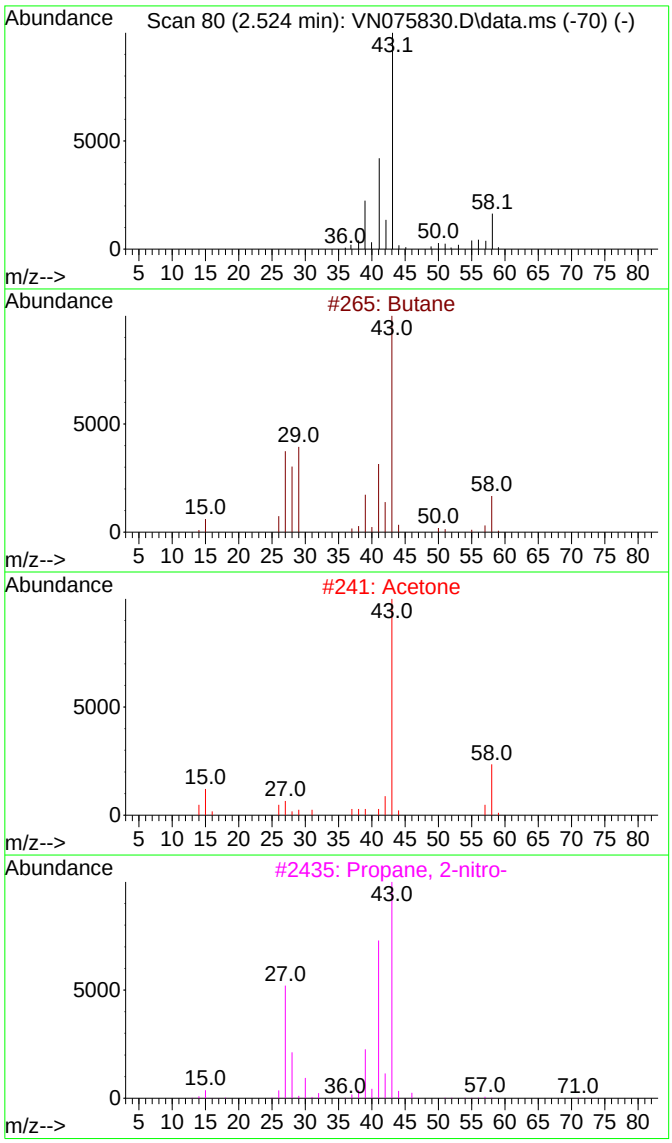
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

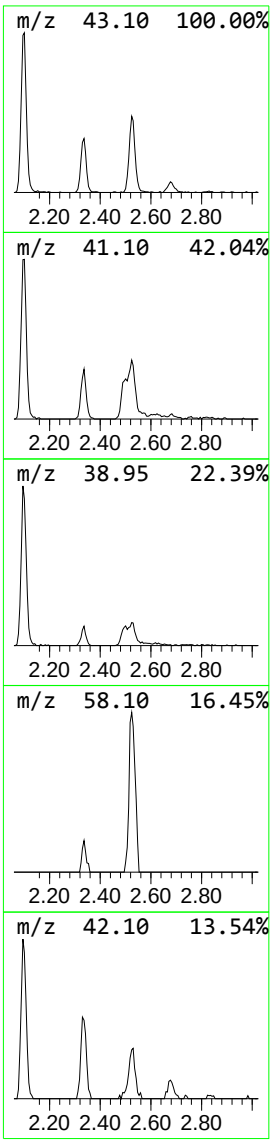
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.524	6.41 ug/l	135787	Pentafluorobenzene	8.229

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	59
2	Acetone	58	C3H6O	000067-64-1	9
3	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	4
4	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	4
5	Propanal	58	C3H6O	000123-38-6	3





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Instrument :
MSVOA_N
ClientSampleId :
ORA-583

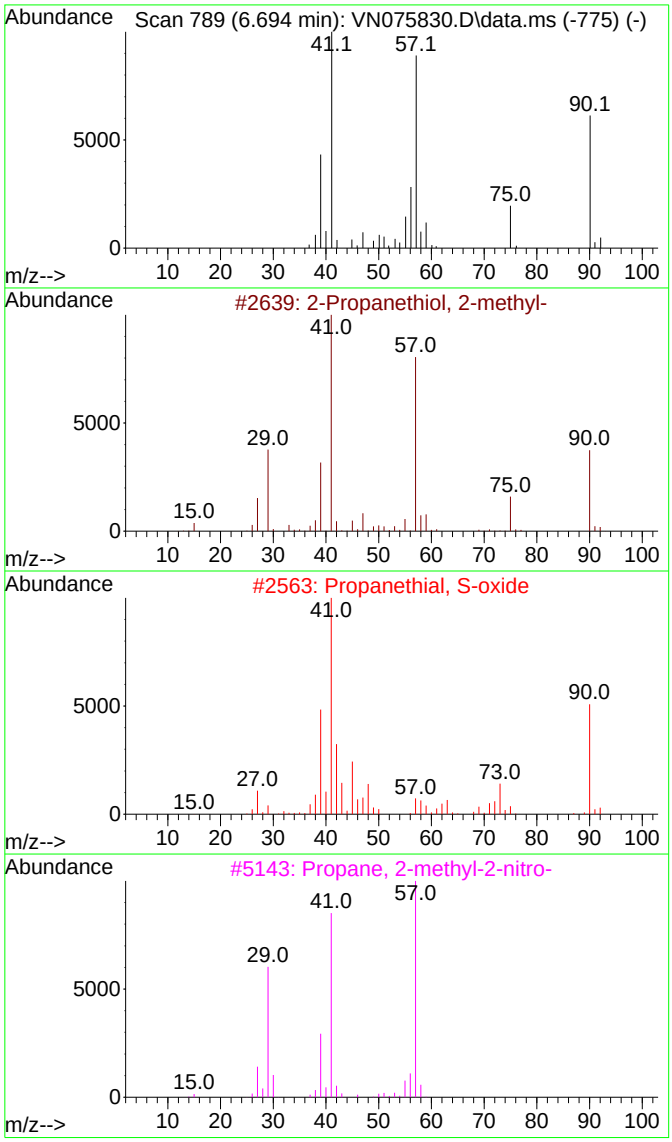
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

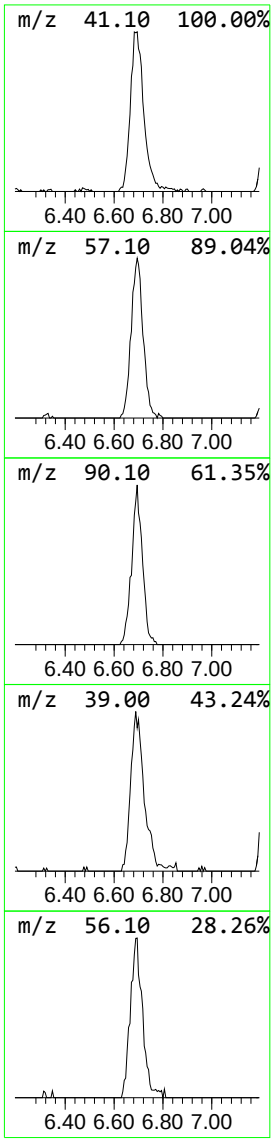
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Propanethiol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.694	13.74 ug/l	291322	Pentafluorobenzene	8.229

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	53
2	Propanethial, S-oxide	90	C3H6OS	032157-29-2	43
3	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	27
4	1-Propene, 2-methyl-	56	C4H8	000115-11-7	27
5	2-Butanethiol	90	C4H10S	000513-53-1	17





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Instrument :
MSVOA_N
ClientSampleId :
ORA-583

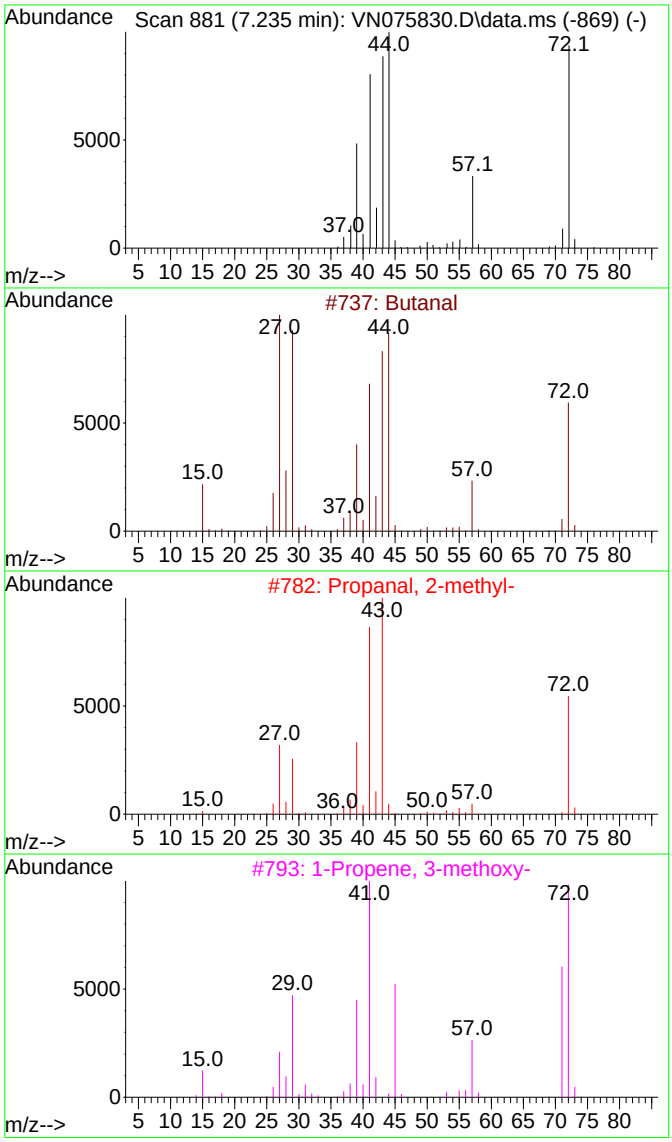
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

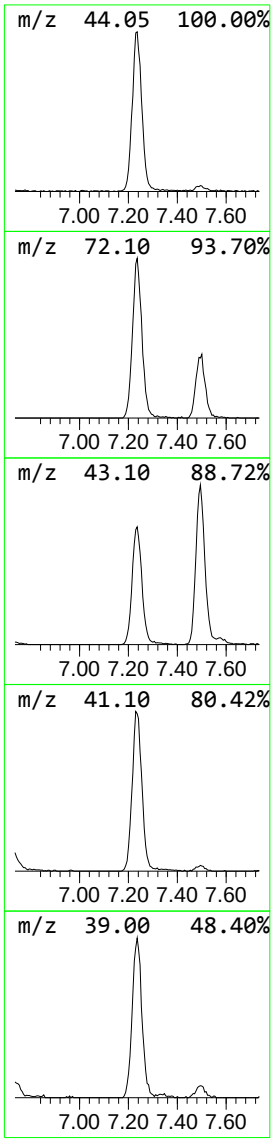
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.235	32.31 ug/l	684891	Pentafluorobenzene	8.229

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Propanal, 2-methyl-	72	C4H8O	000078-84-2	46
3	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	43
4	Isobutylene epoxide	72	C4H8O	000558-30-5	27
5	Cyclopropyl carbinol	72	C4H8O	002516-33-8	12





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Instrument :
MSVOA_N
ClientSampleId :
ORA-583

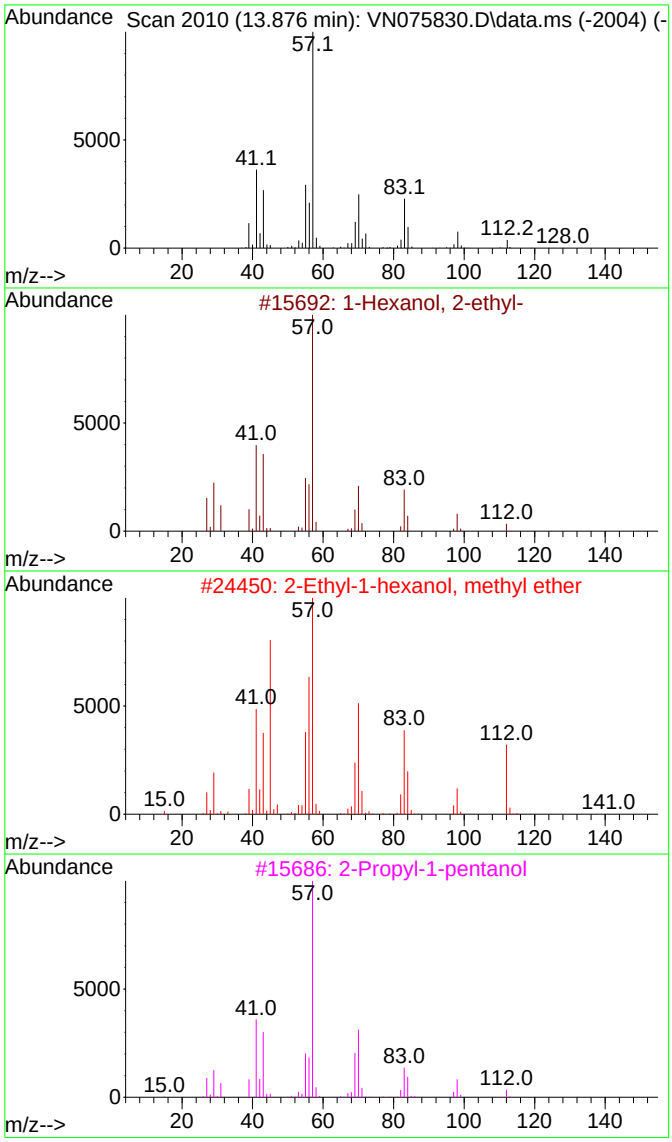
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

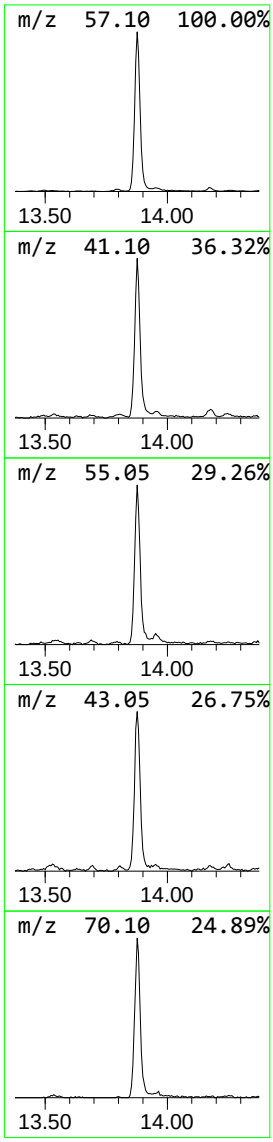
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	30.86 ug/l	795931	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	90
2	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5	Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	45





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane	2.095	14.7	ug/l	310524	1	8.229	1059960	50.0
Butane	2.524	6.4	ug/l	135787	1	8.229	1059960	50.0
2-Propanethiol,...	6.694	13.7	ug/l	291322	1	8.229	1059960	50.0
Butanal	7.235	32.3	ug/l	684891	1	8.229	1059960	50.0
1-Hexanol, 2-et...	13.876	30.9	ug/l	795931	4	13.794	1289520	50.0