LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122022\
Data File : VN075904.D
Acq On : 20 Dec 2022 17:23
Operator : JC\MD
Sample : N6161-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CLI-0667

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: VN075904.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	15	rVB3	26227	38255	2.14%	0.270%
2	2.336	38	48	52	rBV3	21183	41613	2.32%	0.293%
3	2.495	67	75	84	rBV	39365	80185	4.48%	0.565%
4	2.836	126	133	143	rVB4	18291	42079	2.35%	0.297%
5	4.442	394	406	416	rBV2	76280	224549	12.54%	1.583%
6	4.736	446	456	466	rBV3	11781	37993	2.12%	0.268%
7	5.612	600	605	615	rVB5	7890	20773	1.16%	0.146%
8	6.689	777	788	801	rBV3	57719	199712	11.15%	1.408%
9	7.230	870	880	893	rBV2	194632	547893	30.60%	3.863%
10	7.347	893	900	911	rVB6	11201	33053	1.85%	0.233%
11	7.494	917	925	934	rVB	24536	57633	3.22%	0.406%
12	8.171	1029	1040	1045	rBV	249715	604203	33.75%	4.260%
13	8.230	1045	1050	1063	rVB	494051	1098630	61.36%	7.747%
14	8.588	1096	1111	1126	rBV2	260479	725802	40.54%	5.118%
15	9.106	1189	1199	1220	rVB	652444	1324591	73.98%	9.340%
16	9.271	1220	1227	1237	rBV2	16381	38146	2.13%	0.269%
17	9.653	1285	1292	1304	rVB4	25306	66386	3.71%	0.468%
18	10.041	1349	1358	1364	rBV2	10677	19799	1.11%	0.140%
19	10.447	1421	1427	1433	rBV3	14401	27272	1.52%	0.192%
20	10.571	1439	1448	1454	rBV	976728	1790451	100.00%	12.625%
21	10.635	1454	1459	1465	rVB	78160	144396	8.06%	1.018%
22	10.741	1469	1477	1479	rBV	11762	23605	1.32%	0.166%
23	11.865	1656	1668	1680	rBV	835520	1516111	84.68%	10.690%
24	11.971	1680	1686	1693	rVB2	13790	27018	1.51%	0.191%
25	12.071	1697	1703	1714	rVB	43361	87449	4.88%	0.617%
26	12.206	1719	1726	1737	rVB2	169896	294731	16.46%	2.078%
27	12.412	1749	1761	1778	rBV4	167082	379267	21.18%	2.674%
28	12.853	1827	1836	1844	rBV	656971	1157422	64.64%	8.161%
29	13.100	1872	1878	1882	rBV2	12403	22653	1.27%	0.160%
30	13.170	1886	1890	1896	rVB4	14781	23979	1.34%	0.169%
31	13.253	1896	1904	1905	rBV3	12709	22682	1.27%	0.160%
32	13.270	1905	1907	1914	rVV7	14312	27751	1.55%	0.196%
33	13.347	1914	1920	1928	rVB4	32053	62480	3.49%	0.441%
34	13.488	1939	1944	1947	rVV	37688	68054	3.80%	0.480%
35	13.535	1947	1952	1957	rVV4	60256	114080	6.37%	0.804%
36	13.794	1989	1996	2004	rBV	818884	1387001	77.47%	9.780%

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Integration Parameters: RTEINT.P
Integrator: RTE
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Start Thrs: 0.2 Max Peaks: 100
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Peak separation: 5

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

37	13.876	2004	2010	2020	rVV	389625	651159	36.37%	4.591%
38	14.176	2053	2061	2069	rBV	560510	934711	52.21%	6.591%
39	14.294	2077	2081	2085	rVB4	10905	18281	1.02%	0.129%
40	14.464	2102	2110	2115	rBV10	9376	24628	1.38%	0.174%
41	15.123	2216	2222	2227	rVV3	18805	32332	1.81%	0.228%
42	15.211	2229	2237	2245	rVB3	41821	79662	4.45%	0.562%
43	15.323	2250	2256	2264	rVB9	7370	17936	1.00%	0.126%
44	15.641	2305	2310	2318	rVB2	20808	45503	2.54%	0.321%

Sum of corrected areas: 14181909

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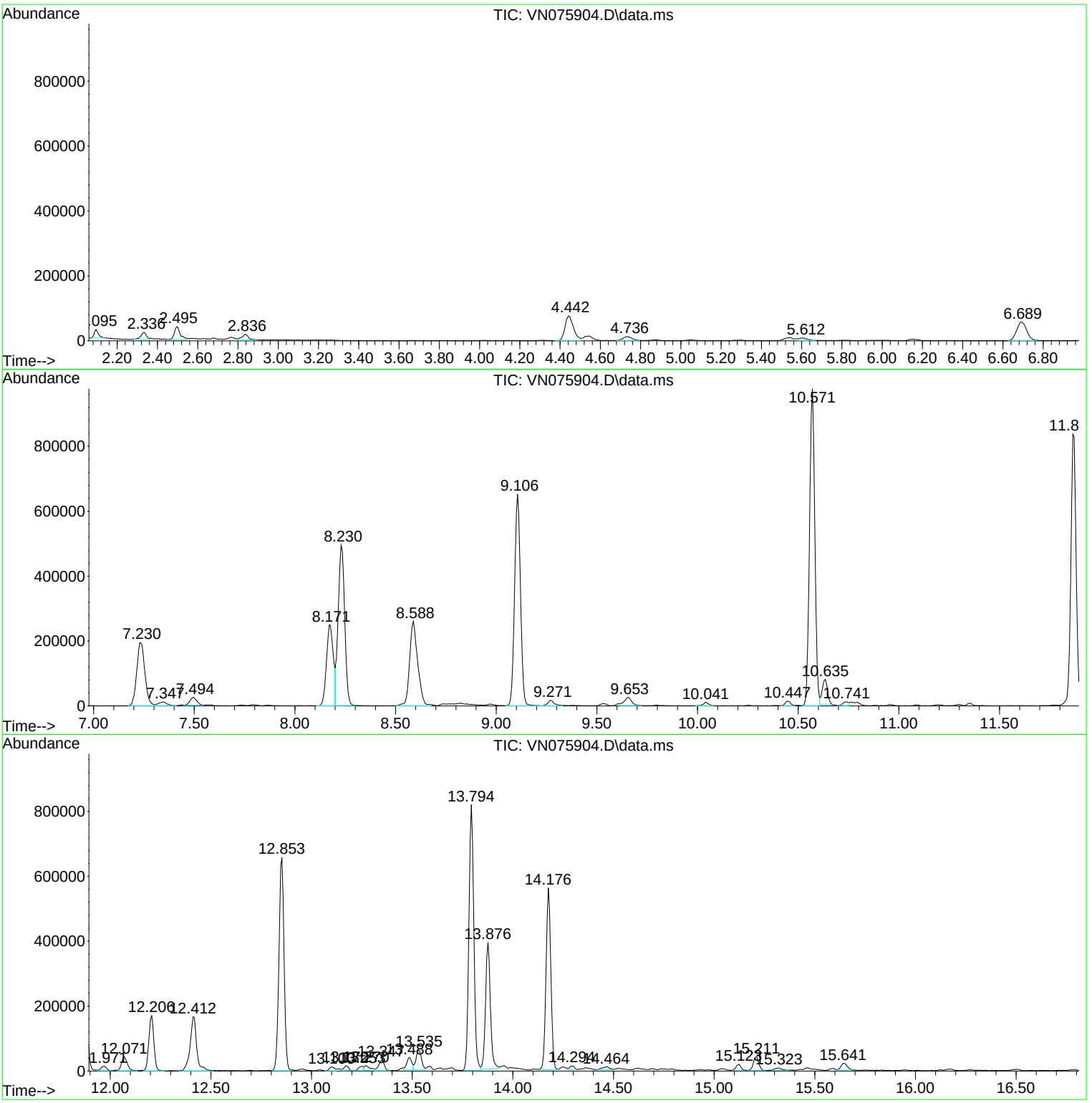
ClientSampleId :
CLI-0667

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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Data File : VN075904.D
Acq On : 20 Dec 2022 17:23
Operator : JC\MD
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CLI-0667

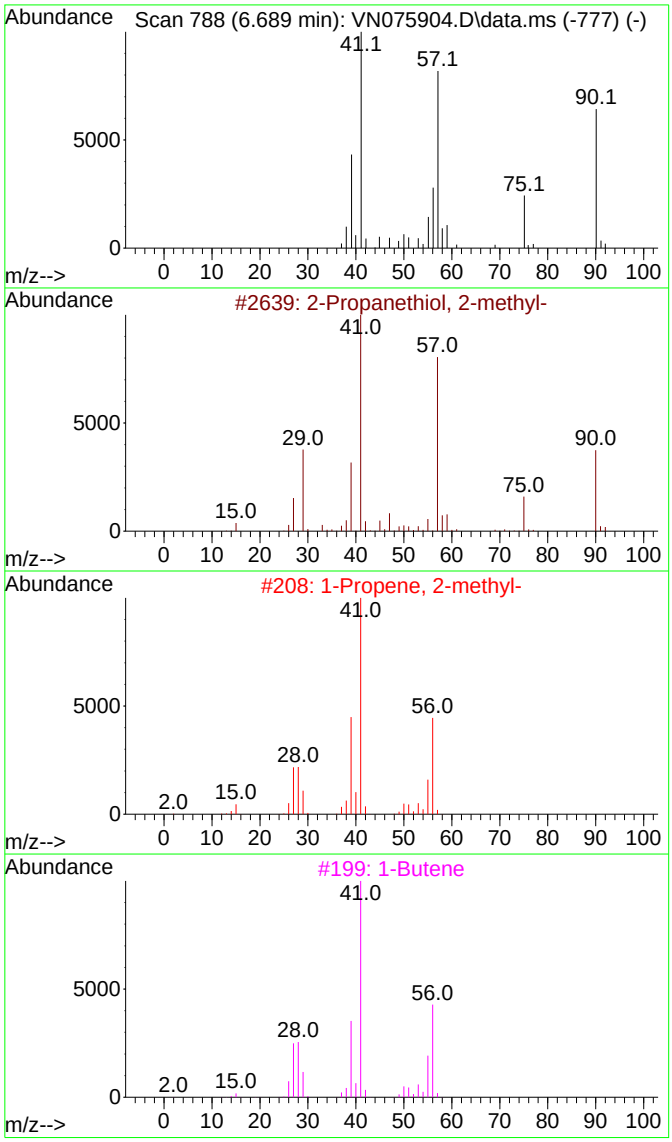
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

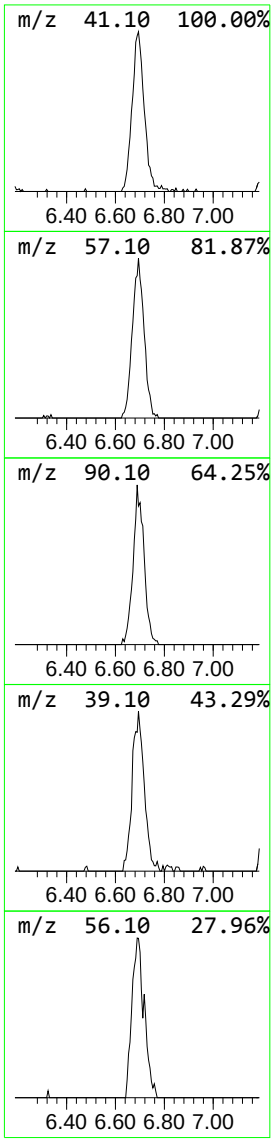
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Propanethiol, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.689	9.09 ug/l	199712	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	50
2	1-Propene, 2-methyl-	56	C4H8	000115-11-7	38
3	1-Butene	56	C4H8	000106-98-9	35
4	2-Butanethiol	90	C4H10S	000513-53-1	32
5	Nitroxide, bis(1,1-dimethylethyl)	144	C8H18NO	002406-25-9	28





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Instrument :
MSVOA_N
ClientSampleId :
CLI-0667

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

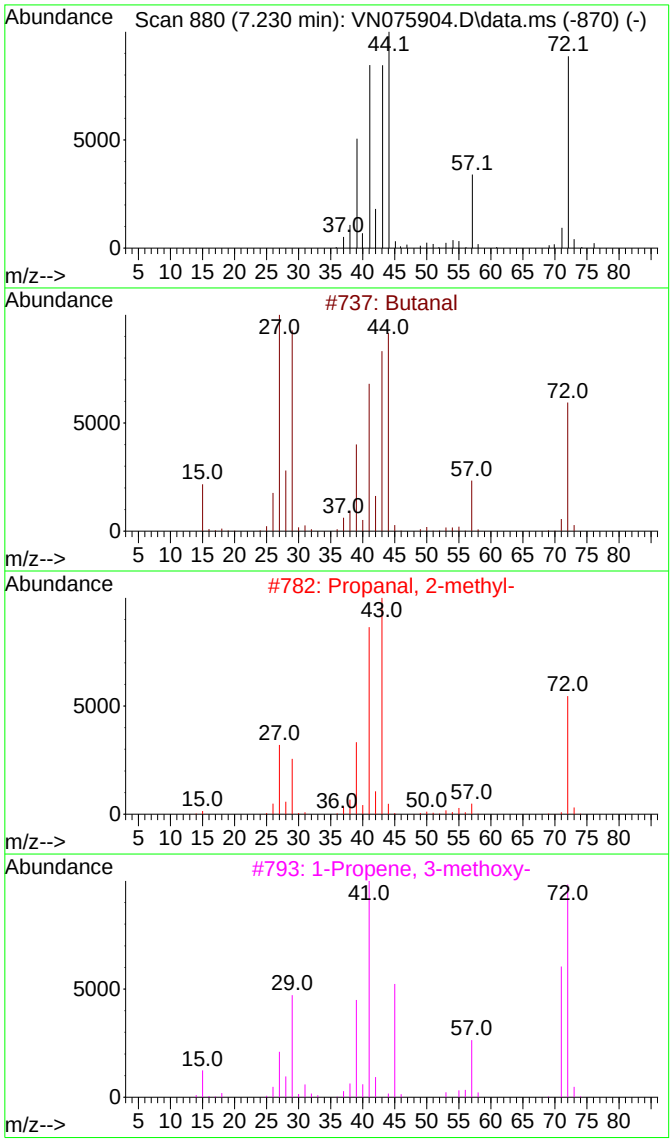
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

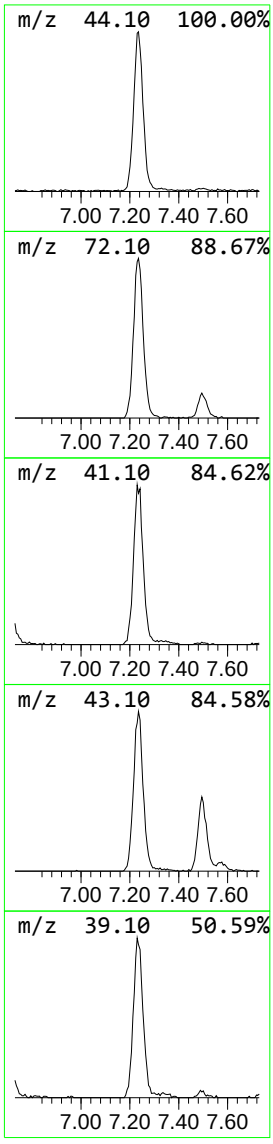
****

Peak Number 2 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.230	24.94 ug/l	547893	Pentafluorobenzene	8.230

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	43
3	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37
4	2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	28
5	Isobutylene epoxide	72	C4H8O	000558-30-5	27





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Data File : VN075904.D
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CLI-0667

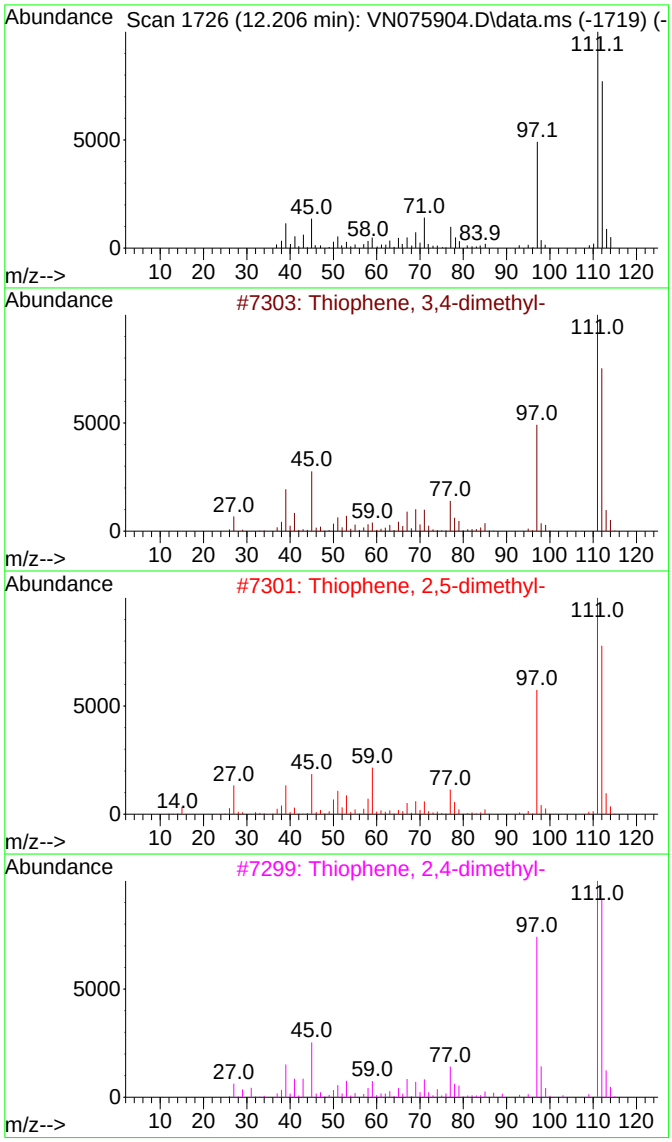
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

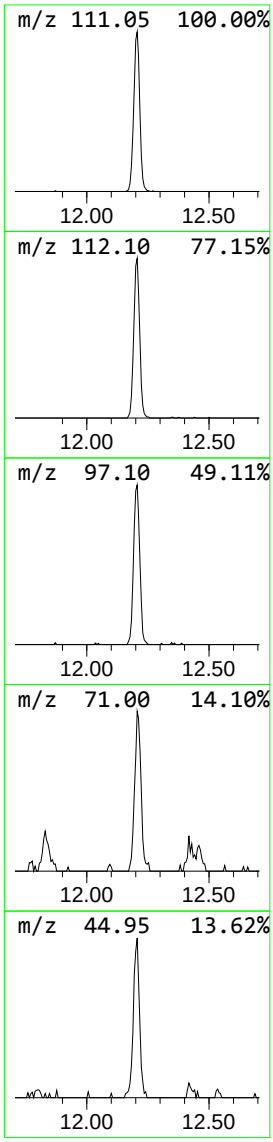
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Thiophene, 3,4-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.206	9.72 ug/l	294731	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, 3,4-dimethyl-	112	C6H8S	000632-15-5	91
2	Thiophene, 2,5-dimethyl-	112	C6H8S	000638-02-8	90
3	Thiophene, 2,4-dimethyl-	112	C6H8S	000638-00-6	90
4	2-Thiophenecarboxaldehyde	112	C5H4OS	000098-03-3	58
5	3-Thiophenecarboxaldehyde	112	C5H4OS	000498-62-4	53





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Sample : N6161-12
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CLI-0667

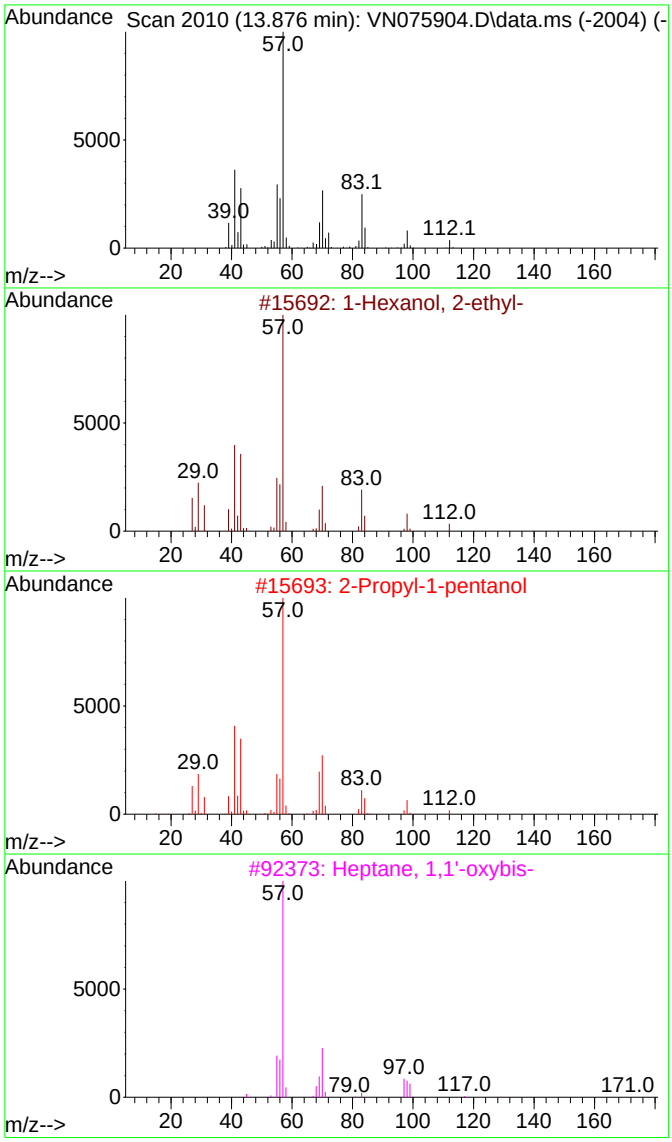
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

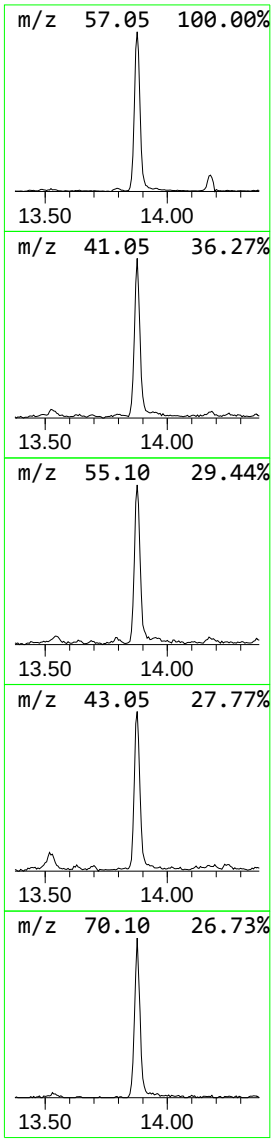
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	23.47 ug/l	651159	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-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
4	Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	45
5	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	42





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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
CLI-0667

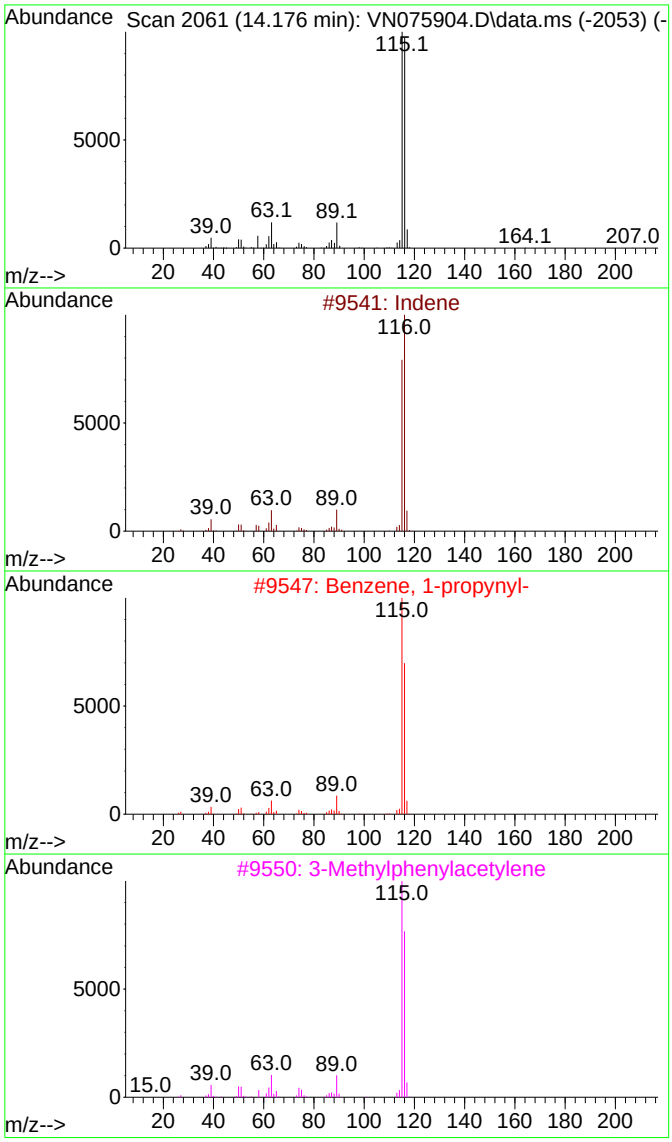
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121422W.M
Quant Title : SW846 8260

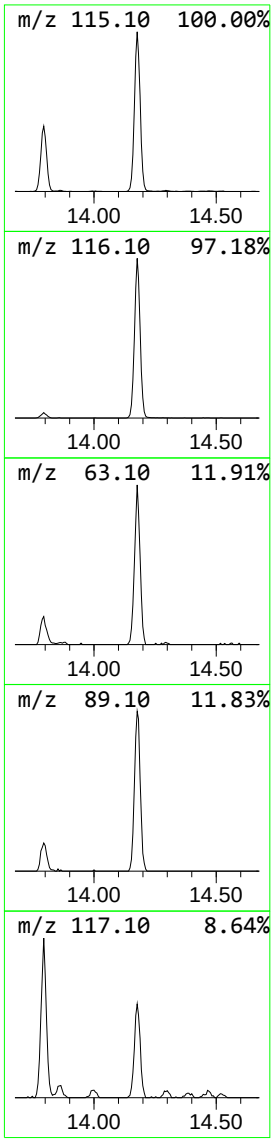
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Indene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.176	33.70 ug/l	934711	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	97
2	Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
3	3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4	2-Methylphenylacetylene	116	C9H8	000766-47-2	91
5	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	87





Tentatively Identified Compound (LSC) summary

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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
2-Propanethiol,...	6.689	9.1	ug/l	199712	1	8.230	1098630	50.0
Butanal	7.230	24.9	ug/l	547893	1	8.230	1098630	50.0
Thiophene, 3,4-...	12.206	9.7	ug/l	294731	3	11.871	1516110	50.0
1-Hexanol, 2-et...	13.876	23.5	ug/l	651159	4	13.794	1387000	50.0
Indene	14.176	33.7	ug/l	934711	4	13.794	1387000	50.0