LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN031221\
Data File : VN066193.D
Acq On : 12 Mar 2021 19:43
Operator : JC/MD
Sample : M1647-21
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP5-30811:15

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\82N031221W.M
Title : SW846 8260

Signal : TIC: VN066193.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.263	199	214	298	rBV	15099913	33325442	100.00%	44.641%
2	6.450	1755	1775	1800	rBV5	110682	336841	1.01%	0.451%
3	7.512	2151	2171	2184	rBV2	293778	730045	2.19%	0.978%
4	7.587	2184	2199	2225	rVB	569758	1340500	4.02%	1.796%
5	7.963	2312	2339	2367	rBV3	1628155	4069910	12.21%	5.452%
6	8.515	2526	2545	2572	rBV	872832	1804093	5.41%	2.417%
7	10.028	3091	3109	3121	rBV	1341162	2437411	7.31%	3.265%
8	10.092	3121	3133	3163	rVB	2167004	3922070	11.77%	5.254%
9	11.350	3582	3602	3629	rBV2	1346038	2501114	7.51%	3.350%
10	11.455	3629	3641	3647	rBV	262629	427239	1.28%	0.572%
11	11.559	3665	3680	3704	rVB	1485371	2711177	8.14%	3.632%
12	11.892	3790	3804	3819	rBV3	1608167	2905081	8.72%	3.891%
13	12.345	3957	3973	3990	rBV	863419	1485156	4.46%	1.989%
14	12.860	4148	4165	4187	rVB4	223588	520899	1.56%	0.698%
15	12.983	4198	4211	4222	rBV	640781	1009734	3.03%	1.353%
16	13.048	4223	4235	4261	rVB3	245659	564802	1.69%	0.757%
17	13.286	4311	4324	4347	rBV2	958007	2075976	6.23%	2.781%
18	13.396	4354	4365	4387	rBV2	787461	1341720	4.03%	1.797%
19	13.665	4452	4465	4485	rBV	837317	1399379	4.20%	1.875%
20	15.067	4969	4988	5001	rBV	4381538	7920640	23.77%	10.610%
21	16.078	5352	5365	5390	rVB	532561	1075000	3.23%	1.440%
22	16.266	5422	5435	5459	rVB	353783	747809	2.24%	1.002%

Sum of corrected areas: 74652038

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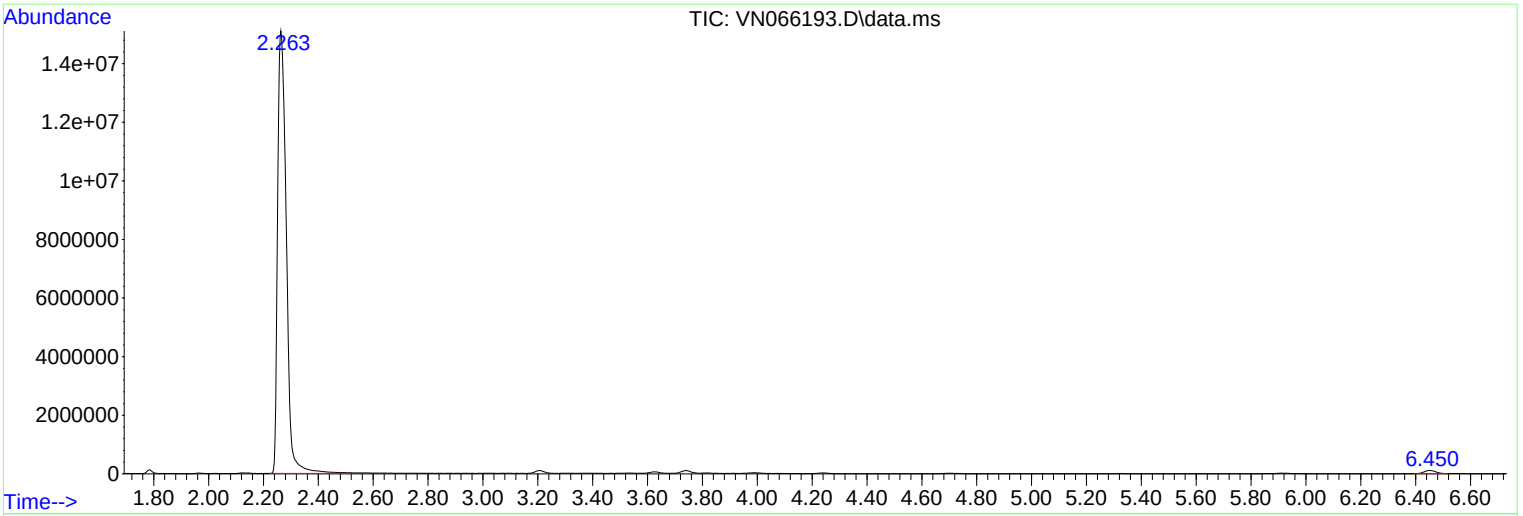
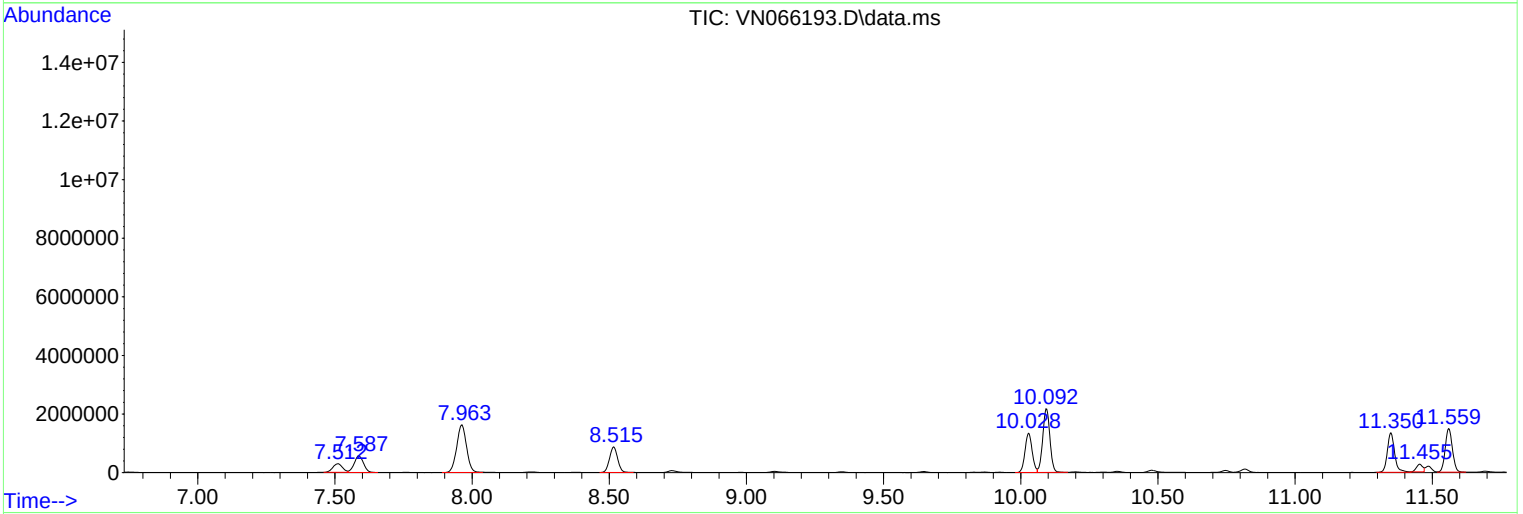
ALS Vial : 20 Sample Multiplier: 1

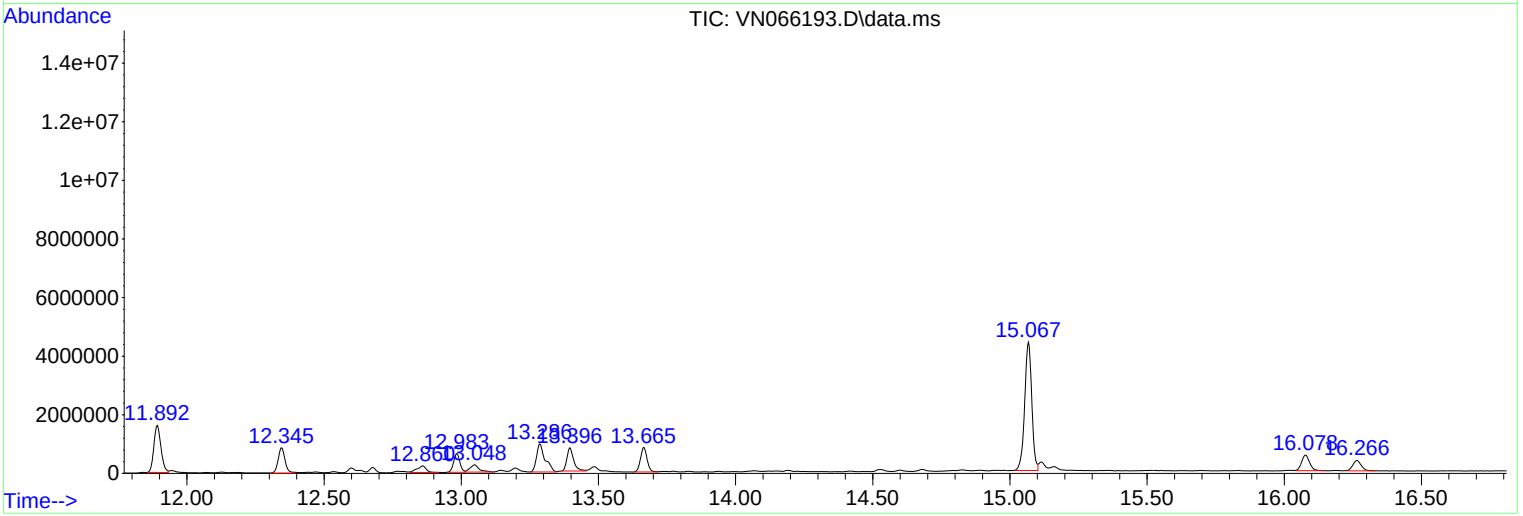
Instrument :
MSVOA_N
ClientSampleId :
COMP5-30811:15

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031221W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







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Data File : VN066193.D
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Operator : JC/MD
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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP5-30811:15

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031221W.M
Quant Title : SW846 8260

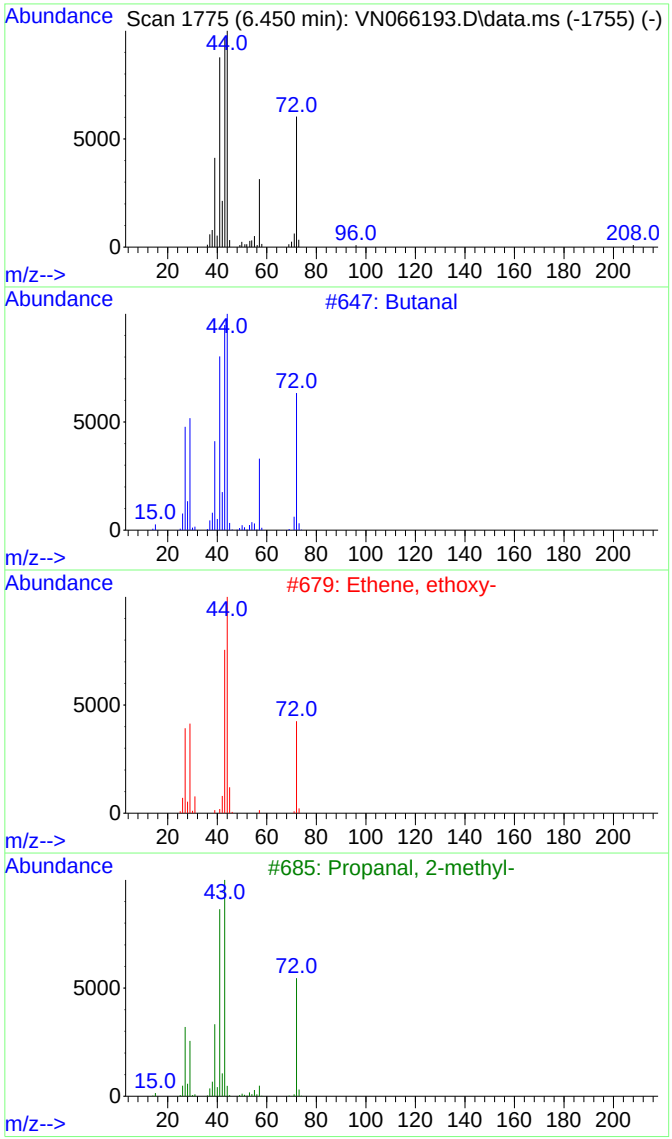
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

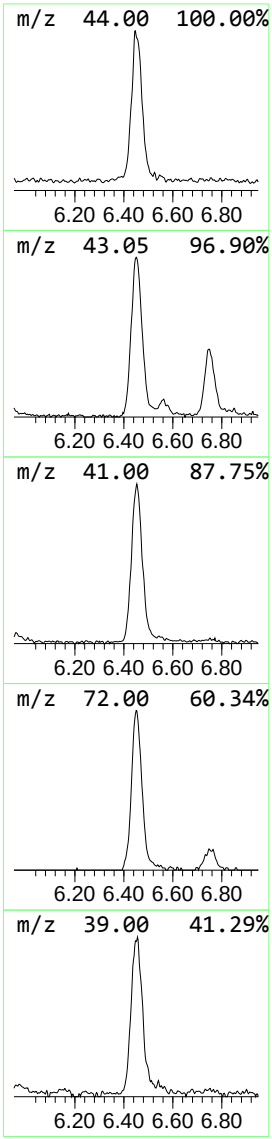
****

Peak Number 2 Butanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.450	12.56 ug/l	336841	Pentafluorobenzene	7.587

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	50
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	49
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	35
5	1,3-Butanediol, (S)-	90	C4H10O2	024621-61-2	32





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Data File : VN066193.D
Acq On : 12 Mar 2021 19:43
Operator : JC/MD
Sample : M1647-21
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP5-30811:15

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031221W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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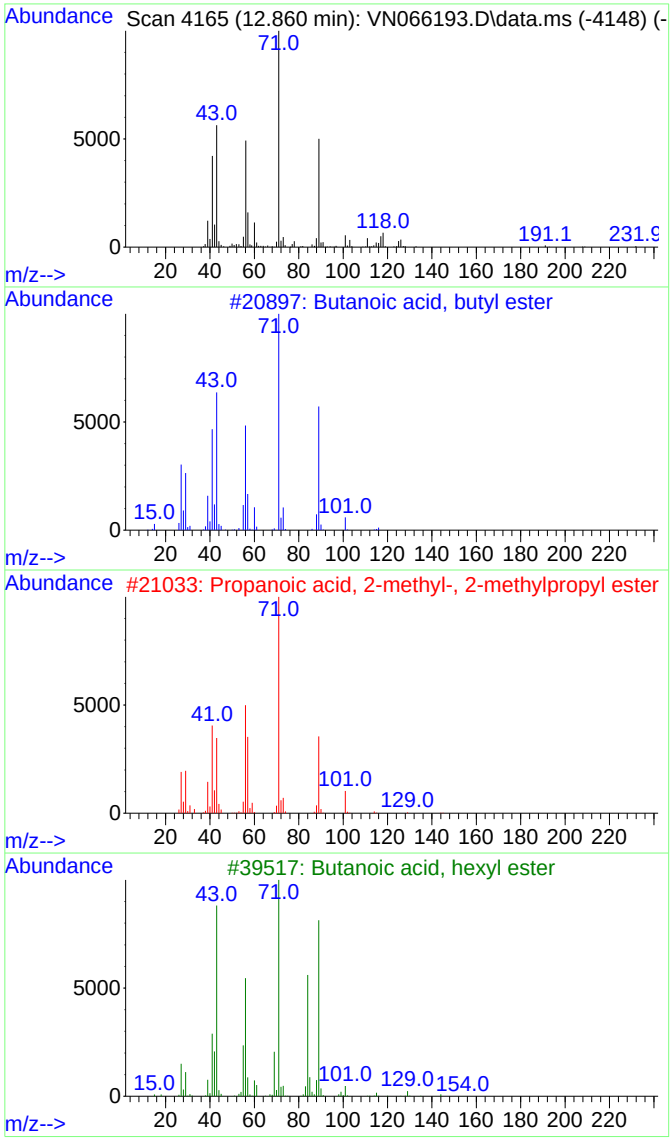
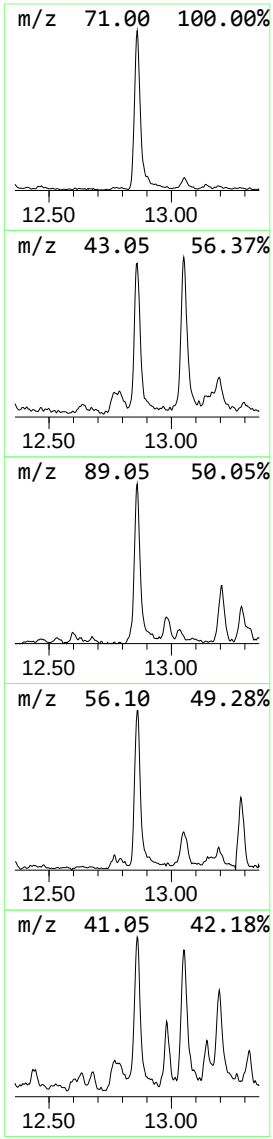
Peak Number 3 Butanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.860	12.55 ug/l	520899	1,4-Dichlorobenzene-d4	13.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	72
2	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	64
3	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	59
4	Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	56
5	Malic Acid	134	C4H6O5	006915-15-7	50





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Operator : JC/MD
Sample : M1647-21
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP5-30811:15

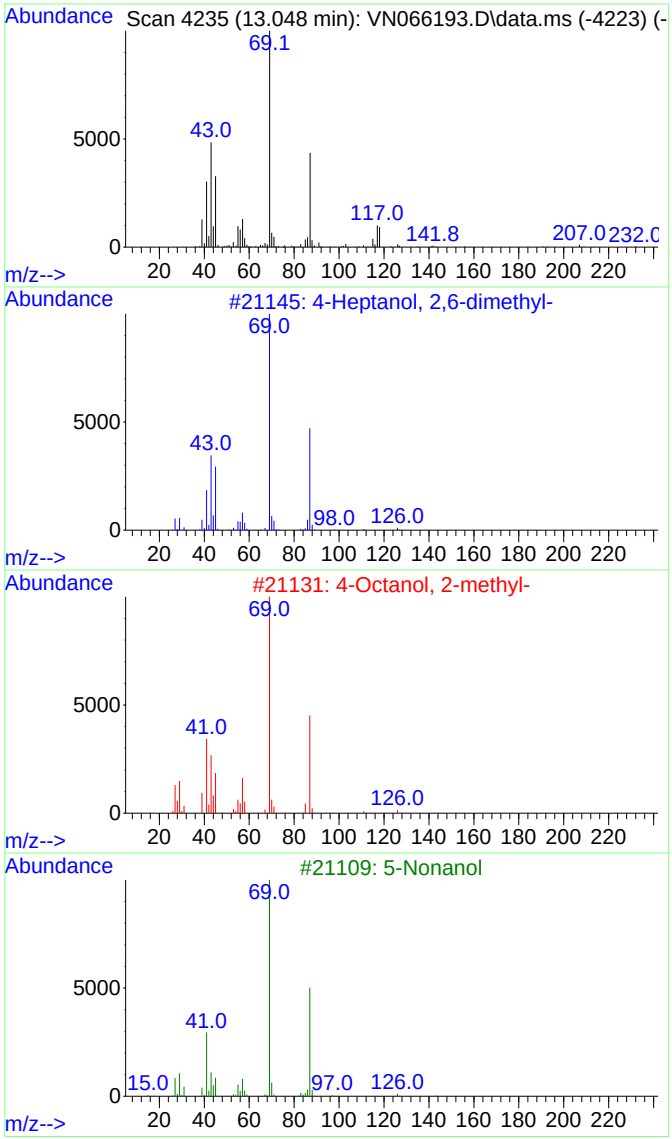
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031221W.M
Quant Title : SW846 8260

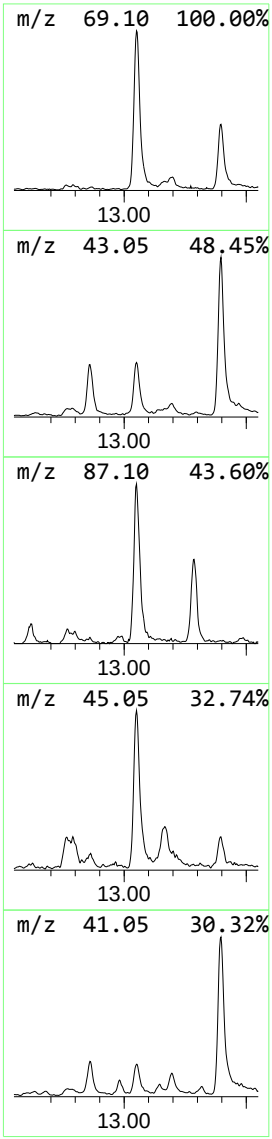
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 4-Heptanol, 2,6-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.048	13.60 ug/l	564802	1,4-Dichlorobenzene-d4	13.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	72
2	4-Octanol, 2-methyl-	144	C9H20O	040575-41-5	64
3	5-Nonanol	144	C9H20O	000623-93-8	64
4	1-Octyn-4-ol	126	C8H14O	052517-92-7	59
5	1,3-Dioxan-4-one, 2-(1,1-dimethy...	172	C9H16O3	113505-75-2	53





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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP5-30811:15

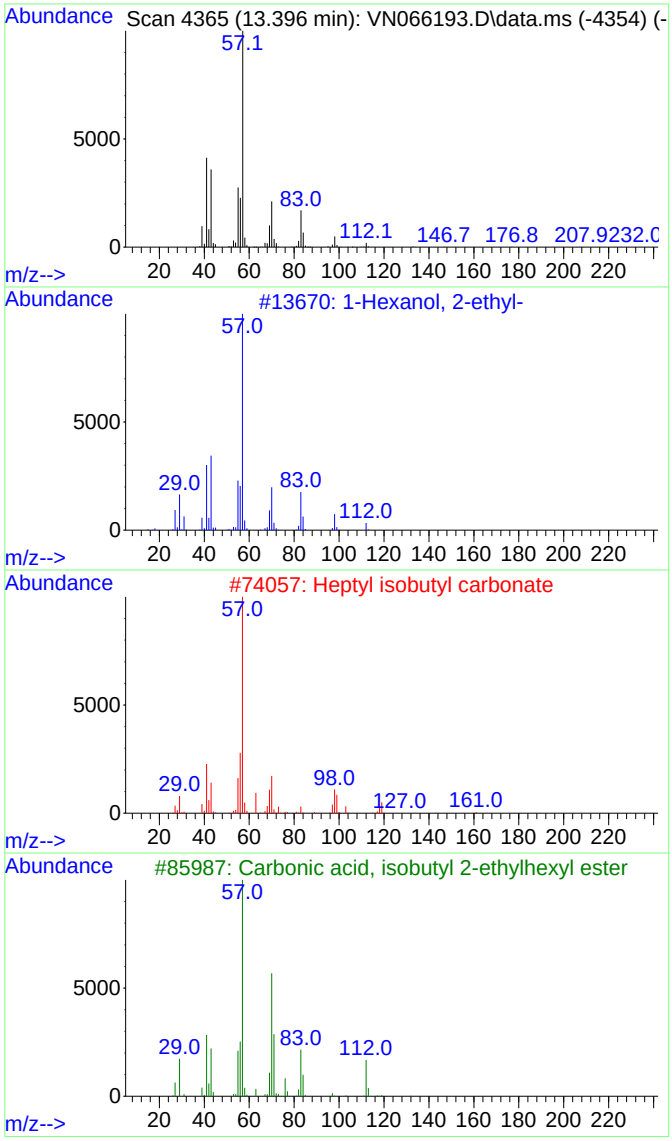
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031221W.M
Quant Title : SW846 8260

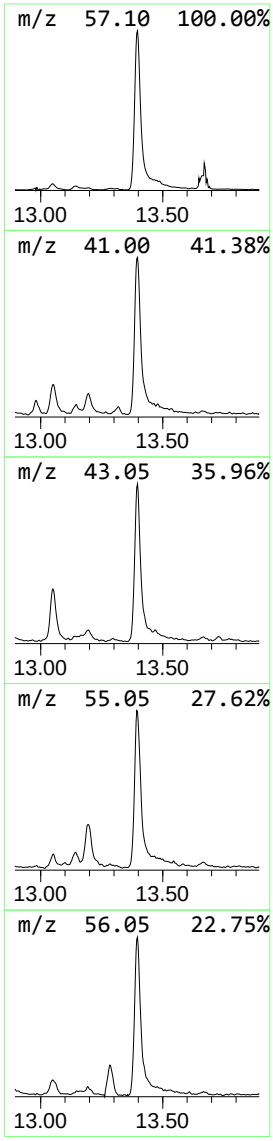
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.396	32.32 ug/l	1341720	1,4-Dichlorobenzene-d4	13.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2	Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	64
3	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	53
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50





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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP5-30811:15

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031221W.M
Quant Title : SW846 8260

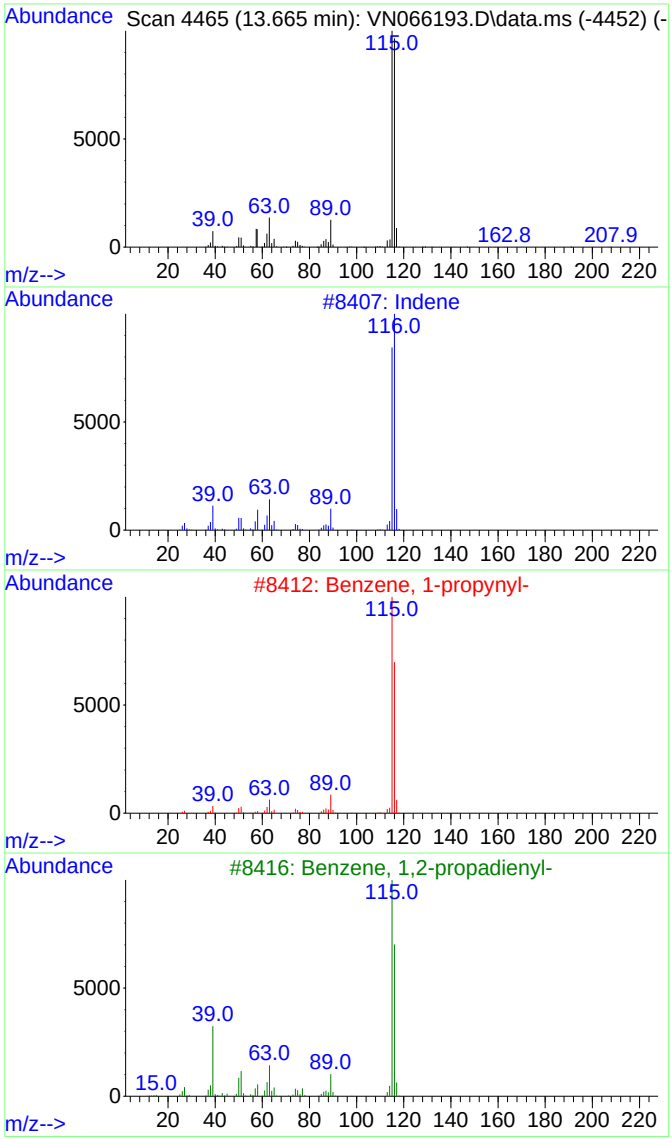
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

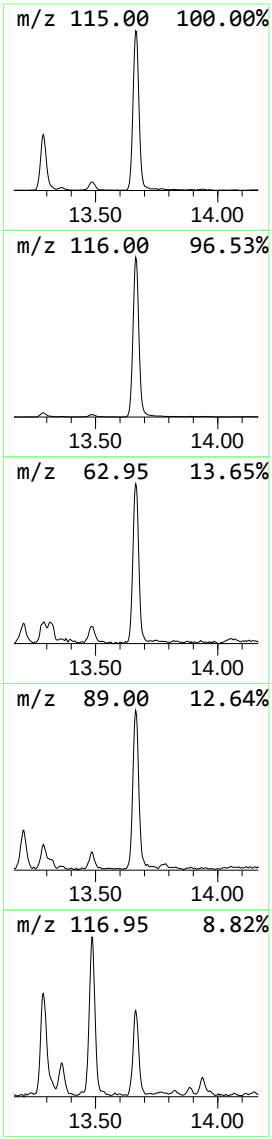
****

Peak Number 6 Indene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.665	33.70 ug/l	1399380	1,4-Dichlorobenzene-d4	13.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	96
2	Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
3	Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91
4	3-Methylphenylacetylene	116	C9H8	000766-82-5	91
5	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	90





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ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP5-30811:15

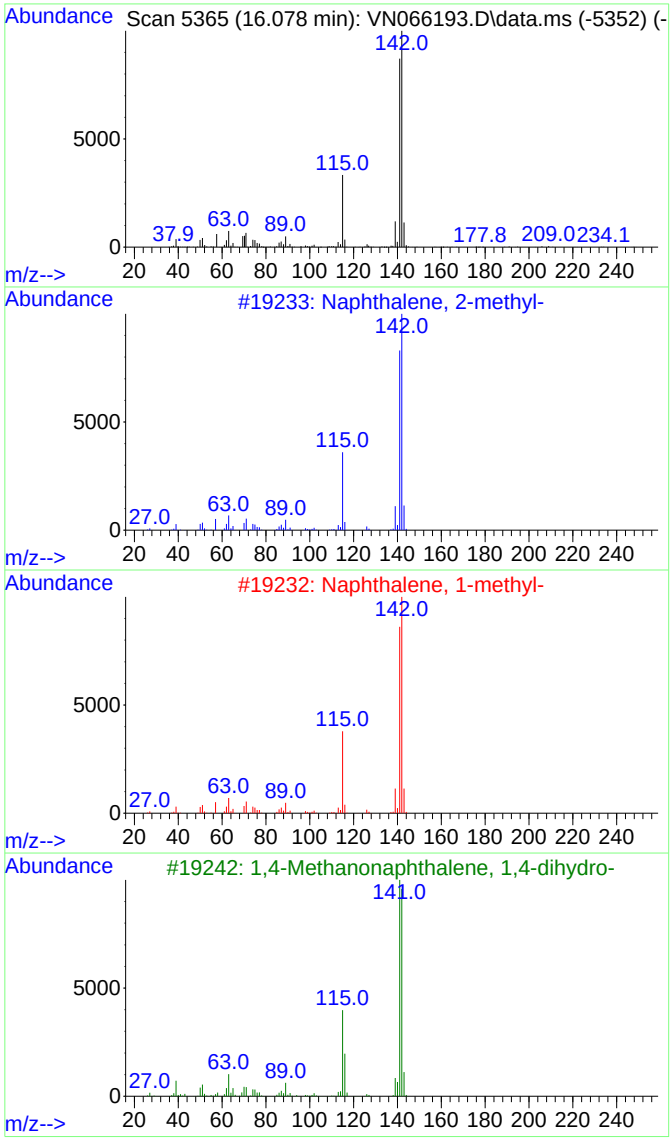
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N031221W.M
Quant Title : SW846 8260

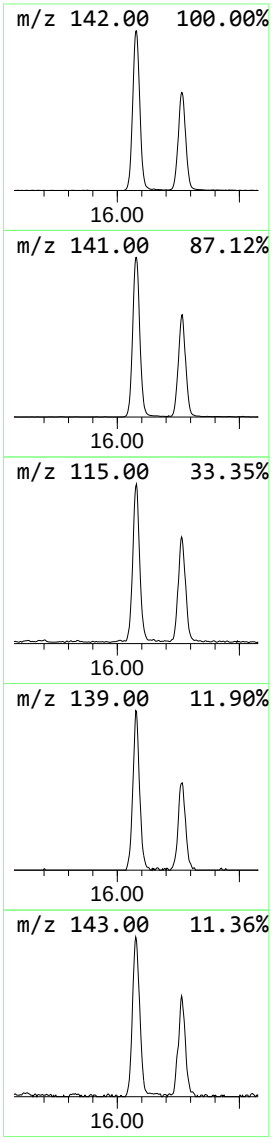
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Naphthalene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.078	25.89 ug/l	1075000	1,4-Dichlorobenzene-d4	13.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91





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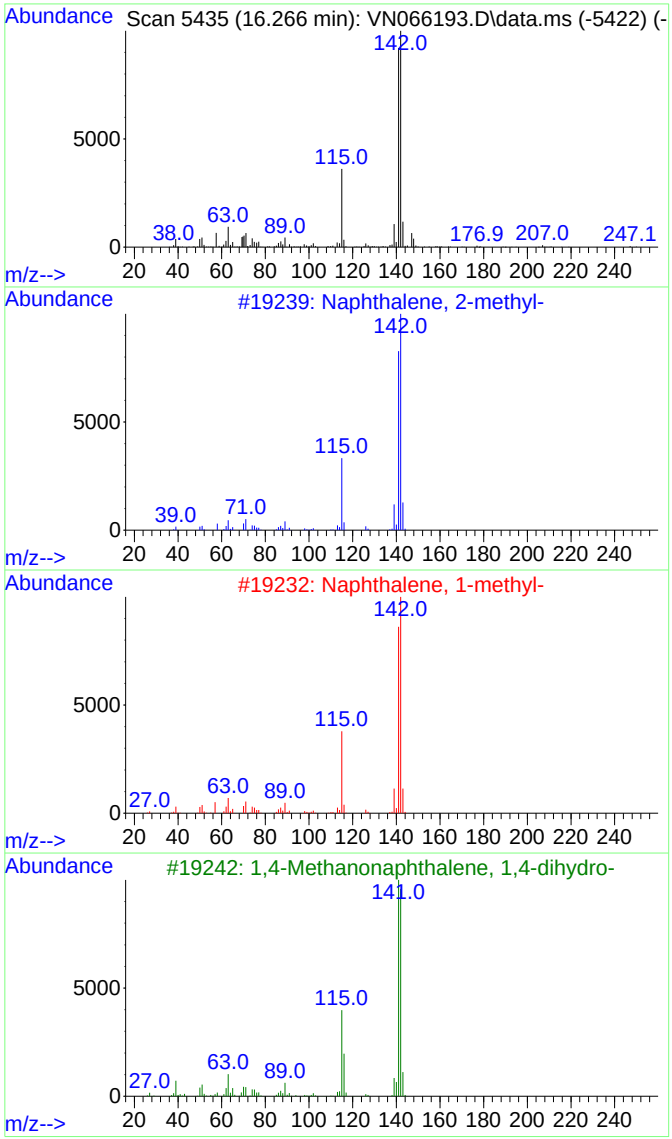
Quant Title : SW846 8260

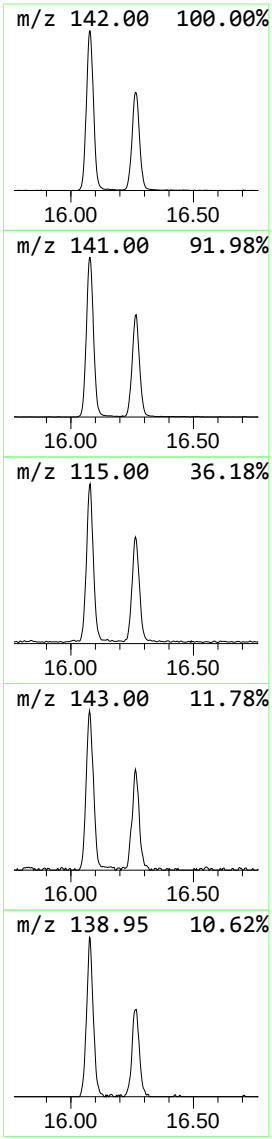
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1,4-Methanonaphthalene, 1,4... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.266	18.01 ug/l	747809	1,4-Dichlorobenzene-d4	13.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	80





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butanal	6.450	12.6	ug/l	336841	1	7.587	1340500	50.0
Butanoic acid, ...	12.860	12.6	ug/l	520899	4	13.286	2075980	50.0
4-Heptanol, 2,6...	13.048	13.6	ug/l	564802	4	13.286	2075980	50.0
1-Hexanol, 2-et...	13.396	32.3	ug/l	1341720	4	13.286	2075980	50.0
Indene	13.665	33.7	ug/l	1399380	4	13.286	2075980	50.0
Naphthalene, 1-...	16.078	25.9	ug/l	1075000	4	13.286	2075980	50.0
1,4-Methanonaph...	16.266	18.0	ug/l	747809	4	13.286	2075980	50.0