LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121120\
Data File : VN065085.D
Acq On : 11 Dec 2020 21:37
Operator : JC/MD
Sample : L4991-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP-2

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\82N121120W.M
Title : SW846 8260

Signal : TIC: VN065085.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.277	155	167	210	rBV	13153447	29673862	100.00%	58.526%
2	3.235	448	465	495	rBV	718733	1721462	5.80%	3.395%
3	3.659	581	597	616	rBV	174069	442152	1.49%	0.872%
4	3.772	616	632	652	rBV	333748	842497	2.84%	1.662%
5	6.492	1452	1478	1506	rBV	620494	1895592	6.39%	3.739%
6	6.785	1552	1569	1591	rBV2	100990	298844	1.01%	0.589%
7	7.550	1788	1807	1818	rBV2	201915	505599	1.70%	0.997%
8	7.627	1818	1831	1857	rVB	323272	783676	2.64%	1.546%
9	7.994	1921	1945	1964	rBV4	323293	884774	2.98%	1.745%
10	8.550	2102	2118	2136	rBV	535188	1102731	3.72%	2.175%
11	9.952	2538	2554	2573	rBV	1467609	2642734	8.91%	5.212%
12	10.058	2574	2587	2598	rVV	874563	1623602	5.47%	3.202%
13	10.122	2598	2607	2630	rVB	329280	604323	2.04%	1.192%
14	11.379	2984	2998	3020	rBV	852033	1520196	5.12%	2.998%
15	11.514	3020	3040	3053	rVV2	482597	873083	2.94%	1.722%
16	12.000	3180	3191	3211	rVB	722621	1186757	4.00%	2.341%
17	12.376	3295	3308	3319	rBV	728830	1215651	4.10%	2.398%
18	13.029	3490	3511	3521	rBV5	122643	348175	1.17%	0.687%
19	13.315	3588	3600	3618	rBV	866812	1531552	5.16%	3.021%
20	13.421	3619	3633	3647	rVV3	180817	332420	1.12%	0.656%
21	15.103	4137	4156	4178	rBV	376206	672051	2.26%	1.325%

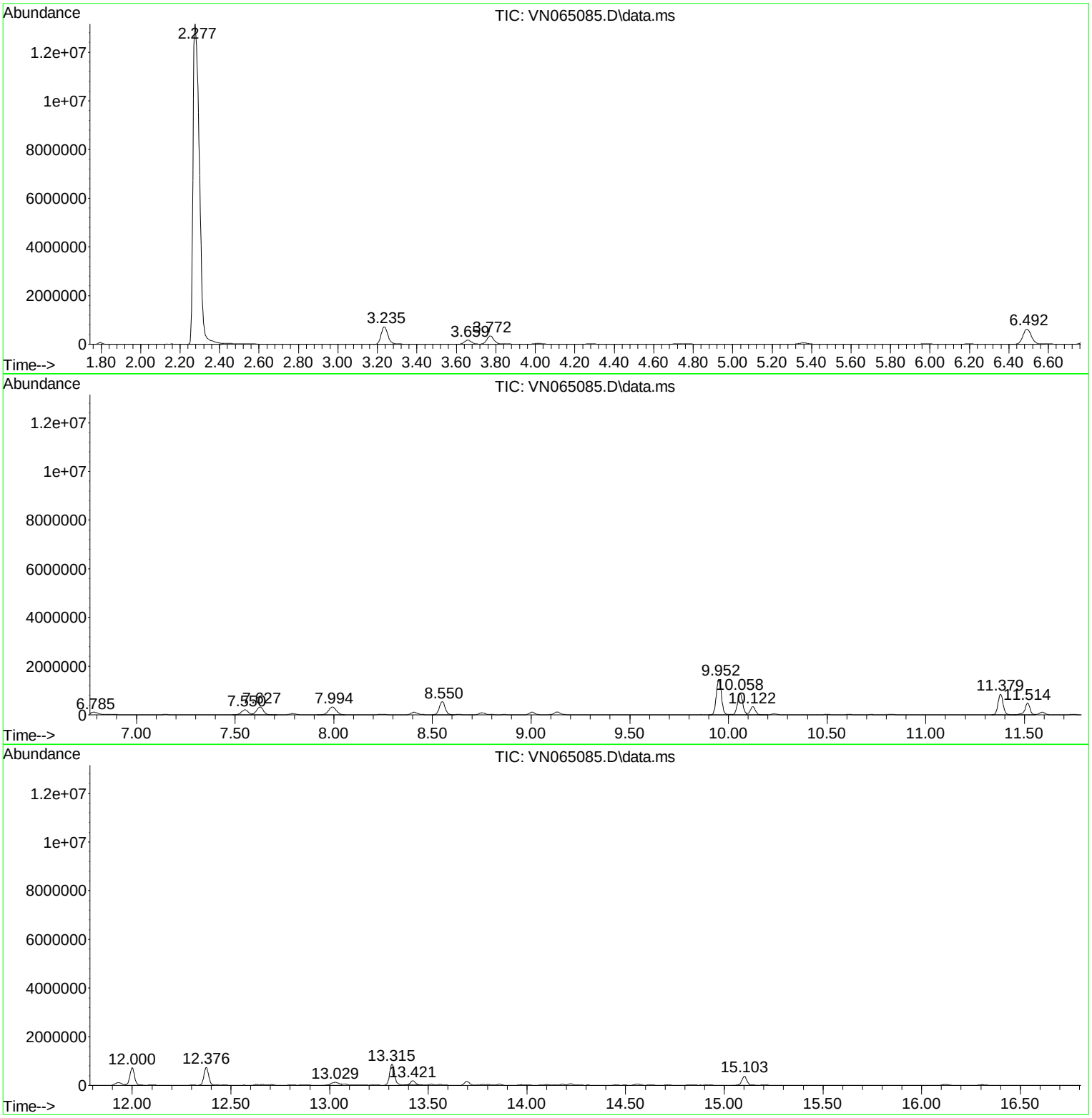
Sum of corrected areas: 50701733

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121120\
Data File : VN065085.D
Acq On : 11 Dec 2020 21:37
Operator : JC/MD
Sample : L4991-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121120W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121120\
Data File : VN065085.D
Acq On : 11 Dec 2020 21:37
Operator : JC/MD
Sample : L4991-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121120W.M
Quant Title : SW846 8260

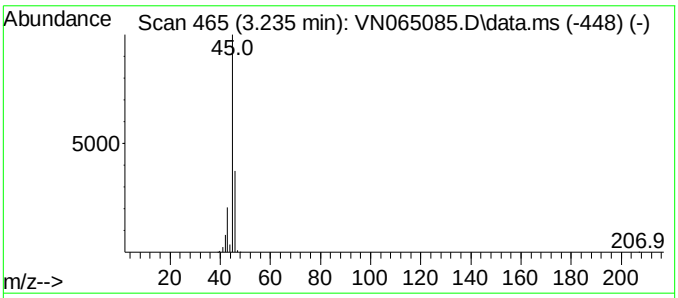
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

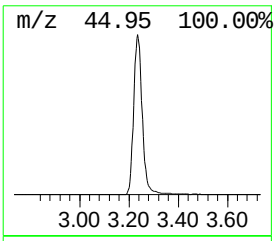
****

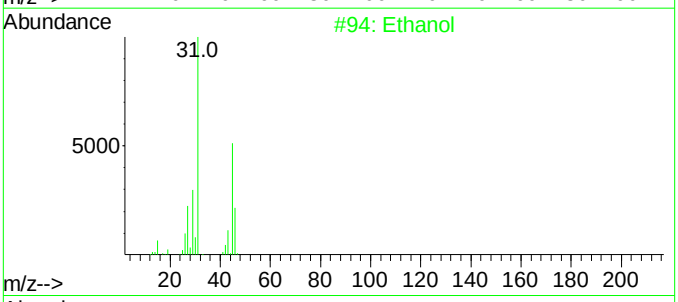
Peak Number 2 Ethanol Concentration Rank 3

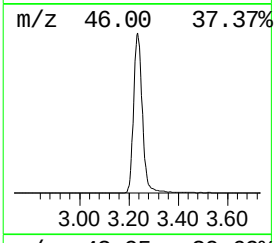
R.T.	EstConc	Area	Relative to ISTD	R.T.
3.235	109.83 ug/l	1721460	Pentafluorobenzene	7.627

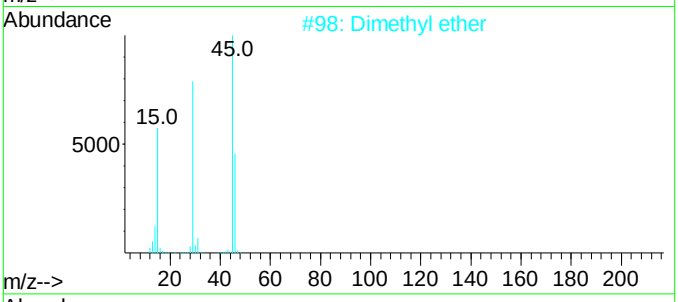
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	64
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Formic acid	46	CH2O2	000064-18-6	4
5	Methyltartronic acid	134	C4H6O5	000595-98-2	2

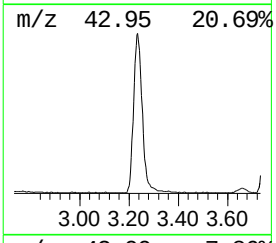


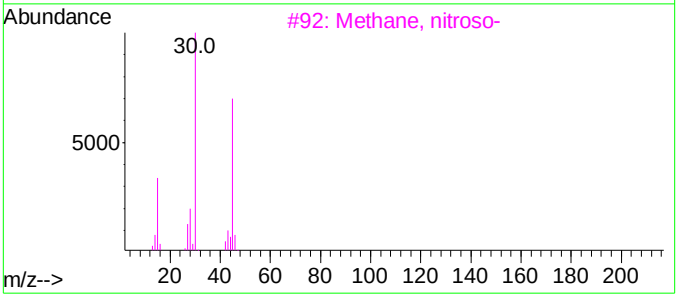


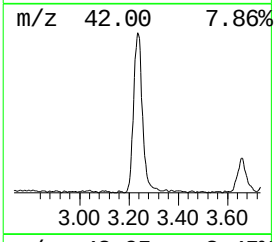


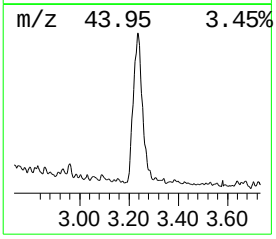












Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121120\
Data File : VN065085.D
Acq On : 11 Dec 2020 21:37
Operator : JC/MD
Sample : L4991-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121120W.M
Quant Title : SW846 8260

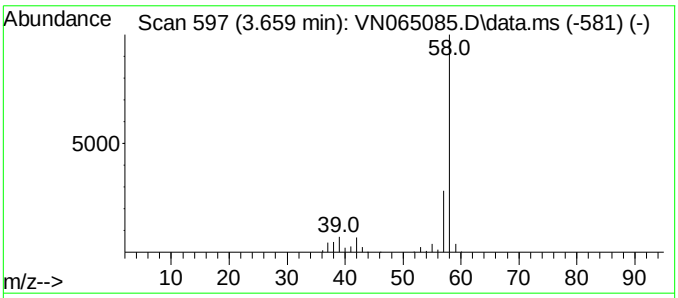
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

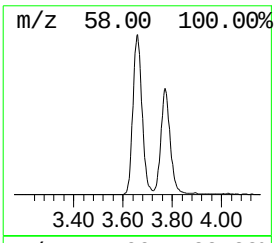
****

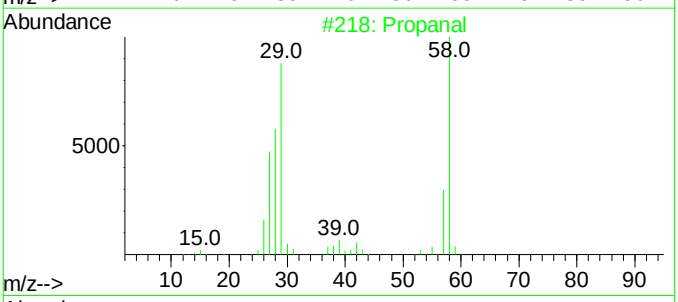
Peak Number 3 Propanal Concentration Rank 5

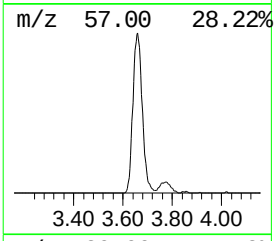
R.T.	EstConc	Area	Relative to ISTD	R.T.
3.659	28.21 ug/l	442152	Pentafluorobenzene	7.627

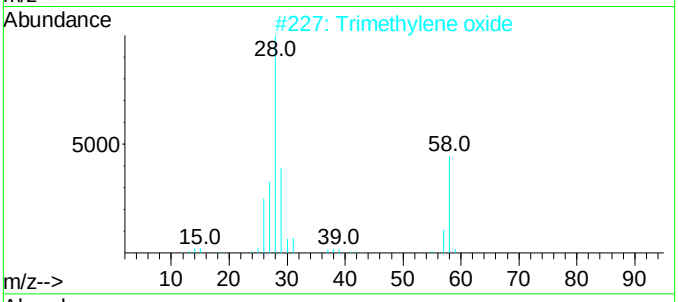
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal	58	C3H6O	000123-38-6	72
2	Trimethylene oxide	58	C3H6O	000503-30-0	56
3	Succindialdehyde	86	C4H6O2	000638-37-9	9
4	.alpha.-Pinene, 10-(dimethylamin...	193	C13H23N	015063-97-5	9
5	Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7

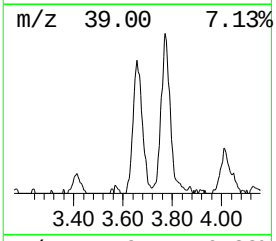


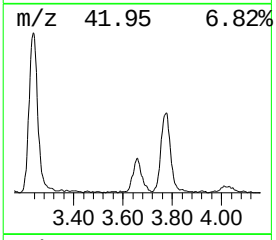


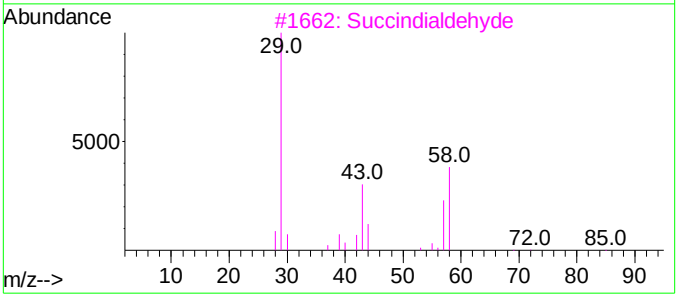


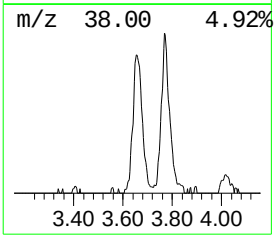












Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121120\
Data File : VN065085.D
Acq On : 11 Dec 2020 21:37
Operator : JC/MD
Sample : L4991-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121120W.M
Quant Title : SW846 8260

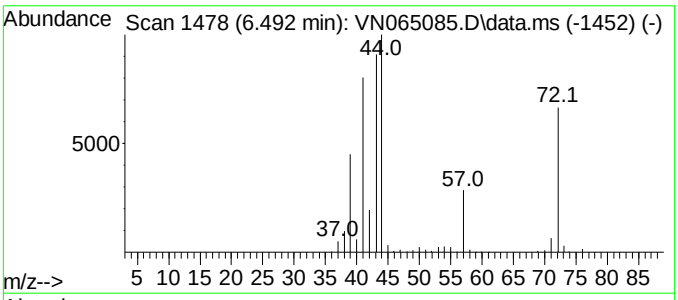
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

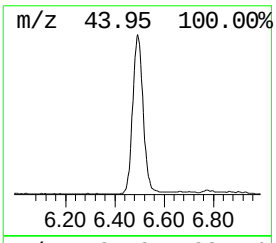
****

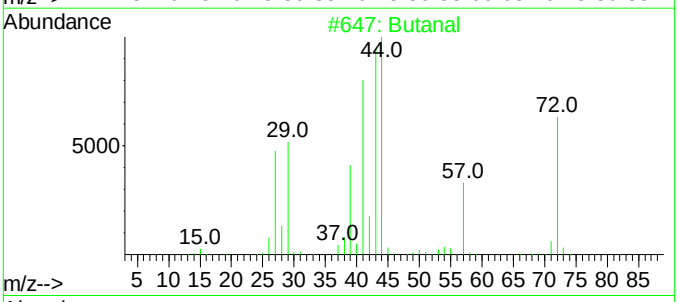
Peak Number 4 Butanal Concentration Rank 2

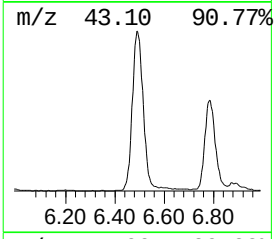
R.T.	EstConc	Area	Relative to ISTD	R.T.
6.492	120.94 ug/l	1895590	Pentafluorobenzene	7.627

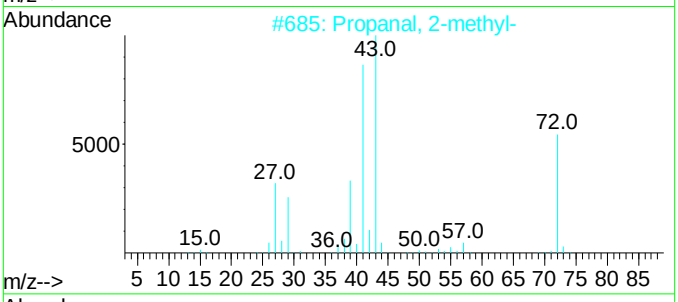
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
3	Ethene, ethoxy-	72	C4H8O	000109-92-2	38
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	25
5	Methacrolein	70	C4H6O	000078-85-3	22

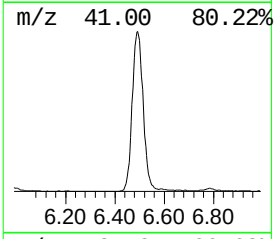


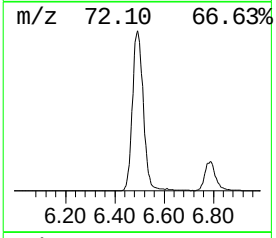


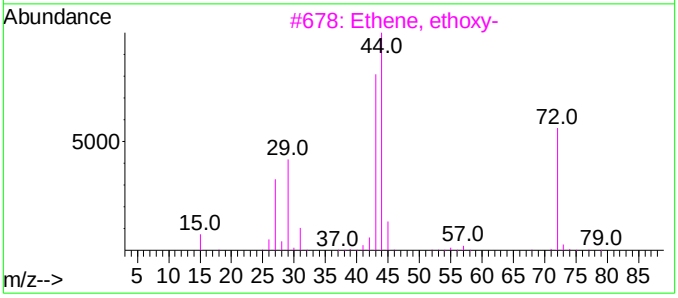


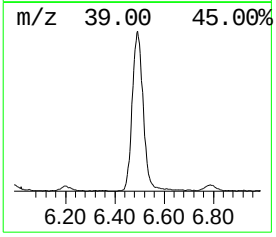












Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121120\
Data File : VN065085.D
Acq On : 11 Dec 2020 21:37
Operator : JC/MD
Sample : L4991-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121120W.M
Quant Title : SW846 8260

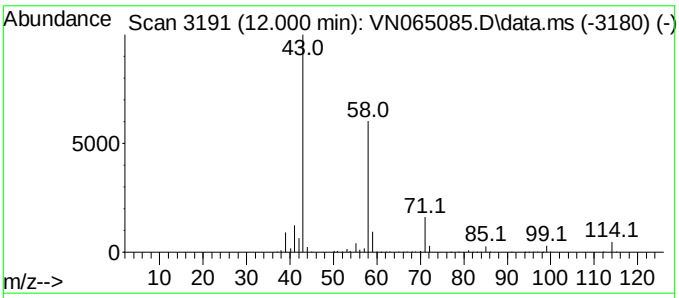
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

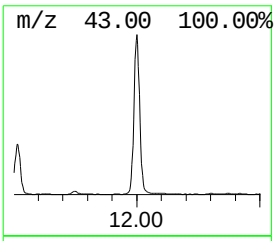
****

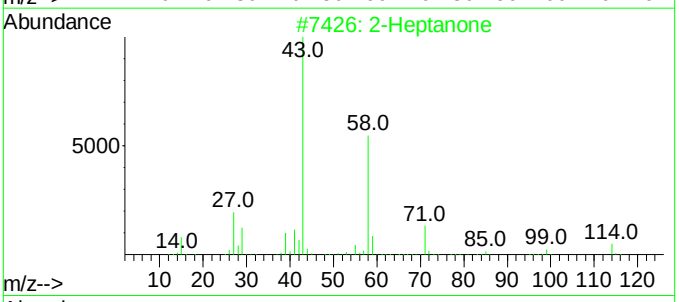
Peak Number 5 2-Heptanone Concentration Rank 4

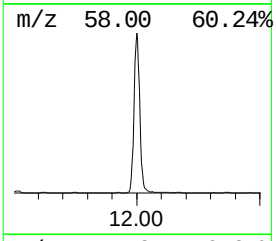
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.000	39.03 ug/l	1186760	Chlorobenzene-d5	11.379

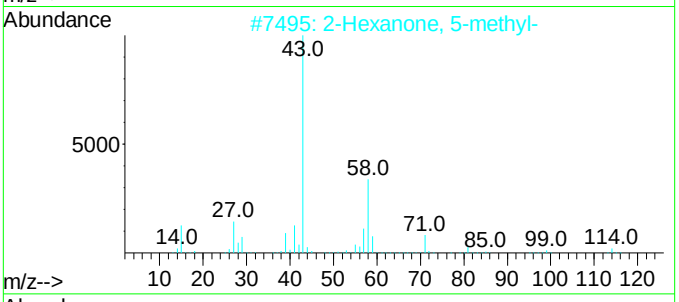
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone	114	C7H14O	000110-43-0	91
2	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	83
3	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	64
4	2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	52
5	2-Hexanone	100	C6H12O	000591-78-6	40

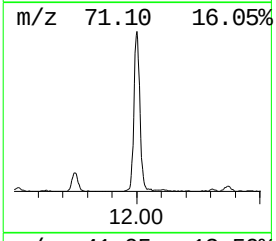


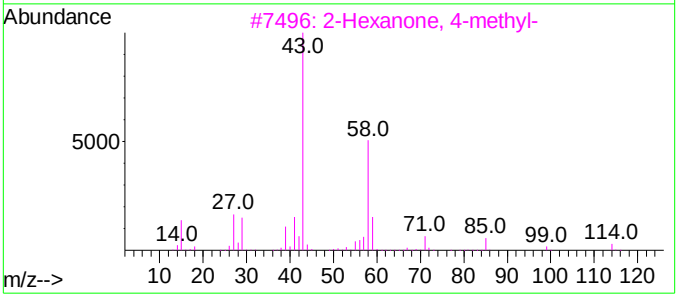


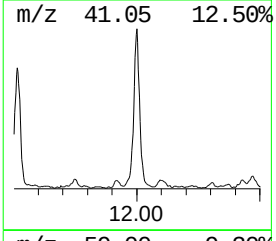


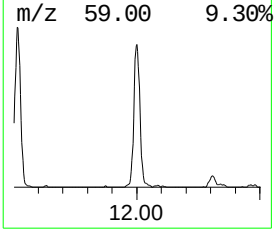












Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121120\
Data File : VN065085.D
Acq On : 11 Dec 2020 21:37
Operator : JC/MD
Sample : L4991-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
COMP-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121120W.M
Quant Title : SW846 8260

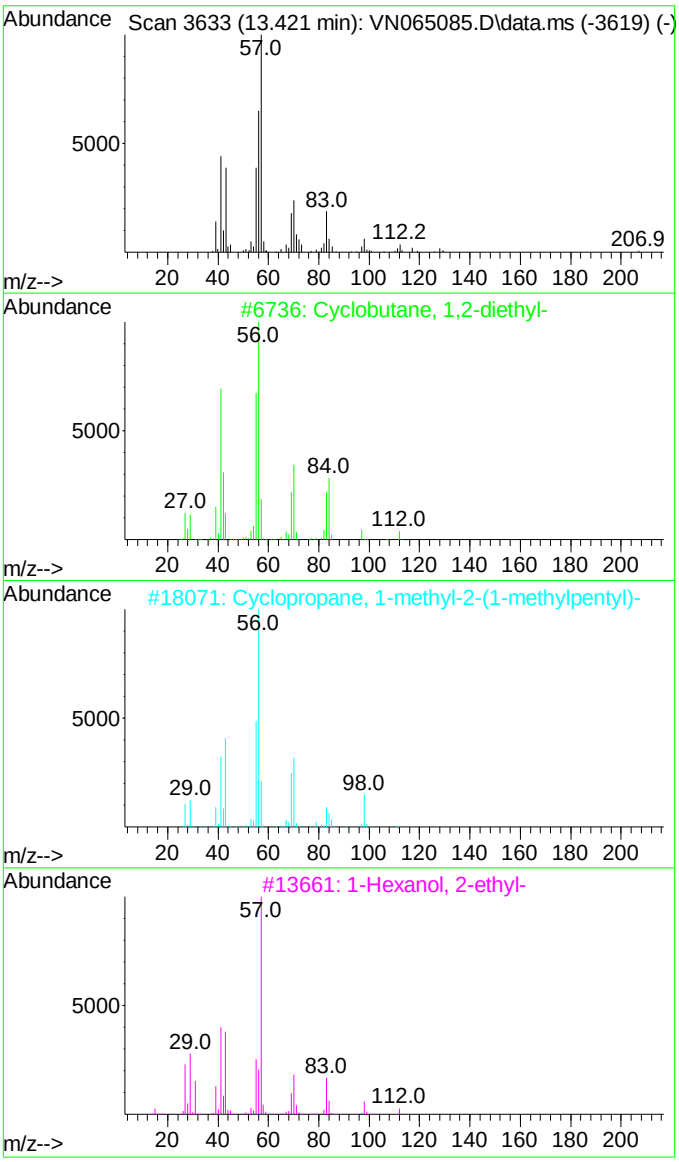
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

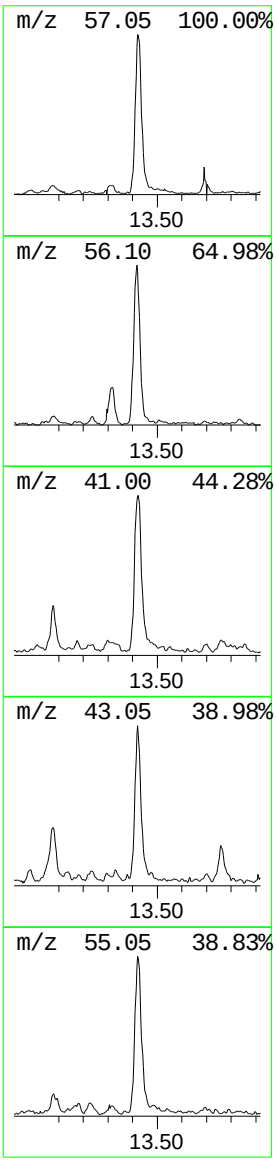
****

Peak Number 6 Cyclobutane, 1,2-diethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.421	10.85 ug/l	332420	1,4-Dichlorobenzene-d4	13.318

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, 1,2-diethyl-	112	C8H16	061141-83-1	64
2	Cyclopropane, 1-methyl-2-(1-meth...	140	C10H20	062238-06-6	59
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5	1-Heptene, 2-methyl-	112	C8H16	015870-10-7	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN121120\
Data File : VN065085.D
Acq On : 11 Dec 2020 21:37
Operator : JC/MD
Sample : L4991-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121120W.M
Quant Title : SW846 8260

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethanol	3.235	109.8	ug/l	1721460	1	7.627	783676	50.0
Propanal	3.659	28.2	ug/l	442152	1	7.627	783676	50.0
Butanal	6.492	120.9	ug/l	1895590	1	7.627	783676	50.0
2-Heptanone	12.000	39.0	ug/l	1186760	3	11.379	1520200	50.0
Cyclobutane, 1,...	13.421	10.9	ug/l	332420	4	13.318	1531550	50.0