LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
Data File : VX025455.D
Acq On : 03 Dec 2021 02:30
Operator : JC/MD
Sample : M4917-19
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-35

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_X\Method\82X111721W.M
Title : SW846 8260

Signal : TIC: VX025455.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	21	26	29	rBV	52975	72966	3.90%	1.179%
2	1.368	41	46	52	rVB	25033	27560	1.47%	0.445%
3	1.752	103	109	117	rVB	44302	63009	3.37%	1.018%
4	2.215	180	185	197	rVB	28475	45766	2.44%	0.740%
5	2.751	266	273	283	rBV2	13180	35186	1.88%	0.569%
6	2.867	283	292	300	rVV	30089	66105	3.53%	1.068%
7	2.959	300	307	321	rVV	61917	130828	6.99%	2.114%
8	3.117	323	333	347	rVB	60327	141173	7.54%	2.281%
9	3.763	427	439	447	rBV3	11636	40085	2.14%	0.648%
10	4.312	519	529	540	rBV4	25156	76218	4.07%	1.232%
11	5.391	694	706	714	rBV	64724	189219	10.11%	3.058%
12	5.477	714	720	725	rVV2	13288	39731	2.12%	0.642%
13	5.556	725	733	758	rVB	106620	307322	16.41%	4.966%
14	5.958	788	799	804	rBV	67037	172149	9.19%	2.782%
15	6.043	804	813	830	rVB	719224	1872292	100.00%	30.255%
16	6.214	831	841	842	rBV4	10217	22958	1.23%	0.371%
17	6.763	921	931	943	rBV	172173	408490	21.82%	6.601%
18	8.427	1198	1204	1211	rBV	13142	21911	1.17%	0.354%
19	8.653	1233	1241	1247	rBV	352869	550971	29.43%	8.903%
20	8.720	1247	1252	1259	rVB2	18559	30281	1.62%	0.489%
21	8.958	1280	1291	1298	rBV	18905	31322	1.67%	0.506%
22	9.049	1299	1306	1312	rBV	22184	32966	1.76%	0.533%
23	9.458	1364	1373	1386	rVB2	32414	53263	2.84%	0.861%
24	10.055	1465	1471	1485	rVV	356198	491772	26.27%	7.947%
25	10.195	1489	1494	1502	rVV	164241	213654	11.41%	3.452%
26	10.963	1614	1620	1625	rBV	35158	43849	2.34%	0.709%
27	11.085	1634	1640	1649	rBV	278053	367391	19.62%	5.937%
28	11.305	1672	1676	1685	rVB	26979	34300	1.83%	0.554%
29	12.024	1789	1794	1802	rBV	367610	449323	24.00%	7.261%
30	12.244	1823	1830	1838	rBV	101257	126775	6.77%	2.049%
31	12.701	1901	1905	1911	rVB	23133	29610	1.58%	0.478%

Sum of corrected areas: 6188445

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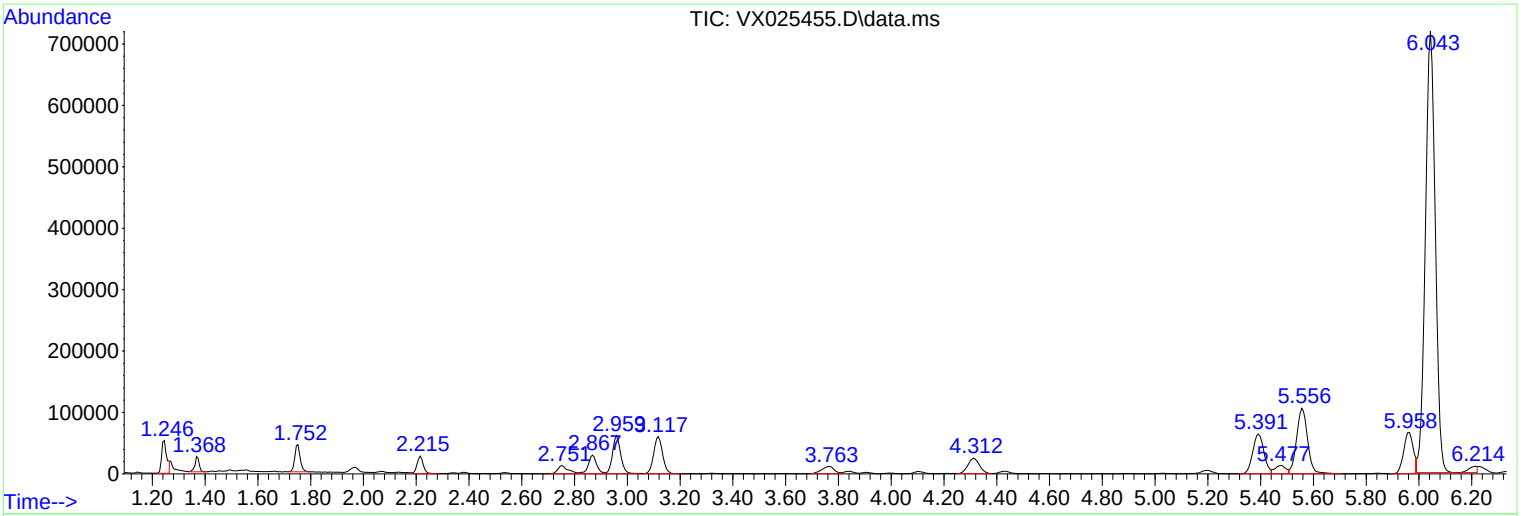
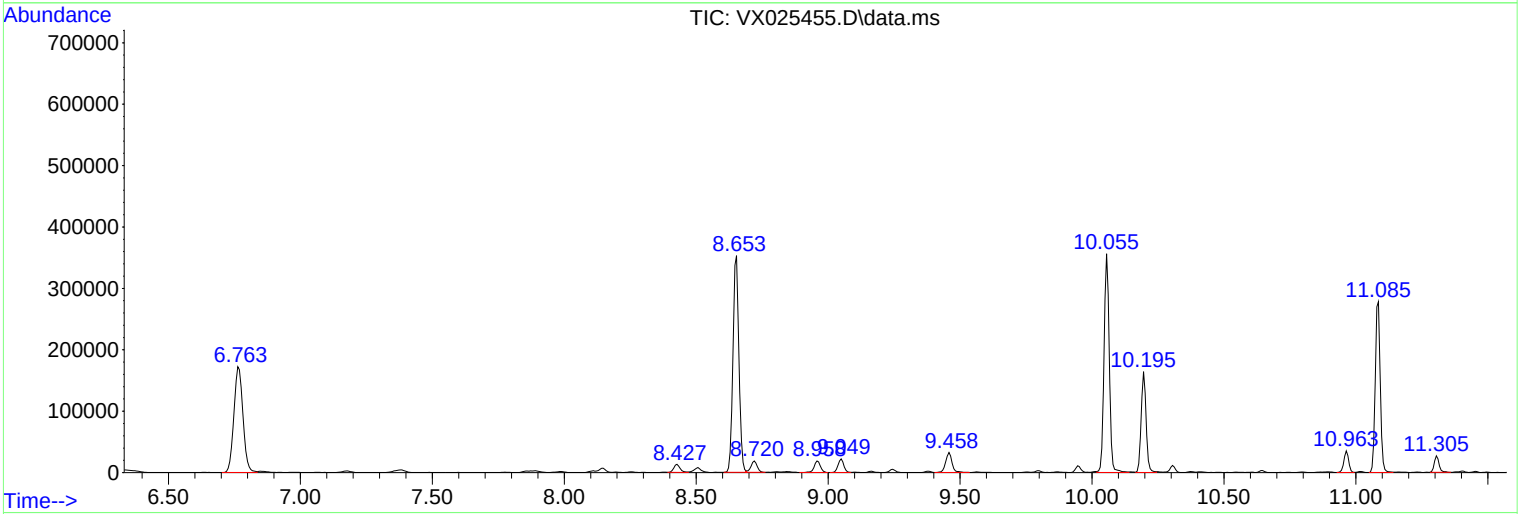
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 43 Sample Multiplier: 1

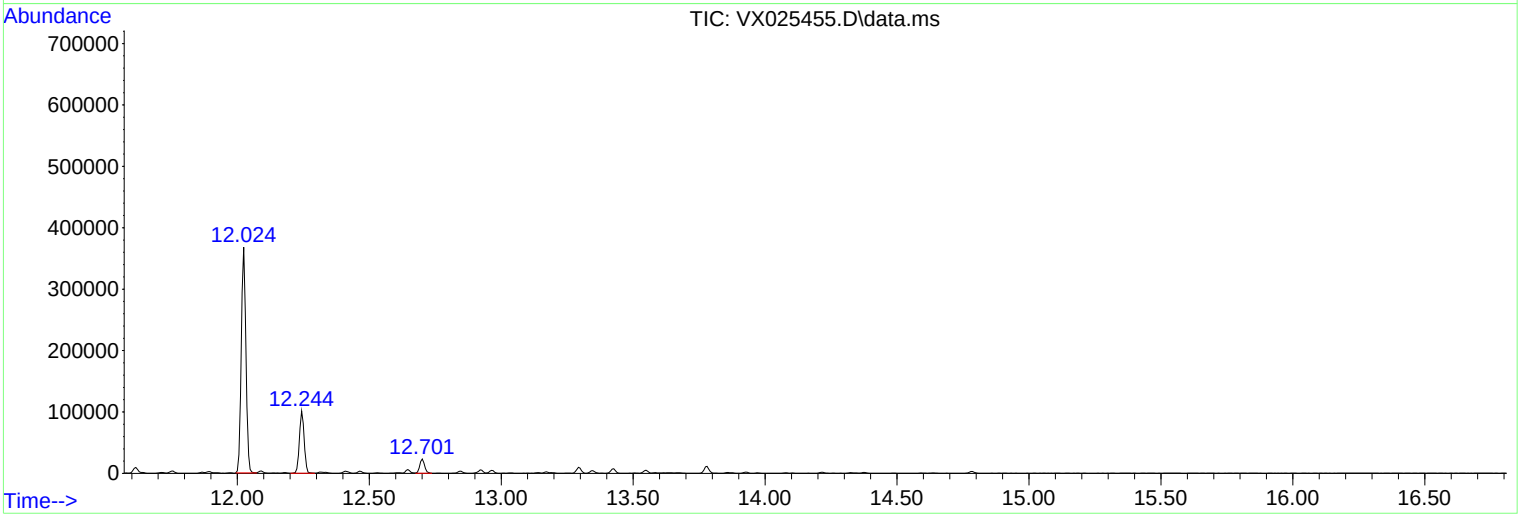
Instrument :
MSVOA_X
ClientSampleId :
MW-35

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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







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Quant Title : SW846 8260

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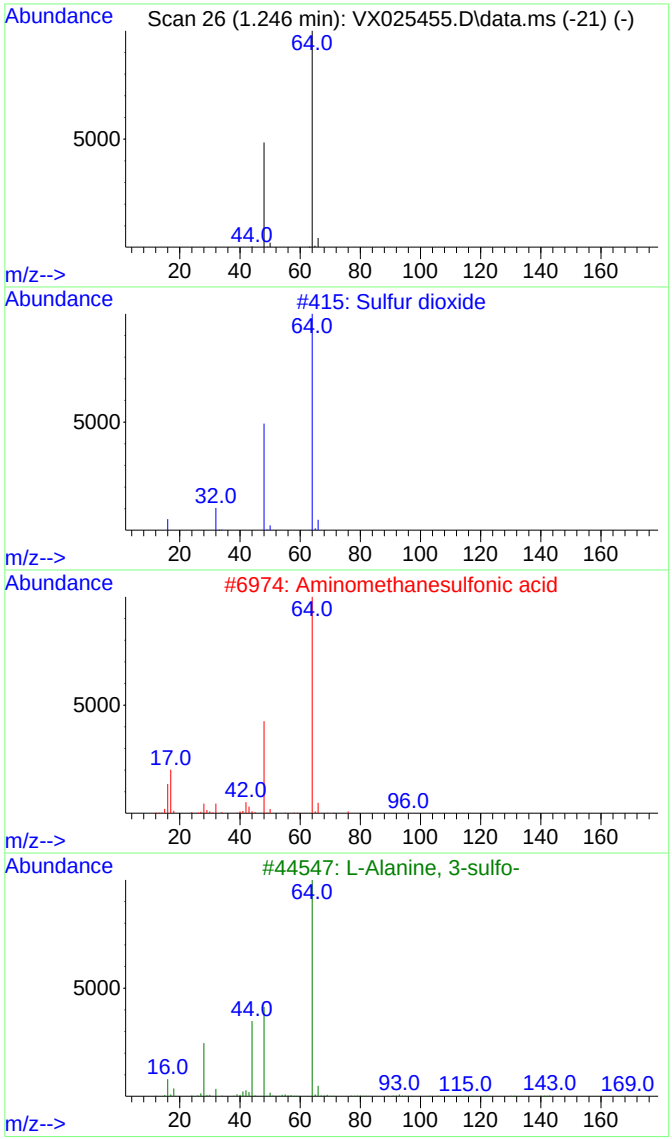
TIC Integration Parameters: LSCINT.P

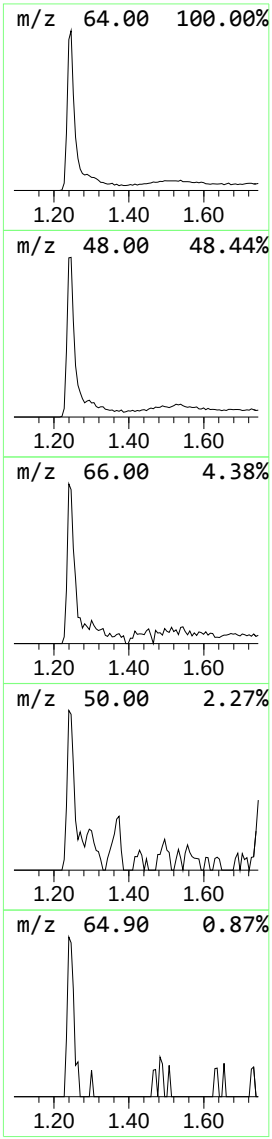
****

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	11.87 ug/l	72966	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





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Data File : VX025455.D
Acq On : 03 Dec 2021 02:30
Operator : JC/MD
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ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-35

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

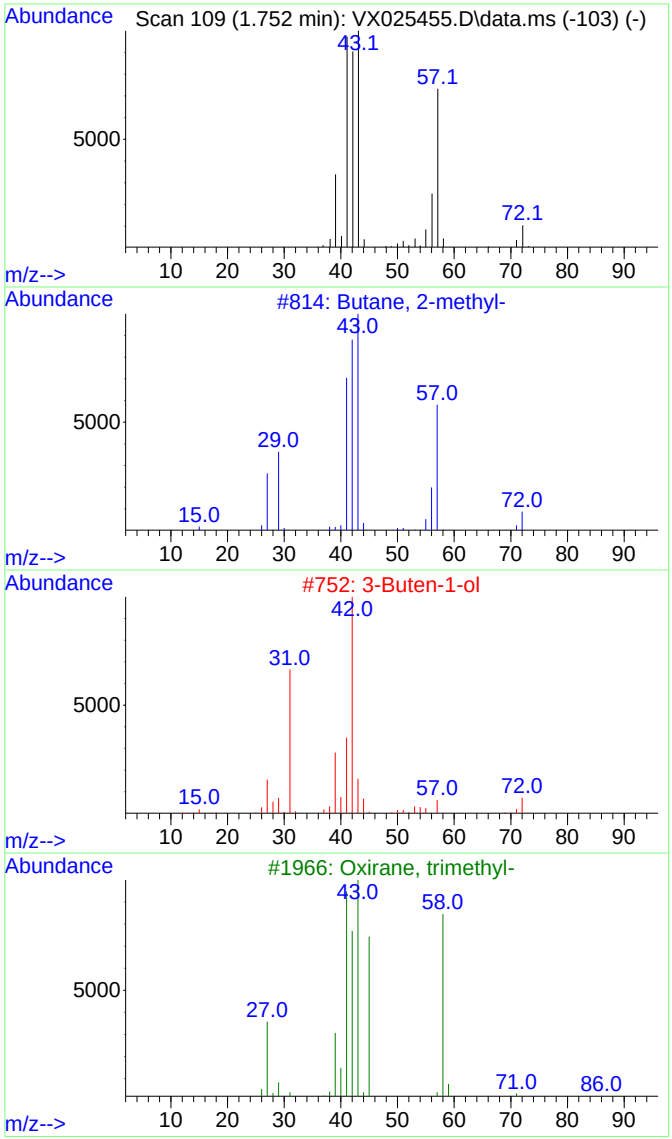
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

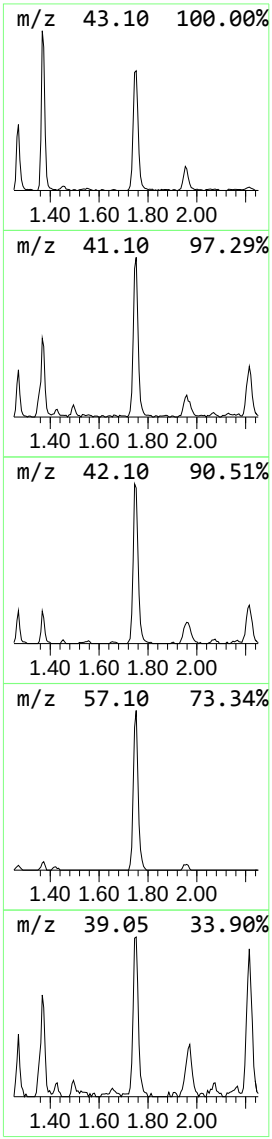
****

Peak Number 2 Butane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	10.25 ug/l	63009	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	90
2	3-Buten-1-ol	72	C4H8O	000627-27-0	43
3	Oxirane, trimethyl-	86	C5H10O	005076-19-7	36
4	Pentane	72	C5H12	000109-66-0	32
5	1-Butene	56	C4H8	000106-98-9	10





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Operator : JC/MD
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ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-35

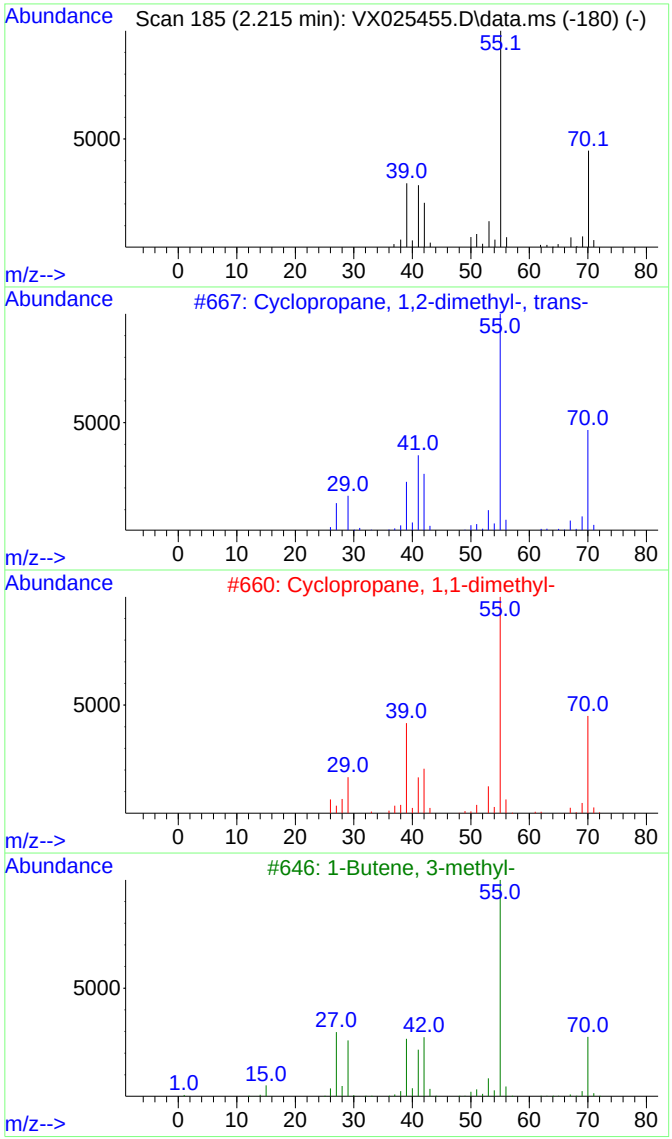
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

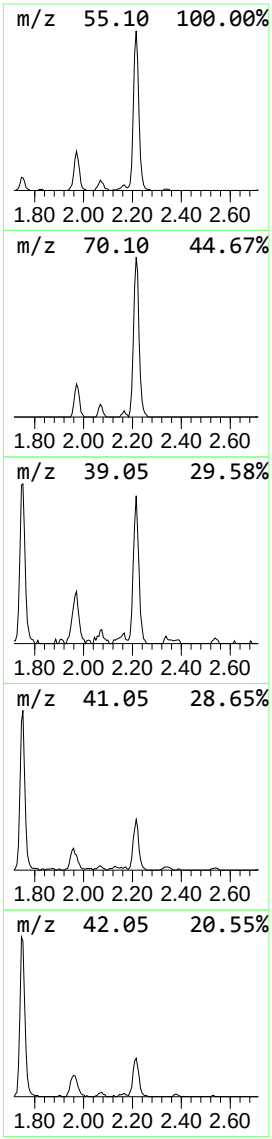
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopropane, 1,2-dimethyl-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.215	7.45 ug/l	45766	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	91
2	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80
3	1-Butene, 3-methyl-	70	C5H10	000563-45-1	78
4	2-Pentene, (Z)-	70	C5H10	000627-20-3	78
5	2-Butene, 2-methyl-	70	C5H10	000513-35-9	78





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Data File : VX025455.D
Acq On : 03 Dec 2021 02:30
Operator : JC/MD
Sample : M4917-19
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-35

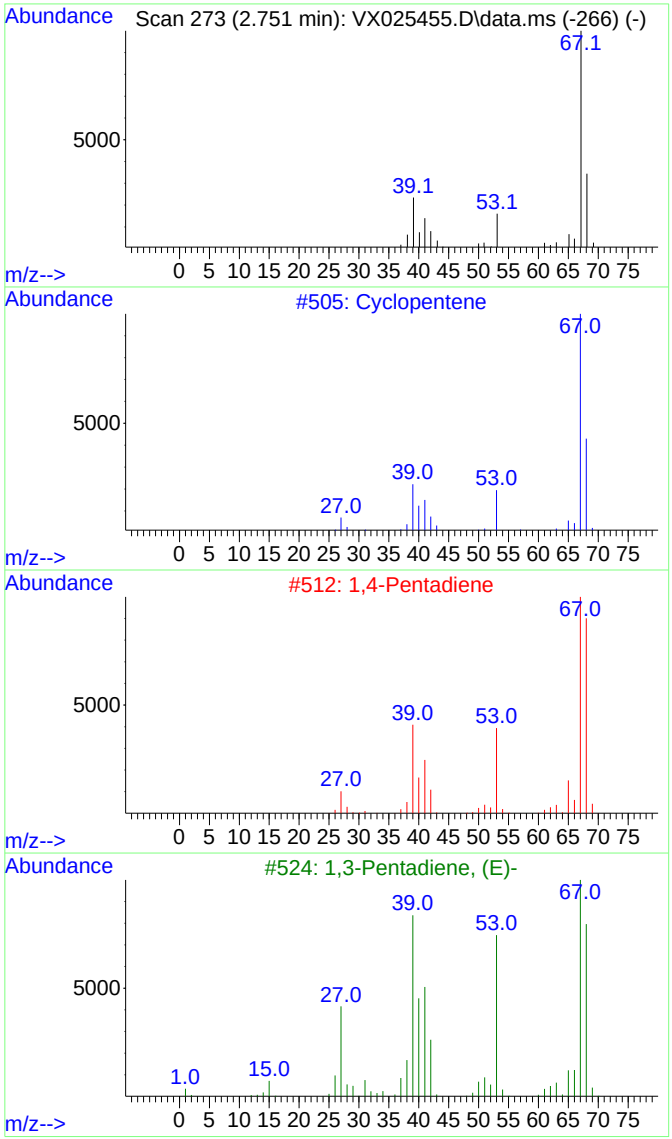
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

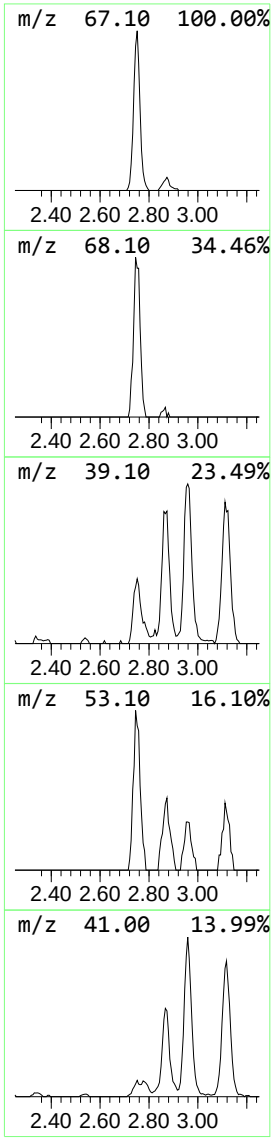
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopentene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.751	5.72 ug/l	35186	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene	68	C5H8	000142-29-0	91
2	1,4-Pentadiene	68	C5H8	000591-93-5	52
3	1,3-Pentadiene, (E)-	68	C5H8	002004-70-8	52
4	1,3-Pentadiene	68	C5H8	000504-60-9	52
5	1,3-Pentadiene, (Z)-	68	C5H8	001574-41-0	52





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Data File : VX025455.D
Acq On : 03 Dec 2021 02:30
Operator : JC/MD
Sample : M4917-19
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-35

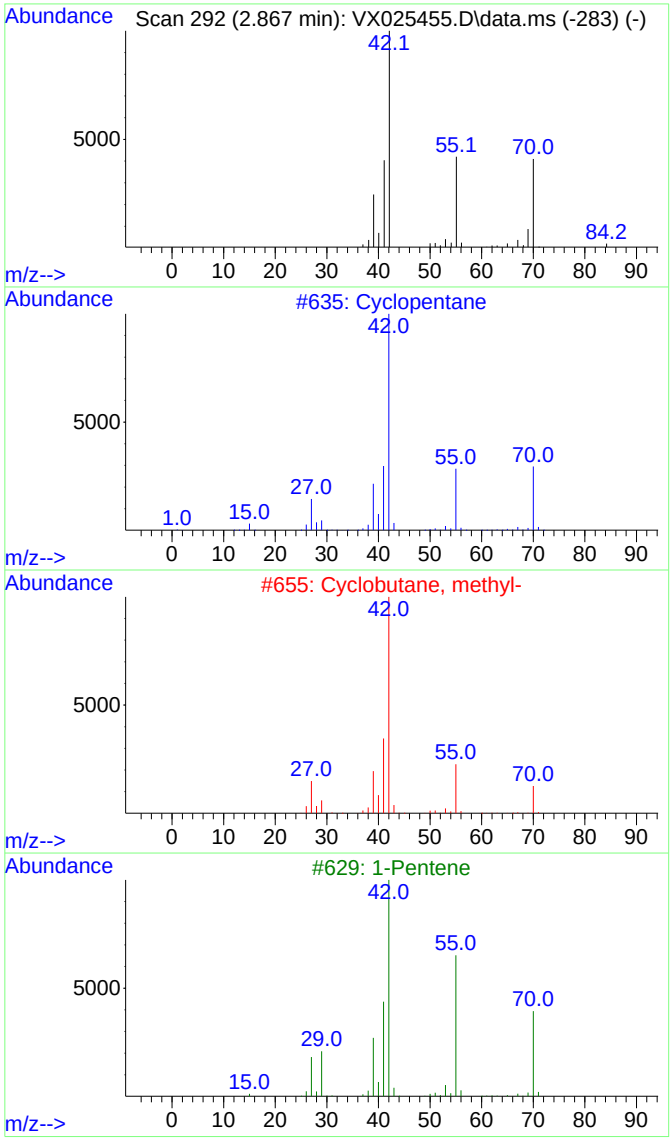
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

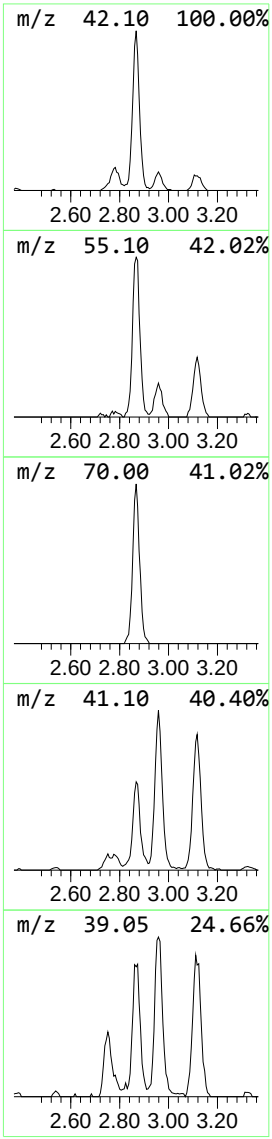
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclopentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	10.76 ug/l	66105	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	90
2	Cyclobutane, methyl-	70	C5H10	000598-61-8	86
3	1-Pentene	70	C5H10	000109-67-1	56
4	3-Buten-1-ol	72	C4H8O	000627-27-0	38
5	Cyclopropane, ethyl-	70	C5H10	001191-96-4	9





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Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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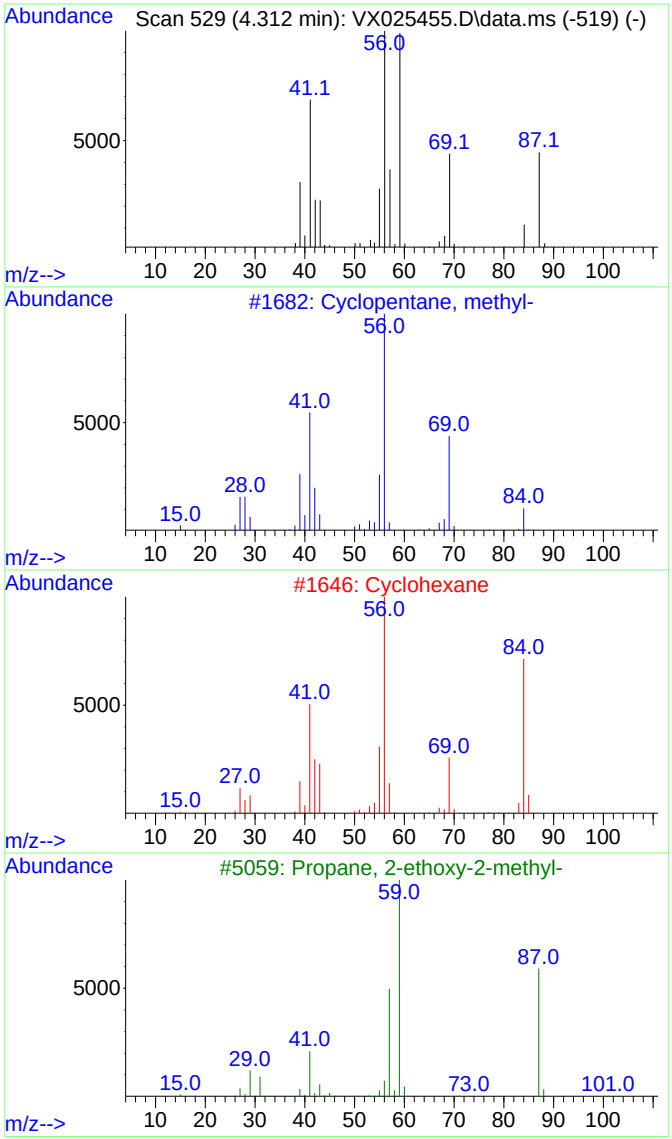
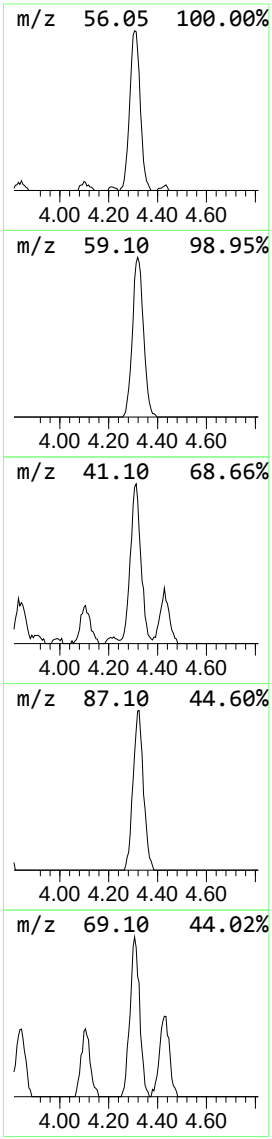
****
Peak Number 6 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.312	12.40 ug/l	76218	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	50
2	Cyclohexane	84	C6H12	000110-82-7	43
3	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	38
4	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	35
5	5-Methyl-5-hexen-3-ol	114	C7H14O	067760-89-8	32





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ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-35

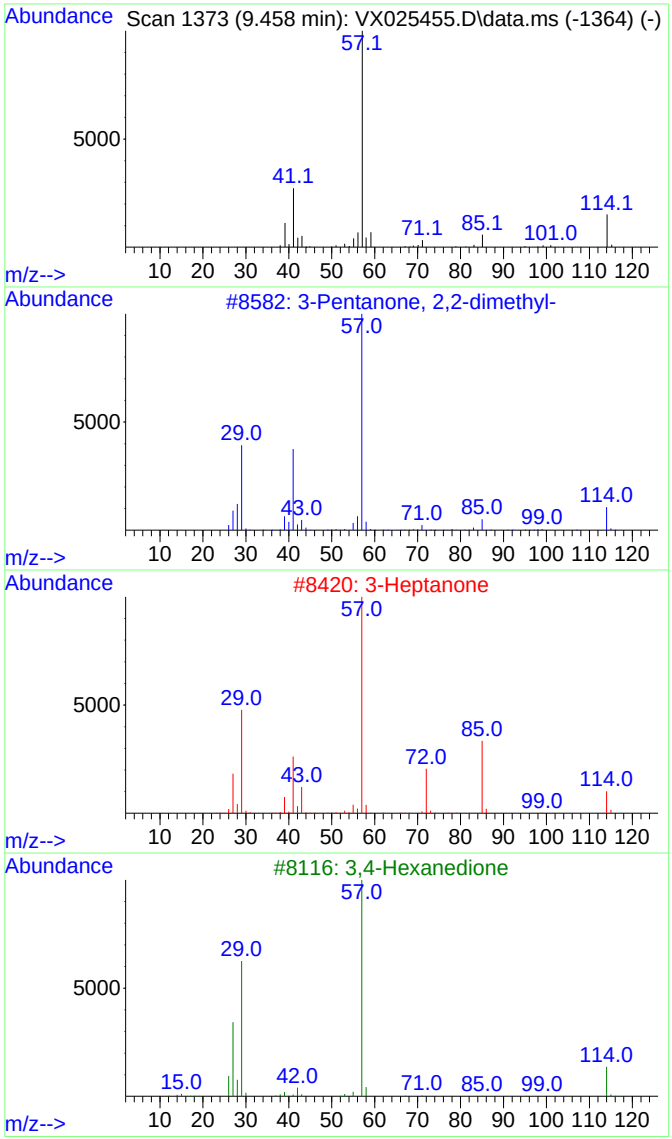
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

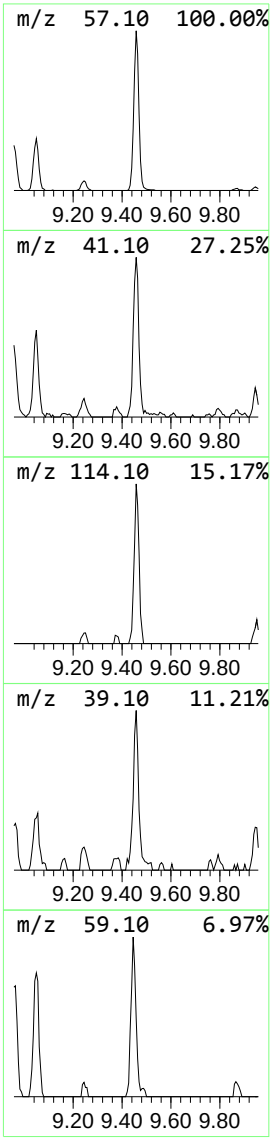
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 3-Pentanone, 2,2-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.458	5.42 ug/l	53263	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,2-dimethyl-	114	C7H14O	000564-04-5	72
2	3-Heptanone	114	C7H14O	000106-35-4	59
3	3,4-Hexanedione	114	C6H10O2	004437-51-8	58
4	3-Hexanone, 5-methyl-	114	C7H14O	000623-56-3	53
5	Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	43





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Instrument :
MSVOA_X
ClientSampleId :
MW-35

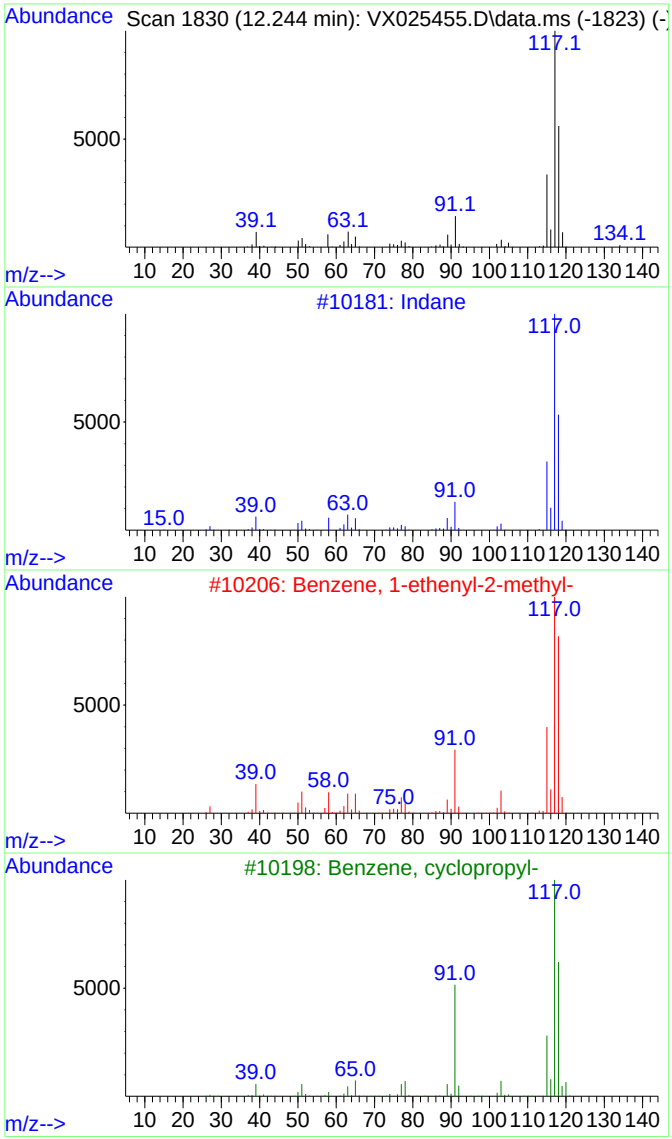
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

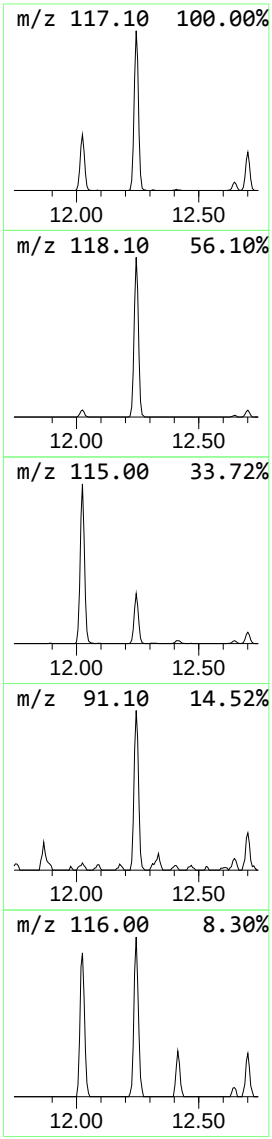
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	14.11 ug/l	126775	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	95
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	87
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	83
4	Deltacyclene	118	C9H10	007785-10-6	72
5	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64





Tentatively Identified Compound (LSC) summary

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Instrument :
MSVOA_X
ClientSampleId :
MW-35

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.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	1.246	11.9	ug/l	72966	1	5.556	307322	50.0
Butane, 2-methyl-	1.752	10.3	ug/l	63009	1	5.556	307322	50.0
Cyclopropane, 1...	2.215	7.5	ug/l	45766	1	5.556	307322	50.0
Cyclopentene	2.751	5.7	ug/l	35186	1	5.556	307322	50.0
Cyclopentane	2.867	10.8	ug/l	66105	1	5.556	307322	50.0
Cyclopentane, m...	4.312	12.4	ug/l	76218	1	5.556	307322	50.0
3-Pentanone, 2,...	9.458	5.4	ug/l	53263	3	10.055	491772	50.0
Indane	12.244	14.1	ug/l	126775	4	12.024	449323	50.0