LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
Data File : VX025454.D
Acq On : 03 Dec 2021 02:06
Operator : JC/MD
Sample : M4917-18
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

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: VX025454.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	21	25	41	rBV	61843	118214	9.12%	2.204%
2	1.368	43	46	52	rVB	18243	20497	1.58%	0.382%
3	1.746	103	108	121	rVB	25683	39772	3.07%	0.741%
4	2.215	180	185	193	rVB	14673	24123	1.86%	0.450%
5	2.867	285	292	299	rVB2	17363	33197	2.56%	0.619%
6	2.959	299	307	322	rVB	70319	148556	11.46%	2.769%
7	3.117	323	333	345	rVB	62406	146459	11.30%	2.730%
8	3.764	428	439	447	rBV3	12632	38536	2.97%	0.718%
9	4.318	519	530	540	rVV5	17693	53842	4.15%	1.004%
10	5.391	694	706	715	rBV	63551	183774	14.18%	3.426%
11	5.471	715	719	724	rVV2	7825	20469	1.58%	0.382%
12	5.556	724	733	760	rVB	102777	302125	23.31%	5.632%
13	5.958	789	799	805	rBV	64862	173324	13.38%	3.231%
14	6.044	805	813	828	rVV	488261	1295846	100.00%	24.156%
15	6.233	831	844	855	rVV8	13098	61339	4.73%	1.143%
16	6.330	855	860	876	rVB8	3305	13619	1.05%	0.254%
17	6.763	921	931	942	rBV	164095	391332	30.20%	7.295%
18	8.110	1144	1152	1155	rBV2	8813	18451	1.42%	0.344%
19	8.427	1199	1204	1210	rVB2	9960	15922	1.23%	0.297%
20	8.507	1210	1217	1225	rVB5	7074	14607	1.13%	0.272%
21	8.653	1228	1241	1248	rBV	331308	535449	41.32%	9.981%
22	8.958	1281	1291	1299	rVB2	16955	29211	2.25%	0.545%
23	9.049	1299	1306	1312	rBV	18837	28562	2.20%	0.532%
24	9.458	1365	1373	1379	rBV	29968	48483	3.74%	0.904%
25	10.055	1465	1471	1483	rVB	335838	455734	35.17%	8.495%
26	10.195	1489	1494	1501	rBV	34960	44296	3.42%	0.826%
27	10.964	1613	1620	1626	rBV	24545	32399	2.50%	0.604%
28	11.085	1634	1640	1650	rBV	256958	340517	26.28%	6.347%
29	11.305	1672	1676	1685	rVB	21227	26921	2.08%	0.502%
30	12.024	1789	1794	1801	rBV	338391	405219	31.27%	7.554%
31	12.244	1825	1830	1838	rBV	98677	124536	9.61%	2.321%
32	12.646	1893	1896	1901	rVV	11287	13327	1.03%	0.248%
33	12.701	1901	1905	1913	rVB	35621	45971	3.55%	0.857%
34	12.920	1933	1941	1945	rBV	19300	25537	1.97%	0.476%
35	12.963	1945	1948	1953	rVB	16244	19402	1.50%	0.362%
36	13.292	1998	2002	2007	rBV2	21941	28001	2.16%	0.522%

LSC Area Percent Report

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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

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

37	13.426	2020	2024	2030	rVB2	9794	13107	1.01%	0.244%
38	13.780	2075	2082	2090	rBV	8133	13152	1.01%	0.245%
39	14.786	2240	2247	2252	rBV2	15290	20761	1.60%	0.387%

Sum of corrected areas: 5364589

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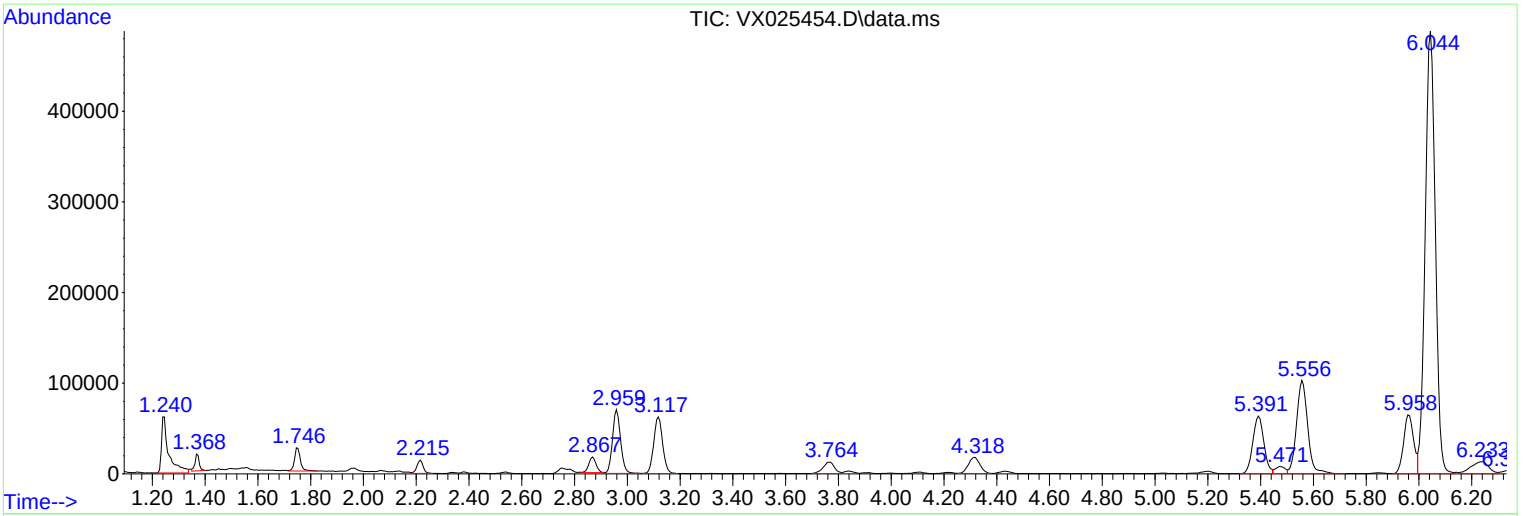
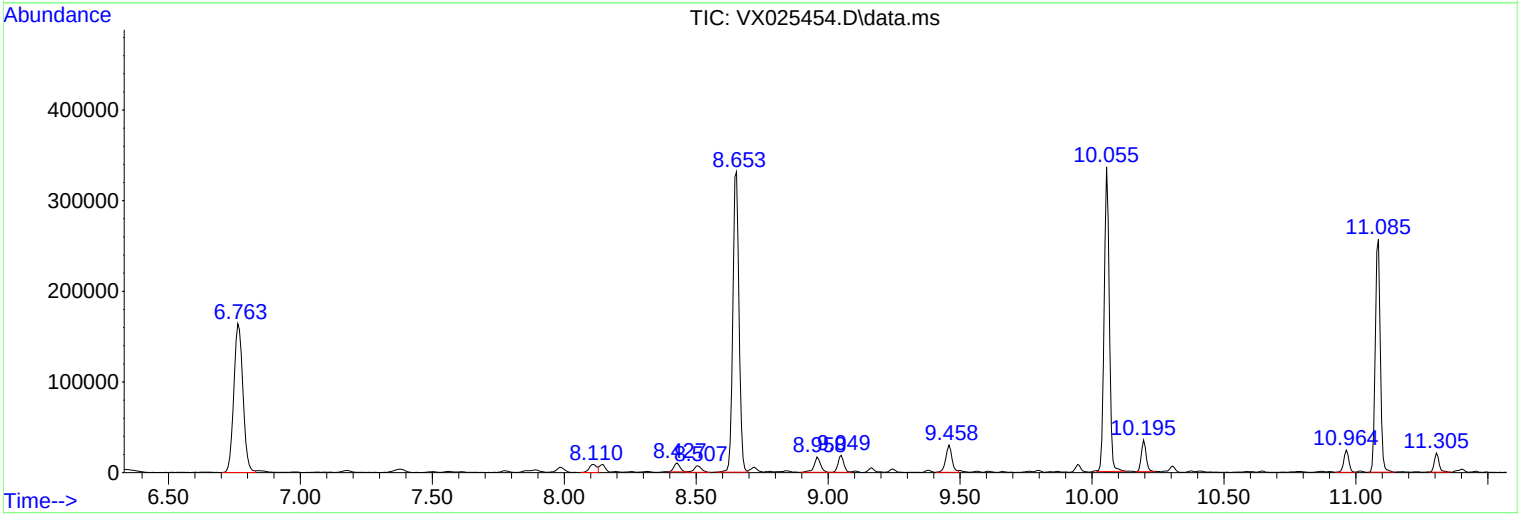
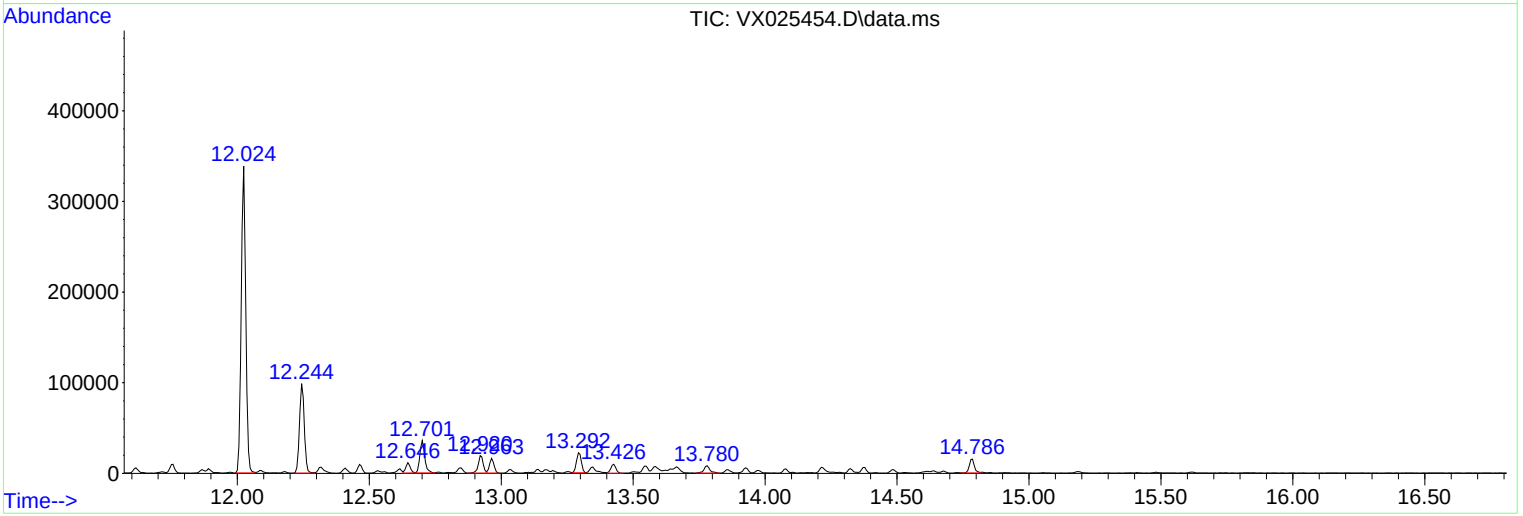
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

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







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Operator : JC/MD
Sample : M4917-18
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Instrument :
MSVOA_X
ClientSampleId :
MW-34

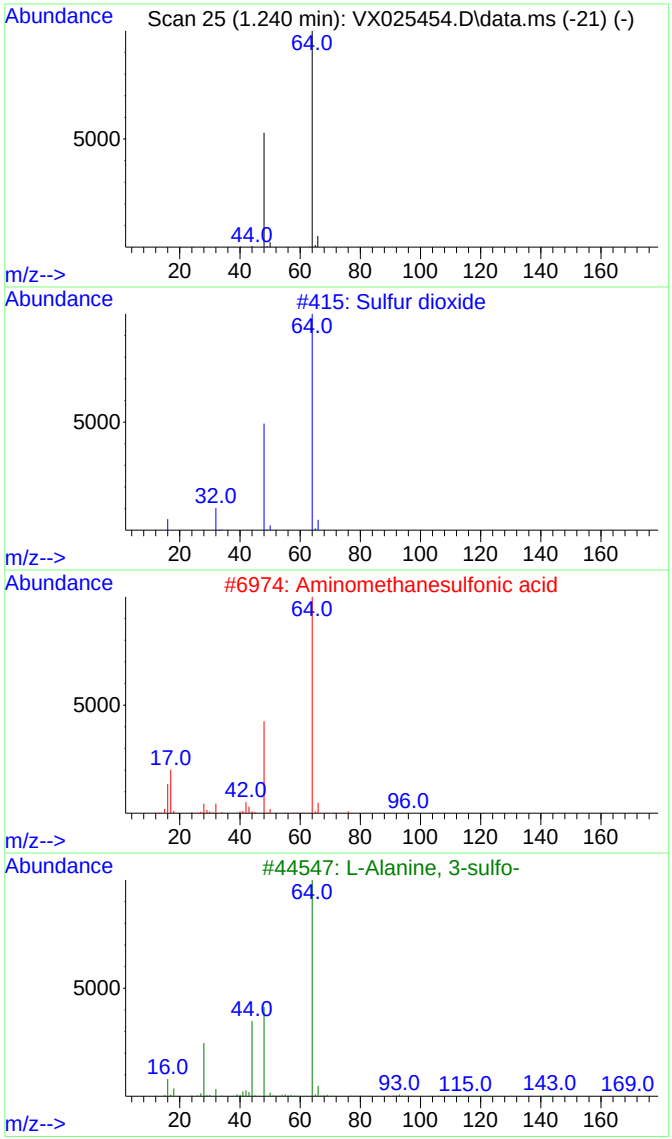
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

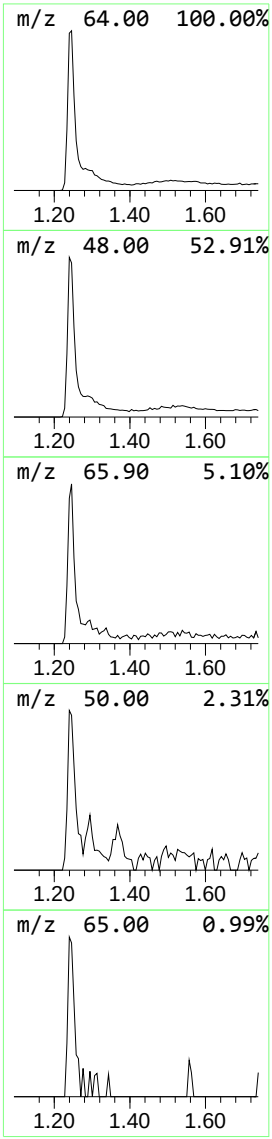
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	19.56 ug/l	118214	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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ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

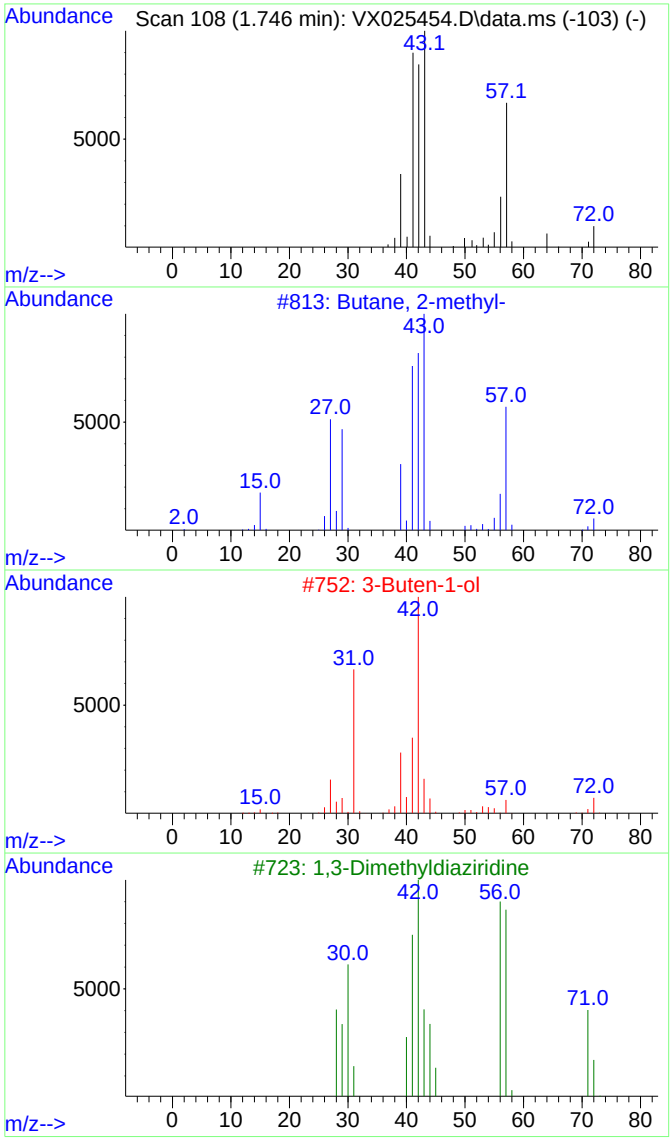
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

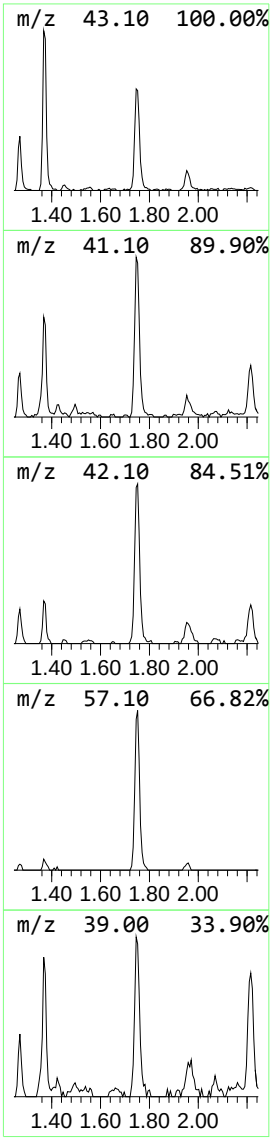
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.746	6.58 ug/l	39772	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	87
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47
3	1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	33
4	Pentane	72	C5H12	000109-66-0	33
5	2,5-Furandione, dihydro-3-methyl-	114	C5H6O3	004100-80-5	23





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
Data File : VX025454.D
Acq On : 03 Dec 2021 02:06
Operator : JC/MD
Sample : M4917-18
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

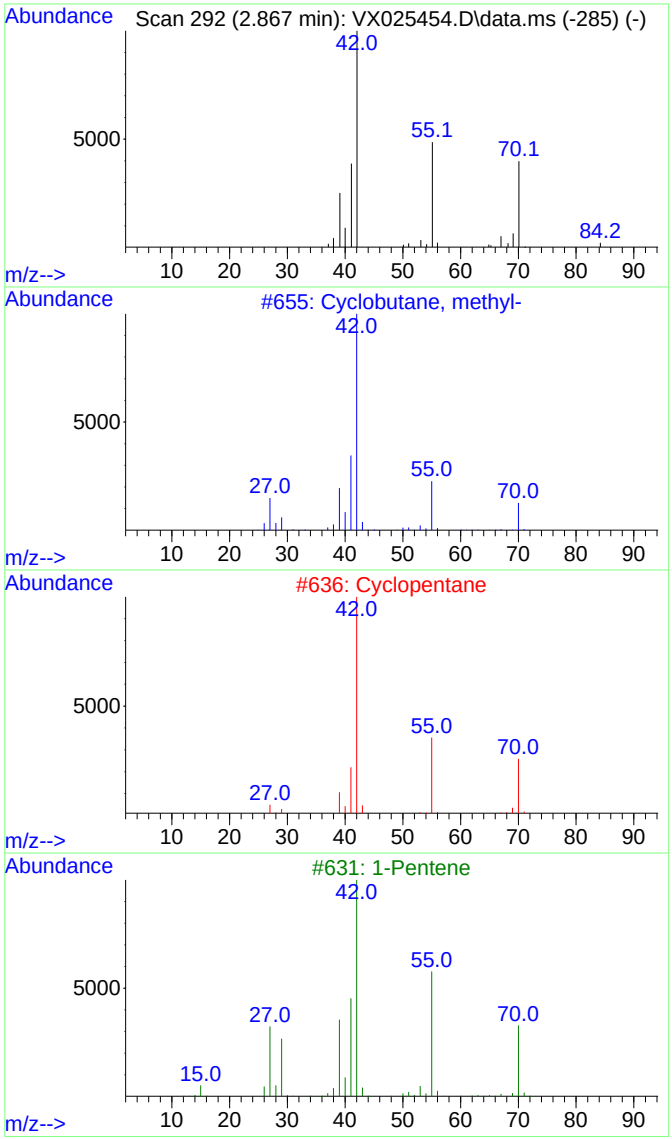
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

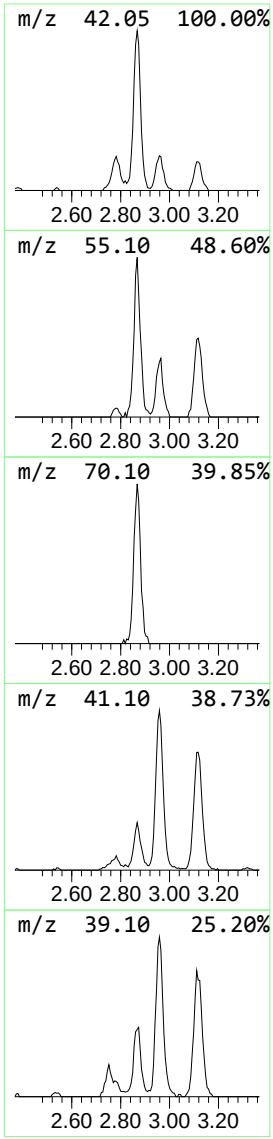
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclobutane, methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	5.49 ug/l	33197	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, methyl-	70	C5H10	000598-61-8	78
2	Cyclopentane	70	C5H10	000287-92-3	78
3	1-Pentene	70	C5H10	000109-67-1	64
4	1-Pentanol	88	C5H12O	000071-41-0	40
5	2H-Tetrazole, 2,5-dimethyl-	98	C3H6N4	004135-93-7	39





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120221\
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Operator : JC/MD
Sample : M4917-18
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

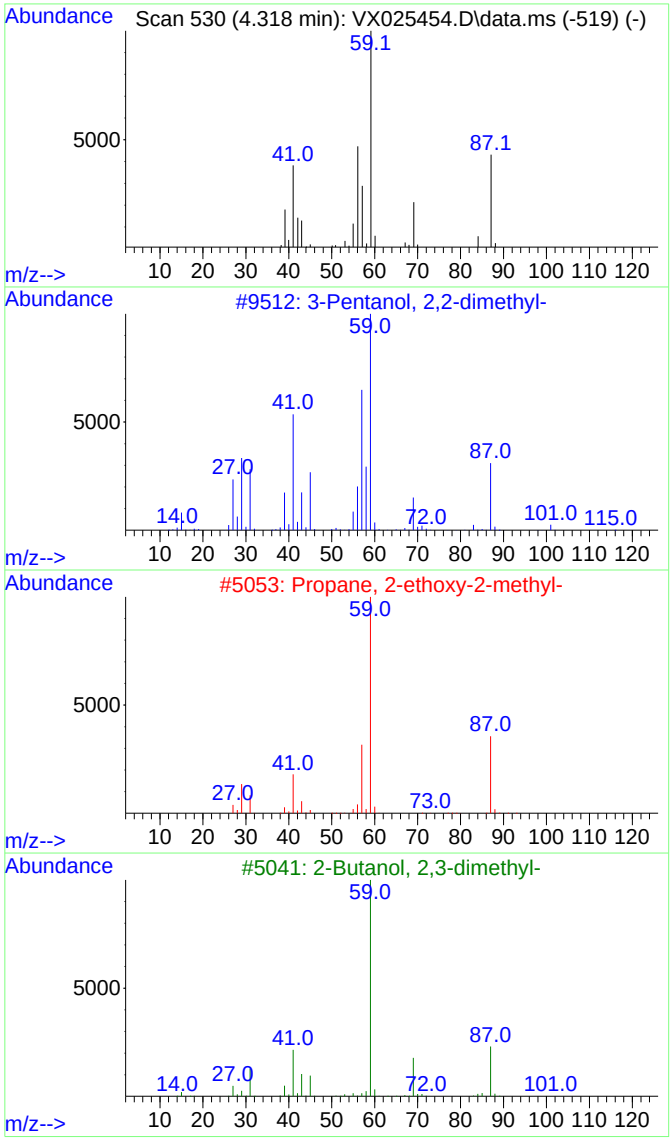
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

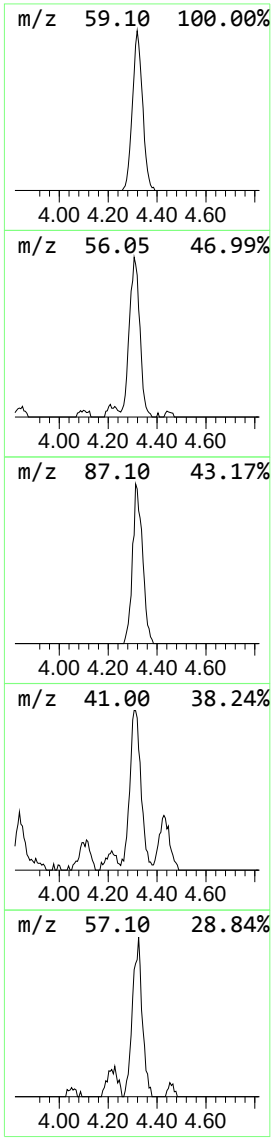
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 3-Pentanol, 2,2-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.318	8.91 ug/l	53842	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	50
2	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	42
3	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	42
4	Hexane, 1-ethoxy-	130	C8H18O	005756-43-4	36
5	HEX-5-EN-3-OL	100	C6H12O	000688-99-3	25





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Operator : JC/MD
Sample : M4917-18
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

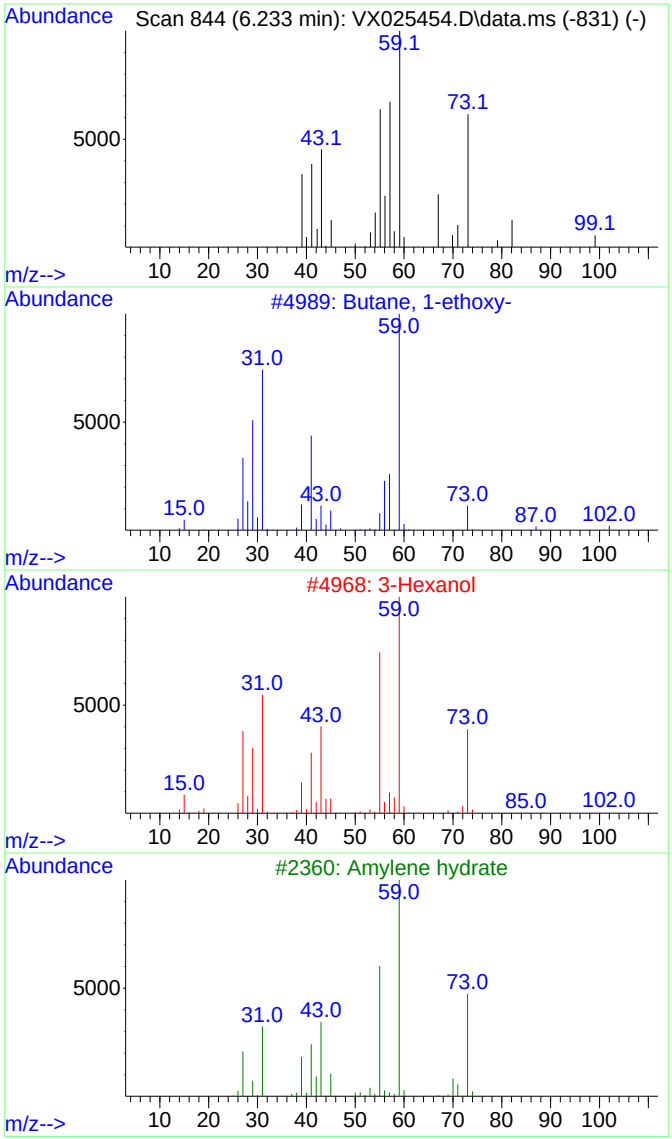
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

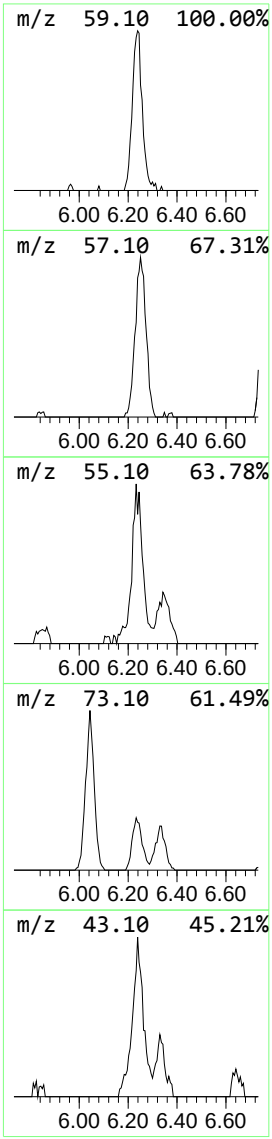
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 unknown6.233 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.233	7.84 ug/l	61339	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	42
2	3-Hexanol	102	C6H14O	000623-37-0	42
3	Amylene hydrate	88	C5H12O	000075-85-4	40
4	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	33
5	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	28





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Sample : M4917-18
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ALS Vial : 42 Sample Multiplier: 1

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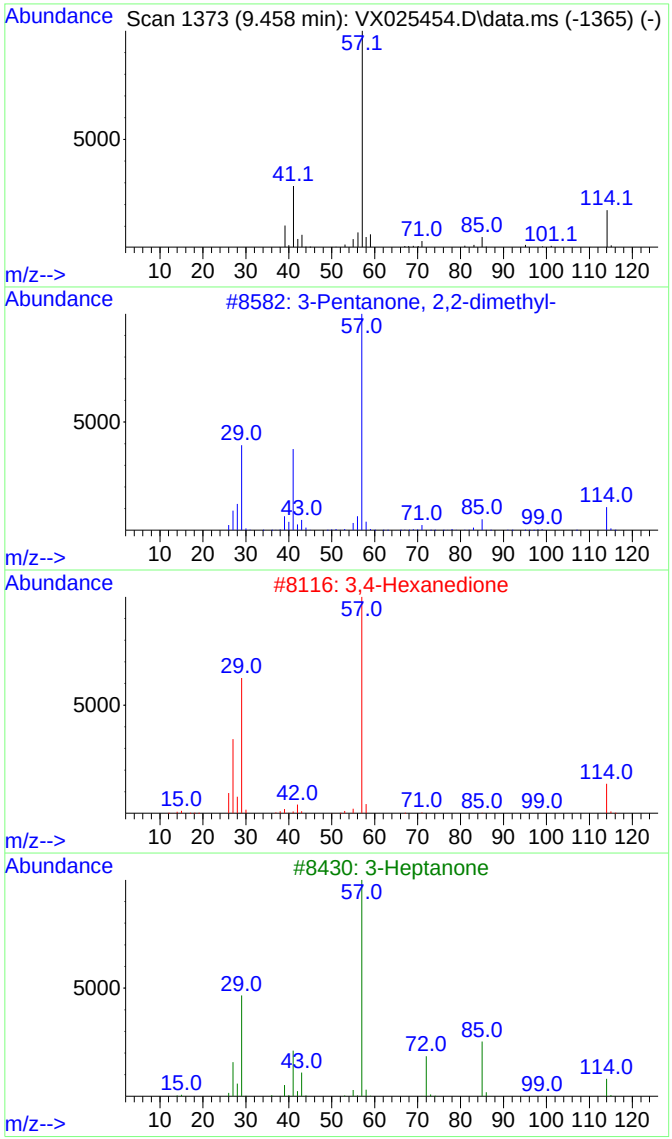
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

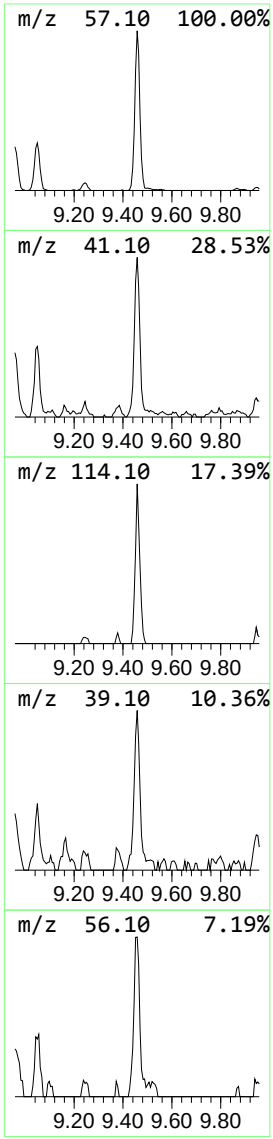
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 3-Pentanone, 2,2-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.458	5.32 ug/l	48483	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,2-dimethyl-	114	C7H14O	000564-04-5	83
2	3,4-Hexanedione	114	C6H10O2	004437-51-8	58
3	3-Heptanone	114	C7H14O	000106-35-4	53
4	3-Hexanone, 5-methyl-	114	C7H14O	000623-56-3	53
5	2,2,5,5-Tetramethyl-3-hexanone	156	C10H20O	000868-91-7	42





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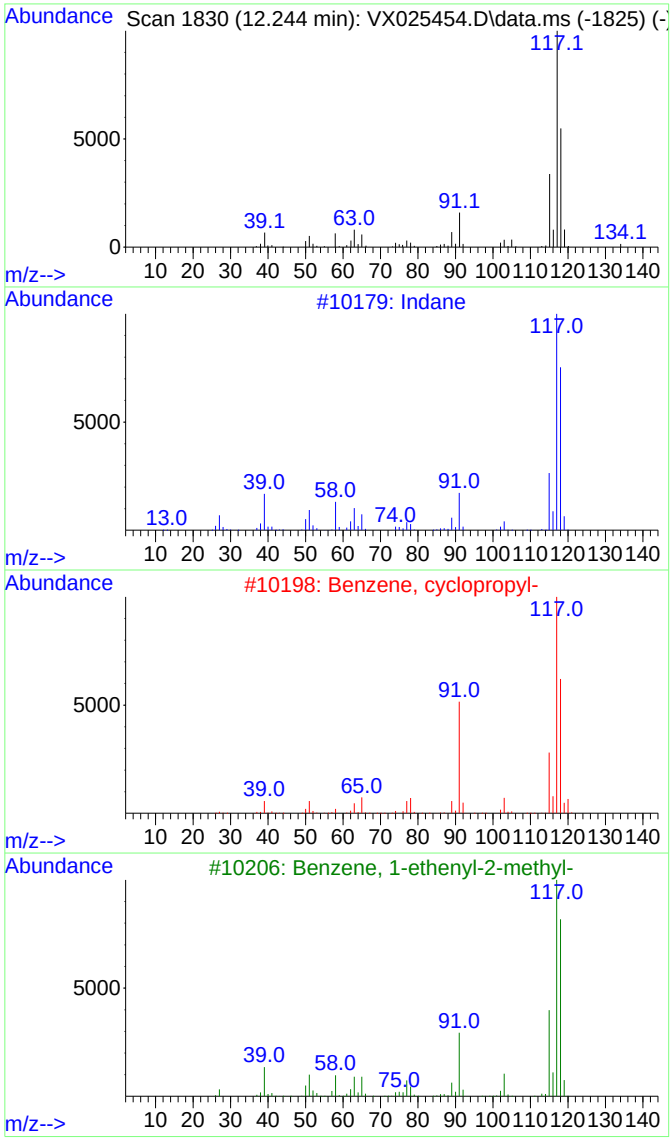
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

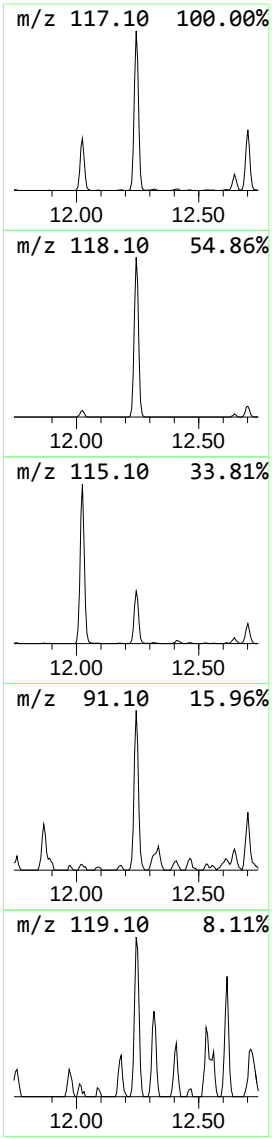
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	15.37 ug/l	124536	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	91
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
3	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	60
4	Benzene, 1,1'-(1,5-hexadiene-1,6...	234	C18H18	004439-45-6	59
5	Benzeneethanol, .beta.-ethenyl-	148	C10H12O	006052-63-7	53





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ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

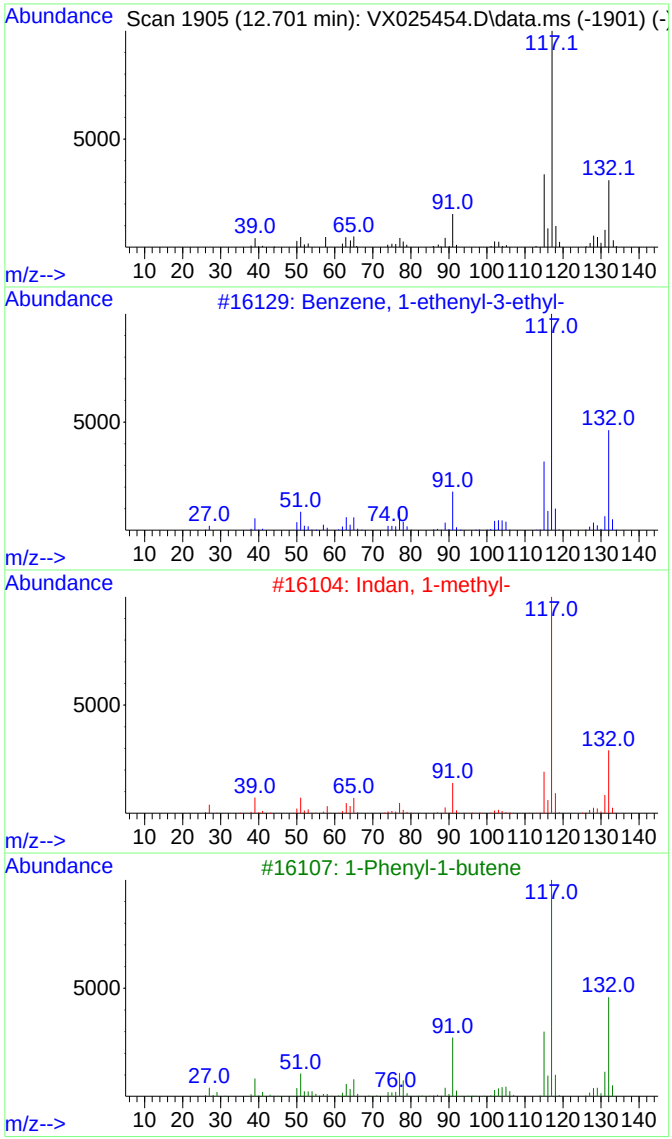
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X111721W.M
Quant Title : SW846 8260

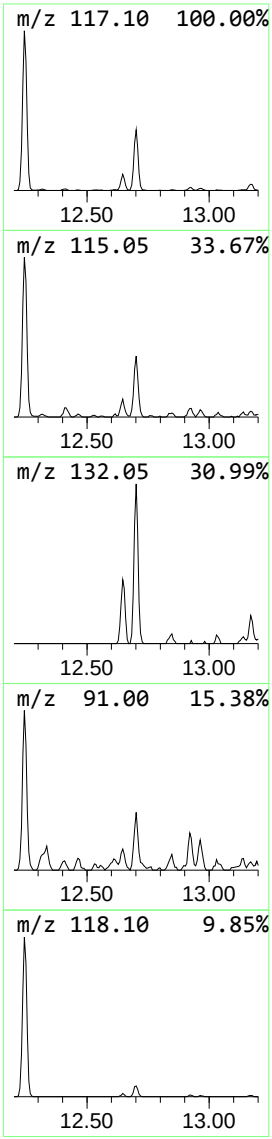
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	5.67 ug/l	45971	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
2	Indan, 1-methyl-	132	C10H12	000767-58-8	87
3	1-Phenyl-1-butene	132	C10H12	000824-90-8	87
4	1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	86
5	1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	86





Tentatively Identified Compound (LSC) summary

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Data File : VX025454.D
Acq On : 03 Dec 2021 02:06
Operator : JC/MD
Sample : M4917-18
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

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	1.240	19.6	ug/l	118214	1	5.556	302125	50.0
Butane, 2-methyl-	1.746	6.6	ug/l	39772	1	5.556	302125	50.0
Cyclobutane, me...	2.867	5.5	ug/l	33197	1	5.556	302125	50.0
3-Pentanol, 2,2...	4.318	8.9	ug/l	53842	1	5.556	302125	50.0
unknown6.233	6.233	7.8	ug/l	61339	2	6.763	391332	50.0
3-Pentanone, 2,...	9.458	5.3	ug/l	48483	3	10.055	455734	50.0
Indane	12.244	15.4	ug/l	124536	4	12.024	405219	50.0
Benzene, 1-ethe...	12.701	5.7	ug/l	45971	4	12.024	405219	50.0