LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052022\
Data File : VX028857.D
Acq On : 20 May 2022 17:43
Operator : JC/MD
Sample : N2943-15
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 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\82X051222W.M
Title : SW846 8260

Signal : TIC: VX028857.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	23	27	43	rBV	212414	488724	13.76%	3.277%
2	1.367	43	46	52	rVB	45004	56799	1.60%	0.381%
3	1.752	104	109	116	rVB	81067	114348	3.22%	0.767%
4	2.215	180	185	195	rVB	49311	74553	2.10%	0.500%
5	2.751	265	273	276	rBV2	18417	38067	1.07%	0.255%
6	2.867	286	292	299	rVB	47198	90624	2.55%	0.608%
7	2.953	299	306	320	rVB	160762	356759	10.04%	2.392%
8	3.117	323	333	348	rVB	174460	413846	11.65%	2.775%
9	3.757	426	438	446	rBV4	31199	93061	2.62%	0.624%
10	4.312	518	529	541	rBV3	52559	159704	4.50%	1.071%
11	5.391	694	706	715	rBV	158599	464397	13.07%	3.114%
12	5.470	715	719	725	rVV3	25817	73595	2.07%	0.493%
13	5.556	725	733	755	rVB	259079	758719	21.36%	5.087%
14	5.958	788	799	805	rBV	171246	464767	13.08%	3.116%
15	6.043	805	813	827	rVV	1364821	3552369	100.00%	23.817%
16	6.239	830	845	855	rVV6	31085	146358	4.12%	0.981%
17	6.342	855	862	878	rVB8	8339	37468	1.05%	0.251%
18	6.763	921	931	945	rBV	416720	997772	28.09%	6.690%
19	8.506	1210	1217	1225	rVB5	18790	37067	1.04%	0.249%
20	8.653	1226	1241	1248	rBV	868564	1353008	38.09%	9.071%
21	8.958	1281	1291	1299	rBV3	41148	70796	1.99%	0.475%
22	9.049	1299	1306	1312	rBV	44201	67533	1.90%	0.453%
23	9.457	1364	1373	1378	rBV	67006	112290	3.16%	0.753%
24	10.055	1465	1471	1477	rBV	1012833	1304631	36.73%	8.747%
25	10.195	1489	1494	1500	rBV	205446	264548	7.45%	1.774%
26	10.305	1504	1512	1518	rVB	36639	58687	1.65%	0.393%
27	10.963	1615	1620	1625	rBV	83899	104673	2.95%	0.702%
28	11.085	1634	1640	1650	rBV	849371	1096903	30.88%	7.354%
29	11.305	1668	1676	1685	rBV	63949	88161	2.48%	0.591%
30	11.756	1746	1750	1756	rVB	36639	46886	1.32%	0.314%
31	12.024	1788	1794	1801	rBV	876531	1079680	30.39%	7.239%
32	12.244	1823	1830	1838	rBV	304226	379776	10.69%	2.546%
33	12.701	1901	1905	1912	rVB	94391	121499	3.42%	0.815%
34	12.920	1935	1941	1945	rBV	48176	64314	1.81%	0.431%
35	12.963	1945	1948	1955	rVB	44664	53601	1.51%	0.359%
36	13.292	1998	2002	2007	rVB2	56553	71653	2.02%	0.480%

LSC Area Percent Report

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Operator : JC/MD
Sample : N2943-15
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ALS Vial : 17 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\82X051222W.M
Title : SW846 8260

37	13.426	2018	2024	2030	rVB2	27966	40697	1.15%	0.273%
38	13.780	2074	2082	2091	rBV	43074	62443	1.76%	0.419%
39	14.780	2241	2246	2250	rBV	41744	54684	1.54%	0.367%

Sum of corrected areas: 14915460

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MSVOA_X
ClientSampleId :
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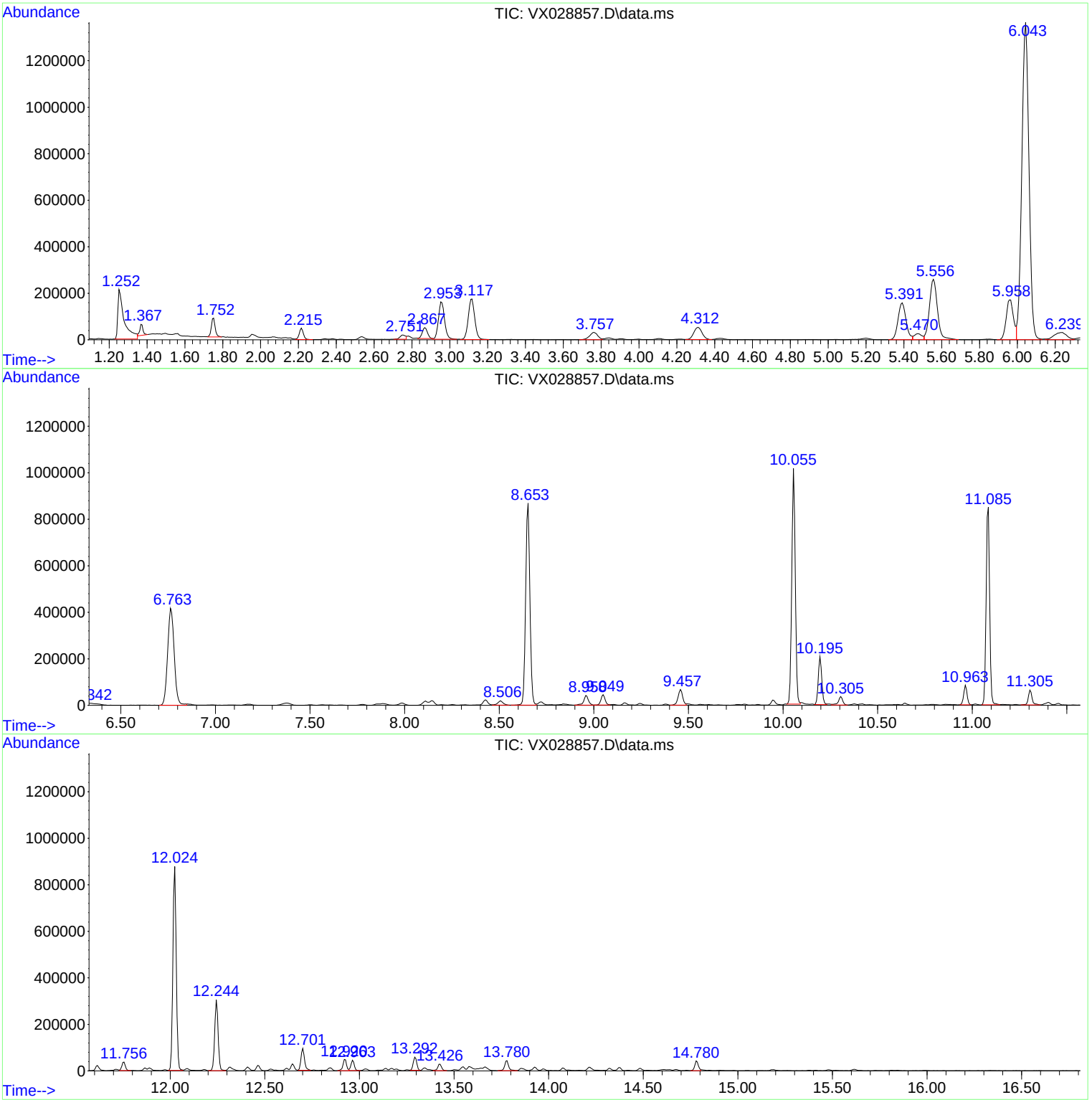
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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



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Data File : VX028857.D
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

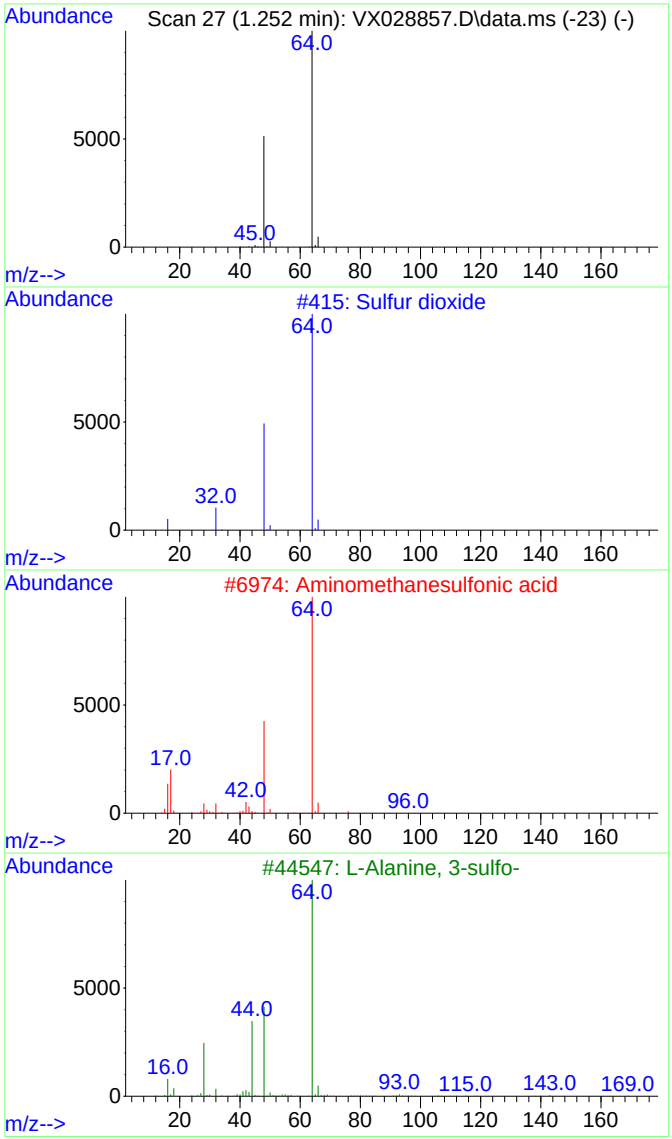
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

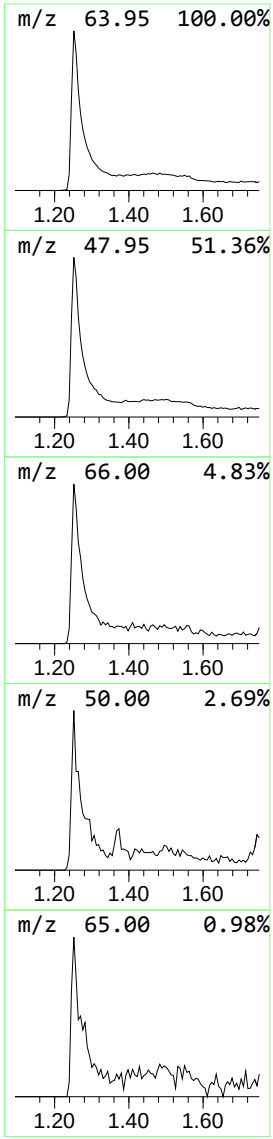
****

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.252	32.21 ug/l	488724	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 : VX028857.D
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Instrument :
MSVOA_X
ClientSampleId :
MW-34

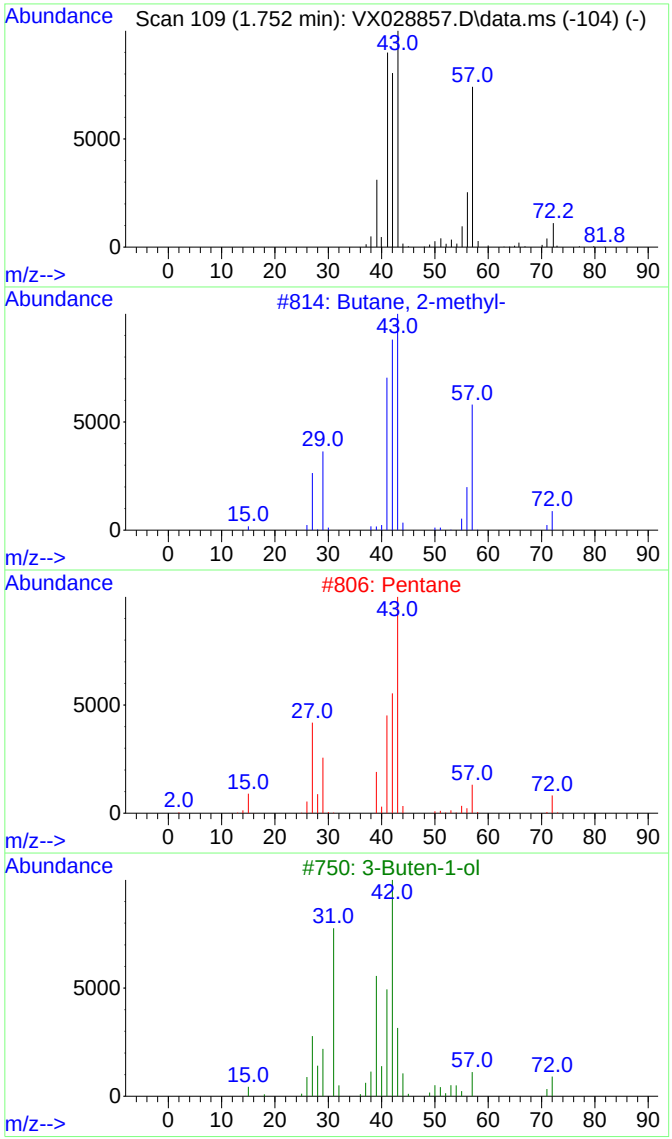
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

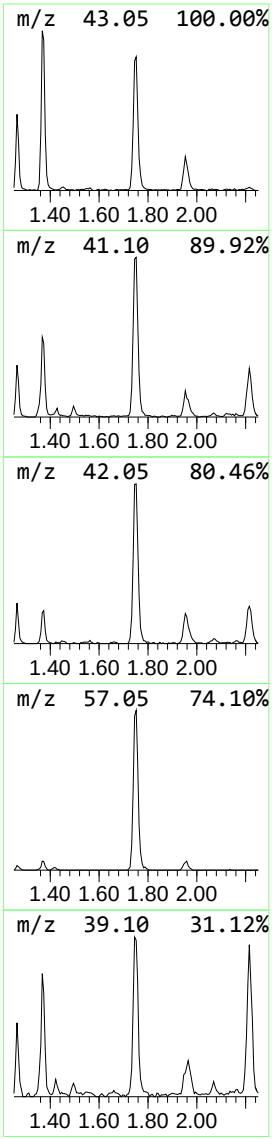
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	7.54 ug/l	114348	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	90
2	Pentane	72	C5H12	000109-66-0	33
3	3-Buten-1-ol	72	C4H8O	000627-27-0	25
4	1-Butene	56	C4H8	000106-98-9	11
5	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052022\
Data File : VX028857.D
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Operator : JC/MD
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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

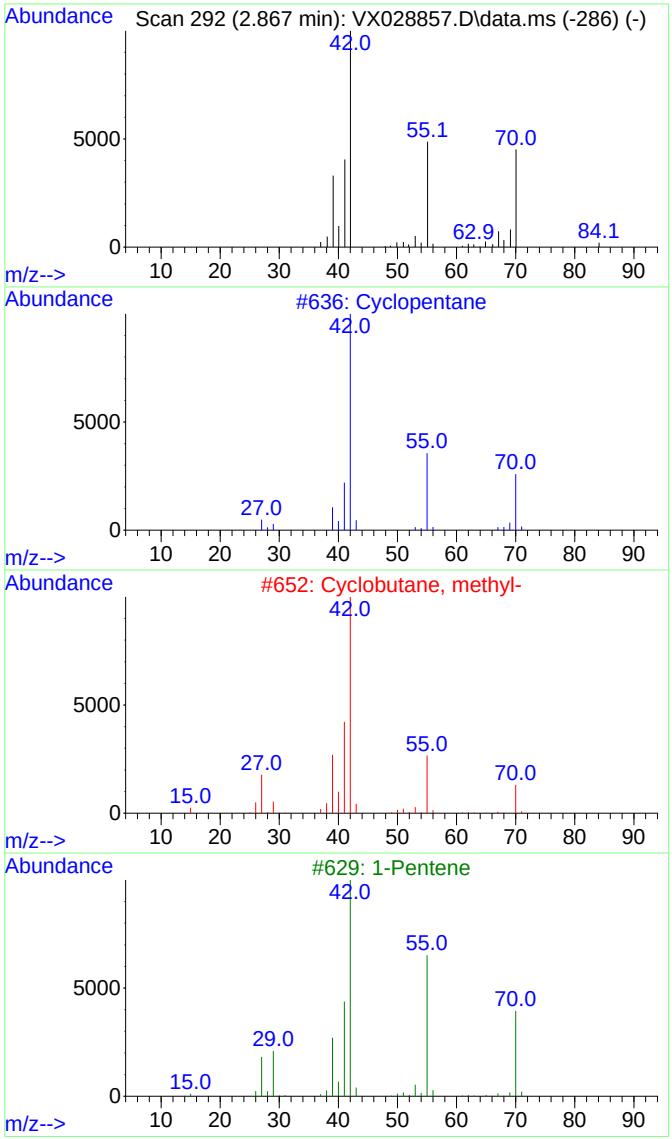
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

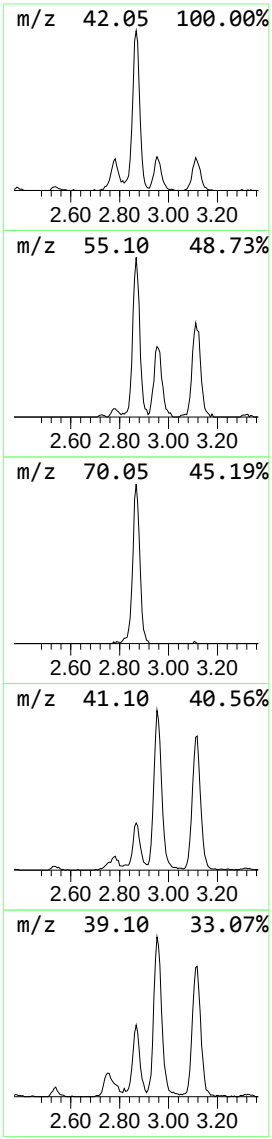
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopentane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	5.97 ug/l	90624	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	86
2	Cyclobutane, methyl-	70	C5H10	000598-61-8	80
3	1-Pentene	70	C5H10	000109-67-1	64
4	Cyclopropane, ethyl-	70	C5H10	001191-96-4	50
5	1-Pentanol	88	C5H12O	000071-41-0	40





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

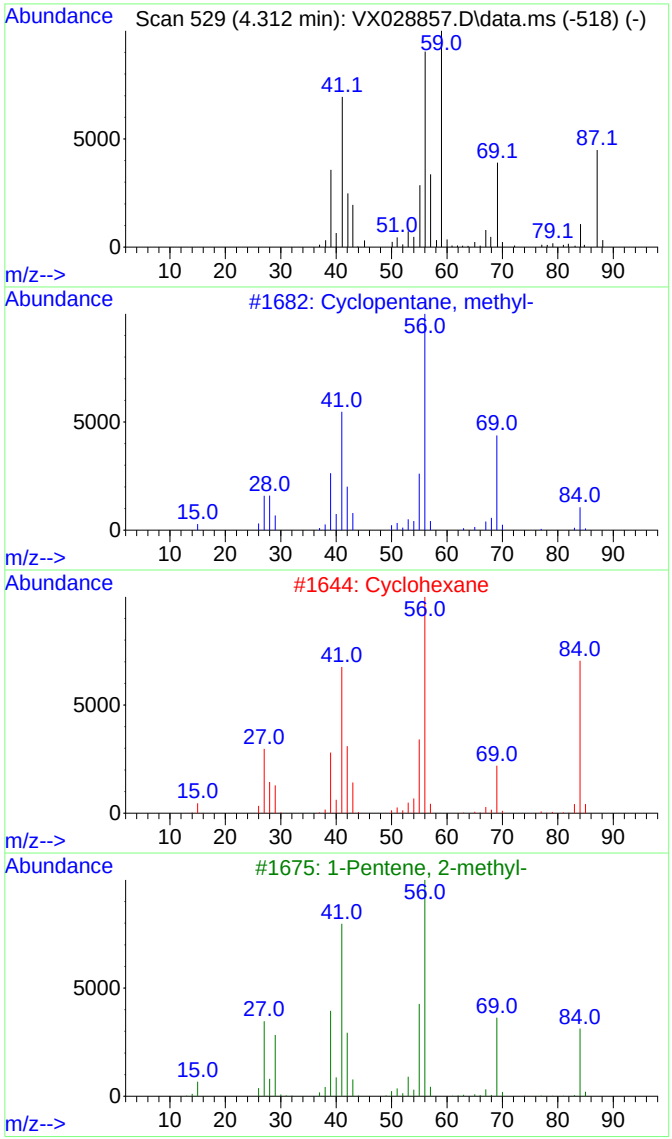
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

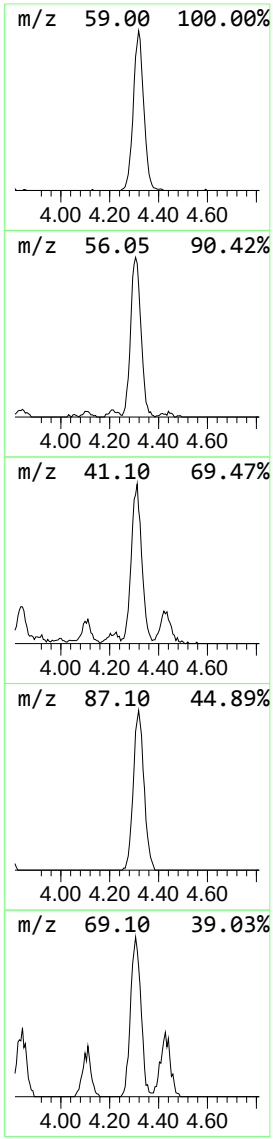
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.312	10.52 ug/l	159704	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	45
2	Cyclohexane	84	C6H12	000110-82-7	35
3	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	35
4	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	32
5	Cyclobutane, 1,2-diethyl-, trans-	112	C8H16	019341-98-1	25





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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-34

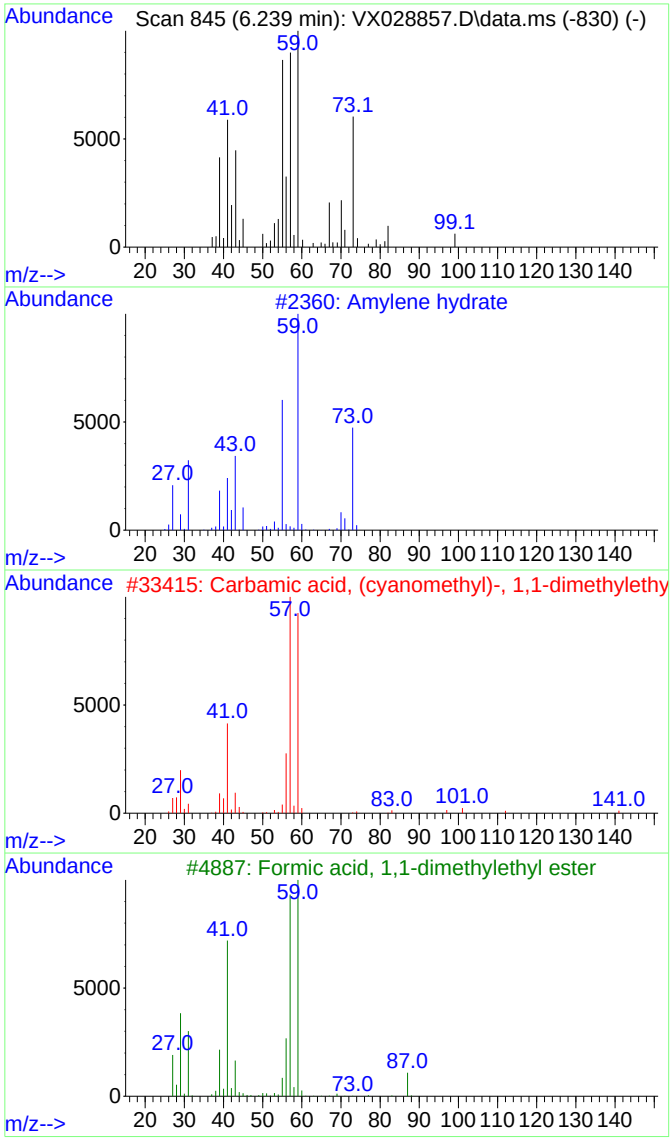
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

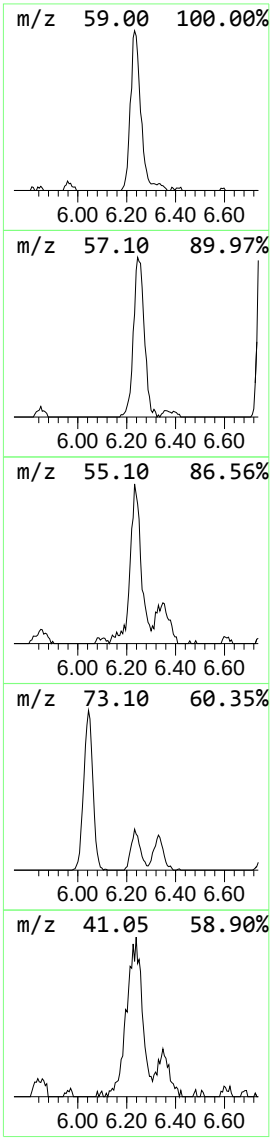
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 unknown6.239 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.239	7.33 ug/l	146358	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Amylene hydrate	88	C5H12O	000075-85-4	38
2	Carbamic acid, (cyanomethyl)-, 1...	156	C7H12N2O2	085363-04-8	32
3	Formic acid, 1,1-dimethylethyl e...	102	C5H10O2	000762-75-4	32
4	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	27
5	Acetaldoxime	59	C2H5NO	000107-29-9	27





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Instrument :
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ClientSampleId :
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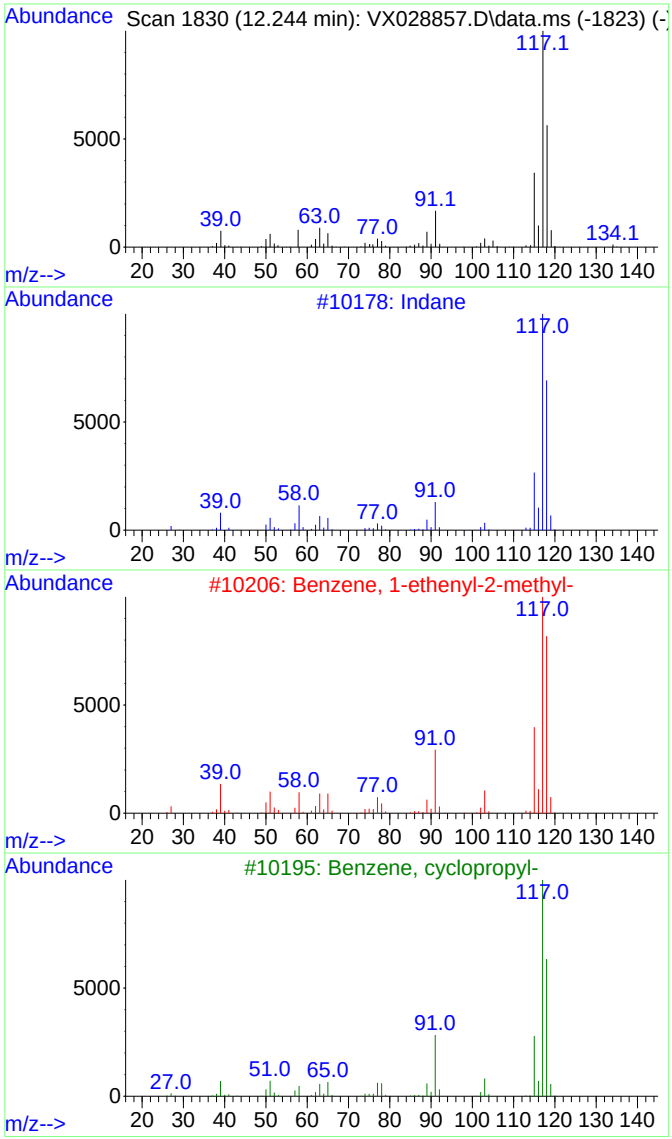
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

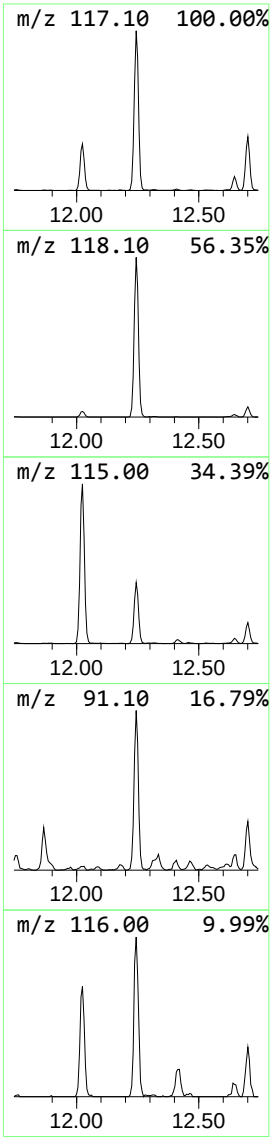
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.243	17.59 ug/l	379776	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	81
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	74
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
5	Deltacyclene	118	C9H10	007785-10-6	72





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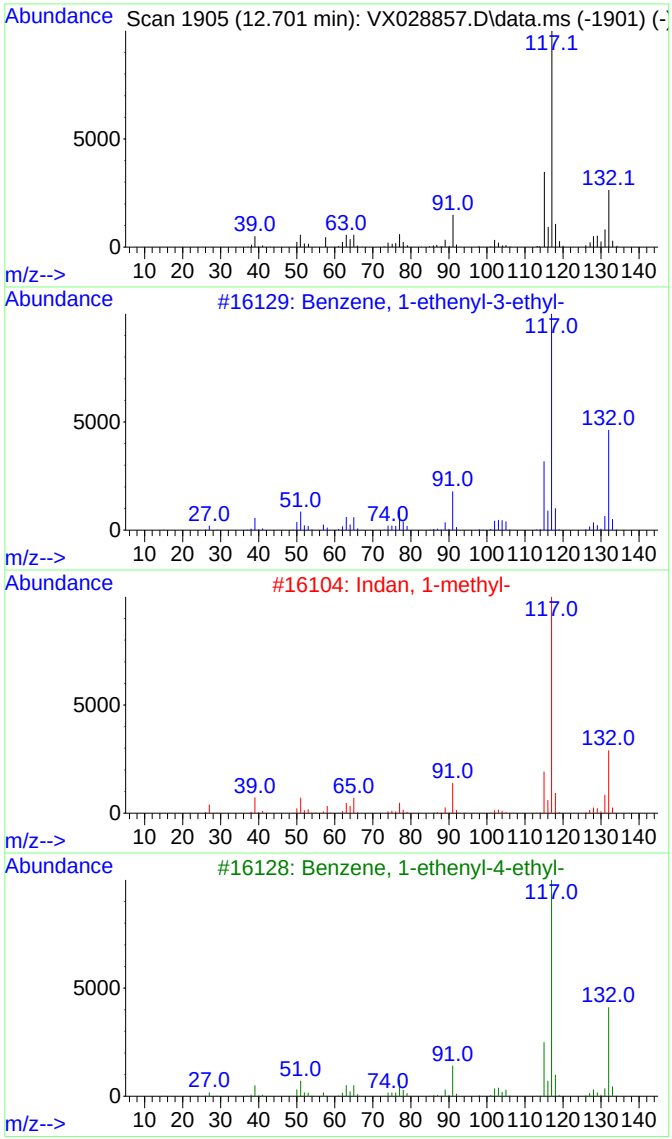
Quant Title : SW846 8260

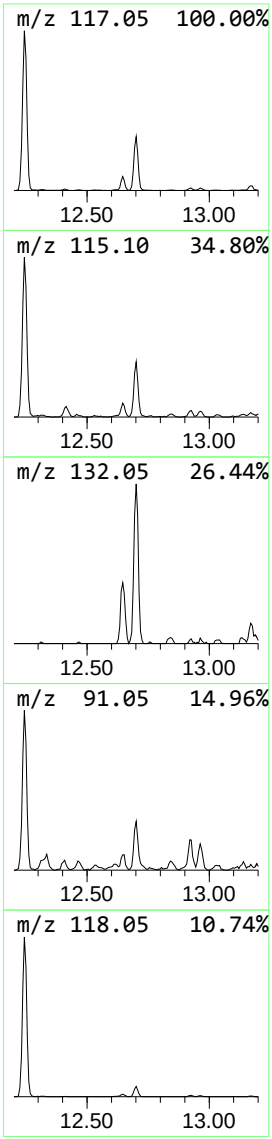
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	5.63 ug/l	121499	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	90
3	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	90
4	Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	83
5	Benzene, 2-butenyl-	132	C10H12	001560-06-1	80





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
Sulfur dioxide	1.252	32.2	ug/l	488724	1	5.556	758719	50.0
Butane, 2-methyl-	1.752	7.5	ug/l	114348	1	5.556	758719	50.0
Cyclopentane	2.867	6.0	ug/l	90624	1	5.556	758719	50.0
Cyclopentane, m...	4.312	10.5	ug/l	159704	1	5.556	758719	50.0
unknown6.239	6.239	7.3	ug/l	146358	2	6.763	997772	50.0
Indane	12.243	17.6	ug/l	379776	4	12.024	1079680	50.0
Benzene, 1-ethe...	12.701	5.6	ug/l	121499	4	12.024	1079680	50.0