LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121322\
Data File : VX033398.D
Acq On : 13 Dec 2022 17:26
Operator : JC/MD
Sample : N6001-13
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

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\82X120722W.M
Title : SW846 8260

Signal : TIC: VX033398.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	22	26	42	rBV	26844	62501	11.62%	1.623%
2	1.374	43	47	52	rVV	18324	18595	3.46%	0.483%
3	1.752	104	109	119	rVB	63406	77876	14.48%	2.023%
4	1.959	138	143	148	rVB2	5434	7893	1.47%	0.205%
5	2.221	179	186	191	rVB	8495	12808	2.38%	0.333%
6	2.343	200	206	218	rVB2	3619	8089	1.50%	0.210%
7	2.782	268	278	282	rBV3	7950	18603	3.46%	0.483%
8	2.867	287	292	303	rVB	23270	49624	9.23%	1.289%
9	3.105	323	331	339	rVB2	7051	15666	2.91%	0.407%
10	3.733	426	434	442	rBV3	3288	7310	1.36%	0.190%
11	4.099	488	494	503	rVB5	2159	5897	1.10%	0.153%
12	4.215	503	513	520	rVV5	2880	9034	1.68%	0.235%
13	4.306	520	528	540	rVB3	14706	42469	7.90%	1.103%
14	4.434	540	549	557	rVB6	1969	6007	1.12%	0.156%
15	5.196	668	674	684	rVB	2615	6811	1.27%	0.177%
16	5.385	694	705	715	rBV	47449	140927	26.20%	3.660%
17	5.550	723	732	754	rVB	127241	373618	69.47%	9.703%
18	5.958	790	799	806	rBV2	37460	98543	18.32%	2.559%
19	6.037	806	812	823	rVV2	51839	139511	25.94%	3.623%
20	6.251	834	847	858	rVB4	13222	49788	9.26%	1.293%
21	6.763	921	931	942	rBV	187142	449847	83.65%	11.683%
22	7.373	1023	1031	1038	rVB5	3147	8543	1.59%	0.222%
23	7.988	1122	1132	1138	rBV3	9101	20582	3.83%	0.535%
24	8.110	1144	1152	1163	rBV3	16126	37675	7.01%	0.978%
25	8.507	1211	1217	1224	rVB3	6920	11843	2.20%	0.308%
26	8.647	1228	1240	1248	rBV	143215	237244	44.11%	6.162%
27	8.720	1248	1252	1259	rVB	6874	10572	1.97%	0.275%
28	8.842	1264	1272	1279	rBV	5170	9704	1.80%	0.252%
29	10.055	1460	1471	1478	rBV	400091	537796	100.00%	13.967%
30	10.146	1481	1486	1489	rVV4	4366	7104	1.32%	0.184%
31	10.195	1489	1494	1502	rVV	221449	287165	53.40%	7.458%
32	10.305	1505	1512	1519	rVB	15422	23958	4.45%	0.622%
33	10.646	1563	1568	1572	rBV2	4891	6555	1.22%	0.170%
34	10.963	1615	1620	1626	rVB	18994	23441	4.36%	0.609%
35	11.079	1634	1639	1649	rBV	271459	346415	64.41%	8.997%
36	11.305	1672	1676	1682	rVB	21639	26996	5.02%	0.701%

LSC Area Percent Report

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Acq On : 13 Dec 2022 17:26
Operator : JC/MD
Sample : N6001-13
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

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\82X120722W.M
Title : SW846 8260

37	11.616	1722	1727	1733	rVB	6790	7928	1.47%	0.206%
38	12.024	1788	1794	1801	rBV	402931	507389	94.35%	13.177%
39	12.244	1825	1830	1836	rBV	67124	82923	15.42%	2.154%
40	12.616	1887	1891	1894	rBV2	5231	6340	1.18%	0.165%
41	12.701	1900	1905	1913	rVB	11612	14341	2.67%	0.372%
42	13.292	1997	2002	2007	rBV2	12290	15039	2.80%	0.391%
43	13.774	2077	2081	2089	rBV	14725	19454	3.62%	0.505%

Sum of corrected areas: 3850424

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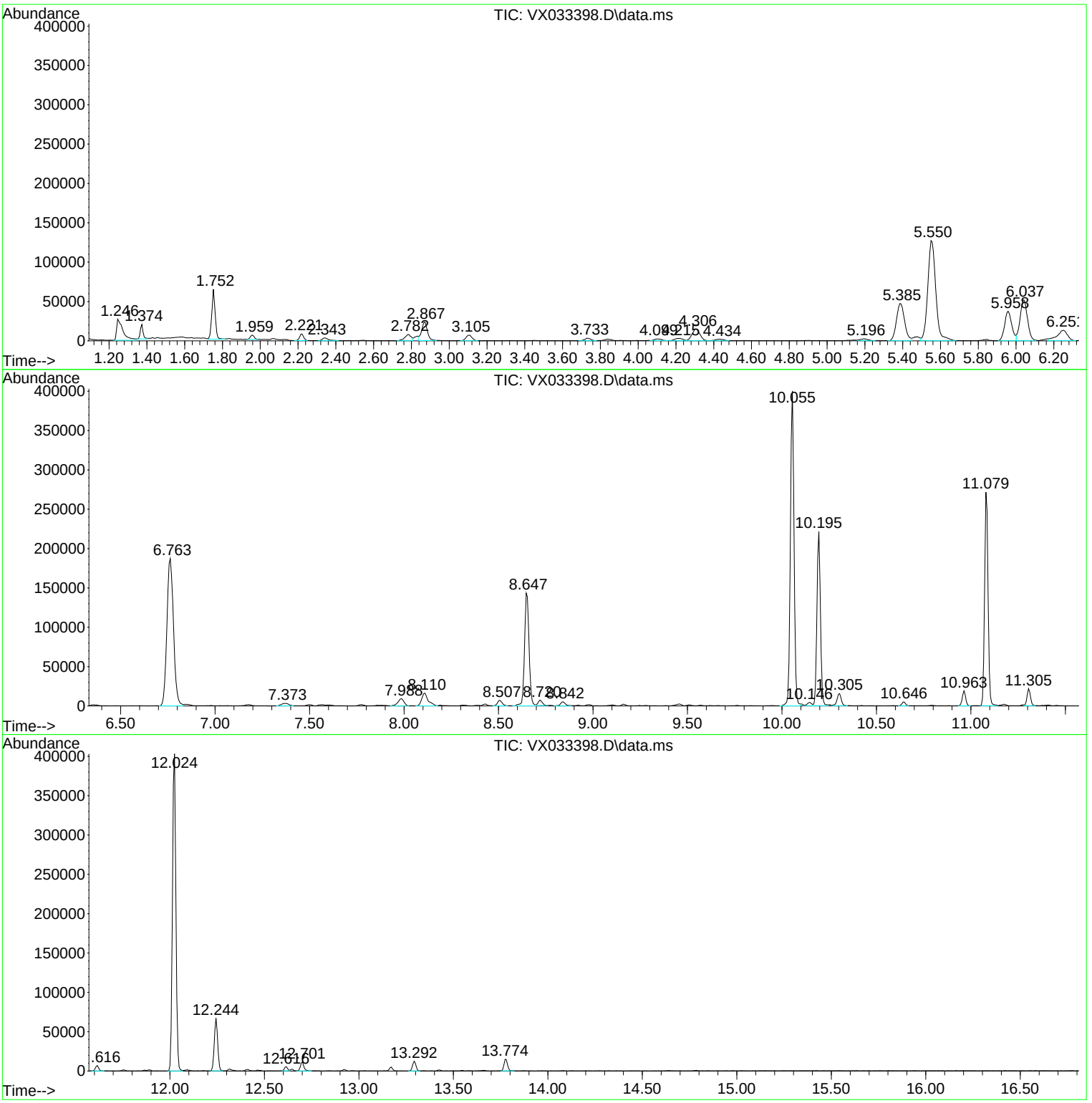
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121322\
Data File : VX033398.D
Acq On : 13 Dec 2022 17:26
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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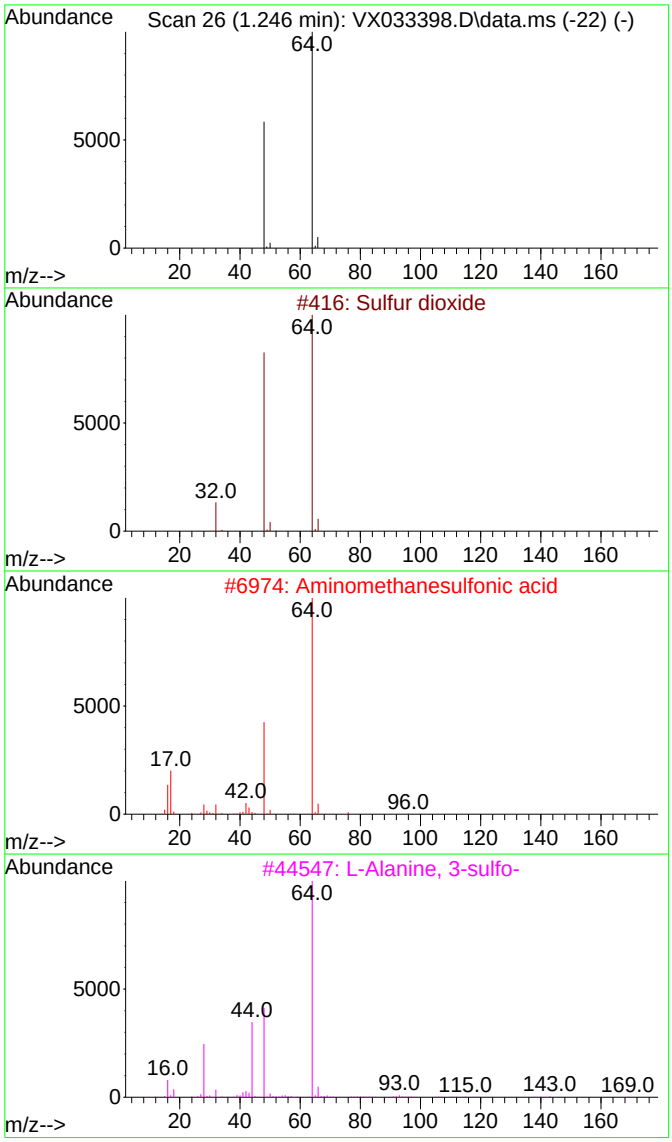
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

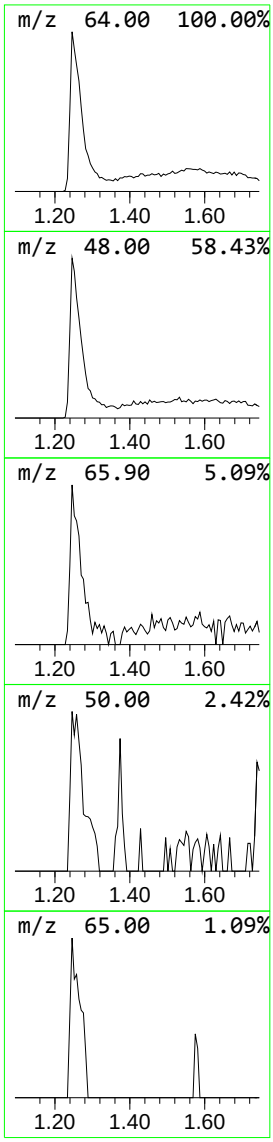
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	8.36 ug/l	62501	Pentafluorobenzene	5.550

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 : VX033398.D
Acq On : 13 Dec 2022 17:26
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

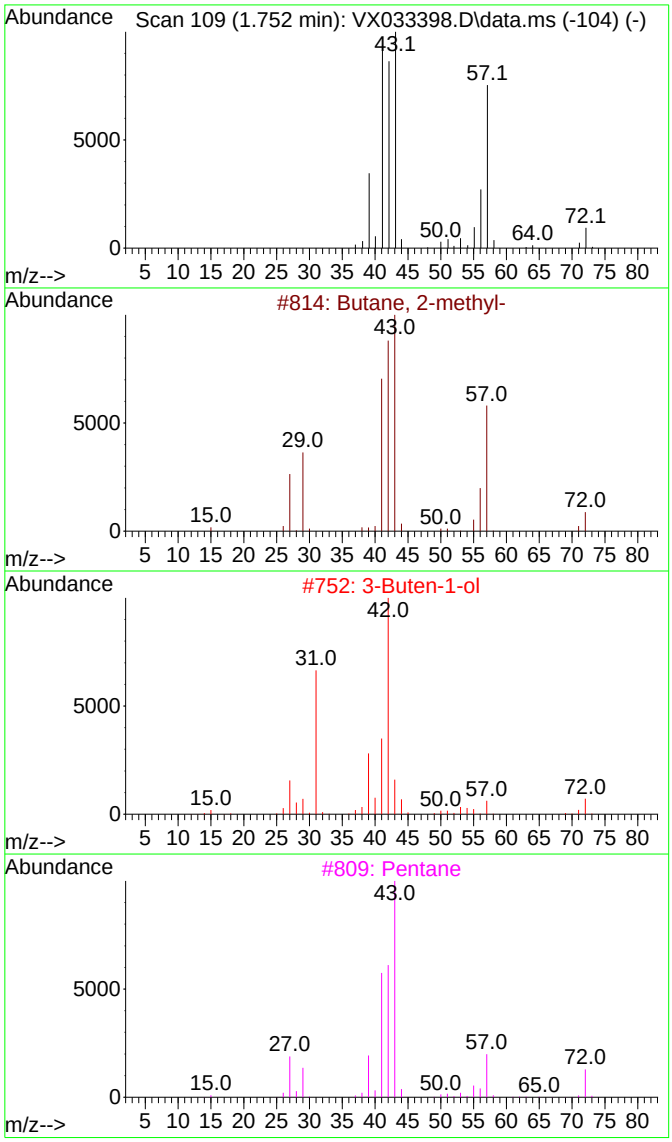
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

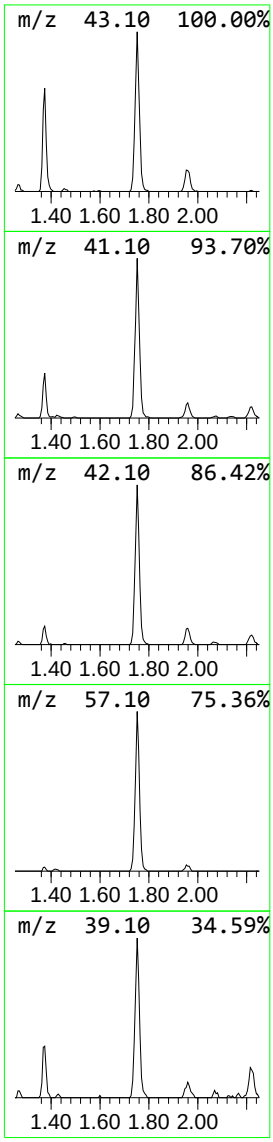
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	10.42 ug/l	77876	Pentafluorobenzene	5.550

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	43
3	Pentane	72	C5H12	000109-66-0	33
4	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	16
5	1-Propene, 2-methyl-	56	C4H8	000115-11-7	11





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121322\
Data File : VX033398.D
Acq On : 13 Dec 2022 17:26
Operator : JC/MD
Sample : N6001-13
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

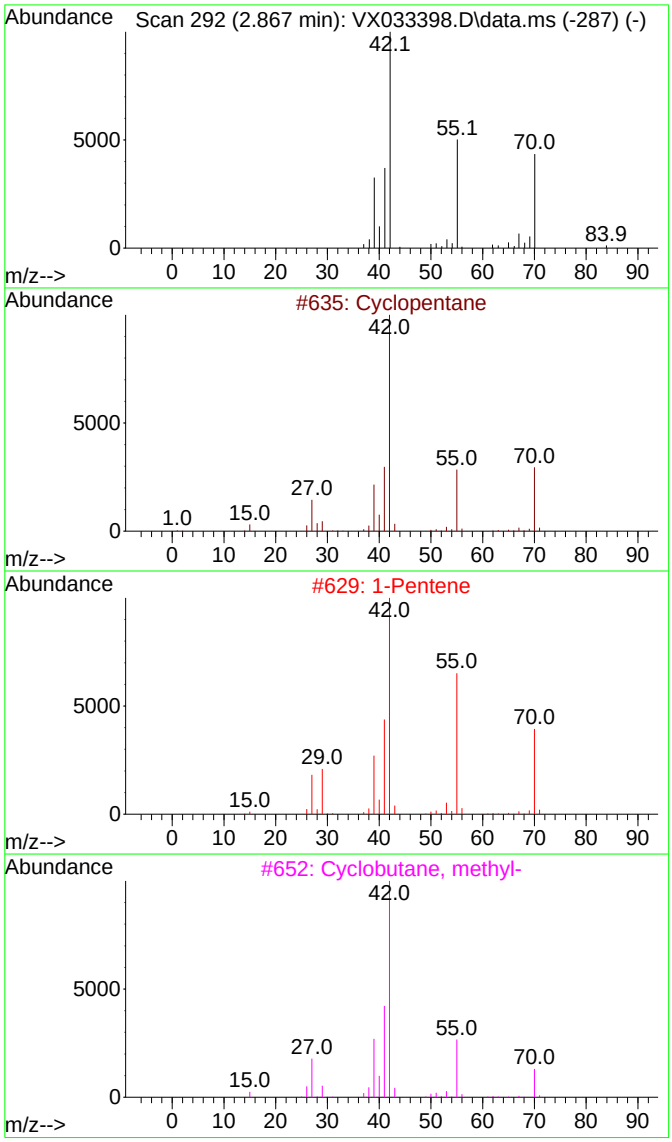
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

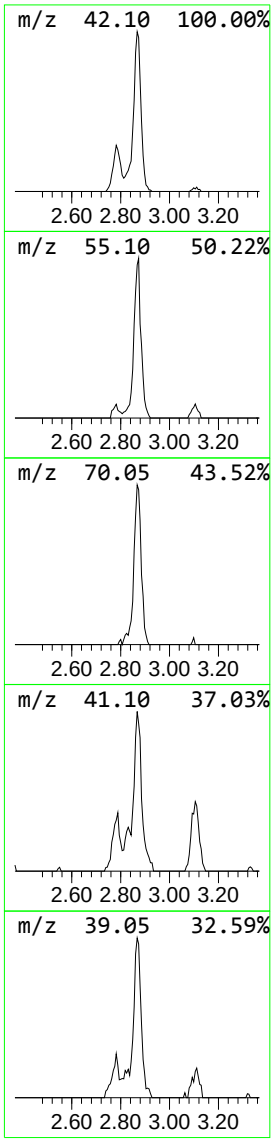
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Cyclopentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.867	6.64 ug/l	49624	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	86
2	1-Pentene	70	C5H10	000109-67-1	86
3	Cyclobutane, methyl-	70	C5H10	000598-61-8	86
4	2-Pentene, (Z)-	70	C5H10	000627-20-3	47
5	2-Pentene, (E)-	70	C5H10	000646-04-8	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121322\
Data File : VX033398.D
Acq On : 13 Dec 2022 17:26
Operator : JC/MD
Sample : N6001-13
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

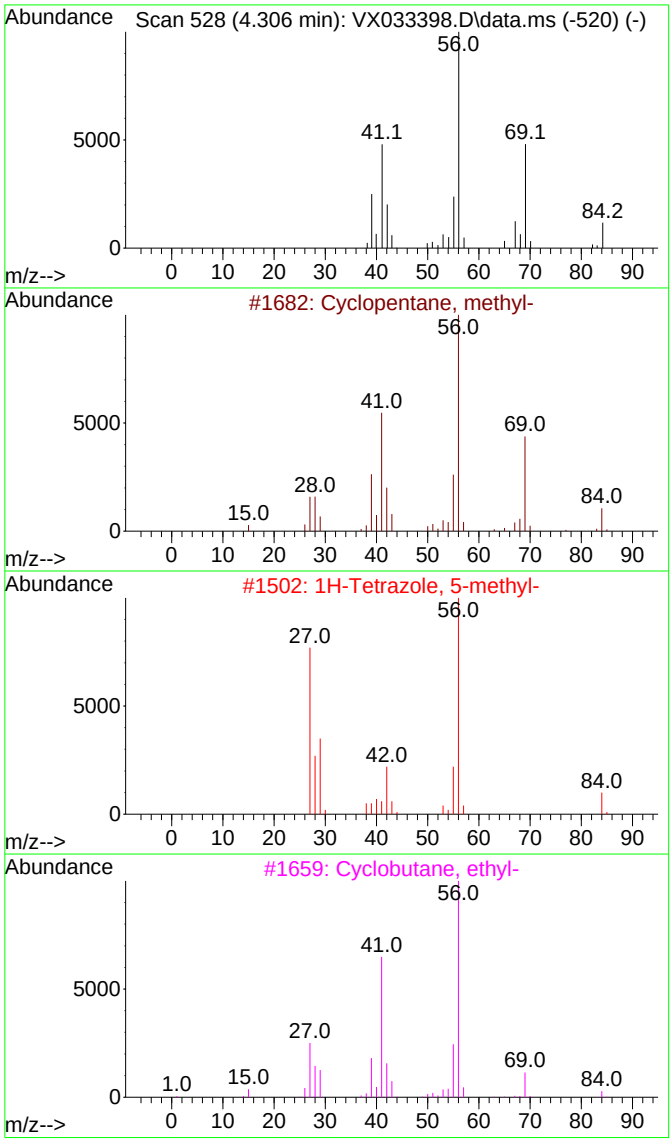
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

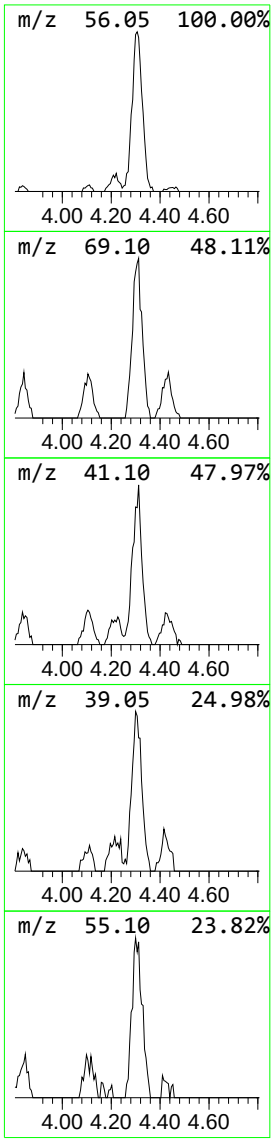
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopentane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	5.68 ug/l	42469	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	59
4	Cyclobutane, butyl-	112	C8H16	013152-44-8	42
5	2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121322\
Data File : VX033398.D
Acq On : 13 Dec 2022 17:26
Operator : JC/MD
Sample : N6001-13
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-12

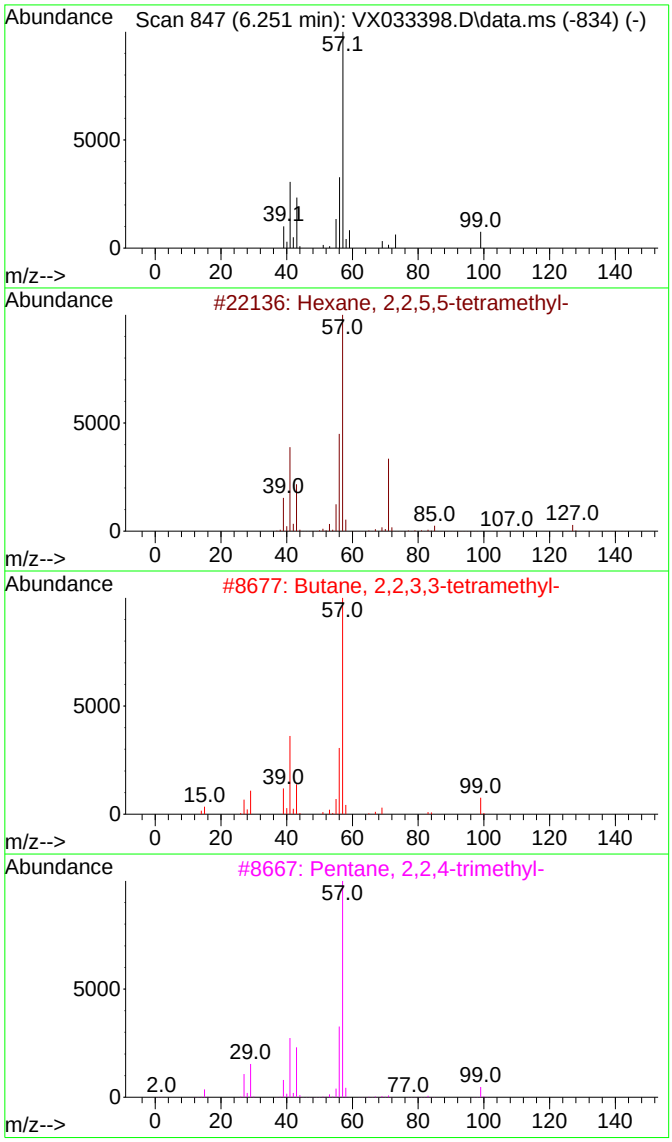
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

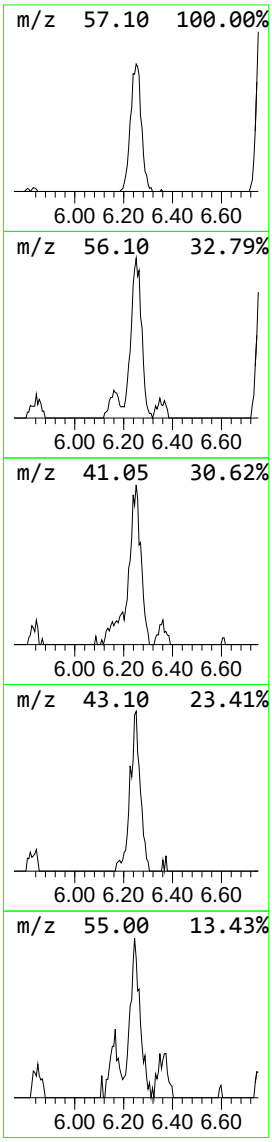
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Hexane, 2,2,5,5-tetramethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.251	5.53 ug/l	49788	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	53
2	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	50
3	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	50
4	Heptane, 3-bromo-	178	C7H15Br	001974-05-6	47
5	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	42





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Instrument :
MSVOA_X
ClientSampleId :
MW-12

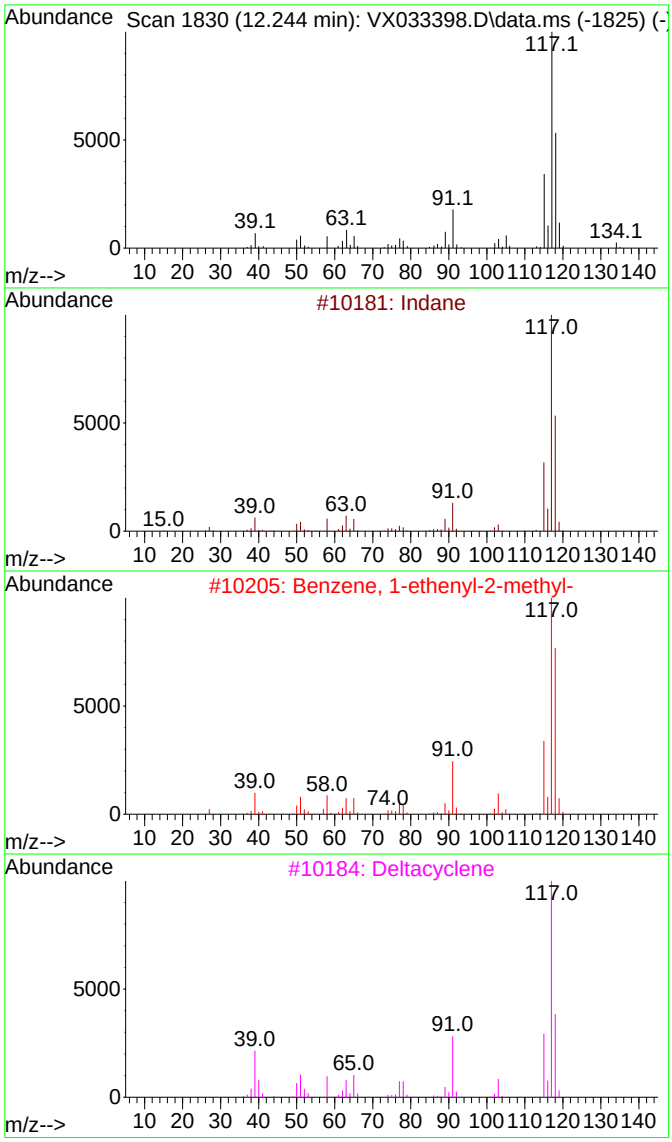
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.M
Quant Title : SW846 8260

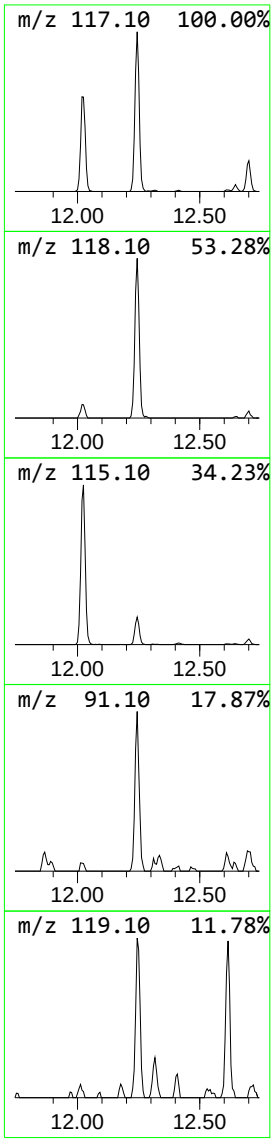
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	8.17 ug/l	82923	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	94
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	81
3	Deltacyclene	118	C9H10	007785-10-6	76
4	Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
5	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	72





Tentatively Identified Compound (LSC) summary

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Instrument :
MSVOA_X
ClientSampleId :
MW-12

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X120722W.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	8.4	ug/l	62501	1	5.550	373618	50.0
Butane, 2-methyl-	1.752	10.4	ug/l	77876	1	5.550	373618	50.0
Cyclopentane	2.867	6.6	ug/l	49624	1	5.550	373618	50.0
Cyclopentane, m...	4.306	5.7	ug/l	42469	1	5.550	373618	50.0
Hexane, 2,2,5,5...	6.251	5.5	ug/l	49788	2	6.763	449847	50.0
Indane	12.244	8.2	ug/l	82923	4	12.024	507389	50.0