LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062122\
Data File : VX029681.D
Acq On : 21 Jun 2022 22:46
Operator : JC/MD
Sample : N3286-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6D

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\82X061822W.M
Title : SW846 8260

Signal : TIC: VX029681.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	22	27	43	rBV2	219500	550828	43.35%	6.123%
2	1.368	43	46	51	rVV	86677	91477	7.20%	1.017%
3	1.752	104	109	119	rVB	65460	93674	7.37%	1.041%
4	2.130	165	171	179	rVB5	11540	31909	2.51%	0.355%
5	2.215	180	185	192	rVB	9608	15681	1.23%	0.174%
6	2.337	198	205	211	rBV2	17179	35400	2.79%	0.393%
7	2.782	263	278	287	rBV2	57757	144468	11.37%	1.606%
8	2.867	287	292	301	rVV2	21574	47313	3.72%	0.526%
9	2.959	301	307	320	rVB	10402	24487	1.93%	0.272%
10	3.111	322	332	344	rVB3	68585	174195	13.71%	1.936%
11	4.215	501	513	520	rBV4	5841	17433	1.37%	0.194%
12	4.306	520	528	537	rVB2	10611	29515	2.32%	0.328%
13	5.391	694	706	716	rBV	149455	423839	33.36%	4.711%
14	5.556	722	733	758	rVB	269716	808726	63.65%	8.989%
15	5.958	789	799	807	rBV	153154	406426	31.98%	4.517%
16	6.043	807	813	824	rVB2	49317	130832	10.30%	1.454%
17	6.239	835	845	857	rVB2	82114	258170	20.32%	2.870%
18	6.763	920	931	945	rBV	406985	972151	76.51%	10.806%
19	7.135	984	992	999	rBV2	9528	22031	1.73%	0.245%
20	7.988	1125	1132	1140	rVB	7534	15400	1.21%	0.171%
21	8.110	1144	1152	1155	rBV2	9671	19290	1.52%	0.214%
22	8.427	1199	1204	1211	rBV3	17836	30581	2.41%	0.340%
23	8.506	1211	1217	1225	rVV	28115	45732	3.60%	0.508%
24	8.653	1234	1241	1249	rBV	823507	1270680	100.00%	14.124%
25	8.842	1262	1272	1281	rVB	39451	66435	5.23%	0.738%
26	9.458	1365	1373	1380	rBV3	19133	34300	2.70%	0.381%
27	10.055	1466	1471	1477	rVV	826757	1081573	85.12%	12.022%
28	10.146	1483	1486	1490	rVB3	10493	14105	1.11%	0.157%
29	10.195	1490	1494	1499	rBV	30605	37484	2.95%	0.417%
30	10.305	1507	1512	1516	rVB	8322	12859	1.01%	0.143%
31	11.085	1634	1640	1650	rBV	630220	817744	64.35%	9.089%
32	12.024	1788	1794	1802	rBV	846599	1021456	80.39%	11.354%
33	12.244	1824	1830	1837	rBV	151819	184410	14.51%	2.050%
34	12.615	1885	1891	1894	rBV	15169	18780	1.48%	0.209%
35	12.701	1900	1905	1912	rVV	17491	23688	1.86%	0.263%
36	13.170	1978	1982	1990	rVB	18444	23634	1.86%	0.263%

LSC Area Percent Report

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Operator : JC/MD
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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6D

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\82X061822W.M
Title : SW846 8260

Sum of corrected areas: 8996706

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062122\
Data File : VX029681.D
Acq On : 21 Jun 2022 22:46
Operator : JC/MD
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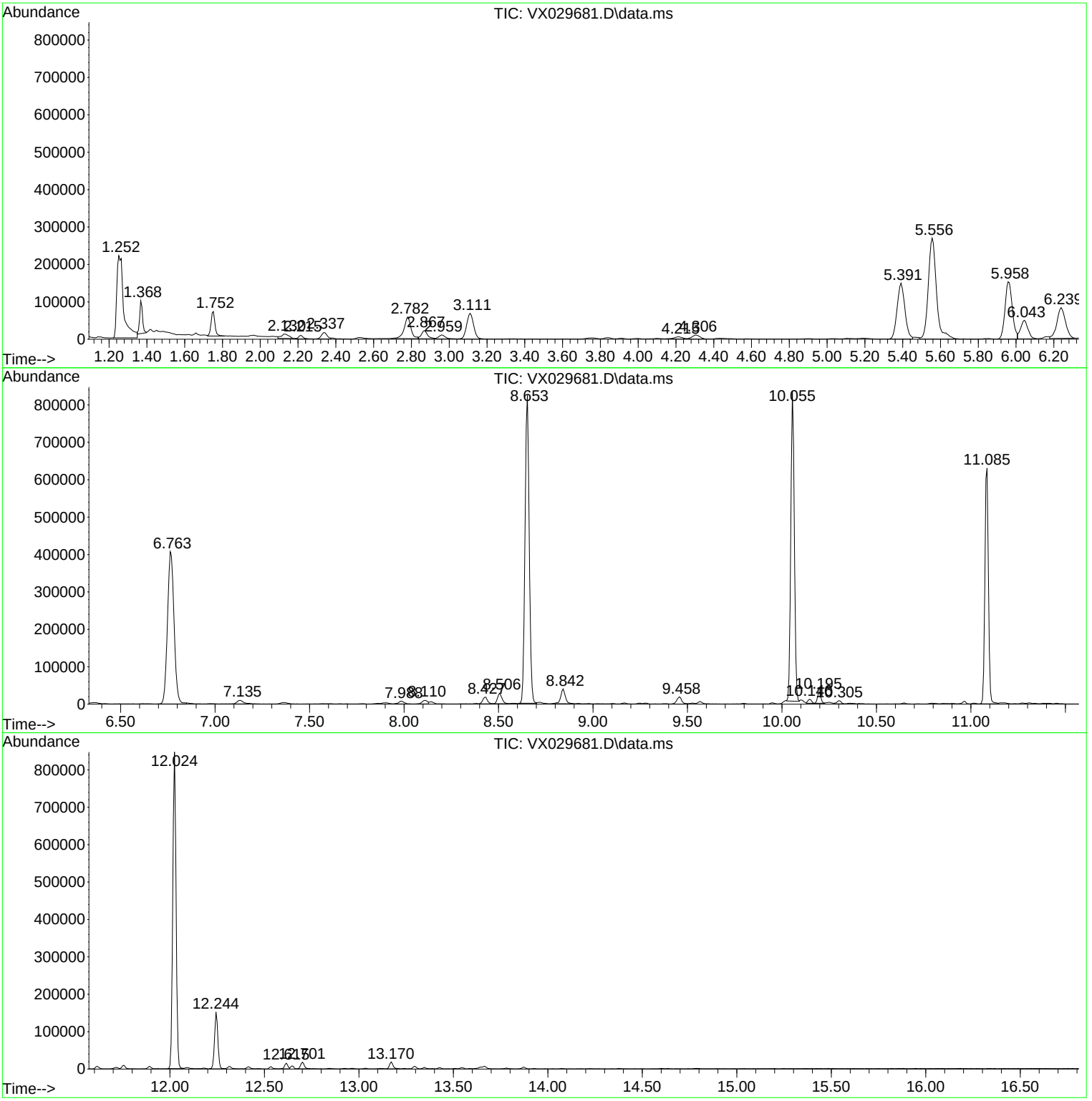
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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



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Data File : VX029681.D
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Operator : JC/MD
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MSVOA_X
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

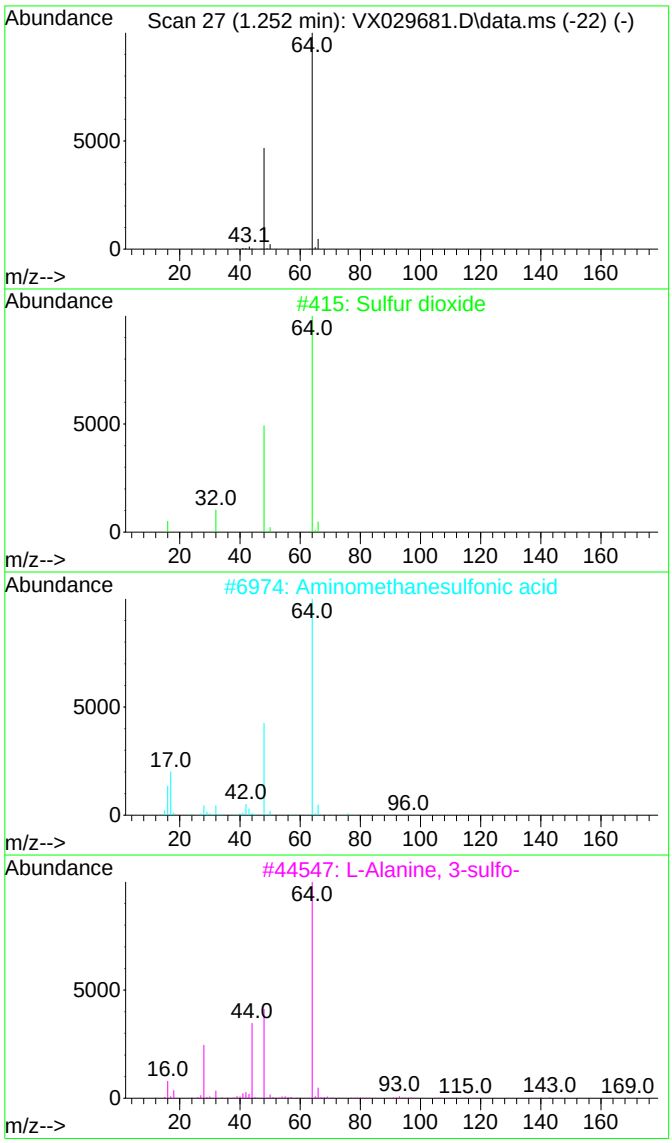
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

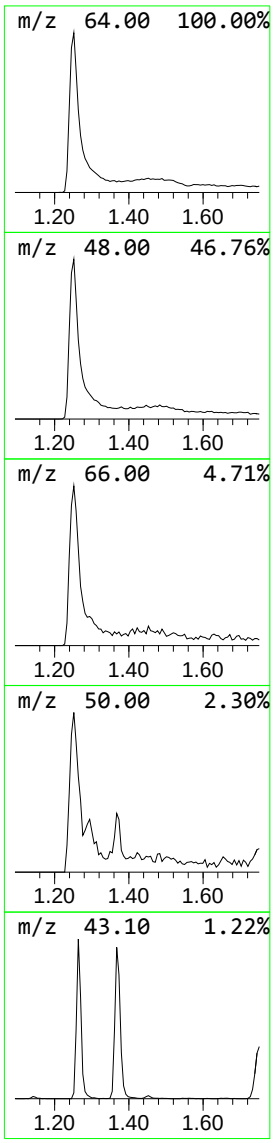
****

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.252	34.06 ug/l	550828	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	5
5	Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	4





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Data File : VX029681.D
Acq On : 21 Jun 2022 22:46
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

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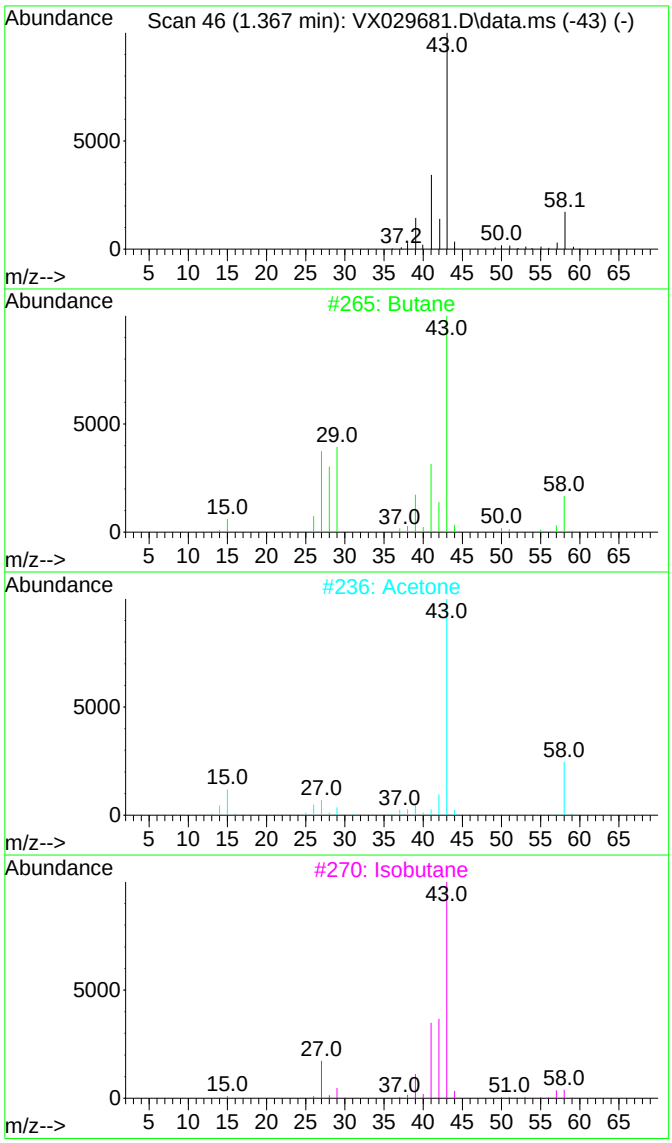
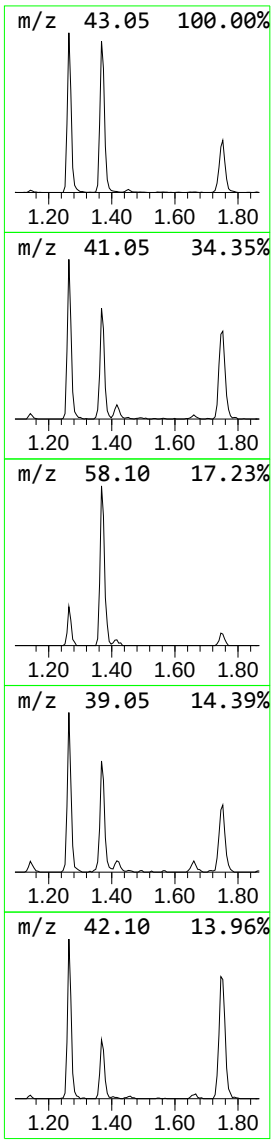
Peak Number 2 Butane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.367	5.66 ug/l	91477	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	80
2	Acetone	58	C3H6O	000067-64-1	9
3	Isobutane	58	C4H10	000075-28-5	9
4	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX062122\
Data File : VX029681.D
Acq On : 21 Jun 2022 22:46
Operator : JC/MD
Sample : N3286-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

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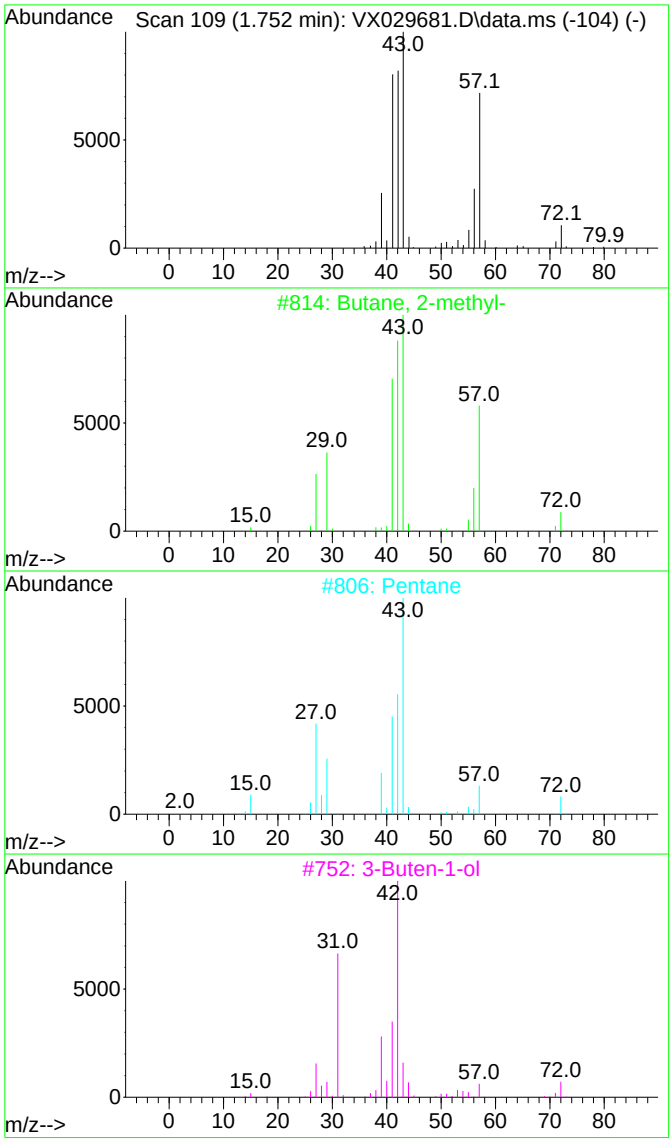
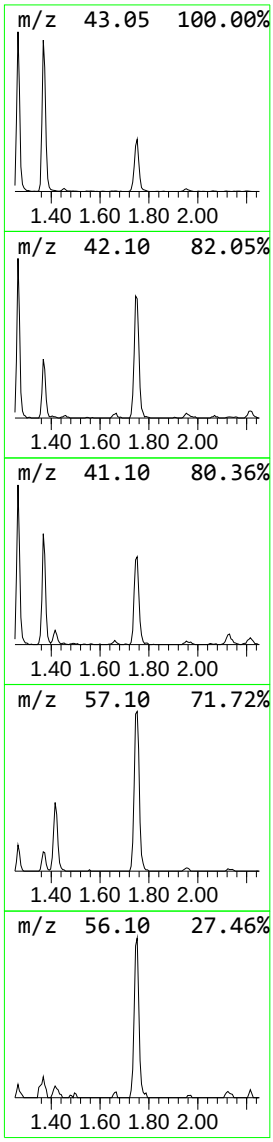
Peak Number 3 Butane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.752	5.79 ug/l	93674	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	87
2	Pentane	72	C5H12	000109-66-0	45
3	3-Buten-1-ol	72	C4H8O	000627-27-0	38
4	Oxirane, trimethyl-	86	C5H10O	005076-19-7	36
5	1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	33





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Data File : VX029681.D
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6D

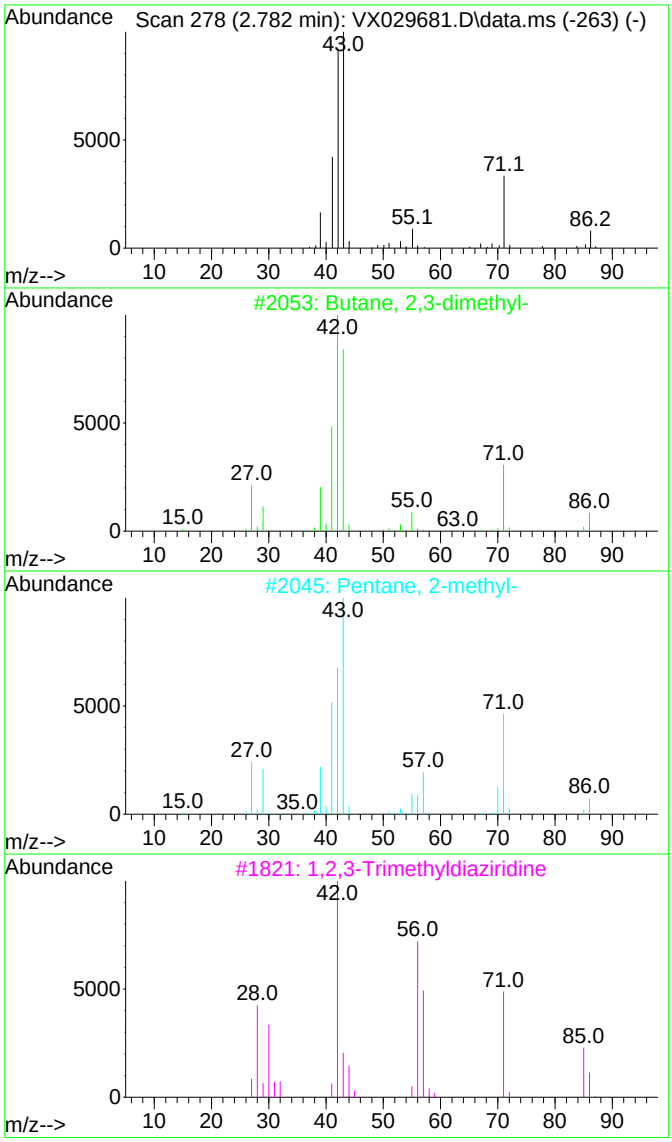
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

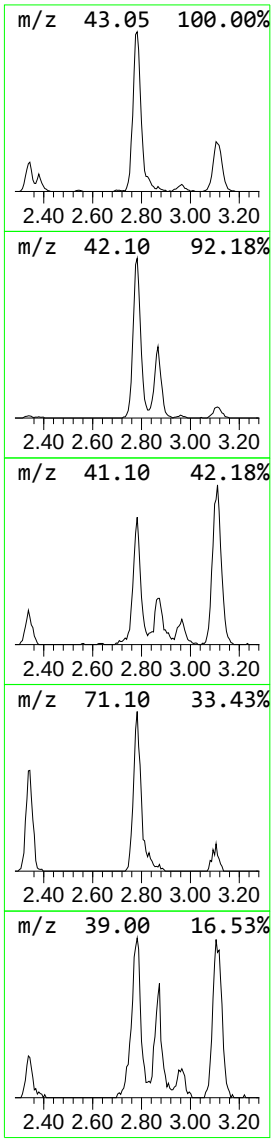
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.782	8.93 ug/l	144468	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	47
3	1,2,3-Trimethyldiaziridine	86	C4H10N2	113604-56-1	38
4	Pyrrolidine	71	C4H9N	000123-75-1	22
5	Butanal, 2,2-dimethyl-	100	C6H12O	002094-75-9	10





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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

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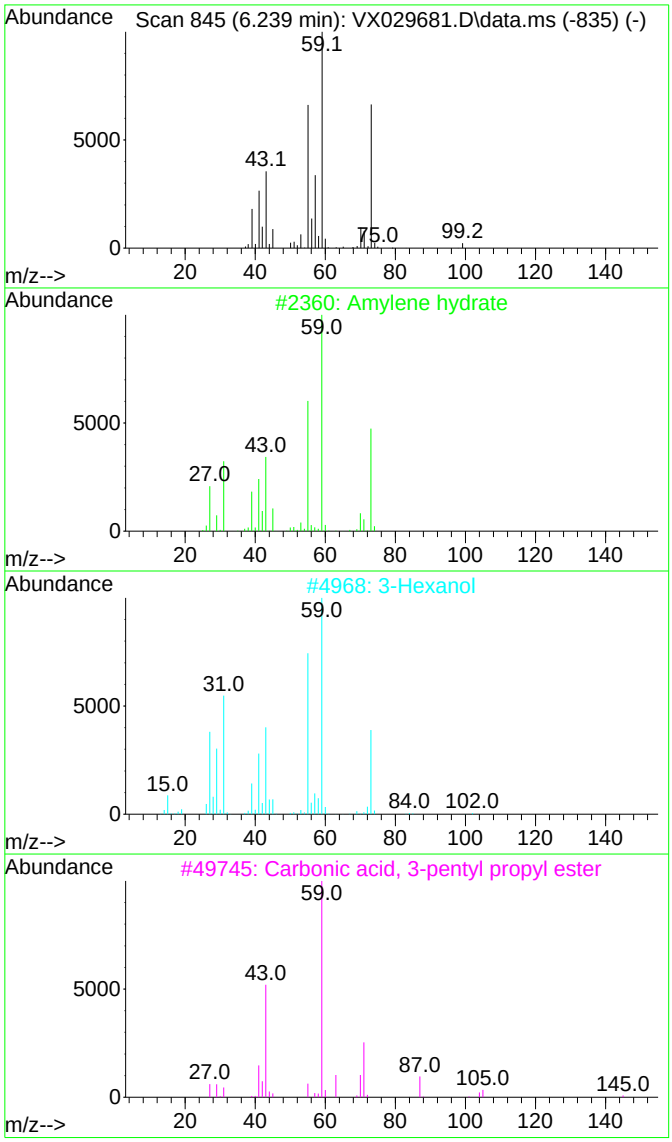
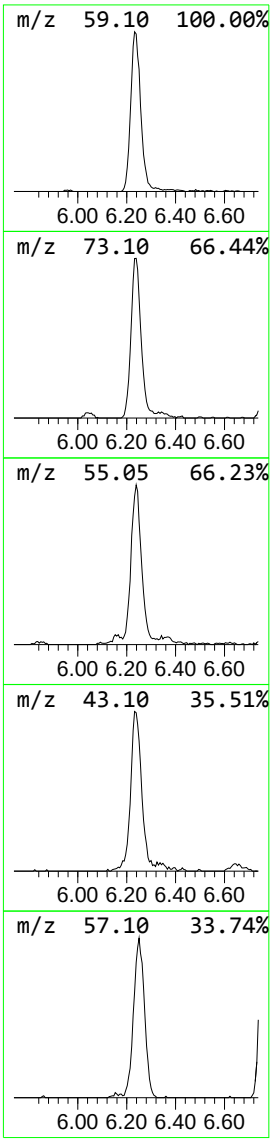
Peak Number 5 Amylene hydrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.239	13.28 ug/l	258170	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Amylene hydrate	88	C5H12O	000075-85-4	56
2	3-Hexanol	102	C6H14O	000623-37-0	40
3	Carbonic acid, 3-pentyl propyl e...	174	C9H18O3	1000325-64-0	38
4	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	38
5	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	38





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ALS Vial : 26 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.M
Quant Title : SW846 8260

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

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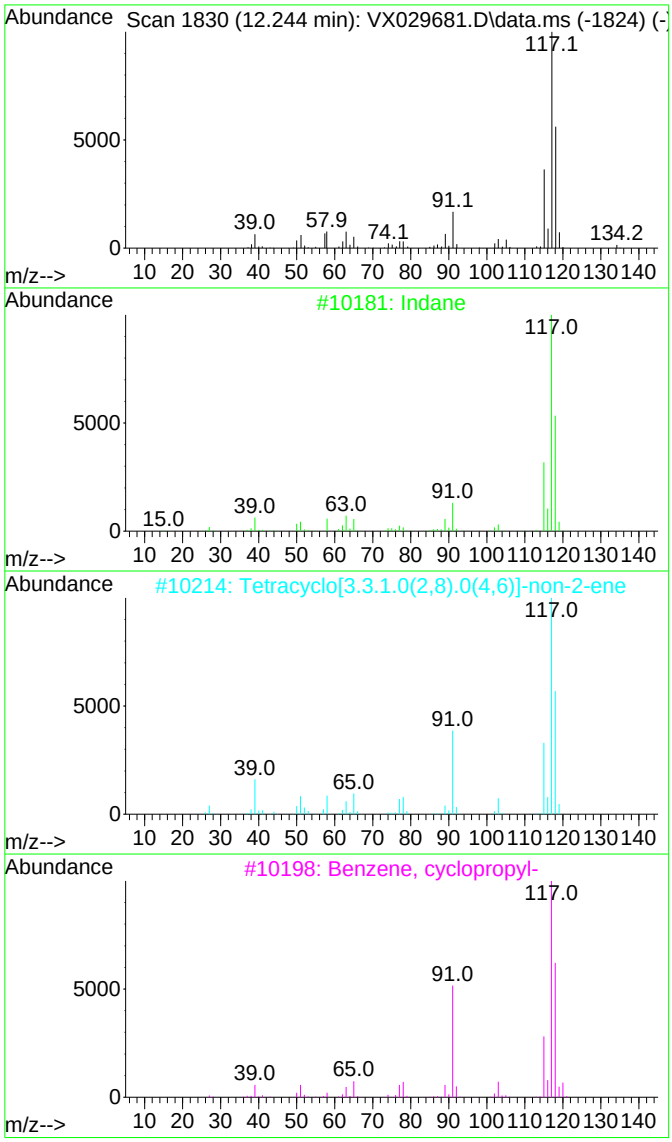
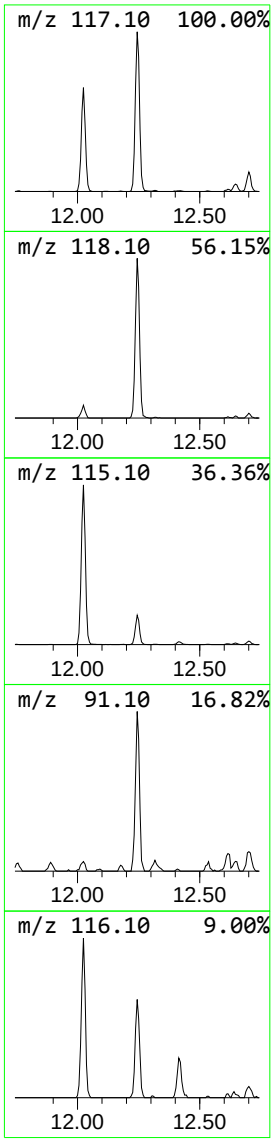
Peak Number 6 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	9.03 ug/l	184410	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	94
2	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	87
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	87
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	83
5	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	81





Tentatively Identified Compound (LSC) summary

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MSVOA_X
ClientSampleId :
MW-6D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X061822W.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	1.252	34.1	ug/l	550828	1	5.556	808726	50.0
Butane	1.367	5.7	ug/l	91477	1	5.556	808726	50.0
Butane, 2-methyl-	1.752	5.8	ug/l	93674	1	5.556	808726	50.0
Butane, 2,3-dim...	2.782	8.9	ug/l	144468	1	5.556	808726	50.0
Amylene hydrate	6.239	13.3	ug/l	258170	2	6.763	972151	50.0
Indane	12.244	9.0	ug/l	184410	4	12.024	1021460	50.0