LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX092818\
Data File : VX004832.D
Acq On : 28 Sep 2018 20:06
Operator : JC/MD
Sample : J5130-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FA18-JBW-7338B

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\82X092618W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.318	18	27	35	rBV2	24879	109359	7.57%	0.912%
2	1.404	37	41	46	rVV	208705	217448	15.05%	1.814%
3	1.788	99	104	120	rVB	991146	1397209	96.72%	11.654%
4	2.001	134	139	153	rVB2	60455	106112	7.35%	0.885%
5	2.617	233	240	250	rBV	83877	154731	10.71%	1.291%
6	2.843	269	277	283	rBV	204253	468798	32.45%	3.910%
7	3.019	301	306	314	rVB2	12239	25906	1.79%	0.216%
8	3.166	323	330	342	rVB	60938	144753	10.02%	1.207%
9	4.300	504	516	524	rBV2	44568	136712	9.46%	1.140%
10	4.397	524	532	543	rVB	41427	123316	8.54%	1.029%
11	4.556	546	558	561	rBV4	6993	21178	1.47%	0.177%
12	4.757	582	591	602	rBV2	5325	18724	1.30%	0.156%
13	5.501	700	713	721	rBV	181593	526991	36.48%	4.396%
14	5.574	721	725	731	rVV2	49501	134178	9.29%	1.119%
15	5.665	731	740	766	rVB	221919	818314	56.65%	6.826%
16	5.940	777	785	796	rVB3	9676	33789	2.34%	0.282%
17	6.068	796	806	815	rVV	191572	504370	34.92%	4.207%
18	6.147	815	819	829	rVV2	14522	34822	2.41%	0.290%
19	6.263	829	838	842	rVV3	12533	37270	2.58%	0.311%
20	6.348	842	852	862	rVV	107628	334683	23.17%	2.792%
21	6.452	862	869	880	rVB3	9557	29290	2.03%	0.244%
22	6.860	926	936	958	rBV	367500	920742	63.74%	7.680%
23	7.458	1023	1034	1045	rBV2	39260	99294	6.87%	0.828%
24	8.055	1123	1132	1144	rVB	52870	111939	7.75%	0.934%
25	8.177	1144	1152	1162	rBV	104064	208097	14.41%	1.736%
26	8.713	1234	1240	1249	rBV	886466	1444535	100.00%	12.049%
27	8.787	1249	1252	1257	rVV	23768	38165	2.64%	0.318%
28	8.835	1257	1260	1266	rVB	12348	20077	1.39%	0.167%
29	9.043	1288	1294	1301	rVB	14322	25673	1.78%	0.214%
30	10.116	1459	1470	1478	rBV	804059	1124965	77.88%	9.383%
31	10.183	1479	1481	1487	rVV3	9342	15910	1.10%	0.133%
32	10.256	1487	1493	1501	rVV	68746	99400	6.88%	0.829%
33	10.359	1501	1510	1515	rVB2	9894	21095	1.46%	0.176%
34	11.018	1613	1618	1624	rBV2	13299	17258	1.19%	0.144%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX092818\
Data File : VX004832.D
Acq On : 28 Sep 2018 20:06
Operator : JC/MD
Sample : J5130-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FA18-JBW-7338B

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\82X092618W.M
Title : SW846 8260

35	11.140	1632	1638	1653	rBV	835386	1047241	72.50%	8.735%
36	11.670	1717	1725	1733	rBV	12431	17895	1.24%	0.149%
37	12.079	1786	1792	1799	rBV	1037774	1256297	86.97%	10.479%
38	12.140	1799	1802	1807	rVB	10725	14684	1.02%	0.122%
39	12.298	1821	1828	1836	rBV2	32533	54475	3.77%	0.454%
40	12.518	1859	1864	1871	rVB	12367	16214	1.12%	0.135%
41	12.755	1898	1903	1911	rVB2	21690	34662	2.40%	0.289%
42	13.353	1996	2001	2005	rBV	17170	22272	1.54%	0.186%

Sum of corrected areas: 11988843

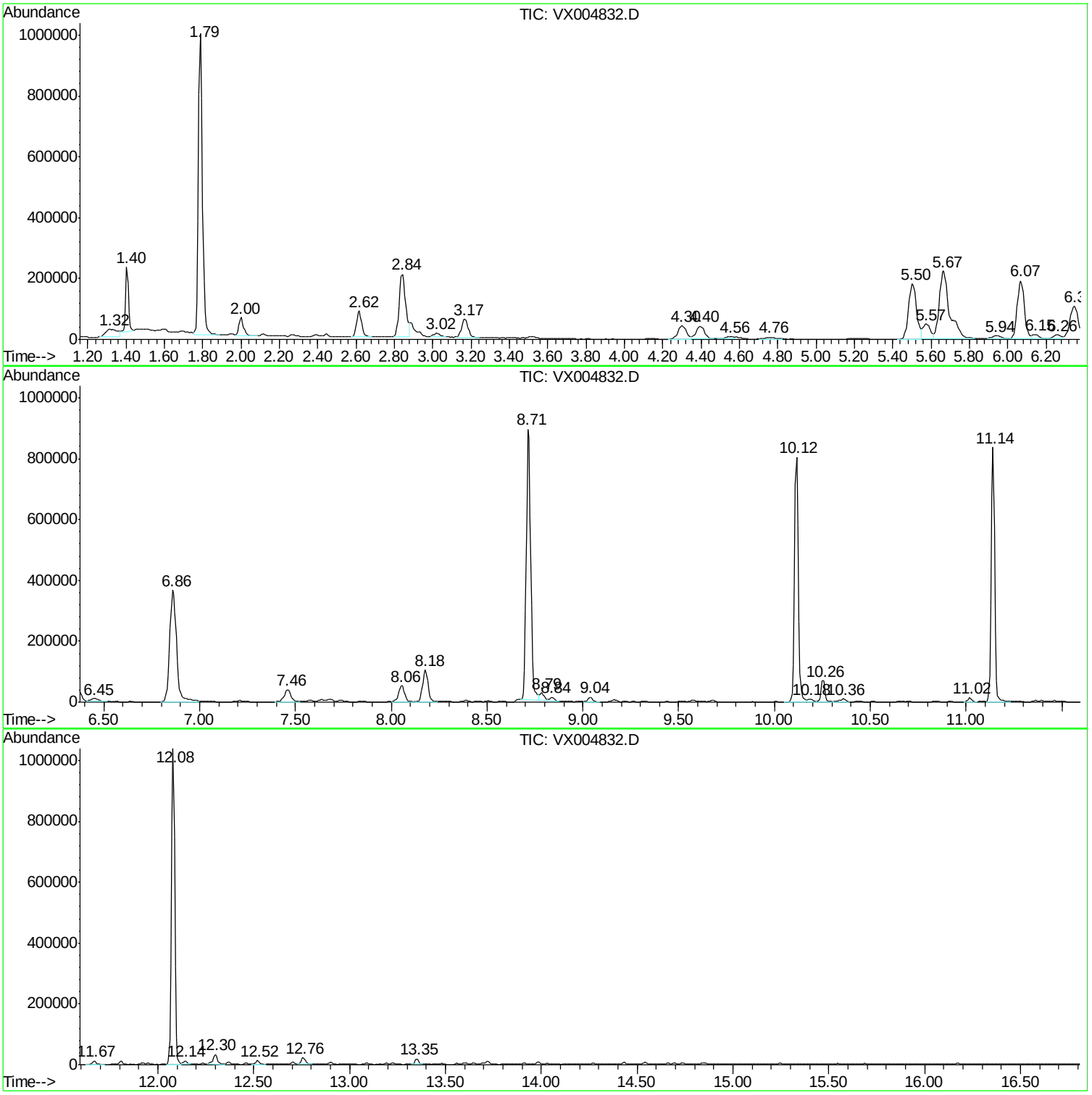
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX092818\
Data File : VX004832.D
Acq On : 28 Sep 2018 20:06
Operator : JC/MD
Sample : J5130-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FA18-JBW-7338B

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX092818\
Data File : VX004832.D
Acq On : 28 Sep 2018 20:06
Operator : JC/MD
Sample : J5130-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FA18-JBW-7338B

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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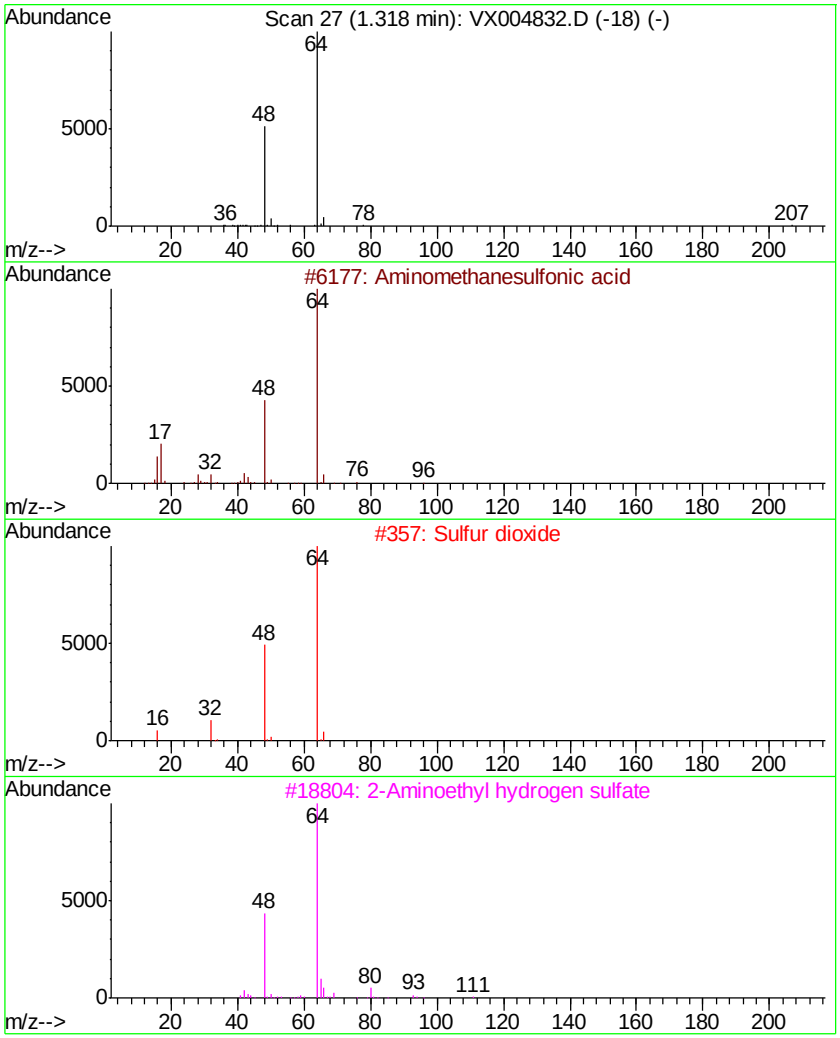
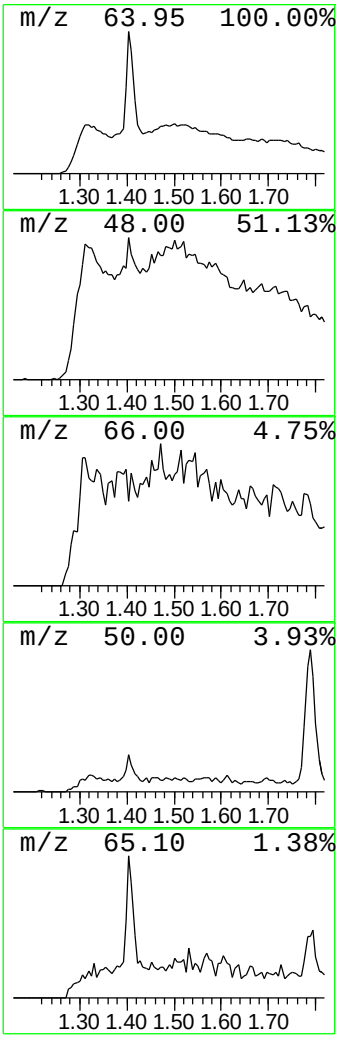
Peak Number 1 Aminomethanesulfonic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.32	6.68 ug/l	109359	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	83
2	Sulfur dioxide	64	O2S	007446-09-5	83
3	2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	74
4	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5	2,4,6-Triamino-5-pyrimidinyl hyd...	221	C4H7N5O4S	071552-23-3	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX092818\
Data File : VX004832.D
Acq On : 28 Sep 2018 20:06
Operator : JC/MD
Sample : J5130-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FA18-JBW-7338B

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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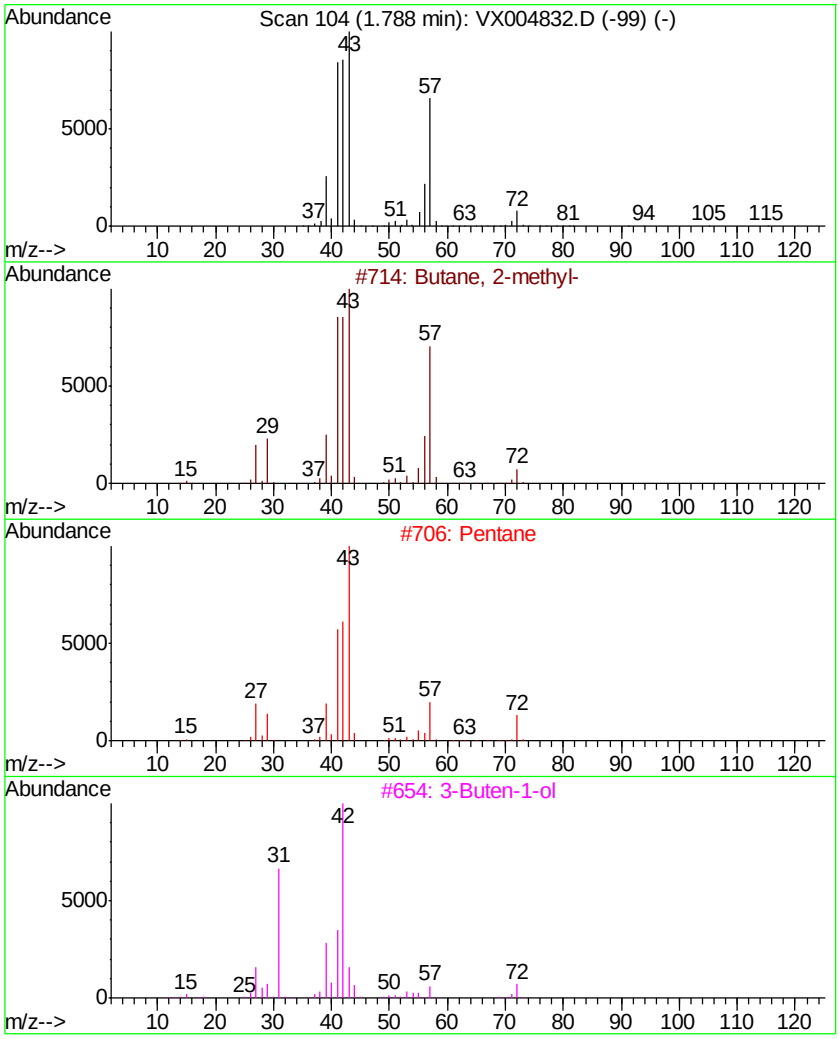
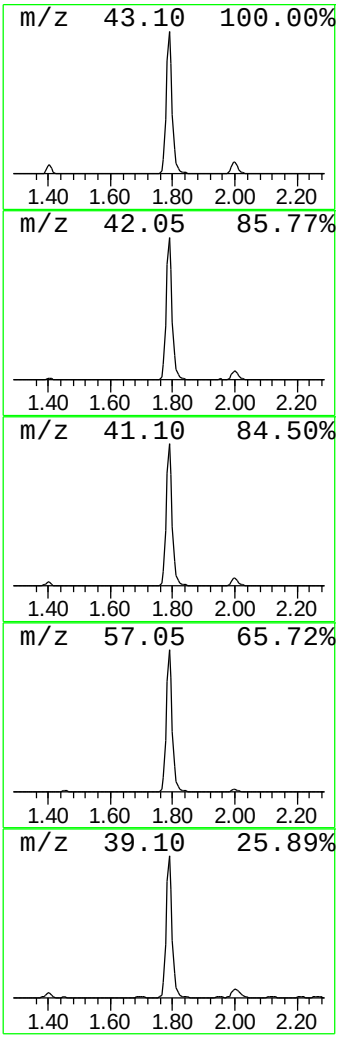
Peak Number 2 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	85.37 ug/l	1397210	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	94
2	Pentane	72	C5H12	000109-66-0	45
3	3-Buten-1-ol	72	C4H8O	000627-27-0	28
4	1-Butene	56	C4H8	000106-98-9	10
5	1-Propene, 2-methyl-	56	C4H8	000115-11-7	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX092818\
Data File : VX004832.D
Acq On : 28 Sep 2018 20:06
Operator : JC/MD
Sample : J5130-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FA18-JBW-7338B

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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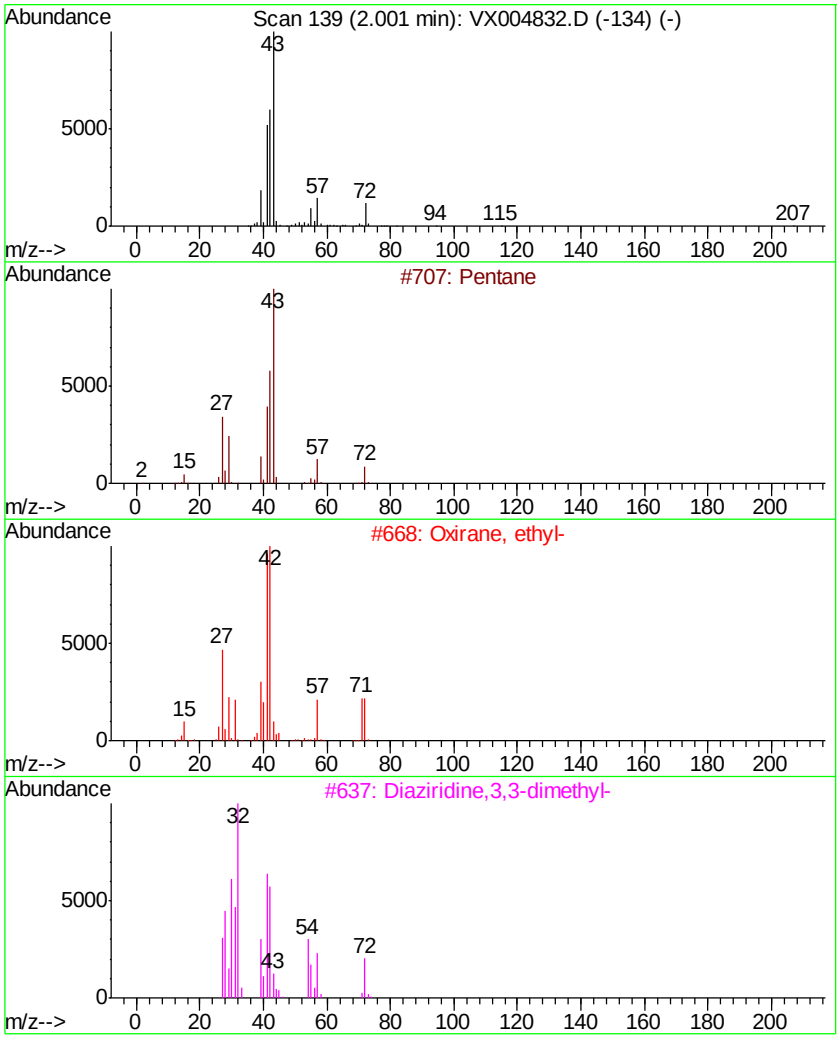
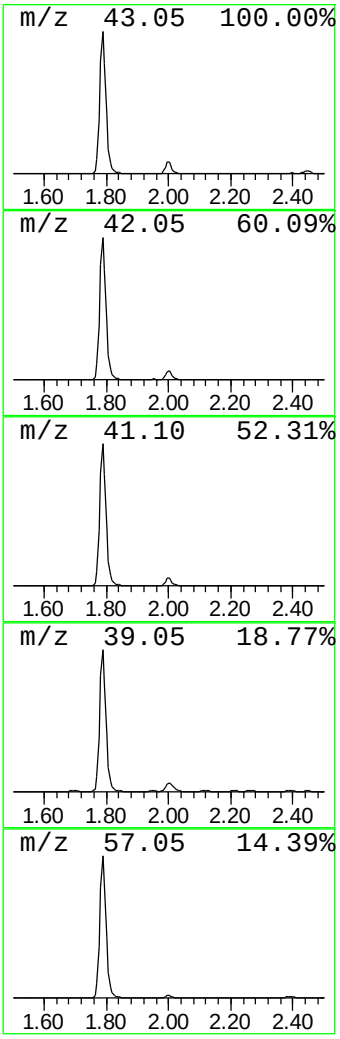
Peak Number 3 Pentane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.00	6.48 ug/l	106112	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	86
2	Oxirane, ethyl-	72	C4H8O	000106-88-7	42
3	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	35
4	Butane, 2-methyl-	72	C5H12	000078-78-4	33
5	Isobutylene epoxide	72	C4H8O	000558-30-5	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX092818\
Data File : VX004832.D
Acq On : 28 Sep 2018 20:06
Operator : JC/MD
Sample : J5130-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FA18-JBW-7338B

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

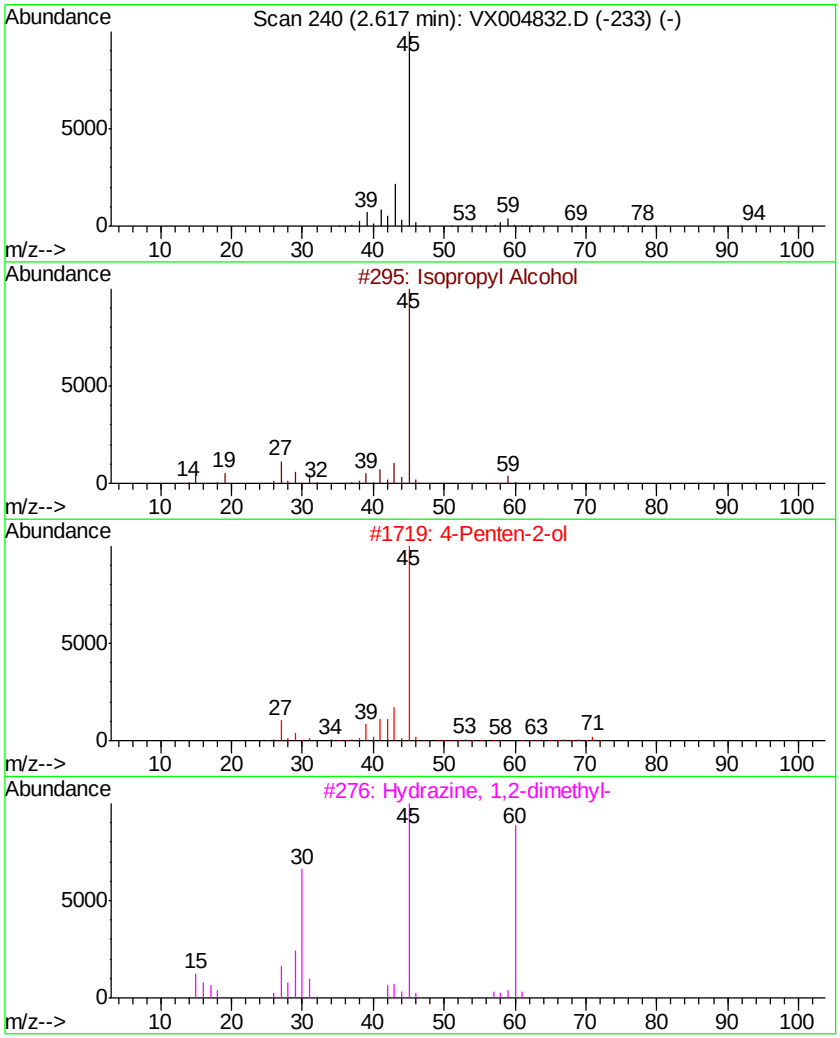
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

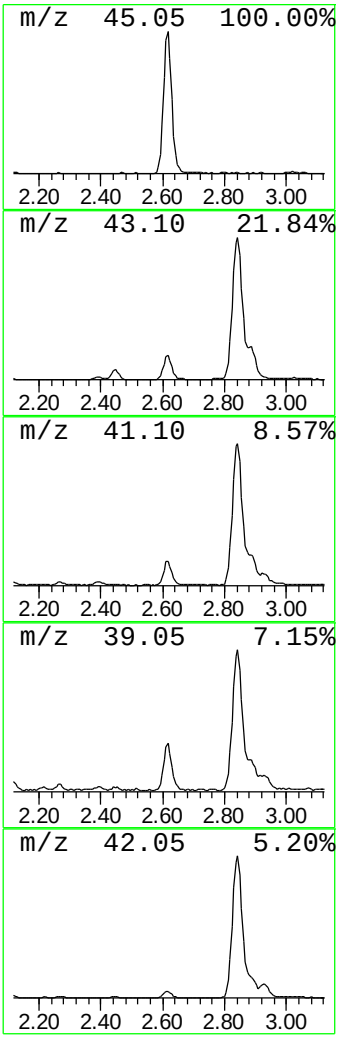
****

Peak Number 4 Isopropyl Alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.62	9.45 ug/l	154731	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	86
2	4-Penten-2-ol	86	C5H10O	000625-31-0	9
3	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4	Hydrazine, ethyl-	60	C2H8N2	000624-80-6	4
5	1-Butene, 4-methoxy	86	C5H10O	004696-30-4	4





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX092818\
Data File : VX004832.D
Acq On : 28 Sep 2018 20:06
Operator : JC/MD
Sample : J5130-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FA18-JBW-7338B

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

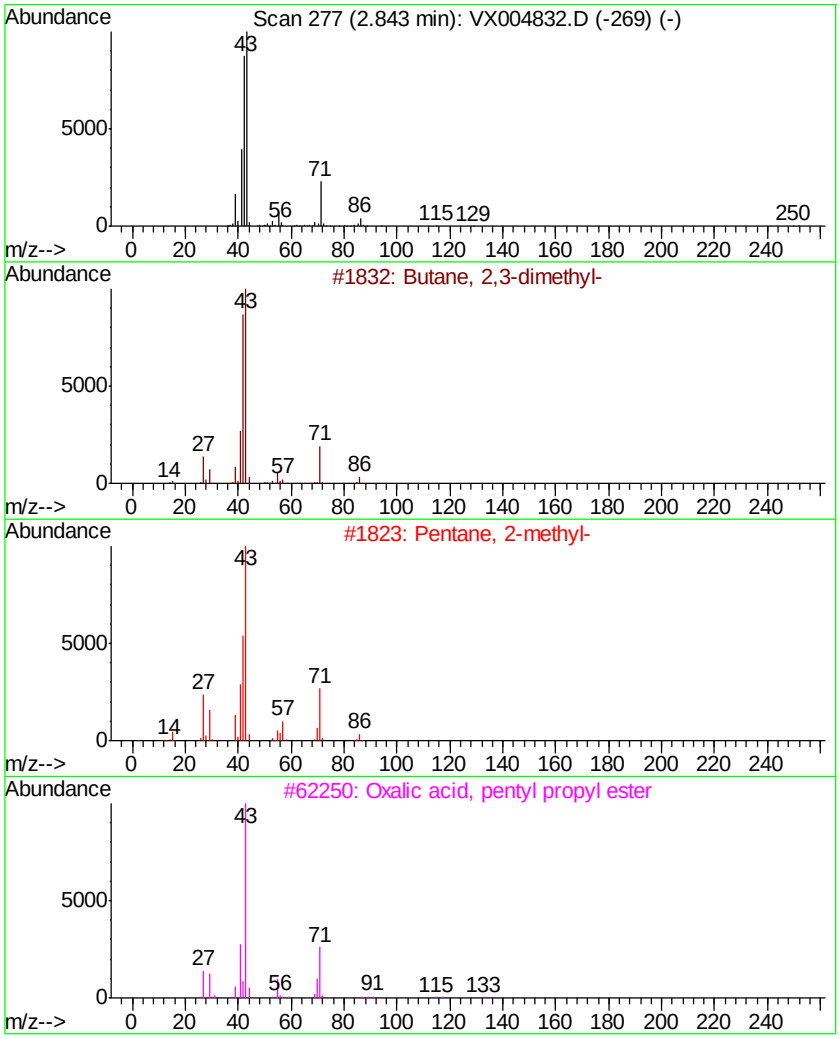
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

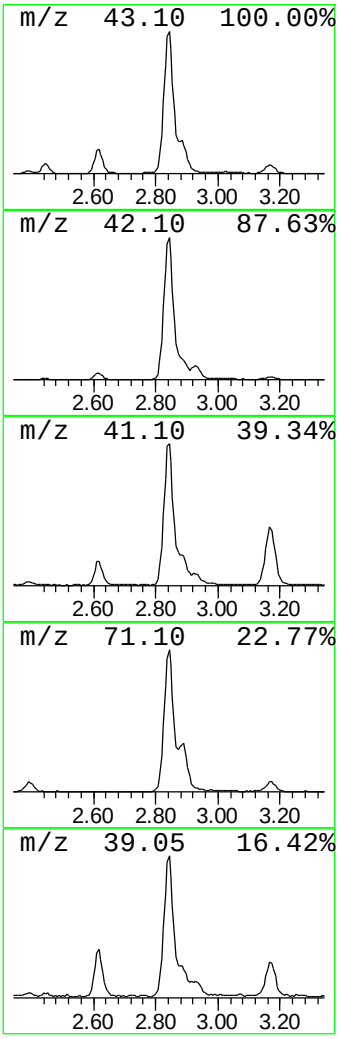
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	28.64 ug/l	468798	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	90
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	32
3	Oxalic acid, pentyl propyl ester	202	C10H18O4	1000309-25-7	12
4	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	9
5	Pyrrolidine	71	C4H9N	000123-75-1	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX092818\
Data File : VX004832.D
Acq On : 28 Sep 2018 20:06
Operator : JC/MD
Sample : J5130-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FA18-JBW-7338B

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

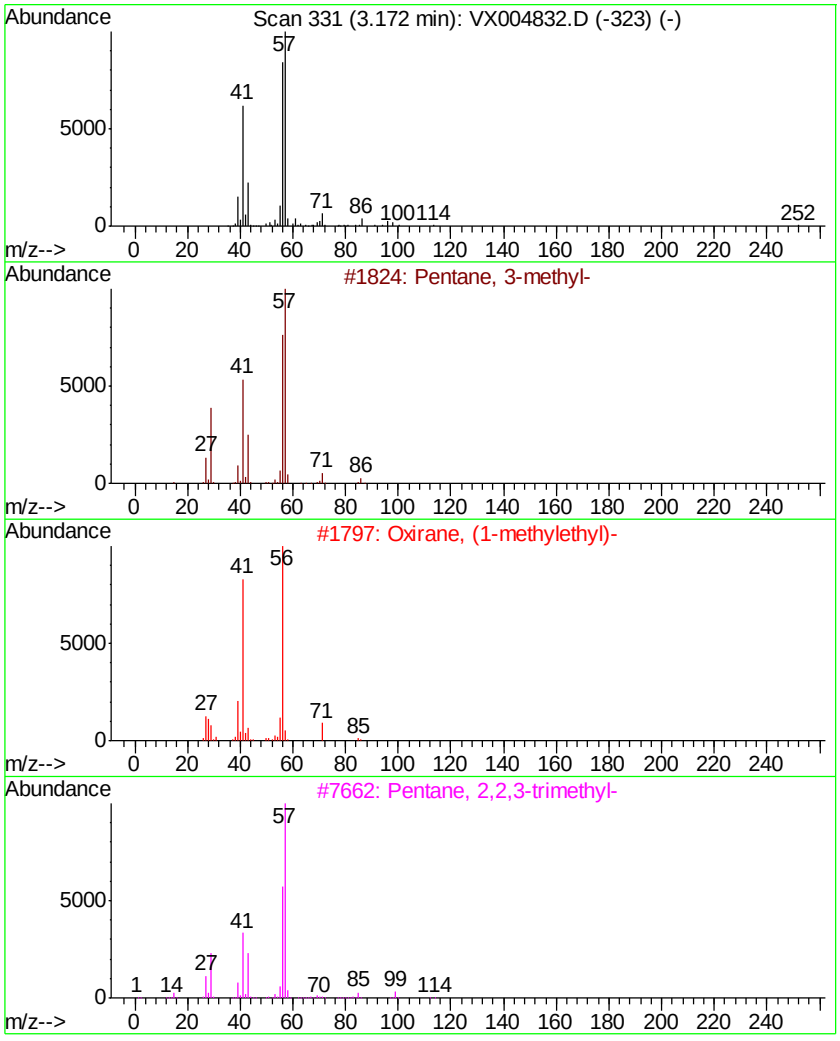
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

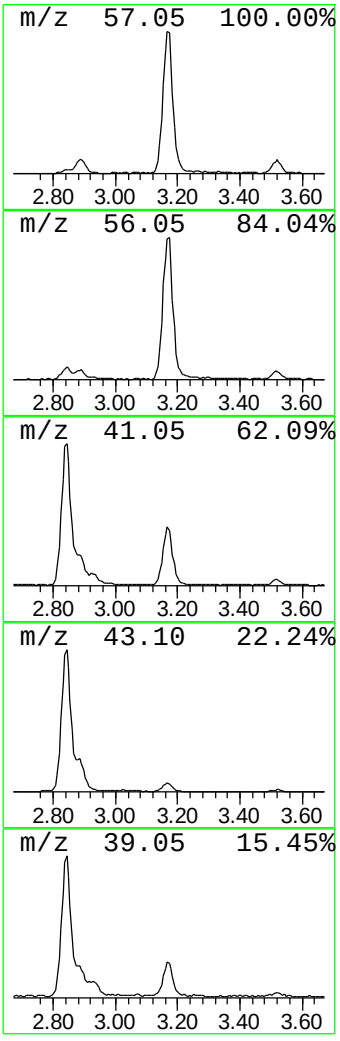
****

Peak Number 6 Pentane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	8.84 ug/l	144753	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	90
2	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	53
3	Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	50
4	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	40
5	Acetamide, N-2-propenyl-	99	C5H9NO	000692-33-1	39





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX092818\
Data File : VX004832.D
Acq On : 28 Sep 2018 20:06
Operator : JC/MD
Sample : J5130-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FA18-JBW-7338B

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

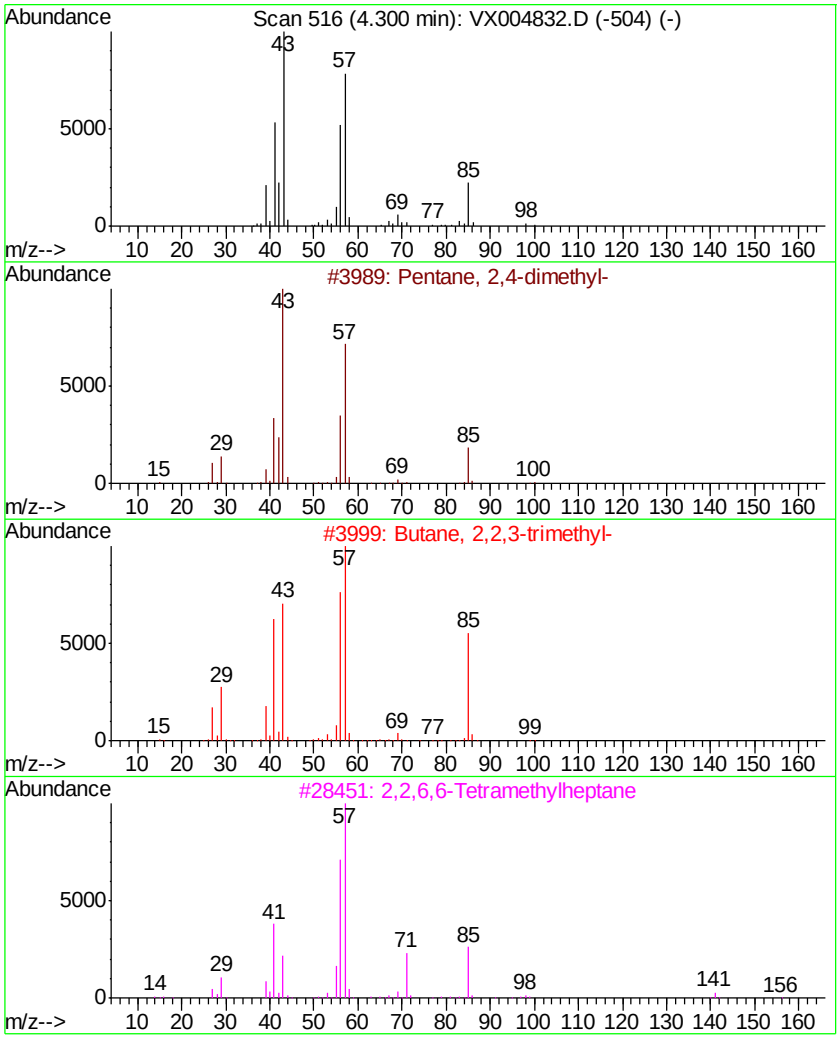
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

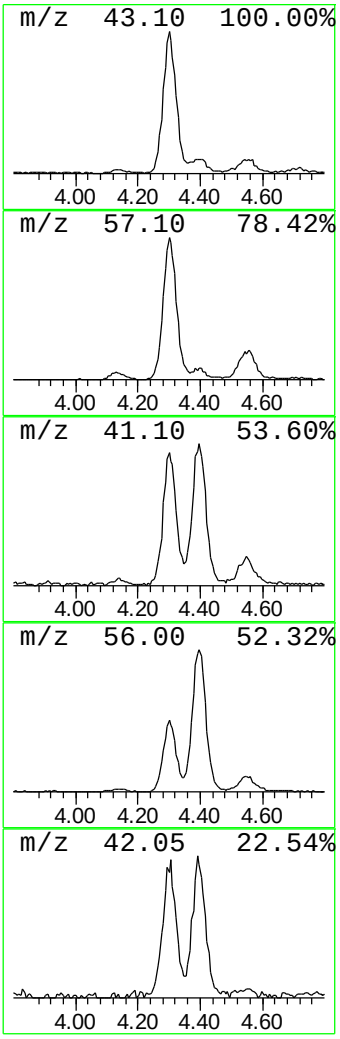
****

Peak Number 7 Pentane, 2,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.30	8.35 ug/l	136712	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	90
2	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	59
3	2,2,6,6-Tetramethylheptane	156	C11H24	040117-45-1	50
4	1-Pentene, 4-methyl-	84	C6H12	000691-37-2	49
5	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	47





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX092818\
Data File : VX004832.D
Acq On : 28 Sep 2018 20:06
Operator : JC/MD
Sample : J5130-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FA18-JBW-7338B

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

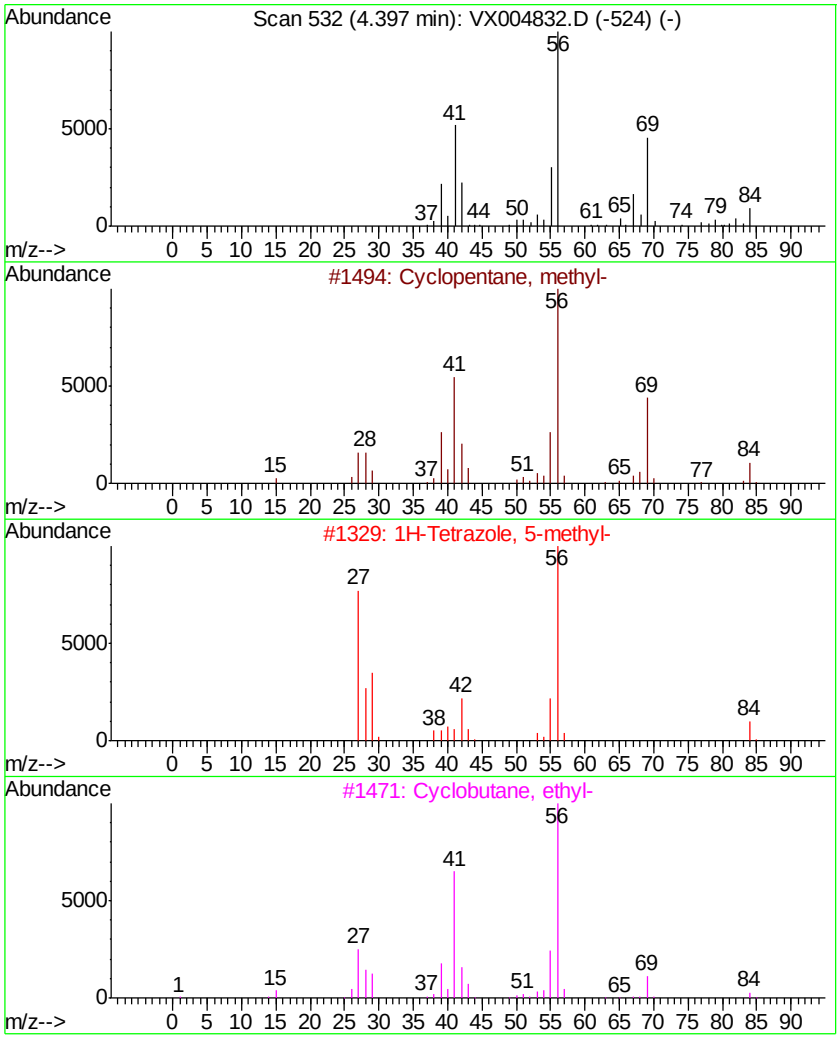
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

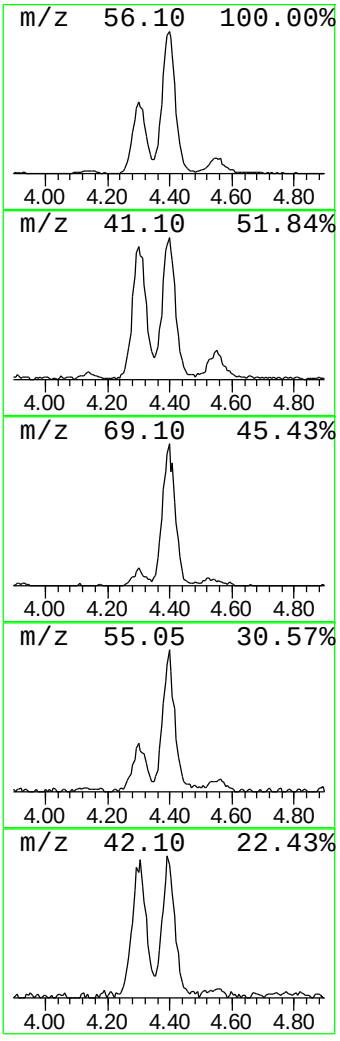
****

Peak Number 8 Cyclopentane, methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	7.53 ug/l	123316	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	87
2	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	53
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	53
4	Cyclobutane	56	C4H8	000287-23-0	43
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	38





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX092818\
Data File : VX004832.D
Acq On : 28 Sep 2018 20:06
Operator : JC/MD
Sample : J5130-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FA18-JBW-7338B

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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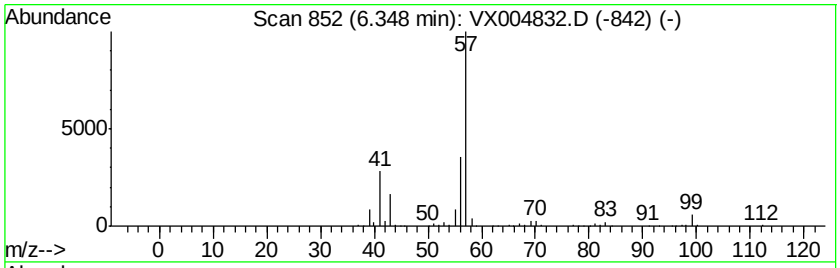
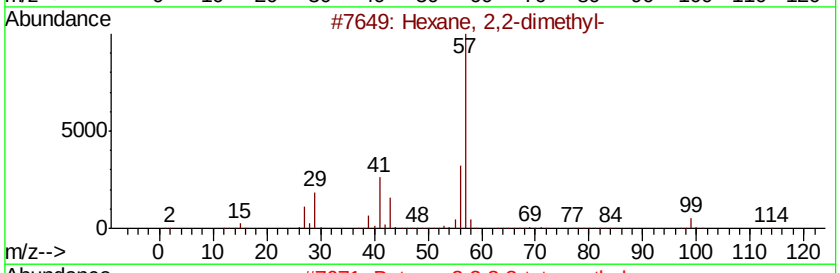
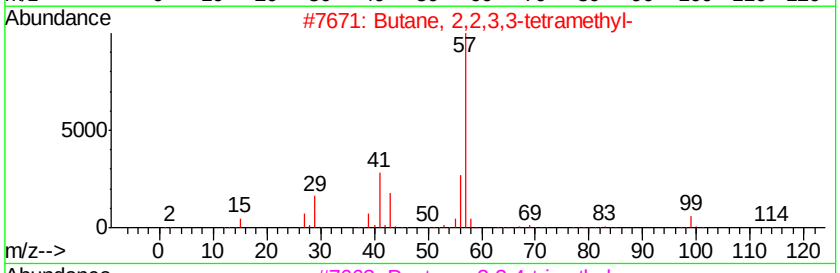
Peak Number 9 Hexane, 2,2-dimethyl- Concentration Rank 3

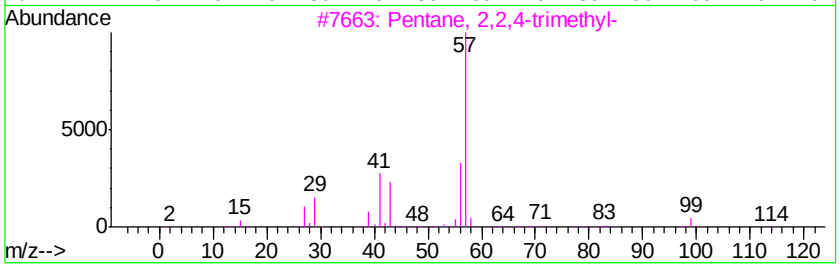
R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	18.17 ug/l	334683	1,4-Difluorobenzene	6.86

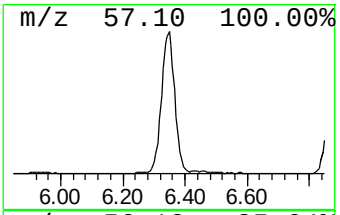
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
2	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
3	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	64
4	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59
5	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59

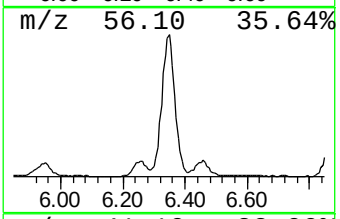


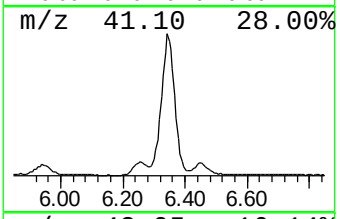


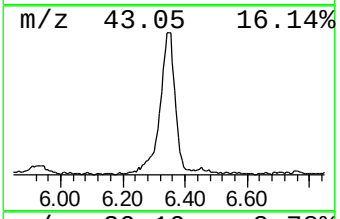


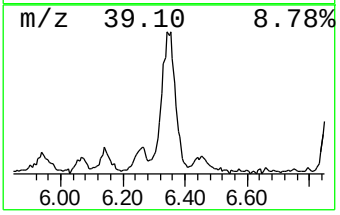












Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX092818\
Data File : VX004832.D
Acq On : 28 Sep 2018 20:06
Operator : JC/MD
Sample : J5130-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FA18-JBW-7338B

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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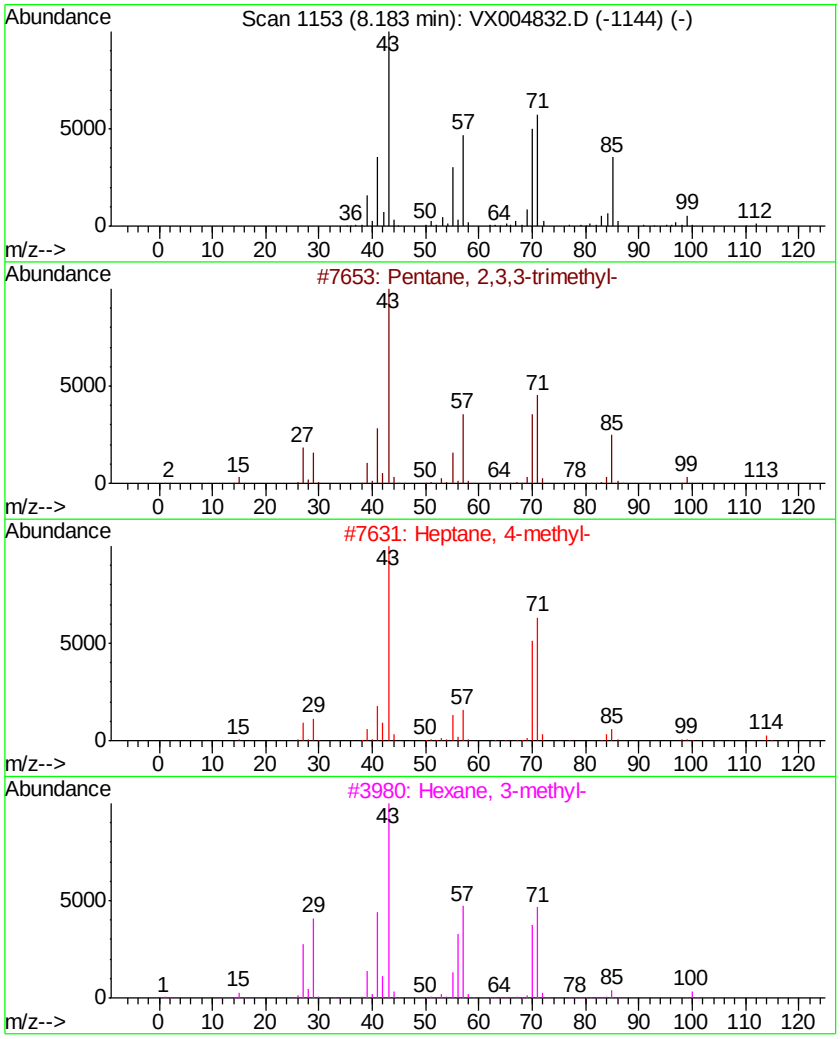
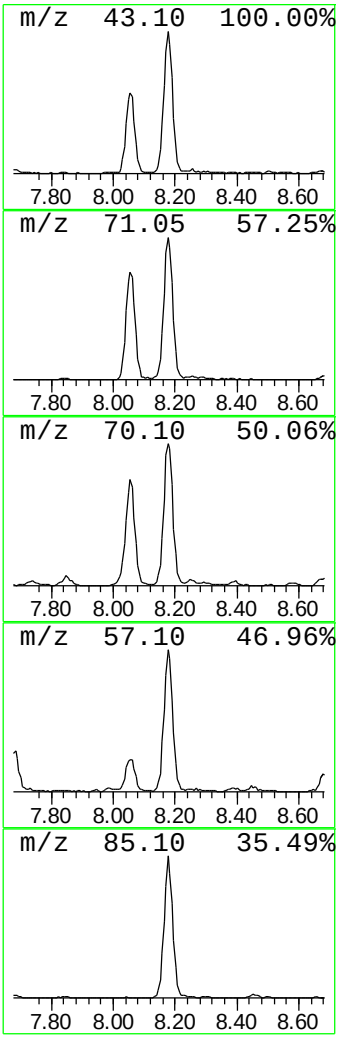
Peak Number 10 Pentane, 2,3,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.18	11.30 ug/l	208097	1,4-Difluorobenzene	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	78
2	Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3	Hexane, 3-methyl-	100	C7H16	000589-34-4	59
4	Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	59
5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	53





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX092818\
Data File : VX004832.D
Acq On : 28 Sep 2018 20:06
Operator : JC/MD
Sample : J5130-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FA18-JBW-7338B

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Aminomethanesulfo...	1.32	6.7	ug/l	109359	1	5.67	818314	50.0
Butane, 2-methyl-	1.79	85.4	ug/l	1397210	1	5.67	818314	50.0
Pentane	2.00	6.5	ug/l	106112	1	5.67	818314	50.0
Isopropyl Alcohol	2.62	9.4	ug/l	154731	1	5.67	818314	50.0
Butane, 2,3-dimet...	2.84	28.6	ug/l	468798	1	5.67	818314	50.0
Pentane, 3-methyl-	3.17	8.8	ug/l	144753	1	5.67	818314	50.0
Pentane, 2,4-dime...	4.30	8.3	ug/l	136712	1	5.67	818314	50.0
Cyclopentane, met...	4.40	7.5	ug/l	123316	1	5.67	818314	50.0
Hexane, 2,2-dimet...	6.35	18.2	ug/l	334683	2	6.86	920742	50.0
Pentane, 2,3,3-tr...	8.18	11.3	ug/l	208097	2	6.86	920742	50.0