LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX032519\
Data File : VX008442.D
Acq On : 26 Mar 2019 03:58
Operator : JC/SP
Sample : K2059-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-7

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\82X032519W.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	1.276	13	20	22	rBV	54652	71247	3.89%	0.532%
2	1.300	22	24	33	rVV2	51823	101347	5.53%	0.757%
3	1.404	37	41	45	rVV	92972	98872	5.39%	0.739%
4	1.788	99	104	115	rVB	406748	595830	32.50%	4.452%
5	1.995	134	138	152	rVB	102630	168800	9.21%	1.261%
6	2.263	176	182	196	rVB	139459	227884	12.43%	1.703%
7	2.391	196	203	209	rBV	19426	38730	2.11%	0.289%
8	2.812	261	272	273	rBV	37149	57717	3.15%	0.431%
9	2.843	274	277	281	rVV	47401	98892	5.39%	0.739%
10	2.891	281	285	288	rVV	68943	143899	7.85%	1.075%
11	2.934	288	292	305	rVB	106812	236033	12.88%	1.764%
12	3.172	322	331	345	rVB2	63988	162772	8.88%	1.216%
13	3.525	379	389	396	rBV2	17505	40972	2.24%	0.306%
14	3.818	429	437	445	rBV	26919	67481	3.68%	0.504%
15	3.928	447	455	462	rVV2	19947	53813	2.94%	0.402%
16	4.196	488	499	508	rBV2	18403	50606	2.76%	0.378%
17	4.403	523	533	545	rVB2	86634	252504	13.77%	1.887%
18	4.531	545	554	564	rBV4	11743	36646	2.00%	0.274%
19	5.299	671	680	690	rVB5	15513	54786	2.99%	0.409%
20	5.501	701	713	721	rBV	140037	411363	22.44%	3.074%
21	5.580	721	726	731	rVV2	29764	84018	4.58%	0.628%
22	5.659	731	739	768	rVB	248295	787117	42.94%	5.881%
23	5.927	772	783	796	rBV5	11261	39622	2.16%	0.296%
24	6.061	796	805	811	rBV	176460	462280	25.22%	3.454%
25	6.141	811	818	830	rVB	711257	1833065	100.00%	13.696%
26	6.305	833	845	847	rBV4	24713	69120	3.77%	0.516%
27	6.458	862	870	880	rVB4	15953	46019	2.51%	0.344%
28	6.860	925	936	945	rBV	404695	968390	52.83%	7.236%
29	7.256	993	1001	1011	rVB4	17344	40139	2.19%	0.300%
30	7.458	1022	1034	1046	rVB3	36916	105499	5.76%	0.788%
31	7.933	1105	1112	1113	rBV4	10457	19307	1.05%	0.144%
32	7.957	1113	1116	1122	rVB3	11780	20863	1.14%	0.156%
33	8.055	1122	1132	1140	rVB	13916	33155	1.81%	0.248%
34	8.177	1144	1152	1153	rBV	19757	30988	1.69%	0.232%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX032519\
Data File : VX008442.D
Acq On : 26 Mar 2019 03:58
Operator : JC/SP
Sample : K2059-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-7

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\82X032519W.M
Title : SW846 8260

35	8.214	1153	1158	1163	rVB	43877	78070	4.26%	0.583%
36	8.494	1193	1204	1210	rBV4	14235	30506	1.66%	0.228%
37	8.567	1210	1216	1223	rVB2	37142	64588	3.52%	0.483%
38	8.713	1234	1240	1247	rVV	859413	1333069	72.72%	9.961%
39	8.781	1247	1251	1258	rVB	65636	104447	5.70%	0.780%
40	8.902	1264	1271	1277	rVB	20131	36142	1.97%	0.270%
41	9.219	1318	1323	1333	rVB	22830	37974	2.07%	0.284%
42	9.512	1363	1371	1376	rVV2	16470	34497	1.88%	0.258%
43	10.110	1464	1469	1475	rBV	776426	1054264	57.51%	7.877%
44	10.250	1488	1492	1497	rBV	112406	143775	7.84%	1.074%
45	10.353	1504	1509	1515	rVB	129867	189974	10.36%	1.419%
46	11.018	1612	1618	1624	rBV	125809	164458	8.97%	1.229%
47	11.134	1632	1637	1643	rBV	639426	803706	43.84%	6.005%
48	11.359	1670	1674	1682	rVB	78947	104864	5.72%	0.784%
49	11.451	1682	1689	1695	rVV	14576	27841	1.52%	0.208%
50	11.664	1720	1724	1735	rVB	59470	81010	4.42%	0.605%
51	12.079	1786	1792	1799	rBV	738988	939003	51.23%	7.016%
52	12.140	1799	1802	1809	rVV	19447	26782	1.46%	0.200%
53	12.298	1820	1828	1833	rBV	225119	289235	15.78%	2.161%
54	12.518	1859	1864	1869	rVB	13307	18643	1.02%	0.139%
55	12.664	1883	1888	1892	rBV	53994	70580	3.85%	0.527%
56	12.755	1899	1903	1910	rVB2	47601	68393	3.73%	0.511%
57	12.975	1932	1939	1943	rBV	37975	49877	2.72%	0.373%
58	13.225	1976	1980	1987	rVB	32450	43842	2.39%	0.328%
59	13.347	1994	2000	2005	rVB2	53866	78159	4.26%	0.584%

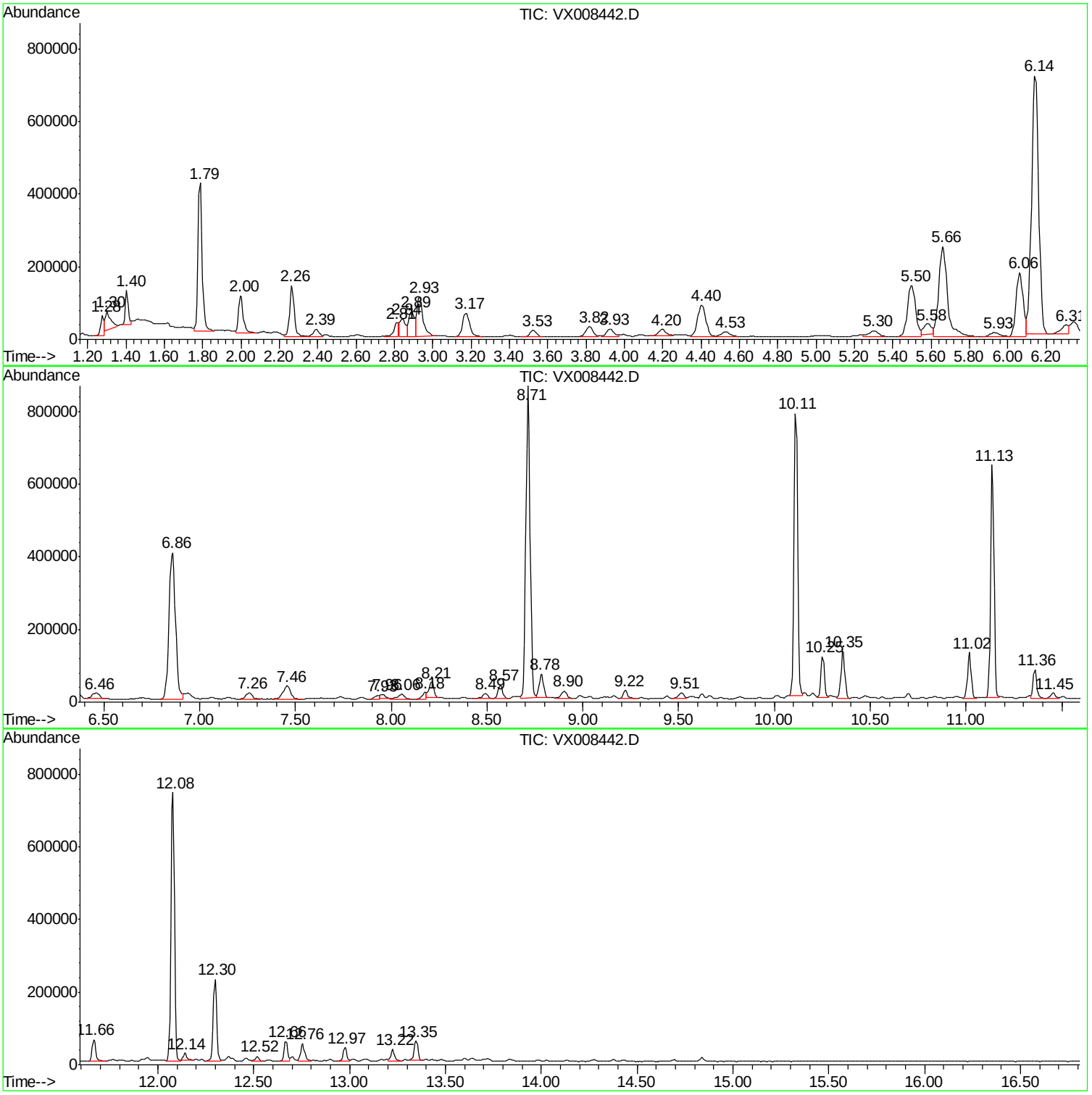
Sum of corrected areas: 13383475

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX032519\
Data File : VX008442.D
Acq On : 26 Mar 2019 03:58
Operator : JC/SP
Sample : K2059-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032519W.M
Quant Title : SW846 8260

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX032519\
Data File : VX008442.D
Acq On : 26 Mar 2019 03:58
Operator : JC/SP
Sample : K2059-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032519W.M
Quant Title : SW846 8260

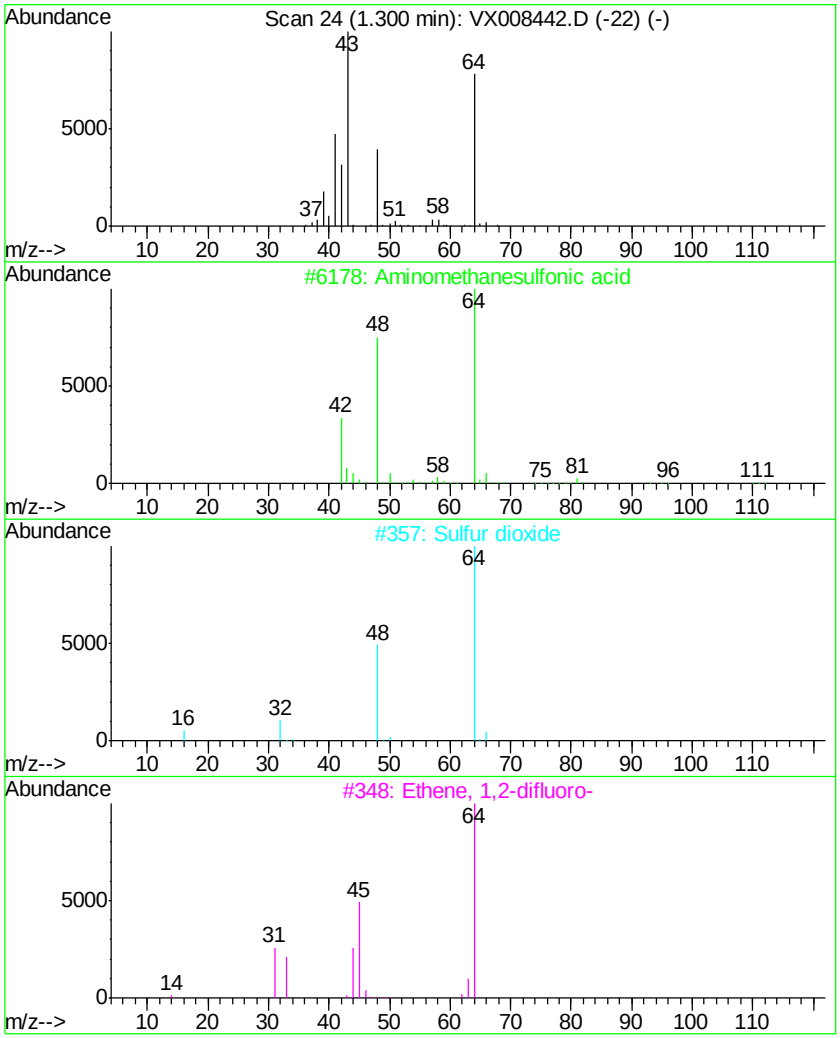
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

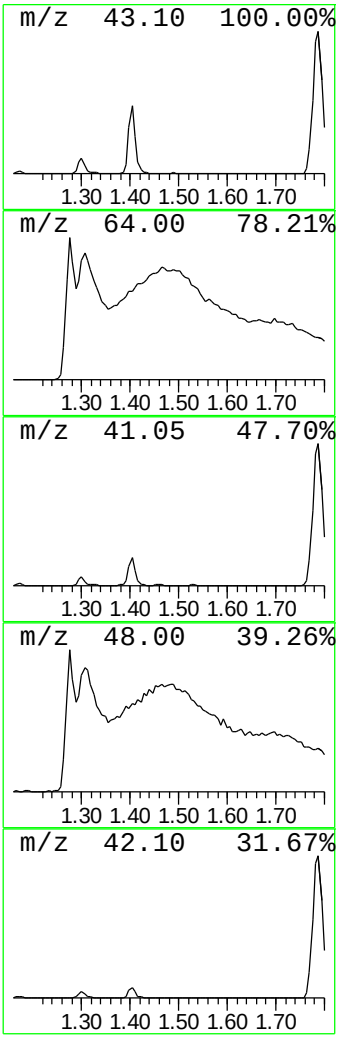
****

Peak Number 1 unknown1.30 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.30	6.44 ug/l	101347	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	43
2	Sulfur dioxide	64	O2S	007446-09-5	9
3	Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	4
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	4





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX032519\
Data File : VX008442.D
Acq On : 26 Mar 2019 03:58
Operator : JC/SP
Sample : K2059-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032519W.M
Quant Title : SW846 8260

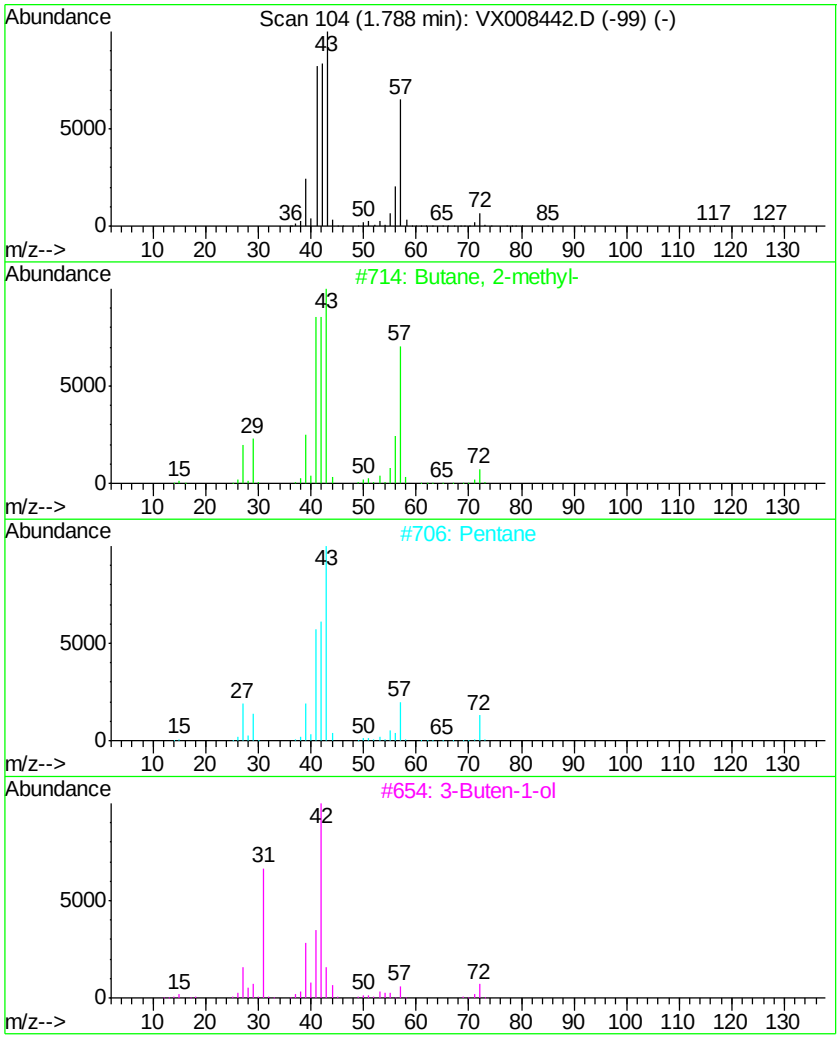
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

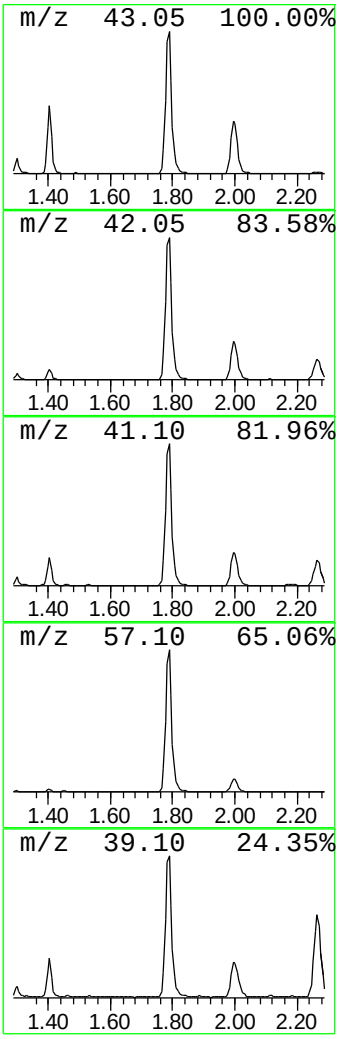
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	37.85 ug/l	595830	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	36
3	3-Buten-1-ol	72	C4H8O	000627-27-0	25
4	1-Propene, 2-methyl-	56	C4H8	000115-11-7	9
5	1-Butene	56	C4H8	000106-98-9	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX032519\
Data File : VX008442.D
Acq On : 26 Mar 2019 03:58
Operator : JC/SP
Sample : K2059-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032519W.M
Quant Title : SW846 8260

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

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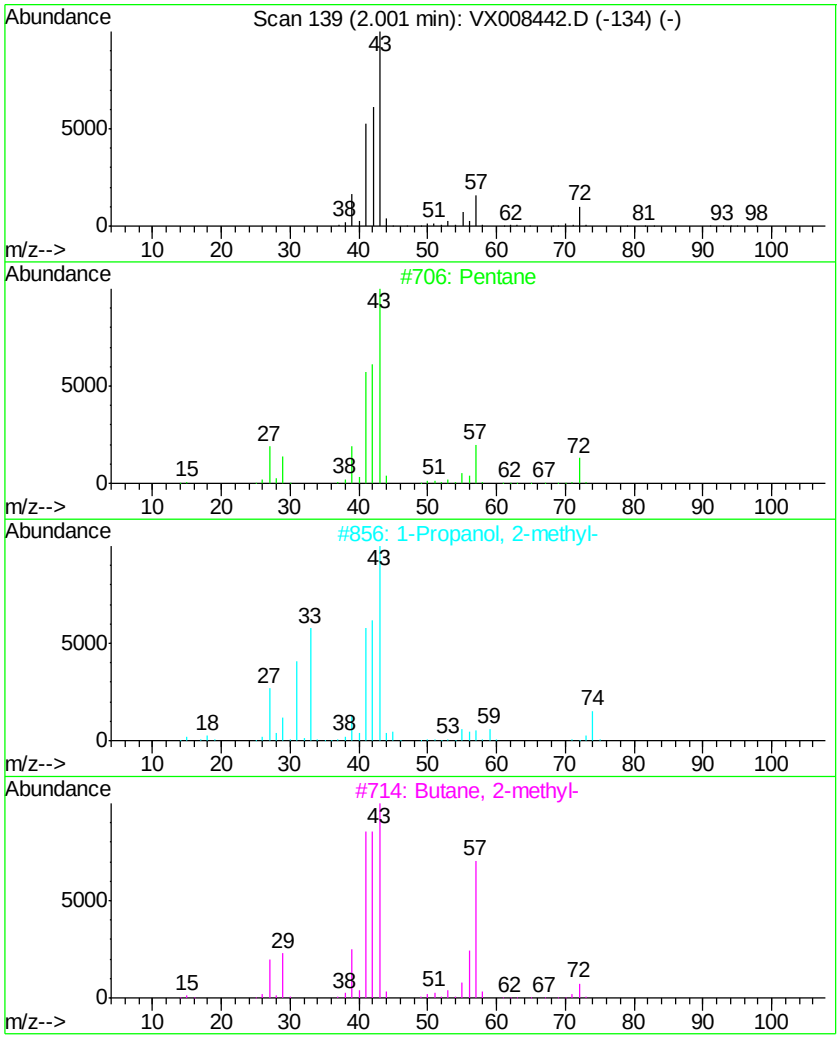
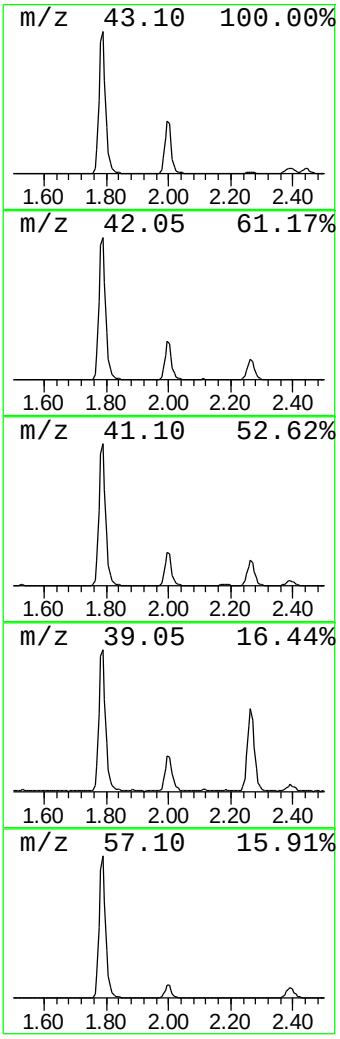
Peak Number 3 Pentane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.00	10.72 ug/l	168800	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	38
3	Butane, 2-methyl-	72	C5H12	000078-78-4	28
4	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9
5	Oxirane, ethyl-	72	C4H8O	000106-88-7	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX032519\
Data File : VX008442.D
Acq On : 26 Mar 2019 03:58
Operator : JC/SP
Sample : K2059-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032519W.M
Quant Title : SW846 8260

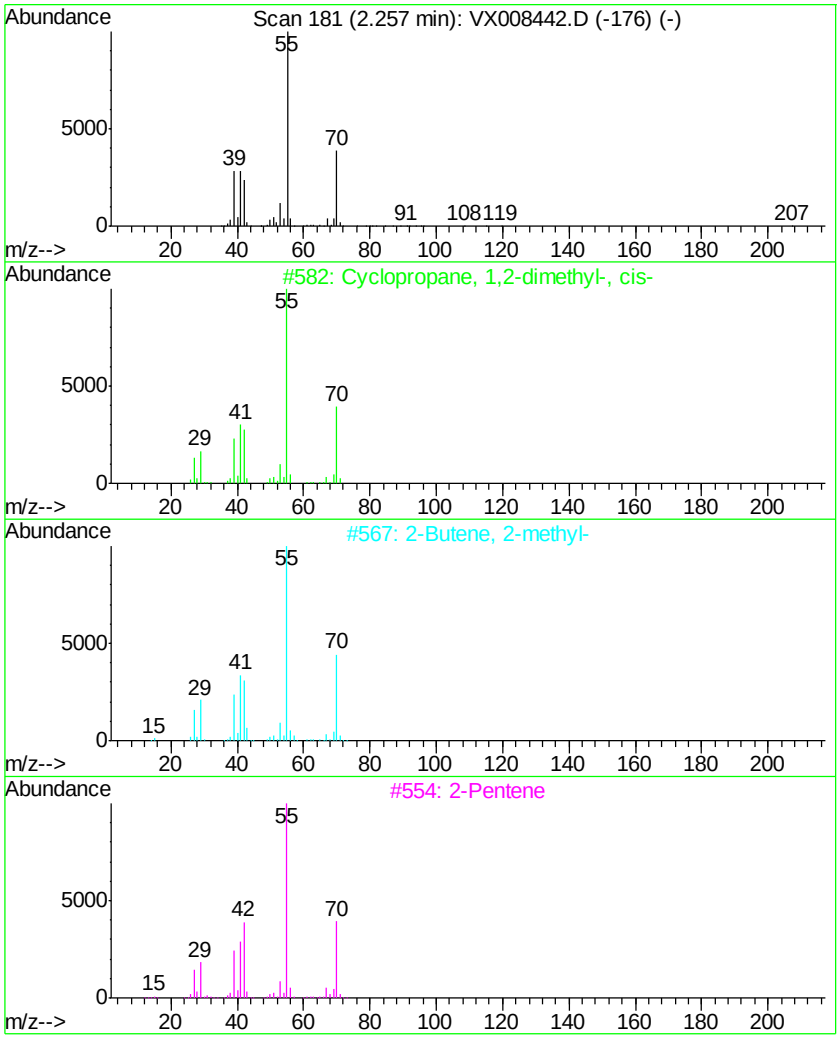
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

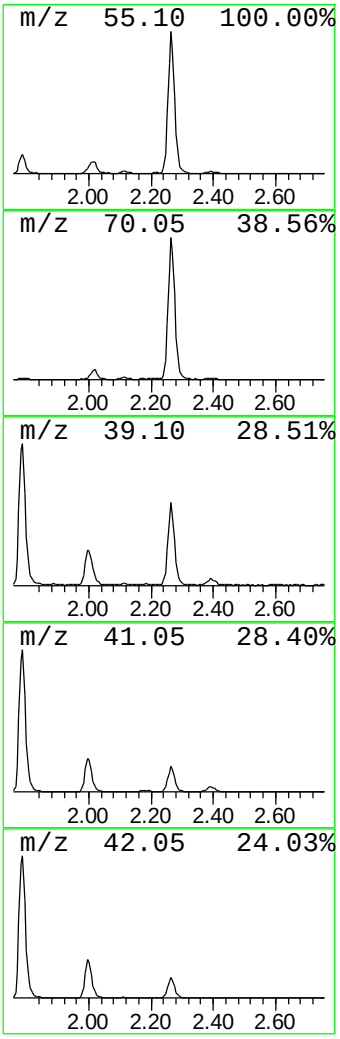
****

Peak Number 4 Cyclopropane, 1,2-dimethyl-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.26	14.48 ug/l	227884	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
2	2-Butene, 2-methyl-	70	C5H10	000513-35-9	91
3	2-Pentene	70	C5H10	000109-68-2	90
4	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	87
5	1-Butene, 3-methyl-	70	C5H10	000563-45-1	86





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX032519\
Data File : VX008442.D
Acq On : 26 Mar 2019 03:58
Operator : JC/SP
Sample : K2059-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032519W.M
Quant Title : SW846 8260

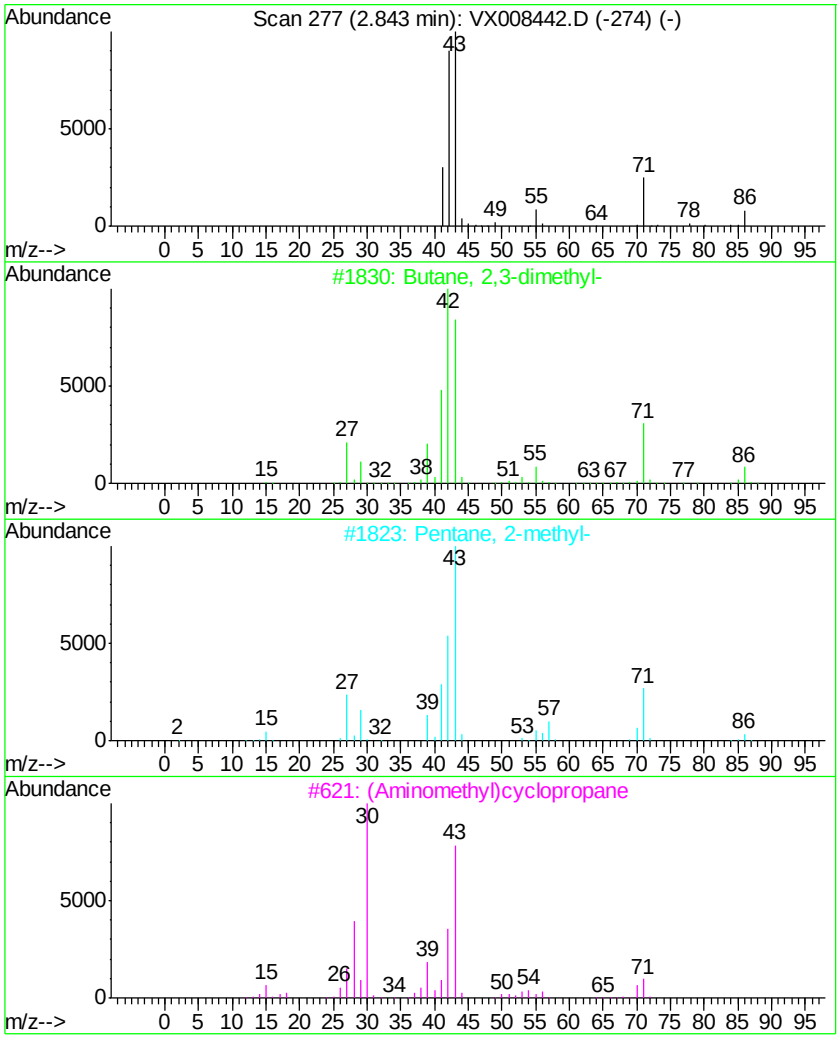
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

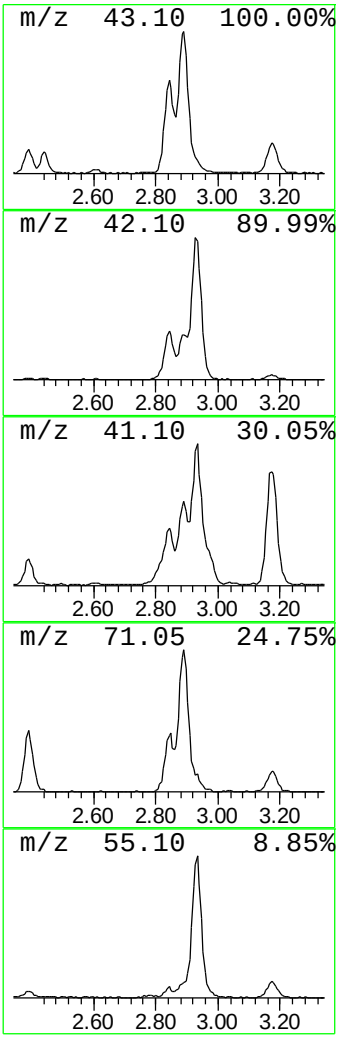
****

Peak Number 5 Butane, 2,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	6.28 ug/l	98892	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	80
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	7
3	(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	4
4	Acetic acid ethenyl ester	86	C4H6O2	000108-05-4	4
5	n-Propyl chloride	78	C3H7Cl	000540-54-5	4





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX032519\
Data File : VX008442.D
Acq On : 26 Mar 2019 03:58
Operator : JC/SP
Sample : K2059-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032519W.M
Quant Title : SW846 8260

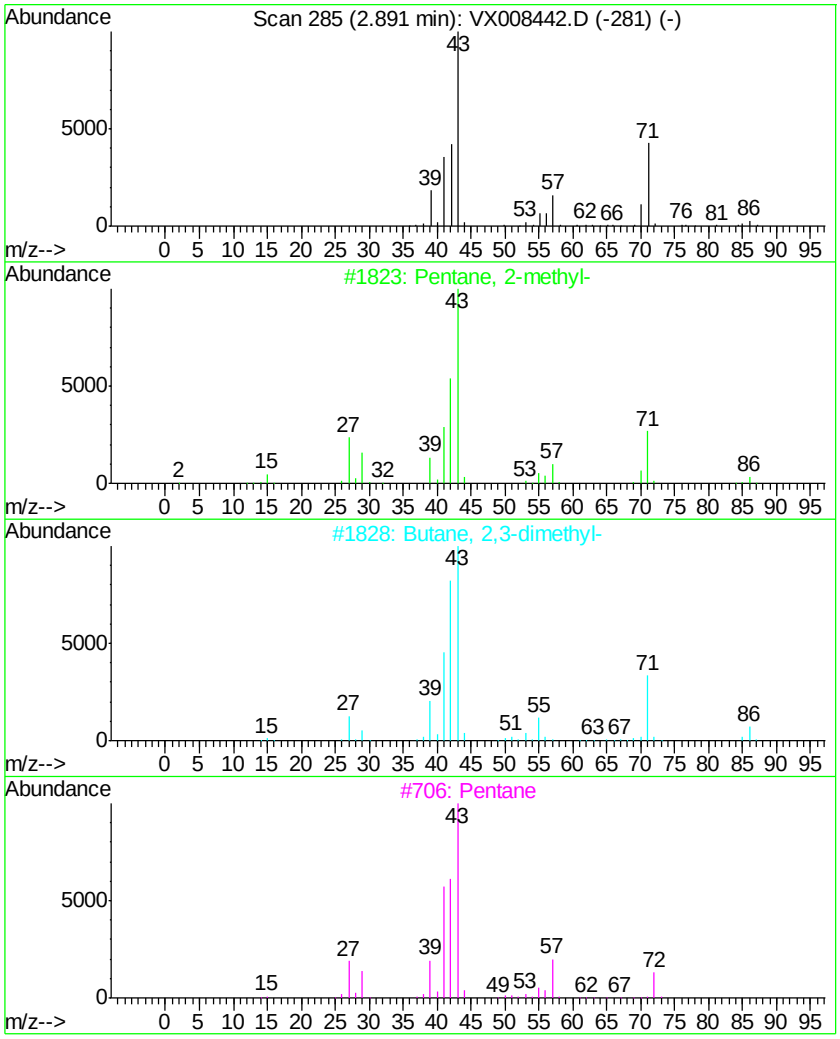
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

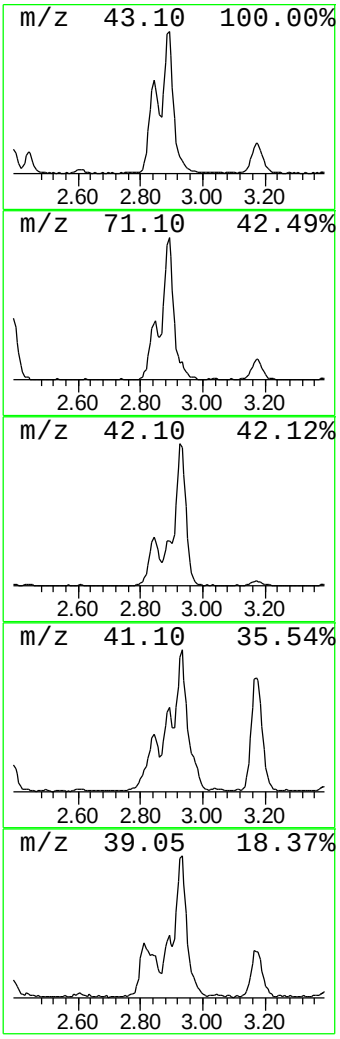
****

Peak Number 6 Pentane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.89	9.14 ug/l	143899	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	64
2	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	38
3	Pentane	72	C5H12	000109-66-0	38
4	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	28
5	Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	12





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX032519\
Data File : VX008442.D
Acq On : 26 Mar 2019 03:58
Operator : JC/SP
Sample : K2059-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032519W.M
Quant Title : SW846 8260

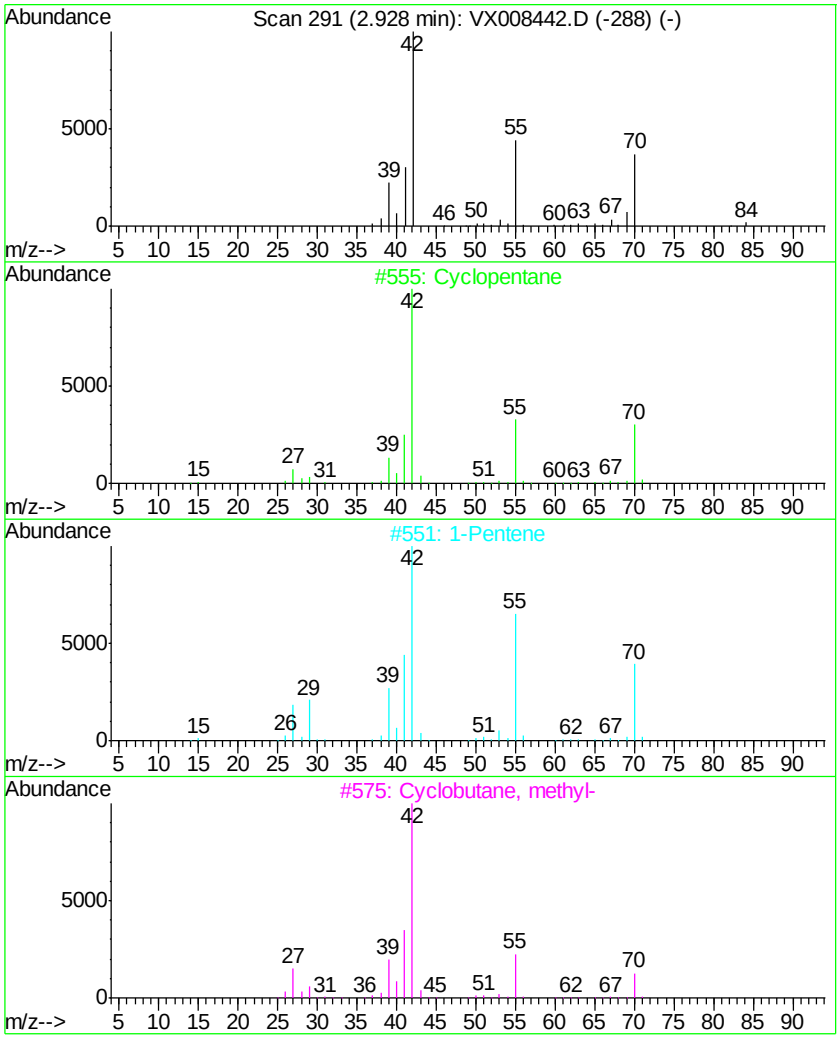
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

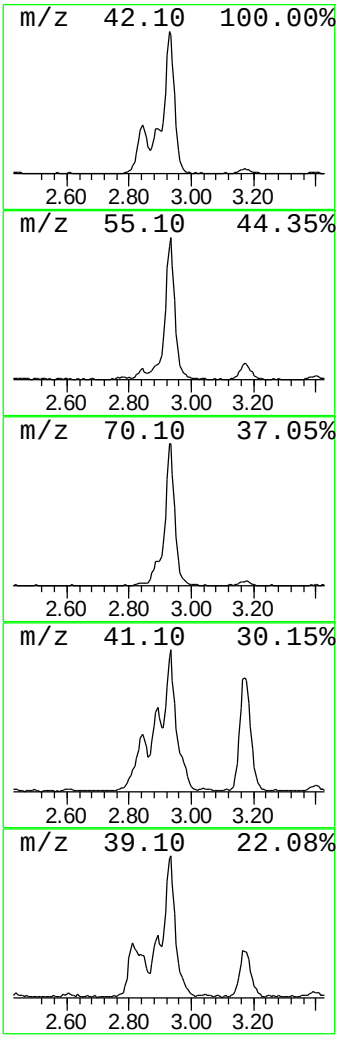
****

Peak Number 7 Cyclopentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.93	14.99 ug/l	236033	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	80
2	1-Pentene	70	C5H10	000109-67-1	72
3	Cyclobutane, methyl-	70	C5H10	000598-61-8	64
4	1-Pentanol	88	C5H12O	000071-41-0	40
5	2-Pentene, (E)-	70	C5H10	000646-04-8	27





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX032519\
Data File : VX008442.D
Acq On : 26 Mar 2019 03:58
Operator : JC/SP
Sample : K2059-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032519W.M
Quant Title : SW846 8260

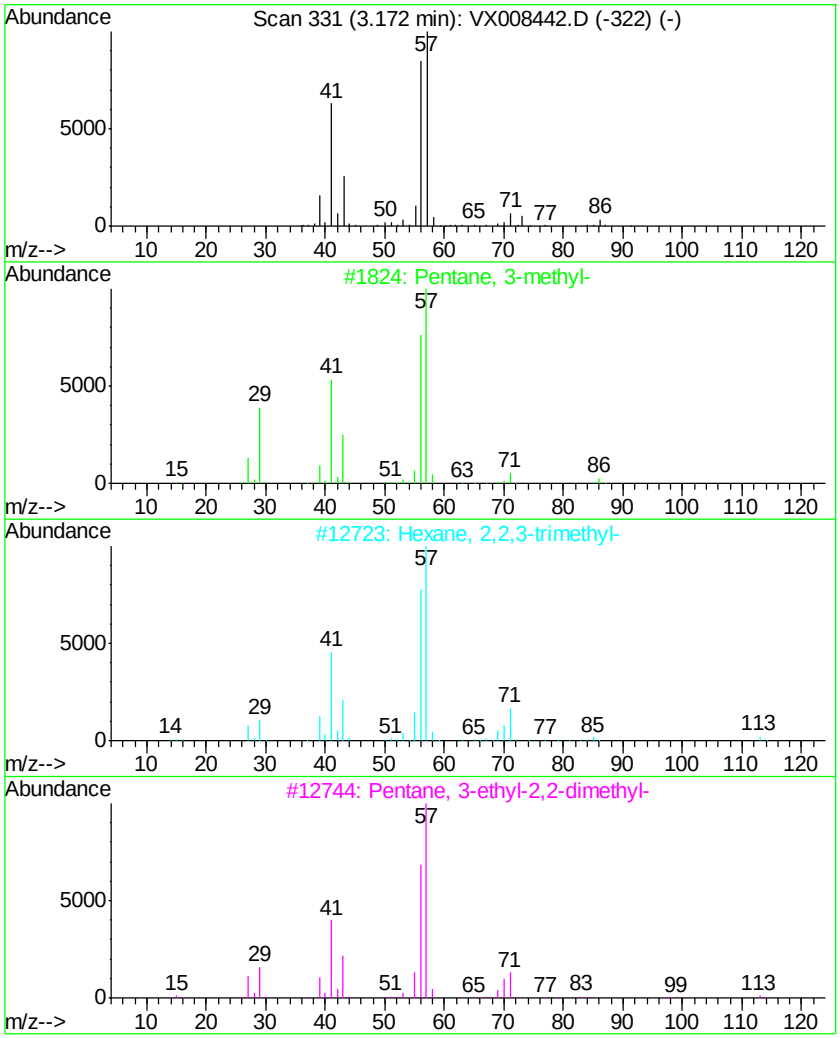
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

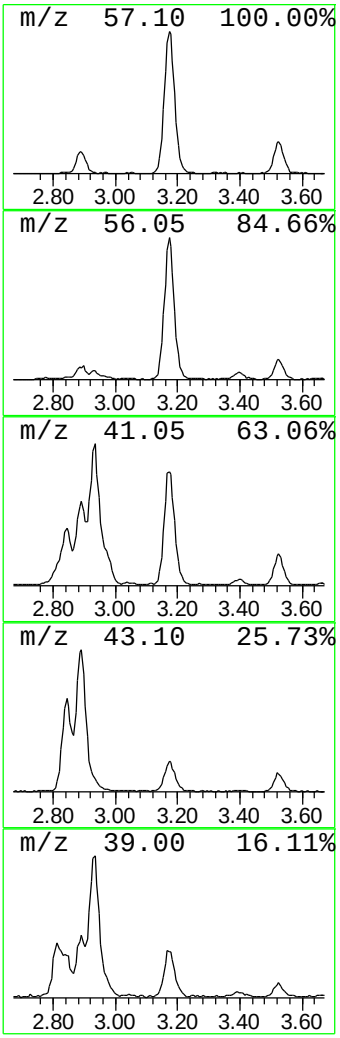
****

Peak Number 8 Pentane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	10.34 ug/l	162772	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	90
2	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	78
3	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	56
4	Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	56
5	Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	50





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX032519\
Data File : VX008442.D
Acq On : 26 Mar 2019 03:58
Operator : JC/SP
Sample : K2059-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032519W.M
Quant Title : SW846 8260

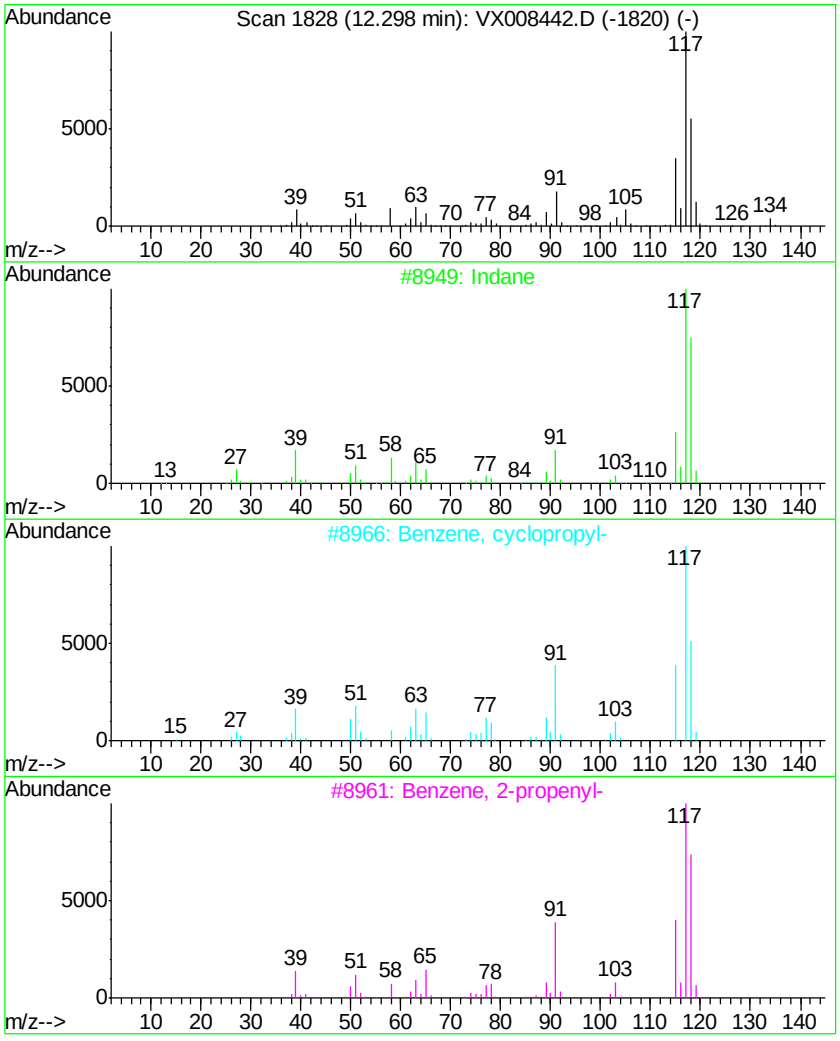
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

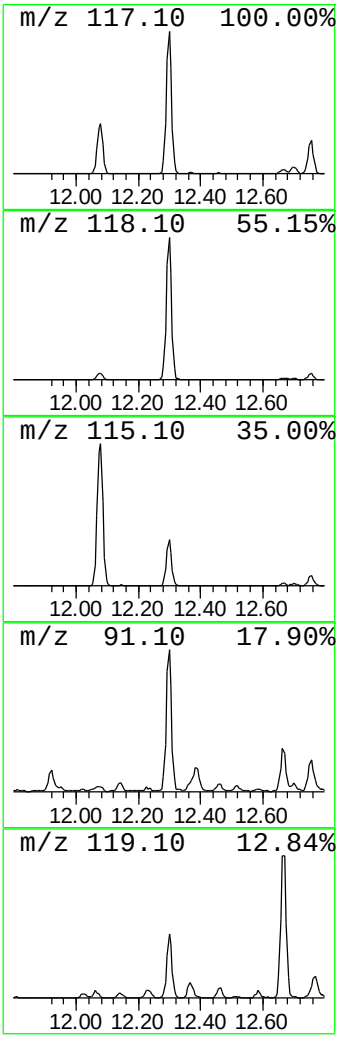
****

Peak Number 10 Indane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	15.40 ug/l	289235	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	93
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	72
4	Deltacyclene	118	C9H10	007785-10-6	64
5	trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX032519\
Data File : VX008442.D
Acq On : 26 Mar 2019 03:58
Operator : JC/SP
Sample : K2059-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 37 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032519W.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
unknown1.30	1.30	6.4	ug/l	101347	1	5.67	787117	50.0
Butane, 2-methyl-	1.79	37.9	ug/l	595830	1	5.67	787117	50.0
Pentane	2.00	10.7	ug/l	168800	1	5.67	787117	50.0
Cyclopropane, 1,2...	2.26	14.5	ug/l	227884	1	5.67	787117	50.0
Butane, 2,3-dimet...	2.84	6.3	ug/l	98892	1	5.67	787117	50.0
Pentane, 2-methyl-	2.89	9.1	ug/l	143899	1	5.67	787117	50.0
Cyclopentane	2.93	15.0	ug/l	236033	1	5.67	787117	50.0
Pentane, 3-methyl-	3.17	10.3	ug/l	162772	1	5.67	787117	50.0
Indane	12.30	15.4	ug/l	289235	4	12.08	939003	50.0