Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX092019\
Data File : VX012588.D
Acq On : 21 Sep 2019 04:02
Operator : JC/SP
Sample : K4978-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : Z2-0162

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\82X091719W.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	1.070	26	30	43	rBV	903437	1054230	15.86%	2.205%
2	1.783	141	147	159	rVB	428840	619471	9.32%	1.296%
3	2.594	273	280	291	rBV	69415	125354	1.89%	0.262%
4	2.838	311	320	326	rBV	340206	793190	11.93%	1.659%
5	2.917	331	333	345	rVB	39208	73912	1.11%	0.155%
6	3.161	363	373	385	rBV	255612	586209	8.82%	1.226%
7	4.301	549	560	568	rBV2	78866	237839	3.58%	0.497%
8	4.393	568	575	587	rVV	52239	150342	2.26%	0.314%
9	5.228	698	712	722	rBV2	18294	67058	1.01%	0.140%
10	5.490	743	755	761	rBV2	102785	289268	4.35%	0.605%
11	5.569	761	768	775	rVV	115895	380684	5.73%	0.796%
12	5.655	775	782	786	rVV	196931	553124	8.32%	1.157%
13	5.716	787	792	810	rVB	252794	750563	11.29%	1.570%
14	5.941	815	829	839	rBV4	123994	413366	6.22%	0.864%
15	6.057	839	848	855	rBV	116583	296438	4.46%	0.620%
16	6.252	869	880	888	rBV2	217995	687444	10.34%	1.438%
17	6.350	888	896	905	rVV3	321689	958023	14.41%	2.004%
18	6.447	905	912	923	rVB2	45642	129819	1.95%	0.271%
19	6.849	966	978	990	rBV	287466	692397	10.42%	1.448%
20	7.453	1066	1077	1088	rVB4	160719	419021	6.30%	0.876%
21	7.843	1133	1141	1150	rVB	87379	176924	2.66%	0.370%
22	8.050	1164	1175	1184	rVB2	180112	531946	8.00%	1.112%
23	8.172	1186	1195	1204	rBV	296161	605846	9.11%	1.267%
24	8.386	1220	1230	1236	rBV2	100702	189455	2.85%	0.396%
25	8.666	1268	1276	1279	rBV3	118272	237472	3.57%	0.497%
26	8.709	1279	1283	1297	rVB	585438	944526	14.21%	1.975%
27	8.837	1297	1304	1308	rBV	250613	425498	6.40%	0.890%
28	9.038	1331	1337	1343	rVB	381543	616757	9.28%	1.290%
29	9.160	1348	1357	1363	rBV	188111	301576	4.54%	0.631%
30	9.569	1418	1424	1428	rBV2	122943	186647	2.81%	0.390%
31	9.617	1428	1432	1436	rVB	55691	75302	1.13%	0.157%
32	9.672	1436	1441	1446	rBV	281956	430252	6.47%	0.900%
33	9.886	1471	1476	1490	rVB4	35512	72687	1.09%	0.152%
34	10.111	1508	1513	1518	rBV	543651	739908	11.13%	1.547%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX092019\
Data File : VX012588.D
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Sample : K4978-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : Z2-0162

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\82X091719W.M
Title : SW846 8260

35	10.184	1518	1525	1529	rBV	149366	219194	3.30%	0.458%
36	10.251	1529	1536	1545	rBV	4862885	6647926	100.00%	13.903%
37	10.355	1545	1553	1559	rVV	3385201	4499893	67.69%	9.411%
38	10.642	1591	1600	1607	rBV2	49836	145163	2.18%	0.304%
39	10.830	1620	1631	1639	rBV2	81699	151532	2.28%	0.317%
40	10.910	1639	1644	1649	rBV3	43500	77752	1.17%	0.163%
41	11.013	1656	1661	1667	rBV	1351403	1675109	25.20%	3.503%
42	11.135	1675	1681	1685	rBV	454102	598710	9.01%	1.252%
43	11.355	1712	1717	1727	rVB	952324	1132099	17.03%	2.368%
44	11.452	1727	1733	1737	rBV	972172	1200604	18.06%	2.511%
45	11.666	1757	1768	1777	rBV	1297301	1779501	26.77%	3.722%
46	11.763	1777	1784	1786	rVV4	43974	95276	1.43%	0.199%
47	11.800	1786	1790	1795	rVB	1067843	1313222	19.75%	2.746%
48	11.916	1801	1809	1810	rBV3	77780	116172	1.75%	0.243%
49	11.940	1810	1813	1821	rVB	271851	367909	5.53%	0.769%
50	12.074	1829	1835	1840	rVB2	607652	867977	13.06%	1.815%
51	12.141	1841	1846	1850	rBV	568263	715185	10.76%	1.496%
52	12.227	1856	1860	1865	rVB	122137	144459	2.17%	0.302%
53	12.294	1865	1871	1876	rBV	1210998	1494021	22.47%	3.125%
54	12.361	1876	1882	1892	rVB	241035	361948	5.44%	0.757%
55	12.458	1892	1898	1902	rBV	205960	268480	4.04%	0.561%
56	12.513	1902	1907	1914	rBV	543398	648578	9.76%	1.356%
57	12.580	1914	1918	1921	rBV	213377	280215	4.22%	0.586%
58	12.666	1926	1932	1935	rVV	376661	471441	7.09%	0.986%
59	12.696	1935	1937	1942	rVV	235781	267908	4.03%	0.560%
60	12.751	1942	1946	1953	rVB2	638863	978025	14.71%	2.045%
61	12.891	1964	1969	1975	rVB2	100127	157936	2.38%	0.330%
62	12.970	1975	1982	1986	rBV	352569	499280	7.51%	1.044%
63	13.013	1986	1989	1995	rVB	247266	304235	4.58%	0.636%
64	13.080	1995	2000	2005	rBV3	68613	104015	1.56%	0.218%
65	13.190	2014	2018	2020	rBV2	76607	87157	1.31%	0.182%
66	13.220	2020	2023	2026	rVB	96378	92996	1.40%	0.194%
67	13.306	2033	2037	2038	rBV	66963	81258	1.22%	0.170%
68	13.342	2038	2043	2048	rVB2	1060990	1468487	22.09%	3.071%
69	13.476	2060	2065	2071	rVB	178193	234895	3.53%	0.491%
70	13.598	2081	2085	2087	rVV	80762	111340	1.67%	0.233%
71	13.635	2087	2091	2096	rVV3	140803	275649	4.15%	0.576%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX092019\
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Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : Z2-0162

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\82X091719W.M
Title : SW846 8260

72	13.696	2097	2101	2102	rVV	80489	115689	1.74%	0.242%
73	13.720	2102	2105	2113	rVB3	131740	243711	3.67%	0.510%
74	13.830	2114	2123	2131	rVB	972824	1297549	19.52%	2.714%
75	13.921	2131	2138	2142	rBV2	57963	106163	1.60%	0.222%
76	13.982	2144	2148	2152	rVB3	57521	77808	1.17%	0.163%
77	14.269	2190	2195	2202	rVB2	69736	115705	1.74%	0.242%
78	14.537	2234	2239	2250	rVB2	71935	115488	1.74%	0.242%
79	14.690	2260	2264	2269	rBV	255479	313271	4.71%	0.655%
80	14.836	2283	2288	2297	rBV	252651	339759	5.11%	0.711%
81	15.269	2349	2359	2364	rBV2	43279	86060	1.29%	0.180%
82	15.543	2399	2404	2410	rBV	47781	79713	1.20%	0.167%
83	15.683	2417	2427	2430	rBV	60466	107114	1.61%	0.224%
84	15.720	2430	2433	2440	rVB	45236	70015	1.05%	0.146%

Sum of corrected areas: 47816140

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX092019\
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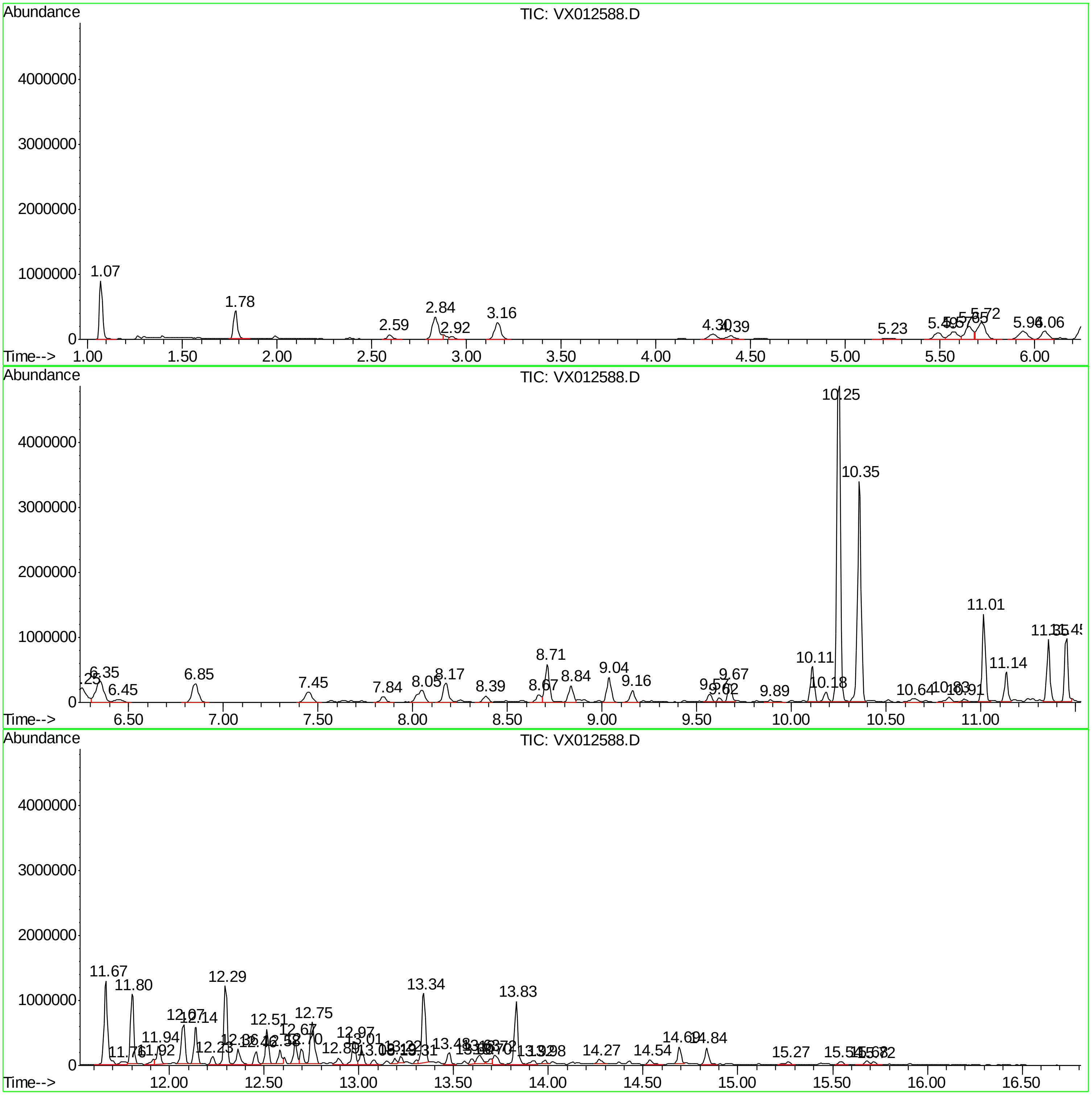
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
Z2-0162

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX092019\
Data File : VX012588.D
Acq On : 21 Sep 2019 04:02
Operator : JC/SP
Sample : K4978-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : Z2-0162

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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

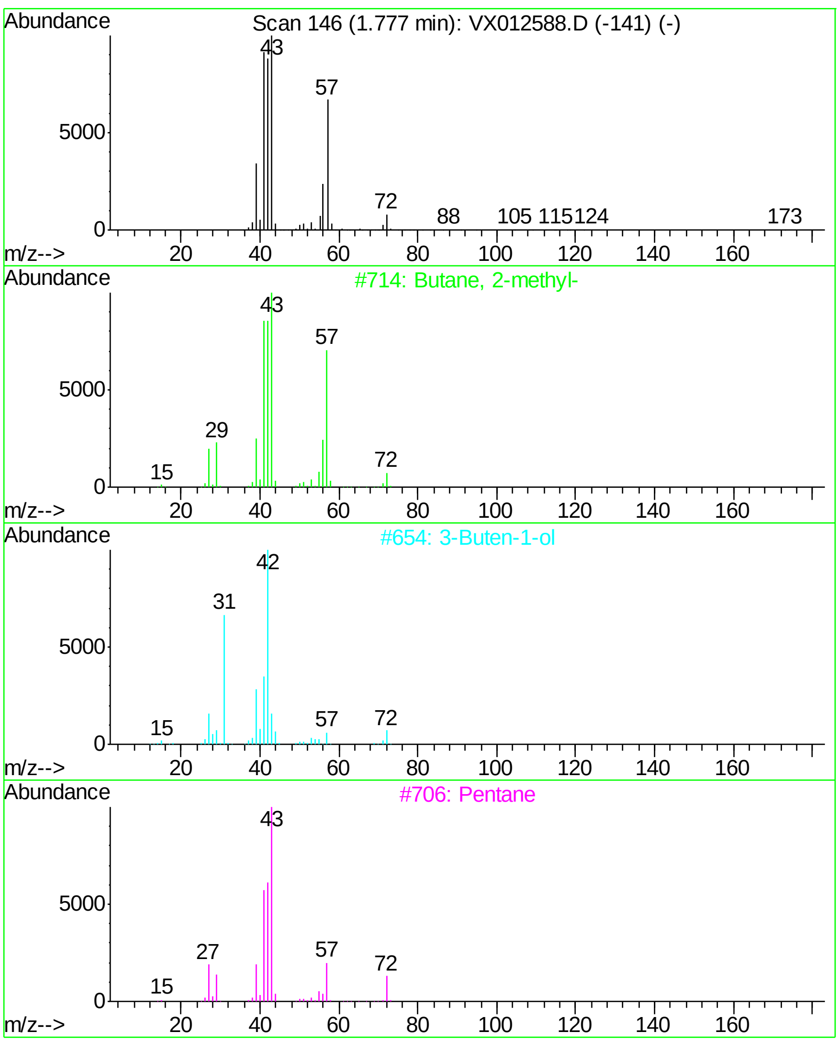
****

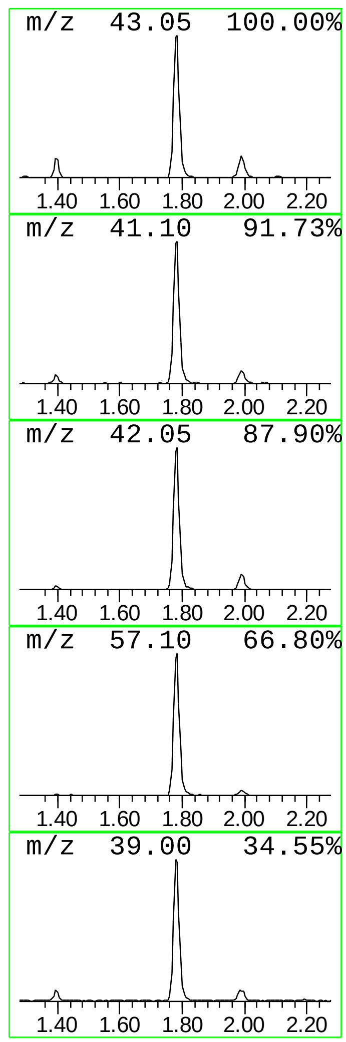
Peak Number 2 Butane, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.78	56.00 ug/l	619471	Pentafluorobenzene	5.65

Hit# of 5

Hit#	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	3-Buten-1-ol	72	C4H8O	000627-27-0	50
3	Pentane	72	C5H12	000109-66-0	36
4	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	30
5	1-Propene, 2-methyl-	56	C4H8	000115-11-7	14





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX092019\
Data File : VX012588.D
Acq On : 21 Sep 2019 04:02
Operator : JC/SP
Sample : K4978-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : Z2-0162

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

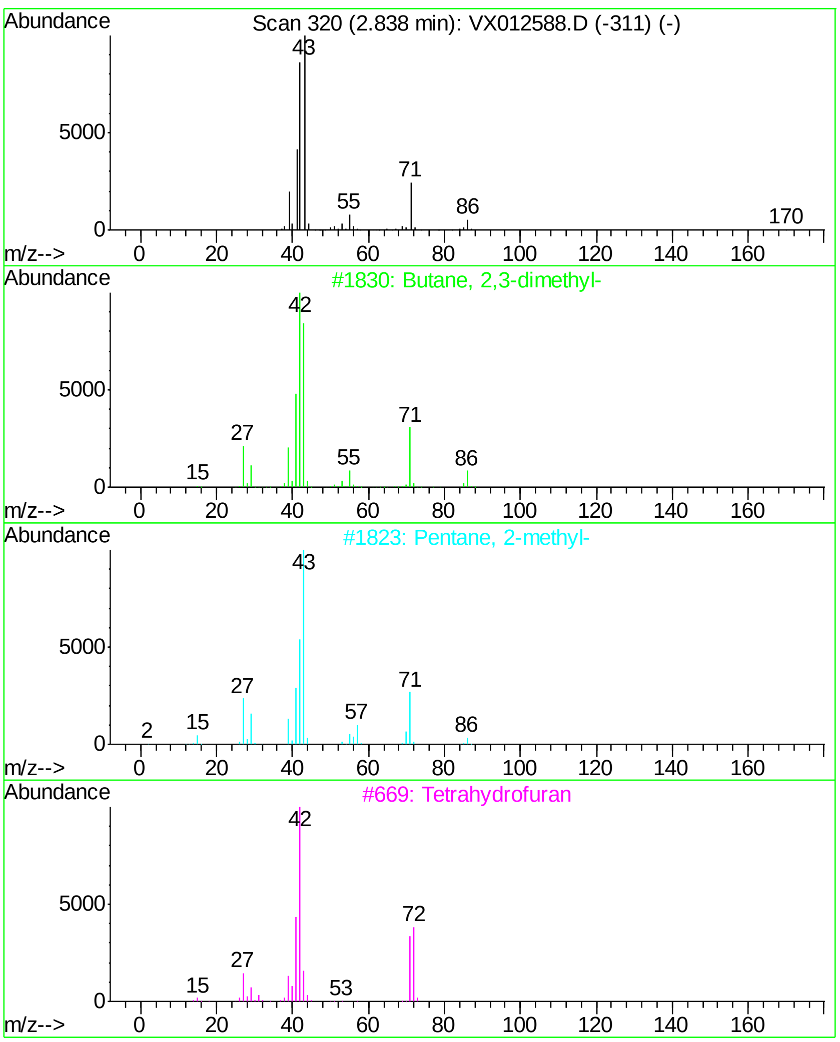
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

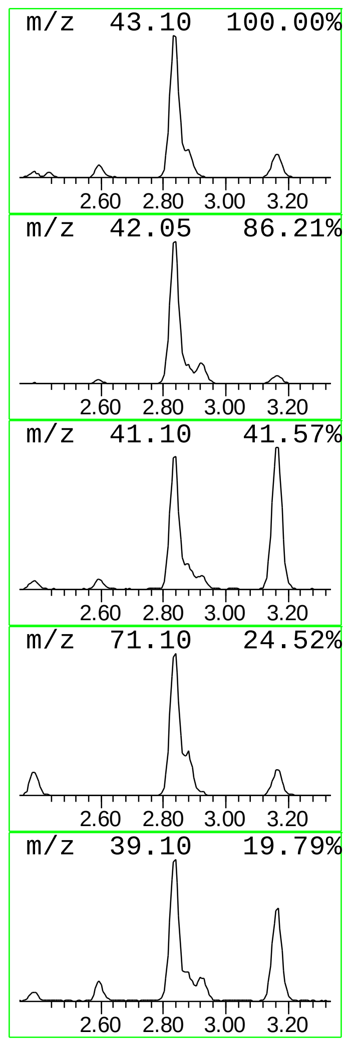
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	71.70 ug/l	793190	Pentafluorobenzene	5.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	87
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	40
3	Tetrahydrofuran	72	C4H8O	000109-99-9	38
4	Butane, 2-methyl-	72	C5H12	000078-78-4	36
5	Pentane	72	C5H12	000109-66-0	23





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX092019\
Data File : VX012588.D
Acq On : 21 Sep 2019 04:02
Operator : JC/SP
Sample : K4978-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : Z2-0162

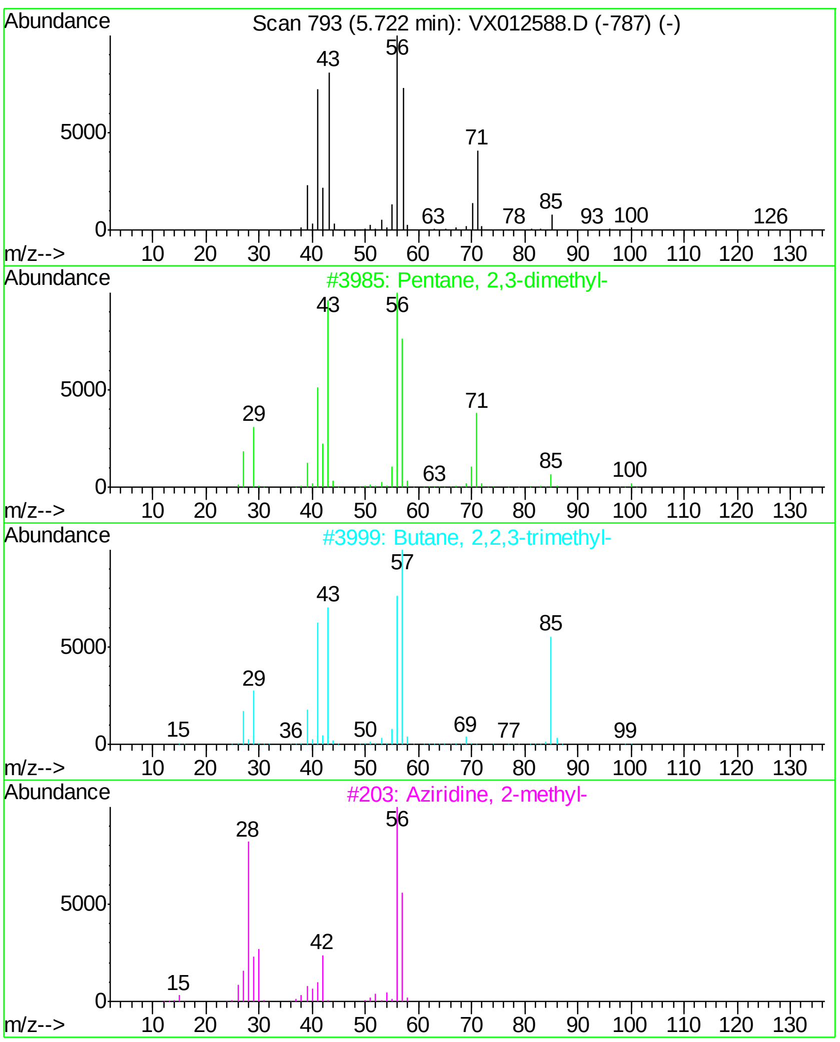
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

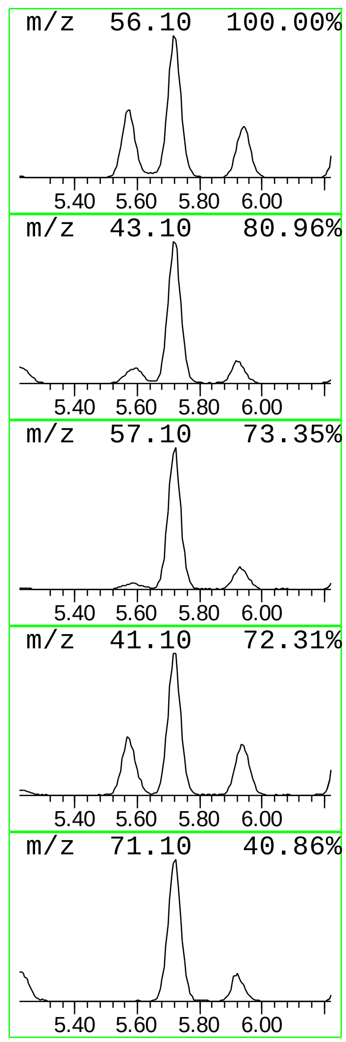
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentane, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	67.85 ug/l	750563	Pentafluorobenzene	5.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	50
3	Aziridine, 2-methyl-	57	C3H7N	000075-55-8	49
4	Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	40
5	Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	40





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX092019\
Data File : VX012588.D
Acq On : 21 Sep 2019 04:02
Operator : JC/SP
Sample : K4978-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : Z2-0162

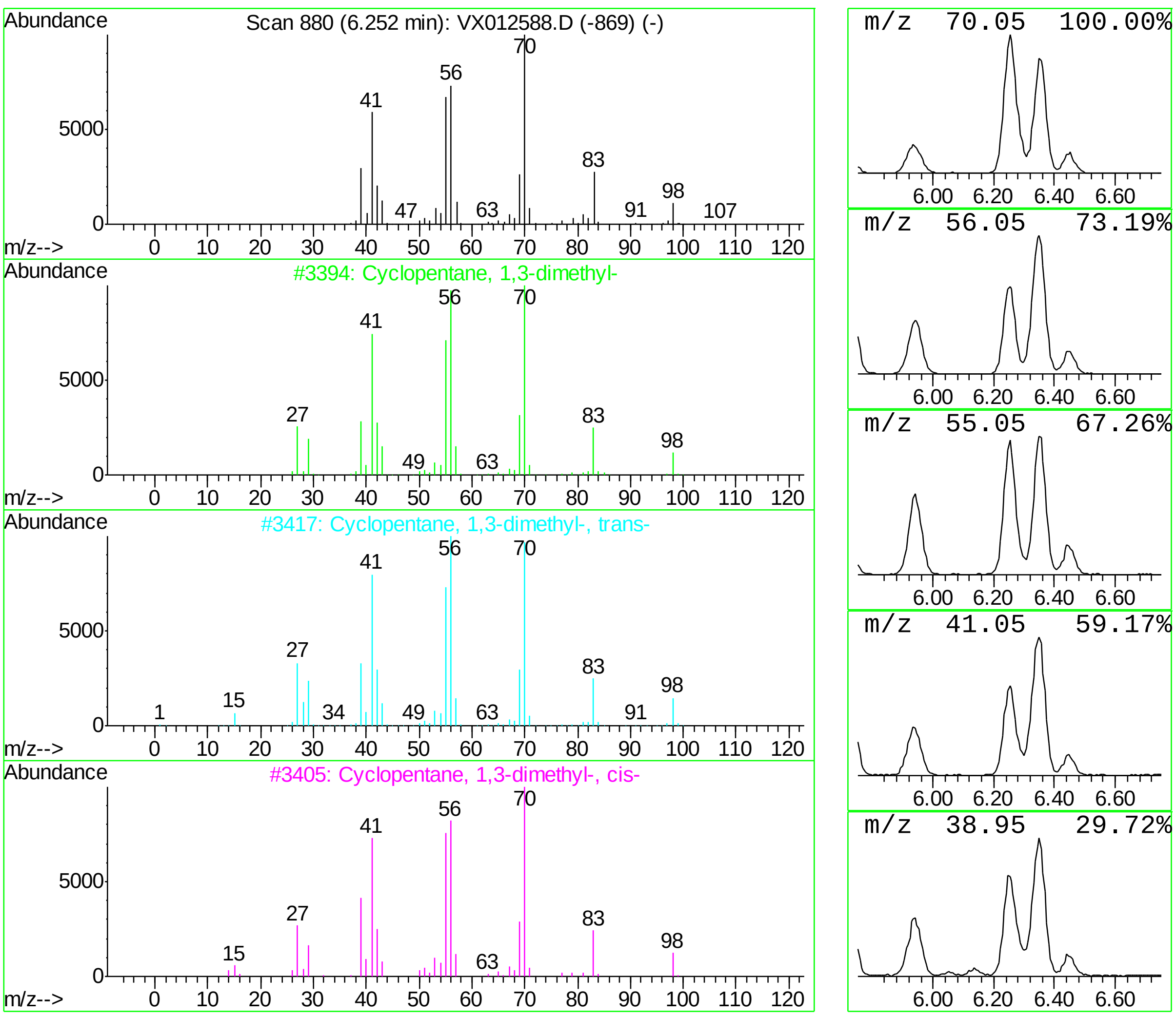
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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

Peak Number 5 Cyclopentane, 1,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.25	62.14 ug/l	687444	Pentafluorobenzene	5.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	94
2	Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	94
3	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	93
4	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	76
5	2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	64



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX092019\
Data File : VX012588.D
Acq On : 21 Sep 2019 04:02
Operator : JC/SP
Sample : K4978-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : Z2-0162

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

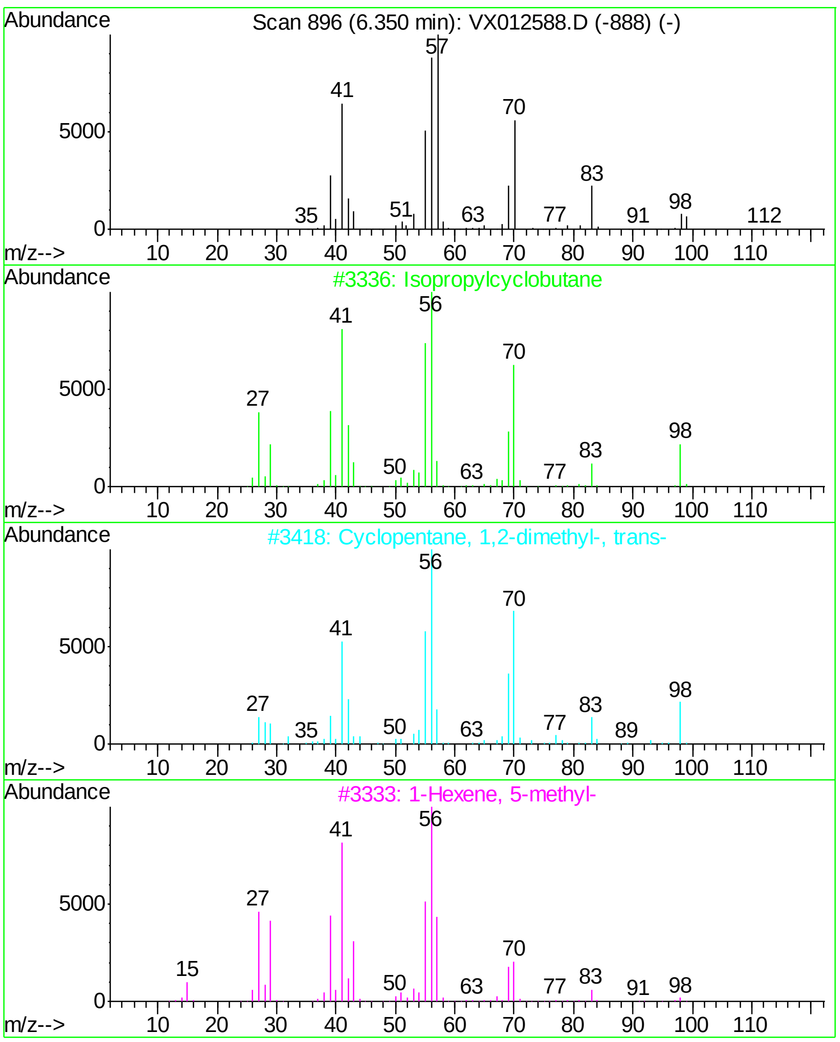
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

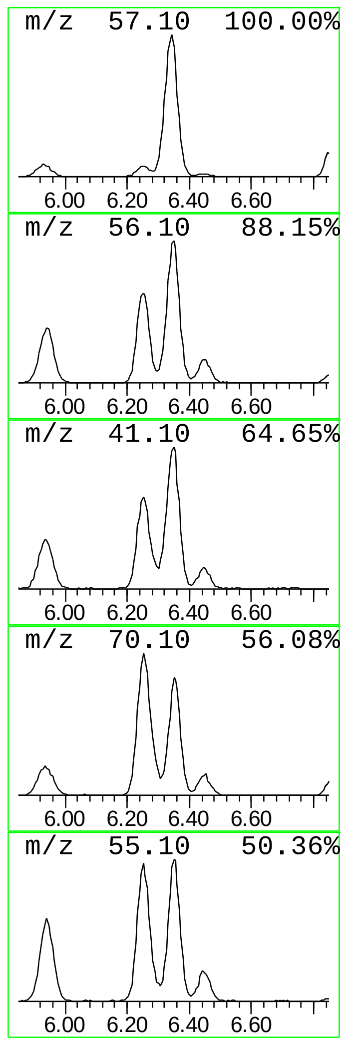
****

Peak Number 6 Isopropylcyclobutane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	69.18 ug/l	958023	1,4-Difluorobenzene	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropylcyclobutane	98	C7H14	000872-56-0	72
2	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	72
3	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	58
4	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	53
5	1-Butanol, 2-methyl-	88	C5H12O	000137-32-6	50





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX092019\
Data File : VX012588.D
Acq On : 21 Sep 2019 04:02
Operator : JC/SP
Sample : K4978-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : Z2-0162

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

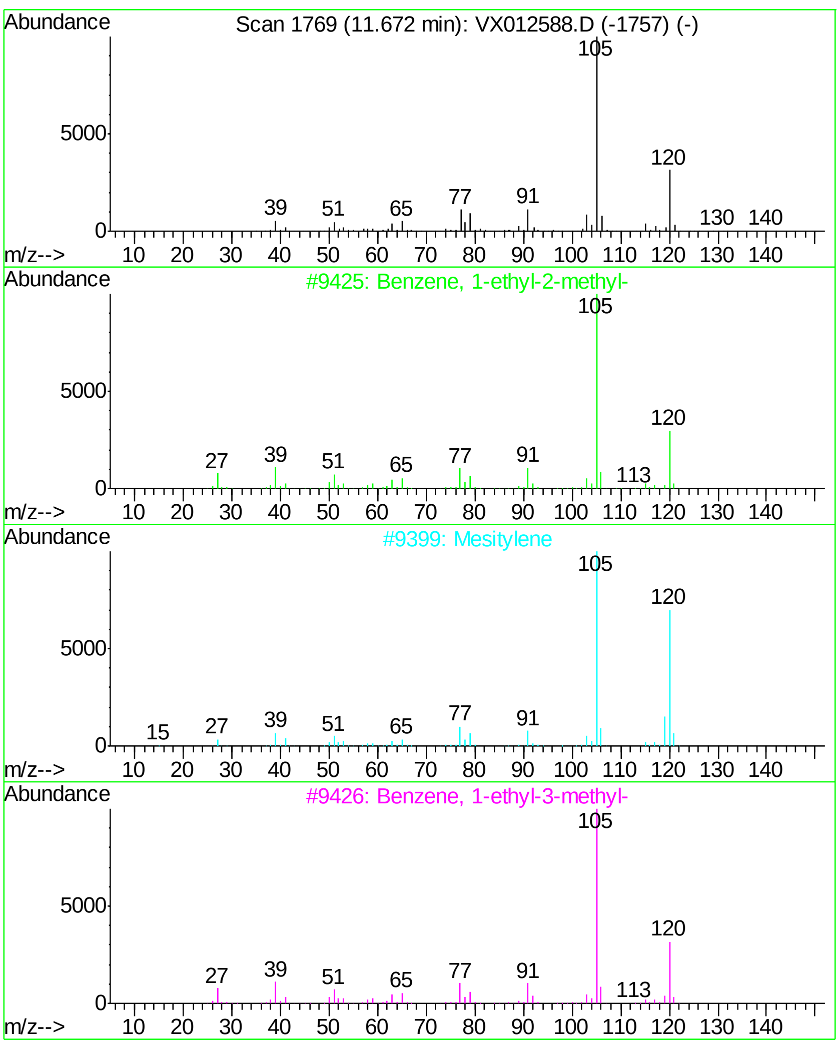
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

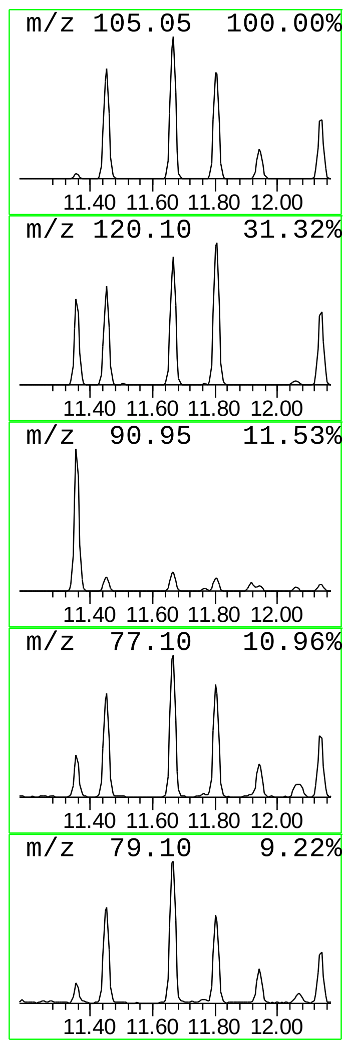
****

Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.67	102.51 ug/l	1779500	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Mesitylene	120	C9H12	000108-67-8	91
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX092019\
Data File : VX012588.D
Acq On : 21 Sep 2019 04:02
Operator : JC/SP
Sample : K4978-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : Z2-0162

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

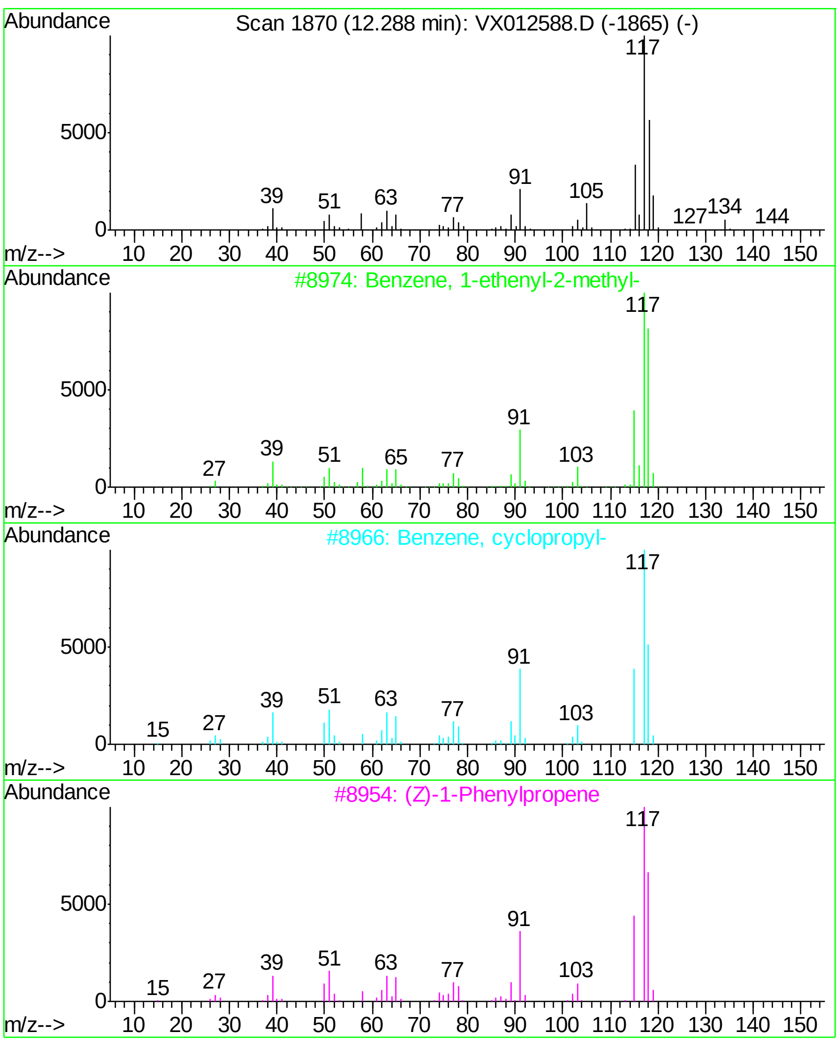
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

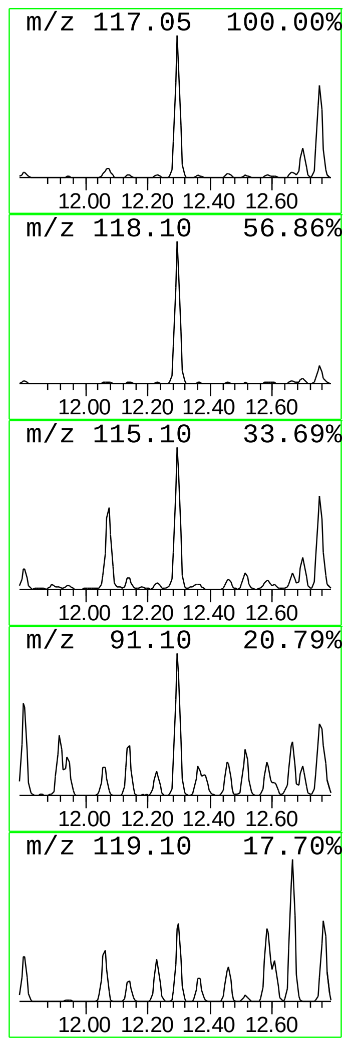
****

Peak Number 8 Benzene, 1-ethenyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	86.06 ug/l	1494020	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	86
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	70
3	(Z)-1-Phenylpropene	118	C9H10	000766-90-5	70
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	70
5	Indane	118	C9H10	000496-11-7	70





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX092019\
Data File : VX012588.D
Acq On : 21 Sep 2019 04:02
Operator : JC/SP
Sample : K4978-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
Z2-0162

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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

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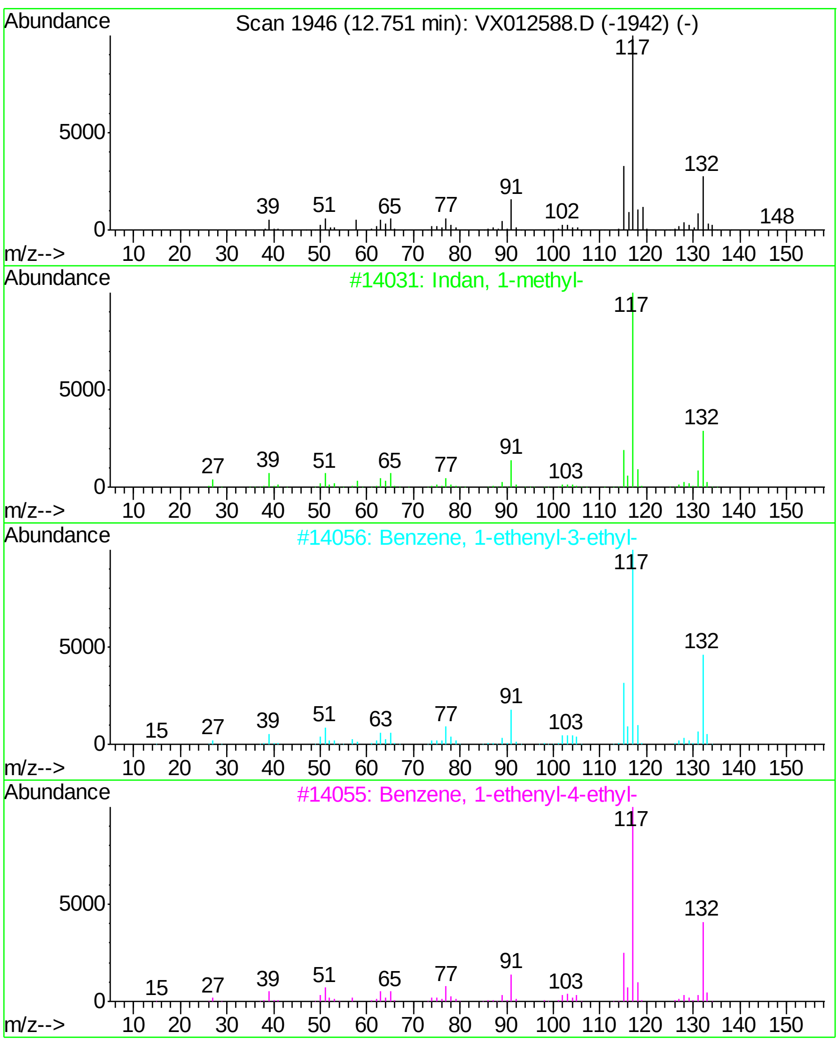
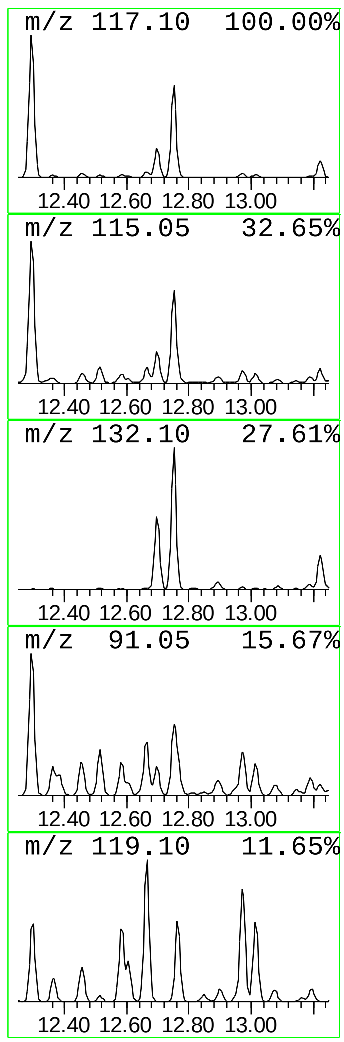
Peak Number 9 Indan, 1-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.75	56.34 ug/l	978025	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indan, 1-methyl-	132	C10H12	000767-58-8	93
2	Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	90
3	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	87
4	Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	87
5	Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	83





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX092019\
Data File : VX012588.D
Acq On : 21 Sep 2019 04:02
Operator : JC/SP
Sample : K4978-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : Z2-0162

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.M
Quant Title : SW846 8260

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

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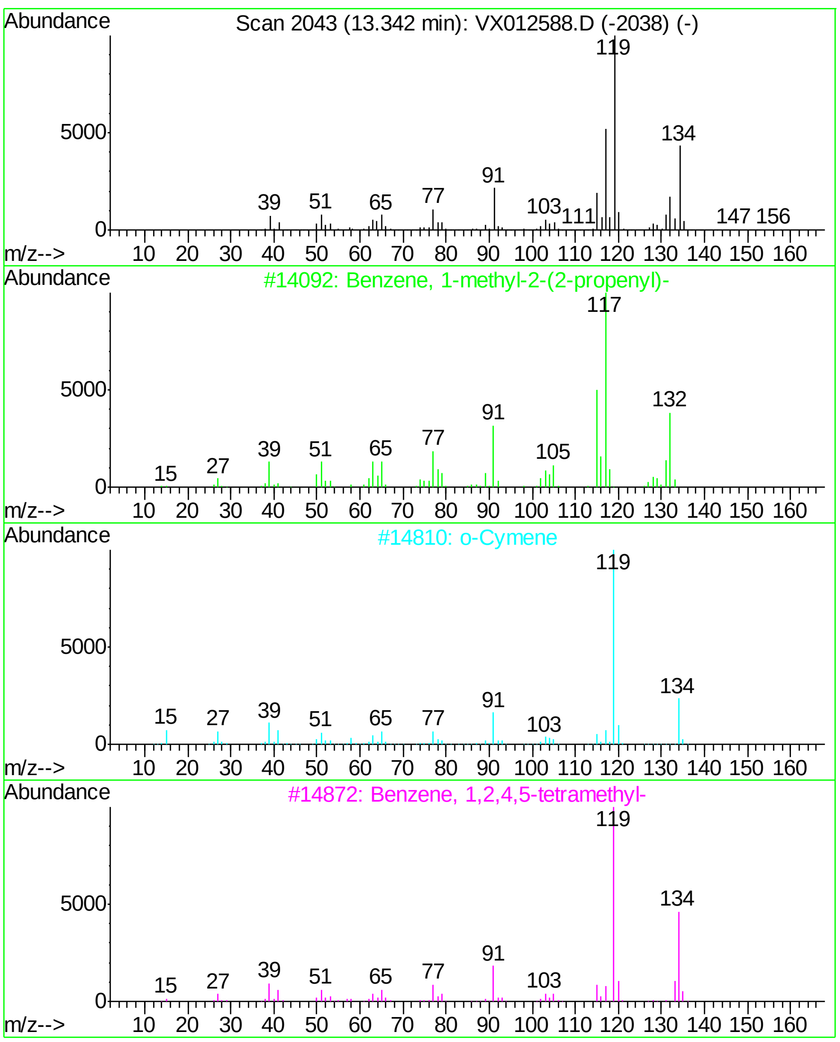
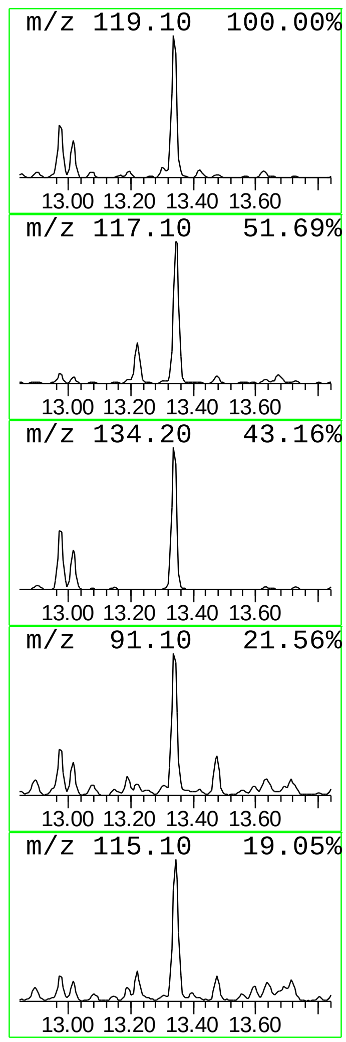
Peak Number 10 Benzene, 1-methyl-2-(2-prop... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.34	84.59 ug/l	1468490	1,4-Dichlorobenzene-d4	12.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	70
2	o-Cymene	134	C10H14	000527-84-4	64
3	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	64
4	Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	64
5	p-Cymene	134	C10H14	000099-87-6	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX092019\
Data File : VX012588.D
Acq On : 21 Sep 2019 04:02
Operator : JC/SP
Sample : K4978-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 47 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : Z2-0162

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091719W.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
Butane, 2-methyl-	1.78	56.0	ug/l	619471	1	5.65	553124	50.0
Butane, 2,3-dimet...	2.84	71.7	ug/l	793190	1	5.65	553124	50.0
Pentane, 2,3-dime...	5.72	67.8	ug/l	750563	1	5.65	553124	50.0
Cyclopentane, 1,3...	6.25	62.1	ug/l	687444	1	5.65	553124	50.0
Isopropylcyclobutane	6.35	69.2	ug/l	958023	2	6.85	692397	50.0
Benzene, 1-ethyl-...	11.67	102.5	ug/l	1779500	4	12.07	867977	50.0
Benzene, 1-etheny...	12.29	86.1	ug/l	1494020	4	12.07	867977	50.0
Indan, 1-methyl-	12.75	56.3	ug/l	978025	4	12.07	867977	50.0
Benzene, 1-methyl...	13.34	84.6	ug/l	1468490	4	12.07	867977	50.0