LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX060120\
Data File : VX016539.D
Acq On : 01 Jun 2020 19:08
Operator : JC/SP
Sample : L2831-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WC-20200529

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\82X052720W.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	1.160	9	12	20	rVB	139075	126058	2.29%	0.403%
2	1.471	59	63	76	rVB	303903	342543	6.23%	1.094%
3	1.715	98	103	109	rBV	58258	74489	1.36%	0.238%
4	2.233	182	188	197	rVV	95654	153225	2.79%	0.489%
5	2.331	198	204	211	rVV	114167	180716	3.29%	0.577%
6	2.416	211	218	234	rVB	961756	1539416	28.02%	4.916%
7	2.575	237	244	253	rVB	43487	78692	1.43%	0.251%
8	2.867	283	292	304	rBV	28780	57390	1.04%	0.183%
9	3.007	305	315	328	rBV	1380864	2952324	53.73%	9.429%
10	3.166	335	341	352	rVB	26427	63210	1.15%	0.202%
11	3.379	368	376	390	rBV	117740	273056	4.97%	0.872%
12	4.300	514	527	545	rBV5	104126	373272	6.79%	1.192%
13	4.635	571	582	597	rBV	129553	367673	6.69%	1.174%
14	5.470	706	719	730	rBV2	145569	417473	7.60%	1.333%
15	5.629	733	745	762	rVB	265258	747767	13.61%	2.388%
16	6.031	802	811	822	rBV	159396	421304	7.67%	1.346%
17	6.306	846	856	868	rBV2	81336	223951	4.08%	0.715%
18	6.708	905	922	930	rBV	118832	342950	6.24%	1.095%
19	6.830	930	942	963	rVB	409612	1008507	18.36%	3.221%
20	7.019	963	973	986	rBV	2477427	5494369	100.00%	17.548%
21	7.513	1046	1054	1067	rVB	365722	684438	12.46%	2.186%
22	7.903	1105	1118	1122	rBV	84430	181769	3.31%	0.581%
23	7.952	1122	1126	1137	rVB	104522	213643	3.89%	0.682%
24	8.549	1219	1224	1230	rVB	53654	81882	1.49%	0.262%
25	8.622	1230	1236	1241	rBV	200428	316180	5.75%	1.010%
26	8.695	1241	1248	1256	rVB	878630	1367800	24.89%	4.368%
27	8.848	1267	1273	1279	rBV	58531	92136	1.68%	0.294%
28	8.982	1289	1295	1301	rBV	768150	1119734	20.38%	3.576%
29	9.049	1301	1306	1319	rVB	101858	168130	3.06%	0.537%
30	9.287	1339	1345	1350	rVV	261437	401180	7.30%	1.281%
31	9.482	1370	1377	1383	rBV3	176007	332184	6.05%	1.061%
32	9.744	1404	1420	1429	rVB	210583	375028	6.83%	1.198%
33	9.872	1437	1441	1454	rVB	684861	914558	16.65%	2.921%
34	9.988	1454	1460	1466	rBV2	72436	121804	2.22%	0.389%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX060120\
Data File : VX016539.D
Acq On : 01 Jun 2020 19:08
Operator : JC/SP
Sample : L2831-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WC-20200529

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\82X052720W.M
Title : SW846 8260

35	10.098	1467	1478	1484	rBV	914858	1346308	24.50%	4.300%
36	10.213	1493	1497	1500	rBV	63488	78726	1.43%	0.251%
37	10.256	1500	1504	1506	rVV	108070	150157	2.73%	0.480%
38	10.311	1506	1513	1521	rVV	1062863	1413807	25.73%	4.515%
39	10.415	1525	1530	1535	rBV2	75052	110626	2.01%	0.353%
40	10.805	1586	1594	1600	rBV3	47202	100401	1.83%	0.321%
41	10.908	1605	1611	1615	rVV	82700	164437	2.99%	0.525%
42	10.951	1615	1618	1629	rVV2	122318	219241	3.99%	0.700%
43	11.049	1629	1634	1637	rVV	163723	247896	4.51%	0.792%
44	11.122	1641	1646	1655	rVV2	850206	1265319	23.03%	4.041%
45	11.207	1655	1660	1667	rVB3	158670	235400	4.28%	0.752%
46	11.329	1673	1680	1685	rBV2	83641	159530	2.90%	0.509%
47	11.378	1685	1688	1696	rVV4	85048	147333	2.68%	0.471%
48	11.445	1696	1699	1703	rVV	119242	154466	2.81%	0.493%
49	11.494	1704	1707	1715	rVV	48285	80878	1.47%	0.258%
50	11.573	1715	1720	1730	rVB	127520	190352	3.46%	0.608%
51	11.792	1751	1756	1761	rVB	107555	143094	2.60%	0.457%
52	11.841	1761	1764	1773	rBV5	22385	56480	1.03%	0.180%
53	11.945	1777	1781	1787	rBV	82812	108828	1.98%	0.348%
54	12.012	1787	1792	1796	rBV	509559	647660	11.79%	2.068%
55	12.061	1796	1800	1805	rBV	1091852	1353230	24.63%	4.322%
56	12.170	1812	1818	1823	rBV5	38253	78777	1.43%	0.252%
57	12.286	1833	1837	1842	rVB3	44899	68263	1.24%	0.218%
58	12.396	1848	1855	1863	rVB5	76271	195243	3.55%	0.624%
59	12.554	1876	1881	1886	rBV3	37229	64547	1.17%	0.206%
60	13.048	1957	1962	1966	rBV4	56220	101802	1.85%	0.325%
61	13.091	1966	1969	1974	rVB	71222	95306	1.73%	0.304%
62	13.170	1976	1982	1986	rBV5	27726	57922	1.05%	0.185%
63	13.414	2017	2022	2028	rBV4	45647	89489	1.63%	0.286%
64	14.133	2136	2140	2144	rBV2	74189	93016	1.69%	0.297%
65	14.194	2144	2150	2152	rBV6	34363	77660	1.41%	0.248%
66	14.548	2202	2208	2212	rBV4	29792	71624	1.30%	0.229%
67	14.737	2234	2239	2244	rBV3	56755	110860	2.02%	0.354%
68	15.109	2297	2300	2309	rVB2	77986	145549	2.65%	0.465%
69	15.188	2309	2313	2322	rVB6	32469	78267	1.42%	0.250%

Sum of corrected areas: 31311345

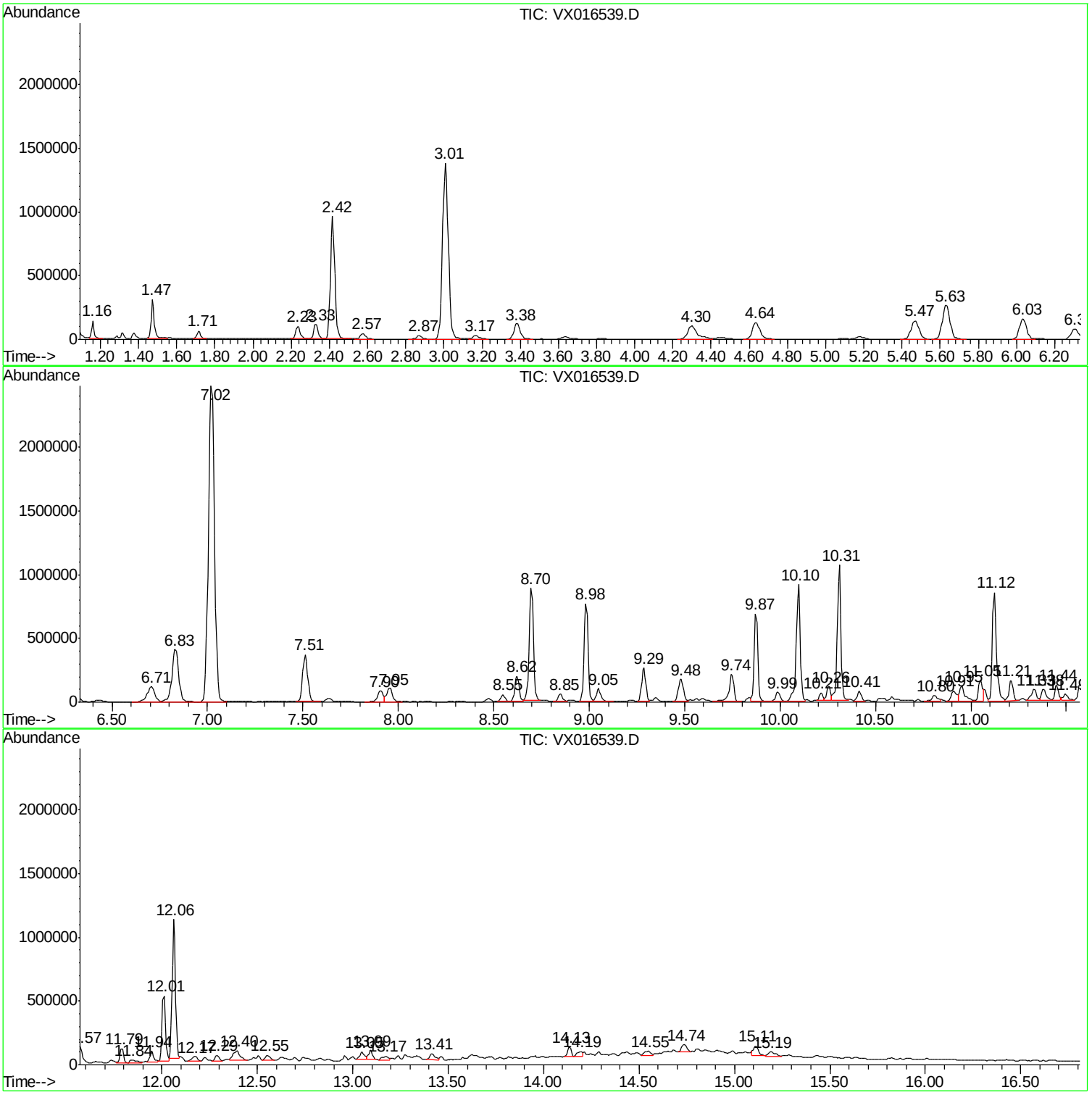
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX060120\
Data File : VX016539.D
Acq On : 01 Jun 2020 19:08
Operator : JC/SP
Sample : L2831-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WC-20200529

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X052720W.M
Quant Title : SW846 8260

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX060120\
Data File : VX016539.D
Acq On : 01 Jun 2020 19:08
Operator : JC/SP
Sample : L2831-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WC-20200529

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X052720W.M
Quant Title : SW846 8260

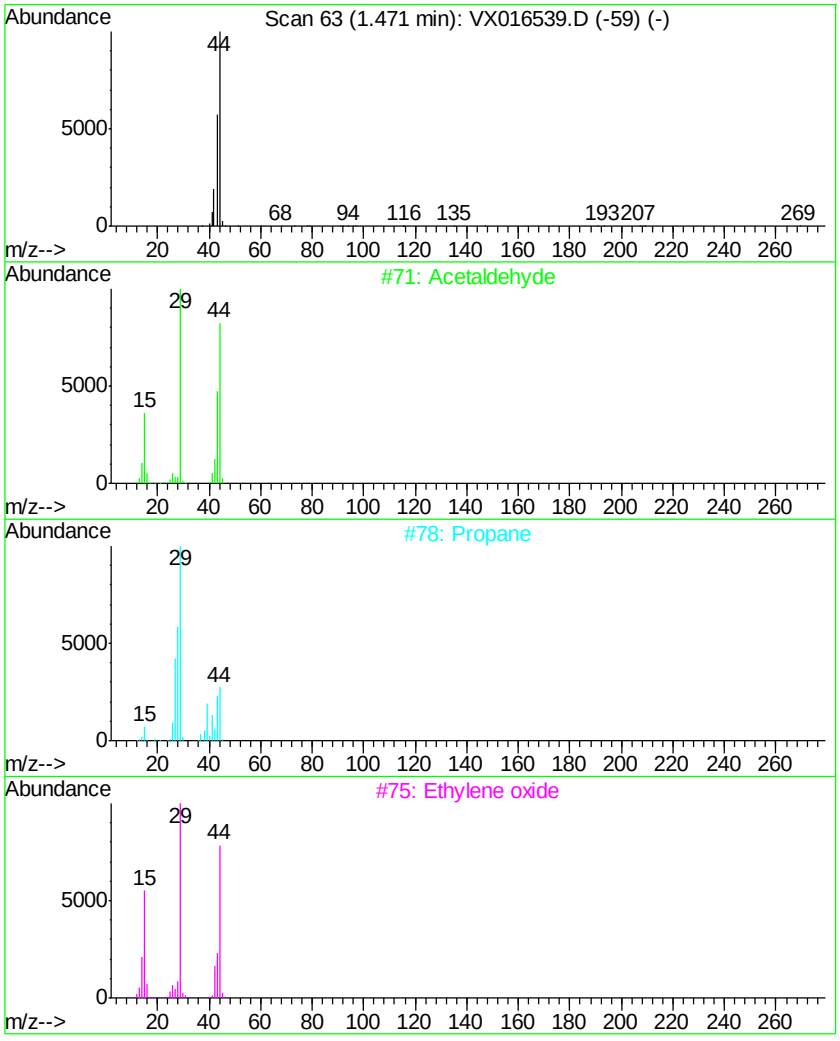
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

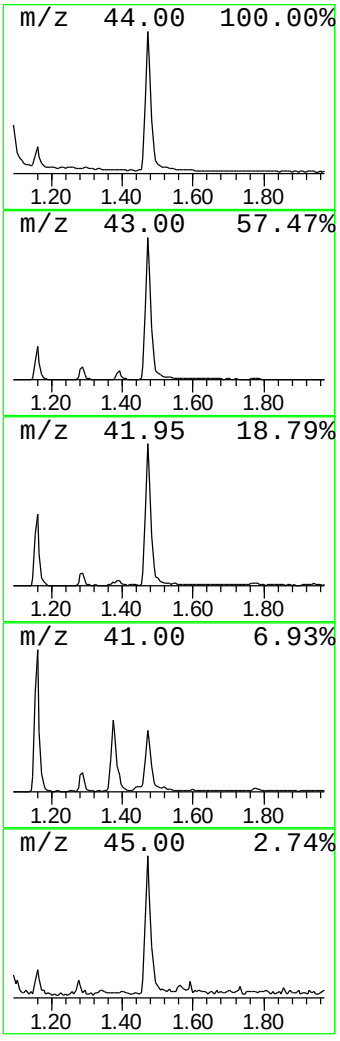
****

Peak Number 1 Acetaldehyde Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.47	22.90 ug/l	342543	Pentafluorobenzene	5.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	64
2	Propane	44	C3H8	000074-98-6	5
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Alanine	89	C3H7NO2	000056-41-7	4
5	1,2-Propanediamine	74	C3H10N2	000078-90-0	4





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX060120\
Data File : VX016539.D
Acq On : 01 Jun 2020 19:08
Operator : JC/SP
Sample : L2831-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WC-20200529

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X052720W.M
Quant Title : SW846 8260

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

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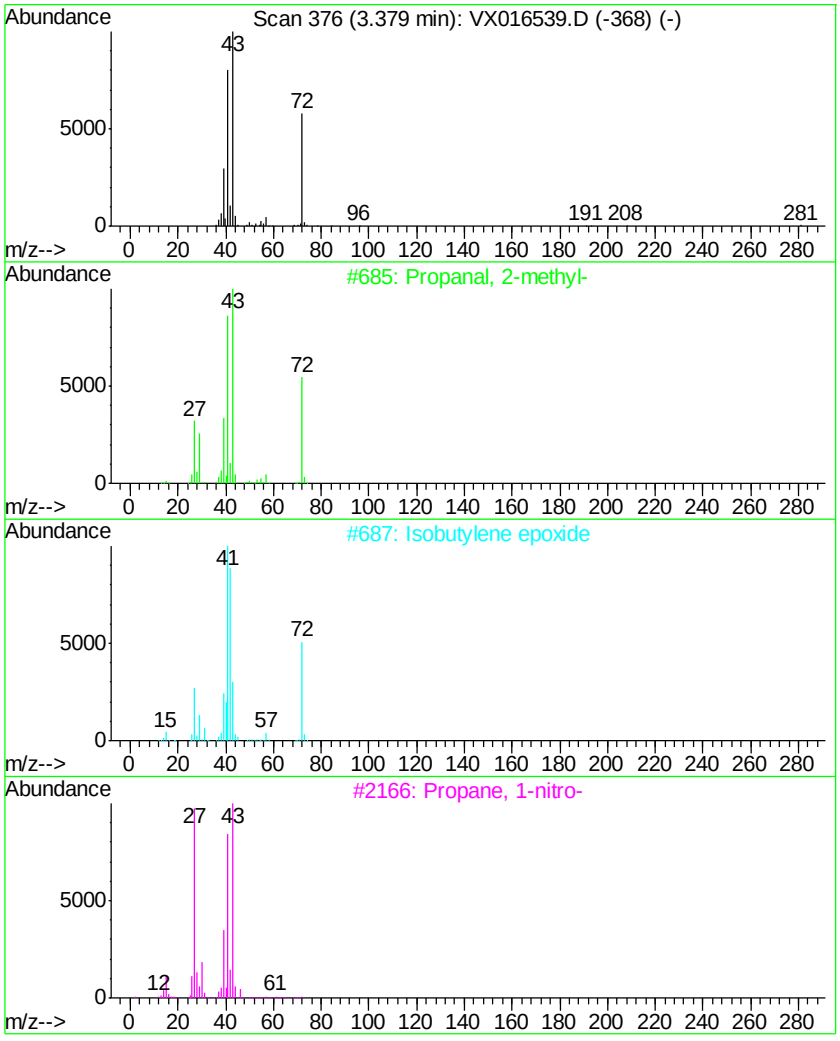
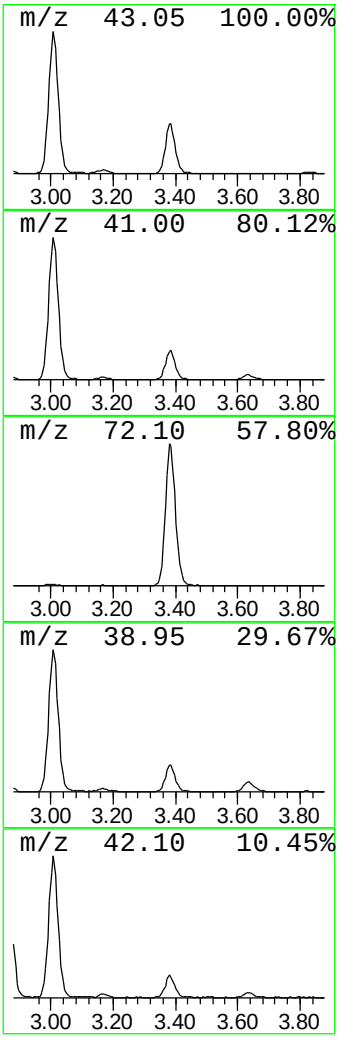
Peak Number 2 Propanal, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.38	18.26 ug/l	273056	Pentafluorobenzene	5.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal, 2-methyl-	72	C4H8O	000078-84-2	90
2	Isobutylene epoxide	72	C4H8O	000558-30-5	42
3	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	32
4	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	32
5	Isobutyl nitrite	103	C4H9NO2	000542-56-3	23





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX060120\
Data File : VX016539.D
Acq On : 01 Jun 2020 19:08
Operator : JC/SP
Sample : L2831-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WC-20200529

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X052720W.M
Quant Title : SW846 8260

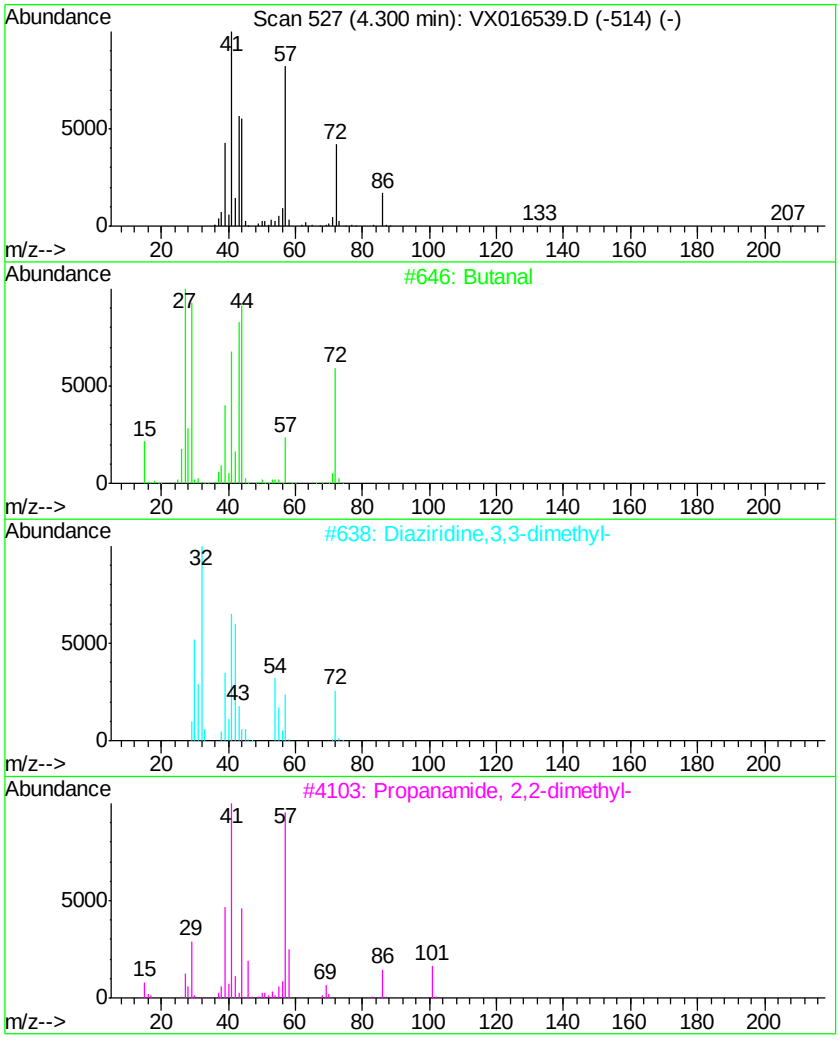
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

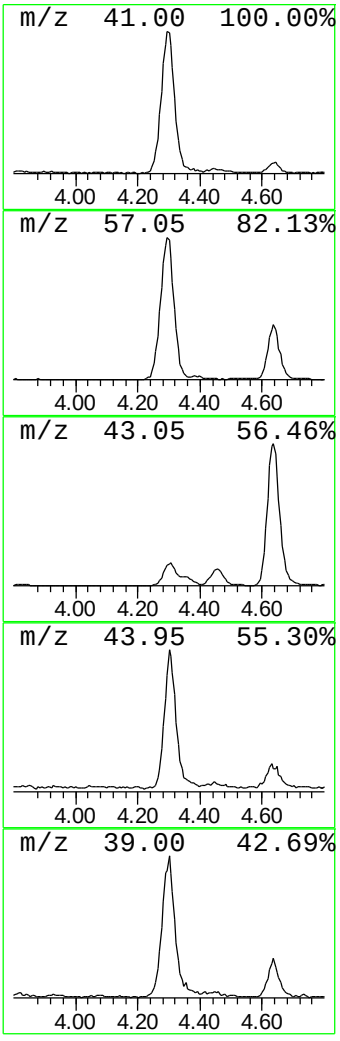
****

Peak Number 3 unknown4.30 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.30	24.96 ug/l	373272	Pentafluorobenzene	5.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	49
2	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	47
3	Propanamide, 2,2-dimethyl-	101	C5H11NO	000754-10-9	45
4	5,9-Dodecadien-2-one, 6,10-dimet...	208	C14H24O	1000132-10-9	35
5	Ethene, ethoxy-	72	C4H8O	000109-92-2	27





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX060120\
Data File : VX016539.D
Acq On : 01 Jun 2020 19:08
Operator : JC/SP
Sample : L2831-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WC-20200529

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X052720W.M
Quant Title : SW846 8260

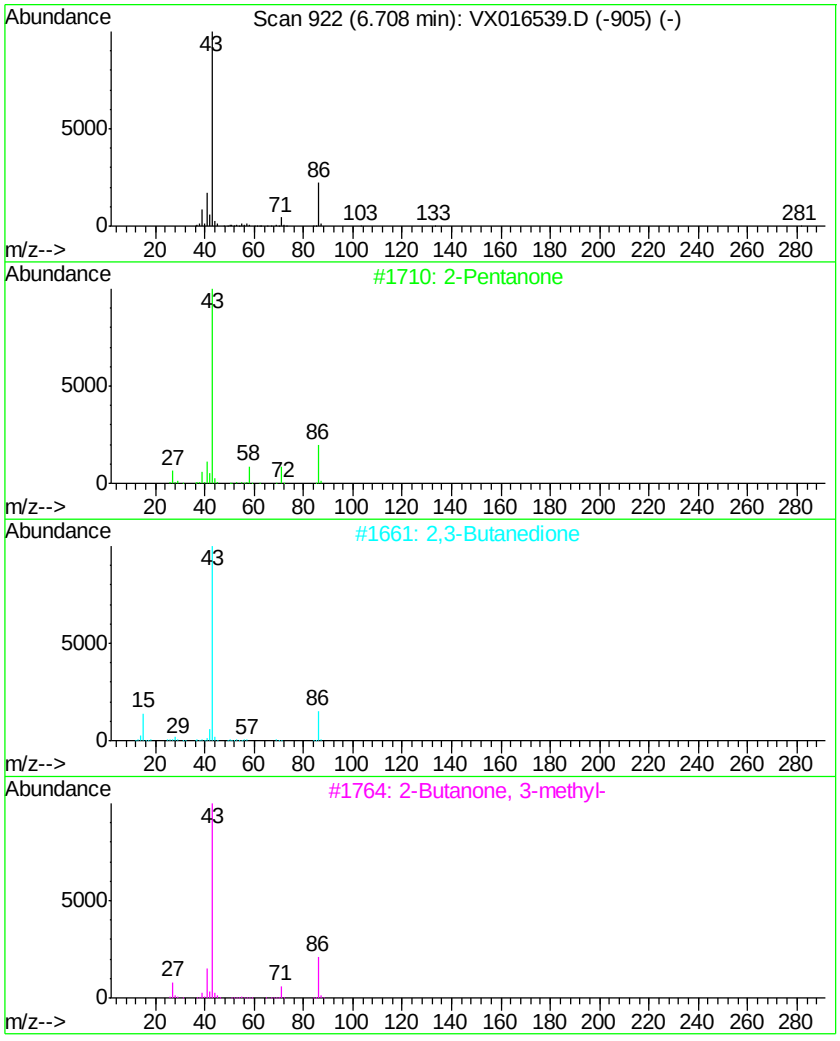
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

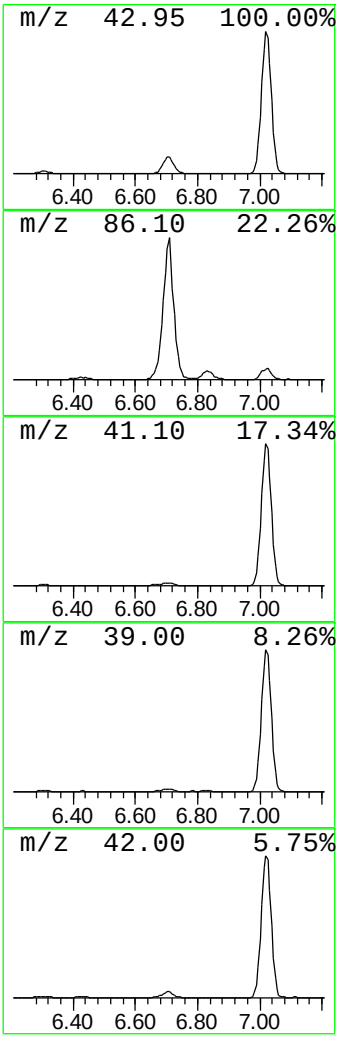
****

Peak Number 4 2-Pentanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.71	17.00 ug/l	342950	1,4-Difluorobenzene	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	59
2	2,3-Butanedione	86	C4H6O2	000431-03-8	58
3	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	53
4	2,3-Hexanedione	114	C6H10O2	003848-24-6	9
5	Propanal, 2-methyl-	72	C4H8O	000078-84-2	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX060120\
Data File : VX016539.D
Acq On : 01 Jun 2020 19:08
Operator : JC/SP
Sample : L2831-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WC-20200529

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X052720W.M
Quant Title : SW846 8260

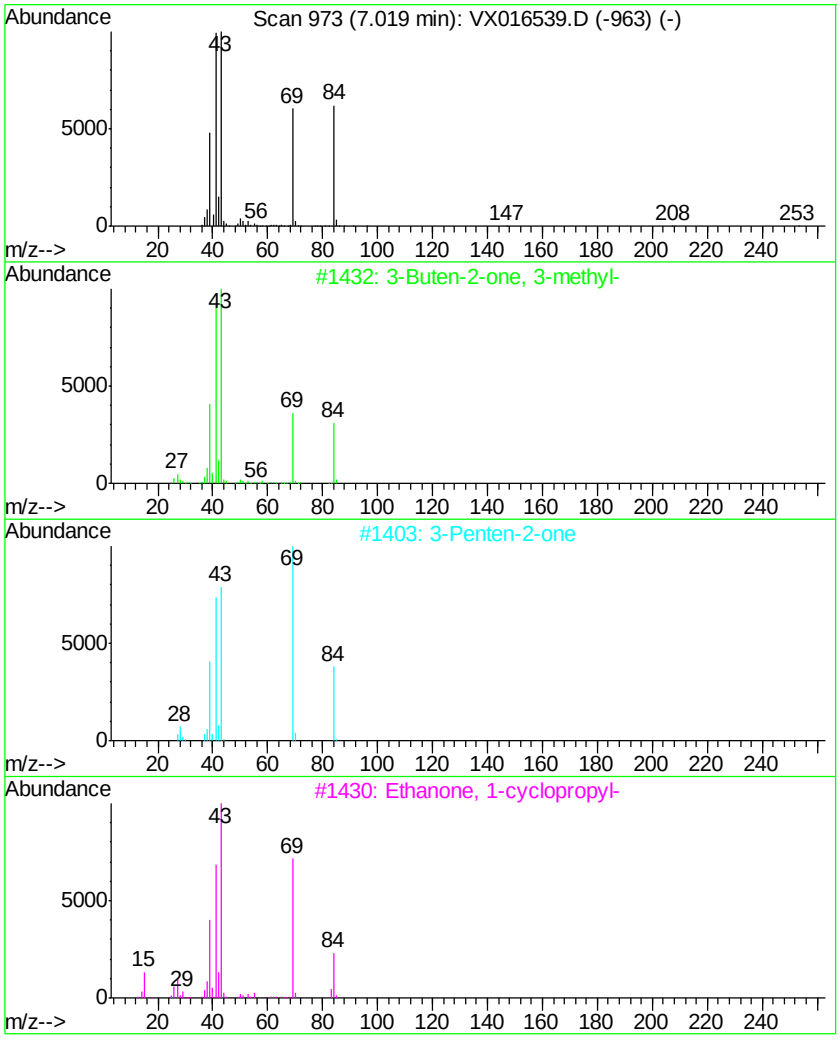
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

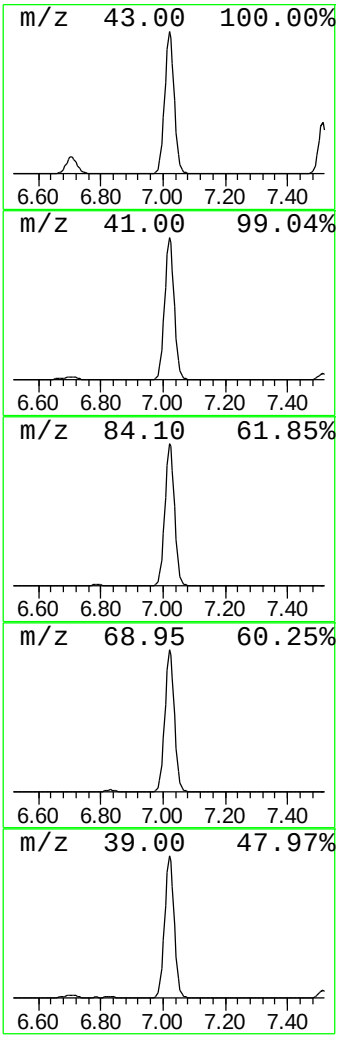
****

Peak Number 5 3-Buten-2-one, 3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.02	272.40 ug/l	5494370	1,4-Difluorobenzene	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-2-one, 3-methyl-	84	C5H8O	000814-78-8	91
2	3-Penten-2-one	84	C5H8O	000625-33-2	90
3	Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	59
4	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	38
5	3-Penten-2-one, (E)-	84	C5H8O	003102-33-8	35





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX060120\
Data File : VX016539.D
Acq On : 01 Jun 2020 19:08
Operator : JC/SP
Sample : L2831-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WC-20200529

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X052720W.M
Quant Title : SW846 8260

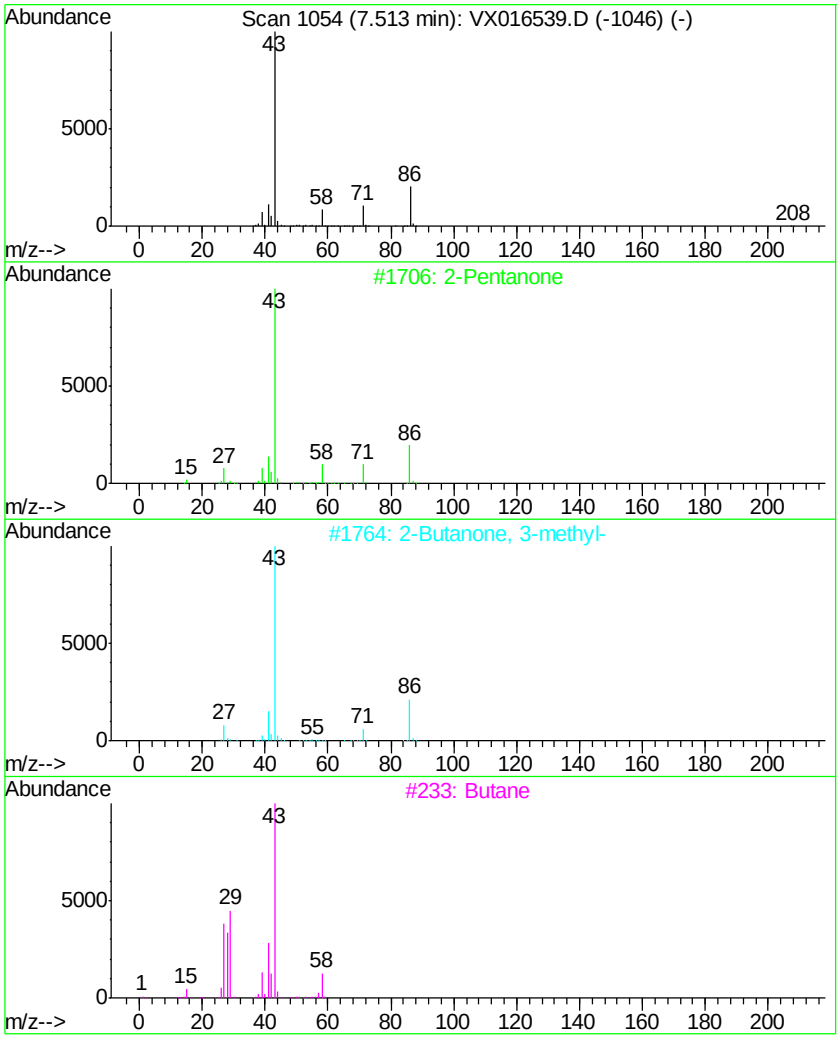
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

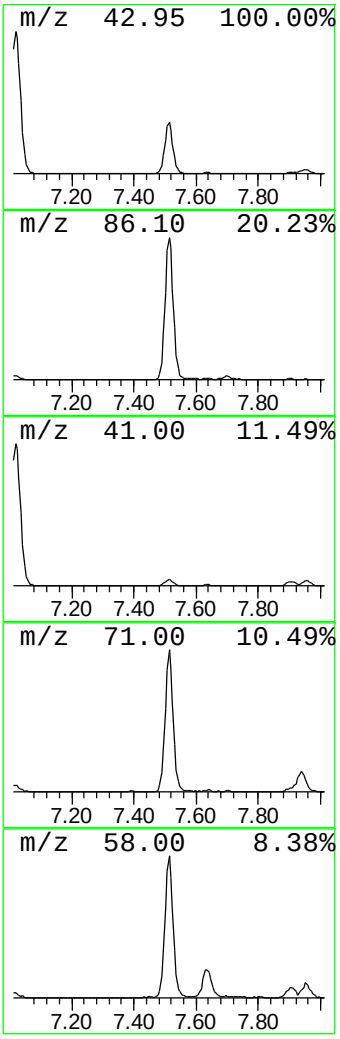
****

Peak Number 6 2-Pentanone, 3-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.51	33.93 ug/l	684438	1,4-Difluorobenzene	6.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	91
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	64
3	Butane	58	C4H10	000106-97-8	9
4	2,3-Butanedione	86	C4H6O2	000431-03-8	9
5	2-Pentanone, 3-ethyl-	114	C7H14O	006137-03-7	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX060120\
Data File : VX016539.D
Acq On : 01 Jun 2020 19:08
Operator : JC/SP
Sample : L2831-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WC-20200529

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X052720W.M
Quant Title : SW846 8260

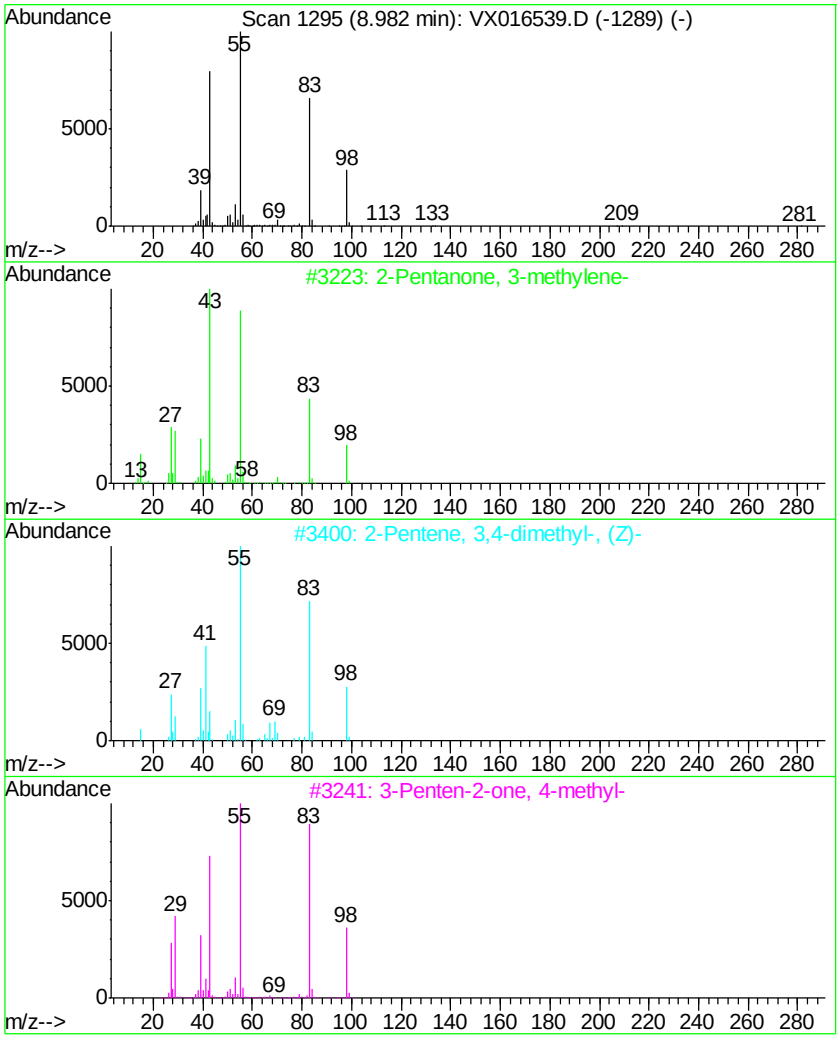
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

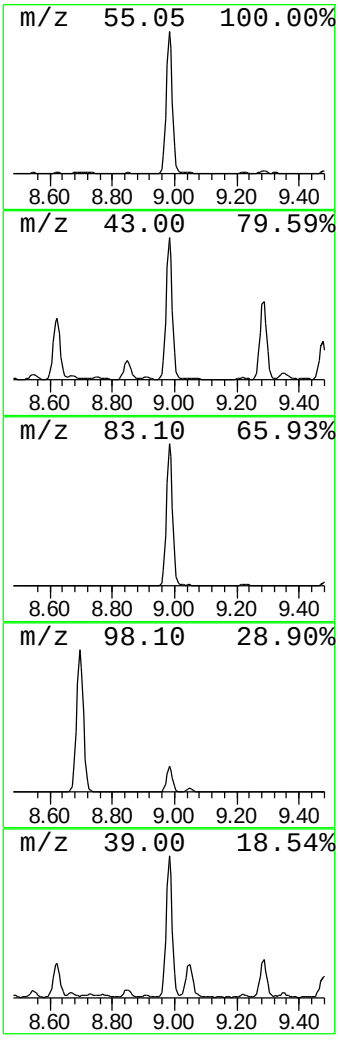
****

Peak Number 7 2-Pentanone, 3-methylene- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.98	41.59 ug/l	1119730	Chlorobenzene-d5	10.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	91
2	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	74
3	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	74
4	3-Hexen-2-one	98	C6H10O	000763-93-9	72
5	2(5H)-Furanone, 5-methyl-	98	C5H6O2	000591-11-7	64





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX060120\
Data File : VX016539.D
Acq On : 01 Jun 2020 19:08
Operator : JC/SP
Sample : L2831-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WC-20200529

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X052720W.M
Quant Title : SW846 8260

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

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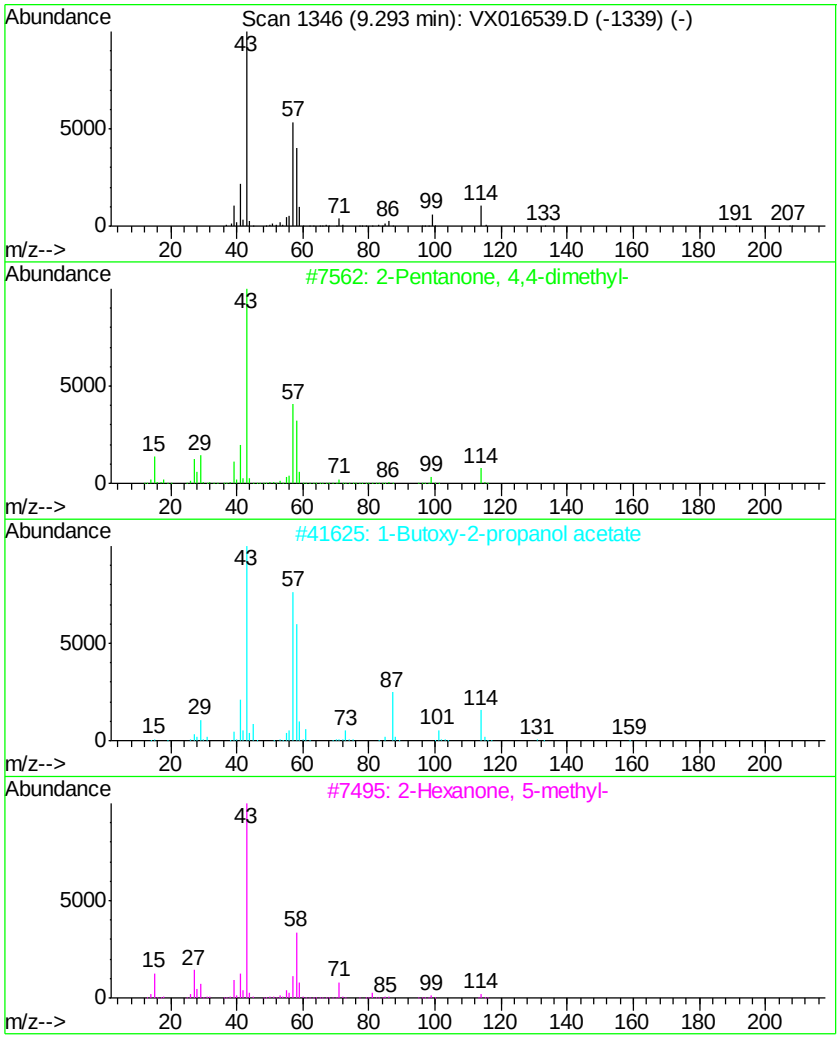
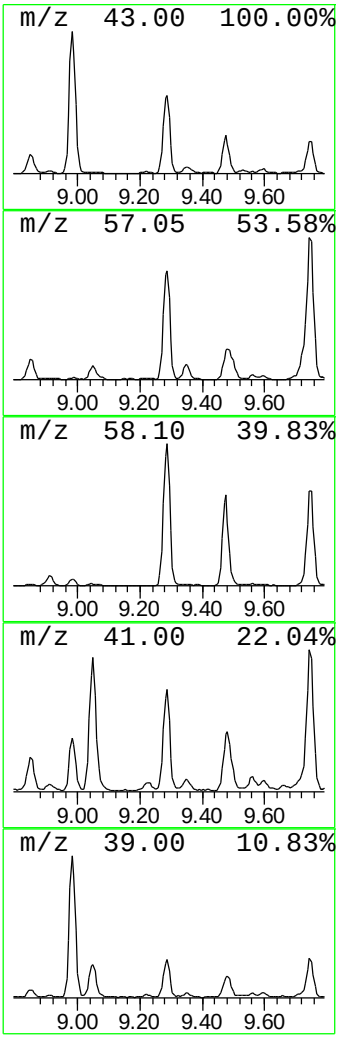
Peak Number 8 2-Pentanone, 4,4-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.29	14.90 ug/l	401180	Chlorobenzene-d5	10.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	91
2	1-Butoxy-2-propanol acetate	174	C9H18O3	085409-76-3	78
3	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	72
4	2-Methoxyethyl 2-methylbutanoate	160	C8H16O3	1000366-96-4	33
5	Butanal, 2-methyl-	86	C5H10O	000096-17-3	28





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX060120\
Data File : VX016539.D
Acq On : 01 Jun 2020 19:08
Operator : JC/SP
Sample : L2831-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WC-20200529

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X052720W.M
Quant Title : SW846 8260

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

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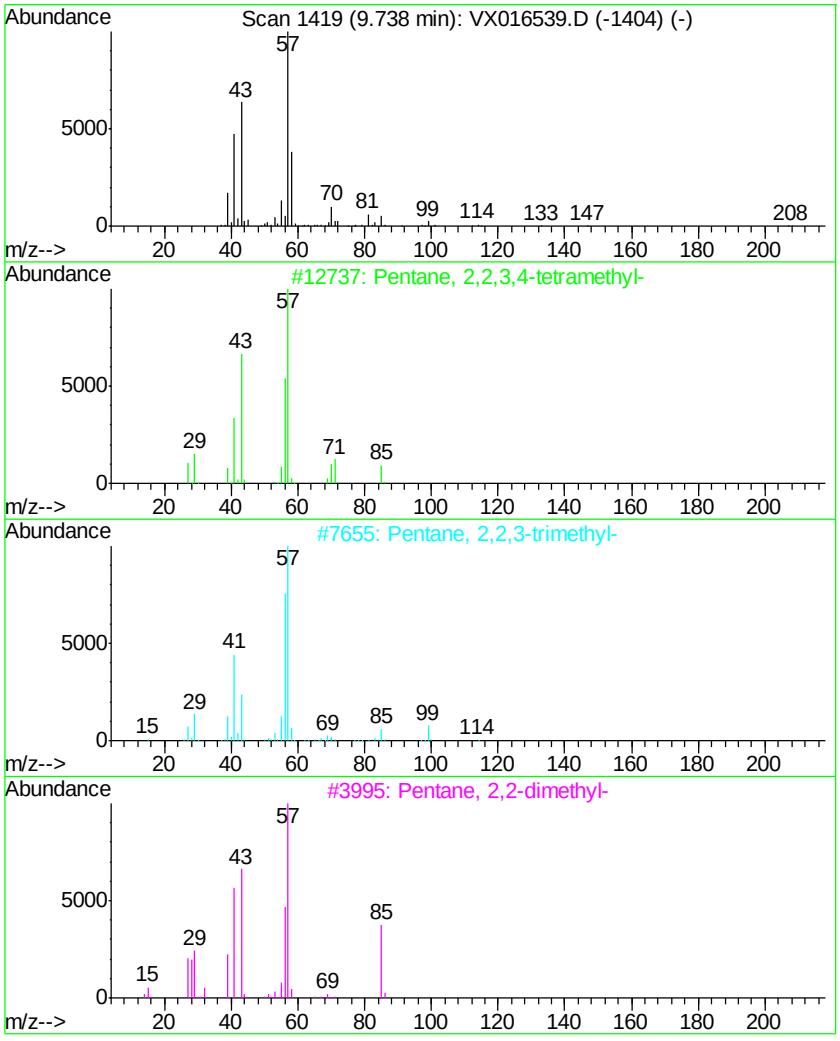
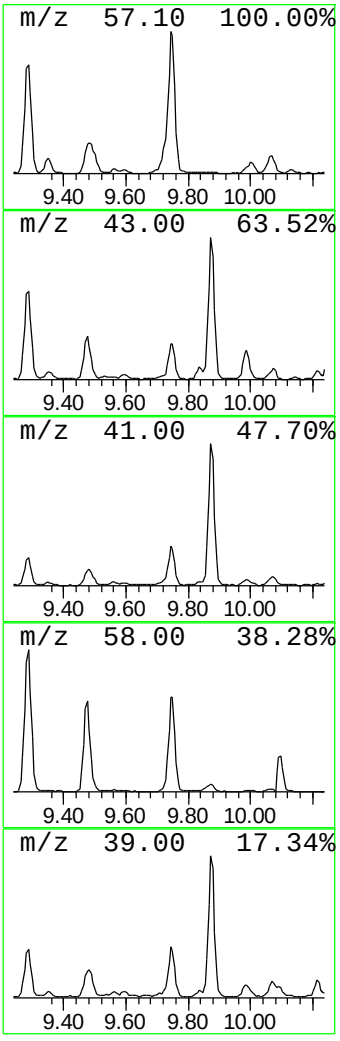
Peak Number 9 unknown9.74 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.74	13.93 ug/l	375028	Chlorobenzene-d5	10.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	22
2	Pentane, 2,2,3-trimethyl-	114	C8H18	000564-02-3	22
3	Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	14
4	Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	12
5	2-Pentanone, 3-ethyl-	114	C7H14O	006137-03-7	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX060120\
Data File : VX016539.D
Acq On : 01 Jun 2020 19:08
Operator : JC/SP
Sample : L2831-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WC-20200529

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X052720W.M
Quant Title : SW846 8260

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

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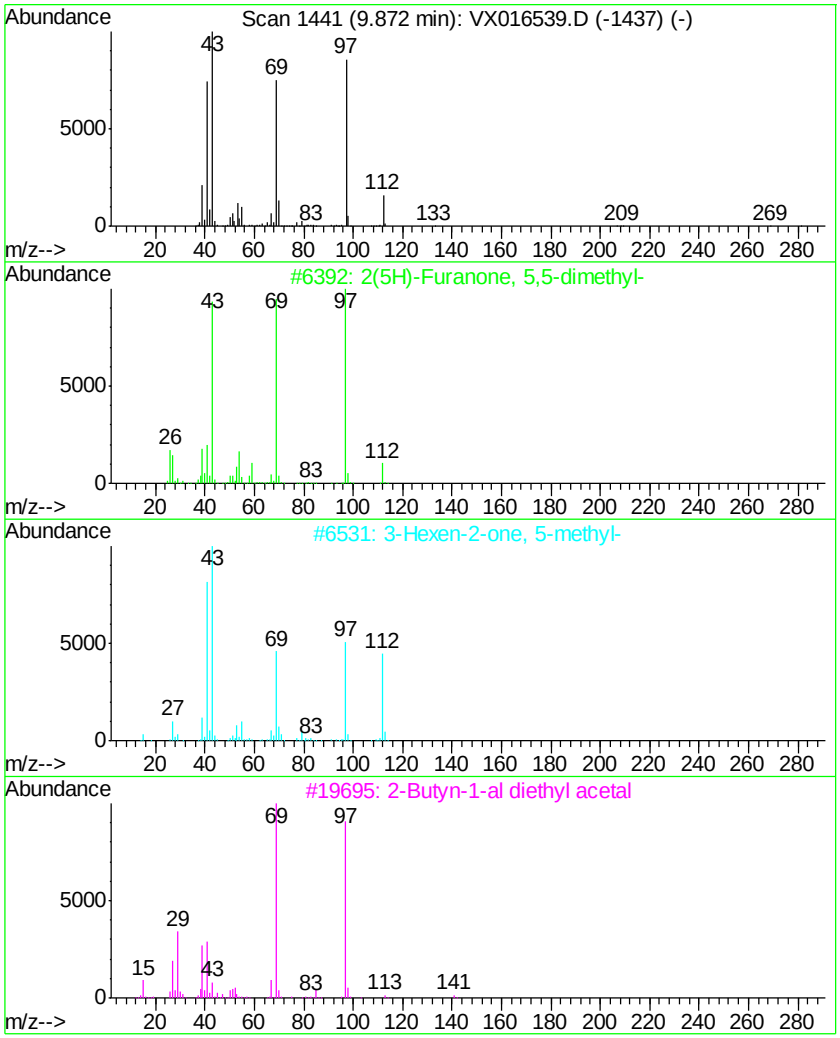
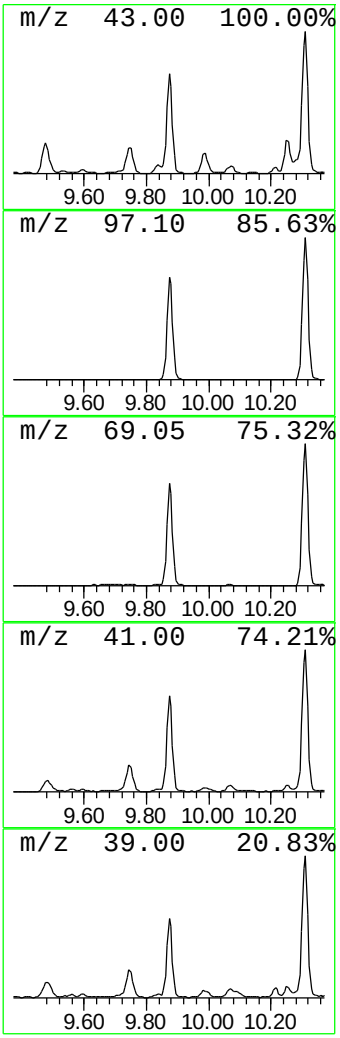
Peak Number 10 2(5H)-Furanone, 5,5-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.87	33.97 ug/l	914558	Chlorobenzene-d5	10.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(5H)-Furanone, 5,5-dimethyl-	112	C6H8O2	020019-64-1	83
2	3-Hexen-2-one, 5-methyl-	112	C7H12O	005166-53-0	59
3	2-Butyn-1-al diethyl acetal	142	C8H14O2	002806-97-5	53
4	5-Hexen-2-one, 5-methyl-	112	C7H12O	003240-09-3	47
5	2-Hexene, 2,5-dimethyl-	112	C8H16	003404-78-2	46





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX060120\
Data File : VX016539.D
Acq On : 01 Jun 2020 19:08
Operator : JC/SP
Sample : L2831-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : WC-20200529

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X052720W.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
Acetaldehyde	1.47	22.9	ug/l	342543	1	5.63	747767	50.0
Propanal, 2-methyl-	3.38	18.3	ug/l	273056	1	5.63	747767	50.0
unknown4.30	4.30	25.0	ug/l	373272	1	5.63	747767	50.0
2-Pentanone	6.71	17.0	ug/l	342950	2	6.83	1008510	50.0
3-Buten-2-one, 3-...	7.02	272.4	ug/l	5494370	2	6.83	1008510	50.0
2-Pentanone, 3-et...	7.51	33.9	ug/l	684438	2	6.83	1008510	50.0
2-Pentanone, 3-me...	8.98	41.6	ug/l	1119730	3	10.10	1346310	50.0
2-Pentanone, 4,4-...	9.29	14.9	ug/l	401180	3	10.10	1346310	50.0
unknown9.74	9.74	13.9	ug/l	375028	3	10.10	1346310	50.0
2(5H)-Furanone, 5...	9.87	34.0	ug/l	914558	3	10.10	1346310	50.0