LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100418\
Data File : VX004973.D
Acq On : 03 Oct 2018 17:06
Operator : JC/MD
Sample : J5214-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : N48719

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	1.483	50	54	76	rBV	13027239	16068915	7.50%	0.412%
2	2.477	205	217	237	rVV3	35245267	102978399	48.05%	2.641%
3	3.099	306	319	327	rBV	2466986	6678724	3.12%	0.171%
4	4.367	507	527	547	rBV4	2307776	9567021	4.46%	0.245%
5	4.830	572	603	610	rBV2	28212443	177254178	82.71%	4.547%
6	4.952	610	623	637	rVB2	3671019	12030679	5.61%	0.309%
7	5.592	709	728	738	rBV2	2868423	10452466	4.88%	0.268%
8	6.159	797	821	828	rBV	19325453	55046727	25.69%	1.412%
9	6.793	914	925	932	rVB	13869214	39523424	18.44%	1.014%
10	7.464	1017	1035	1043	rBV	2762740	7818955	3.65%	0.201%
11	7.628	1043	1062	1067	rVV2	38754262	143643939	67.03%	3.685%
12	7.769	1077	1085	1093	rVB	14209239	28650862	13.37%	0.735%
13	7.854	1093	1099	1103	rBV	3396388	5669827	2.65%	0.145%
14	8.012	1111	1125	1136	rBV4	3020834	9624745	4.49%	0.247%
15	8.384	1175	1186	1196	rBV3	12917399	29913851	13.96%	0.767%
16	8.500	1196	1205	1210	rBV2	5496957	12022727	5.61%	0.308%
17	8.561	1210	1215	1220	rVB2	6459367	10876167	5.07%	0.279%
18	8.634	1222	1227	1230	rBV	6478730	9631901	4.49%	0.247%
19	8.695	1230	1237	1246	rVB	19619567	44932600	20.97%	1.153%
20	8.823	1246	1258	1263	rBV4	71391449	182475244	85.14%	4.681%
21	8.903	1263	1271	1274	rBV	19222349	32156200	15.00%	0.825%
22	9.390	1342	1351	1357	rVB	20604835	33044325	15.42%	0.848%
23	9.530	1366	1374	1378	rVV2	35884374	71470879	33.35%	1.833%
24	9.573	1378	1381	1385	rVV	14440485	21304017	9.94%	0.546%
25	9.628	1385	1390	1400	rVB	37537919	68702394	32.06%	1.762%
26	9.732	1400	1407	1412	rVB2	3199311	7074283	3.30%	0.181%
27	9.847	1419	1426	1429	rBV2	3399037	6891836	3.22%	0.177%
28	9.927	1434	1439	1443	rVB4	5178294	7818948	3.65%	0.201%
29	10.043	1451	1458	1460	rBV2	6310500	14177498	6.62%	0.364%
30	10.073	1461	1463	1467	rVB3	5847507	7013290	3.27%	0.180%
31	10.128	1467	1472	1476	rVB4	5818577	11509866	5.37%	0.295%
32	10.219	1476	1487	1490	rBV3	7950614	25588570	11.94%	0.656%
33	10.274	1490	1496	1501	rVB4	57939222	105073674	49.03%	2.695%
34	10.323	1501	1504	1505	rBV	6724239	7865937	3.67%	0.202%

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Integrator: RTE
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Title : SW846 8260

35	10.372	1505	1512	1513	rBV3	65819721	101768406	47.49%	2.610%
36	10.469	1525	1528	1531	rBV	11559695	16011796	7.47%	0.411%
37	10.591	1543	1548	1550	rBV2	8088549	11926202	5.56%	0.306%
38	10.664	1555	1560	1563	rVV2	10202298	17152195	8.00%	0.440%
39	10.738	1563	1572	1580	rVV4	83020870	196136591	91.52%	5.031%
40	10.847	1580	1590	1595	rVV2	44138556	71673288	33.44%	1.838%
41	10.902	1596	1599	1604	rVV3	6661330	12728268	5.94%	0.326%
42	10.963	1605	1609	1615	rVV3	24608287	41367944	19.30%	1.061%
43	11.030	1615	1620	1627	rVB3	38873354	67816963	31.64%	1.740%
44	11.103	1627	1632	1637	rBV4	8461183	17453628	8.14%	0.448%
45	11.170	1637	1643	1647	rVV6	6470274	14431175	6.73%	0.370%
46	11.213	1647	1650	1652	rVV2	5639723	8265523	3.86%	0.212%
47	11.256	1652	1657	1662	rVV3	24509684	46027250	21.48%	1.181%
48	11.311	1662	1666	1670	rVV2	11079523	19382941	9.04%	0.497%
49	11.378	1670	1677	1683	rVB2	34279374	70642063	32.96%	1.812%
50	11.463	1683	1691	1697	rBV2	90556302	214313573	100.00%	5.497%
51	11.536	1697	1703	1710	rVB5	70164745	126517949	59.03%	3.245%
52	11.640	1713	1720	1723	rBV3	15522509	27689700	12.92%	0.710%
53	11.689	1723	1728	1733	rBV	50081234	69724927	32.53%	1.788%
54	11.743	1733	1737	1740	rBV2	14419225	19774493	9.23%	0.507%
55	11.780	1740	1743	1746	rVB3	8387159	10076437	4.70%	0.258%
56	11.847	1746	1754	1758	rVB3	86723270	202516244	94.50%	5.195%
57	11.914	1761	1765	1777	rBV4	20671893	40502629	18.90%	1.039%
58	12.048	1777	1787	1792	rBV5	25138932	54192092	25.29%	1.390%
59	12.164	1800	1806	1810	rBV2	55349522	93268481	43.52%	2.392%
60	12.207	1810	1813	1818	rVB5	7294290	14425098	6.73%	0.370%
61	12.317	1827	1831	1833	rBV	33803797	45887599	21.41%	1.177%
62	12.341	1833	1835	1839	rVV2	32957393	36893580	17.21%	0.946%
63	12.390	1839	1843	1849	rVB4	45126584	74109141	34.58%	1.901%
64	12.469	1853	1856	1857	rVV2	8134239	8408410	3.92%	0.216%
65	12.493	1857	1860	1864	rVV	19369982	25305400	11.81%	0.649%
66	12.536	1864	1867	1873	rVB2	21527335	33470362	15.62%	0.859%
67	12.603	1873	1878	1880	rBV	27840643	39548423	18.45%	1.014%
68	12.634	1880	1883	1887	rVB3	23555446	30494705	14.23%	0.782%
69	12.688	1887	1892	1895	rVB2	32068352	39476929	18.42%	1.013%
70	12.719	1895	1897	1900	rVB2	5933869	6206091	2.90%	0.159%
71	12.774	1903	1906	1909	rBV2	4775039	6259100	2.92%	0.161%

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Title : SW846 8260

72	12.877	1920	1923	1927	rVB	32611148	44250930	20.65%	1.135%
73	12.920	1927	1930	1933	rVB	9849519	9540357	4.45%	0.245%
74	12.993	1938	1942	1945	rVV	19474267	22426910	10.46%	0.575%
75	13.036	1945	1949	1954	rVB2	38992944	50723301	23.67%	1.301%
76	13.091	1954	1958	1960	rBV	9976784	14220359	6.64%	0.365%
77	13.140	1964	1966	1970	rVB2	7262465	6734672	3.14%	0.173%
78	13.231	1977	1981	1985	rVB2	17569510	24797695	11.57%	0.636%
79	13.280	1985	1989	1992	rBV2	8288783	9697406	4.52%	0.249%
80	13.335	1992	1998	2000	rBV3	32210328	45437908	21.20%	1.166%
81	13.359	2000	2002	2007	rVB2	28050467	33886294	15.81%	0.869%
82	13.420	2007	2012	2020	rVB6	15633307	31840081	14.86%	0.817%
83	13.493	2020	2024	2030	rVB5	7602985	14285038	6.67%	0.366%
84	13.572	2033	2037	2041	rVB5	5449680	7412719	3.46%	0.190%
85	13.652	2046	2050	2051	rBV3	9434967	11423620	5.33%	0.293%
86	13.670	2051	2053	2057	rVB	10009651	10855242	5.07%	0.278%
87	13.749	2062	2066	2067	rBV2	5240824	7042569	3.29%	0.181%
88	13.786	2068	2072	2076	rVV	37501460	47675676	22.25%	1.223%
89	13.859	2077	2084	2087	rVV2	52064246	84274239	39.32%	2.162%
90	13.902	2087	2091	2094	rVV	20469766	28833263	13.45%	0.740%
91	13.938	2094	2097	2103	rVV	12884995	18105838	8.45%	0.464%
92	14.097	2120	2123	2126	rVB2	9393435	10623601	4.96%	0.273%
93	14.243	2142	2147	2150	rBV3	5965348	8155236	3.81%	0.209%
94	14.334	2157	2162	2166	rVB2	7847243	10674481	4.98%	0.274%
95	14.469	2181	2184	2192	rVB3	6840759	13303734	6.21%	0.341%
96	14.578	2198	2202	2205	rVB	5576180	5814032	2.71%	0.149%
97	14.706	2219	2223	2228	rVV	25973822	32220578	15.03%	0.826%
98	14.847	2243	2246	2253	rVB2	11030998	13947260	6.51%	0.358%
99	14.944	2258	2262	2269	rVB	5232486	7726991	3.61%	0.198%
100	15.231	2305	2309	2314	rVV	4302180	6219602	2.90%	0.160%

Sum of corrected areas: 3898548296

LSC Report - Integrated Chromatogram

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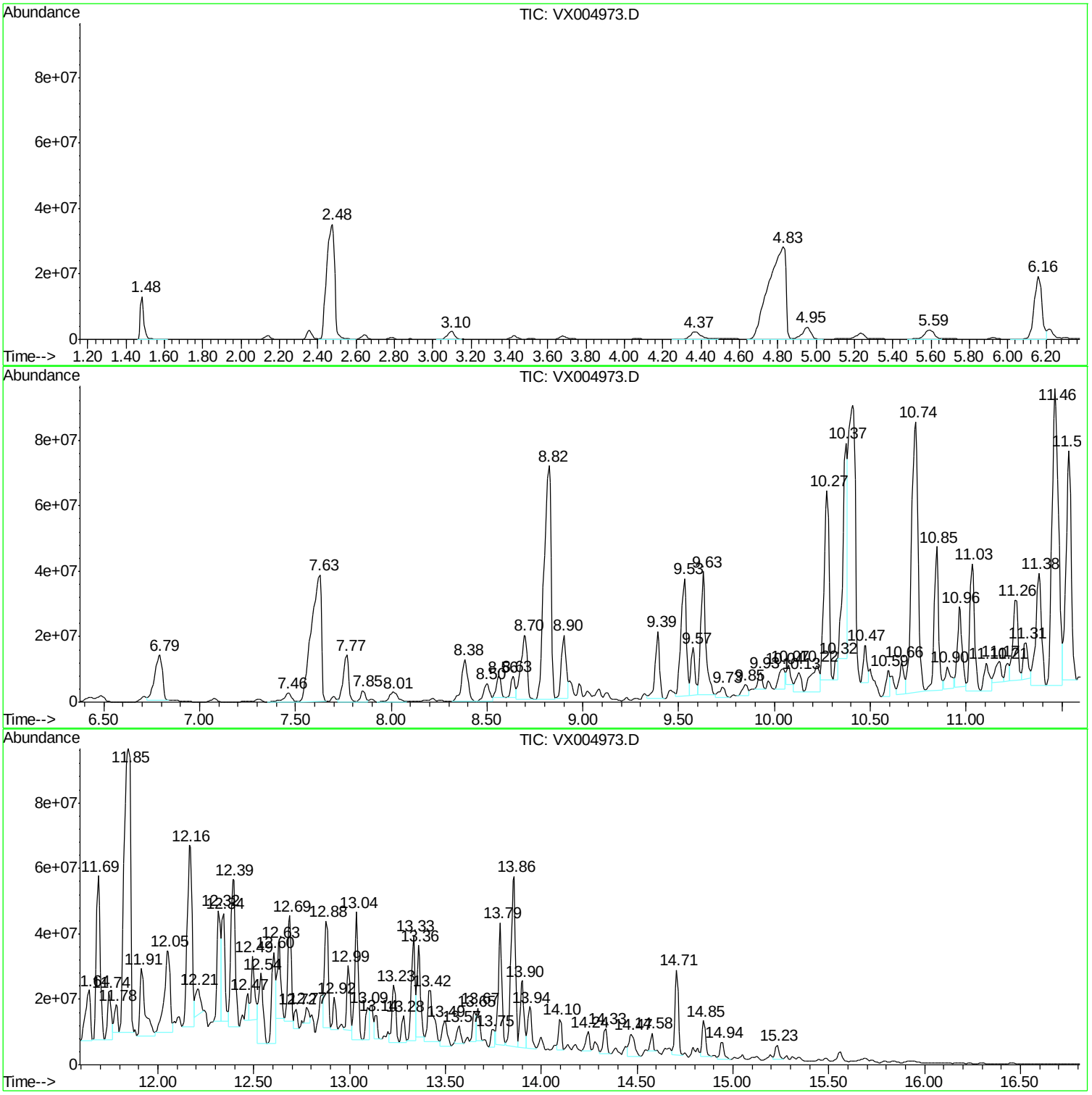
Instrument : MSVOA_X
ClientSampleId : N48719

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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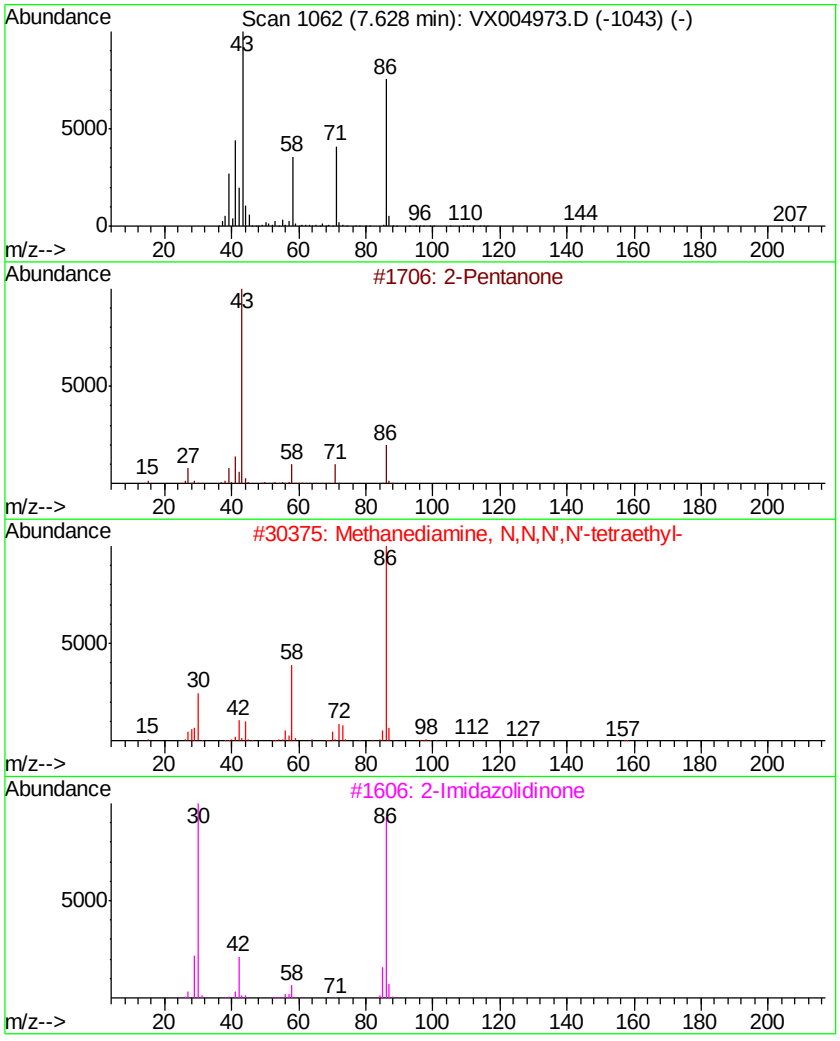
TIC Integration Parameters: LSCINT.P

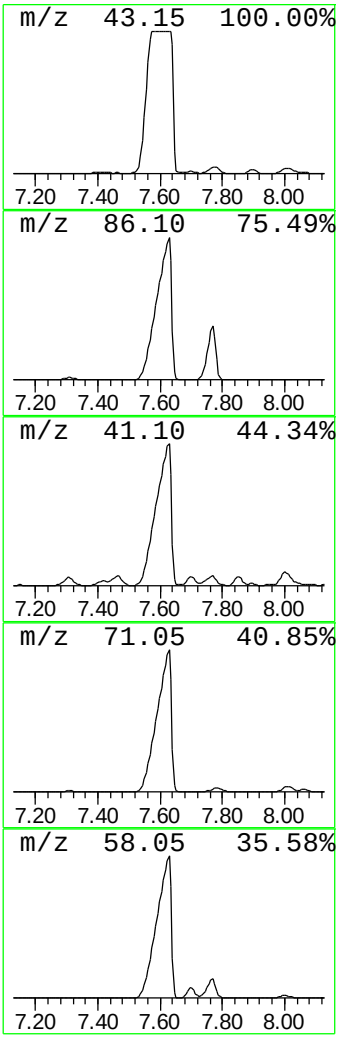
****

Peak Number 2 2-Pentanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.63	181.72 ug/l	143644000	1,4-Difluorobenzene	6.88

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	80
2	Methanediamine, N,N,N',N'-tetrae...	158	C9H22N2	000102-53-4	38
3	2-Imidazolidinone	86	C3H6N2O	000120-93-4	37
4	Imidazole, 4-fluoro-	86	C3H3FN2	030086-17-0	35
5	Ethanamine, N-ethyl-N-[(ethylthi...	147	C7H17NS	003492-79-3	28





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Instrument : MSVOA_X
ClientSampleId : N48719

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

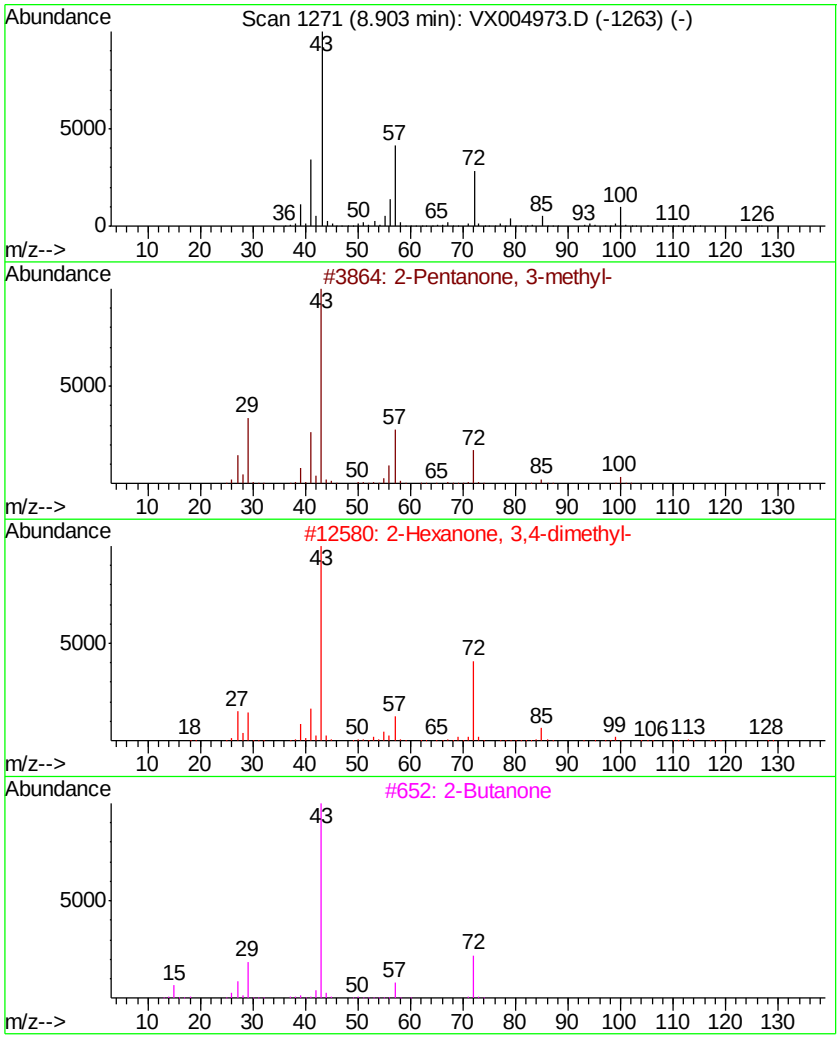
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

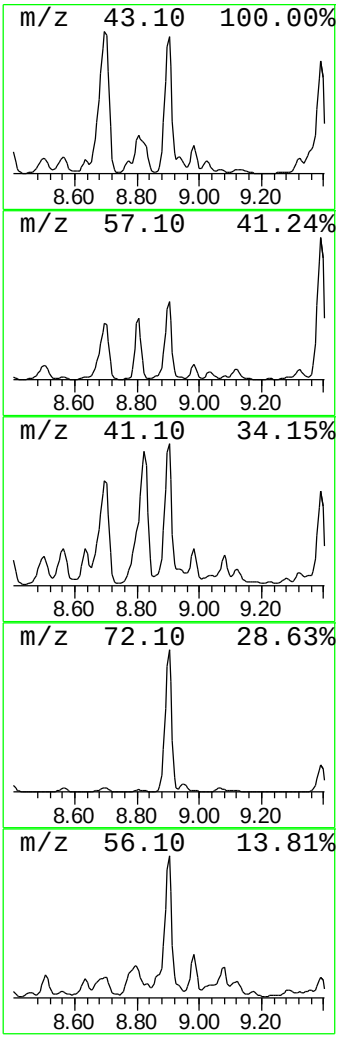
****

Peak Number 3 2-Pentanone, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.90	139.69 ug/l	32156200	Chlorobenzene-d5	10.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	87
2	2-Hexanone, 3,4-dimethyl-	128	C8H16O	019550-10-8	50
3	2-Butanone	72	C4H8O	000078-93-3	47
4	2-Heptanone, 3-methyl-	128	C8H16O	002371-19-9	40
5	Butanal, 2-ethyl-	100	C6H12O	000097-96-1	38





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TIC Library : C:\DATABASE\NIST11.L
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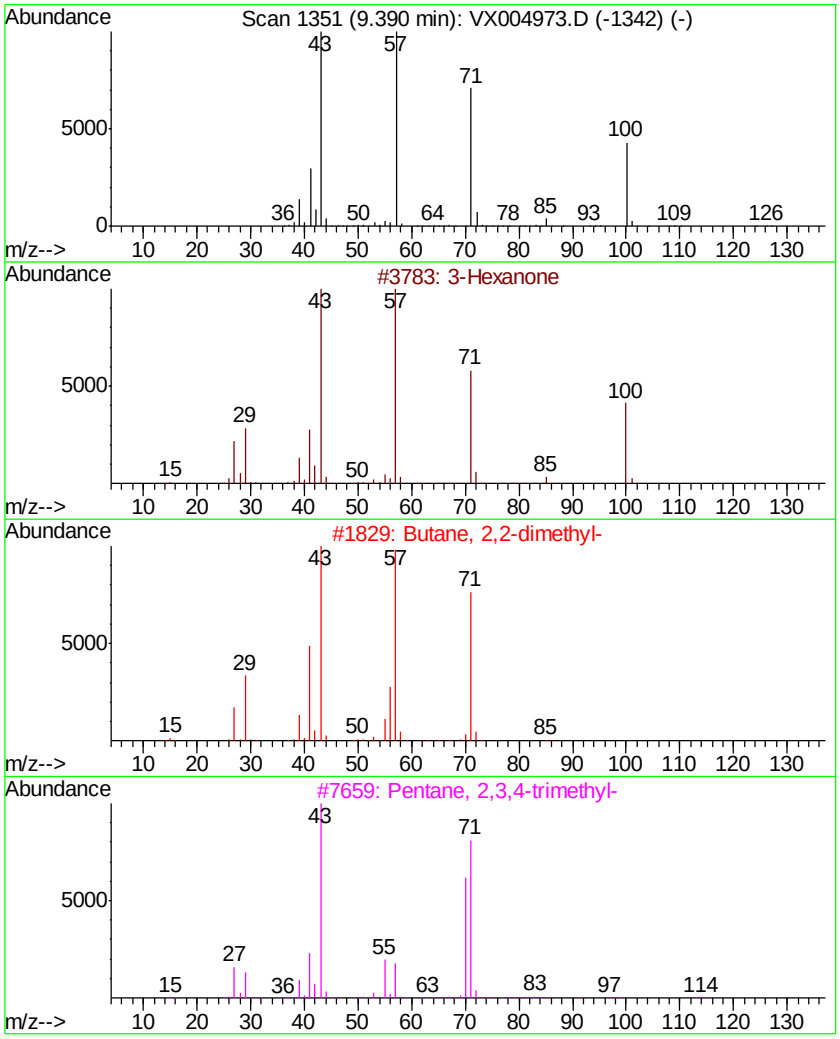
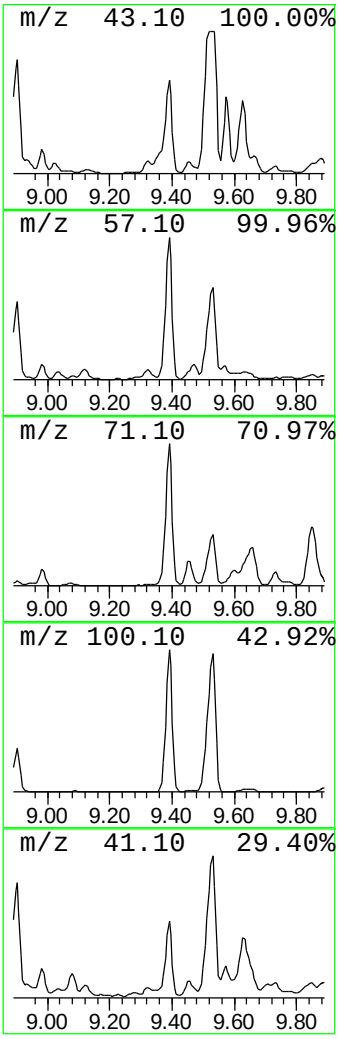
Peak Number 4 3-Hexanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.39	143.55 ug/l	33044300	Chlorobenzene-d5	10.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexanone	100	C6H12O	000589-38-8	91
2	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	40
3	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	37
4	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	33
5	Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	32





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Quant Title : SW846 8260

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

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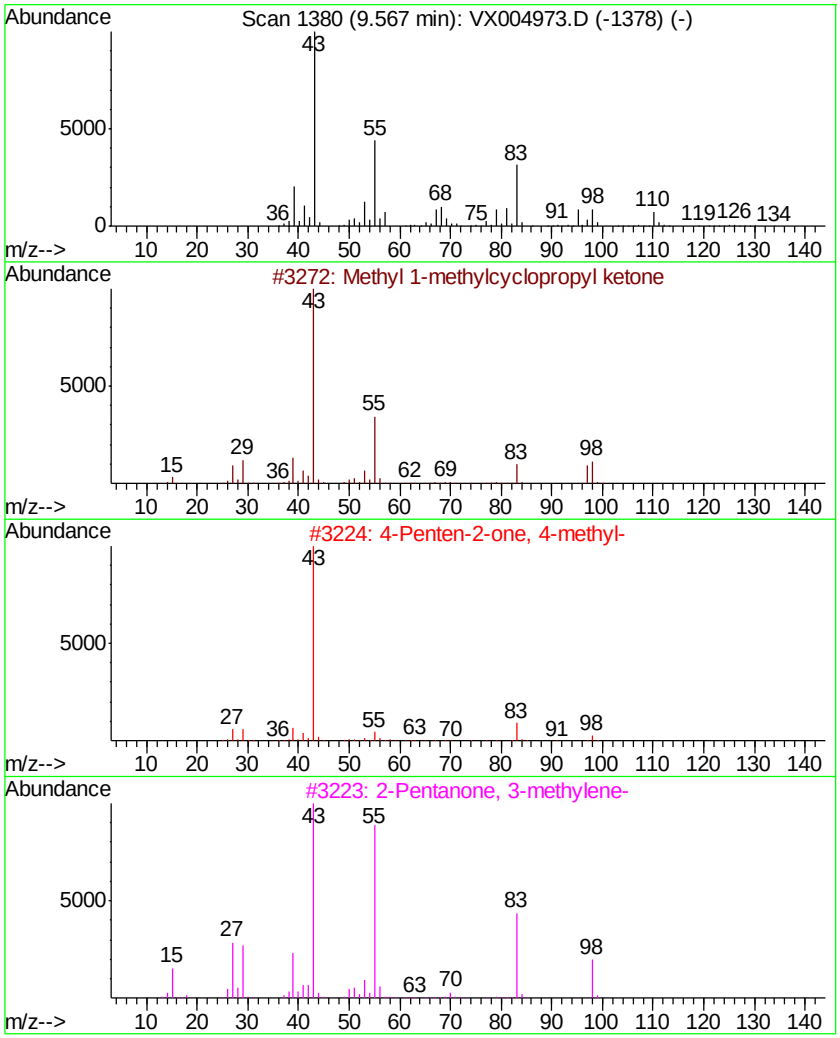
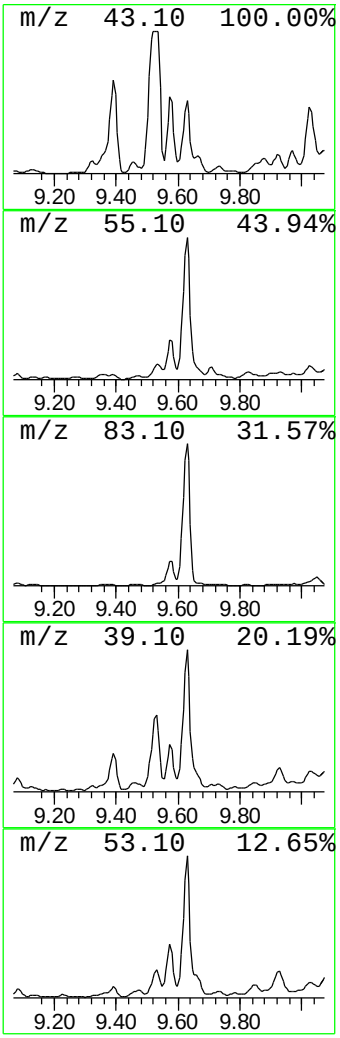
Peak Number 5 Methyl 1-methylcyclopropyl ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.57	92.55 ug/l	21304000	Chlorobenzene-d5	10.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl 1-methylcyclopropyl ketone	98	C6H10O	001567-75-5	58
2	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	50
3	2-Pentanone, 3-methylene-	98	C6H10O	004359-77-7	49
4	3-Hexene-2,5-diol	116	C6H12O2	007319-23-5	38
5	2-Propanone, 1-cyclopropyl-	98	C6H10O	004160-75-2	38





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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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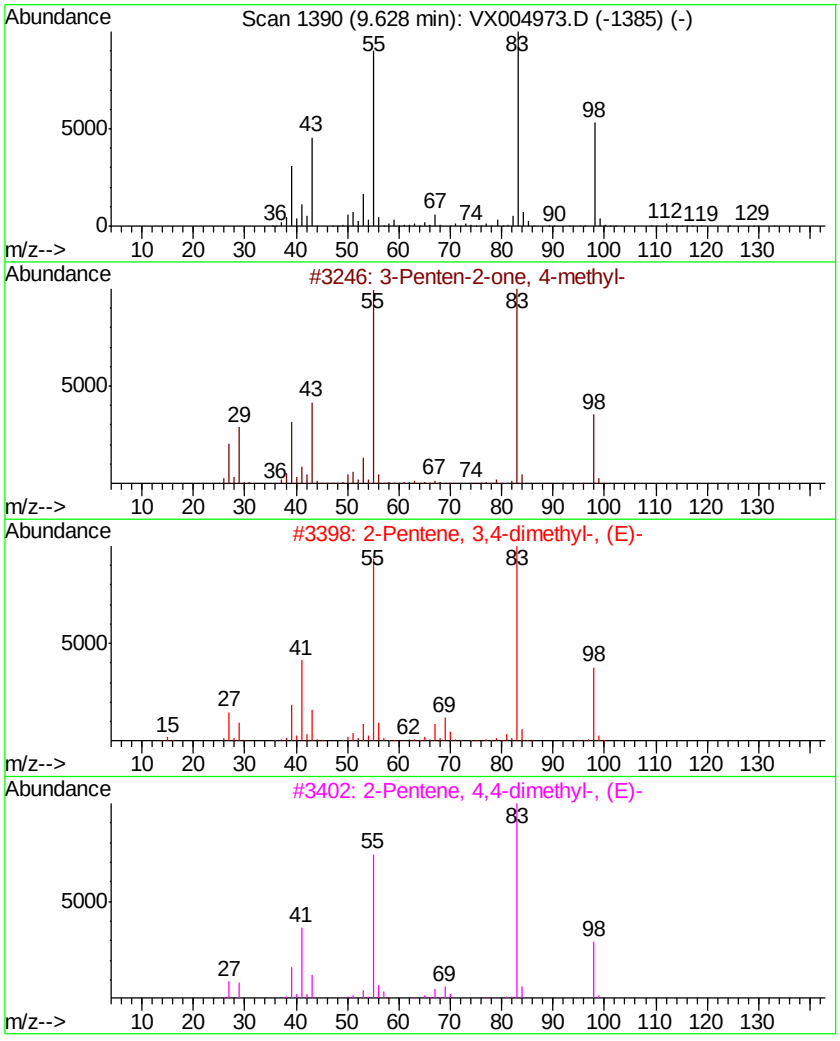
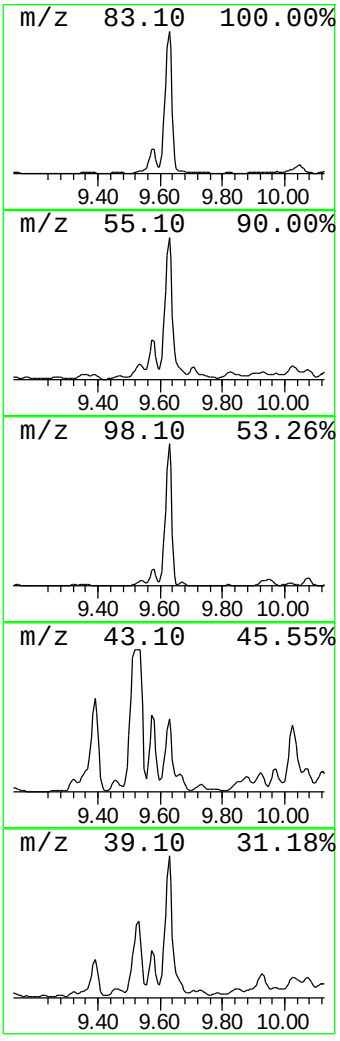
Peak Number 6 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.63	298.45 ug/l	68702400	Chlorobenzene-d5	10.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
3	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	78
4	2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	78
5	1H-Pyrazole, 4,5-dihydro-4,5-dim...	98	C5H10N2	028019-94-5	59





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX100418\
Data File : VX004973.D
Acq On : 03 Oct 2018 17:06
Operator : JC/MD
Sample : J5214-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : N48719

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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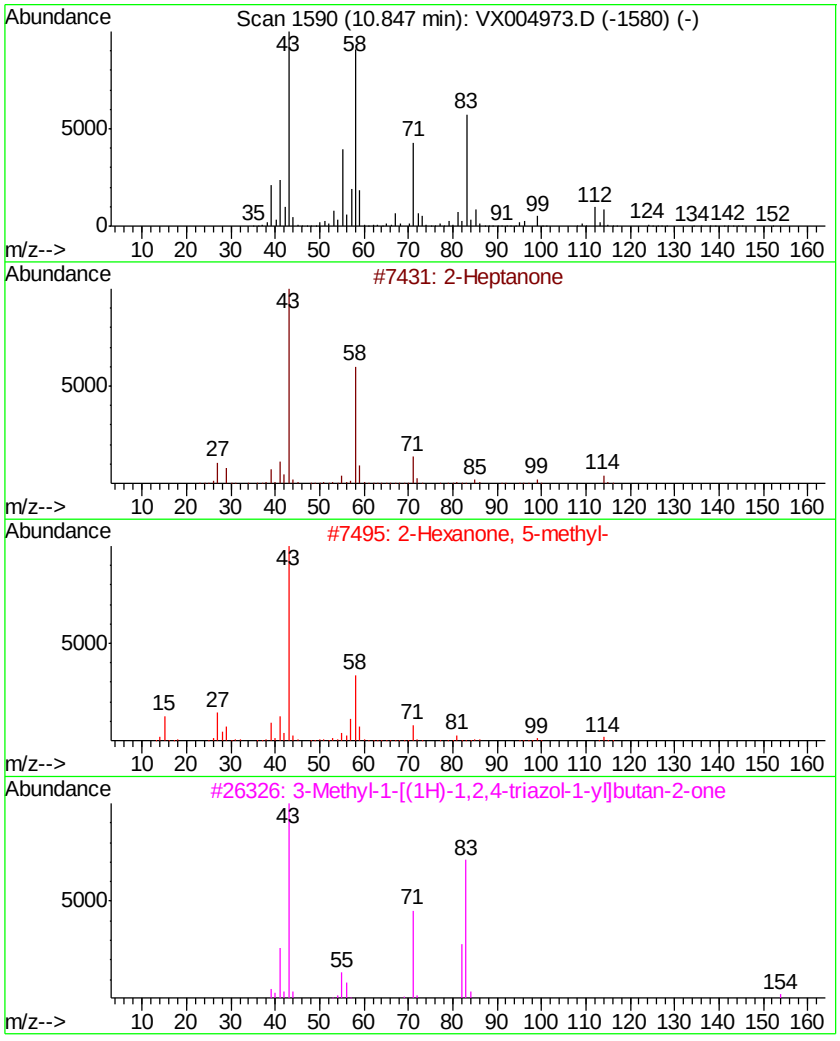
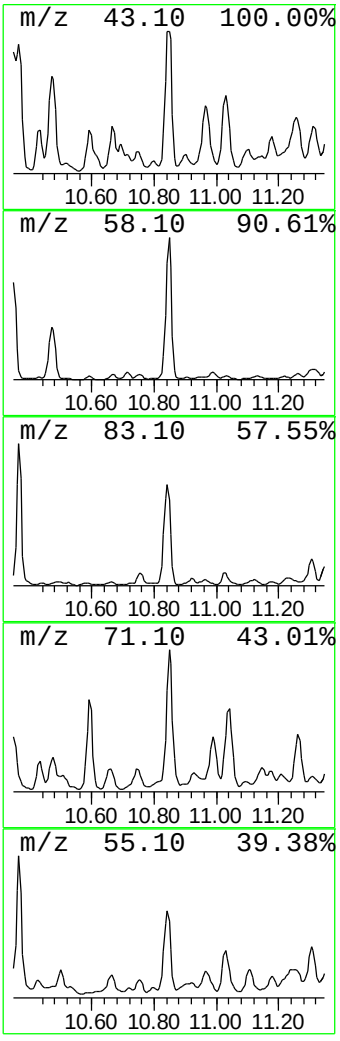
Peak Number 7 unknown10.85 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.85	311.36 ug/l	71673300	Chlorobenzene-d5	10.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone	114	C7H14O	000110-43-0	49
2	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	43
3	3-Methyl-1-[(1H)-1,2,4-triazol-1...	153	C7H11N3O	064922-02-7	27
4	4-Pentenylamine, N,N-dimethyl-	113	C7H15N	001001-91-8	27
5	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	14





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX100418\
Data File : VX004973.D
Acq On : 03 Oct 2018 17:06
Operator : JC/MD
Sample : J5214-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : N48719

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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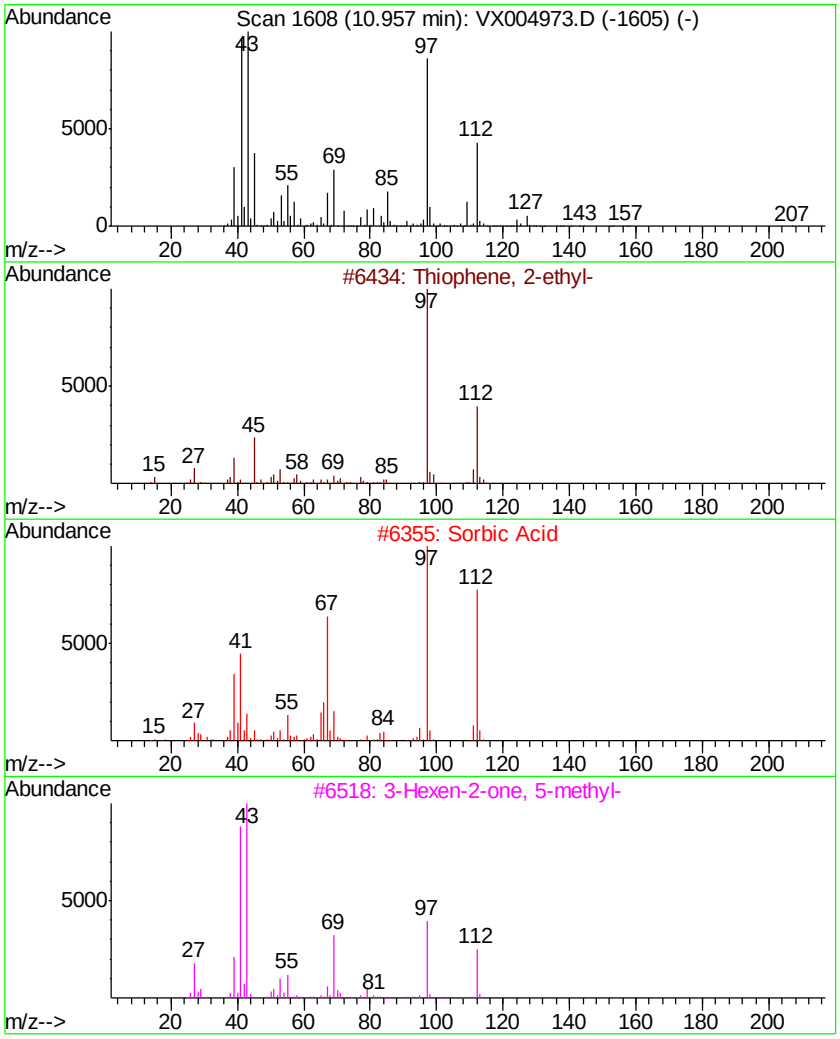
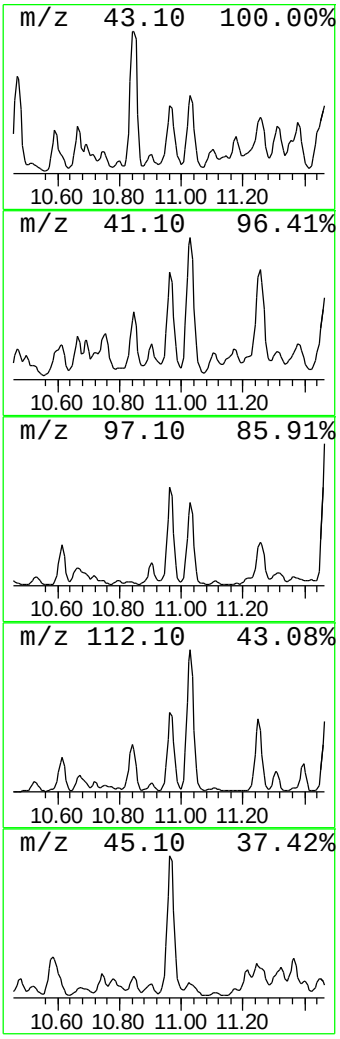
Peak Number 8 Thiophene, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.96	179.71 ug/l	41367900	Chlorobenzene-d5	10.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, 2-ethyl-	112	C6H8S	000872-55-9	64
2	Sorbic Acid	112	C6H8O2	000110-44-1	52
3	3-Hexen-2-one, 5-methyl-	112	C7H12O	005166-53-0	52
4	3-Hexene-2,5-dione	112	C6H8O2	004436-75-3	52
5	1H-Pyrazole, 4,5-dihydro-3,5,5-t...	112	C6H12N2	003975-85-7	50





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX100418\
Data File : VX004973.D
Acq On : 03 Oct 2018 17:06
Operator : JC/MD
Sample : J5214-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : N48719

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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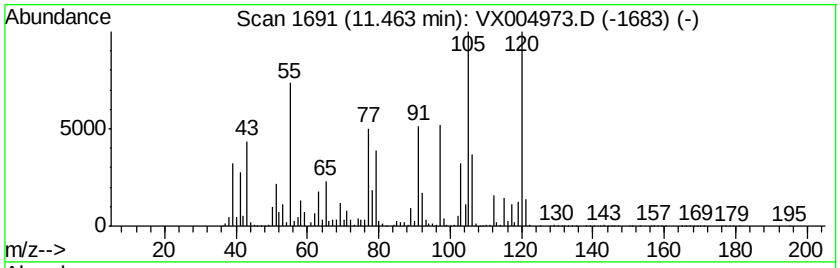
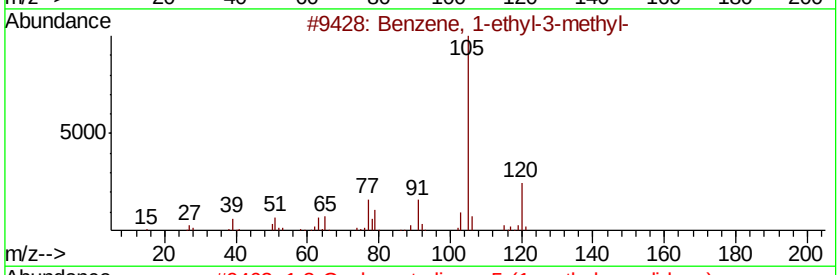
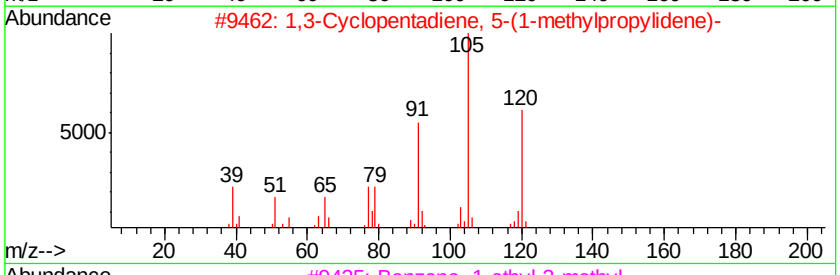
Peak Number 9 Benzene, 1-ethyl-3-methyl- Concentration Rank 4

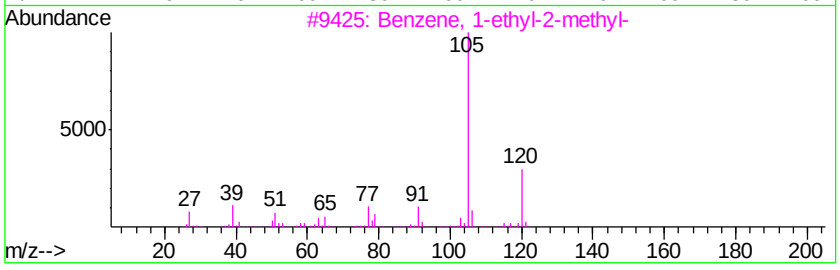
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.46	197.74 ug/l	214314000	1,4-Dichlorobenzene-d4	12.10

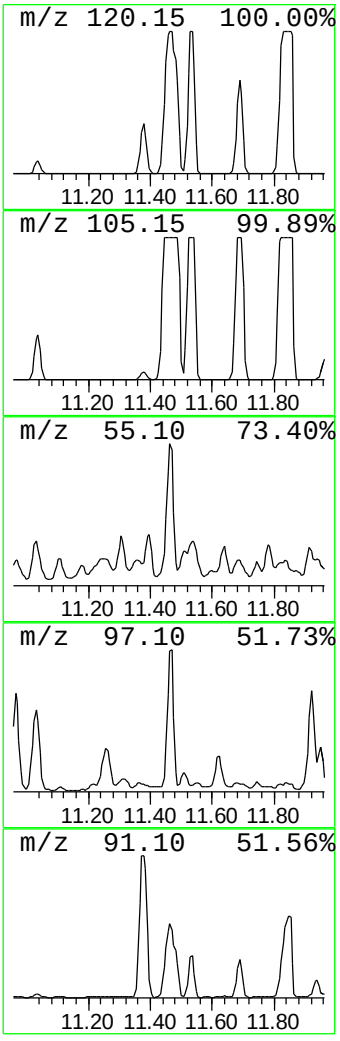
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	81
2	1,3-Cyclopentadiene, 5-(1-methyl...	120	C9H12	003141-02-4	70
3	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	70
4	Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	68
5	2,3-Heptadien-5-yne, 2,4-dimethyl-	120	C9H12	041898-89-9	62











Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX100418\
Data File : VX004973.D
Acq On : 03 Oct 2018 17:06
Operator : JC/MD
Sample : J5214-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : N48719

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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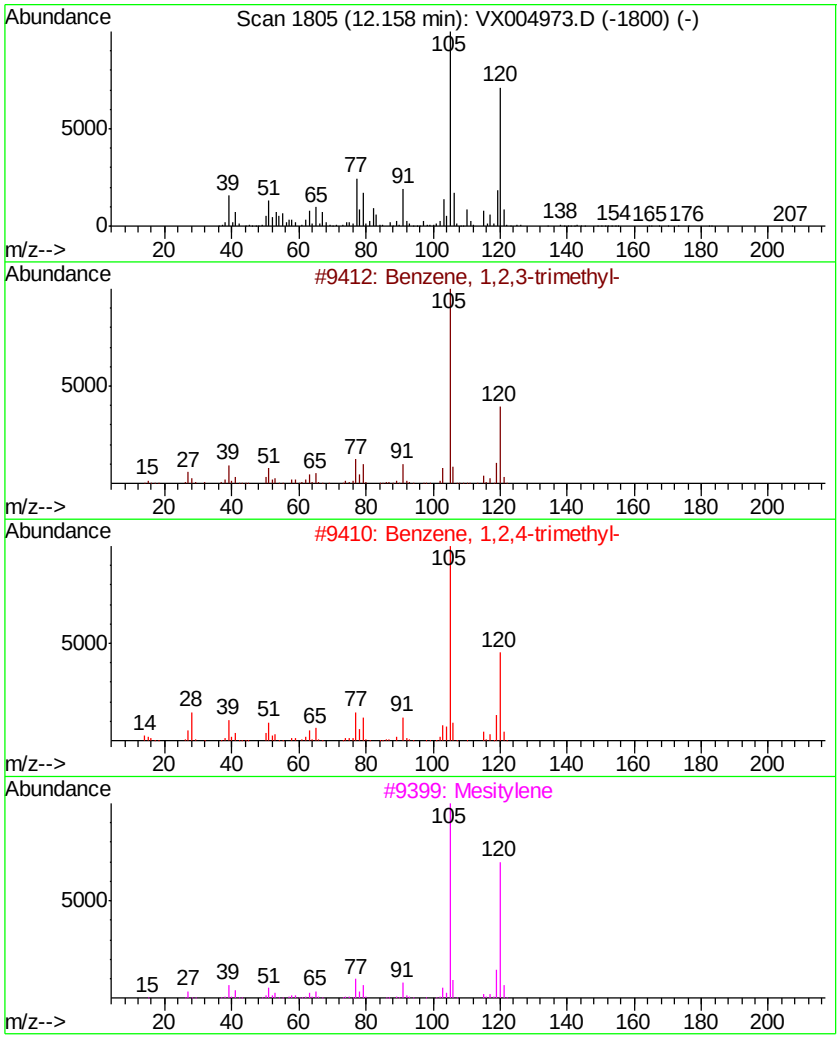
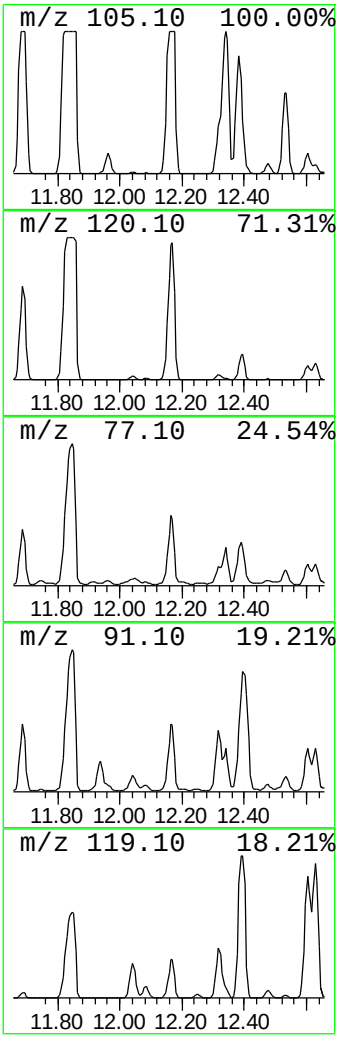
Peak Number 10 Benzene, 1,2,3-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.16	86.05 ug/l	93268500	1,4-Dichlorobenzene-d4	12.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	93
2	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
3	Mesitylene	120	C9H12	000108-67-8	87
4	2,3-Heptadien-5-yne, 2,4-dimethyl-	120	C9H12	041898-89-9	83
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX100418\
Data File : VX004973.D
Acq On : 03 Oct 2018 17:06
Operator : JC/MD
Sample : J5214-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : N48719

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
2-Pentanone	7.63	181.7	ug/l	143644000	2	6.88	39523400	50.0
2-Pentanone, 3-me...	8.90	139.7	ug/l	32156200	3	10.13	11509900	50.0
3-Hexanone	9.39	143.6	ug/l	33044300	3	10.13	11509900	50.0
Methyl 1-methylcy...	9.57	92.5	ug/l	21304000	3	10.13	11509900	50.0
3-Penten-2-one, 4...	9.63	298.4	ug/l	68702400	3	10.13	11509900	50.0
unknown10.85	10.85	311.4	ug/l	71673300	3	10.13	11509900	50.0
Thiophene, 2-ethyl-	10.96	179.7	ug/l	41367900	3	10.13	11509900	50.0
Benzene, 1-ethyl-...	11.46	197.7	ug/l	214314000	4	12.10	54192100	50.0
Benzene, 1,2,3-tr...	12.16	86.0	ug/l	93268500	4	12.10	54192100	50.0