LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX091818\
Data File : VX004659.D
Acq On : 18 Sep 2018 15:49
Operator : JC/MD
Sample : J4906-05
Misc : 4.08g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP-PIT-1

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\82X091118W.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	2.849	273	278	291	rVB	252283	539678	11.82%	0.371%
2	3.483	372	382	400	rVB	357536	785304	17.20%	0.540%
3	4.367	518	527	541	rVB	233263	686729	15.04%	0.472%
4	5.507	695	714	717	rBV	148621	436240	9.56%	0.300%
5	5.574	717	725	733	rVV4	366104	1452066	31.81%	0.998%
6	5.653	733	738	766	rVB5	232992	1008239	22.09%	0.693%
7	5.909	766	780	796	rBV	441276	1317610	28.86%	0.905%
8	6.244	823	835	844	rBV3	204184	684089	14.99%	0.470%
9	6.342	844	851	858	rVV2	198608	541339	11.86%	0.372%
10	6.433	858	866	880	rVB2	322478	899873	19.71%	0.618%
11	6.695	895	909	926	rBV	868551	2063577	45.20%	1.418%
12	6.860	926	936	943	rBV	343518	867345	19.00%	0.596%
13	7.451	1019	1033	1044	rBV2	1884290	4325249	94.75%	2.972%
14	7.842	1090	1097	1105	rVB2	345156	695648	15.24%	0.478%
15	8.024	1120	1127	1143	rVB2	373464	825631	18.09%	0.567%
16	8.335	1173	1178	1182	rVV	1336120	2243778	49.15%	1.542%
17	8.378	1182	1185	1192	rVB2	510521	826540	18.11%	0.568%
18	8.500	1200	1205	1213	rBV	831306	1472107	32.25%	1.012%
19	8.567	1213	1216	1225	rVB2	228921	432043	9.46%	0.297%
20	8.665	1225	1232	1235	rBV	1350046	2340794	51.28%	1.609%
21	8.713	1235	1240	1249	rVB2	913667	2036947	44.62%	1.400%
22	8.835	1249	1260	1264	rBV	457238	791255	17.33%	0.544%
23	8.908	1269	1272	1277	rVB	402480	592855	12.99%	0.407%
24	8.969	1277	1282	1288	rBV	917777	1382401	30.28%	0.950%
25	9.036	1288	1293	1305	rVB2	928019	1708408	37.42%	1.174%
26	9.165	1305	1314	1319	rBV	477394	825502	18.08%	0.567%
27	9.445	1354	1360	1364	rBV	1006558	1474120	32.29%	1.013%
28	9.561	1374	1379	1385	rBV3	735573	1651263	36.17%	1.135%
29	9.622	1385	1389	1393	rVB	1388031	1881625	41.22%	1.293%
30	9.677	1393	1398	1403	rBV	1661539	2631290	57.64%	1.808%
31	9.817	1416	1421	1426	rBV2	546746	838354	18.36%	0.576%
32	9.878	1426	1431	1437	rBV3	916224	2170249	47.54%	1.491%
33	9.963	1440	1445	1449	rVB	1767897	2472783	54.17%	1.699%
34	10.067	1455	1462	1466	rVB	1879239	2587459	56.68%	1.778%

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Integrator: RTE
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Title : SW846 8260

35	10.116	1466	1470	1474	rBV	655975	842252	18.45%	0.579%
36	10.183	1474	1481	1486	rBV3	279956	650223	14.24%	0.447%
37	10.237	1486	1490	1497	rVB2	346959	714364	15.65%	0.491%
38	10.335	1497	1506	1509	rBV2	846097	1804491	39.53%	1.240%
39	10.378	1509	1513	1516	rVB	958532	1287613	28.21%	0.885%
40	10.414	1516	1519	1530	rVB2	894742	1710489	37.47%	1.175%
41	10.512	1530	1535	1543	rBV2	478166	832118	18.23%	0.572%
42	10.640	1550	1556	1561	rBV2	1321652	2311862	50.64%	1.589%
43	10.725	1565	1570	1575	rBV2	614670	1065026	23.33%	0.732%
44	10.835	1580	1588	1592	rBV2	2967194	4564992	100.00%	3.137%
45	10.914	1592	1601	1604	rBV3	2192422	3539946	77.55%	2.433%
46	10.951	1604	1607	1612	rVB	1199756	1572527	34.45%	1.081%
47	11.018	1612	1618	1621	rBV3	485001	899213	19.70%	0.618%
48	11.060	1621	1625	1626	rBV2	397791	513030	11.24%	0.353%
49	11.085	1626	1629	1632	rVB	706846	799842	17.52%	0.550%
50	11.140	1632	1638	1641	rBV3	2168270	3283803	71.93%	2.257%
51	11.243	1649	1655	1658	rBV	1436118	2212371	48.46%	1.520%
52	11.280	1658	1661	1669	rVB4	1419551	1974933	43.26%	1.357%
53	11.365	1671	1675	1677	rBV	448936	589344	12.91%	0.405%
54	11.396	1677	1680	1685	rVV3	368354	542412	11.88%	0.373%
55	11.451	1685	1689	1692	rVV3	522150	807861	17.70%	0.555%
56	11.487	1692	1695	1700	rVV	1447525	2001545	43.85%	1.375%
57	11.536	1700	1703	1708	rVB3	920020	1400344	30.68%	0.962%
58	11.682	1721	1727	1732	rVB7	675109	1494318	32.73%	1.027%
59	11.737	1732	1736	1738	rBV2	602578	723555	15.85%	0.497%
60	11.768	1738	1741	1745	rBV	2040786	2174457	47.63%	1.494%
61	11.896	1758	1762	1764	rBV2	415029	639165	14.00%	0.439%
62	11.945	1764	1770	1775	rVV5	1296955	2425410	53.13%	1.667%
63	11.999	1775	1779	1782	rVV	1798575	2439000	53.43%	1.676%
64	12.030	1782	1784	1787	rVV3	643589	759498	16.64%	0.522%
65	12.091	1787	1794	1798	rVV3	1342674	2762346	60.51%	1.898%
66	12.127	1798	1800	1802	rVV	893928	891094	19.52%	0.612%
67	12.158	1802	1805	1809	rVB3	1131933	1267675	27.77%	0.871%
68	12.225	1812	1816	1824	rVB3	1230911	2216736	48.56%	1.523%
69	12.304	1824	1829	1836	rBV	1350330	2193763	48.06%	1.508%
70	12.371	1836	1840	1847	rBV3	1751808	3175961	69.57%	2.182%
71	12.475	1847	1857	1862	rBV3	932457	2652219	58.10%	1.823%

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Title : SW846 8260

72	12.524	1862	1865	1871	rVB4	1101015	1819642	39.86%	1.250%
73	12.615	1873	1880	1881	rBV4	628196	1225926	26.85%	0.842%
74	12.670	1886	1889	1893	rVB	1147300	1198387	26.25%	0.824%
75	12.761	1897	1904	1912	rBV5	1035549	3349971	73.38%	2.302%
76	12.877	1920	1923	1929	rVB3	1101914	1705500	37.36%	1.172%
77	12.944	1929	1934	1938	rBV4	1570897	2961776	64.88%	2.035%
78	13.042	1945	1950	1954	rVB4	820425	1407539	30.83%	0.967%
79	13.097	1954	1959	1963	rBV4	928218	1464941	32.09%	1.007%
80	13.152	1966	1968	1973	rVB2	362887	511381	11.20%	0.351%
81	13.225	1973	1980	1984	rBV5	638393	1291499	28.29%	0.887%
82	13.316	1991	1995	1996	rBV2	422967	554221	12.14%	0.381%
83	13.353	1996	2001	2006	rVV3	2550767	4102204	89.86%	2.819%
84	13.438	2011	2015	2018	rVV2	752272	1109564	24.31%	0.762%
85	13.481	2018	2022	2031	rVB7	946203	2355636	51.60%	1.619%
86	13.566	2031	2036	2039	rBV2	437642	711651	15.59%	0.489%
87	13.603	2039	2042	2045	rBV	538176	653621	14.32%	0.449%
88	13.639	2045	2048	2053	rVB3	584240	867525	19.00%	0.596%
89	13.725	2059	2062	2066	rVB2	584560	813478	17.82%	0.559%
90	13.859	2081	2084	2087	rVB3	397439	440878	9.66%	0.303%
91	13.901	2087	2091	2098	rVB5	555191	976331	21.39%	0.671%
92	13.987	2098	2105	2110	rVB6	480141	1053969	23.09%	0.724%
93	14.133	2125	2129	2132	rBV3	398979	552786	12.11%	0.380%
94	14.273	2149	2152	2161	rVB2	541742	828540	18.15%	0.569%
95	14.548	2192	2197	2201	rBV4	231823	536859	11.76%	0.369%
96	14.700	2218	2222	2225	rVB	1199905	1408970	30.86%	0.968%
97	14.840	2242	2245	2253	rVB	691280	993624	21.77%	0.683%
98	15.554	2357	2362	2369	rVB	314169	500829	10.97%	0.344%
99	15.694	2380	2385	2388	rBV	305134	488979	10.71%	0.336%
100	15.730	2388	2391	2400	rVV	234027	412599	9.04%	0.284%

Sum of corrected areas: 145523014

LSC Report - Integrated Chromatogram

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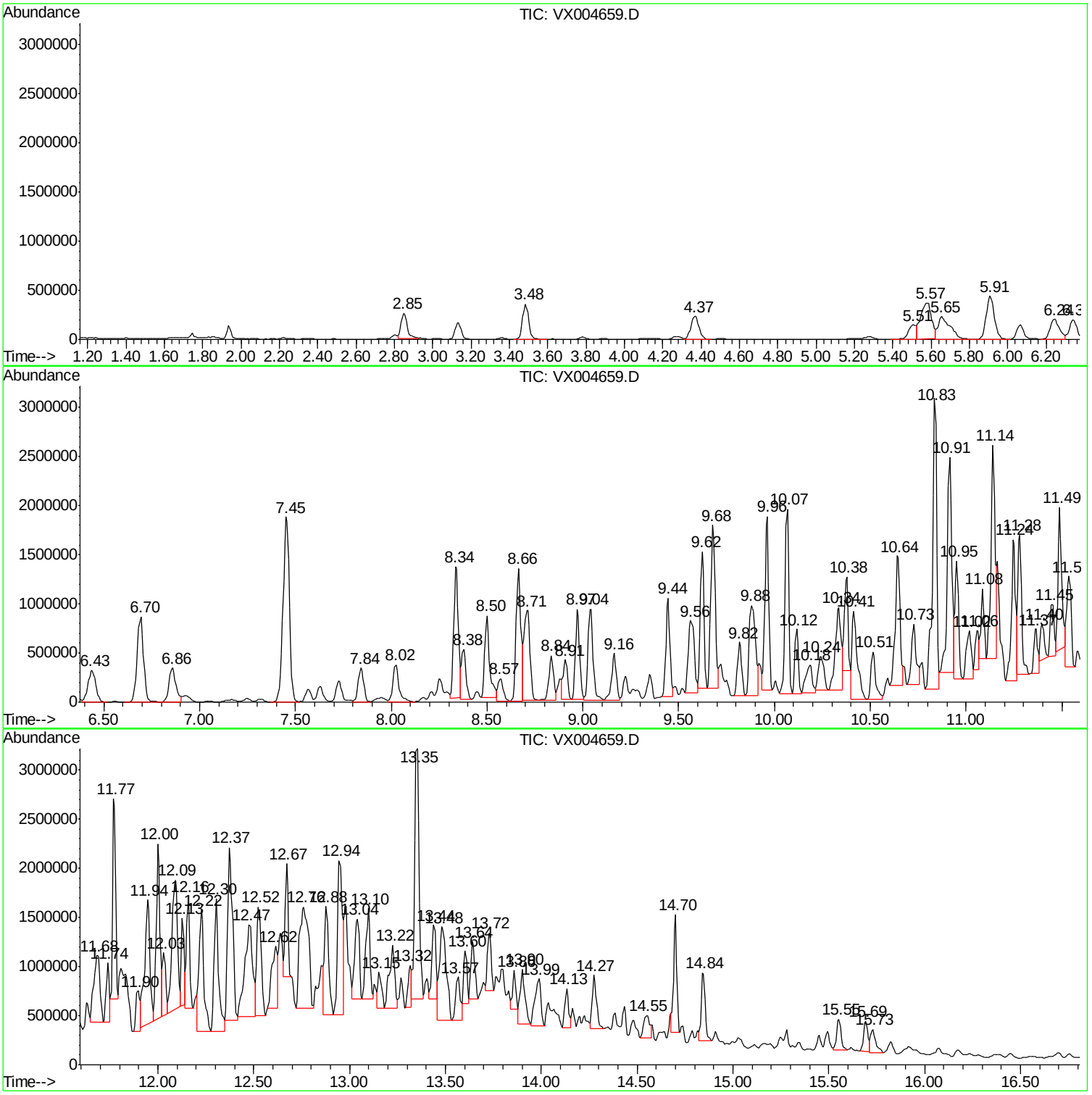
ClientSampleId : SP-PIT-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

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



Library Search Compound Report

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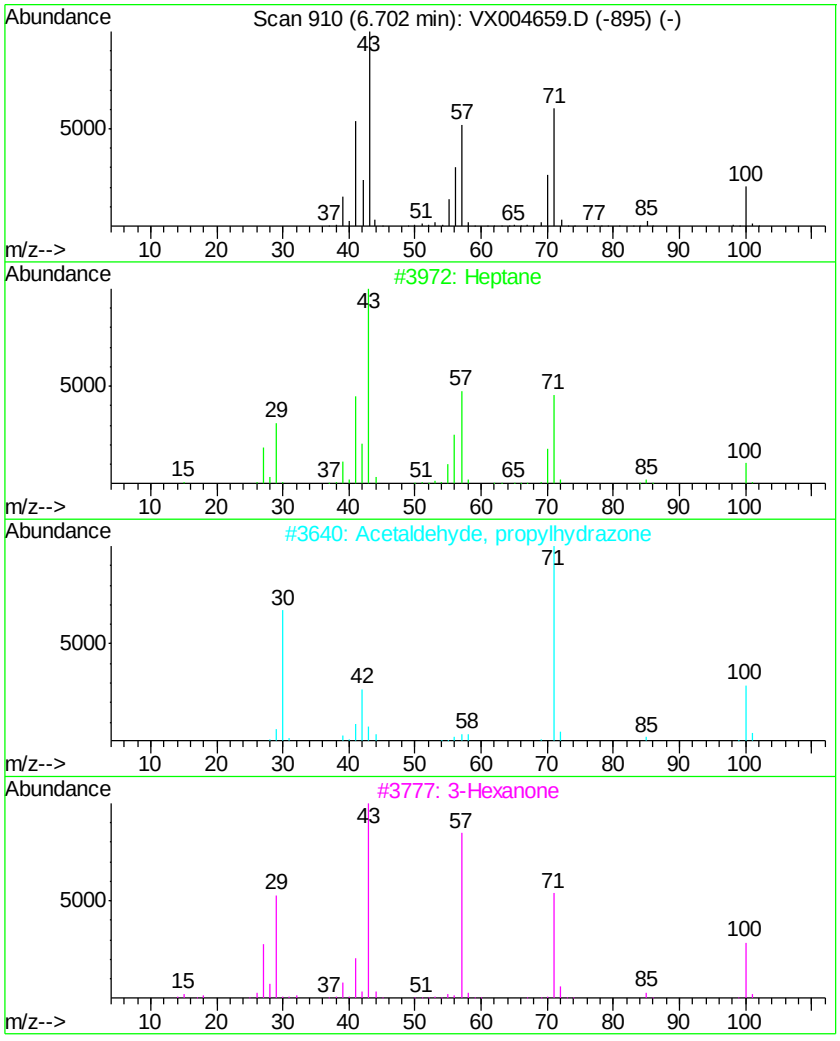
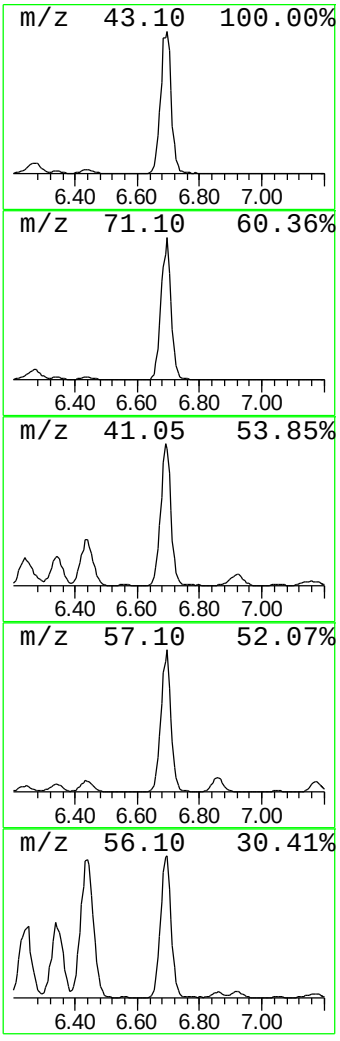
****

Peak Number 1 Heptane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.70	118.96 ug/l	2063580	1,4-Difluorobenzene	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	91
2	Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	47
3	3-Hexanone	100	C6H12O	000589-38-8	46
4	Hexane, 3-methyl-	100	C7H16	000589-34-4	38
5	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	37





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ClientSampleId : SP-PIT-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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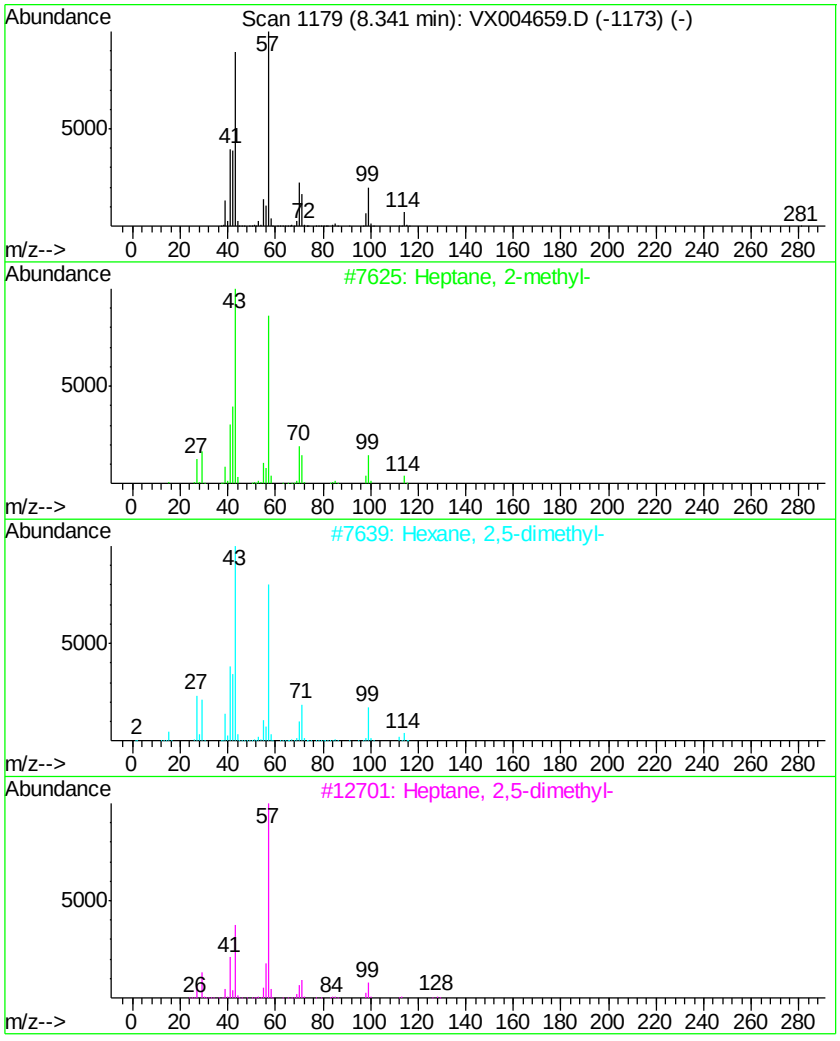
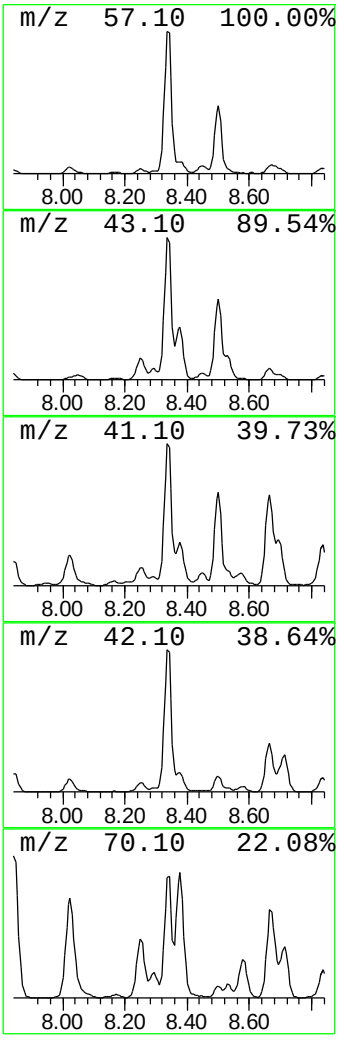
Peak Number 2 Heptane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.34	129.35 ug/l	2243780	1,4-Difluorobenzene	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 2-methyl-	114	C8H18	000592-27-8	94
2	Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	87
3	Heptane, 2,5-dimethyl-	128	C9H20	002216-30-0	38
4	Isobutane	58	C4H10	000075-28-5	35
5	Butane, 1-(ethenyloxy)-3-methyl-	114	C7H14O	039782-38-2	35





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TIC Library : C:\DATABASE\NIST11.L
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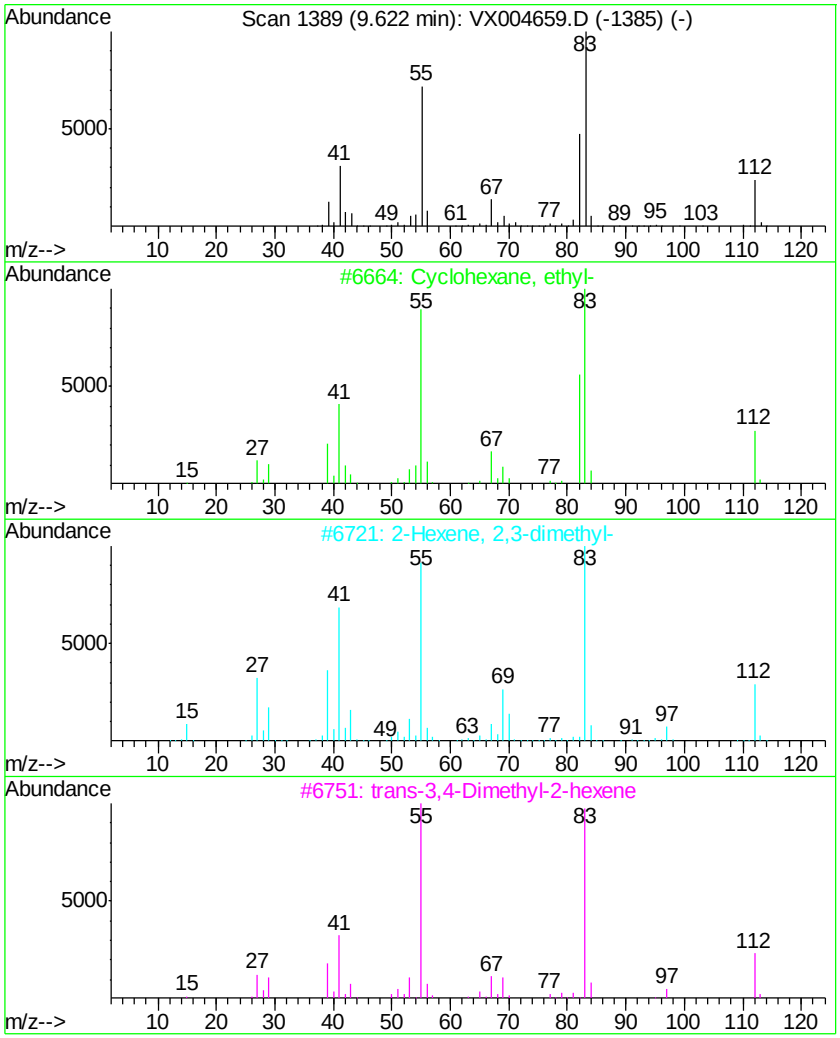
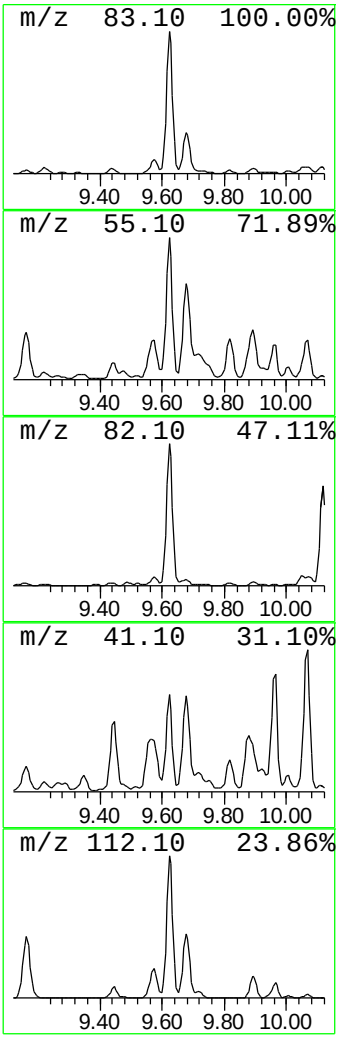
Peak Number 3 Cyclohexane, ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.62	111.70 ug/l	1881630	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, ethyl-	112	C8H16	001678-91-7	93
2	2-Hexene, 2,3-dimethyl-	112	C8H16	007145-20-2	58
3	trans-3,4-Dimethyl-2-hexene	112	C8H16	019550-82-4	53
4	2-Pentene, 3-ethyl-2-methyl-	112	C8H16	019780-67-7	53
5	Oxalic acid, cyclohexyl dodecyl ...	340	C20H36O4	1000309-31-4	53





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Quant Title : SW846 8260

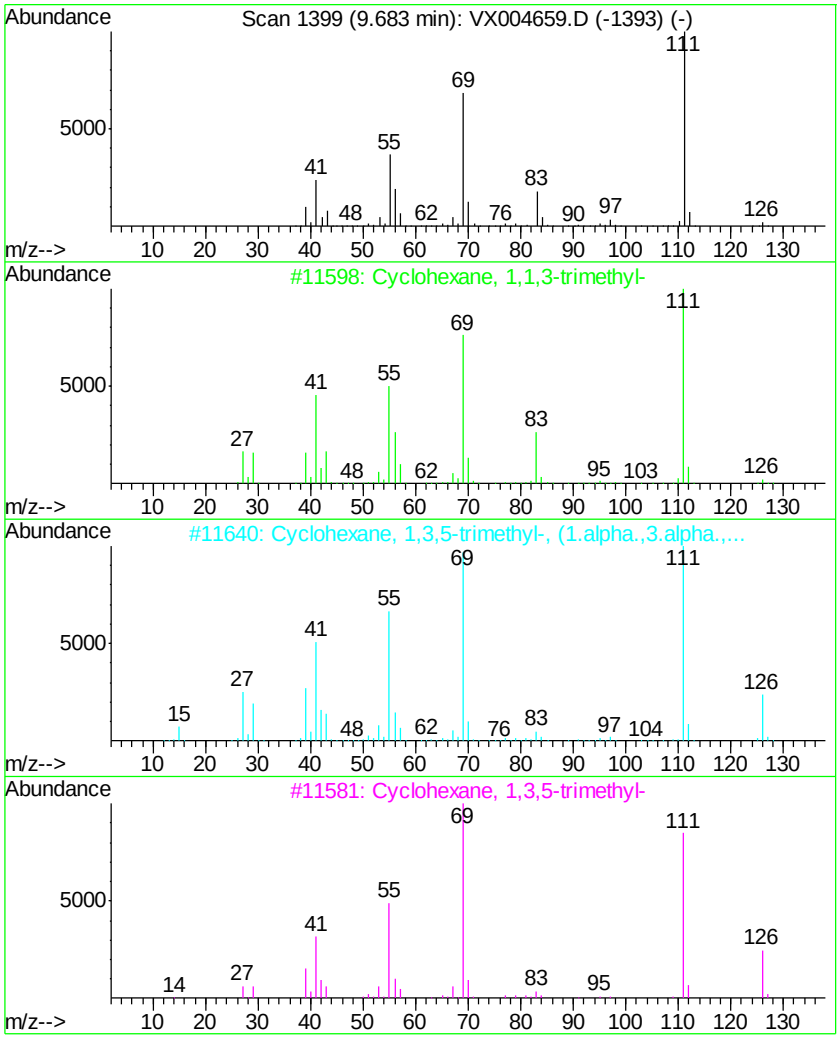
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

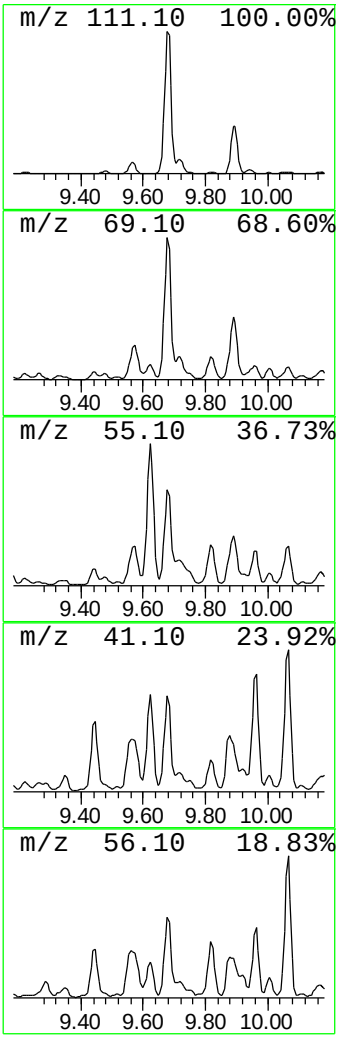
****

Peak Number 4 Cyclohexane, 1,1,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.68	156.21 ug/l	2631290	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	97
2	Cyclohexane, 1,3,5-trimethyl-, (...	126	C9H18	001795-27-3	64
3	Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	64
4	Cyclooctane, (1-methylpropyl)-	168	C12H24	016538-89-9	59
5	Isocytosine	111	C4H5N3O	000108-53-2	53





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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

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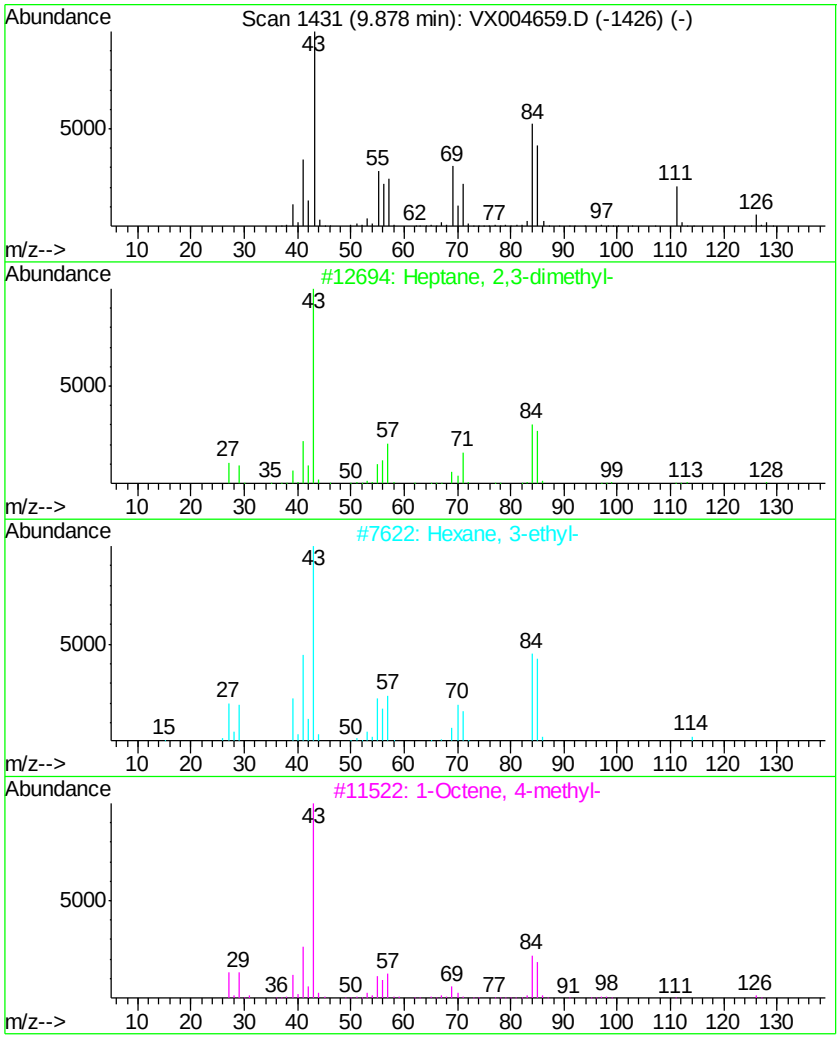
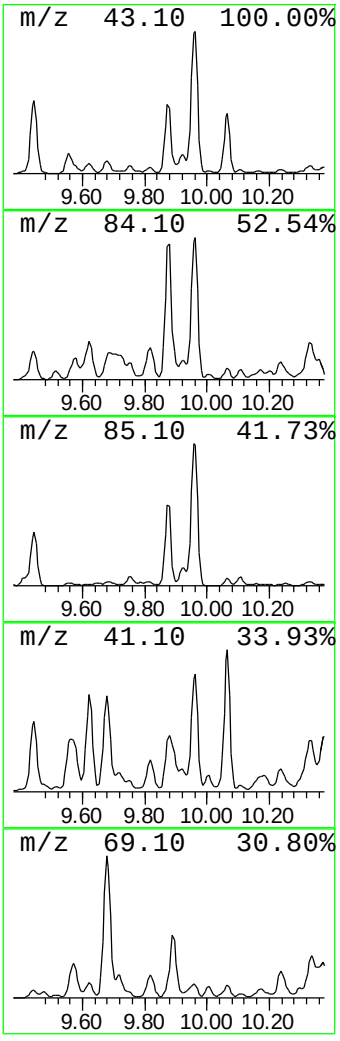
****

Peak Number 5 Heptane, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.88	128.84 ug/l	2170250	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 2,3-dimethyl-	128	C9H20	003074-71-3	68
2	Hexane, 3-ethyl-	114	C8H18	000619-99-8	50
3	1-Octene, 4-methyl-	126	C9H18	013151-12-7	50
4	Decane, 5,6-dimethyl-	170	C12H26	001636-43-7	50
5	Nonane	128	C9H20	000111-84-2	47





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX091818\
Data File : VX004659.D
Acq On : 18 Sep 2018 15:49
Operator : JC/MD
Sample : J4906-05
Misc : 4.08g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP-PIT-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

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

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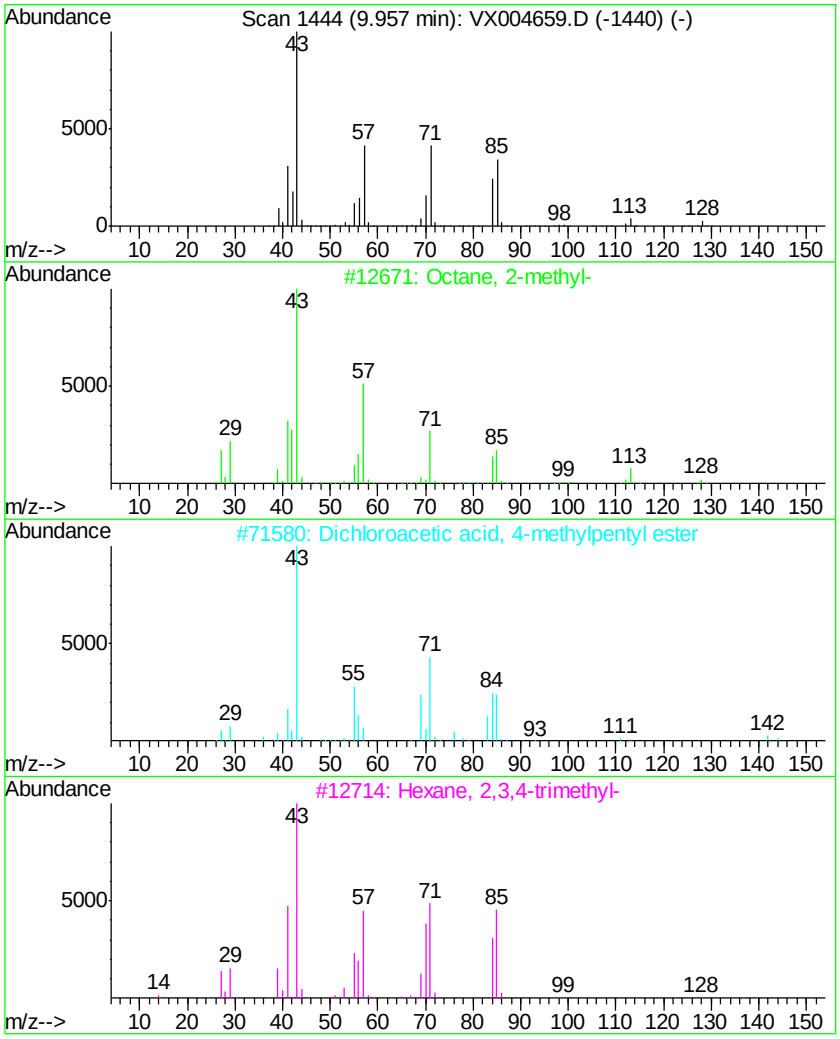
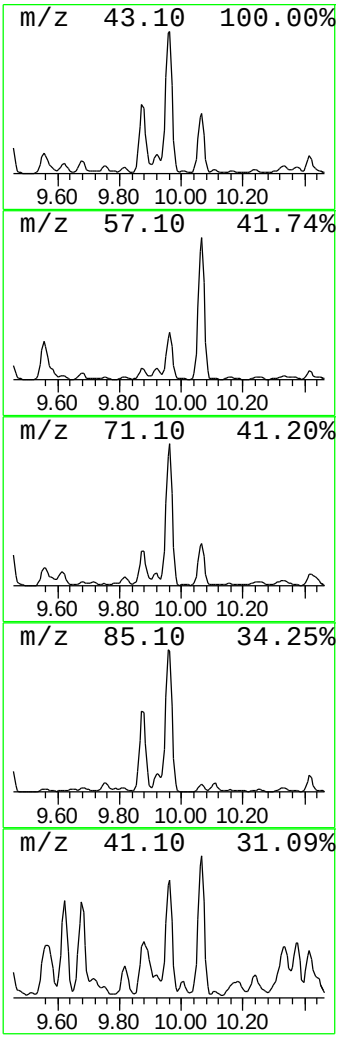
Peak Number 6 Octane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.96	146.80 ug/l	2472780	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-methyl-	128	C9H20	003221-61-2	90
2	Dichloroacetic acid, 4-methylpen...	212	C8H14Cl2O2	1000282-43-7	64
3	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59
4	Octane, 4-methyl-	128	C9H20	002216-34-4	53
5	Octane, 6-ethyl-2-methyl-	156	C11H24	062016-19-7	50





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX091818\
Data File : VX004659.D
Acq On : 18 Sep 2018 15:49
Operator : JC/MD
Sample : J4906-05
Misc : 4.08g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP-PIT-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

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

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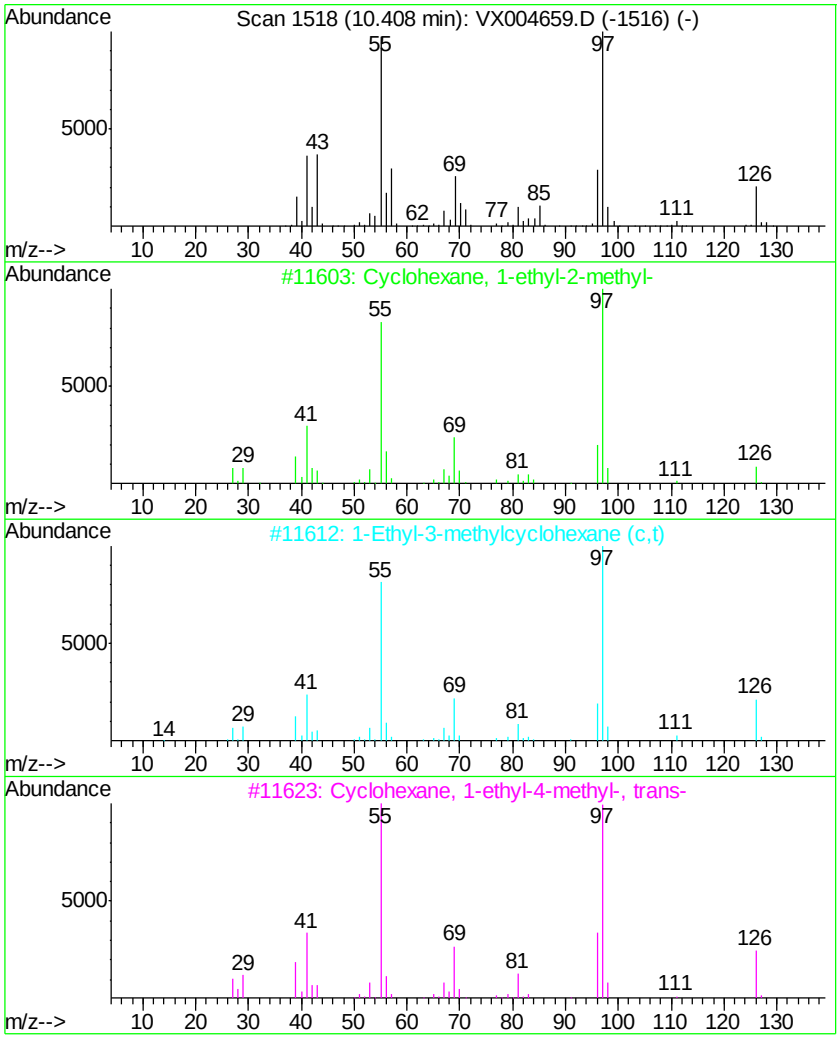
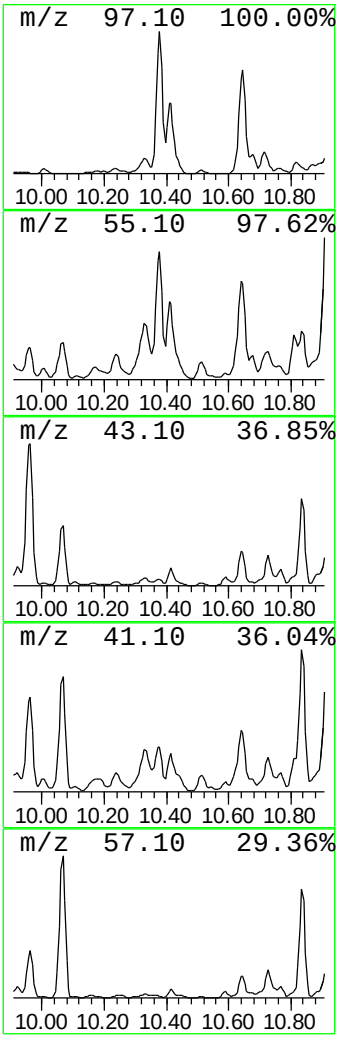
Peak Number 7 Cyclohexane, 1-ethyl-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.41	101.54 ug/l	1710490	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	86
2	1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	81
3	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	81
4	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	72
5	cis-1-Ethyl-3-methyl-cyclohexane	126	C9H18	019489-10-2	68





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX091818\
Data File : VX004659.D
Acq On : 18 Sep 2018 15:49
Operator : JC/MD
Sample : J4906-05
Misc : 4.08g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP-PIT-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

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

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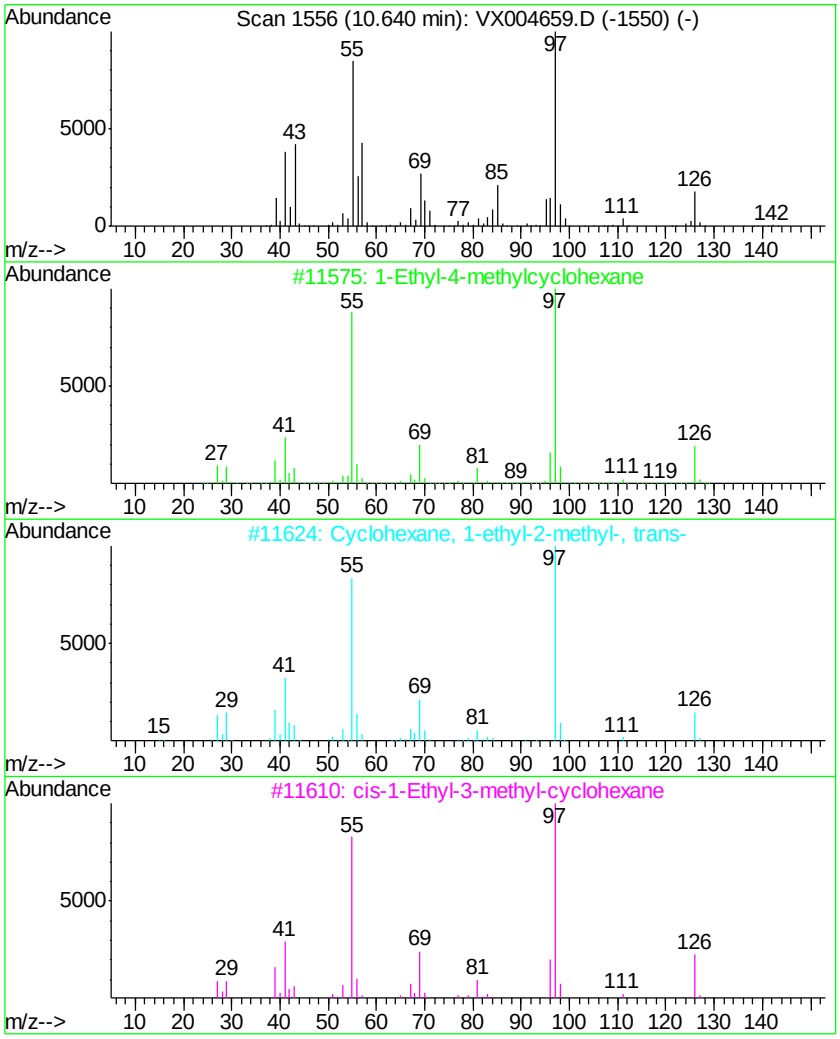
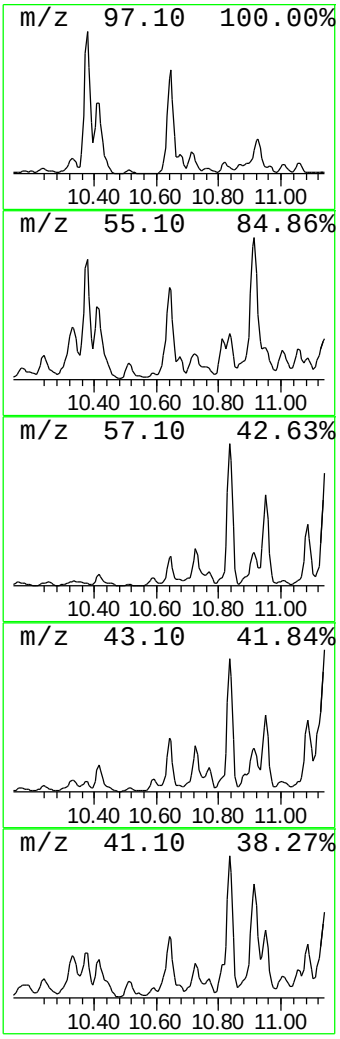
Peak Number 8 1-Ethyl-4-methylcyclohexane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.64	137.24 ug/l	2311860	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Ethyl-4-methylcyclohexane	126	C9H18	003728-56-1	76
2	Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	62
3	cis-1-Ethyl-3-methyl-cyclohexane	126	C9H18	019489-10-2	62
4	1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	62
5	Sulfurous acid, cyclohexylmethyl...	402	C23H46O3S	1000309-22-4	59





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX091818\
Data File : VX004659.D
Acq On : 18 Sep 2018 15:49
Operator : JC/MD
Sample : J4906-05
Misc : 4.08g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP-PIT-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

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

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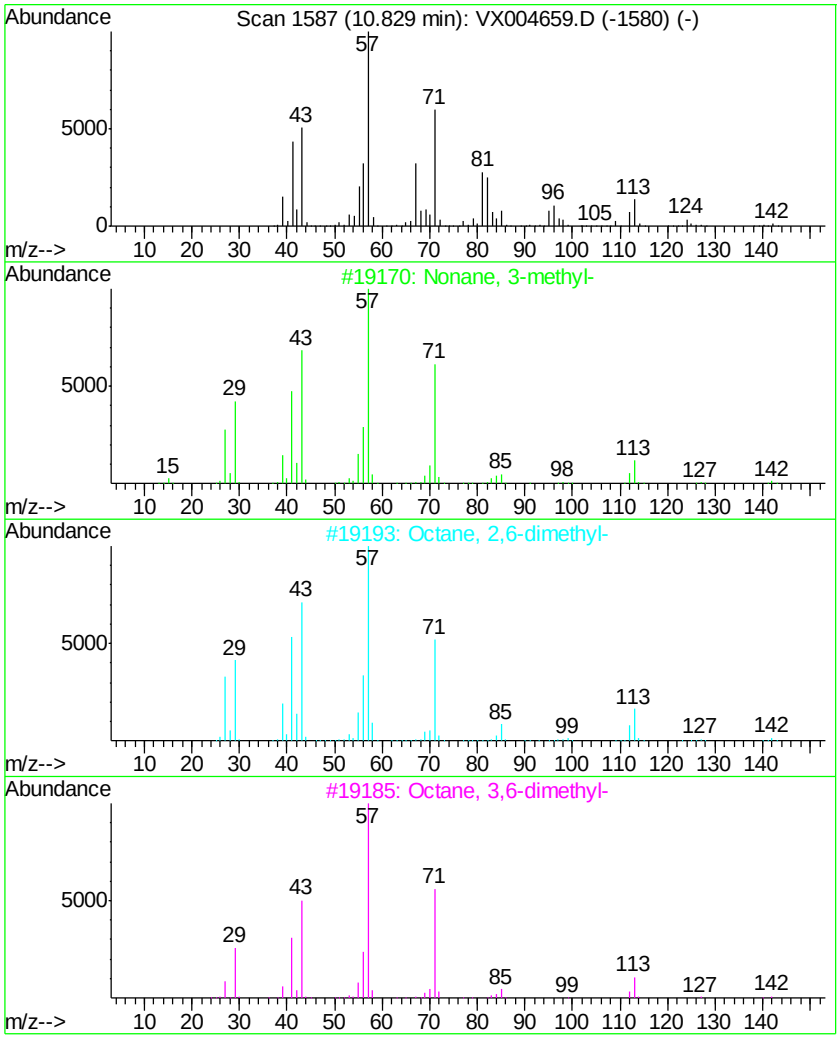
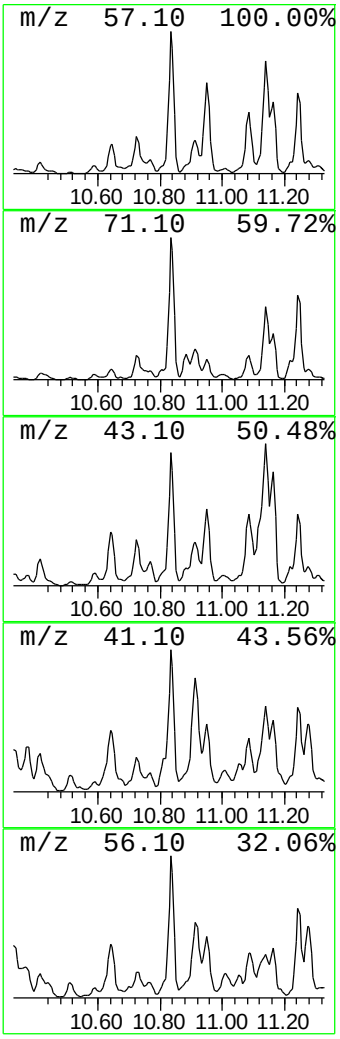
Peak Number 9 Nonane, 3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.83	271.00 ug/l	4564990	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 3-methyl-	142	C10H22	005911-04-6	60
2	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	60
3	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	60
4	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	46
5	Sulfurous acid, di(2-ethylhexyl)...	306	C16H34O3S	1000309-19-1	43





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX091818\
Data File : VX004659.D
Acq On : 18 Sep 2018 15:49
Operator : JC/MD
Sample : J4906-05
Misc : 4.08g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP-PIT-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.M
Quant Title : SW846 8260

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

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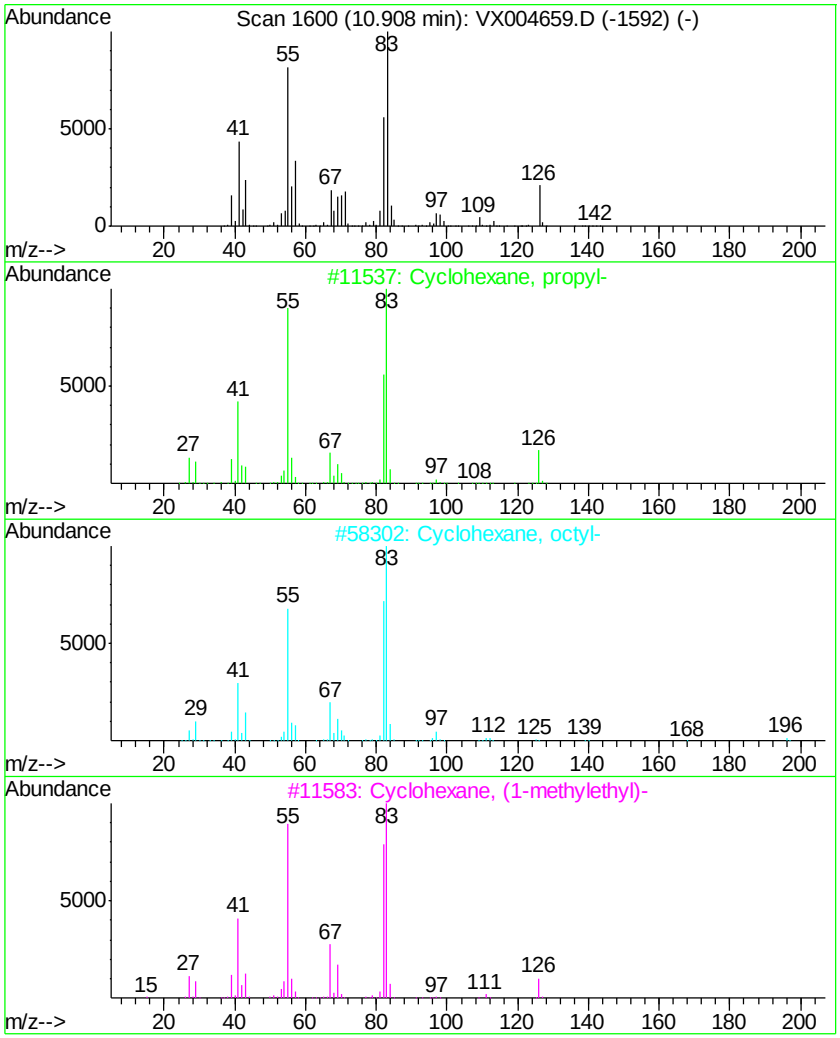
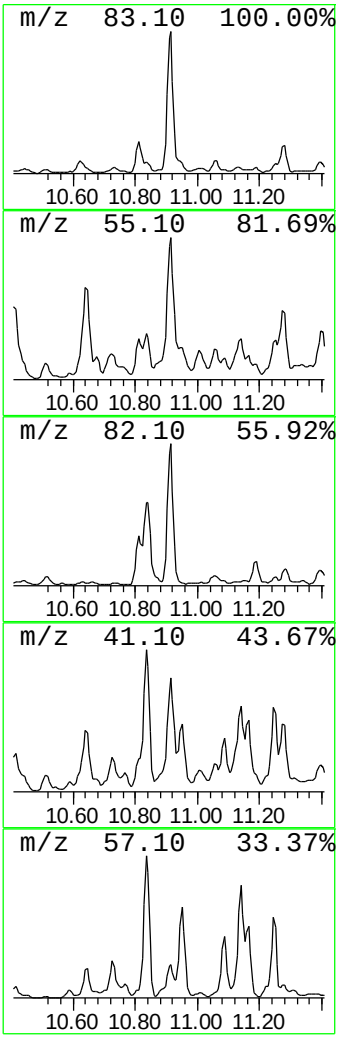
Peak Number 10 Cyclohexane, propyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.91	210.15 ug/l	3539950	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, propyl-	126	C9H18	001678-92-8	74
2	Cyclohexane, octyl-	196	C14H28	001795-15-9	53
3	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	53
4	Cyclohexane, butyl-	140	C10H20	001678-93-9	53
5	Cyclopentane, 1-ethyl-1-methyl-	112	C8H16	016747-50-5	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX091818\
Data File : VX004659.D
Acq On : 18 Sep 2018 15:49
Operator : JC/MD
Sample : J4906-05
Misc : 4.08g/5mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SP-PIT-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X091118W.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
Heptane	6.70	119.0	ug/l	2063580	2	6.85	867345	50.0
Heptane, 2-methyl-	8.34	129.3	ug/l	2243780	2	6.85	867345	50.0
Cyclohexane, ethyl-	9.62	111.7	ug/l	1881630	3	10.12	842252	50.0
Cyclohexane, 1,1,...	9.68	156.2	ug/l	2631290	3	10.12	842252	50.0
Heptane, 2,3-dime...	9.88	128.8	ug/l	2170250	3	10.12	842252	50.0
Octane, 2-methyl-	9.96	146.8	ug/l	2472780	3	10.12	842252	50.0
Cyclohexane, 1-et...	10.41	101.5	ug/l	1710490	3	10.12	842252	50.0
1-Ethyl-4-methylc...	10.64	137.2	ug/l	2311860	3	10.12	842252	50.0
Nonane, 3-methyl-	10.83	271.0	ug/l	4564990	3	10.12	842252	50.0
Cyclohexane, propyl-	10.91	210.2	ug/l	3539950	3	10.12	842252	50.0